Probing the Carbon-Hydrogen Activation of Alkanes Following Photolysis of Tp'Rh(CNR)(carbodiimide): A Computational and Time-resolved Infrared Spectroscopic Study

Jia Guan,[†] Alisdair Wriglesworth,[‡] Edward N. Brothers,[&] Snežana D. Zarić,[&,¶]

William D. Jones,[#] Michael B. Hall,*[,†] and Michael W. George*[,‡]

[†]*Department of Chemistry, Texas A&M University, College Station, Texas 77843-3255, United States*

[‡]*School of Chemistry, University of Nottingham, University Park NG7 2RD, U.K.*

[&]*Science Program, Texas A&M University at Qatar, P. O. Box 23874, Doha, Qatar*

[¶]*Department of Chemistry, University of Belgrade, Belgrade, Serbia*

[#]*Department of Chemistry, University of Rochester, Rochester, New York 14627, United States*

Abstract

Carbon–hydrogen bond activation reactions of alkanes by Tp'Rh(CNR) (Tp' = Tp = trispyrazolylborate or Tp* = tris(3,5-dimethylpyrazolyl)borate) were followed by time-resolved infrared spectroscopy (TRIR) in the υ(CNR) and υ(BH) spectral regions on Tp*Rh($CNCH_2CMe_3$), and their reaction mechanisms were modelled by density functional theory on TpRh(CNMe). The major intermediate species were analogs of those in the previously studied Tp'Rh(CO) alkane activations: κ^3-η^1-alkane complex (**1**); κ^2-η^2-alkane complex (**2**); and κ^3-alkyl hydride (**3**). Calculations predict that the barrier between **1** and **2** arises from a triplet-singlet crossing and leads to the singlet κ^2-Tp'Rh(CNR)(η^2-alkane) with one pyrazolyl arm dechelated, and a strongly bonded alkane. Intermediate **2** proceeds over the rate-determining C-H activation barrier to give the final product **3**. The carbon-hydrogen

activation lifetimes measured for the Tp*Rh(CNR) and Tp*Rh(CO) fragments with four cycloalkanes (C_5H_{10}, C_6H_{12}, C_7H_{14}, and C_8H_{16}) increase with alkanes size and show a dramatic increase between C_6H_{12} and C_7H_{14}, indicating the control that the alkane has on the rate of C-H activation. Similar step-like behaviour was observed previously in studies on cycloalkane reactions with CpRh(CO) and Cp*Rh(CO) fragments and is attribute to the wider difference in C-H bonds that appear at C_7H_{14}. However, these rhodium fragments are significantly different in terms of their absolute lifetimes, as Tp'Rh(CNR) and Tp'Rh(CO) fragments have much slower rates of C-H activation and longer lifetimes compared to those of CpRh(CO) and Cp*Rh(CO) fragments. This is in accordance with reduced electron density in dechelated κ^2-η^2-alkane Tp' complexes, which stabilizes the d^8 Rh(I) in a square-planar geometry and weakens the metal's ability for oxidative addition of the C-H bond. Further, the Tp'Rh(CNR) fragment has significantly slower rates of C-H activation in comparison to the Tp'Rh(CO) fragment especially for the larger cycloalkanes. This behaviour can be attributed to steric bulk of the neopentyl isocyanide ligand, which hinders the rechelation in κ^2-Tp'Rh(CNR)(cycloalkane) species and results in the C-H activation without the assistance of the rechelation. On the other hand, the C-H activation in κ^2-Tp'Rh(CNR)(alkane) is assisted by CNR weaker backbonding, which increases electron density on metal centre in comparison to κ^2-Tp'Rh(CO)(alkane).

Introduction

The control of organometallic reactions is a complex interplay between sterics and electronics.[1,2] Even though the C-H activation of alkanes by rhodium complexes such as Cp'Rh(CO)$_2$ (Cp' is Cp = C_5H_5 or Cp* = C_5Me_5) and Tp'Rh(CO)$_2$ (Tp' is Tp = tris(pyrazolyl)borate), Tp* = tris(3,5-dimethylpyrazolyl)borate), or Tp^{tBu} = tris(3,5-dimethyl 4-*t*-butylpyrazolyl)borate)) has been extensively studied, understanding all of the factors that control the barriers to activation and how these depend upon the nature of the metal centre

and the alkane is still incomplete.[3-8] Complications include the varying strength of structurally different σ-bonded alkane complexes, electronic and steric barriers to activation over a number of closely related but different barriers, and whether the barriers for migration to alternative C-H activation sites are higher or lower than activation barrier thereby providing slower or faster routes to additional σ-bonded alkane complexes as resting states.

Previous experimental and theoretic reports have provided insight into answering some of these questions.[3-8] Cp'Rh(CO)(alkane) forms the alkyl hydride Cp'Rh(CO)(R)H rapidly on the 1-20 ns timescale depending on the alkanes.[3] Varying the nature of the alkane from methane to decane showed a nearly linear increase with respect to the alkane which was initially surprising because a difference was expected upon the introduction of secondary C-H i.e. going from ethane to propane. A more pronounced clearly oscillatory behaviour upon changing the alkane was observed for Cp*Rh(CO)(alkane) and an understanding of the barriers to primary and secondary alkane activation, the rates of 1,2- and 1,3-migrations of the coordination centre along the chain, and the importance of the conformation (trans vs. gauche) of the coordinated alkane is required in order to predict the behavior of these reactions. In other words, the observed variation in lifetimes arises from a subtle competition between activation and migration rates for truly linear alkanes being 1,3-migrations > 1,2-migrations > primary C-H activation > secondary C-H activation. Longer alkanes such as decane have a tendency to fold upon themselves in solution and this additional complexity makes unraveling the behavior of these more sterically crowed systems difficult. Studies on the activation of Cp'Rh(CO)(alkane) for cyclic alkanes (C_5H_{10}, C_6H_{12}, C_7H_{14}, and C_8H_{16}) showed an unexpectedly large increase in the lifetimes of the σ-complexes from cyclohexane to cycloheptane.[4,5] It was concluded that the different C−H bonds formed a range of σ-complex stabilities and activation barriers, and these ranges widen with ring size and it is this large number of inequivalent C−H bonds and the larger steric crowding for the cycloheptane

ring that leads to its large increase in lifetime. There have also been extensive studies on the activation of related Tp'Rh(CO)(alkane) where two distinct σ-complexes were observed κ^3-Tp'Rh(CO)(alkane) and κ^2-Tp'Rh(CO)(alkane) where the latter has one arm of the Tp' ligand dechelated as a result of loss of a CO π-acceptor from the parent Tp'Rh(CO)$_2$ which is key to stabilizing the 5-coordinate d^8 complexes.[6-8] The activation of the C-H bond occurs on a slower timescale compared to the analogous Cp'Rh(CO)(alkane) complexes. Initial interpretations reported that C-H activation occurs to form κ^2-Tp'Rh(CO)(alkyl)H but subsequent studies suggested that prior recoordination was essential to lowering the barrier for C-H activation.[7] However, these studies only examined a limited number of linear alkanes. Although fast time-resolved studies have not been reported for Tp*Rh(CNR)(alkane), activation and reductive elimination for small linear alkane complexes have been studied both experimentally and computationally, where the results parallel those of Tp*Rh(CO)(alkane).[9-12]

In this paper we investigate photochemistry of Tp*Rh(CNR)(carbodiimide) in cyclic alkanes in order to elucidate the factors controlling the stability and activation of alkanes to Tp' versus Cp' complexes and the interplay between activation between κ^2-Tp'RhL(alkane) and κ^3-Tp'RhL(alkane) and how the sterics and electronics govern this important reaction.

Results and discussion

Initially, the photochemistry of Tp*Rh(CNR)(carbodiimide) in n-heptane was studied using TRIR spectroscopy and DFT calculations, following the process of the activation of heptane as well as other processes observed at earlier time measurements. The detailed study of n-heptane established appropriate computational methodology capable of complementing the

experimental data. Then this combination of experimental and theoretical methodology was used to study the photochemical reaction of Tp*Rh(CNR)(carbodiimide) in cycloalkanes.

Photochemistry of Tp*Rh(CNR)(carbodiimide) in n-heptane

TRIR spectroscopy of the activation of heptane. The Tp*Rh(CNR)(carbodiimide) (R = neopentyl) compound has two important infrared active groups: an isocyanide (CNR) and a BH, which are present in *n*-heptane at 2178 and 2524 cm^{-1}, respectively (see **Table 1**). CNR is a π-acceptor group bound to the metal through the carbon and can act as a reporter group, which has been followed by TRIR spectroscopy. Additionally, the ν(BH) band in the IR can provide additional information to aid the elucidation of the mechanism of C-H activation as it reports on the coordination (κ^2 or κ^3) of the Tp* ligand to the rhodium centre, **Figure 1**.

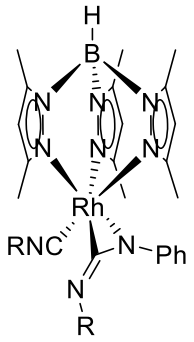

Figure 1: Structure of Tp*Rh(CNR)(carbodiimide).

The ps-TRIR spectra obtained in the isocyanide spectral region after 355 nm photolysis of Tp*Rh(CNR)(carbodiimide) in *n*-heptane is shown in **Figure 2(a)**. The TRIR spectrum obtained 1 ps after irradiation clearly shows that the parent band at 2178 cm^{-1} is bleached together with the production of several positive peaks relating to the formation of new species. A major transient band at 2076 cm^{-1} was also observed, which undergoes a small shift to 2083 cm^{-1} due to vibrational cooling over *ca*. 15 ps. This band, referred to as species

1, decays away [τ = 430 (± 30) ps] at the same rate a new peak at 2108 cm^{-1} (referred to as species **2**) grows in [τ = 360 (± 60) ps], **Figure 2(c)**. All of the observed υ(CNR) frequencies of the major species are summarised in **Table 1**. A number of species at low concentrations observed in the early time but not included in Table 1 are discussed in the next section. The conversion of **1** to **2** appears to fit with a dechelation step from a κ^3-Tp* intermediate to a κ^2-Tp* species, similarly observed with Tp'$Rh(CO)_2$ in previous time-resolved IR experiments.[7,8] As one of the pyrazolyl arms dechelates, removing electron density from the metal, back-donation into the CNR anti-bonding orbitals decreases and the CNR bonding is strengthened. Therefore, a $\kappa^3 \rightarrow \kappa^2$ dechelation step is consistent with the observed increase in υ(CNR) frequency from 2083 to 2108 cm^{-1}. The measured lifetimes for the conversion of **1** to **2** are also on a similar timescale to the lifetimes observed with Tp'$Rh(CO)_2$, again consistent with a $\kappa^3 \rightarrow \kappa^2$ dechelation step.[7,8] We therefore tentatively assign **1** to be κ^3-Tp*Rh(CNR)(alkane) and **2** to be κ^2-Tp*Rh(CNR)(alkane).

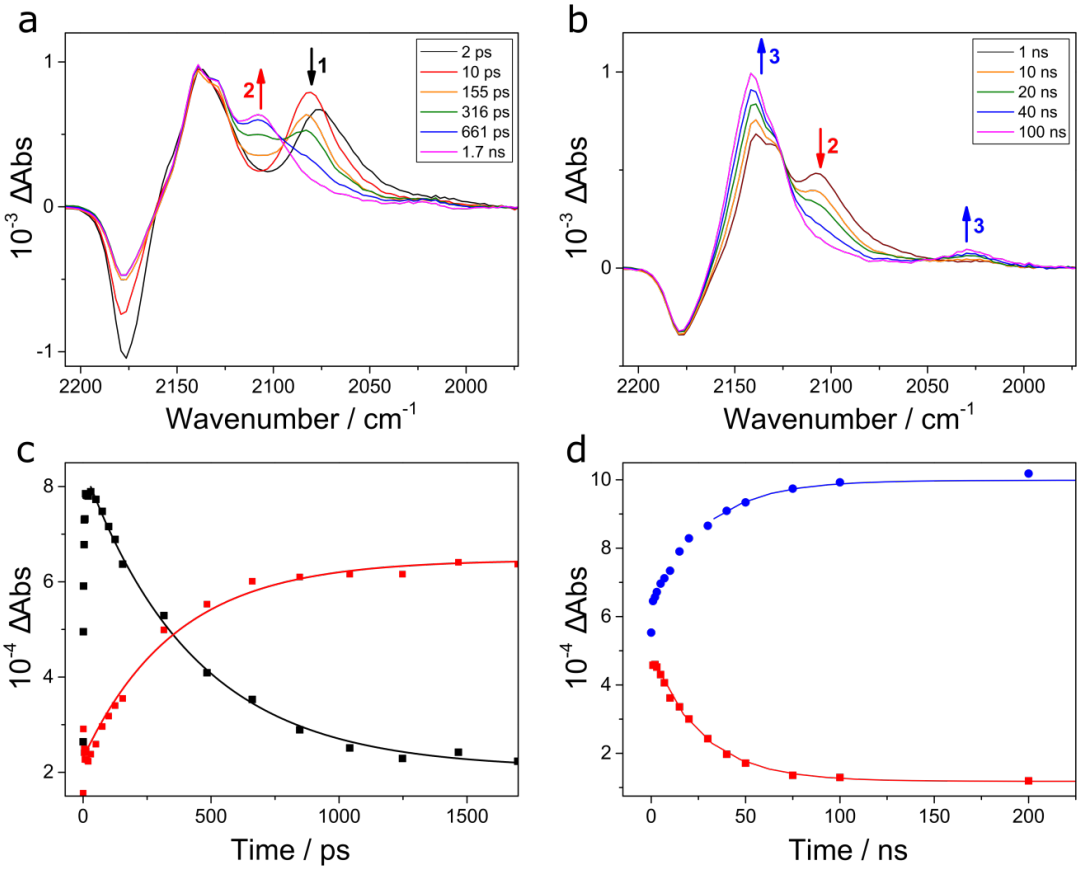

Figure 2: Photolysis (355 nm) of Tp*Rh(CNR)(carbodiimide) in *n*-heptane. (a) ps-TRIR and (b) ns-TRIR spectra in the υ(CNR) region at selected time delays. (c) Corresponding ps-TRIR kinetics: τ = 430 ± 30 ps for the decay of 1 at 2083 cm^{-1} (black); and τ = 360 ± 60 ps for the growth of 2 at 2108 cm^{-1} (red). (d) Corresponding ns-TRIR kinetics: τ = 28 (± 2) ns for the decay of 2 at 2108 cm^{-1} (red); and τ = 27 (± 2) ns for the growth of 3 at 2142 cm^{-1} (blue).

Table 1: Frequencies for the species observed by TRIR spectroscopy of Tp*Rh(CNR) species in the υ(CNR) and υ(BH) spectral region in *n*-heptane.

Species	υ(CNR) region (cm^{-1})	υ(BH) (cm^{-1})
Tp*Rh(CNR)(carbodiimide)	2178[a]	2524[a]
κ^3-η^1-alkane complex (1)	2083	2520
κ^2-η^2-alkane complex (2)	2108	2485
alkyl hydride (3)	2142, 2029	2518
free carbodiimide	2138[b]	-

[a] *lit.* 2186 cm^{-1} / 2525 cm^{-1} (KBr).[9] [b] *lit.* 2137 cm^{-1} (C_6H_6).[9]

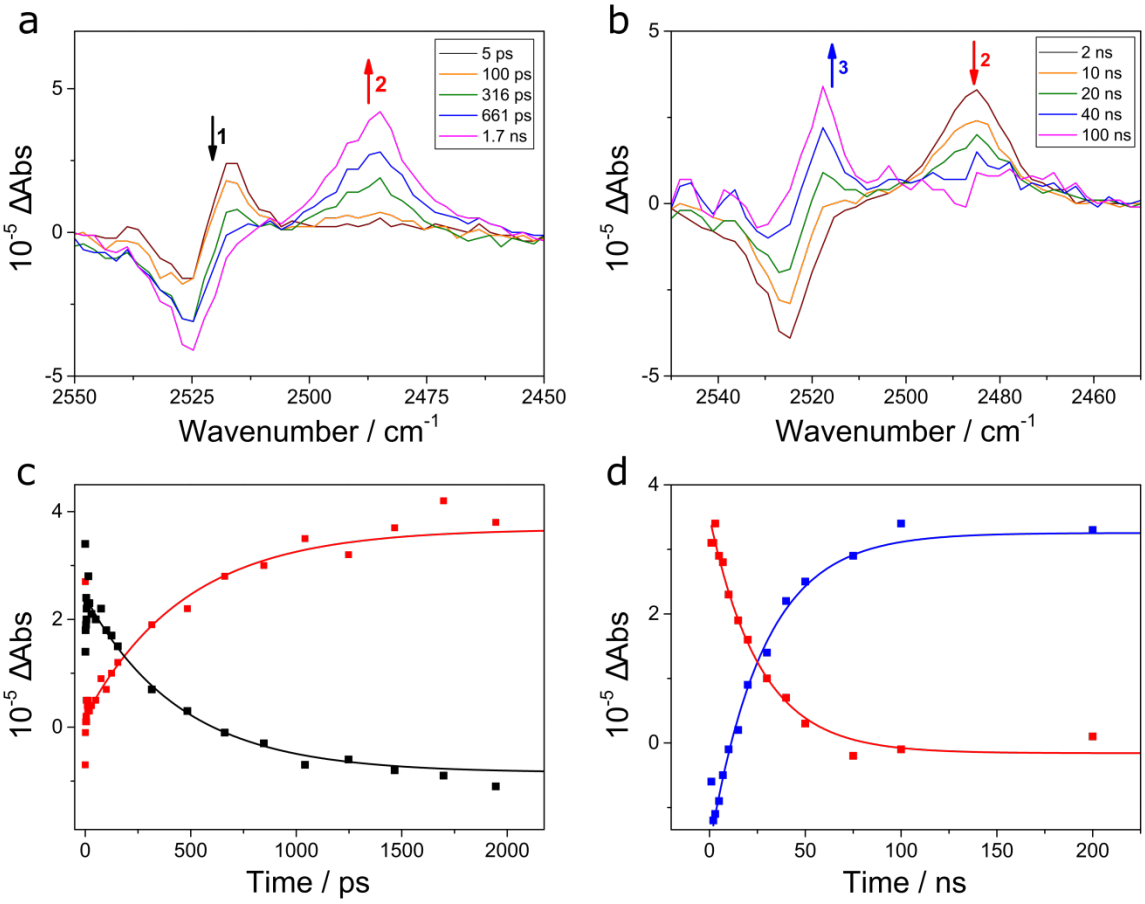

Figure 3: Photolysis (355 nm) of Tp*Rh(CNR)(carbodiimide) in *n*-heptane. (a) ps-TRIR and (b) ns-TRIR spectra in the υ(BH) region at selected time delays. (c) Corresponding ps-TRIR kinetics: τ = 450 ± 50 ps for the decay of 1 at 2520 cm^{-1} (black); and τ = 470 ± 50 ps for the growth of 2 at 2485 cm^{-1} (red). (d) Corresponding ns-TRIR kinetics: τ = 26 ± 3 ns for the decay of 2 at 2485 cm^{-1} (red); and τ = 28 ± 2 ns for the growth of 3 at 2518 cm^{-1} (blue).

We have investigated the assignment of **1** and **2** further by repeating the ps-TRIR measurements in the B-H region. The ν(B-H) band is sensitive to mode of coordination (κ^2 or κ^3) to the metal centre (see Suplementary information).[13] ps-TRIR spectra of the υ(B-H) spectral region of Tp*Rh(CNR)(carbodiimide) after photolysis are shown in **Figure 3(a)**. At a time delay of 1 ps, there is a clear parent bleach at 2524 cm^{-1} and a transient band at 2520 cm^{-1}, which decays [τ = 450 (± 50) ps] at the same rate [470 (± 50) ps] as a new transient peak grows-in to lower wavenumber at 2485 cm^{-1}. This behaviour mirrors the υ(CNR) TRIR experiments described above, **Figure 2(a)**, and these bands in the υ(B-H) TRIR spectra are

also assigned to the same intermediates, **1** and **2**, respectively. Additionally, in the υ(B-H) TRIR spectra, the position of the peaks relative to the parent bleach is reversed when compared to the isocyanide spectral region (**Figure 2(a)**). For **1**, the Tp* ligand is still in a κ^3-configuration, so the ν(B-H) is relatively unaffected relative to parent and its υ(BH) frequency of 2520 cm^{-1} is diagnostic of κ^3-Tp* coordination.[13] Upon conversion of **1** to the κ^2-Tp* intermediate **2**, there should be a decrease of υ(BH) upon conversion and the shift in υ(BH) from 2520 to 2485 cm^{-1} is consistent with our assignment,[13] and provides very strong evidence for the structure of the intermediates.

The photochemistry of Tp*Rh(CNR)(carbodiimide) was also investigated on the nanosecond timescale by TRIR spectroscopy in both the CNR and B-H region, **Figures 2(b) and 3(b)**. The difference TRIR spectrum obtained 2 ns after photolysis (355) nm in *n*-heptane shows the same profile as the later time delays of the ps-TRIR experiment in both regions. In the CNR region a parent bleach is seen at 2178 cm^{-1}, as well as the presence of intermediate **2** (a κ^2- alkane σ-complex) at 2108 cm^{-1}. **2** decays [τ =28 (± 2) ns] on the ns-timescale at the same rate [27 (± 2) ns] a new species, **3**, grows in and this is observed at higher wavenumber overlapping with the free carbodiimide peak at 2138 cm^{-1}. By analogy to the C-H activation of Cp'Rh$(CO)_2$,[3,4] and Tp'Rh$(CO)_2$,[8] **3** was assigned to a rhodium alkyl hydride. As C-H activation occurs, the rhodium is oxidised from +1 to +3, resulting in a decrease in electron donation from the metal to the CNR antibonding orbitals. Therefore, the CNR bonding is strengthened and there is an associated increase in wavenumber of the stretching vibration. Concurrently with the formation of this new isocyanide peak, the rise of a small peak to lower wavenumber is observed at 2029 cm^{-1}. This peak is assigned to the metal-hydride stretch of the alkyl hydride **3** and consistent with the low oscillator strength of the ν(M-H) band compared to CO or CN stretches.[14] The similar timescale to the C-H activation of the

more widely studied Tp'Rh(CO)$_2$[8] and Cp'Rh(CO)$_2$[3,4] also indicates that the conversion of **2** to **3** corresponds to that of an alkane σ-complex to an alkyl hydride.

We also observed similar processes in the B-H region. The transient peak **2** decays over the course of the time delays displayed in **Figure 3(b)** and there is a concurrent growth at 2518 cm^{-1}, which was assigned to the alkyl hydride, **3**. The υ(B-H) frequency of **3** is indicative of the Tp* ligand in a κ^3 configuration.[13] Furthermore, the position of **3** relative to the parent fits with an alkyl hydride in a similar κ^3 environment to the parent. As the alkane is C-H activated the pyrazolyl arm is proposed to rechelate resulting in a κ^3-configuration and **3** having a similar υ(B-H) frequency to the parent. **Figure 3(d)** shows kinetic traces obtained from the ns-TRIR spectra in the υ(B-H) region, and the traces for the decay of **2** and formation of **3** match within error, with measured lifetimes of 26 (± 3) and 29 (± 2 ns), respectively.

Density Functional Theory (DFT) calculations on the activation of *n*-heptane. DFT calculations are performed, to gain insights into the different intermediates observed by TRIR spectroscopy and to help confirm the assignment of each peak to a specific intermediate (see Experimental section for detailed computational methodology). To decrease the computational time, Tp* was replaced by Tp as in previous investigations[8,12] and CNMe was used as CNR; these change are not thought to dramatically affect the electronic structure or the relative accuracy. The optimized geometries are shown in **Figure 4** with selected distances in **Table 2**. The κ^3-η^1-alkane complex (**1**) with the alkane weakly bound in an η^1-fashion, analogous to previous calculations on the closely related Tp'Rh(CO)(alkane) complexes,[8] has the alkane relatively far from the metal with a Rh-H1 distance of 3.11 Å and an almost unaffected C1-H1 bond (1.10 Å). The κ^3-Tp ligand has three nearly equal Rh-N1 distances, 2.14 to 2.23 Å. In the κ^2-η^2-alkane complex (**2**), the alkane is much closer to the metal, the Rh-H1 decreases to 1.85 Å, and C1-H1 bond elongates to 1.14 Å. The alkane's strong binding to the metal is accompanied by the Tp ligand changing to a κ^2-coordination, as

shown in **Figure 4**, with the unbound nitrogen N1 3.58 Å away from the metal and N2 and N3 both closer to the metal than in **1**. Thus, **2** is the square planar structure expected for a d^8 metal without strong π acceptors. After oxidative addition of the alkane, the Tp returns to a κ^3-configuration in the alkyl hydride (**3**), as expected. All these observations correspond with those for the similar Tp'Rh(CO)(alkane) systems.[8]

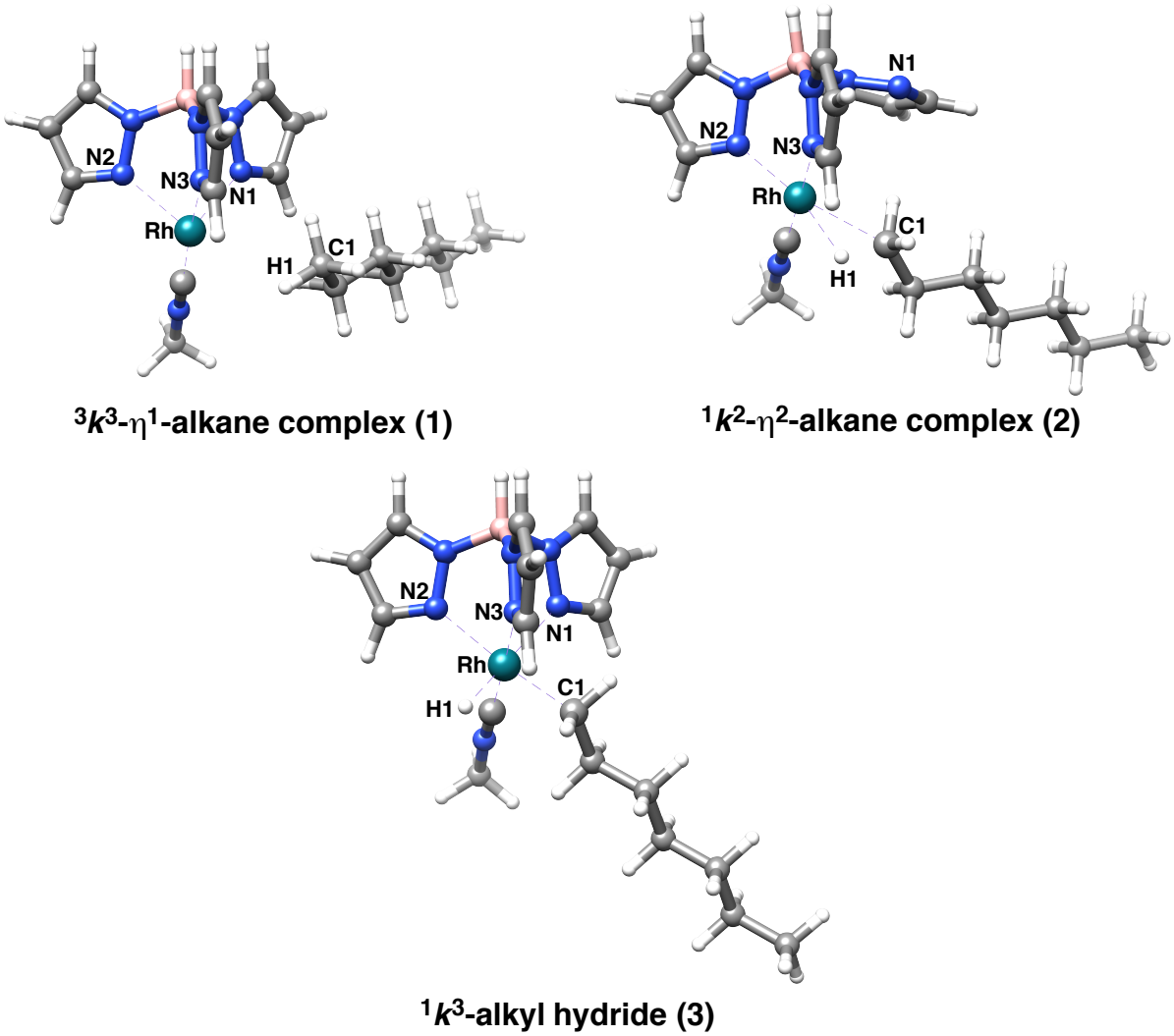

Figure 4: DFT calculated optimized geometries of the κ^3-η^1-alkane complex (1, triplet), the κ^2-η^2-alkane complex (2, singlet) and the κ^3-alkyl hydride (3, singlet) in *n*-heptane.

Table 2: Selected bond lengths from the optimized geometries of the different intermediates calculated with DFT. The specific atoms are denoted in Figure 4.

Calculated Species	Bond Lengths (Å)					
	Rh-H1	**Rh-C1**	**C1-H1**	**Rh-N1**	**Rh-N2**	**Rh-N3**
κ^3-η^1-alkane complex (1)	3.11	3.50	1.10	2.22	2.23	2.14
κ^2-η^2-alkane complex (2)	1.85	2.40	1.14	3.58	2.02	2.07
alkyl hydride (3)	1.55	2.06	2.54	2.18	2.16	2.08

Vibrational frequencies were also computed for these intermediates, **Table 3**. Important information can be obtained from their value relative to the parent frequencies, which were also computed. Examination of the calculated υ(CNR) frequencies in **Table 3** indicates the following order: **parent** > **3** > **2** > **1**. This replicates the trend in wavenumber observed by TRIR spectroscopy.

Table 3: DFT calculated and experimentally observed frequencies in the υ(CNR) and υ(BH) spectral regions for the different C-H activation intermediates.

Calculated Species	υ(CNR) [RhH] (cm^{-1})		υ(BH) (cm^{-1})	
	Calc.[a]	**Exp.**	**Calc.**[b]	**Exp.**
Tp'Rh(CNR)(carbodiimide) (parent)	2163	2177	2524	2523
κ^3-η^1-alkane complex (1)	2090	2083	2510	2514
κ^2-η^2-alkane complex (2)	2108	2108	2480	2483
alkyl hydride (3)	2146 [2069[c]]	2142 [2029]	2518	2518

[a,b]Scaling factors of 0.928 and 0.970, respectively (from calculated to experimental values). [c]Scaling factor of 0.928 is uncalibrated for Rh-H frequency.

The frequencies obtained from DFT calculations add further support to the assignments of **1**, **2** and **3** to a κ^3-η^1-alkane complex, a κ^2-η^2-alkane complex and an alkyl hydride, respectively. Furthermore, calculations predict a weak Rh-H stretch at 2069 cm^{-1}, which corresponds to the ns-TRIR spectra described in **Figure 2(b)**, where a small peak at 2029 cm^{-1} appears to grow in concurrently with the ν(CNR) of **3** at 2142 cm^{-1}.

Frequencies calculated in the ν(B-H) region for the different intermediates of C-H activation also correlate well with the peaks observed by TRIR spectroscopy. Upon conversion of **1** to **2**, a decrease of 30 cm^{-1} was predicted by the calculations, corresponding to a downshift of 31 cm^{-1} observed by TRIR spectroscopy. The C-H activation of **2** to **3** leads to an increase in the predicted frequency of 38 cm^{-1}, resulting in a peak on the lower frequency shoulder of the parent. The matching of these predicted trends and relative positions to the parent frequency with those observed by TRIR spectroscopy provide further evidence for the proposed C-H activation mechanism.

In summary, like Tp'Rh(CO), dechelation of one arm of the Tp' occurs to form the κ^2-Tp'(CNR*)*(*n*-heptane) complex, which then activates the C-H bond with synchronization of the rechelation of the Tp'. However, there are clearly additional processes occurring in the early times of the spectra that are discussed below.

Early time observations in the TRIR spectra. At early times in both the CNR and B-H regions, there are several other features. An intense band to lower frequency of the parent remains constant on the ps-timescale at 2138 cm^{-1} and is consistent with production of free carbodiimide ligand after it is photo-ejected from the rhodium by comparison to the literature.[9] There are several other bands that are either present at 1 ps or grow-in over the first 10-20 ps. These are tentatively assigned to in-cage re-coordination of the photo-ejected carbodiimide ligand to the rhodium to form η^2-arene complexes or to reform the parent complex.

The TRIR spectra at early time around the parent ν(CNR) band is complicated and there is some spectroscopic evidence for a transient with a band which is present as a small shoulder at 2156 cm^{-1} and this band decays [6 (± 1) ps] at the same rate as the apparent parent recovery at 2178 cm^{-1}, which can be fitted to a biexponential growth [5 (± 1) and 50 (± 10) ps].

Therefore, the band at 2156 cm^{-1} is tentatively assigned to a κ^2-parent complex with one dechelated pyrazolyl arm (see DFT results below) formed after photoexcitation that rearranges to reform the parent. As stated above, the partial reformation of the parent can be fitted to a biexponential with the slower part occurring with a 50 ps process and we also observe the growth of a shoulder at 2130 cm^{-1}, which occurs on a similar timescale [50 (± 10) ps]. The slower processes can be assigned to the re-coordination of the free ligand to the κ^2-Tp*Rh(CNMe) residue after the photolysis, where the κ^2-η^2-arene complex are generated. The migration of the Rh about the aryl ring and the re-chelation of the κ^2-η^2-arene complex to the κ^3-η^2-arene complex give rise to the two growths on the 50 ps timescale, where the calculated bands (see DFT results below) agree well with the spectra.

DFT calculations on early time observations. Figure 5 summarizes the results of the DFT calculations that were performed to understand these early-time spectral features; in addition to the structure and the relative energy, Figure 5 displays the ν(CNR) values as 'predicted(*measured*)'. The parent complex, κ^3-Tp'Rh(CNR)(carbodiimide), is excited to the excited state, [parent]*, which mainly decays to the longer-lived unsaturated triplet κ^3-Tp'Rh(CNR)(alkane) fragment after vibrational cooling, and this fragment will subsequently proceed to activate the alkane. In addition, [parent]* may decay by two distinct minor pathways: on the one hand, it can render a stable κ^2-parent with a ν(CNMe) of 2151 cm^{-1}, which agrees well with the observed band of 2156 cm^{-1} in the TRIR spectra. The dechelated pyrazolyl arm of this κ^2-parent rechelates via a small rotation barrier of 1.7 kcal/mol to render the κ^3-parent, here this shallow barrier corresponds to a estimated lifetime of 3 ps, which fits well with the observed fast recovery of parent at 2178 cm^{-1} band on a timescale of [6 (± 1) ps] in spectra.

On the other hand, ejection of the carbodiimide ligand from the [parent]* could also generate the κ^2-Tp'Rh(CNR) residue in the singlet state, where the adjacent free ligand can re-

coordinate to form the κ^2-1,2-η^2-arene complexes. Through a rechelation TS with a barrier of 2.9 kcal/mol, this arene complex can rearrange to generate the corresponding more stable κ^3-1,2-η^2-arene complex that has a calculated band of 2150 cm^{-1}, which fits reasonably well with the observed recovery at 2178 cm^{-1} in spectra, as its calculated ν(CNR) is similar to the calculated ν(CNR) of the parent, 2163 cm^{-1}. Further, this initial arene complex can undergo an arene migration with a barrier of 2.4 kcal/mol to form a more stable κ^2-2,3-η^2-arene complex that has a calculated band of 2119 cm^{-1}, corresponding the growth of a shoulder at 2130 cm^{-1}. Note that this κ^2-2,3-η^2-arene complex does not rearrange to the κ^3 conformation due to steric issues, validating the spectral observation of no decay in both growths. Furthermore, these 1,2-η^2-arene complexes are quite stable and will not evolve further in the short time scale; however, in longer times they may undergo aryl C-H activation of the phenyl ring on the carbodiimide ligand on the ns timescale, the products of which have also been observed by NMR experiments in previous studies.[9,10]

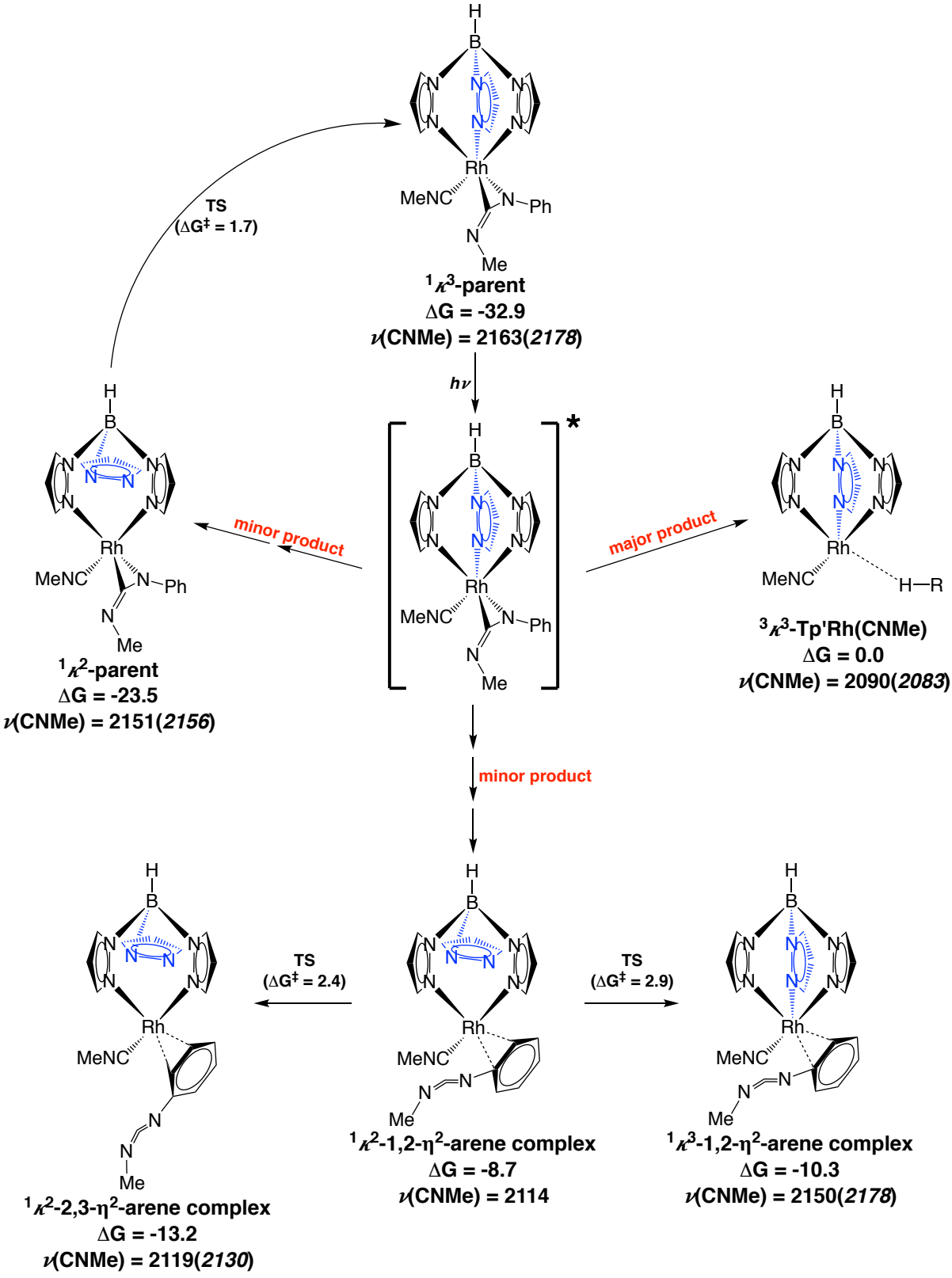

Figure 5: DFT calculations on the proposed species seen in the early stages after photolysis. ν(CNR) frequencies presented as predicted (*measured*).

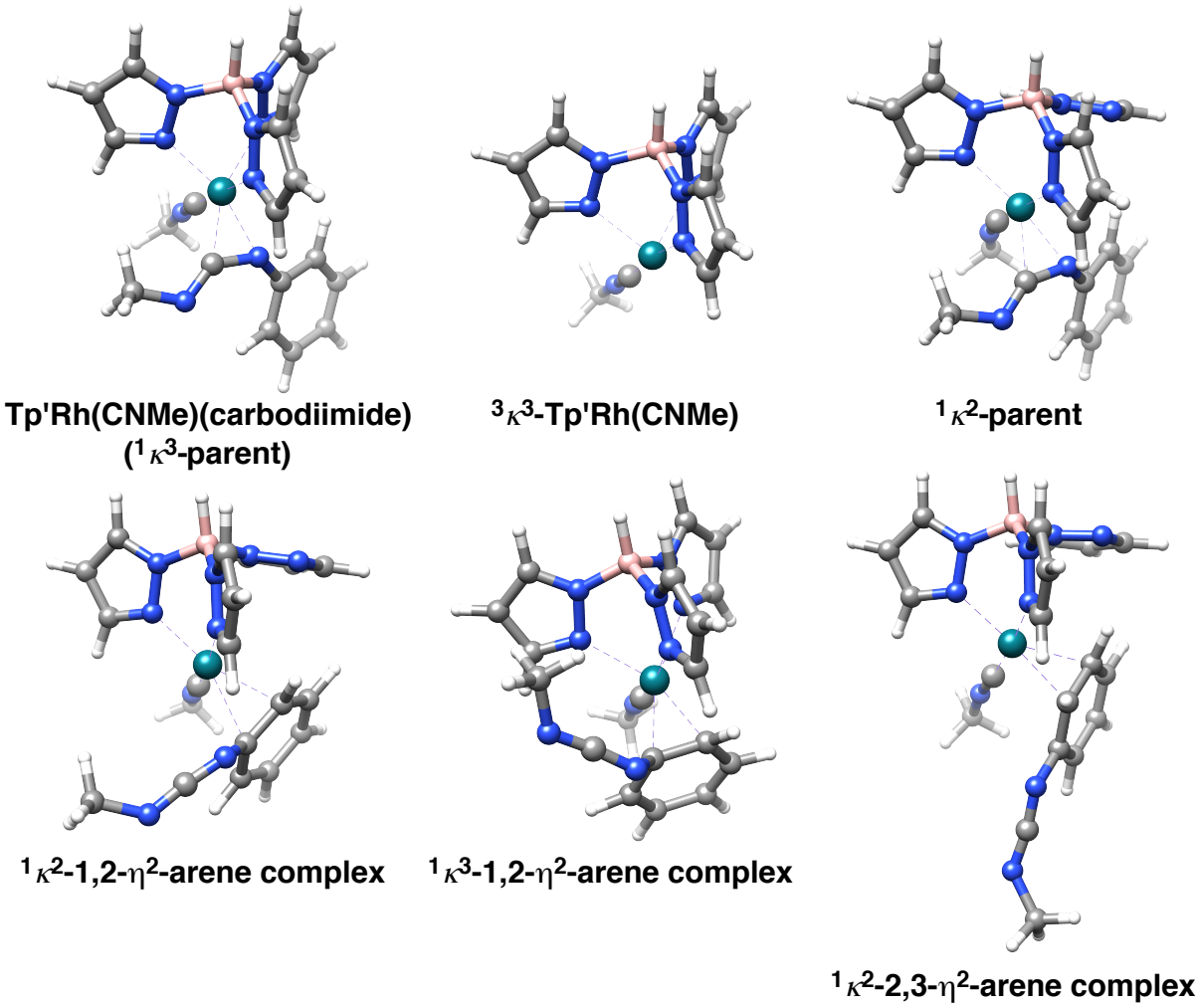

Figure 6: Optimized molecular structures of the parent Tp'Rh(CNMe)(carbodiimide) and other species generated in the early stage.

Table 4: Relative energies and frequencies (cm^{-1}) of DFT calculated parent Tp'Rh(CNMe)(carbodiimide), Tp'Rh(CNMe) residue, and η^2-arene complexes in κ^3 and κ^2 conformations, respectively, in the early stage after photolysis. Structures are shown in Figures 5 and 6.

Calculated Species	ΔG	Wavenumber (cm^{-1})	
		***ν*(CNMe)**	***ν*(B-H)**
Tp'Rh(CNMe)(carbodiimide) ($^1\kappa^3$-parent)	-32.9	2163	2525
$^1\kappa^2$-parent	-23.5	2151	2500
$^3\kappa^3$-Tp'Rh(CNMe)	[a]0.0	2090	2509
$^1\kappa^3$-1,2-η^2-arene complex	-10.3	2150	2515
$^1\kappa^2$-1,2-η^2-arene complex	-8.7	2114	2477
$^1\kappa^2$-2,3-η^2-arene complex	-13.2	2119	2477

[a]Total energies of the triplet κ^3-Tp'Rh(CNMe) residue and free carbodiimide are set as zero.

Although one might expect a high degree of similarity in the photo-initiated C-H activation reaction between Tp'Rh(CO)$_2$ and the Tp'Rh(CNR)(carbodiimide), there are significant differences in the early-time dynamics from additional reactions arising from the slow ejection of the heavier carbodiimide that results in the formation of other species especially η^2-arene π-complexes. In spite of these interesting differences, the major reaction paths of both involve ligand loss, σ-alkane complex formation and C-H activation, but with significant differences in the rates as described below for the cycloalkanes.

Rates of C-H activation of Cyclic Alkanes by Tp'Rh(CNR)

We have previously investigated the effect of changing the nature of the alkane on the reactivity of Cp'Rh(CO)(alkane)[3-5] and Tp'Rh(CO)(alkane)[8] and as stated above different factors affect the rate depending upon the nature of the complex and the alkane.

The C-H activation lifetimes of four cycloalkanes (*c*-pentane, *c*-hexane, *c*-heptane and *c*-octane) with the Tp*Rh(CNR) fragment was determined by looking at the growth of **3**. Normalised kinetic traces for the C-H activation reactions of the different cycloalkanes, **Figure 7**, show a significant increase in the lifetime as the size of the cycloalkane increases. *C*-octane, the largest cycloalkane studied in this work, has the longest lifetime of 1570 (± 70) ns and *c*-pentane has the shortest at 220 (± 10) ns. Furthermore, the rates for *c*-pentane and *c*-hexane are similar, as are those of *c*-heptane and *c*-octane. Thus, a step-like lifetime trend is observed, **Figure 8**. Similar step-like trends with a dramatic change in lifetime between *c*-hexane and *c*-heptane have been reported for the CpRh(CO) and Cp*Rh(CO) fragments[5] and the latter is compared with Tp*Rh(CNR) in **Figure 8**.

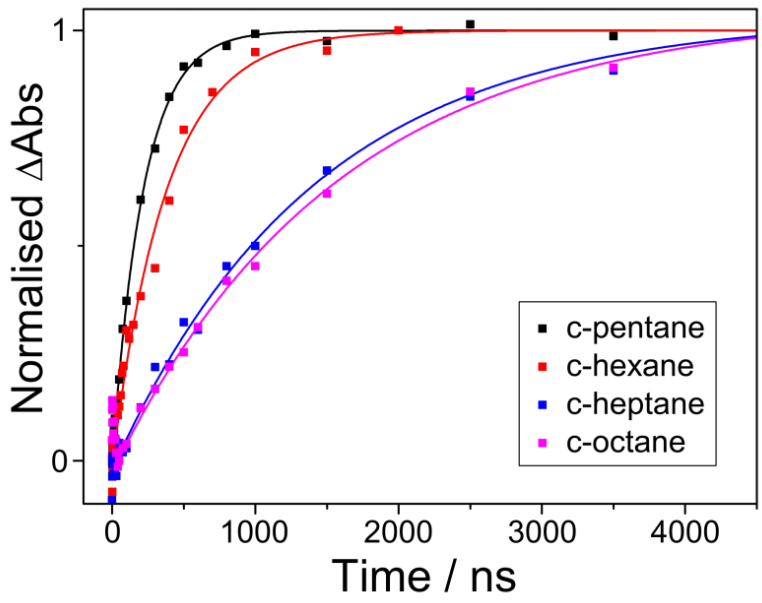

Figure 7: Kinetic traces and mono-exponential fits for the room temperature C-H activation of cyclic alkanes by the Tp*Rh(CNR) fragment.

The similarity of the lifetime trend for the Tp*Rh(CNR) fragment to that of the Cp*Rh(CO) fragment with the same step-like feature observed, demonstrates the inherent control that the nature of the alkane has on the relative rate of C-H activation. However, the absolute lifetimes for the Tp*Rh(CNR) fragment are considerably longer than their $Cp^*Rh(CO)_2$ counterparts. These lifetimes shows that although the specific alkane exerts influence on the relative rate when compared to other alkanes, the metal fragment initiating the C-H activation still has significant control as well.

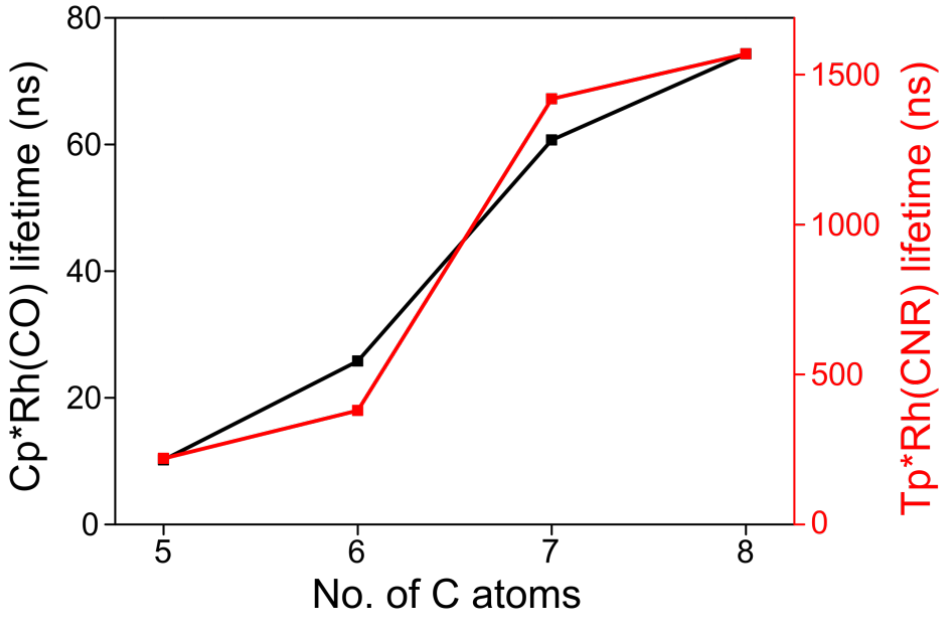

Figure 8: Scaled lifetime trends for the C-H activation of cycloalkanes by Tp*Rh(CNR) (red) and Cp*Rh(CO)[5] (black).

Lifetimes of the C-H activation of cycloalkanes by the Tp*Rh(CO) fragment were also measured at room temperature, see Supplemental Information (SI), and are summarised in **Table 5** along with the lifetimes for the Tp*Rh(CNR) fragment, and those previously reported for the Cp'Rh(CO) fragments. Although the lifetimes measured for *c*-pentane and *c*-hexane with the Tp*Rh(CNR) fragment are similar to those with the Tp*Rh(CO) fragment the lifetimes for *c*-heptane and *c*-octane are much longer with the Tp*Rh(CNR) fragment. This observation may be related to the appearance of significant steric problems between CNR and larger cycloalkane.

Using these values, lifetime trends for all four rhodium fragments were normalised and plotted together for comparison, **Figure 9**. Upon examination of the normalised lifetime trends, those of the Cp*Rh(CO) and Tp*Rh(CNR) fragments are very similar in nature, although there is more exaggerated step between the *c*-hexane and *c*-heptane lifetimes for the Tp*Rh(CNR) fragment. In a similar manner to all of the other rhodium fragments,

Tp*Rh(CO) also exhibits a step-like C-H activation lifetime trend with a large increase in lifetime between *c*-hexane and *c*-heptane, again showing the influence that the nature of the alkane has on the relative rate of C-H activation. However, there are considerable differences between the fragments. CpRh(CO) shows a relatively linear relationship, particularly between *c*-hexane and *c*-octane, whereas Cp*Rh(CO) and Tp'Rh(CNR) have very pronounced steps in their trends.

Table 5: Room temperature lifetimes for the C-H activation of cycloalkanes by the different rhodium fragments studied: CpRh(CO); Cp*Rh(CO); Tp*Rh(CNR); and Tp*Rh(CO).

	C-H activation lifetime (ns)			
	CpRh(CO)[a]	**Cp*Rh(CO)[a]**	**Tp*Rh(CNR)**	**Tp*Rh(CO)**
***c*-pentane**	5.9 (± 0.2)	10.2 (± 0.8)	220 (± 10)	230 (± 10)
***c*-hexane**	8.6 (± 0.3)	25.8 (± 2.0)	380 (± 40)	280 (± 15)
***c*-heptane**	22.7 (± 0.7)	60.7 (± 2.4)	1415 (± 50)	550 (± 45)
***c*-octane**	31.7 (± 0.9)	74.3 (± 4.0)	1570 (± 70)	640* (± 60)

[a] from Ref. [5] * Unidentified peak due to suspected *c*-octene complex from impurity or side-reaction was present, but lifetime was obtained from unobscured alkyl hydride peak.

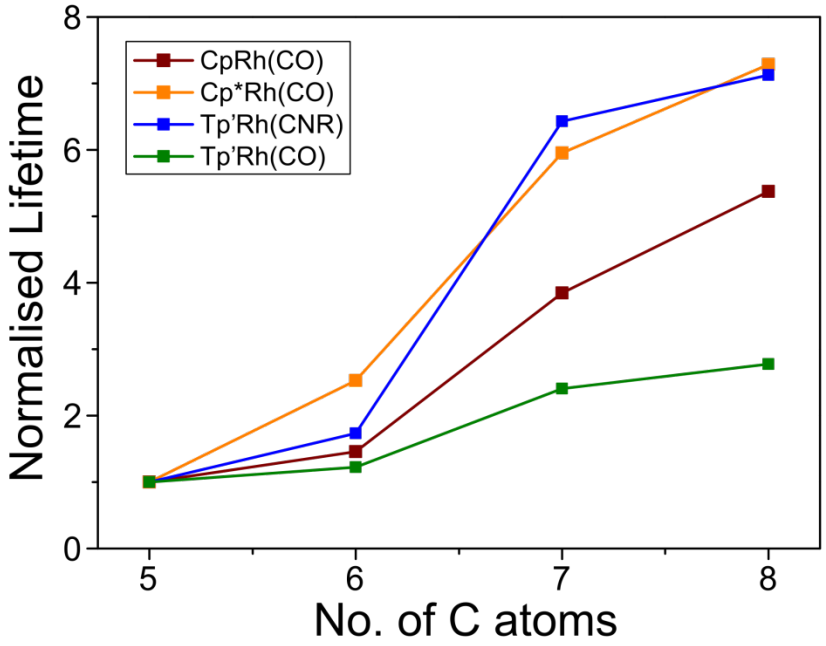

Figure 9: Lifetime trends for the CpRh(CO)[5] (red), Cp*Rh(CO)[5] (orange), Tp*Rh(CNR) (blue) and Tp*Rh(CO) (green) fragments with the cycloalkanes (*c*-pentane to *c*-octane). All of the lifetimes with *c*-pentane were normalised to 1.

Although the Tp* complexes are only differentiated by a CO or a CNR ligand, this has a large effect on their lifetime trends. For *c*-pentane, Tp'Rh(CO) and Tp'Rh(CNR) have similar lifetimes of 230 (± 10) and 220 (± 10) ns, respectively, but for the larger *c*-octane, there is a large difference between their lifetimes of 640 (± 60) and 1570 (± 70) ns, respectively. These changes are proposed to be due to the sterics of the two fragments. Tp'Rh(CNR) is much more sterically crowded than the analogous Tp'Rh(CO) due to the bulky isocyanide neopentyl group. This steric difference may hinder the rechelation of the Tp' arm, which has been proposed to be crucially important for C-H activation,[8] or simply make the transition state for the larger cycloalkanes more crowded. All of these differences between the rhodium fragments highlight how the nature of the metal fragment and its environment also plays a crucial role in determining the rate of C-H activation.

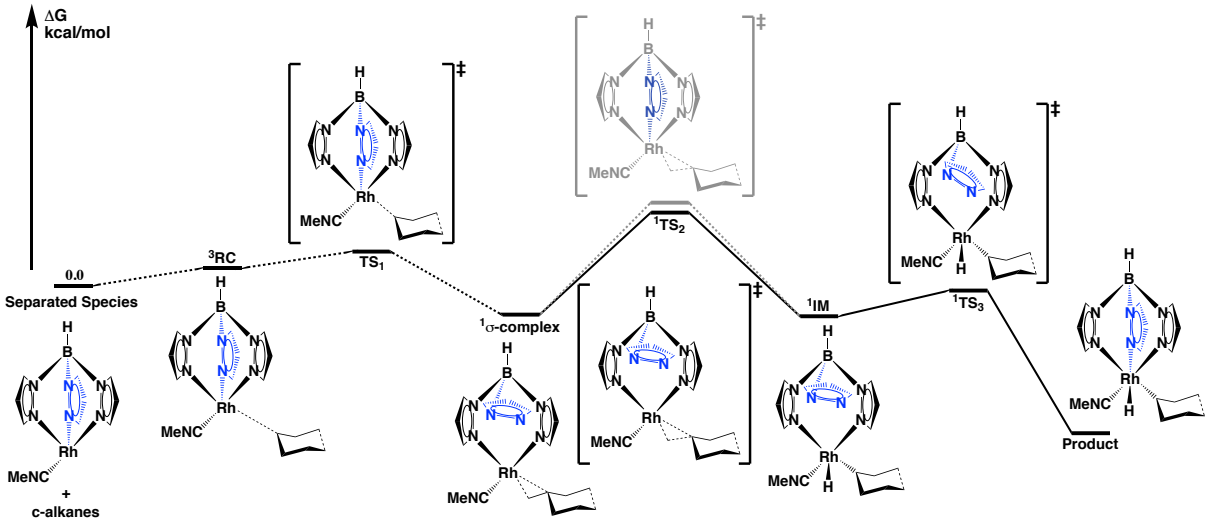

Figure 10: DFT results for the proposed mechanism C-H activation of *c*-alkanes by TpRh(CNMe). The grey-coloured $^1TS_2$ indicates the less stable κ^3 C-H activation transition state.

DFT calculations indicate that the main product of photolysis, the triplet κ^3-Tp'Rh(CNMe) complex, is in rapid equilibrium with respect to the weak binding of the *c*-alkane (^{3}RC, an enthalpically stable intermediate, but the free energy favours the free fragment) (**Figure 10**). Going through a triplet-singlet crossing barrier brings this Tp'Rh(CNMe)(*c*-alkane) complex to a singlet state with one pyrazolyl arm dechelated, which strongly binds the *c*-alkane as the κ^2-σ-complex, κ^2-Tp'Rh(CNMe)(*c*-alkane). The conversion barrier of 4.0 kcal/mol was estimated here,[3,5,7] which corresponds to the **1** to **2** decay at ~400 ps in experiment. Table 6: Relative free energies (lowest/highest) of DFT calculated species to the separated species (RC) in the proposed mechanism of Tp*Rh(CNMe) catalysed C-H activation of *c*-pentane, *c*-hexane, *c*-heptane, and *c*-octane.

	Separated Species	$^1\kappa^2$-σ-complex	$^1TS_2$	^{1}IM	$^1TS_3$	Product
c-pentane	0.0	-3.6/-2.5	6.2/7.6	-5.1/-3.2	-2.4/-1.1	-20.1/-18.1
c-hexane	0.0	-2.9/-2.6	6.7/7.2	-3.9/-2.2	-2.1/0.7	-20.4/-16.0
c-heptane	0.0	-4.3/-2.4	7.4/8.2	-3.3/-1.6	-1.6/1.5	-20.0/-15.2
c-octane	0.0	-4.3/-2.6	6.9/13.4	-3.8/4.6	-1.8/7.9	-19.2/-7.7

Subsequently, the κ^2-σ-complex proceeds over the rate-determining C-H activation barrier (^{1}**TS$_2$** in **Figure 10**) which ranges from of 9.6-11.7 kcal/mol (**Table 6**) to render the alkyl hydride with Tp* in the κ^2 conformation; finally, the dechelated pyrazolyl rechelates to the Rh via a very shallow barrier (^{1}**TS$_3$**) to form the final product.

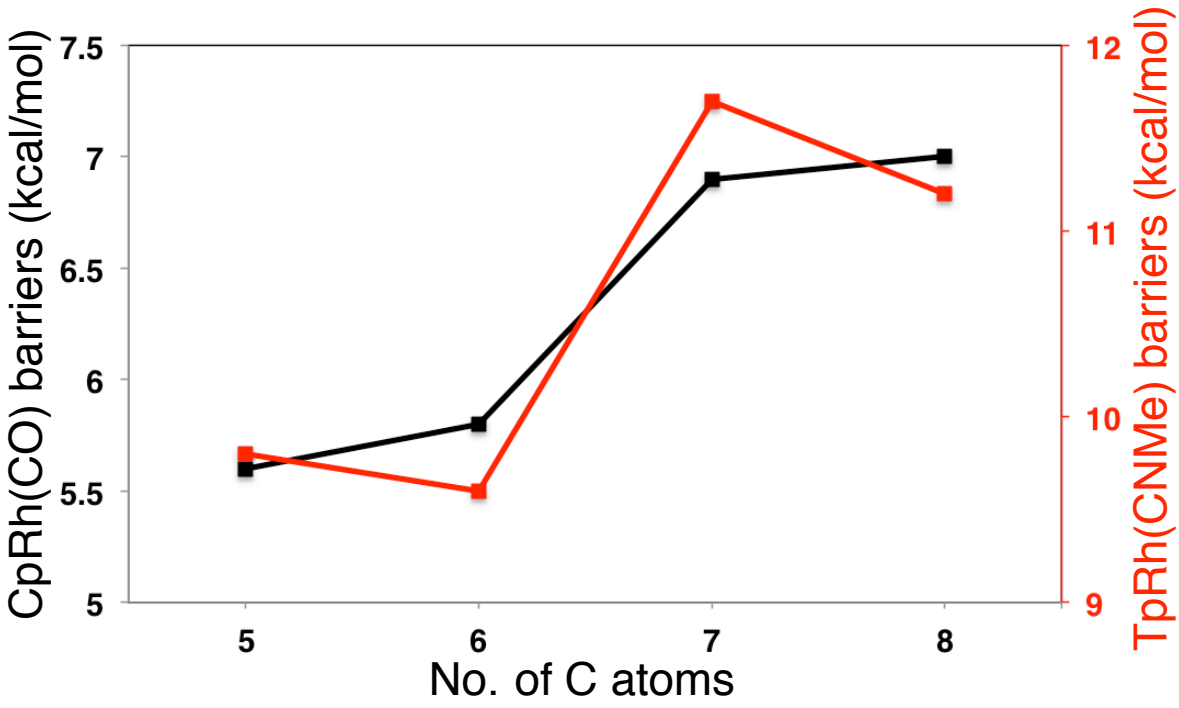

Figure 11: Calculated C-H bond activation barriers for the four cycloalkanes catalysed by TpRh(CNMe) (red) and CpRh(CO) (black).

In contrast to the barrier of 8.1 kcal/mol calculated for the activation of *n*-heptane, the barriers of activating *c*-alkanes in the range of 9.6-11.7 kcal/mol, which correlates with the measured lifetimes of ~ 20 ns and more than 200 ns, respectively. This difference can be attributed to a combination of the larger barrier for the secondary C-H bond activation vs the primary C-H bond activation in *n*-heptane and the greater steric hindrance between the Tp*Rh(CNMe) residue and the cyclic alkane than that of the linear alkane, which contributes to the increase in lifetimes from *c*-pentane to *c*-octane, as shown in Figure 8, while those of *n*-pentane to *n*-nonane do not change as much (see SI Table S1).

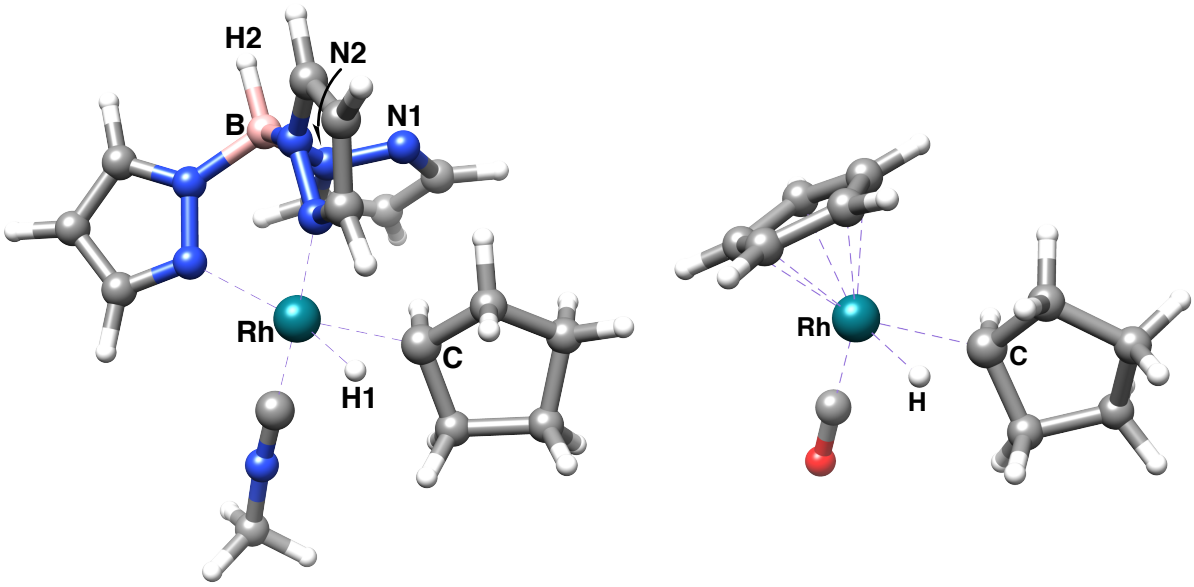

Figure 12: Sampled optimized geometries of the C-H activation TSs catalysed by TpRh(CNMe) and CpRh(CO), respectively.

Table 7: Geometric parameters of the lowest-energy σ-complexes and activation TSs in TpRh(CNMe) and CpRh(CO) catalysed C-H activation step of *c*-pentane, *c*-hexane, *c*-heptane, and *c*-octane, respectively.

	TpRh(CNMe)								CpRh(CO)		
	σ-complex				$TS_{activation}$				$TS_{activation}$		
	[a]B_{C-H1}	B_{Rh-H1}	B_{Rh-C}	[b]D	B_{C-H1}	B_{Rh-H1}	B_{Rh-C}	D	B_{C-H}	B_{Rh-H}	B_{Rh-C}
c-pentane	1.144	1.848	2.386	89.12	1.586	1.551	2.110	79.84	1.461	1.576	2.191
c-hexane	1.147	1.847	2.448	89.30	1.607	1.552	2.140	79.59	1.480	1.577	2.212
c-heptane	1.142	1.881	2.439	87.31	1.634	1.551	2.142	76.98	1.507	1.573	2.214
c-octane	1.148	1.878	2.465	89.31	1.631	1.553	2.146	74.19	1.489	1.576	2.219

[a]B: bond length, in Å; [b]D: dihedral angle $D_{N1-N2-B-H2}$, in °.

The plot (**Figure 11**) of the calculated barriers for the lowest energy pathway in the series of *c*-alkanes activated by TpRh(CNMe) produces the trend like that seen in the experiment, especially a pronounced step from *c*-hexane to *c*-heptane, but they do not correctly reproduce

the much smaller difference between *c*-pentane and *c*-hexane or between *c*-heptane and *c*-octane. A similar increasing trend was also calculated for CpRh(CO), although the lifetime difference between *c*-hexane and *c*-heptane is not as dramatic as that for TpRh(CNMe) (**Figure 11**). **Table 7** summarizes the C-H, Rh-H, and Rh-C bond lengths in the activation TSs of the four *c*-alkanes by TpRh(CNMe) and CpRh(CO), respectively, as shown in **Figure 12**. The much longer C-H bonds and shorter Rh-H and Rh-C bonds in the TpRh(CNMe) transition state (TS) than those in the CpRh(CO) TS indicate a later TS for TpRh(CNMe) in comparison to CpRh(CO), consistent with the former's higher barrier, as more geometric distortion is needed before the electronic rearrangement begins to stabilize the energy.[15]

Table 8: Calculated ranges of activation and methylene migration barriers (lowest/highest) in the C-H activation of *c*-pentane, *c*-hexane, *c*-heptane, and *c*-octane.

	Activation Barriers	Migration Barriers[a]
c-pentane	9.8/10.1	6.7/7.8
c-hexane	9.6/9.8	6.2/6.5
c-heptane	10.3/11.6	4.5/8.0
c-octane	9.8/16.0	5.4/8.7

[a]Much lower barriers (<2 kcal/mol) for 1,1-migrations between the two H atoms on the same C are not listed.

As reported in our previous study on the CpRh(CO)(alkane) activations,[5] ring-migration can play a role in influencing the rate of C-H activation. The numerous migration barriers (TSs) between different κ^2-σ-complexes have been located for the TpRh(CNMe)(c-alkane) systems and these always have lower barriers than the activation (**Table 8**), which facilitates the C-H activation to proceed via the lowest energy pathway, i.e. from the most stable κ^2-σ-complex over the lowest C-H activation TS even if this TS involves a migration to a different CH_2 group. Thus, the kinetics of the entire C-H reaction are dominated by the C-H activation barriers (^{1}**TS$_2$**), like the CpRh(CO) case.

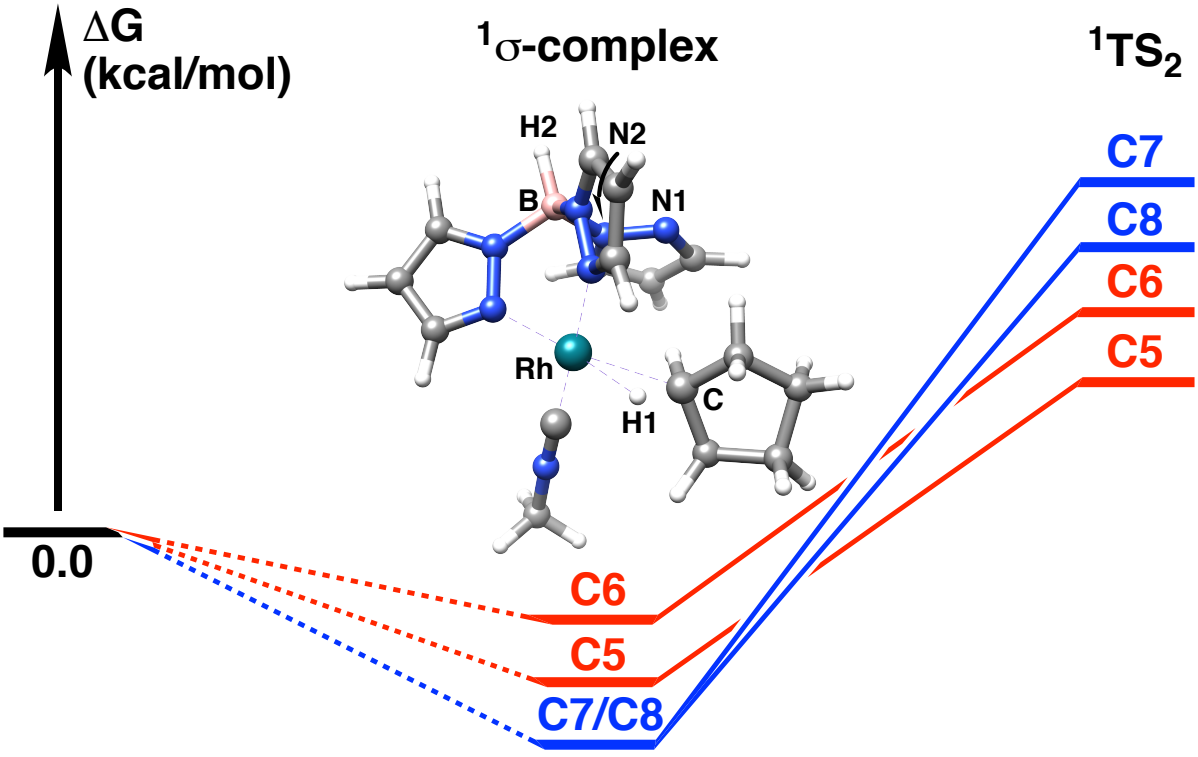

Figure 13: Comparative illustration of the relative energies of the rate-determining step of *c*-pentane, *c*-hexane (in red), *c*-heptane, and *c*-octane (in blue) activation. Depicted is the optimized geometry of a sampled σ-complex.

Figure 13 illustrates that the smaller activation barriers in *c*-pentane and *c*-hexane originate from the combination of the relatively high-energy σ-complexes and the low-energy transition states, whereas in *c*-heptane and *c*-octane the σ-complexes become more stable and the transition states become more unfavourable, a combination that lead to their larger barriers. Similar enhanced stability of σ-complexes as a function of the the alkane size has been observed in experiments,[16] and was attributed to the larger number of alkane-metal interaction sites.[17] Nevertheless, as illustrated in Figure 13 and Table 7, the σ-complexes in *c*-pentane and *c*-hexane have much shorter Rh-H1 bonds (1.848 and 1.847 Å) than the larger *c*-heptane and *c*-octane (1.881 and 1.878 Å), especially an obvious jump from 1.847 Å in *c*-hexane to 1.881 Å in *c*-heptane, as well as a general trend of longer Rh-C bonds for larger *c*-

alkanes from 2.386 Å in *c*-pentane to 2.465 Å in *c*-octane, yet the C-H1 bond lengths are all around 1.145 Å. The greater distance between C-H bond of the larger *c*-alkanes and the Rh should reflect a weaker interaction but the overall binding energy is larger. This dilemma is resolved when dispersion is considered as it stabilizes the larger *c*-alkanes at longer distances from the Rh, without dispersion effects the larger *c*-alkanes are bound more weakly (see **Table S1** in **SI** for more discussion on the effect of dispersion correction). With relative to the σ-complexes, the TSs require closer proximity of the *c*-alkane and the Rh in order to cleave the C-H bond; here steric hindrance between *c*-alkane skeleton and Tp ligand, increases and contributes to the higher barriers for the larger *c*-alkanes. The dihedral angle $D_{N1\text{-}N2\text{-}B\text{-}H2}$ reflects the position of the dechelated pyrazolyl arm with respect to its original κ^3 conformation (180), and the smaller it is, the larger the arm deviates. $D_{N1\text{-}N2\text{-}B\text{-}H2}$ should indicate the steric influence of the alkane ring on the Tp ligand, which is another factor that affects the stability of the geometric structures. Thus, $D_{N1\text{-}N2\text{-}B\text{-}H2}$ in the C-H activation TSs (^{1}**TS$_2$**) parallels well the expected steric influence of the c-alkanes.

Table 9: Relative free energies ($\Delta G^{\ddagger}_{\kappa 3} - \Delta G^{\ddagger}_{\kappa 2}$, kcal/mol) of the C-H activation TSs in linear/cyclo heptane catalyzed by TpRh(CO) and TpRh(CNMe), respectively.

	n-heptane	c-heptane
TpRh(CO)	-1.7	-0.6
TpRh(CNMe)	-0.5	0.2

Conclusions

TRIR spectroscopy has been successfully utilised to investigate the mechanism of C-H activation by Tp*Rh(CNR) in the υ(CNR) and υ(BH) spectral regions. Intermediate species with matching kinetics were observed in both spectral windows. These were assigned to

analogous species to those of the widely studied Tp*Rh(CO) C-H activation mechanism:[6-8] κ^3-η^1-alkane complex (**1**); κ^2-η^2-alkane complex (**2**); and κ^3-alkyl hydride (**3**). Identification of the intermediates in the υ(BH) spectral region afforded direct evidence that **1** and **3** are in a κ^3-configuration, while **2** is in a κ^2-configuration since the υ(BH) stretch is very characteristic of the environment of the Tp' ligand.[13] DFT calculations support the assignment of the these species with optimised structures and calculated frequencies for all the intermediates observed, including several low-concentration intermediates seen at very short times, in which the carbodiimide has recoiled rather than replaced by the cycloalkane. Calculations predict that the photolysis product (**1**) is a triplet κ^3-Tp'Rh(CNR) residue that only weakly binds the alkane as an η^1-alkane, as indicated by a long Rh-H1 contact in its optimized geometry. Subsequently, **1** dechelates one pyrazolyl arm to form κ^2-Tp'Rh(CNR)(η^2-alkane) with a strongly bound alkane, a singlet σ-complex with short Rh-H1 and Rh-C1 contacts and a stretched C1-H1. Intermediate **2** proceeds over the rate-determining C-H activation barrier to give the final product **3.** Good agreement has been made between their calculated frequencies and those observed experimentally.

Room temperature C-H activation rates were measured for Tp*Rh(CNR)(cycloalkane) and also for Tp*Rh(CO)(cycloalkane) for comparison to each other, as well as to the Cp and Cp* fragments examined previously. The lifetime trends for the C-H activation of the cyclic alkanes by all four rhodium fragments displayed similar step-like behaviour, showing the subtle control that the alkane has on the rate of C-H activation. As for the Cp and Cp* rhodium fragments, this control is thought to be a result of a number of discrete σ-complexes for each cyclic alkane, all with different activation barriers and various possible ring migrations between these σ-complexes. The large change occurs between cyclohexane and cycloheptane because the latter has a much larger number of more stable σ-complexes and more sterically crowded higher-energy transition states.

However, there were differences between the rhodium fragments in terms of their absolute lifetimes. This clearly demonstrates that the specific ligand environment has a much more significant influence on the absolute rate of C-H activation. Much slower rates of C-H activation with the cyclic alkanes were measured for the Tp*Rh(CNR) and Tp*Rh(CO) fragments compared to the CpRh(CO) and Cp*Rh(CO) fragments. This fits with the previous report of how dechelation of the Tp's third pyrazolyl arm stabilizes the 4-coordinate, square-planar κ^2-η^2-alkane complex and reduces the electron density available for the oxidative addition of the C-H bond.[8] The DFT calculations here show that the key, rate-determining C-H activation step in the more crowded cyclic alkanes may occur before the rechelation of the third pyrazolyl arm, while for the less crowded linear alkane rechelation is predicted to proceed first and lower the activation barrier.

Furthermore, the rates of C-H activation for the Tp*Rh(CNR) fragment compared to the closely related Tp*Rh(CO) fragment are similar for small cycloalkanes as the extra steric bulk of the neopentyl isocyanide ligand is offset by the higher Rh electron density from the weaker backbonding of the CNR ligand. However, the extra steric bulk of the neopentyl isocyanide ligand, along with the already bulky Tp* ligand, may hinder the rechelation of the Tp' arm,[8] such that the C-H activation takes place over a barrier without the assistance of the rechelation.

Table 9 compares the relative energies of the κ^3-TSs, where the third pyrazolyl arm rechelates before the TS, and the κ^2-TSs, where C-H activation occurs before the third pyrazolyl arm rechelates. In the case of linear alkanes, where primary C-H bonds are activated, the calculations predict that κ^3-TSs are strongly favoured over the corresponding κ^2-TSs for Tp'Rh(CO), where Rh needs the additional electron density from the rechelation because of the strong backbonding by CO, while κ^3-TSs are only weakly favoured over the corresponding κ^2-TSs for Tp'Rh(CNMe), where the poorer backbonding CNR ligand leaves

the Rh with more electron density. However, in the case of cycloalkanes, the scenario bifurcates, where κ^3-TSs are only weakly preferred in Tp'Rh(CO) activation because now the greater steric bulk of the cycloalkanes raises the relative energy of the κ^3-TSs, while finally in Tp'Rh(CNR) the combination of a more electron-rich Rh and less steric crowding in the κ^2-TSs renders them more stable than the κ^3-TSs. Thus, the balance between the sterics and the electronics in the reactive species tunes the preference of κ^2- or κ^3-TS geometries, where the carbon skeleton of cycloalkanes favors the dechelation of the pyrazol arm to reduce sterics while the electron-withdrawing ligand CO facilitates the rechelation of the pyrazol arm to the Rh to promote the oxidative addition of the C-H bonds. Thus, the less sterically demanding linear alkanes always favor rechelation of the pyrazol arm before the C-H activation.

Experimental

Tp'Rh(CNR)(carbodiimide)[9] and Tp'Rh$(CO)_2$[18,19] were synthesised *via* adapted literature procedures. The following solvents were all dried over CaH_2 under an argon atmosphere prior to use: *c*-pentane (Sigma Aldrich, ≥ 99%); *c*-hexane (Sigma Aldrich, ≥ 99.9%); *c*-heptane (Alfa Aesar, 99%); *c*-octane (Alfa Aesar, 99%); *n*-pentane (Alfa Aesar, 99+%); *n*-hexane (Sigma Aldrich, ≥ 99%); *n*-heptane (Sigma Aldrich, 99%); *n*-octane (Lancaster, 99%) and *n*-nonane (Sigma Aldrich).

For the TRIR experiments a recirculating flow system consisting of a peristaltic pump, Teflon tubing, and an infrared solution cell (Harrick Corp.) with CaF_2 windows (25x2 mm, Crystran) typically at a pathlength of 0.5 mm was used. The samples were placed under a positive pressure of argon. The TRIR experiments were performed at the ULTRA facility at the Rutherford Appleton Laboratory, which has been discussed in detail elsewhere,[20] therefore, only a brief summary is given here. A Ti:sapphire laser amplifier (Thales Laser) produces 800 nm laser pulses (0.8 mJ, 10 kHz with a pulsewidth of 50 fs). This laser output is split and one portion is used to generate the 267 nm pump beam by harmonic generation. The second portion is sent through an optical parametric amplifier (Light Conversion) and a difference frequency generator to produce a tuneable mid-IR probe. The diameter of the pump and probe beams were around 150 μm and 80 μm, respectively. After transmission through the sample, the IR probe is dispersed onto two linear 128 element MCT detector arrays (Infrared Associates). By the use of a chopper, the pump-on and pump-off infrared intensities can be measured and difference spectra generated. A small portion of the IR probe beam is taken before the sample and dispersed onto a 64 element MCT detector array (Infrared Associates) to provide a reference for beam intensity fluctuations. The cell is rastered in the plane

perpendicular to the pump and probe beams again and usually the sample is continually flowed through the cell to avoid degradation of the sample.

All the Density Functional-Theory (DFT) calculations were performed with the Gaussian 09 suite of programs.[21] MN12SX functional[22] was employed with using the 6-311++G**[23,24] basis set for the C, H, B, N, and O atoms, and the Stuttgart quasi-relativistic basis set and effective core potential[25] for Rh. Each species was optimized in the gas phase with tight convergence criteria and on an ultrafine grid as specified in Gaussian 09. Analytical frequency calculations were performed on all optimized structures to ensure that either a minimum or a first-order saddle point was achieved. To decrease the computational time, the methyl groups of Tp'Rh(CNMe)(carbodiimide) were omitted. Scaling factors of 0.928 and 0.970 were used for the calculated frequencies of υ(CNMe) and υ(BH) regions, respectively.

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Supplementary Information

Probing the Carbon-Hydrogen Activation of Alkanes Following Photolysis of Tp'Rh(CNR)(carbodiimide): A Computational and Time-resolved Infrared Spectroscopic Study

Alisdair Wriglesworth,[†,§] Jia Guan,[‡,§] Michael W. George,[*,†] Edward N. Brothers,[&] Michael B. Hall,[*,‡] William D. Jones,[#] and Snežana D. Zarić[&,¶]

[†]*School of Chemistry, University of Nottingham, University Park NG7 2RD, U.K.*

[‡]*Department of Chemistry, Texas A&M University, College Station, Texas 77843-3255, United States*

[&]*Science Program, Texas A&M University at Qatar, P. O. Box 23874, Doha, Qatar*

[#]*Department of Chemistry, University of Rochester, Rochester, New York 14627, United States*

[¶]*Department of Chemistry, University of Belgrade, Belgrade, Serbia*

The experimental results below are taken from the Ph.D dissertation of Alisdair Wriglesworth, University of Nottingham. Table S1: Lifetimes for the C-H activation of linear alkanes by the different rhodium fragments studied: CpRh(CO); Cp*Rh(CO); Tp*Rh(CNR); and Tp*Rh(CO).

	CpRh(CO) lifetime (ns)	**Cp*Rh(CO) lifetime (ns)**	**Tp'Rh(CNR) lifetime (ns)**	**Tp*Rh(CO) lifetime (ns)**
***n*-pentane**	9.8 (± 0.2)	8.8 (± 0.5)	24.1 (± 1.5)	11.4 (± 0.4)
***n*-hexane**	9.8 (± 0.2)	8.8 (± 0.2)	25.5 (± 1.3)	11.5 (± 0.3)
***n*-heptane**	11.0 (± 0.3)	10.8 (± 0.4)	27.4 (± 2.0)	11.6 (± 0.3)
***n*-octane**	12.5 (± 0.6)	12.5 (± 0.3)	28.6 (± 0.9)	12.2 (± 0.2)
***n*-nonane**	13.4 (± 0.5)	14.1 (± 0.8)	27.1 (± 1.3)	12.6 (± 0.4)

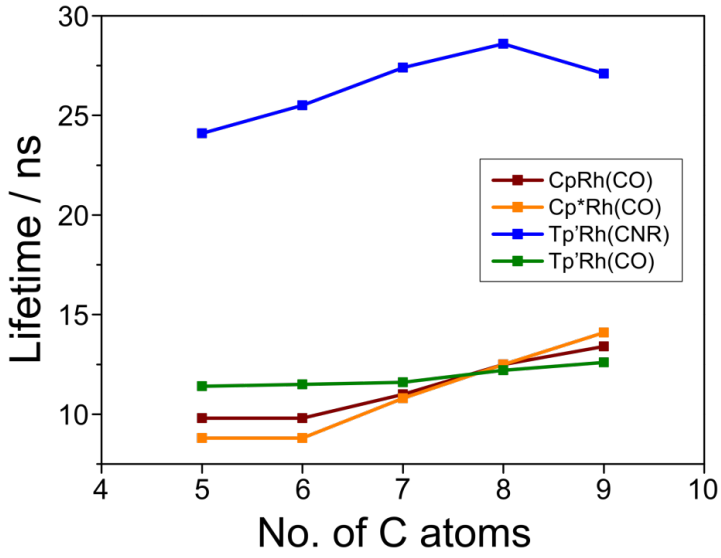

Figure S1: Lifetime trends for the CpRh(CO) (red), Cp*Rh(CO) (orange), Tp'Rh(CNR) (blue) and Tp'Rh(CO) (green) fragments with the linear alkanes (*n*-pentane to *n*-nonane).

Table S2: Infrared frequencies (cm^{-1}) for a number of Tp complexes in κ^3 and κ^2 configurations. Reproduced from Ref [13].

Complex	Hapticity (κ) of Tp^{iPr}	ν(B−H) (cm^{-1})[a]	Ref.
$Tp^{iPr}Ru(H)(cod)$	2	2471	13
$Tp^{iPr}Rh(nbd)$	2	2472	13
$Tp^{iPr}Rh(cod)$	2	2475	13
$Tp^{iPr}Pd(OO^tBu)py$	2	2476	13
$Tp^{iPr,tBu}Rh(coe)(CO)$	2	2486	13
$Tp^{iPr}M(\mu\text{-}OH)_2MTp^{iPr}$ (M = Mn, Fe, Co, Ni, Cu)	3	2527−2543	26-29
$Tp^{iPr}Fe(OC_6H_4Me\text{-}p)_2$	3	2538	30
$Tp^{iPr}Rh(nbd)$	3	2539	13
$Tp^{iPr}Cu(\mu\text{-}O_2)CuTp^{iPr}$	3	2539	29
$Tp^{iPr}Fe\text{-}OC_6F_5$	3	2540	30
$Tp^{iPr}Rh(coe)(NCMe)$	3	2544	13
$Tp^{iPr}FeCl$	3	2550	30
$Tp^{iPr}RhI_2(NCMe)$	3	2554	13

[a]Observed as KBr pellets. Tp^{iPr} = tris(3,5-diisopropylpyrazolyl)borate; $Tp^{iPr,tBu}$ = tris(3-*tert*-butyl-5-isopropylpyrazolyl)borate; coe = cyclooctene; nbd = norbornadiene; cod = 1,5-cyclooctadiene.

Supporting Information

Probing the Carbon-Hydrogen Activation of Alkanes Following Photolysis of Tp'Rh(CNR)(carbodiimide): A Computational and Time-resolved Infrared Spectroscopic Study

Jia Guan,[†] Alisdair Wriglesworth,[‡] Xue Zhong Sun,[‡] Edward N. Brothers,[&] Snežana D. Zarić,[&] Meagan E. Evans,[#] William D. Jones,[#] Michael Towrie,[%] Michael B. Hall,[*,†] and Michael W. George[*,‡,§]

[†]Department of Chemistry, Texas A&M University, College Station, TX 77843-3255, USA
[‡]School of Chemistry, University of Nottingham, University Park NG7 2RD, UK
[&]Science Program, Texas A&M University at Qatar, P. O. Box 23874, Doha, QATAR
[¶]Department of Chemistry, University of Belgrade, Belgrade, SERBIA
[#]Department of Chemistry, University of Rochester, Rochester, NY 14627, USA
[%]Central Laser Facility, Research Complex at Harwell, Rutherford Appleton Laboratory, Chilton, Oxfordshire OX11 0QX, UK
[§]Department of Chemical and Environmental Engineering, University of Nottingham Ningbo China, 199 Taikang East Road, Ningbo 315100, CHINA

Table of Contents

XYZ-Coordinates Cyclopentane

XYZ-Coordinates Cyclohexane

XYZ-Coordinates Cycloheptane

XYZ-Coordinates Cyclooctane

XYZ-Coordinates N-heptane

XYZ-Coordinates **$^{3}\kappa^{3}$-η^{1}-alkane complex (1)**

XYZ-Coordinates TpRh(CNMe)-N-heptane σ-complex-(1) **[$^{1}\kappa^{2}$-η^{2}-alkane complex (2)]**

XYZ-Coordinates TpRh(CNMe)-N-heptane TS_2-(1)-κ^3

XYZ-Coordinates TpRh(CNMe)-N-heptane TS_2-(1)-κ^2

XYZ-Coordinates TpRh(CNMe)-N-heptane IM-(1)

XYZ-Coordinates TpRh(CNMe)-N-heptane TS_3-(1)

XYZ-Coordinates TpRh(CNMe)-N-heptane product-(1) **[$^{1}\kappa^{3}$-alkyl hydride (3)]**

XYZ-Coordinates TpRh(CNMe)(carbodiimide) ($^{1}\kappa^{3}$-parent)

XYZ-Coordinates $^{1}\kappa^{2}$-parent

XYZ-Coordinates TS between $^{1}\kappa^{2}$-parent and $^{1}\kappa^{3}$-parent

XYZ-Coordinates $^{3}\kappa^{3}$-TpRh(CNMe)

XYZ-Coordinates Free carbodiimide

XYZ-Coordinates $^{1}\kappa^{3}$-1,2-η^{2}-arene complex

XYZ-Coordinates $^{1}\kappa^{2}$-1,2-η^{2}-arene complex

XYZ-Coordinates $^{1}\kappa^{2}$-2,3-η^{2}-arene complex

XYZ-Coordinates TS between $^{1}\kappa^{2}$-1,2-η^{2}-arene complex and $^{1}\kappa^{3}$-1,2-η^{2}-arene complex

XYZ-Coordinates TS between $^{1}\kappa^{2}$-1,2-η^{2}-arene complex and $^{1}\kappa^{2}$-2,3-η^{2}-arene complex

XYZ-Coordinates TpRh(CNMe)-Cyclopentane σ-complex-(1)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane σ-complex-(2)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane TS_2-(1)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cyclopentane TS_2-(1)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cyclopentane TS_2-(2)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cyclopentane TS_2-(2)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cyclopentane IM-(1)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane IM-(2)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane TS_3-(1)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane TS_3-(2)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane product-(1)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane product-(2)

XYZ-Coordinates TpRh(CNMe)-Cyclopentane 1,2-migration

XYZ-Coordinates TpRh(CNMe)-Cyclohexane σ-complex-(axi)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane σ-complex-(equ)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane TS_2-(axi)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cyclohexane TS_2-(axi)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cyclohexane TS_2-(equ)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cyclohexane TS_2-(equ)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cyclohexane IM-(axi)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane IM-(equ)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane TS_3-(axi)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane TS_3-(equ)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane product-(axi)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane product-(equ)

XYZ-Coordinates TpRh(CNMe)-Cyclohexane 1,2-migration

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(1)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(2)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(3)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(4)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(5)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(6)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane σ-complex-(7)

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XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(3)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(4)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(4)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(5)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(5)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(6)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(6)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(7)-κ^3

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_2-(7)-κ^2

XYZ-Coordinates TpRh(CNMe)-Cycloheptane IM-(1)

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XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_3-(4)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_3-(5)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane TS_3-(6)

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XYZ-Coordinates TpRh(CNMe)-Cycloheptane product-(1)

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XYZ-Coordinates TpRh(CNMe)-Cycloheptane product-(6)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane product-(7)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(1/2-ie)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(1/2-ii)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(1/3-ii)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(1/3-ie)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(2/5-ii)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(5/7-ie)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(5/6-ii)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(6/7-ie)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,2-migration-(7/7-ii)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,3-migration-(1/4)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,3-migration-(3/7)

XYZ-Coordinates TpRh(CNMe)-Cycloheptane 1,3-migration-(4/7)

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XYZ-Coordinates TpRh(CNMe)-Cyclooctane σ-complex-(1)

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Experimental Section:

Table S1: Infrared frequencies (cm^{-1}) for a number of Tp complexes in κ^3 and κ^2 configurations. Reproduced from Ref [13,27-31].

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$Tp^{iPr}Pd(OO^tBu)py$	2	2476	13
$Tp^{iPr,tBu}Rh(coe)(CO)$	2	2486	13
$Tp^{iPr}M(\mu\text{-}OH)_2MTp^{iPr}$ (M = Mn, Fe, Co, Ni, Cu)	3	2527−2543	27-30
$Tp^{iPr}Fe(OC_6H_4Me\text{-}p)_2$	3	2538	31
$Tp^{iPr}Rh(nbd)$	3	2539	13
$Tp^{iPr}Cu(\mu\text{-}O_2)CuTp^{iPr}$	3	2539	30
$Tp^{iPr}Fe\text{-}OC_6F_5$	3	2540	31
$Tp^{iPr}Rh(coe)(NCMe)$	3	2544	13
$Tp^{iPr}FeCl$	3	2550	31
$Tp^{iPr}RhI_2(NCMe)$	3	2554	13

[a]Observed as KBr pellets. Tp^{iPr} = tris(3,5-diisopropylpyrazolyl)borate; $Tp^{iPr,tBu}$ = tris(3-*tert*-butyl-5-isopropylpyrazolyl)borate; coe = cyclooctene; nbd = norbornadiene; cod = 1,5-cyclooctadiene. [b]Ref. here refer to **References** Section in the paper.

The experimental results below are taken from the Ph.D dissertation of Alisdair Wriglesworth, University of Nottingham.

Table S2: Lifetimes for the C-H activation of linear alkanes by the different rhodium fragments studied: CpRh(CO); Cp*Rh(CO); Tp*Rh(CNR); and Tp*Rh(CO).

	CpRh(CO) lifetime (ns)	Cp*Rh(CO) lifetime (ns)	Tp'Rh(CNR) lifetime (ns)	Tp*Rh(CO) lifetime (ns)
***n*-pentane**	9.8 (± 0.2)	8.8 (± 0.5)	24.1 (± 1.5)	11.4 (± 0.4)
***n*-hexane**	9.8 (± 0.2)	8.8 (± 0.2)	25.5 (± 1.3)	11.5 (± 0.3)
***n*-heptane**	11.0 (± 0.3)	10.8 (± 0.4)	27.4 (± 2.0)	11.6 (± 0.3)
***n*-octane**	12.5 (± 0.6)	12.5 (± 0.3)	28.6 (± 0.9)	12.2 (± 0.2)
***n*-nonane**	13.4 (± 0.5)	14.1 (± 0.8)	27.1 (± 1.3)	12.6 (± 0.4)

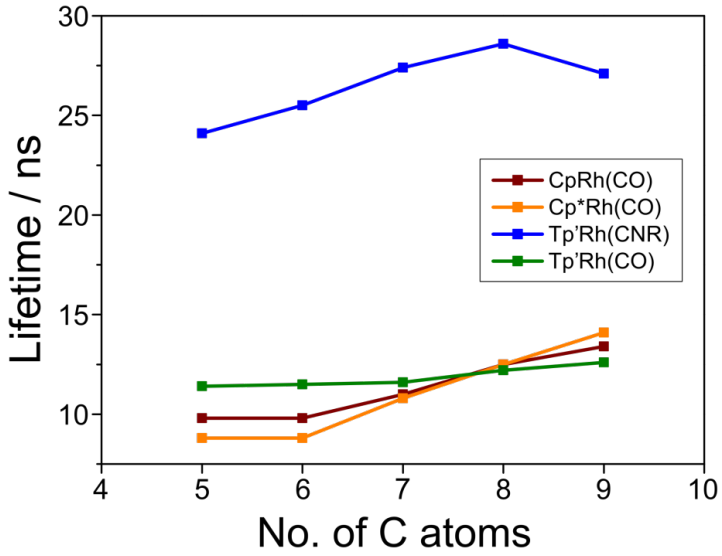

Figure S1: Lifetime trends for the CpRh(CO) (red), Cp*Rh(CO) (orange), Tp'Rh(CNR) (blue) and Tp'Rh(CO) (green) fragments with the linear alkanes (*n*-pentane to *n*-nonane).

Theoretical Section:

Frequency Scaling Procedure from Calculated to Experimental Values

υ(CNMe) and υ(BH) of the experimentally observed species, including the parent TpRh(CNR)(carbodiimide), complexes **1**, **2** and **3**, were calculated, and a ratio of $\upsilon(CNMe)_{exp}$ and $\upsilon(CNMe)_{calc}$ was calculated by $\upsilon(CNMe)_{exp}/\upsilon(CNMe)_{calc}$, which yielded a scaling factor for that specific species. Same method was utilized for the scaling factor of υ(BH). As shown in **Table S3**, the data of the four reaction species generates two sets of 4 different scaling factors for υ(CNMe) and υ(BH), respectively, where averaged scaling factors of 0.928 and 0.970 were obtained for υ(CNMe) and υ(BH) regions, respectively. All the υ(CNMe) and υ(BH) reported in this work are scaled using these scaling factors.

Table S3. Experimentally measured and calculated υ(CNMe) and υ(BH) of reaction species in the C-H activation of n-heptane catalyzed by TpRh(CNMe). SSF are the specific scaling factors calculated for each species.

Reaction Species	**υ(CNMe) (cm^{-1})**			**υ(BH) (cm^{-1})**		
	exp	*calc*	*SSF**	*exp*	*calc*	*SSF*
TpRh(CNR)(carbodiimide)	2178	2331	***0.934***	2524	2603	***0.970***
κ^3-η^1-alkane complex (1)	2083	2252	***0.925***	2520	2587	***0.974***
κ^2-η^2-alkane complex (2)	2108	2269	***0.929***	2485	2571	***0.967***
alkyl hydride (3)	2142	2314	***0.926***	2518	2597	***0.970***
Averaged Scaling Factor	-	-	***0.928***	-	-	***0.970***

*SSF: specific scaling factor.

Effect of Dispersion Correction on the Stability of σ-Complexes

Under BMK functional that doesn't include dispersion correction, the lowest σ-complexes exhibit a general trend of destabilized as a function of the c-alkanes size, whereas the inclusion of dispersion correction with GD3BJ model significantly lowers their relative energies, especially, the σ-complexes in c-heptane and c-octane get even more stabilized than those in c-pentane and c-hexane, as shown in **Table S4**. MN12SX functional used in this work has also produced similar trend of enhanced stability as c-alkanes get larger, which validates the significance of dispersion correction on evaluating the stabilities of σ-complexes due to the dispersion effects implicitly built into its parametrization scheme.

Table S4. Relative energies (kcal/mol) of the lowest-energy σ-complexes calculated using BMK[1] (with and without dispersion corrections (modeled by GD3BJ[2])) and MN12SX functionals.

	BMK	BMK (GD3BJ)	MN12SX
***c*-pentane**	14.9	5.8	-3.6
***c*-hexane**	15.9	5.9	-2.9
***c*-heptane**	15.3	3.6	-4.3
***c*-octane**	16.4	4.6	-4.3

[1]Boese, A. D.; Martin, J. M. L. *J. Chem. Phys.* **2004**, *121*, 3405.
[2]Grimme, S.; Ehrlich, S.; Goerigk, L. *J. Comput. Chem.* **2011**, *32*, 1456.

XYZ-Coordinates

TpRh(CNMe)

G = -944.399269

B	-0.262797935884	-0.259674502845	-0.176048745662
H	0.703176182455	-0.398340749447	-0.868220131665
N	0.071883416147	0.674193809088	0.997631928160
C	1.241695319658	1.255624265800	1.312052185568
C	-0.284635055704	1.809367929135	2.788010346764
C	1.063169933216	2.000148620555	2.461900143255
H	2.115646154262	1.096608334465	0.693136519498
H	-0.860523422340	2.208998107987	3.614387425270
N	-0.713391171958	-1.626578664012	0.362656164112
C	-0.154475551679	-2.835198683518	0.183127253175
C	-1.932880603327	-3.019590566026	1.455154037861
C	-0.905940869217	-3.769189147965	0.869642189960
H	0.737606539042	-2.941294233906	-0.421079673907
H	-2.755620659081	-3.342979179384	2.081870419811
N	-1.404925875485	0.358200867840	-1.002416629979
C	-1.414015323955	0.717906231435	-2.294692188898
C	-3.372161594912	1.139476159535	-1.400360204255
C	-2.661722989431	1.228093127094	-2.600291055617
H	-0.529397035189	0.584117110253	-2.904021677402
H	-4.392441300349	1.425895278681	-1.176310279999
N	-1.807516087596	-1.736076499768	1.144212655580
N	-2.608766946747	0.615540987123	-0.445972725994
N	-0.869256303153	1.012687429620	1.902954858564
Rh	-2.898508142393	0.145149619772	1.616710949794
C	-3.407587098345	-0.184061671377	3.439060714530
N	-3.622734159570	-0.421728285024	4.566251166164
C	-3.911917610727	-0.694907259774	5.912642209535
H	-3.050225544474	-1.168106426466	6.398504416934
H	-4.149222273355	0.233282582146	6.446398618885
H	-4.771785682527	-1.371587870444	5.987132560536
H	1.798363866710	2.594487746220	2.984218734451
H	-3.005762864004	1.607802180341	-3.550785306988
H	-0.737012190086	-4.834026627132	0.934066411962

Cyclopentane

G = -196.297617

C	0.013627519129	0.003267141417	0.009415265063
C	0.007951363767	-0.013695747404	1.538552815357
C	1.494152281144	0.003969073444	1.880705989487

C	2.079432687482	-1.007281459139	0.894106588762
C	1.245394478139	-0.836295922338	-0.394423768073
H	-0.918770507796	-0.371576960543	-0.427992606025
H	0.132391537715	1.038571617970	-0.339446139346
H	-0.441079405121	-0.949029910970	1.906451133257
H	-0.558122973273	0.815940805447	1.978065210854
H	1.902972167318	1.006972471982	1.684034062980
H	1.711008967512	-0.238152331549	2.927729657345
H	3.154026980844	-0.871769645761	0.726526603725
H	1.947863147779	-2.021443969213	1.296391332027
H	1.821635722917	-0.334761714544	-1.181198424826
H	0.950144852443	-1.810111128800	-0.803218800587

Cyclohexane

G = -235.561595

C	-4.321028589449	-0.868503727351	1.456407044976
C	-2.795153458094	-0.872333862469	1.461611149108
C	-2.242340884401	0.549764870086	1.457384337931
C	-2.793895386112	1.357093342873	2.628797515068
C	-4.319770517467	1.360923477992	2.623593410937
C	-4.872583091160	-0.061175254563	2.627820222114
H	-1.144284354733	0.535794233296	1.482798878886
H	-2.439169733322	-1.394815105172	2.364795314259
H	-2.408932143000	-1.438039367266	0.602914883473
H	-4.677009859401	-0.423290187220	0.512723106583
H	-4.708593931669	-1.896001023983	1.480779480505
H	-2.437914116160	0.911879802742	3.572481453462
H	-2.406330043892	2.384590639506	2.604425079540
H	-4.705991832561	1.926628982789	3.482289676571
H	-4.675754242239	1.883404720695	1.720409245785
H	-4.588753710262	-0.555352609322	3.571577767056
H	-5.970639620828	-0.047204617773	2.602405681158
H	-2.526170265299	1.043942224844	0.513626792988

Cycloheptane

G = -274.809027

C	-0.301708268263	1.498994304843	0.408049857857
C	-1.536274476005	0.755511726344	-0.102932730960
C	-1.536176554453	-0.755711512459	0.102941122133
C	0.955369397747	1.224371549246	-0.422043964054

C	-0.301517112330	-1.499034969658	-0.408047695713
C	1.771413638652	0.000113272389	-0.000004088628
C	0.955529339552	-1.224250230356	0.422039784244
H	-0.121696338797	1.257406333420	1.468289834486
H	-1.640484054897	0.972154210243	-1.178799660080
H	-1.640352770514	-0.972367418342	1.178808580301
H	-0.121541674248	-1.257423820321	-1.468288585083
H	0.650387526277	1.119047396195	-1.474849819529
H	2.436521931691	-0.274888180382	-0.831885181792
H	-0.518238571732	2.575857868515	0.380116485702
H	-2.435785746636	1.170133159209	0.374772564642
H	-2.435636785936	-1.170448896069	-0.374759624209
H	1.617200227669	2.101008982402	-0.398669620291
H	-0.517908492003	-2.575926430294	-0.380113213885
H	2.436490528963	0.275200495842	0.831873753507
H	1.617473044848	-2.100802343581	0.398662010431
H	0.650539210416	-1.118965497185	1.474847190923

Cyclooctane

G = -314.059934

C	-0.012439806309	1.599459073696	0.637739127779
C	-1.181048752295	1.317199682363	-0.319120113464
C	1.382604604188	-1.301861471516	0.076728356370
C	-1.924263146280	-0.000013672480	-0.086342240037
C	-0.012415375588	-1.599452535500	0.637749490473
C	-1.181028397540	-1.317217011684	-0.319111804186
H	-0.175263387413	1.054371603516	1.577011769209
H	-2.297185190067	-0.000013281570	0.951765774075
H	2.115339798028	-1.338591469103	0.897822730695
H	-0.175247408856	-1.054361522580	1.577018612049
H	-0.027260722316	2.660862427075	0.921648604024
H	1.656278865881	-2.124817051242	-0.601731404374
H	-2.821642871269	-0.000022606002	-0.722782335571
H	-0.027220168910	-2.660854301844	0.921665743933
C	1.382584659150	1.301885657906	0.076719688144
H	2.115319425735	1.338632375236	0.897813694222
H	1.656246200451	2.124840916082	-0.601745591970
C	1.557110422344	0.000010842682	-0.698439251836
H	0.882019627196	0.000002761098	-1.566464719189
H	2.569066258051	0.000017156034	-1.128899768459
H	-1.923149231948	2.121124346113	-0.215835678662
H	-1.923116522435	-2.121152471268	-0.215822631971
H	-0.837169650761	-1.376348407073	-1.363640141049

H	-0.837191229036	1.376329960061	-1.363648910203

N-heptane

G = -275.995247

C	-2.802202641208	1.651358821526	0.001194747784
C	-1.282376501254	1.623230973103	0.001646536665
H	-3.192513338206	2.675350840681	0.001922540779
H	-3.206429039292	1.142838098949	-0.883493074268
H	-3.206981843070	1.141370601984	0.884784393692
C	-0.715258843969	0.210347330079	0.000651275623
H	-0.899924877324	2.166802024225	-0.876099220587
H	-0.900474040300	2.165344192287	0.880532259921
C	0.805748568127	0.165488316882	0.001089548570
H	-1.097305698796	-0.335551045991	0.878949072555
H	-1.096756189531	-0.334092294781	-0.878790096263
H	1.186901045187	0.711603214986	-0.877314989888
H	1.186351469245	0.710144286772	0.880637461995
C	1.371616701178	-1.247051359036	0.000094182358
C	2.893377312866	-1.292965035286	0.000531815505
H	0.991524950577	-1.792472600772	-0.879347564753
H	0.990975441312	-1.793931351982	0.878391604064
H	3.271694398051	-0.746506571275	-0.877212838029
H	3.271145235074	-0.747964403213	0.879418642479
C	3.443130741747	-2.710156989308	-0.000472449466
H	4.538900409463	-2.723989952332	-0.000141366934
H	3.104033163205	-3.266014888021	0.883099662674
H	3.104585966982	-3.264547391056	-0.885177805285

$^{3}\kappa^{3}$-η^{1}-alkane complex (1)

G = -1220.384910

B	-1.918270385991	-1.247749551712	1.122127882024
H	-2.366077167050	-2.001396919121	1.936381211505
N	-0.429697440503	-0.996858118498	1.415390531432
C	0.319477049824	-1.441132334092	2.438250089581
C	1.517834064067	-0.122894010058	1.157365766386
C	1.587628084117	-0.906428140344	2.315072301174
H	-0.105855943244	-2.105030579786	3.180208901773
H	2.282261500264	0.483073501413	0.683860237036
N	-2.684410389885	0.084169189453	1.172895919728
C	-3.680268048642	0.455187185801	1.995253749312

C	-3.204352872471	2.095005276840	0.617327966768
C	-4.051074697325	1.746963914923	1.676240032908
H	-4.052245913200	-0.228892300910	2.747441915828
H	-3.145229439961	3.017788315461	0.052395474079
N	-2.063189586674	-1.859046887760	-0.281790785375
C	-2.582958137223	-3.042128440595	-0.641978931320
C	-1.899881819600	-1.964478408176	-2.426709014982
C	-2.500299752883	-3.157833752361	-2.017017776593
H	-2.974433156110	-3.717089227390	0.108287205442
H	-1.638722650691	-1.625526489403	-3.422129243204
N	-2.389116586679	1.090787344165	0.323239367485
N	-1.640966763047	-1.190635087031	-1.376964190599
N	0.304452496145	-0.187300080725	0.623783079029
Rh	-0.732365773664	0.724963579604	-1.118908266659
C	0.137639696056	2.436566264855	-1.168958100932
N	0.679709967620	3.473324948636	-1.102108526677
C	1.330517490191	4.717094959391	-1.071128968548
H	1.354783449978	5.108828407945	-0.047244950777
H	2.360991304376	4.615106737234	-1.432144380064
H	0.804570928555	5.436906866502	-1.709935477160
H	2.434711272226	-1.059616747692	2.967441229616
H	-2.828198935811	-3.983128739877	-2.631298499496
H	-4.821314284570	2.345985621045	2.139296568060
C	1.623847950256	-1.291771786996	-2.742893058904
C	2.741961145617	-0.371491420405	-2.283619502396
H	0.873778554108	-0.747943150601	-3.333419801958
H	2.009542405436	-2.115239804200	-3.359220678086
H	1.102927343715	-1.730386723815	-1.880717816099
C	3.773219819424	-1.082729584019	-1.419414835686
H	3.242450436585	0.082429932863	-3.153536703832
H	2.303251437761	0.467670961653	-1.717610016382
C	4.868691472922	-0.163643820311	-0.899056044702
H	3.261454912959	-1.561648865109	-0.568493531234
H	4.229712697190	-1.905085564633	-1.994526858240
H	5.402631467375	0.291246576958	-1.749659205239
H	4.410824478263	0.679883439619	-0.354123761218
C	5.867177970318	-0.863066598691	0.011114326055
C	6.961934360465	0.054911909326	0.537073571463
H	6.327496270090	-1.705407417617	-0.530859692128
H	5.329047120551	-1.314399727013	0.861137767875
H	7.497341912462	0.503726074245	-0.313962719158
H	6.499985451873	0.895509818891	1.078073002779
C	7.949294051787	-0.659555421046	1.445565411580
H	8.729287771108	0.015954440479	1.814817049002
H	7.442394368250	-1.090047161615	2.318731318449
H	8.446489923290	-1.483435765698	0.917719321277

TpRh(CNMe)-N-heptane σ-complex-(1)

[$^{1}\kappa^{2}$-η^{2}-alkane complex (2)]

G = -1220.400208

B	-2.868693388438	-1.117678971536	1.057095992366
H	-3.721547066417	-1.681533167215	1.684853840323
N	-1.546156765377	-0.929615973374	1.807894997692
C	-1.167787054350	0.101112640987	2.592056981259
C	0.408944997216	-1.417019699660	2.500715429906
C	0.098729824578	-0.168169538576	3.066047786690
H	-1.818614454396	0.954223651319	2.744350491943
H	1.309413246963	-2.010764316591	2.615435649053
N	-3.399387029908	0.281999243219	0.669189236491
C	-4.531226284175	0.891044353150	1.052484731989
C	-3.405742788609	2.222710097575	-0.280784603351
C	-4.580363325562	2.143916429056	0.470779895143
H	-5.219569764102	0.382310473592	1.714997516825
H	-3.034208501918	3.018981348813	-0.913435122584
N	-2.591349626041	-1.899730435258	-0.231564490161
C	-2.991176130682	-3.123672590119	-0.593848966205
C	-1.676217964045	-2.295576152781	-2.141606147274
C	-2.429739422228	-3.425721247173	-1.821383062788
H	-3.641348963743	-3.695992165579	0.054910775663
H	-1.080706144925	-2.086369827859	-3.022243107642
N	-2.704661137134	1.099228008751	-0.153696814596
N	-1.777741437080	-1.385498026997	-1.175583216446
N	-0.582334033508	-1.872360577522	1.746136164578
Rh	-0.934365735814	0.491135803755	-0.913469161670
C	-0.195086732257	2.208238561974	-0.643475942193
N	0.250493723219	3.274142019229	-0.457438736040
C	0.821239641570	4.526299959485	-0.174675121714
H	0.479276048844	4.884385850093	0.803458784979
H	1.914565408824	4.445901234492	-0.156089027760
H	0.536017083775	5.259188668490	-0.938867699350
H	0.702022945638	0.443605439805	3.721704979773
H	-2.549700822801	-4.329775773451	-2.399171487427
H	-5.356222801489	2.888398538386	0.568674130768
C	1.186512219319	-0.517438899613	-1.397398436444
C	2.519201745968	0.209380327901	-1.333977445097
H	0.466469566774	0.079467283697	-2.054243988584
H	1.250285002091	-1.475644039385	-1.928729444018
H	0.826693636842	-0.757036761985	-0.380887081931
C	3.567449804267	-0.600611668199	-0.583005690888

H	2.882235988747	0.436524831052	-2.347942963169
H	2.381382597628	1.178337818813	-0.831125615958
C	4.914411613756	0.100114754916	-0.485519723060
H	3.190215969087	-0.822362635079	0.428505724085
H	3.697311875014	-1.577305619128	-1.076749512321
H	5.283715428086	0.327064723811	-1.499176989455
H	4.782643502490	1.075314739926	0.011613283270
C	5.963835322591	-0.708177011522	0.263347718313
C	7.312003618004	-0.008183777292	0.364469584498
H	6.096433982221	-1.683308703010	-0.233190226406
H	5.594622681850	-0.936346319114	1.276469300904
H	7.678374009660	0.219105371706	-0.648654413026
H	7.177463392494	0.965394406329	0.860896010929
C	8.349692225494	-0.827730393307	1.114253381026
H	9.312792247414	-0.308833615353	1.177807912055
H	8.019339396207	-1.041182602043	2.138839931251
H	8.524230628370	-1.791800071598	0.619674005785

TpRh(CNMe)-N-heptane TS_2-(1)-κ^3

G = -1220.388008

B	-3.383434839973	-0.876605888121	0.553001524121
H	-4.463344557789	-1.323906831142	0.811485501988
N	-2.548366699635	-0.763318877054	1.824292419412
C	-2.828897355022	-1.185174971392	3.071726003517
C	-0.828185442447	-0.289810951145	2.999954161987
C	-1.742448695584	-0.899362364520	3.873375122904
H	-3.778814215216	-1.654340634767	3.295742091325
H	0.162571946426	0.097915998574	3.209828814812
N	-3.547034023633	0.508038004894	-0.098208246086
C	-4.659867303220	1.252220197909	-0.189885430441
C	-2.976334578770	2.339040831071	-1.078878439694
C	-4.343598901452	2.443743003917	-0.813798123645
H	-5.598270700929	0.875579316768	0.196027159909
H	-2.309002449619	3.034699982719	-1.572422256240
N	-2.689076649382	-1.809304611339	-0.460742208149
C	-3.104748610986	-3.009803992227	-0.889434256804
C	-1.198522759342	-2.513566250548	-1.849449732687
C	-2.176611895810	-3.506390170950	-1.785019774269
H	-4.035716238992	-3.423234446674	-0.523786288760
H	-0.294675868968	-2.472574761197	-2.443787169444
N	-2.507239356186	1.173437482260	-0.644093221935
N	-1.512106773865	-1.499769935414	-1.046440371876
N	-1.319486256155	-0.211523217394	1.771281642083

Rh	-0.576092818441	0.332046594982	-0.699642610566
C	0.211346462693	2.037453966787	-0.524877529089
N	0.677957568636	3.104252206343	-0.424945096634
C	1.286606307513	4.360559406569	-0.269523188543
H	0.778680273277	4.931339127731	0.516445060898
H	2.339357326018	4.235089430536	0.010690832553
H	1.237548664494	4.928417702972	-1.206361233007
H	-1.630990950736	-1.097720365123	4.929556806950
H	-2.207920178015	-4.444026137991	-2.319337075079
H	-5.006915364843	3.261899607822	-1.051425784548
C	1.339467374048	-0.669040364715	-0.724057810174
C	2.612652261090	0.144701821191	-0.542436583237
H	0.570630865434	-0.033176159214	-1.726783017608
H	1.533728474170	-1.494481451654	-1.428623964694
H	1.057772206538	-1.166027646705	0.218373756027
C	3.838963241690	-0.723380379178	-0.287797949485
H	2.793626462601	0.772818462221	-1.430471584169
H	2.485768416753	0.843704362639	0.298405611900
C	5.116735413588	0.078752204143	-0.087081320260
H	3.660056046264	-1.356472302536	0.596229951280
H	3.973808738763	-1.418912455910	-1.132265507697
H	5.290063201805	0.715557638958	-0.970333973451
H	4.983648101338	0.770895055158	0.760790412141
C	6.344888257148	-0.785530561472	0.158138775317
C	7.623711827244	0.016147367590	0.357463272166
H	6.478509388635	-1.478720759254	-0.688522414835
H	6.173106141119	-1.422243906278	1.041409337908
H	7.793620958882	0.651082012150	-0.525915663898
H	7.488568901772	0.707922538581	1.203381494646
C	8.841006807397	-0.861082849509	0.601104662469
H	9.751611887531	-0.267826636455	0.741705776315
H	8.707764700663	-1.481723998996	1.496443158037
H	9.014274551481	-1.539660595608	-0.243944523659

TpRh(CNMe)-N-heptane TS_2-(1)-κ^2

G = -1220.387277

B	-3.004973634348	-1.167422068517	1.085108794990
H	-3.886012302954	-1.750250021462	1.651157673894
N	-1.724410700633	-0.982824275886	1.908944157235
C	-1.312363609263	0.089565139405	2.623927169111
C	0.106598599671	-1.568049931446	2.829010111614
C	-0.123248380467	-0.242370493789	3.236681926193
H	-1.890565418714	1.005902755089	2.641660535680

H	0.934020873842	-2.222332668129	3.080769624497
N	-3.507076526920	0.239445460741	0.696992035191
C	-4.652030320721	0.857663059926	1.016058874656
C	-3.395176442519	2.211971375677	-0.167939440005
C	-4.629658410349	2.132886995384	0.479972543148
H	-5.400197767227	0.342732541100	1.605182310424
H	-2.958192223208	3.025463309828	-0.734387555572
N	-2.635444550630	-1.928594761437	-0.195524664292
C	-3.056297339213	-3.121373910420	-0.631127412289
C	-1.542321011073	-2.334397340975	-2.009107720277
C	-2.384294898041	-3.427142515794	-1.800669607276
H	-3.797718600611	-3.672971808954	-0.067848026813
H	-0.841895306001	-2.141593423097	-2.812413551922
N	-2.728424026008	1.069007151503	-0.031909272400
N	-1.698958452866	-1.440507736536	-1.036015756645
N	-0.857684202457	-2.009958163939	2.034455272901
Rh	-0.828088303355	0.405726133180	-0.685163397561
C	-0.066946838593	2.118606963526	-0.415557172834
N	0.396186509190	3.177267516047	-0.251546983334
C	1.046356709079	4.401271410000	-0.016256386407
H	0.687510946643	4.843877139733	0.919815650228
H	2.128111767485	4.239263279034	0.060104188076
H	0.849754629061	5.100621960721	-0.837062246763
H	0.481838519370	0.378562019027	3.881866292404
H	-2.486689694125	-4.312166128694	-2.410376129872
H	-5.396662656248	2.890176651092	0.544346512164
C	1.052050871739	-0.543106506449	-0.830766434006
C	2.321308263840	0.278851756055	-0.682530055184
H	0.149287437435	0.198972477895	-1.870293296284
H	1.189552661195	-1.305681661443	-1.614625802470
H	0.840511573988	-1.110564235686	0.093439164016
C	3.566224069883	-0.591868023505	-0.553557835579
H	2.445549737823	0.961582508523	-1.539521866413
H	2.241289800851	0.918869086339	0.209803539342
C	4.845848735120	0.210706103043	-0.366448356256
H	3.437679953647	-1.282953839909	0.294806380659
H	3.660704580091	-1.228198388753	-1.448465499001
H	4.966348841460	0.908547850533	-1.211749319695
H	4.751953590651	0.841214157331	0.533148264316
C	6.093275610054	-0.652394965375	-0.246372339693
C	7.372540592794	0.150656832766	-0.055217192105
H	6.189919082931	-1.281991612568	-1.146018689637
H	5.973231706426	-1.352148467934	0.596734491921
H	7.490068578404	0.849647178915	-0.897894678900
H	7.274315645142	0.777999428183	0.844338324947
C	8.609790956106	-0.724667524401	0.062051135767

H	9.520186879127	-0.130380898464	0.199791208270
H	8.528834233766	-1.410411895308	0.915107809952
H	8.746622049733	-1.337609481726	-0.838050952113

TpRh(CNMe)-N-heptane IM-(1)

G = -1220.405134

B	-2.942630382347	-1.025011103792	0.987187918007
H	-3.730272270666	-1.570629313005	1.703330130387
N	-1.600857766194	-0.661547869834	1.666235413814
C	-1.210455756048	0.511755336925	2.243627234763
C	0.170063350583	-1.109203534083	2.770600739882
C	-0.058569614780	0.268026987027	2.954990471658
H	-1.791792032052	1.416516070573	2.108486442608
H	0.978739336504	-1.718504846906	3.159232945323
N	-3.544522414905	0.287076716808	0.452359206272
C	-4.748569752296	0.845649641692	0.648293784118
C	-3.573130035553	2.082580958283	-0.736046077029
C	-4.815662055783	2.008553123889	-0.096171649938
H	-5.470043773818	0.372993868087	1.302561508265
H	-3.190473437282	2.828067320865	-1.422966857280
N	-2.585701260659	-1.927403966218	-0.201886250139
C	-3.019439604349	-3.140876548346	-0.562079394454
C	-1.481903762093	-2.461399885659	-1.978341973566
C	-2.341793130500	-3.527628843165	-1.704459635838
H	-3.771156854177	-3.648003410210	0.028757691431
H	-0.760959869486	-2.332596661881	-2.776177371362
N	-2.819313886014	1.042711007758	-0.401755007464
N	-1.638760750647	-1.507730377056	-1.068218558170
N	-0.757504214979	-1.664950796814	2.011223107529
Rh	-0.788426492906	0.333942937245	-0.699733306972
C	0.018578260190	2.026237052727	-0.383402863696
N	0.515361809636	3.061716536152	-0.195190027867
C	1.265979334913	4.227273579980	0.043737214820
H	0.907013988096	4.726462872405	0.950366210127
H	2.322415443506	3.963788266864	0.173770961584
H	1.170233619160	4.916618480510	-0.802398288541
H	0.528017638323	0.977180543499	3.521574864607
H	-2.447600405082	-4.451138378778	-2.253593329215
H	-5.643432636099	2.698355096126	-0.168944500145
C	1.042210321182	-0.584546856553	-0.799611600961
C	2.296430179205	0.197397789747	-0.436809772246
H	-0.632178046348	0.641522720068	-2.178083593789
H	1.176126446464	-1.037366090069	-1.797018200723

H	0.930426785933	-1.428651788152	-0.095240367216
C	3.561941287907	-0.654064191467	-0.426386028479
H	2.443282869438	1.035985243605	-1.140101100875
H	2.174628351363	0.653829113057	0.562001048112
C	4.817621428712	0.125430400560	-0.061792136372
H	3.428638669472	-1.488648262209	0.280876967610
H	3.694084819000	-1.119295060641	-1.416980557730
H	4.947015553072	0.960892400161	-0.770330995316
H	4.682836883224	0.590613290724	0.929130250986
C	6.082527920543	-0.720480847302	-0.049840770486
C	7.336431784477	0.062348989565	0.314832191247
H	6.219588842131	-1.186391129336	-1.039477479909
H	5.956327790525	-1.555741274230	0.658330739898
H	7.461326280394	0.895631583495	-0.394202182854
H	7.197522569663	0.527332405126	1.303329490414
C	8.590928420792	-0.796201586950	0.323665942808
H	9.482763955285	-0.216530703332	0.587922489285
H	8.502282920002	-1.617000188514	1.046901599623
H	8.767875345372	-1.246860819024	-0.661356686547

TpRh(CNMe)-N-heptane TS_3-(1)

G = -1220.402037

B	-2.949368063822	-0.941649605847	1.134691607502
H	-3.749746586661	-1.441901689284	1.872290583500
N	-1.690395235077	-0.380620623145	1.836264036390
C	-1.622389174978	0.741416393185	2.592327446894
C	0.250418041700	-0.392387693553	2.733610005371
C	-0.382629600539	0.778562343743	3.189226116398
H	-2.458445790916	1.429611940128	2.637268780080
H	1.249331904284	-0.754802290672	2.950377384580
N	-3.578607589353	0.265977993134	0.416093474952
C	-4.817280569007	0.780186041389	0.437200047759
C	-3.550771479422	1.942994210007	-0.931052100246
C	-4.849880032481	1.868547100203	-0.415203647008
H	-5.583900686878	0.335240602585	1.058949297895
H	-3.127836497579	2.639432036763	-1.645305471799
N	-2.505815244944	-1.966933618479	0.083460678014
C	-2.869077514002	-3.245262843307	-0.082594967596
C	-1.425056249372	-2.688148966684	-1.641657013658
C	-2.203199002328	-3.753393549207	-1.182812234301
H	-3.574202699234	-3.702679704347	0.599225648896
H	-0.732679371049	-2.635348970354	-2.472917205532
N	-2.796602492985	0.976333784903	-0.422962531106

N	-1.618900779093	-1.621665098212	-0.876342883040
N	-0.535245477540	-1.093161419385	1.930013486631
Rh	-0.764941997431	0.242344466097	-0.691781781141
C	0.037612120856	1.945959677011	-0.435498670441
N	0.523238723078	2.987766555867	-0.256825707634
C	1.237397005485	4.173611668656	-0.009144169974
H	0.903807327319	4.620893227479	0.933559138423
H	2.308830421259	3.951028692722	0.058901918641
H	1.071271977418	4.889986954310	-0.821239314275
H	0.006023812915	1.536934088338	3.854121382982
H	-2.268168436671	-4.750849966743	-1.590781818319
H	-5.689667420845	2.512036971113	-0.632144686204
C	1.068540889365	-0.657822899487	-0.923611464616
C	2.323788982630	0.116182122577	-0.545573186573
H	-0.723763058278	0.538919264263	-2.176821231841
H	1.172943266730	-1.020173802896	-1.961030497867
H	0.998926656042	-1.555152916757	-0.285927714990
C	3.595917261746	-0.723574891761	-0.603917364895
H	2.449893554564	0.990055408447	-1.208574352367
H	2.219667952381	0.523806523344	0.476108122383
C	4.855531210120	0.048527862583	-0.237111524948
H	3.486911536483	-1.589639106862	0.068872558913
H	3.706068834946	-1.144041602834	-1.617012718430
H	4.963893210707	0.912874245910	-0.913741612530
H	4.741901116568	0.472364051837	0.774760533898
C	6.124357700216	-0.790017526842	-0.289428839373
C	7.383514614502	-0.015842330199	0.075516537434
H	6.239240273421	-1.215651063211	-1.299839015634
H	6.019224472479	-1.653422247792	0.387786970384
H	7.487900161986	0.845216539971	-0.602973886623
H	7.266799399957	0.409286707969	1.084583970258
C	8.641173492560	-0.868044276558	0.020282039539
H	9.537014688524	-0.294957108405	0.285380471911
H	8.573316129612	-1.716941651120	0.712688300600
H	8.795750910631	-1.278984830593	-0.985663647265

TpRh(CNMe)-N-heptane product-(1)

[$^{1}\kappa^{3}$-alkyl hydride (3)]

G = -1220.429052

B	-3.217173189489	-0.696054944890	1.111288552882
H	-4.164642874107	-1.058859444037	1.743212939460
N	-2.111298257890	-0.190334738700	2.049264639574
C	-2.069897438249	-0.125611795916	3.389914756298

C	-0.154726522623	0.548114061308	2.553122032383
C	-0.826884098406	0.348187337622	3.764454658281
H	-2.927154012202	-0.424847486101	3.979327992820
H	0.852892259042	0.901942043588	2.365428511020
N	-3.621318348818	0.430070985575	0.146367795786
C	-4.814404910358	1.018698479612	-0.035717548709
C	-3.351048508937	1.856534067886	-1.441132548983
C	-4.690796408834	1.950191890891	-1.048545224860
H	-5.665101065252	0.728213201148	0.567365692412
H	-2.813703872896	2.394536770246	-2.212860524701
N	-2.655203378192	-1.863812185458	0.280530558541
C	-3.087613859530	-3.130316859005	0.186070187478
C	-1.348747172464	-2.849606511512	-1.125533543832
C	-2.277228027094	-3.806106010655	-0.706128263916
H	-3.942953756392	-3.457454724467	0.763093234533
H	-0.527573063231	-2.933872404813	-1.826051187401
N	-2.719752375727	0.941938209434	-0.716772379026
N	-1.584873523135	-1.689769047116	-0.525603738894
N	-0.937043392299	0.222824139918	1.532733212502
Rh	-0.696793666461	0.183975975620	-0.629666628734
C	0.110956924210	1.886811766403	-0.804692634420
N	0.600303409749	2.937015857592	-0.923059633287
C	1.306165195098	4.143502993162	-1.071773266930
H	0.954127647282	4.879583748907	-0.340536172269
H	2.377030615117	3.967536687411	-0.914076091819
H	1.157203908179	4.546238627839	-2.080038801414
H	-0.460796954660	0.520377438772	4.765733913610
H	-2.348687301921	-4.839312195420	-1.011284151391
H	-5.458238013052	2.596351080150	-1.448189528796
C	1.139827936499	-0.739379735020	-0.466529185289
C	2.409425923111	0.101013267211	-0.447324242900
H	-0.553017308347	0.070620828357	-2.172168624414
H	1.232248895930	-1.477629109063	-1.280487184796
H	1.088774337482	-1.325116503295	0.469210748242
C	3.685085624213	-0.713981044834	-0.259644071091
H	2.494436352548	0.677551179105	-1.384876800926
H	2.358021916649	0.854857574663	0.359839962057
C	4.952363694184	0.129241619216	-0.237782016304
H	3.611809699805	-1.290771423763	0.676842433523
H	3.756762938057	-1.461875097811	-1.066153653501
H	5.023649237755	0.704932191855	-1.175817736225
H	4.878393743255	0.878382870691	0.568523631132
C	6.225852883337	-0.682485243073	-0.050452475114
C	7.491316990031	0.163750446728	-0.027385588162
H	6.303471206268	-1.430870994253	-0.856134791590
H	6.156793694714	-1.258984137975	0.886657009464

H	7.559329651796	0.737959966769	-0.964532614288
H	7.411872904130	0.911001213000	0.777583262393
C	8.754065083421	-0.661324820895	0.161613344579
H	9.654230971071	-0.036233387351	0.175706697566
H	8.722946959267	-1.219732374826	1.106033988811
H	8.871518698365	-1.394086300430	-0.647064901364

TpRh(CNMe)(carbodiimide) ($^1\kappa^3$-parent)

G = -1363.240347

B	-3.145680939149	-0.763199528297	-0.244826778693
H	-4.282094492513	-1.108503928105	-0.371431126997
N	-2.347433483765	-1.806890393194	0.548949110049
C	-2.726686201673	-2.984308230054	1.071422041106
C	-0.608459532167	-2.618649555652	1.517208560160
C	-1.637523935259	-3.547696673779	1.708453115188
H	-3.743829481075	-3.335367776321	0.951950656760
H	0.424219270429	-2.649953913149	1.846861764759
N	-3.071890567587	0.573987537424	0.513044088704
C	-4.048759737095	1.314382425001	1.057752726697
C	-2.108360017849	2.274153218813	1.424245663526
C	-3.477847002375	2.420866878397	1.657972936874
H	-5.081013590525	0.998887317506	0.977171279673
H	-1.280574702518	2.912706866805	1.708227326228
N	-2.488906109617	-0.572442448490	-1.620498742706
C	-2.978669608086	-0.807837092721	-2.847172980247
C	-0.900384746829	-0.108575716159	-3.013701232679
C	-1.995620893545	-0.522839834232	-3.775619714094
H	-3.994272048970	-1.162435739066	-2.967535628571
H	0.091348456922	0.205452930876	-3.316741999467
N	-1.878079581499	1.160972530901	0.735886269767
N	-1.212314431933	-0.143543155272	-1.723187470619
N	-1.046788943154	-1.578309819515	0.819834330678
Rh	-0.135199687155	0.277294395960	-0.014918756941
C	0.985689309960	0.618339083954	1.508604946268
N	1.817217066715	0.741639524445	2.308385677856
C	3.007599448854	0.758417908395	3.067041216100
H	2.844369846191	0.263838608602	4.030056521790
H	3.786619082589	0.228210101724	2.502566013211
H	3.322384447980	1.792544331116	3.242118222282
H	-1.594686894088	-4.491487583924	2.231668289675
H	-2.060362327140	-0.602108362657	-4.850455488461
H	-3.979436815259	3.219903147889	2.183089281540
C	3.959531463854	0.511574929924	-0.697104043419

C	2.831667097178	-0.318722696409	-0.624671771516
C	2.965958345786	-1.595262559629	-0.060530724607
C	4.190724486984	-2.025607590066	0.426565291596
C	5.310678288116	-1.197949305803	0.360053403920
C	5.182015554126	0.065857527826	-0.208201470958
H	3.858255138132	1.498766145434	-1.142945937440
H	2.083673891844	-2.233517463717	-0.015182122365
H	4.276161091205	-3.021989675160	0.858463669660
H	6.272603866004	-1.540394252851	0.734572894002
H	6.051045651632	0.719452098418	-0.276619897321
N	1.585592517346	0.087694450698	-1.093369359531
C	1.155626024267	1.360366835969	-1.062720559288
N	1.512145441033	2.477200329579	-1.519037914375
C	0.689506789737	3.623572827556	-1.212302427082
H	-0.217047467002	3.365693677359	-0.639633977942
H	1.270524784721	4.359926736968	-0.639483629549
H	0.382311310284	4.120099298313	-2.142571758218

$^{1}\kappa^{2}$-parent

G = -1363.225406

B	3.054855066633	0.697124175563	-0.339877926941
H	4.179792154083	1.064268468737	-0.521692528783
N	2.014118612234	1.822628534927	-0.223985541646
C	1.522174917850	2.428758290875	0.885654741752
C	0.771319995031	3.404958353455	-0.928568063550
C	0.702938653622	3.457605360121	0.475837075015
H	1.792339308610	2.085542211556	1.877564820812
H	0.277009532062	4.038661163938	-1.656822139175
N	2.986317159431	-0.101109376287	0.979819730865
C	3.922314432640	-0.349517477153	1.904450737382
C	2.018502625745	-1.245131092950	2.535708721260
C	3.348663801579	-1.085091972411	2.927122763054
H	4.930985884124	0.019236160962	1.768124176816
H	1.202623700708	-1.759218776226	3.029474874325
N	2.615028553728	-0.221109746307	-1.486165435012
C	3.214816537847	-0.503017469129	-2.648484485706
C	1.215164381170	-1.412916636093	-2.623177170900
C	2.358265323920	-1.275389009860	-3.411641425888
H	4.206077284430	-0.119815291390	-2.853422591551
H	0.284428293965	-1.929157743510	-2.826517530410
N	1.813931413080	-0.650194000893	1.362809177750
N	1.382963409750	-0.774580010184	-1.468901543535
N	1.559782502147	2.426364027827	-1.344137980715
Rh	0.155894444024	-0.450481817704	0.149573371918

C	-1.067379537622	-0.060055667932	1.578702951608
N	-1.929724640278	0.208849525946	2.309152160918
C	-3.120914046561	0.641879366234	2.929916785173
H	-2.930781339951	1.557628611283	3.499502925453
H	-3.867825791456	0.841668529267	2.150010885265
H	-3.494139527622	-0.132444827462	3.608220833585
H	0.146163337794	4.143954355280	1.097977217533
H	2.531162989899	-1.672791957110	-4.400418753086
H	3.825028514585	-1.452871965527	3.823600336124
C	-3.893152588720	-0.712630298609	-0.739094028043
C	-2.703747479709	0.006420012071	-0.893209387289
C	-2.731113364046	1.404456441880	-0.861567262467
C	-3.933730219652	2.069831040179	-0.674202176460
C	-5.122525476437	1.358048360063	-0.522746785933
C	-5.092058681522	-0.032369601352	-0.558768710752
H	-3.865098355707	-1.800533125743	-0.768516668080
H	-1.791677282667	1.946665025492	-0.973287184538
H	-3.945087074248	3.158506212751	-0.651956684470
H	-6.064975922860	1.884027484287	-0.387318615995
H	-6.015389743083	-0.599334087416	-0.448650056420
N	-1.473529204577	-0.637077548335	-1.082920874988
C	-1.173034794224	-1.798187762841	-0.548908744261
N	-1.430803824958	-3.014583853186	-0.523962624753
C	-0.689655130145	-3.912858273250	0.328862378709
H	0.097399248434	-3.403218943571	0.906349111708
H	-1.377384497259	-4.411604217483	1.023644573842
H	-0.224851625819	-4.696774352778	-0.282234589518

TS between $^{1}\kappa^{2}$-parent and $^{1}\kappa^{3}$-parent

G = -1363.222767

B	-3.006249327186	0.912446132773	0.427778376661
H	-4.129462938114	1.276587673622	0.632214307119
N	-1.989396521797	2.058899806623	0.291937114317
C	-1.956220102072	2.985200001424	-0.689798407268
C	-0.368410106608	3.360876042325	0.771314627880
C	-0.919541698556	3.852978761228	-0.423869343955
H	-2.670312382816	2.957219985176	-1.504761615338
H	0.466736294376	3.748618730323	1.344432920436
N	-2.969696324171	0.148190905013	-0.917135502122
C	-3.921630141878	-0.068854495599	-1.832894660711
C	-2.011010540477	-0.866794952492	-2.563988407197
C	-3.354081091539	-0.722252777774	-2.913625947014
H	-4.935607139286	0.264508227828	-1.651408574691
H	-1.194543859691	-1.327916471367	-3.106741525351

N	-2.557603458674	-0.035663477024	1.539061202806
C	-3.141738823308	-0.306196716648	2.713682325675
C	-1.234708599904	-1.388295964585	2.583909662415
C	-2.332496426396	-1.176278879675	3.419506521447
H	-4.093497397072	0.145444233096	2.961941724282
H	-0.345474092750	-1.988086269399	2.736471906937
N	-1.793064668419	-0.337368217706	-1.361657483118
N	-1.384345662861	-0.699777087628	1.457463525669
N	-1.011069546668	2.283882521621	1.202053431168
Rh	-0.135440364067	-0.342288291955	-0.135581826710
C	1.120135935506	0.080042312614	-1.525748522087
N	2.007035168239	0.342001861817	-2.228526586555
C	3.231132687642	0.728435367209	-2.814498095597
H	3.119523026149	1.705683248242	-3.295857278674
H	3.991782146807	0.790703697729	-2.024810321418
H	3.538161721471	-0.008558193453	-3.563879639708
H	-0.615073310461	4.714120064579	-1.001591767561
H	-2.508795813396	-1.594603080209	4.398985198426
H	-3.841692755271	-1.044973127406	-3.821321239774
C	3.869198218396	-1.123852289659	0.647293959767
C	2.763427251634	-0.311323082251	0.918222713323
C	2.939828757356	1.068003934963	1.067773259738
C	4.204193408821	1.624172022794	0.942858800721
C	5.309452215996	0.818671824374	0.673731160731
C	5.131711799747	-0.553768903900	0.530442010217
H	3.726646955727	-2.197473761401	0.537208002036
H	2.061514785076	1.680766188426	1.270281297126
H	4.331102952438	2.699217000055	1.061518023257
H	6.301155909898	1.256901533420	0.586227385491
H	5.988894420809	-1.194343863336	0.327668563942
N	1.472553104870	-0.838046147523	1.048102540997
C	1.049526855946	-1.888879917069	0.381819213822
N	1.183041693409	-3.113573392272	0.209604498118
C	0.353349448923	-3.825030092960	-0.732904715774
H	-0.391591699781	-3.177484909324	-1.221435737646
H	0.984194133959	-4.288362126700	-1.502416887939
H	-0.172475759979	-4.637551297959	-0.216011938314

$^{3}\kappa^{3}$-TpRh(CNMe)

G = -1363.180961

B	-3.332846264319	-0.162926204363	-0.007502735724
H	-4.515765672273	0.004342619106	-0.041393935700
N	-2.985036976363	-1.317157986695	0.947658633155
C	-3.789669050746	-2.057479102473	1.725582761502

C	-1.710610469771	-2.712485759234	1.980674441033
C	-3.014399281108	-2.972263043125	2.412652401874
H	-4.857348151461	-1.879182153065	1.732383412282
H	-0.779421864593	-3.193668289647	2.254670286370
N	-2.631710931693	1.114380144343	0.480495664125
C	-3.145730129126	2.321811292291	0.770441613655
C	-0.971272765151	2.345785459402	1.074269126683
C	-2.112152304797	3.152209758081	1.159990365697
H	-4.210119478259	2.500087395924	0.683171841041
H	0.066522695025	2.587261006946	1.274258281721
N	-2.816631703743	-0.526537749136	-1.411555994259
C	-3.478237411732	-0.595925746394	-2.576383160250
C	-1.357829286024	-1.062392402756	-2.913187710249
C	-2.582837981618	-0.939833301756	-3.572229196291
H	-4.541602596816	-0.396327899306	-2.610909747163
H	-0.372633011266	-1.296490242124	-3.299556009424
N	-1.296317212577	1.126665999997	0.667191749904
N	-1.512777065476	-0.814078236180	-1.616572098942
N	-1.705748642033	-1.717429307191	1.100966435561
Rh	-0.188636688036	-0.712536732174	-0.022468562822
C	1.119335177630	-0.722807809114	1.401884181588
N	1.944057081697	-0.694575488766	2.221810491715
C	3.069956020619	-0.628846835219	3.066666218797
H	2.920701709369	0.143782278074	3.828804786947
H	3.221395007311	-1.593676888096	3.562973853377
H	3.956850794073	-0.383518877934	2.468613500615
H	-3.344595339550	-3.719343026599	3.118938174654
H	-2.787130942944	-1.080946861572	-4.623004759720
H	-2.176435570689	4.187092460535	1.462577415388
C	3.629914262732	1.193136940042	-0.088025302826
C	3.490357050837	-0.135148283316	-0.582362688984
C	4.600510866731	-1.013093949455	-0.442947898279
C	5.779076392786	-0.584836710598	0.132983748898
C	5.897296854477	0.725258474919	0.607243892423
C	4.815098276990	1.601989640890	0.493129137635
H	2.793330685314	1.879926108678	-0.188633314586
H	4.486277270691	-2.028031691104	-0.818885515637
H	6.621910246670	-1.268984736723	0.216850576055
H	6.828186075278	1.062010872721	1.058876745815
H	4.909302261843	2.622762386363	0.861383683737
N	2.372801054843	-0.635291065067	-1.141191448891
C	1.224255128784	0.141586429263	-1.252314672886
N	1.189284023222	1.095908275685	-2.097690058011
C	0.004972293215	1.883333119793	-2.319980466234
H	-0.858522448836	1.634263617209	-1.690616980844
H	0.249441647168	2.944525705905	-2.164852302260

H	-0.299268202248	1.791904764646	-3.373179077288

Free carbodiimide

G = -418.788687

C	-4.216319323009	-0.403295018284	-0.887379730813
C	-3.021644321813	0.308701891657	-0.750073160713
C	-3.054247601996	1.627505507462	-0.299769553124
C	-4.266981976988	2.224039947261	0.015442616517
C	-5.456156640378	1.516284836967	-0.117857124549
C	-5.423797404465	0.201536453717	-0.571572714340
H	-4.191736720101	-1.430607499318	-1.249043460563
H	-2.115730763702	2.168474242543	-0.203824446714
H	-4.282478073254	3.253837068784	0.367263574493
H	-6.405261330946	1.986681359010	0.128860021944
H	-6.349721064887	-0.359814838424	-0.682987033631
N	-1.770139305296	-0.241063393726	-1.062194025190
C	-1.533697998474	-1.401485299584	-1.370490193927
N	-1.202689747387	-2.479072653899	-1.804952557599
C	-0.728102991629	-3.647035958392	-1.105595386663
H	-0.675475134070	-3.502222206553	-0.018854071239
H	-1.390473754734	-4.492840429706	-1.320980052672
H	0.269449153128	-3.906229009515	-1.477784701218

$^{1}\kappa^{3}$-1,2-η^{2}-arene complex

G = -1363.204397

B	2.649788484526	-1.431647416442	0.351102983103
H	3.579713057926	-2.148728599786	0.576347405540
N	3.120606610247	-0.164311312414	-0.374678769329
C	4.353657418928	0.249748233552	-0.706352453383
C	2.863903606562	1.701389914389	-1.409910116096
C	4.240979495687	1.454085475098	-1.375546325909
H	5.220357456641	-0.344511654560	-0.446103836331
H	2.317209684830	2.530011191001	-1.845318791326
N	1.953639643335	-1.041728670703	1.660555559298
C	2.257654311981	-1.351211470890	2.931165181060
C	0.445490860964	-0.113119584718	2.879773763707
C	1.313636327245	-0.771740765850	3.757330689110
H	3.121518470569	-1.964515803222	3.153709171927
H	-0.448124199572	0.463400683796	3.088586185281
N	1.639828717404	-2.156787813220	-0.553613616263
C	1.770505073577	-3.375769010010	-1.096396296223

C	-0.125891732652	-2.487745526570	-1.746143250905
C	0.659926175895	-3.633917059385	-1.874007215833
H	2.648843096929	-3.971223793950	-0.883132942274
H	-1.099772280052	-2.275473558615	-2.163927495446
N	0.840926678348	-0.283149220848	1.624175720463
N	0.467904892450	-1.600638281007	-0.951332312986
N	2.202886486530	0.720436911349	-0.807495379321
Rh	0.078435391731	0.378847458548	-0.313846970271
C	-0.041806871285	2.163085925287	0.308876758350
N	-0.022369803721	3.252671695454	0.714863133204
C	-0.188291766631	4.590049556706	1.113208588413
H	0.629614938170	5.205288677601	0.722021977577
H	-1.141323163310	4.968851668055	0.724269861512
H	-0.192088524642	4.661303115917	2.206595262559
H	5.037147630068	2.057761640779	-1.785683783237
H	0.441737459620	-4.524873992530	-2.443425086683
H	1.256597617777	-0.826731113317	4.834371787337
C	-2.004451741729	0.274070356498	-0.612719457579
C	-2.839758321649	1.287555535101	0.018022515568
C	-1.309994081545	0.663457180110	-1.852306494977
C	-2.967153261092	2.534996196110	-0.498160433505
C	-1.539100306468	1.990612636142	-2.372816946526
C	-2.305440912810	2.900711536829	-1.715807031436
H	-1.126915073923	-0.108918331751	-2.600836813579
N	-2.475969400569	-1.074600303342	-0.517805630827
C	-3.222355120370	-1.543271446529	0.321248667680
N	-3.857263022431	-2.139016438394	1.174191465840
C	-5.287809126025	-2.345670511047	1.160295674766
H	-5.727144384768	-1.917324080214	2.069075241614
H	-5.783143844312	-1.901403379745	0.286017404249
H	-5.497044710564	-3.422095629591	1.173771254610
H	-1.104804639269	2.243353752790	-3.340543699040
H	-2.462221392570	3.893167671009	-2.134191868719
H	-3.609881042702	3.260565098011	-0.000211054395
H	-3.401930863280	0.997298658516	0.907192819632

$^{1}\kappa^{2}$-1,2-η^{2}-arene complex

G = -1363.200729

B	2.792666193456	-1.298987446958	0.007404793529
H	3.834797415322	-1.894211010028	0.004372032761
N	2.809277194958	-0.020817653836	-0.836889562286
C	3.120478445737	1.234485493829	-0.452504990841
C	2.799838986199	1.148116189693	-2.617492702599
C	3.122890661159	2.034625842664	-1.575755145485

H	3.308313246514	1.468264551541	0.589049873056
H	2.699233775798	1.353399771923	-3.678082342400
N	2.462242134926	-0.908483800047	1.461947783857
C	3.209310211175	-1.021509564746	2.569012845536
C	1.272022493900	-0.126924403999	3.083619812223
C	2.487369672778	-0.529914180608	3.641220557907
H	4.203094489642	-1.446281323646	2.509102281727
H	0.398829863343	0.307096951301	3.554702907211
N	1.690414737656	-2.233434855313	-0.496024000336
C	1.828924758243	-3.456368393633	-1.020038775228
C	-0.296456923583	-2.920391068929	-0.967746092487
C	0.576459231062	-3.942864363860	-1.340635463284
H	2.815604555089	-3.886356965524	-1.132902376707
H	-1.374058737861	-2.870691389005	-1.034698685027
N	1.268543794355	-0.362808009945	1.773592488808
N	0.381275954809	-1.890126360141	-0.461005899219
N	2.610186313491	-0.085618848176	-2.169889979492
Rh	-0.124290541084	0.017402471799	0.304859201290
C	-0.313146135489	1.738196799518	1.046184432719
N	-0.338431298461	2.793902512582	1.546705688389
C	-0.368589007999	4.137890193820	1.952476657511
H	0.624672517888	4.589592560121	1.843813073496
H	-1.080289432212	4.696607649989	1.332003456228
H	-0.678404158134	4.215796739468	3.001085647819
H	3.331609151023	3.093608387320	-1.631992837612
H	0.328871547087	-4.897543186750	-1.779962159090
H	2.792054697041	-0.478930856358	4.675861136618
C	-2.209388848069	0.244142719938	-0.768001151091
C	-2.926355800240	1.412055441551	-0.371197502809
C	-1.114116773810	0.385149575947	-1.653091393548
C	-2.561904685017	2.645533225990	-0.841945139928
C	-0.741154871788	1.683389489968	-2.089153579432
C	-1.449629109898	2.792510154079	-1.696832873964
H	-0.726948843378	-0.481937558309	-2.183544590436
N	-2.767611973002	-1.033485086155	-0.568136662783
C	-3.778293311159	-1.289405134974	0.074072612193
N	-4.678542586447	-1.676634705942	0.781885520745
C	-6.066640989970	-1.890446170329	0.451369041559
H	-6.693079310887	-1.269528534049	1.101471610438
H	-6.298137354793	-1.658509875802	-0.596224891964
H	-6.323295642846	-2.937232636301	0.649063413475
H	0.105282559563	1.772107375084	-2.766623263775
H	-1.164299015751	3.779563277340	-2.053951107069
H	-3.140721160970	3.521343932744	-0.550640719909
H	-3.790018089367	1.297258075152	0.282542019707

$^{1}\kappa^{2}$-2,3-η^{2}-arene complex

G = -1363.208986

B	3.268259642750	-0.834474610892	-0.111375185557
H	4.417191518272	-1.179673390082	-0.141389404517
N	2.937098363593	0.290691006178	-1.093016444498
C	2.935320476437	1.622873128647	-0.878840265914
C	2.591782233513	1.181782447322	-2.997539982779
C	2.712474038612	2.246720895892	-2.088197352946
H	3.083296082981	2.028851839949	0.114944779026
H	2.412542032946	1.217028148619	-4.066845917653
N	2.950960197074	-0.344336155949	1.317715997409
C	3.793173423154	-0.116477793231	2.335608371721
C	1.749146413787	0.382869382493	2.956849432158
C	3.067677720489	0.353137712690	3.415040198990
H	4.852011047947	-0.305396476219	2.213203990067
H	0.840638640606	0.674078796144	3.469637023905
N	2.386482929812	-2.053913649760	-0.407117444699
C	2.768255541055	-3.288558075808	-0.752208001630
C	0.590217137681	-3.236346533292	-0.519876847697
C	1.645435681131	-4.089748340092	-0.840329395181
H	3.816061717907	-3.504293983845	-0.915464754811
H	-0.464637483302	-3.462561347684	-0.435810408638
N	1.690185790572	-0.039114053011	1.695731817256
N	1.043350701105	-2.007967314169	-0.267889311459
N	2.729253246665	0.007498643686	-2.396056521966
Rh	0.124664844032	-0.234962782764	0.358778275581
C	-0.633715884395	1.358749197349	1.034849585748
N	-1.063574897453	2.341046843142	1.497714648723
C	-1.663384552336	3.556643844477	1.866001052605
H	-2.236987817350	3.956366731445	1.020467235608
H	-2.341350811726	3.406560154293	2.714386468239
H	-0.897136922772	4.286762696185	2.150865660129
H	2.647298072666	3.308306480851	-2.280758579933
H	1.596328352313	-5.137507157185	-1.095772188124
H	3.437832873069	0.626803149768	4.391740177375
C	-2.837794805517	-0.093356450944	-0.549558343973
C	-3.090391590035	1.211396822225	-0.915229610159
C	-1.614284676033	-0.721912363680	-0.932580308609
C	-2.145097017715	1.928355491842	-1.677252644766
C	-0.672332544412	0.007646229492	-1.698583098029
C	-0.961492000436	1.351414599271	-2.063287496361
H	-1.602869438555	-1.807318174416	-0.899322413344
N	-3.740588772553	-0.882838871706	0.170980954772
C	-4.862845038911	-0.565178739306	0.543580456618

N	-5.920437418671	-0.317680968442	1.071356545923
C	-7.265460561127	-0.513685561212	0.590395444761
H	-7.798077613968	0.443597651843	0.602678679670
H	-7.298521727590	-0.928139481007	-0.425270858277
H	-7.792959727754	-1.193967322376	1.268540384784
H	0.138535364493	-0.505906388046	-2.215687003329
H	-0.241470943587	1.897652184512	-2.668268371041
H	-2.371594178371	2.952458714619	-1.971405290930
H	-4.030528660094	1.680455192185	-0.626494734247

TS between $^{1}\kappa^{2}$-1,2-η^{2}-arene complex and $^{1}\kappa^{3}$-1,2-η^{2}-arene complex

G = -1363.195661

B	-2.750977386137	1.275244071508	0.101107664493
H	-3.748962168170	1.931590625769	0.206501193343
N	-3.079409381923	-0.062152722210	-0.561253157536
C	-4.228269953420	-0.758669568352	-0.450643727658
C	-2.737373023317	-1.915169358297	-1.562565688484
C	-4.057472591541	-1.970424190036	-1.086474798966
H	-5.083026249866	-0.337063786768	0.064191718106
H	-2.189635031099	-2.657504604261	-2.133151054784
N	-2.184235944602	1.066072817865	1.522959454885
C	-2.751039398075	1.367416271129	2.699908330323
C	-0.806321437897	0.415518118454	3.049227286184
C	-1.902099502481	0.966695998045	3.715200403342
H	-3.720748977567	1.847339031242	2.727199397541
H	0.107637738107	-0.010214348784	3.444086773217
N	-1.712495781458	2.051039464606	-0.716429731455
C	-1.942390683443	3.153002376417	-1.444150065214
C	0.181641928147	2.630105251595	-1.564578781443
C	-0.754098852077	3.562999720393	-2.013593230378
H	-2.941190891684	3.566558281316	-1.497007263989
H	1.244826025407	2.573471726763	-1.752071705015
N	-0.988249605067	0.482746706967	1.731978158795
N	-0.399741473232	1.719675471608	-0.784602388596
N	-2.153329192008	-0.767713283813	-1.245964021760
Rh	0.225636696461	-0.089259391493	0.152074215474
C	0.518300461867	-1.706835648426	1.065987680163
N	0.606908612785	-2.699430997303	1.674516713326
C	0.729527039643	-3.973417992521	2.251163018804
H	-0.236039859984	-4.492664230924	2.232843519938
H	1.461531353000	-4.566128008388	1.688641266603
H	1.066108451699	-3.892628810292	3.291348060011
H	-4.783229283277	-2.762217746475	-1.205310919483
H	-0.584451079442	4.418208767193	-2.650425436675

H	-2.050161709641	1.068441747208	4.779904105744
C	2.339402300569	-0.178585195728	-0.723415712967
C	3.170752912386	-1.209587533547	-0.177729043151
C	1.342683195926	-0.546791866416	-1.671436420044
C	3.000482569864	-2.514566221374	-0.545994529644
C	1.179484127661	-1.920777896906	-2.004012086338
C	1.982104812243	-2.886330300597	-1.455894311962
H	0.928270461770	0.204042973281	-2.339882706673
N	2.773229166320	1.164176574870	-0.678667392047
C	3.674400693150	1.613775276759	0.015644989664
N	4.448260977256	2.191093301519	0.745738352838
C	5.847053563685	2.470725618334	0.527382504752
H	6.436944616763	2.019576614810	1.333273751649
H	6.214912860349	2.095997437414	-0.436797095709
H	6.006048738020	3.554185921045	0.571022972641
H	0.416789489256	-2.181764197393	-2.736111252356
H	1.855130570389	-3.930603207329	-1.732395006869
H	3.660520042122	-3.277129250973	-0.134085849841
H	3.966205042565	-0.923900877502	0.509698497201

TS between $^{1}\kappa^{2}$-1,2-η^{2}-arene complex and $^{1}\kappa^{2}$-2,3-η^{2}-arene complex

G = -1363.197984

B	-2.908922812140	1.215568797966	-0.195505128164
H	-3.954860648468	1.803009493731	-0.225382809608
N	-2.843597935385	0.023911803307	-1.155096902321
C	-3.119840559281	-1.273195662147	-0.908529368662
C	-2.722118936914	-0.961128843203	-3.040358091007
C	-3.049595091133	-1.957261309830	-2.104314795626
H	-3.334576552837	-1.616374292032	0.096659926887
H	-2.572507518487	-1.056362964219	-4.110627395957
N	-2.687162342461	0.697439153556	1.241233750602
C	-3.532761273781	0.712592848325	2.282225489876
C	-1.628016478146	-0.182108203565	2.904002601257
C	-2.899053235148	0.153600678380	3.375924500240
H	-4.526706637276	1.124345718116	2.163781152272
H	-0.789784008280	-0.633060438189	3.420215593847
N	-1.779861086727	2.197124971145	-0.521794151811
C	-1.860139453090	3.473102970473	-0.915939820373
C	0.248782061718	2.896140415304	-0.730552506932
C	-0.578320977185	3.969582192076	-1.064857672271
H	-2.828134460674	3.931470285506	-1.070946222895
H	1.329562090261	2.830296725046	-0.694824843387
N	-1.511631048261	0.150847462927	1.620566056691
N	-0.485577604481	1.831543622282	-0.409166444927

N	-2.597011660654	0.227976636306	-2.465912528886
Rh	0.009308302658	-0.085814174838	0.276763456645
C	0.330179589442	-1.786229677592	1.015949374250
N	0.472166831644	-2.832331538460	1.520258226682
C	0.662710908606	-4.154868759598	1.950692544817
H	1.042225116729	-4.767330294439	1.122969175054
H	1.384747437379	-4.190451657601	2.775356836605
H	-0.285901457113	-4.581768019909	2.296976149211
H	-3.214561101070	-3.012194337481	-2.271936099860
H	-0.285112592366	4.962368214900	-1.371743449475
H	-3.294487212957	0.017714366711	4.371425473272
C	2.465362752244	-0.214283805877	-0.712035636232
C	3.085357638748	-1.443759482414	-0.413672964042
C	1.348390333592	-0.193746340116	-1.569186651932
C	2.597961645272	-2.613731616221	-0.963739031767
C	0.823638161254	-1.409306070507	-2.052154764215
C	1.452568908809	-2.610711082468	-1.764974508302
H	1.016631011812	0.747328308677	-1.999020323556
N	3.008742501375	1.014853960411	-0.314335364092
C	4.014689353974	1.173795606146	0.368994063533
N	4.903801077485	1.451456859549	1.134735550883
C	6.296553202072	1.729854714662	0.889448352287
H	6.912069912942	1.021191448605	1.454375939898
H	6.562323628845	1.668053992702	-0.173512609528
H	6.529229387336	2.735466860906	1.256929842838
H	-0.057183939060	-1.377329622246	-2.691164393491
H	1.057440413507	-3.542366802348	-2.162884719890
H	3.109579055748	-3.552487996713	-0.752992661369
H	3.963212299921	-1.454726115703	0.230355802931

TpRh(CNMe)-Cyclopentane σ-complex-(1)

G = -1140.700859

B	-2.157897056715	-1.031041296762	0.803148696977
H	-3.105101167846	-1.584802928444	1.288037630065
N	-2.654641381691	0.271717078561	0.130226772316
C	-3.878720457161	0.819956226564	0.165080910161
C	-2.564313978362	2.058813552157	-1.081990249016
C	-3.871083453687	1.973743909583	-0.595480245928
H	-4.667689151092	0.342017143391	0.731328150843
H	-2.108449141968	2.794694922936	-1.732376216785
N	-1.549626275803	-1.922170471113	-0.283777790109
C	-1.823504266014	-3.187788376044	-0.617745488220
C	-0.212871474837	-2.424162030749	-1.896532068181
C	-0.987203133446	-3.559760711178	-1.655398936560

H	-2.590156991766	-3.736029315031	-0.085898655848
H	0.564152543574	-2.258570896429	-2.632889176676
N	-1.054095801009	-0.671870063604	1.804955425748
C	-0.894675417291	0.467555714769	2.509246384080
C	0.694124944717	-0.962893852797	2.988914381503
C	0.231579751751	0.329197850523	3.293138941349
H	-1.581806409333	1.297013169411	2.389907141709
H	1.555874853330	-1.488349293711	3.386863389078
N	-0.555017837366	-1.447313907663	-1.060166559944
N	-0.080882788844	-1.561972206428	2.094275319896
N	-1.843525715484	1.031668061891	-0.641519656638
Rh	0.099799792987	0.508844266488	-0.827873340302
C	0.648983053933	2.309442591834	-0.662655575708
N	0.980350212818	3.426426014729	-0.554485300534
C	1.392641935325	4.758187082508	-0.382262636213
H	1.222605389684	5.333760431367	-1.300077749104
H	0.831911579634	5.224630917731	0.436279292088
H	2.461244409991	4.792871593669	-0.139543682865
H	-4.692559020906	2.649929215447	-0.779251508441
H	0.649871007181	1.050281180505	3.980945807094
H	-0.946124398097	-4.511727342331	-2.162981657867
C	4.143576464820	-1.784032679222	0.219580999531
C	2.740806270007	-1.773860173196	-0.431354705154
C	2.311549430274	-0.297512883950	-0.403304779700
C	3.595290911295	0.509946661344	-0.235238826942
C	4.367880721237	-0.362692324461	0.749674545459
H	4.233015961783	-2.542396699434	1.005265481653
H	4.907396629553	-2.018500289133	-0.534116628135
H	2.014548881416	-2.389813247860	0.112495335848
H	2.788195845881	-2.162959305679	-1.456224192721
H	1.803658874115	-0.011561845764	-1.386151945603
H	1.690132112453	-0.136262310599	0.498569933678
H	4.141340249732	0.582967306883	-1.188388478571
H	3.410814386953	1.529317989132	0.125314678960
H	5.428350179719	-0.098633902791	0.834840330706
H	3.918142517858	-0.255377246616	1.748118664893

TpRh(CNMe)-Cyclopentane σ-complex-(2)

G = -1140.702637

B	-2.372679316871	-0.895900149770	0.749438846881
H	-3.390705818663	-1.384846824649	1.154034272022
N	-2.698959934378	0.515519061910	0.205015863768
C	-3.852744191513	1.196738240701	0.272197307290

C	-2.358128613138	2.403554375018	-0.789480859197
C	-3.683916725300	2.419299258210	-0.349827320291
H	-4.712091157100	0.755411526304	0.760378875481
H	-1.796148123596	3.148467169527	-1.338705589534
N	-1.828609257780	-1.738760324678	-0.407717679767
C	-2.214403279851	-2.936802013553	-0.859817711025
C	-0.481024712931	-2.242321256343	-2.010994325101
C	-1.376496166376	-3.306551238190	-1.896927493623
H	-3.054318019072	-3.444653153389	-0.403949710551
H	0.341834637717	-2.099338350884	-2.701202718278
N	-1.269213484962	-0.760845865771	1.805012827609
C	-1.026678213538	0.273143657300	2.636861881262
C	0.409894819295	-1.344857029050	2.980138936889
C	0.058485442194	-0.057128192157	3.420834071328
H	-1.631647963220	1.171564314553	2.600061326324
H	1.207688268648	-1.989873340816	3.332303746530
N	-0.759057293284	-1.307604793988	-1.105425066125
N	-0.390246162688	-1.765297650150	2.009193780437
N	-1.776810207371	1.255960981665	-0.451631101075
Rh	0.097707209042	0.532120748979	-0.676606404639
C	0.855340460369	2.226542261035	-0.320171932408
N	1.328901597170	3.272046439931	-0.093129247351
C	1.920244768419	4.501591529849	0.241065854882
H	1.429631602598	4.929830885498	1.123093264761
H	2.983615955267	4.357529097294	0.466017668670
H	1.830362712557	5.209281779511	-0.591744174939
H	-4.414985199952	3.203967348935	-0.474952663611
H	0.521193880578	0.540323521911	4.193477949137
H	-1.410724293237	-4.211869738096	-2.484129998802
C	4.641135255658	-0.820681244616	-0.221217468821
C	3.547354770399	0.259394888545	-0.200345067430
C	2.223478696515	-0.513055453041	-0.389952354761
C	2.590661943145	-1.985619884006	-0.609223426546
C	3.906813170730	-2.106611702996	0.154359326484
H	5.048949022069	-0.922605413810	-1.237423160506
H	5.482687620827	-0.587641406340	0.441054993478
H	3.702101439964	1.018213402498	-0.977246853828
H	3.534880612336	0.790758550071	0.760756709213
H	1.618968203804	-0.449519570401	0.533157505034
H	1.700039402959	-0.118787904942	-1.327467552161
H	1.802856717306	-2.659340073996	-0.253317245683
H	2.763809668743	-2.199398107408	-1.675186785242
H	3.701838748965	-2.120845078970	1.235621944343
H	4.468503507547	-3.015966277231	-0.088198040527

TpRh(CNMe)-Cyclopentane TS_2-(1)-κ^3

G = -1140.683528

B	-2.622749012254	-0.592157928940	0.164452926903
H	-3.766501048059	-0.946014439292	0.153418163589
N	-2.464071561351	0.653403083998	-0.727982910970
C	-3.428716296005	1.414296760388	-1.266372370702
C	-1.466747202110	2.206778755135	-1.838336273111
C	-2.836527822584	2.431361288191	-1.990608174454
H	-4.469747976393	1.171481918661	-1.096757263392
H	-0.624394275105	2.750995438859	-2.247129935053
N	-1.755109823877	-1.711015904572	-0.447312836600
C	-2.171950728230	-2.891940235948	-0.926117279508
C	-0.040076983706	-2.641711728041	-1.360516261170
C	-1.100926250814	-3.533320760687	-1.518941322939
H	-3.206816078005	-3.187629393534	-0.812351660566
H	0.986242641570	-2.723332523894	-1.694630251407
N	-2.190263427988	-0.279209091074	1.591255107368
C	-2.832176436160	-0.525439389169	2.749072722662
C	-0.869330695403	0.371383411358	3.138950466356
C	-2.015174259081	-0.119251240180	3.784410197052
H	-3.820743270720	-0.967441068437	2.749484210646
H	0.029122330930	0.796413228528	3.573208485443
N	-0.437177621566	-1.553110395647	-0.705611725453
N	-0.983010642069	0.272824803099	1.821918075437
N	-1.253012756813	1.136539549353	-1.078501029161
Rh	0.529395497051	0.271925038255	-0.341783794026
C	1.336002307218	1.975195700270	-0.269246486281
N	1.792995879983	3.050607810695	-0.242379522792
C	2.355428660171	4.336190257773	-0.177265781369
H	1.722491577882	4.995484079731	0.428119893768
H	3.351032755436	4.287299050260	0.279468123932
H	2.451421586656	4.763289020634	-1.182694268882
H	-3.324594497410	3.211510342352	-2.555432328194
H	-2.220623646205	-0.164170825606	4.844157959082
H	-1.091121069618	-4.499222586263	-2.001176620989
C	3.633751659447	-2.259644381718	-0.427175749516
C	2.569610034737	-2.067954207587	0.662340403979
C	2.273509105712	-0.568477864110	0.655955316006
C	3.689176020362	0.003383168316	0.514723728266
C	4.365720394130	-0.899306967273	-0.527194308895
H	4.314728266060	-3.086573768338	-0.194701670869
H	3.165806265604	-2.507209677132	-1.389859412527
H	3.005454114943	-2.315010480932	1.643583426931
H	1.689084536347	-2.704838030058	0.543700772148
H	1.914172096258	-0.358561040604	-0.760760658215

H	1.799143323762	-0.249769023494	1.596445678593
H	3.722539696567	1.063806257075	0.242018356938
H	4.201065137857	-0.097379820224	1.484735799689
H	4.242717207148	-0.472003497931	-1.531128200787
H	5.444449285693	-0.989975692243	-0.354926716960

TpRh(CNMe)-Cyclopentane TS_2-(1)-κ^2

G = -1140.684753

B	-2.359863827393	-0.947807412016	0.405875096597
H	-3.422951059729	-1.451383972149	0.639169686528
N	-2.604597839243	0.402128775046	-0.306645406897
C	-3.755031483054	1.056694958164	-0.511145134242
C	-2.091446776768	2.238190176769	-1.315790725208
C	-3.478423276947	2.247095527314	-1.160372369824
H	-4.690017294966	0.625588856135	-0.176383234587
H	-1.440162977519	2.967782976626	-1.781920012462
N	-1.569590535692	-1.854263322368	-0.543282759899
C	-1.891296441443	-3.052780205551	-1.042713290538
C	0.048812575273	-2.421763491614	-1.847617511200
C	-0.877752223131	-3.463626610938	-1.890069948875
H	-2.817695121160	-3.530378986094	-0.751429178945
H	0.993715989348	-2.310971676870	-2.364814722836
N	-1.502650484839	-0.674370925965	1.645290318869
C	-1.421170643071	0.451320563551	2.388907111189
C	-0.243749739853	-1.160673895589	3.294396046921
C	-0.609503985453	0.185847523487	3.471032578930
H	-1.938379705737	1.356076999913	2.091357979521
H	0.392377509694	-1.779213112703	3.918120767009
N	-0.372727738774	-1.462216377959	-1.027056741246
N	-0.782953891713	-1.674252136216	2.198259224798
N	-1.575004997838	1.125283790923	-0.800435837759
Rh	0.405170660212	0.411639495066	-0.581404273299
C	1.068167877326	2.172144956470	-0.365464920509
N	1.457682790944	3.266839835427	-0.247771848902
C	1.972863676566	4.561520626052	-0.062046181517
H	2.035211407262	5.087821441385	-1.021671627391
H	1.325169063114	5.131556179796	0.613791288772
H	2.976608450020	4.504929461201	0.375312256882
H	-4.178972825887	3.004625220157	-1.478683254942
H	-0.326767352147	0.862069842737	4.265297125452
H	-0.819032736520	-4.382093386057	-2.454445352209
C	3.505912377066	-1.968896154341	-0.451861943829
C	2.375004620905	-1.806799353278	0.570995292484

C	2.060474804520	-0.315813738389	0.568171554085
C	3.464008552744	0.288589131614	0.506666089597
C	4.228112469399	-0.599544095130	-0.487057118763
H	4.181215128462	-2.792295054206	-0.192407109427
H	3.095586338333	-2.207722573775	-1.442341985487
H	2.751960640613	-2.047737044974	1.578780990953
H	1.508918468798	-2.451692209297	0.403076141294
H	1.821328112841	-0.096123999974	-0.993228059034
H	1.504612811985	-0.006394308212	1.468683727706
H	3.490522926985	1.350611144650	0.238486314635
H	3.911304061276	0.199313914217	1.509339539528
H	4.182255897353	-0.165422201773	-1.494844696265
H	5.290990537839	-0.679184091259	-0.230891615658

TpRh(CNMe)-Cyclopentane TS_2-(2)-κ^3

G = -1140.686488

B	-2.600802906488	-0.680664394587	0.391265752305
H	-3.719334827800	-1.075357367030	0.553359164314
N	-2.623651991320	0.576195505092	-0.497708690804
C	-3.684892808319	1.302123012108	-0.880924659879
C	-1.856196270366	2.185171479239	-1.706835376747
C	-3.242026489026	2.352918372795	-1.661336993194
H	-4.680892595849	1.013148202150	-0.571196477742
H	-1.102227125036	2.770251196667	-2.218858949129
N	-1.795375850692	-1.765795536252	-0.352375692778
C	-2.224379019715	-2.972679333016	-0.748208787642
C	-0.188105287306	-2.645373421121	-1.487308866951
C	-1.222038632451	-3.581844403403	-1.479044512142
H	-3.218141086187	-3.308411517846	-0.481594907279
H	0.782174786069	-2.692118227163	-1.964071367199
N	-1.960343218036	-0.359593779054	1.737010257254
C	-2.405156292040	-0.618706156190	2.980899746832
C	-0.424330766729	0.320015923794	3.058298321980
C	-1.443168040119	-0.194328358457	3.875134571273
H	-3.371425870537	-1.081981863697	3.136875262713
H	0.522888380912	0.763787507781	3.345004113270
N	-0.536036699956	-1.560090445648	-0.799877162976
N	-0.743704008539	0.217833076560	1.775652261474
N	-1.494657190415	1.115439676513	-1.004993192039
Rh	0.402842104983	0.295287721596	-0.563390773327
C	1.180477907771	2.014892230045	-0.570792426115
N	1.635109116947	3.090846403319	-0.593304907597
C	2.232338538263	4.361989375674	-0.584893010273

H	2.247836464559	4.784426638692	-1.596719121294
H	1.673240465352	5.038391995610	0.071965026377
H	3.263579727822	4.287782578741	-0.219319851751
H	-3.835708001216	3.119437061168	-2.136618259030
H	-1.477578278552	-0.242669553876	4.953915490346
H	-1.239719727133	-4.556238621468	-1.943702617920
C	4.751833508345	-0.685774893680	0.255736953350
C	3.585827930156	0.294595259692	-0.003584498487
C	2.297700299917	-0.554634755930	0.032933250232
C	2.787185101338	-1.987736398899	-0.208650969229
C	4.086646356477	-2.024925979620	0.589663137232
H	5.362652524700	-0.794315529565	-0.650781440806
H	5.426579786165	-0.341900112636	1.048308872272
H	3.707167113265	0.790815695825	-0.976861989315
H	3.542201194853	1.095462112505	0.746106684391
H	1.898969137462	-0.535625885968	1.062357658624
H	1.707500549309	-0.261966599840	-1.252762031576
H	2.061362851536	-2.743629490321	0.110347626482
H	3.007132581899	-2.162055250965	-1.275599380440
H	3.848380580871	-2.076012538952	1.662185897373
H	4.720694824858	-2.888464580380	0.355168735566

TpRh(CNMe)-Cyclopentane TS_2-(2)-κ^2

G = -1140.687070

B	-2.284793998490	-0.991964998463	0.713063025207
H	-3.274485473188	-1.532380400440	1.120763181143
N	-2.660938365997	0.434892094306	0.253547444777
C	-3.812469513558	1.099454561401	0.415331532644
C	-2.359401041640	2.395190471936	-0.594906917232
C	-3.670420100703	2.368893406311	-0.117110887509
H	-4.651589275604	0.618278232632	0.901619608418
H	-1.819968554123	3.187439793866	-1.100045217372
N	-1.746446082343	-1.766930582117	-0.493302888227
C	-2.169705494111	-2.917911428354	-1.026897646797
C	-0.430835577919	-2.188902585709	-2.147299589677
C	-1.354150724323	-3.233147884534	-2.099155492565
H	-3.016883057043	-3.435705554269	-0.596328857747
H	0.392167529080	-2.020490336798	-2.830850685315
N	-1.158813422417	-0.871720016387	1.746199588898
C	-0.867059261464	0.157462436687	2.572572123399
C	0.428657079899	-1.560376912813	2.990591665108
C	0.162335769182	-0.241025511708	3.398325356471
H	-1.406930628181	1.095077994012	2.509189360354

H	1.167306206222	-2.254769549584	3.376238342861
N	-0.671131376277	-1.315588981098	-1.172425381683
N	-0.367452338496	-1.936188816329	1.999526880852
N	-1.760575043737	1.228496555602	-0.368666814694
Rh	0.203431041160	0.508709399976	-0.716568457952
C	0.970758968287	2.221984158139	-0.457001560021
N	1.449220962017	3.277050359256	-0.314177039926
C	2.103676504513	4.503481807319	-0.105700084199
H	1.641197211189	5.040296999348	0.730337750456
H	3.159987209895	4.325820131958	0.128528633496
H	2.040696658679	5.126312241931	-1.005519808394
H	-4.409522110135	3.155043448183	-0.157694322322
H	0.645180014995	0.334446303121	4.175281488067
H	-1.417926465175	-4.093715294811	-2.747902271737
C	4.457598959874	-0.722252575480	0.007209489737
C	3.380511470279	0.368119916916	-0.195494500837
C	2.031707485344	-0.376677821688	-0.145285479314
C	2.373924330423	-1.833279089297	-0.452121169548
C	3.679166211615	-2.005223902775	0.320472787010
H	5.033490980763	-0.858293682757	-0.918289600435
H	5.179462970151	-0.463486522977	0.790538819383
H	3.526495931668	0.884771529818	-1.154028309744
H	3.423067809279	1.141899004940	0.582685691248
H	1.658483259501	-0.351956656912	0.896170553324
H	1.447718321491	0.091462467664	-1.543499197062
H	1.581204742667	-2.519938025838	-0.135059219834
H	2.556368421196	-1.990382566940	-1.527999405579
H	3.451486320881	-2.061104389052	1.395397561022
H	4.229587534672	-2.915632228194	0.054824921848

TpRh(CNMe)-Cyclopentane IM-(1)

G = -1140.703664

B	-2.236389566325	-0.785791153308	0.498673917459
H	-3.240626290020	-1.267827035659	0.935114028854
N	-2.568382917646	0.470976603769	-0.328095992823
C	-3.739440894229	1.043103683025	-0.646841516051
C	-2.088593035804	2.158980491440	-1.574497534529
C	-3.483016937096	2.139062227363	-1.449625153049
H	-4.669396986690	0.627704272137	-0.279745865995
H	-1.452183270145	2.843532785614	-2.122563973634
N	-1.510087961950	-1.782551898504	-0.413101476818
C	-1.895251254480	-2.954859042779	-0.932781826100
C	0.022864441540	-2.351282640414	-1.821749093615
C	-0.938630874146	-3.365083519873	-1.843902589403

H	-2.821155806250	-3.415058306764	-0.612977830564
H	0.945981237065	-2.252117205193	-2.379012711508
N	-1.215573797116	-0.336030617401	1.573895900434
C	-1.180001904284	0.858782122549	2.240236948785
C	-0.107388659584	-0.687665711919	3.367378293381
C	-0.457596346991	0.680341979852	3.391691749237
H	-1.671238511281	1.733385683022	1.829171396395
H	0.473104039914	-1.248862539805	4.091876650220
N	-0.329180375735	-1.411054721691	-0.953700470308
N	-0.573134499897	-1.296658010781	2.296431021762
N	-1.550315206439	1.151345431799	-0.899541957567
Rh	0.415514280939	0.400225410574	-0.301436019928
C	1.097613803849	2.092246796400	0.237111631993
N	1.547073399933	3.112814358751	0.568767750924
C	2.136420741307	4.319943529747	0.986471290657
H	1.939858065864	5.108642559553	0.251844405066
H	1.721876313510	4.623522313978	1.954087975573
H	3.219505511306	4.188752412594	1.088213066949
H	-4.199602950565	2.819837713509	-1.884972074262
H	-0.212902758632	1.422184752021	4.138610116719
H	-0.934644559391	-4.268822708826	-2.434671513661
C	3.182749413724	-2.368988661584	-0.461973155549
C	2.253851818277	-1.901607042506	0.683294752583
C	2.140264716442	-0.368764945444	0.558513120093
C	3.458760405310	-0.005956648752	-0.134588610203
C	3.606148684405	-1.089991826536	-1.198855693483
H	4.068116120103	-2.875012609270	-0.053966823736
H	2.699494436295	-3.095666446758	-1.126684475141
H	2.719526366615	-2.141809321274	1.652370062502
H	1.286184083718	-2.411346494641	0.690350475294
H	1.167519861214	0.618897750087	-1.606052040655
H	2.096172292564	0.070646739270	1.572765865524
H	3.492664271143	1.011619377959	-0.545573243204
H	4.298127564132	-0.098166374924	0.579220330688
H	2.915973423185	-0.874491657551	-2.028553639772
H	4.615053072339	-1.154334852857	-1.625048469532

TpRh(CNMe)-Cyclopentane IM-(2)

G = -1140.704957

B	-2.188521529982	-0.908944601217	0.769890785534
H	-3.084989076640	-1.439452538722	1.358609182052
N	-2.675923984056	0.415482642360	0.152270188683
C	-3.883139848822	1.000829341029	0.142873049340

C	-2.462340643382	2.206249871009	-1.022959545150
C	-3.796709803811	2.162658259522	-0.601582342394
H	-4.715466671044	0.546627842103	0.665397451474
H	-1.953095611235	2.940455532652	-1.635850165032
N	-1.675875472119	-1.806868122686	-0.360029787339
C	-2.180825474195	-2.921591238609	-0.901261076068
C	-0.455525246060	-2.246074756931	-2.082691768631
C	-1.427051918573	-3.247210055565	-2.014361603993
H	-3.036215086533	-3.407366917311	-0.449895273865
H	0.344833704043	-2.104056171136	-2.797257461634
N	-0.960158964194	-0.558219141653	1.645519892842
C	-0.772526550962	0.562649479809	2.407079548365
C	0.486703468815	-1.082169568101	3.128153606840
C	0.167986928306	0.273577128177	3.361984355190
H	-1.328537460676	1.469479961642	2.197382096967
H	1.195754743111	-1.709470402215	3.657898374016
N	-0.610712410141	-1.389991018740	-1.079650158839
N	-0.195184303709	-1.582331328447	2.117901502697
N	-1.799952513878	1.150442775186	-0.567498179692
Rh	0.243631477206	0.391844641633	-0.456497912935
C	0.995124900329	2.056563994144	0.068634231206
N	1.454301640264	3.077543166549	0.385848801878
C	2.103871373189	4.267154117497	0.761642066691
H	1.858604664664	4.516450273734	1.799840263903
H	3.189052964757	4.141083815982	0.671659346976
H	1.785366895660	5.090981590272	0.113414734638
H	-4.584476672816	2.870561891711	-0.813087924649
H	0.571050275924	0.937304530869	4.113656564365
H	-1.555604527935	-4.091236477718	-2.675253268363
C	4.488326212596	-0.795847369943	-0.322166565715
C	3.355718749287	0.212033377628	-0.621610114031
C	2.082392999681	-0.427213312833	-0.052957399483
C	2.318970067812	-1.903068409527	-0.365157705238
C	3.774855489978	-2.112328470352	0.057755033532
H	5.142357650970	-0.930659673741	-1.193333128089
H	5.132244034756	-0.445279971547	0.494494466053
H	3.246451694798	0.344832835747	-1.708175391467
H	3.564341532374	1.207102423037	-0.205106922198
H	2.129081597414	-0.330345247715	1.054432829224
H	0.724569927360	0.722572369572	-1.861936765323
H	1.614064225037	-2.573746219474	0.140604462860
H	2.228176490186	-2.075957389407	-1.449366149528
H	3.813944115073	-2.264728860003	1.145562119657
H	4.238447947171	-2.993787598271	-0.402733345327

TpRh(CNMe)-Cyclopentane TS_3-(1)

G = -1140.698555

B	-2.078797778683	-1.101519812571	0.865674176479
H	-2.967981860224	-1.657844972812	1.444333871955
N	-2.629000726319	-0.386256605594	-0.383151543857
C	-3.853320994327	-0.329748669601	-0.928377004284
C	-2.432804691617	0.803891289562	-2.163558177957
C	-3.780014894345	0.432201828698	-2.080078612045
H	-4.686844314056	-0.834554594761	-0.456395662198
H	-1.923397562094	1.396498125994	-2.914207984363
N	-1.039434510956	-2.131646169120	0.404277264799
C	-1.104200429174	-3.469841209816	0.431894160840
C	0.631664041735	-2.846960078339	-0.760291853513
C	-0.047642574001	-3.977713872845	-0.300488308508
H	-1.902407558222	-3.963677408659	0.970734113416
H	1.520607561343	-2.770659263732	-1.373197922022
N	-1.373551447722	0.001458265196	1.684059190646
C	-1.897230842371	1.201053846636	2.030322740599
C	-0.003252733175	0.859083362806	3.084068632789
C	-1.042716449124	1.794140637048	2.932336084034
H	-2.832625099153	1.540965738883	1.601394050727
H	0.891359213510	0.927375225622	3.693137282237
N	0.031860257246	-1.745572927354	-0.326744980997
N	-0.204085447543	-0.220623378077	2.343427907433
N	-1.752417120469	0.306700473972	-1.138430935912
Rh	0.329142699975	0.297551370073	-0.451911895304
C	0.535510652967	2.183374766596	-0.573622654365
N	0.680951089303	3.335510493768	-0.634400150152
C	0.873525491021	4.728427132526	-0.673312986648
H	0.104667077847	5.196721662617	-1.297647005974
H	0.810066825788	5.140744191115	0.339720763375
H	1.860618074453	4.956704815413	-1.090321091279
H	-4.581924837209	0.679729388003	-2.759884268926
H	-1.154678656272	2.757063312687	3.410399419049
H	0.197059925316	-5.014620262132	-0.475330777945
C	3.737777898211	-1.628528681015	0.004268560930
C	2.762116205751	-0.968452337496	1.008463904488
C	2.252281792698	0.324186573820	0.338018663604
C	3.371961603703	0.642313059911	-0.660584755147
C	3.724359829427	-0.725606134831	-1.236321908856
H	4.752816315378	-1.658771246845	0.423409187401
H	3.474819670870	-2.669096419392	-0.223628943666
H	3.307340759389	-0.705740497178	1.928578412387
H	1.953850984992	-1.633486894282	1.326862158869
H	0.903326881292	0.227032703205	-1.854279317406

H	2.181467790971	1.117073087575	1.103291030923
H	3.101025849532	1.381090299446	-1.426196521127
H	4.256468565356	1.035411897973	-0.126057423303
H	2.931798010242	-1.033573173324	-1.935526783698
H	4.671035498741	-0.743535149373	-1.790476387529

TpRh(CNMe)-Cyclopentane TS_3-(2)

G = -1140.700701

B	-2.173489714788	-0.820406039858	1.090725538072
H	-3.066585476213	-1.266897546402	1.752759999988
N	-2.709855888556	0.294644221137	0.171812296661
C	-3.941928656973	0.783722499642	-0.032565629597
C	-2.507143289419	1.801603498243	-1.349270098946
C	-3.863364944132	1.764402908577	-1.004553748763
H	-4.783841236248	0.399211346107	0.529296417612
H	-1.994969229832	2.416407334363	-2.079917850603
N	-1.587981827785	-1.925661671764	0.203599002415
C	-2.058622548091	-3.161056488081	-0.013859809211
C	-0.466536369331	-2.721355041644	-1.459207296941
C	-1.366249695323	-3.716972631459	-1.072762082983
H	-2.856037106737	-3.554148693963	0.603358597416
H	0.268986487264	-2.724289321962	-2.252808599178
N	-1.040363671092	-0.165319025535	1.907690925219
C	-1.124062355530	0.989765044944	2.607159535574
C	0.768844123311	-0.031139889850	3.039164907234
C	0.026464571101	1.120793214384	3.352531882497
H	-1.993417962675	1.630269193929	2.515124158070
H	1.749592851775	-0.326894828354	3.394878534981
N	-0.602249964241	-1.652734599873	-0.683782731580
N	0.127621483627	-0.808435567195	2.178373633943
N	-1.825162833619	0.914539736570	-0.635421135953
Rh	0.246558289169	0.230547247030	-0.514060596846
C	0.961942566806	1.980109307500	-0.316978850159
N	1.400957277541	3.047694262966	-0.176891450467
C	1.980111573776	4.315843504808	0.009084303854
H	2.067520566087	4.531135117053	1.079679274922
H	2.978275448331	4.338644489170	-0.442627309672
H	1.357852283792	5.086064014365	-0.459686663190
H	-4.668658808744	2.361589090140	-1.406178366978
H	0.287991833280	1.926064040733	4.024387941636
H	-1.490565578156	-4.700195298092	-1.500961589977
C	4.517279553647	-0.778863645021	-0.891582667288
C	3.266389003074	0.051895758156	-1.250505672756

C	2.182035663427	-0.427222023385	-0.278900039453
C	2.466082675723	-1.926296783637	-0.234963735941
C	3.988874113161	-1.981741703609	-0.074357822694
H	5.057350664828	-1.104298368459	-1.789973585229
H	5.229471047551	-0.187354077639	-0.301816000291
H	2.954564809072	-0.163532974850	-2.283703488588
H	3.451527260715	1.133968015462	-1.200220793637
H	2.451797610538	-0.037430430083	0.726122041488
H	0.499627246064	0.376388011895	-2.002238413718
H	1.916049125538	-2.451144228666	0.555497373322
H	2.193818990562	-2.389223946967	-1.195372078315
H	4.247538029577	-1.862878478397	0.986943322121
H	4.422028898147	-2.935999662429	-0.399582748070

TpRh(CNMe)-Cyclopentane product-(1)

G = -1140.725655

B	-2.176472065958	-1.077557293503	0.795885035891
H	-3.106555391387	-1.663986030823	1.265178212774
N	-2.632245030086	-0.239742109755	-0.411219774853
C	-3.858683766341	-0.072034286530	-0.931537095729
C	-2.382648022476	1.009345629234	-2.144203419586
C	-3.750847366955	0.730742207689	-2.050927442139
H	-4.717883634180	-0.541012743807	-0.469231250499
H	-1.841434381587	1.594607740982	-2.877975517051
N	-1.118898718018	-2.075535784211	0.296248537178
C	-1.203526870653	-3.412230267313	0.215653609489
C	0.617954906872	-2.730026411185	-0.799202939296
C	-0.103837913337	-3.881546705641	-0.475343677024
H	-2.046890243329	-3.930232915933	0.653767049604
H	1.540866936694	-2.624941059095	-1.352754465181
N	-1.545323433744	-0.158620113355	1.847520283873
C	-1.894714147087	0.056135064489	3.125695483073
C	-0.122748950985	1.252182864492	2.627209277323
C	-1.006421152952	0.962165319663	3.672280968778
H	-2.748365696148	-0.454586545342	3.552568007559
H	0.737039222501	1.911041833532	2.612216760902
N	0.006003892175	-1.651414442606	-0.325063474500
N	-0.456806565150	0.573253623979	1.536697269300
N	-1.722119938863	0.421053169345	-1.155496661452
Rh	0.345679844555	0.411088662974	-0.484333430594
C	0.625279410340	2.255748722443	-0.784160660204
N	0.824905779413	3.386954390597	-0.975209560536
C	1.084230505299	4.745289906961	-1.230517078061

H	1.072056356302	4.934284523716	-2.309971292767
H	0.322363030416	5.370366448585	-0.751444171486
H	2.068653842850	5.018617487157	-0.834441695088
H	-4.543667883819	1.058023606361	-2.707131881754
H	-0.996758615216	1.352296530686	4.679187093648
H	0.140174906132	-4.905848939271	-0.714051101106
C	3.654355553403	-1.603152253332	0.215015185803
C	2.678881086301	-0.812848705704	1.121618086281
C	2.265021233032	0.444266696820	0.326437797286
C	3.424878346014	0.617455648332	-0.661259991243
C	3.741262519160	-0.808718102624	-1.095672862140
H	4.648343426003	-1.650559329414	0.680433612705
H	3.341674342550	-2.643806741144	0.062857993402
H	3.197315872930	-0.516286173030	2.046664370843
H	1.821107884469	-1.416372465995	1.441650718846
H	0.919535218022	0.199718101532	-1.912918539361
H	2.244584489911	1.305841996183	1.015653142865
H	3.199531766742	1.285821588925	-1.502059011252
H	4.308373007133	1.031038296636	-0.140087390356
H	2.974476131521	-1.136575170996	-1.811958758694
H	4.713964277533	-0.913269470700	-1.592372355469

TpRh(CNMe)-Cyclopentane product-(2)

G = -1140.728891

B	-1.872410077804	-1.559087040435	0.967964673888
H	-2.607444065568	-2.331871378523	1.507692894793
N	-2.676885587621	-0.583616658270	0.090618546772
C	-4.002846561152	-0.491492797013	-0.100189276568
C	-2.967670979666	0.978384598170	-1.359586173308
C	-4.241851188181	0.506056962643	-1.025779282194
H	-4.678978350919	-1.146614322833	0.434120136829
H	-2.674943076455	1.753472954889	-2.057684596437
N	-0.891836767661	-2.310627767814	0.050718714044
C	-0.863536550306	-3.610523256622	-0.280369383967
C	0.612427122871	-2.515682715650	-1.481029412516
C	0.094532765518	-3.794047114994	-1.259541020232
H	-1.530884069313	-4.310348702192	0.205820247490
H	1.383648442137	-2.181934404485	-2.164888498778
N	-1.076696189075	-0.763728987648	2.011471046207
C	-1.099910948111	-0.828829122837	3.352423605416
C	0.359225703297	0.679372995044	2.706124169346
C	-0.189280795618	0.085070237027	3.847946272716
H	-1.761951399990	-1.521963010694	3.855414158137

H	1.123874573521	1.442853770417	2.617682753554
N	0.018157644042	-1.635612957892	-0.685354897567
N	-0.181936438910	0.161259682823	1.611565830355
N	-2.037243801036	0.317035242271	-0.683896694966
Rh	0.121215730309	0.435087642637	-0.520244585327
C	0.204721975897	2.325781195681	-0.518421279709
N	0.284402106596	3.487559473530	-0.532167821717
C	0.387912648140	4.889122238270	-0.582736361343
H	-0.413764704015	5.347030513911	0.007443359741
H	1.354151786849	5.208168014146	-0.176313596093
H	0.308711564190	5.234849814638	-1.619727660060
H	-5.196040298494	0.836863404637	-1.408291533047
H	0.043857226589	0.289493528292	4.882375060604
H	0.376211528200	-4.717350358447	-1.743128130134
C	4.499003362203	0.364058847116	-0.956231588791
C	3.067845703065	0.614656930487	-1.471573045202
C	2.171516764382	0.473325723014	-0.239839195171
C	2.827120068212	-0.716758528403	0.467629440553
C	4.325067870635	-0.395300986562	0.382098082460
H	5.098803372904	-0.207703416545	-1.676004186726
H	5.029860089757	1.312095436535	-0.798300814493
H	2.791694444640	-0.154786089527	-2.209868385969
H	2.954831777024	1.581580967146	-1.979933344751
H	2.387726951421	1.350888777627	0.408101747384
H	0.340095142532	0.538818567502	-2.055101215681
H	2.478429485130	-0.866345480215	1.497412070619
H	2.621895173621	-1.648045714939	-0.077832912339
H	4.611851890923	0.250538348563	1.223740385474
H	4.957772306354	-1.289744215020	0.444513581483

TpRh(CNMe)-Cyclopentane 1,2-migration

G = -1140.692109

B	-2.360005451923	0.927821772265	-0.103248030088
H	-3.454045119427	1.404156123081	-0.229491703763
N	-2.517197837010	-0.470491942011	0.540428260638
C	-3.641734905187	-1.159909656425	0.786118340699
C	-1.909721296274	-2.351836658108	1.417926849395
C	-3.304317513839	-2.377348949220	1.346043079601
H	-4.602904552654	-0.727358909609	0.540178996180
H	-1.216076728059	-3.088861324358	1.802016043733
N	-1.534458041515	1.803191585403	0.846357955370
C	-1.767859308791	3.040247533371	1.297956724341
C	0.192397792638	2.359781352107	2.009684096428

C	-0.683747980594	3.444889593315	2.056455696756
H	-2.687561235023	3.548275445323	1.038628068171
H	1.163672749783	2.230229666728	2.473595933334
N	-1.582132714793	0.763708233125	-1.412209491714
C	-1.576034448035	-0.288680136914	-2.255964649427
C	-0.259736537642	1.299263598379	-2.994325327125
C	-0.728643996332	0.010312727653	-3.301825381587
H	-2.160649328365	-1.176496888707	-2.044828970726
H	0.427261294132	1.924360628333	-3.554333946529
N	-0.328935976641	1.380153304534	1.274305972353
N	-0.774978707299	1.749380954675	-1.858519272175
N	-1.449382420257	-1.202271569600	0.930903804363
Rh	0.395732795754	-0.470870730407	0.706730371402
C	1.043012061829	-2.157882739675	0.149281281826
N	1.445065978104	-3.196703907524	-0.210240666126
C	1.960216025721	-4.383337389759	-0.758590629424
H	1.999569486594	-5.172166129797	0.001783662322
H	1.328569267325	-4.722441601537	-1.588202206761
H	2.974873496523	-4.209009605286	-1.137061986334
H	-3.969534412091	-3.166045958240	1.664147621467
H	-0.490408775257	-0.607758960536	-4.155853079486
H	-0.549397081205	4.385556032398	2.568949915740
C	2.567561904578	1.064710085347	-0.264447469689
C	3.176098725635	0.427753957271	1.002114364509
C	4.101164501158	-0.704053917318	0.495518302676
C	4.070217103712	-0.604691258029	-1.038943279375
C	3.653616105637	0.837923376657	-1.311125682519
H	1.656994124178	0.550915109799	-0.650700087667
H	2.272050699205	2.110476703167	-0.126607442867
H	2.444181007627	0.060707124586	1.743838139867
H	3.761910010397	1.193022076075	1.530547526004
H	5.121513684234	-0.560392813724	0.872409797828
H	3.773017112870	-1.688872070807	0.849835604206
H	5.022251476610	-0.883488538723	-1.505288661863
H	3.297597362081	-1.275377979893	-1.445597368180
H	4.498140656226	1.519308076324	-1.121218927445
H	3.306905375607	1.010144075832	-2.336148107925

TpRh(CNMe)-Cyclohexane σ-complex-(axi)

G = -1179.964922

B	-2.601431204277	-0.939506765212	0.409074878151
H	-3.660363279580	-1.466423915605	0.610461675550
N	-1.772976547673	-0.674693391577	1.669779860033

C	-1.803880464231	0.403572725127	2.479762321965
C	-0.369630475613	-1.076821234272	3.222063540173
C	-0.905779303927	0.191600235083	3.504394731028
H	-2.449353707843	1.246247526596	2.261205770851
H	0.373597271556	-1.639430399706	3.776703469071
N	-2.865095802801	0.414451320333	-0.294677997641
C	-4.035895780662	1.018527314537	-0.547372644369
C	-2.399393783973	2.248361913147	-1.339254520768
C	-3.789865455581	2.204047815398	-1.213849727353
H	-4.961395021843	0.554238225587	-0.231940062868
H	-1.764158090820	2.990081330694	-1.806840533689
N	-1.773680112049	-1.808420714973	-0.542000360292
C	-2.010265938095	-3.035559603021	-1.018176830221
C	-0.110785666921	-2.289957231027	-1.823203753825
C	-0.964389619684	-3.393616992992	-1.850436432686
H	-2.904941456767	-3.568989934588	-0.724561973283
H	0.826523780488	-2.125032222717	-2.340826579568
N	-1.855080817565	1.168832418624	-0.784687140791
N	-0.603817166449	-1.345351814157	-1.025454564129
N	-0.892713614940	-1.594963094146	2.119087663446
Rh	0.051336206736	0.560588687744	-0.521378500189
C	0.595483317226	2.328612702783	-0.139587470578
N	0.910393485616	3.431457492382	0.094086177715
C	1.289820385878	4.739263194577	0.438905780605
H	0.569790664061	5.167937941048	1.145959857685
H	2.280520239888	4.731994093991	0.908723020506
H	1.329931188210	5.374962660320	-0.453755021086
H	-0.677090577759	0.851731641165	4.329025176208
H	-0.840812108216	-4.315890547995	-2.397924139663
H	-4.510882517529	2.926697329341	-1.565547318127
C	4.451662097308	0.123071670047	-0.508808982440
C	3.424662972097	0.525451796838	0.545219261329
C	2.151860887792	-0.306609402440	0.415580815569
C	2.446140616598	-1.801651258567	0.468988550779
C	3.477138221376	-2.199601728929	-0.581323044829
C	4.752405613849	-1.372017712194	-0.443388878613
H	1.424950387631	-0.043971555239	1.201253792058
H	3.844859918014	0.355205094511	1.549520106879
H	3.193809383816	1.596732716337	0.476497856539
H	4.054809230816	0.369562045866	-1.507728845425
H	5.374100072732	0.706866352118	-0.387627192979
H	2.847736164999	-2.023327984195	1.471343034341
H	1.516813097086	-2.375934894607	0.376077887758
H	3.702972726058	-3.271874554423	-0.510358581172
H	3.054888942217	-2.037147401709	-1.587372759957
H	5.226617625518	-1.601541867455	0.524901617696

H	5.478449534666	-1.650092989132	-1.219056957531
H	1.779678482567	-0.088115033316	-0.652648031865

TpRh(CNMe)-Cyclohexane σ-complex-(equ)

G = -1179.965523

B	-2.246539759377	-1.304050811808	0.840415788646
H	-3.118645865654	-1.979647343117	1.312064963498
N	-1.110829710299	-0.966232543582	1.811703435006
C	-1.023866774462	0.078212835563	2.661037944033
C	0.720602864777	-1.229818139624	2.868249967274
C	0.152376019273	-0.046114299265	3.369501866793
H	-1.794969894945	0.839116006472	2.689210585202
H	1.648170738469	-1.712362893116	3.156675723683
N	-2.876030110480	0.023460376550	0.352913159018
C	-4.130426010998	0.470413536514	0.514816385608
C	-2.975654212195	1.947091627871	-0.626977117491
C	-4.244146300294	1.705855190299	-0.094175363022
H	-4.851248212371	-0.130041637916	1.054639994290
H	-2.608429536279	2.788853019788	-1.200457727271
N	-1.653356770403	-2.018492078826	-0.377255333974
C	-1.872794284934	-3.250413522718	-0.849218215687
C	-0.422865598313	-2.220416861156	-2.133733799890
C	-1.100302196766	-3.431005478088	-1.983147284538
H	-2.559221997977	-3.913299126762	-0.338745630691
H	0.285832187617	-1.911572513566	-2.893053460378
N	-2.162997091525	0.930334937419	-0.353017155032
N	-0.757991929348	-1.380606183308	-1.156983626548
N	-0.040199700412	-1.780577858242	1.931401118987
Rh	-0.211753554048	0.576852371268	-0.733779040757
C	0.217451614005	2.387682125676	-0.407012538525
N	0.463665080929	3.513219703467	-0.200944844655
C	0.781317256094	4.848003648992	0.100295380363
H	1.868685302876	4.968581078373	0.172590849193
H	0.406111207744	5.517464211320	-0.683021775604
H	0.331915630584	5.137279561140	1.057665206134
H	0.536534007314	0.615279043807	4.133034910525
H	-1.039364019221	-4.308676019560	-2.608912019673
H	-5.118583798164	2.336579872872	-0.151983776873
C	3.312351781731	0.926552773286	-0.767771466656
C	2.150368729585	-0.047007112283	-0.587082355035
C	2.585946154995	-1.505947602519	-0.687365486710
C	3.715723985115	-1.783840916432	0.300575027154
C	4.885809604249	-0.825594954166	0.109307271838

C	4.424757658172	0.622921544346	0.231023596226
H	1.734927190710	-2.163926955811	-0.475928876921
H	1.696708422927	0.106302665232	0.410396346915
H	1.437125577246	0.169702063697	-1.459323700793
H	3.709391278668	0.835318724264	-1.791990007180
H	2.961038501490	1.961347505383	-0.658044737406
H	3.319872810795	-1.672672111446	1.322588302733
H	4.047411992435	-2.826204910211	0.205555375424
H	5.680306335719	-1.037615794893	0.837332703823
H	5.326803903534	-0.981666687975	-0.889147953703
H	4.048381569866	0.797506711509	1.252269323568
H	5.266332354174	1.313181277175	0.082647194969
H	2.930809567371	-1.723690055892	-1.712091125889

TpRh(CNMe)-Cyclohexane TS_2-(axi)-κ^3

G = -1179.948030

B	1.957171592519	-0.142134146522	1.151085652442
H	2.884009474772	-0.490329624216	1.824367643426
N	1.343257276978	1.125596325826	1.729103532198
C	1.802489749528	1.926230939732	2.709442391012
C	-0.054273254752	2.735312927318	1.868084999377
C	0.928356160942	2.986313378634	2.838513135872
H	2.712792588372	1.681045867574	3.242212150079
H	-0.937904254683	3.315528126466	1.625281556681
N	0.909567300550	-1.271016026035	1.102291025338
C	0.861220795796	-2.386907478872	1.844994978485
C	-0.833190370104	-2.359074741349	0.455062354613
C	-0.246451709735	-3.121604724293	1.466962808611
H	1.625182435899	-2.578254960849	2.587453612278
H	-1.715818197621	-2.557908337528	-0.140085308974
N	2.454343777574	0.083710179110	-0.291350702721
C	3.698488766790	-0.105614416404	-0.753758853676
C	2.351985052222	0.299520241425	-2.432159848606
C	3.686314969634	0.029889730726	-2.128726394373
H	4.503486988113	-0.328984681655	-0.065715445246
H	1.883655002266	0.452188864225	-3.395671894814
N	-0.131626548912	-1.249361640303	0.242780070780
N	1.617353004205	0.342651119292	-1.322606335069
N	0.201950371194	1.615016216796	1.207005615644
Rh	-0.467166952407	0.403188558021	-1.037747117883
C	-2.324332226793	0.139514301479	-0.868037140629
N	-3.462951717273	-0.096123325706	-0.745655418618
C	-4.842794275400	-0.313986261241	-0.599562928807

H	-5.155861457671	-1.190707613526	-1.179174630828
H	-5.089050052074	-0.481318417697	0.455435851422
H	-5.400858289636	0.560093675504	-0.956480461716
H	0.988808660758	3.810770377317	3.534143465392
H	4.517980279686	-0.059909367420	-2.811313248732
H	-0.573070731244	-4.073788220769	1.857512373567
C	-2.464964492876	2.058694477667	-4.012731954194
C	-2.174256303837	2.630009447697	-2.628490554831
C	-0.771351197543	2.266486004080	-2.137461114361
C	0.244279178539	2.784742939924	-3.158049101932
C	-0.007910351429	2.228879488807	-4.557571330664
C	-1.427986437174	2.539789350024	-5.025093436447
H	-0.584306375889	2.765483337776	-1.173249803107
H	-2.233319500580	3.731276622524	-2.688304386784
H	-2.942235350399	2.325185447474	-1.908267963101
H	-2.447997102010	0.957282429948	-3.962477256382
H	-3.474663472785	2.342195508515	-4.340937672293
H	0.141874043580	3.883293531035	-3.199088260165
H	1.270008116149	2.592047376174	-2.827542599549
H	0.725377661584	2.632515382435	-5.269486284211
H	0.129511132739	1.134637770358	-4.553236745393
H	-1.532200443050	3.630114221896	-5.149762238128
H	-1.614825863275	2.094094585021	-6.011519221847
H	-0.711503491234	0.822659153585	-2.533572683135

TpRh(CNMe)-Cyclohexane TS_2-(axi)-κ^2

G = -1179.949368

B	-2.409922762948	-1.184097908925	0.483789114381
H	-3.417661322129	-1.787553410702	0.725687296099
N	-1.573074442320	-0.835815316823	1.717429107268
C	-1.576820681644	0.296116635132	2.456136914245
C	-0.297041516710	-1.225558167193	3.379087426010
C	-0.757361238664	0.092848210419	3.545842256147
H	-2.154149109907	1.160772728835	2.150130723069
H	0.376247553450	-1.794904481756	4.010532076863
N	-2.790553233101	0.135759172574	-0.224106759717
C	-4.001528579882	0.676519551950	-0.410988965331
C	-2.472558313443	2.004335042312	-1.253045024151
C	-3.851037372953	1.882876373328	-1.072032836241
H	-4.885194162641	0.160749152493	-0.057131769246
H	-1.902326896384	2.789043435164	-1.735524827197
N	-1.548004420336	-2.010042781286	-0.475747182595
C	-1.775638133528	-3.224953154269	-0.986844592304

C	0.090742562511	-2.422440600508	-1.811557043981
C	-0.744910078843	-3.538251109493	-1.854618106780
H	-2.653938292913	-3.782264883775	-0.688179384526
H	1.013931308216	-2.228549913882	-2.342336111893
N	-1.843146032664	0.949356345128	-0.741050160874
N	-0.395922900550	-1.511302961977	-0.971502762960
N	-0.790078876329	-1.780676577827	2.281140604349
Rh	0.207384620320	0.437566377636	-0.548339331020
C	0.674950177043	2.265174654729	-0.414618585768
N	0.920313377911	3.406987045926	-0.383920720264
C	1.286566861093	4.760391391181	-0.284001970892
H	0.514599127063	5.321028610060	0.255347218269
H	2.234248490990	4.852166317934	0.260075429007
H	1.409075554324	5.196533377746	-1.282283796698
H	-0.527665317727	0.791257570108	4.337939742187
H	-0.617146225492	-4.441558126586	-2.431933267160
H	-4.625997214526	2.567982021661	-1.381957855378
C	4.134981188427	0.653859600709	-0.334495372104
C	3.101335645315	0.799914567255	0.777190828505
C	1.915708595479	-0.146968853060	0.612837941480
C	2.425878082094	-1.580391380025	0.508056513873
C	3.459802258018	-1.758504518707	-0.599672249931
C	4.626052746618	-0.788130860791	-0.432435136685
H	1.249924204143	-0.062418304704	1.489277603168
H	3.585992418417	0.544356533382	1.736244397030
H	2.774004005201	1.841459833275	0.875733667483
H	3.683857342956	0.955709272171	-1.294432350189
H	4.980647343758	1.333629586897	-0.160509238233
H	2.909841096843	-1.813819186298	1.473412627153
H	1.595056069772	-2.286645495339	0.413465464383
H	3.822845408921	-2.795112386464	-0.618783489923
H	2.988628573829	-1.576994430221	-1.579223950722
H	5.173889552303	-1.041019810338	0.489978360664
H	5.341170919186	-0.896746402721	-1.259154504922
H	1.663751181434	0.097271065664	-0.979438233944

TpRh(CNMe)-Cyclohexane TS_2-(equ)-κ^3

G = -1179.949569

B	1.991432051449	-0.103308929485	1.075449823595
H	2.972791704700	-0.386113678200	1.699989814276
N	1.429665297512	1.227613970144	1.562372346740
C	1.971171130619	2.126772121943	2.405575282381
C	0.068369054510	2.874497867624	1.611052426624

C	1.123605691024	3.214077889142	2.472016474499
H	2.915850581206	1.925796740612	2.895345554930
H	-0.823381957374	3.441422496666	1.365997910569
N	0.942437708868	-1.220213012058	1.237097321497
C	0.960050721179	-2.252472814905	2.093630178199
C	-0.857668593918	-2.346319334151	0.872502153650
C	-0.180834388252	-3.007600374601	1.899273437900
H	1.789519237230	-2.375995368260	2.777895865914
H	-1.793125999687	-2.593416109027	0.385970232443
N	2.357246489568	-0.023028685032	-0.419444982772
C	3.561346206017	-0.204091373030	-0.980742162184
C	2.056664407434	0.062043345252	-2.550923228200
C	3.421214638277	-0.151619361809	-2.354817940979
H	4.432035695266	-0.360734354523	-0.357294076751
H	1.496063934155	0.150524651764	-3.472498606476
N	-0.175142013049	-1.274344627816	0.480853269388
N	1.424809019470	0.147534932805	-1.382945229824
N	0.259815053987	1.679607026817	1.069950388635
Rh	-0.621471557534	0.243828248058	-0.920200210510
C	-2.466244958576	0.036357343625	-0.592400287380
N	-3.601662985869	-0.124543910020	-0.364006165713
C	-4.970282743905	-0.308392353972	-0.106974768373
H	-5.558171702368	0.438311674028	-0.653724491600
H	-5.289239480928	-1.307894089258	-0.426548591126
H	-5.172494852312	-0.198514446607	0.964867237994
H	1.247100257705	4.112173604636	3.059762042576
H	4.191440479483	-0.260522182031	-3.103527546389
H	-0.472505683591	-3.909748793507	2.415921025141
C	-2.304686840387	2.111897145409	-3.047379985258
C	-1.073983997050	1.985881682032	-2.139724941467
C	0.119201466433	2.701538229646	-2.766265284719
C	-0.214624726099	4.164497026304	-3.057853859441
C	-1.442198635988	4.292871778115	-3.951546617624
C	-2.635832190038	3.573732951890	-3.334442367546
H	0.991578310385	2.641406178059	-2.104527690469
H	-1.314103173593	2.508493572806	-1.194991583856
H	-0.932752425595	0.550952916566	-2.432470957276
H	-2.114194664635	1.593902282055	-4.003013881273
H	-3.168126464424	1.606591727860	-2.594151660120
H	-0.404118023168	4.683266564321	-2.103943930330
H	0.650907509216	4.663156008441	-3.515861048228
H	-1.679409052331	5.349568538518	-4.135612868582
H	-1.222245411429	3.846063049409	-4.935234446892
H	-2.911231839161	4.073347608922	-2.391109711307
H	-3.512970053973	3.642693760458	-3.993259400263
H	0.400357819540	2.207912584367	-3.711728964020

TpRh(CNMe)-Cyclohexane TS_2-(equ)-κ^2

G = -1179.950233

B	-2.124567265560	-1.404371794719	0.816908079240
H	-2.958230630760	-2.130258040994	1.281471537305
N	-1.004372729629	-1.020835222210	1.789418428629
C	-0.905001984435	0.070615719558	2.581501957493
C	0.742873284426	-1.320092941491	2.972782238386
C	0.218465522288	-0.076100352722	3.366225306694
H	-1.634096523671	0.870379815730	2.525103894508
H	1.626322795021	-1.831337694977	3.339712061859
N	-2.809672186351	-0.097259695211	0.358898856626
C	-4.067258602643	0.318722641183	0.555744475448
C	-2.947162312616	1.866556390457	-0.521930640808
C	-4.207830889703	1.580195133928	0.004094738404
H	-4.772190268361	-0.315487306569	1.078206864205
H	-2.600731424768	2.743585552348	-1.055408143539
N	-1.502340977562	-2.075277508206	-0.412929948404
C	-1.739193565112	-3.284104093360	-0.935000345005
C	-0.280925464949	-2.222180498408	-2.182809745398
C	-0.973765620507	-3.428223757996	-2.078572845624
H	-2.432249294714	-3.958081669293	-0.448502256645
H	0.433847009952	-1.893193197706	-2.927074977161
N	-2.113398754972	0.852277423836	-0.304406859157
N	-0.600674302843	-1.417911603066	-1.172211217854
N	0.004959728100	-1.885447614518	2.027995427039
Rh	-0.059519212870	0.539123144782	-0.740152867297
C	0.303466065243	2.384586829067	-0.511692108068
N	0.477111341801	3.532305176916	-0.383663592962
C	0.765283893563	4.897119218283	-0.209433385797
H	1.848399821698	5.041366406922	-0.118705930130
H	0.402935803150	5.475054876352	-1.067570033949
H	0.281601231998	5.271506395331	0.699970505710
H	0.598878626094	0.610747239098	4.108861037402
H	-0.924407604340	-4.281686263733	-2.737941558333
H	-5.094097369106	2.196652444503	-0.018406580587
C	3.125299462754	1.020744564400	-0.634183097349
C	1.977718229793	0.074147095897	-0.276376118259
C	2.407156336406	-1.377929405969	-0.462938895330
C	3.661152035926	-1.675594767764	0.360375704090
C	4.805322791931	-0.730238116053	0.019755303077
C	4.368227602866	0.717581710608	0.200447095411
H	1.605336552610	-2.055892930493	-0.154146949799

H	1.724951998389	0.220300433642	0.793197328644
H	1.191025752561	0.375189006993	-1.644895389959
H	3.377963335003	0.911705914694	-1.702628111390
H	2.827721988871	2.067689897268	-0.493645581514
H	3.410329626082	-1.571223589158	1.428564464683
H	3.961800396346	-2.721867638306	0.211731495512
H	5.687682775773	-0.948472667873	0.636799780671
H	5.109155130485	-0.887537541745	-1.028433033384
H	4.140252975662	0.896862017378	1.263901713844
H	5.180435931867	1.407939146052	-0.067991799418
H	2.617640988816	-1.576032802686	-1.528208271759

TpRh(CNMe)-Cyclohexane IM-(axi)

G = -1179.964287

B	-2.511201626129	-0.929679566249	0.513696512411
H	-3.563188402271	-1.372704429225	0.872145416840
N	-1.568280843050	-0.517310584152	1.663093010796
C	-1.395889040709	0.710934171285	2.233332338469
C	-0.567588110222	-0.862926892219	3.515929977304
C	-0.735932734596	0.532538134847	3.426083661300
H	-1.771937291767	1.604563317476	1.748602319037
H	-0.090101405933	-1.436771506340	4.302700608120
N	-2.742920475870	0.321778487668	-0.354636855456
C	-3.872097990916	0.944308538060	-0.724571799691
C	-2.140763399253	1.938954407966	-1.641875708560
C	-3.536319851774	1.997767780873	-1.554987698358
H	-4.832316825043	0.589993129724	-0.371667075824
H	-1.453368591427	2.568938740339	-2.194068896060
N	-1.760216865905	-1.960703646385	-0.337932762995
C	-2.189126696723	-3.095483698183	-0.901783800832
C	-0.174000034217	-2.627753955449	-1.637919075004
C	-1.200659846591	-3.567032120855	-1.746731271449
H	-3.165611540466	-3.490478957774	-0.652940868333
H	0.792224966373	-2.597746983097	-2.126158074227
N	-1.675949755605	0.925845787517	-0.920704630982
N	-0.515899034454	-1.670432750668	-0.780955517481
N	-1.074258759847	-1.488964323922	2.468589961444
Rh	0.252790946316	0.180980606285	-0.229158364184
C	0.852074568620	1.945940959079	0.133897853978
N	1.176218777438	3.051956357387	0.296487131117
C	1.710061851270	4.326197108974	0.562296568600
H	0.984851256181	4.929373171142	1.119244678204
H	2.625544866834	4.225945572534	1.157461409771

H	1.949585135573	4.836173525120	-0.377347968439
H	-0.422954104390	1.293553102163	4.126566319067
H	-1.215584520429	-4.465111755733	-2.345832678843
H	-4.203703125014	2.699554074455	-2.033032195181
C	3.896723214425	0.648819396471	-0.197003701150
C	3.079003191776	0.320999034131	1.050225136397
C	1.909025433739	-0.617744778304	0.743379697389
C	2.510247190196	-1.898873073498	0.165677741356
C	3.321910989056	-1.638400729555	-1.101444837486
C	4.436746181351	-0.628793963051	-0.836725967051
H	1.412031259421	-0.872448106307	1.699892055244
H	3.752732239238	-0.182650361914	1.769282531080
H	2.746505389956	1.236553346217	1.558888732485
H	3.261009494651	1.177851465314	-0.925385761378
H	4.728685769422	1.325065506097	0.049419689622
H	3.199002546595	-2.324899296023	0.920095669759
H	1.748194505422	-2.666927205498	0.003000296996
H	3.749096800855	-2.575842874173	-1.486683007854
H	2.661072066058	-1.243029726324	-1.889342775463
H	5.170539840661	-1.083629265157	-0.151120482455
H	4.979652011902	-0.397768299383	-1.763993353978
H	1.031614379271	0.303075128313	-1.527156188070

TpRh(CNMe)-Cyclohexane IM-(equ)

G = -1179.967110

B	-2.162254140591	-1.008693881373	1.035221300599
H	-2.937450647657	-1.516250581881	1.792148443057
N	-1.011306462964	-0.228352720015	1.718419883688
C	-1.032509831975	1.069115529971	2.152929652662
C	0.524797222702	-0.069773275227	3.196569567266
C	-0.044152340128	1.218584648347	3.090929816941
H	-1.750999567328	1.773205810748	1.748704978480
H	1.345397811100	-0.395680746250	3.826856856630
N	-2.889756232866	0.006093170806	0.133550374418
C	-4.181271240971	0.359274917209	0.047674179145
C	-3.007811095791	1.454347499144	-1.454153307651
C	-4.309070996404	1.294484133978	-0.962651577849
H	-4.914821970799	-0.081686471103	0.710711200954
H	-2.642812962972	2.085485045127	-2.255752741408
N	-1.512844007065	-2.068202490492	0.137686709112
C	-1.822293780381	-3.353658237021	-0.071292158323
C	-0.287601814969	-2.723587886419	-1.512442954749
C	-1.056657642647	-3.822735643859	-1.123426455052

H	-2.562081491059	-3.843499543031	0.548486886292
H	0.454140212639	-2.637111943467	-2.296259217369
N	-2.164882912046	0.673420286305	-0.790436338924
N	-0.565613432888	-1.677426673177	-0.744246413063
N	-0.062004716153	-0.934656366933	2.394790162900
Rh	-0.013292614507	0.313708304772	-0.617563990812
C	0.420126113351	2.162634208940	-0.527980801916
N	0.678158025888	3.295421470662	-0.463906104994
C	1.069946573677	4.644095818555	-0.384875255173
H	2.082567692436	4.760982682016	-0.787506694723
H	0.381399985401	5.270797700210	-0.962280073290
H	1.061532942975	4.974979335514	0.659530929441
H	0.232571306646	2.119155799949	3.620528082098
H	-1.050238589615	-4.817414968718	-1.543328560808
H	-5.211600987022	1.783776985879	-1.298104011857
C	3.013262156135	0.570789264096	-1.103866058251
C	1.974068357987	-0.052863672978	-0.166607279518
C	2.335728995053	-1.521759665712	0.057211097444
C	3.747294615338	-1.667512721398	0.627967476682
C	4.782734038944	-1.028697172750	-0.289619882588
C	4.436283964083	0.430263594019	-0.560893510912
H	1.610826215709	-2.006280275848	0.722599876938
H	2.074603842840	0.450532003731	0.821338825212
H	0.377700166624	0.369271624575	-2.087690809887
H	2.954162660867	0.071610764391	-2.086247075486
H	2.799301795733	1.632376685647	-1.295275231071
H	3.785495668083	-1.178368130708	1.615756369055
H	3.983935019847	-2.728209890193	0.796131297405
H	5.792119340880	-1.115038258896	0.136999101471
H	4.800756942063	-1.577075875821	-1.246332472917
H	4.516551733816	0.999208301213	0.380619479205
H	5.161484744482	0.875930102445	-1.257975775998
H	2.297786139444	-2.059668110668	-0.904863819544

TpRh(CNMe)-Cyclohexane TS_3-(axi)

G = -1179.959743

B	-2.608620977047	-0.568814226717	0.601649853819
H	-3.710376390163	-0.860413324483	0.971829435133
N	-1.832229647534	0.341605060376	1.570036986567
C	-2.081966393730	1.648758560529	1.813123005048
C	-0.576647606676	0.882196733601	3.211707585033
C	-1.289575783598	2.043874402629	2.868051393999
H	-2.799171895173	2.196545126945	1.213096351481

H	0.171595914996	0.746740118993	3.984735315749
N	-2.693296731589	0.219539877045	-0.719284936102
C	-3.725224253485	0.595817615831	-1.488560569759
C	-1.836355816706	1.249245908432	-2.401371591816
C	-3.223362762584	1.269472020318	-2.587583876203
H	-4.740571790473	0.357497575034	-1.197610616264
H	-1.047353662048	1.650632625632	-3.026525241279
N	-1.809174405831	-1.850586429297	0.329438973012
C	-2.281346848781	-3.102397393056	0.258954235100
C	-0.247923396042	-3.045345211029	-0.560513016395
C	-1.312230855891	-3.910754398306	-0.302935486952
H	-3.279164643779	-3.324905903801	0.614190975913
H	0.717928614374	-3.255236085509	-1.001431497972
N	-1.531832931414	0.615847873207	-1.274995173625
N	-0.548946532822	-1.811357781985	-0.170009240633
N	-0.906869585048	-0.141967912290	2.437447705325
Rh	0.322153418827	0.080783048926	-0.244174571908
C	0.923549455025	1.875865068324	-0.380080598057
N	1.219047480556	2.993133221378	-0.511689889067
C	1.669868526301	4.323579057573	-0.578559925241
H	0.948853665883	4.987021999474	-0.088650444847
H	2.639225446429	4.412002862109	-0.074017333642
H	1.782660612222	4.630070576793	-1.624272658334
H	-1.236343493181	3.023147076882	3.322329444370
H	-1.364073794193	-4.971939112477	-0.494554656350
H	-3.778816812184	1.706304420572	-3.404336657111
C	3.952106753623	0.318123739816	-0.654202987431
C	3.259028406831	0.486928489311	0.695066531162
C	2.034442781285	-0.423534423650	0.842432976391
C	2.539206010645	-1.858509917036	0.693148343431
C	3.211027355879	-2.098425404946	-0.657398144090
C	4.377549306263	-1.134039417358	-0.862601611595
H	1.641935532733	-0.306041836839	1.867557196101
H	3.989348872124	0.215811082567	1.481274524246
H	3.014217013166	1.541529154036	0.880532146785
H	3.264049031592	0.618031900789	-1.460796935739
H	4.829190269110	0.978050827700	-0.725487323187
H	3.298786550911	-2.039569352696	1.477711533177
H	1.746057644958	-2.587027272506	0.886466025566
H	3.565284222767	-3.136953901255	-0.736645404674
H	2.479680700547	-1.949479382284	-1.467779887115
H	5.168607689529	-1.376966331428	-0.134122247233
H	4.821374063932	-1.268413865698	-1.859054728142
H	1.057795029462	-0.169467460176	-1.543715836645

TpRh(CNMe)-Cyclohexane TS_3-(equ)

G = -1179.964135

B	-2.225331452263	-1.055705683609	1.076660958045
H	-3.052893644210	-1.611719735136	1.740743692841
N	-1.206988005903	-0.225618610627	1.887234999551
C	-1.456875238490	0.937525158264	2.533692924061
C	0.532273068423	0.178573547065	3.064158585070
C	-0.357362787790	1.240741655077	3.304928278952
H	-2.394385810202	1.461241750130	2.387720734052
H	1.529950775531	0.022216020656	3.459423333598
N	-2.900454226286	-0.045572520846	0.129220156883
C	-4.185175876196	0.264598500742	-0.100005895764
C	-2.884143024884	1.451420124569	-1.414622677544
C	-4.227674542424	1.231481233463	-1.087838347852
H	-4.974647543964	-0.223996504978	0.457104838559
H	-2.450674044676	2.120297011375	-2.148686424720
N	-1.479040986384	-2.085526348911	0.217686364735
C	-1.771724227659	-3.377521761661	0.016251484513
C	-0.242772887730	-2.742589105797	-1.425269432612
C	-0.999140795867	-3.847590073851	-1.028979826181
H	-2.512953290846	-3.868559895878	0.633351758774
H	0.497916632254	-2.654608720481	-2.209703446467
N	-2.097278577302	0.678907810470	-0.676238857205
N	-0.532840943963	-1.692315418210	-0.667941850427
N	0.020603961899	-0.706678309224	2.221706509384
Rh	0.053016300933	0.286790037739	-0.502623316681
C	0.505238984238	2.121315982625	-0.294901045764
N	0.784250533784	3.239660840877	-0.140958362005
C	1.156881451316	4.579224234176	0.071396261241
H	2.127484160708	4.774603827130	-0.398049374679
H	0.408066173014	5.251075378158	-0.362327684695
H	1.233693714935	4.777177268754	1.146175818618
H	-0.220191964840	2.098856782349	3.947692146820
H	-0.982518755122	-4.844891480492	-1.442111622438
H	-5.101485739451	1.704686259400	-1.510923853433
C	3.007505537395	0.492428079768	-1.294326372385
C	2.073450196187	-0.091844867787	-0.230134887649
C	2.447697838007	-1.554210798517	0.009315598983
C	3.909618184656	-1.688190570568	0.439342544948
C	4.844451399204	-1.093054520139	-0.607521318238
C	4.479437703457	0.357653178721	-0.900418939815
H	1.783510533386	-2.006731452166	0.756606942683
H	2.290885118484	0.440891955513	0.720937837729
H	0.321386165539	0.454225154982	-1.986307737446
H	2.841915625406	-0.036334691743	-2.248931643071

H	2.775222579885	1.549224804609	-1.494049846623
H	4.053709266309	-1.160967518315	1.397232193500
H	4.160812784368	-2.742938856714	0.623526785744
H	5.893119247212	-1.171526615382	-0.287387392931
H	4.758449209521	-1.679295314741	-1.537801690175
H	4.662671859138	0.962698647803	0.003484973980
H	5.130169808719	0.767303583049	-1.687258035098
H	2.318251672545	-2.126962731687	-0.923177771368

TpRh(CNMe)-Cyclohexane product-(axi)

G = -1179.986304

B	-2.714691908553	-0.497332079192	0.539224065135
H	-3.839039290532	-0.774127013463	0.836303930818
N	-2.057897493468	0.326362918301	1.649284978983
C	-2.561250993303	0.780091034524	2.808359846758
C	-0.472789529231	1.424768759330	2.599409209805
C	-1.574962757426	1.497153412651	3.458511930759
H	-3.583228723873	0.556516644618	3.086529108162
H	0.523936652831	1.836579553751	2.711147427288
N	-2.696946312783	0.313118460059	-0.770453519386
C	-3.712455403937	0.750712243498	-1.531654644749
C	-1.799777492378	1.280270683816	-2.469599232158
C	-3.184514806852	1.385848011482	-2.639685632329
H	-4.737166401691	0.573304346732	-1.230980084126
H	-0.993012082871	1.627910994969	-3.103914076098
N	-1.903837262681	-1.781026403791	0.288701399717
C	-2.377244307418	-3.027894790230	0.140516853931
C	-0.288715102938	-2.956364342070	-0.524025688220
C	-1.372323026994	-3.824083653935	-0.371970369169
H	-3.401287034709	-3.254297238726	0.408353040835
H	0.702977857469	-3.151129447356	-0.911609568262
N	-1.520012611552	0.633752266687	-1.345119932389
N	-0.610653954953	-1.734228325715	-0.114206589308
N	-0.776738488983	0.719849418059	1.517063191015
Rh	0.310625153427	0.142362407278	-0.284403904024
C	1.037551548038	1.847666115005	-0.653816712746
N	1.435094127748	2.902985191721	-0.944523999244
C	2.044364358151	4.134221866145	-1.243562044606
H	1.381564138098	4.960944187621	-0.965045101726
H	2.985013842816	4.227106850686	-0.687474208207
H	2.259342450439	4.197374823905	-2.316274333374
H	-1.642464236473	1.994632614675	4.414632659594
H	-1.414611886024	-4.878133155821	-0.601971332099

H	-3.722253265543	1.847937383493	-3.454269486486
C	3.972088241807	0.379166452985	-0.508568450257
C	3.203149992513	0.568835514702	0.797263368324
C	1.980212844246	-0.352139710179	0.896985402975
C	2.510335290351	-1.784934977846	0.790245769079
C	3.276865332225	-2.046660862119	-0.503625949549
C	4.440258103884	-1.067946876059	-0.649560510638
H	1.568787680131	-0.243659047341	1.915274561875
H	3.894514535545	0.326761871593	1.627570791521
H	2.933987860567	1.625293657957	0.943484647169
H	3.323140549348	0.631590442544	-1.361281999311
H	4.836496174594	1.058635263369	-0.550792233460
H	3.215279572597	-1.948424610829	1.628697774337
H	1.714052507131	-2.521060243800	0.940613640656
H	3.652641860207	-3.080455522800	-0.525340443024
H	2.604067756009	-1.932368114952	-1.366803060213
H	5.183287910333	-1.278263499829	0.137645006877
H	4.953922738060	-1.216322364425	-1.609913047909
H	1.050331296603	-0.331082111678	-1.562123452551

TpRh(CNMe)-Cyclohexane product-(equ)

G = -1179.993428

B	-2.426255572138	-1.128685434706	0.637690326830
H	-3.363521790926	-1.756898671482	1.032274114115
N	-1.559554327113	-0.670531297430	1.817648106319
C	-1.713154167670	-0.879873209324	3.135022616947
C	0.099491147969	0.306266480729	2.776721864872
C	-0.666034943664	-0.268045406812	3.797414094863
H	-2.556426258198	-1.449642193897	3.503862786468
H	1.020599476258	0.874653381331	2.835225547250
N	-2.905340457562	0.104124956979	-0.149427992373
C	-4.152702666869	0.536925412425	-0.394436610177
C	-2.702649885679	1.841383998731	-1.401375245979
C	-4.074929143380	1.659383246053	-1.196283252671
H	-5.004746359573	0.010509093880	0.016377708004
H	-2.180733315965	2.595089726112	-1.978773659145
N	-1.575796033403	-1.986520834193	-0.315057784433
C	-1.839402428511	-3.199256853726	-0.824908493369
C	-0.059473130594	-2.364696763901	-1.800849933129
C	-0.885771615274	-3.490862001843	-1.781717018558
H	-2.690967213759	-3.765098558029	-0.469655533411
H	0.815156116618	-2.149350654905	-2.402682721482
N	-2.011316548979	0.902317624447	-0.769133980991

N	-0.477666195865	-1.472357623796	-0.912084499587
N	-0.447969196297	0.057912270038	1.593889359318
Rh	0.099539496196	0.478002107383	-0.466502492788
C	0.618807105082	2.279526030227	-0.209905756777
N	0.968894196584	3.380585199065	-0.062796297318
C	1.402265722897	4.710583898766	0.081974880782
H	2.426873731519	4.729947885323	0.469845879870
H	1.381463886030	5.220689259555	-0.887813437511
H	0.748290816032	5.245697494804	0.779583335287
H	-0.483341812054	-0.242276726875	4.861441804968
H	-0.801389202177	-4.386328338313	-2.378995997639
H	-4.890648852690	2.252773272146	-1.582004331903
C	3.086810973776	0.316479258273	-1.143359578420
C	2.076689303640	-0.000167733688	-0.039652635842
C	2.290231511281	-1.437920012232	0.440292954030
C	3.720140851339	-1.651862021042	0.938758071372
C	4.727603235441	-1.329524543156	-0.159961990499
C	4.528700684830	0.087636558600	-0.686397824975
H	1.566288560564	-1.701880997016	1.224987190645
H	2.347744116526	0.644725999864	0.824543711101
H	0.471963315938	0.690092690882	-1.960137728944
H	2.877475224947	-0.324809660221	-2.017536410933
H	2.964614190519	1.350747571056	-1.497889522954
H	3.905900303107	-0.996304998571	1.806189278471
H	3.856256121093	-2.684337501264	1.292736335169
H	5.756915857460	-1.468474093962	0.200075467641
H	4.589470244999	-2.043109522371	-0.989585642075
H	4.764278133232	0.803913971772	0.118946066628
H	5.234022715246	0.296408689931	-1.504440510696
H	2.114018738517	-2.140824561340	-0.387762333730

TpRh(CNMe)-Cyclohexane 1,2-migration

G = -1179.955270

B	-2.535611079088	-1.038565394413	-0.037699763773
H	-3.573143956717	-1.588265753025	0.209885847487
N	-1.698419119587	-0.676755518441	1.191603732399
C	-1.754162953307	0.443803289543	1.940416888886
C	-0.233662370571	-0.927878591501	2.718087236357
C	-0.818210672085	0.329613770130	2.946532649980
H	-2.443236512394	1.244067401243	1.696771928504
H	0.549090106673	-1.426195229106	3.279892962317
N	-2.857849333393	0.268958569478	-0.801503834548
C	-4.051258198394	0.833638757321	-1.038523406594

C	-2.471928460741	2.094379065443	-1.897352773596
C	-3.856536418809	2.010646316822	-1.736420476188
H	-4.954359858054	0.350678211083	-0.688311697801
H	-1.869596402194	2.842889786201	-2.396071504878
N	-1.698663223514	-1.933249070201	-0.958489140067
C	-1.865232952245	-3.218945892322	-1.286340351170
C	-0.035769875167	-2.456377166985	-2.225194429736
C	-0.818223718691	-3.605068635063	-2.103833707215
H	-2.716111666775	-3.769735270603	-0.907063599822
H	0.873915693337	-2.296230121924	-2.791096270783
N	-1.884456219623	1.042821103729	-1.331547575713
N	-0.572011302020	-1.457658780443	-1.526610679294
N	-0.765145244859	-1.530556739871	1.663274744654
Rh	0.021951761396	0.493781157872	-1.161524543441
C	0.535730722710	2.270054610265	-0.765717971651
N	0.848417845587	3.366780390850	-0.501935150725
C	1.231434847752	4.646354638136	-0.065659279405
H	2.171642950610	4.585547216642	0.495384124289
H	1.374493980335	5.316919226767	-0.921225668247
H	0.459113228331	5.067427562456	0.588664771647
H	-0.596202738652	1.044792885178	3.725841456379
H	-0.648746286534	-4.573986801206	-2.548766662436
H	-4.606759323819	2.704081493536	-2.085751464005
C	4.573523294864	-0.139106057441	-1.403818670077
C	3.050670439013	-0.246760471300	-1.374199681086
C	2.560411704414	-0.590608674388	0.034006691412
C	3.066300542267	0.414385709838	1.063388130967
C	4.586851723547	0.523489305350	1.023494402834
C	5.073007383598	0.874979816875	-0.379481870900
H	1.459251607138	-0.678146359040	0.116461340465
H	2.628641012944	0.721009590028	-1.703168212387
H	2.710521100907	-0.998684340136	-2.099481689533
H	5.003904941863	-1.127364732015	-1.172835382558
H	4.919404854986	0.125512653825	-2.412012551768
H	2.625033948304	1.401663885031	0.848145259582
H	2.714394942814	0.134381553368	2.064958006156
H	4.939199680373	1.267426491703	1.750995258494
H	5.027589792199	-0.440468758194	1.326046888301
H	4.696469478998	1.875420359935	-0.652043839096
H	6.169281346631	0.937493624770	-0.405446655051
H	2.922691675642	-1.598716535801	0.295365922436

TpRh(CNMe)-Cycloheptane σ-complex-(1)

G = -1219.213133

B	-2.456606746913	-1.488449775595	0.614361643500
H	-3.324869160230	-2.241997474412	0.957439594672
N	-1.533522727390	-1.024675953710	1.745977571356
C	-1.683253272041	0.036081877987	2.565711201497
C	0.143164206750	-1.067598185353	3.061084386867
C	-0.616059078680	0.053411032245	3.438683119888
H	-2.526740830648	0.707956179542	2.458670665850
H	1.068758979817	-1.437900471180	3.488939186050
N	-3.123859250723	-0.239295707243	-0.011830114936
C	-4.425835303703	0.077945285168	-0.075003205946
C	-3.249198573346	1.640861234129	-1.070330606034
C	-4.558454366503	1.280875545349	-0.742371608634
H	-5.163654102864	-0.582276921033	0.362395208857
H	-2.876518577099	2.503150367903	-1.608759808852
N	-1.603075996323	-2.155652990019	-0.468083875364
C	-1.625302589571	-3.408280025669	-0.936035452434
C	-0.089085733981	-2.256441802955	-1.997060750674
C	-0.664750936502	-3.525495056181	-1.925243704087
H	-2.320612669138	-4.129105926489	-0.525972177104
H	0.698807174417	-1.887978857328	-2.643012867514
N	-2.396816239190	0.720831764633	-0.627452758533
N	-0.656109752482	-1.442309274078	-1.110093553553
N	-0.411303052415	-1.713858611490	2.044064264623
Rh	-0.384283190273	0.567273651554	-0.662496718413
C	-0.205197204887	2.415742664557	-0.316756378044
N	-0.114879452836	3.562503248830	-0.100491908340
C	0.009347434153	4.921643881783	0.232226944688
H	-0.679149893999	5.175901586904	1.046774975942
H	1.033661379113	5.136606687571	0.558978048663
H	-0.221547432782	5.551542675137	-0.635181357437
H	-0.419934074164	0.765583782198	4.227563515290
H	-0.420410547584	-4.399911707253	-2.509427596283
H	-5.469274227206	1.815496930174	-0.966773907750
C	4.268868959116	1.057108015673	-0.918264649183
C	5.356813153968	0.284739784252	-0.172794810514
C	5.052626738173	-1.183009047445	0.106854195172
C	3.018490907532	1.309787354727	-0.072570085587
C	3.721862045236	-1.467712405362	0.803188203465
C	1.973033232720	0.189730305238	-0.092908785826
C	2.498626941394	-1.247912355558	-0.090802688018
H	4.000057061700	0.534967212073	-1.850936259036
H	5.545832738776	0.802275794187	0.782125836761
H	5.063950538040	-1.740314668433	-0.844210576195
H	3.633754450610	-0.869616259953	1.724846375128
H	3.332939532565	1.484889356854	0.967799493250
H	1.314664049127	0.310728074196	0.786489309309

H	4.687384148556	2.024817238754	-1.227863588422
H	6.297993796324	0.344742389204	-0.738122623453
H	5.874829836824	-1.598314728419	0.707311485703
H	2.529855041452	2.239213097938	-0.393460618248
H	3.723794189574	-2.516439845668	1.129608849343
H	1.416183074586	0.331433411028	-1.086276774463
H	1.676045948525	-1.898323478514	0.232582073016
H	2.759689424427	-1.564072900445	-1.113028340011

TpRh(CNMe)-Cycloheptane σ-complex-(2)

G = -1219.215114

B	-2.363773165255	-1.117576146306	1.082247182959
H	-3.227855171916	-1.707810285211	1.669033719680
N	-1.132279023490	-0.789671636292	1.931674019205
C	-0.897833784660	0.313461709479	2.671982142369
C	0.750972440137	-1.114110483110	2.873105007582
C	0.318096818771	0.152333232233	3.302011778112
H	-1.603719011042	1.135578252930	2.686592952123
H	1.654881905436	-1.649170968756	3.142503309730
N	-2.954620981122	0.213964264459	0.562441914134
C	-4.158326999158	0.755572116343	0.801684288902
C	-3.015398944445	2.081727320566	-0.522689470490
C	-4.244946754396	1.959773716915	0.128963285535
H	-4.865801444816	0.238359250465	1.436906262063
H	-2.646385415004	2.861741891404	-1.176676990704
N	-1.924003830005	-1.944026515041	-0.130818012139
C	-2.263188594067	-3.185802971518	-0.493152033581
C	-0.889856956171	-2.339110425554	-1.979067263281
C	-1.620436807812	-3.489518671165	-1.680358056982
H	-2.934343333138	-3.767363435523	0.125361075250
H	-0.245966652500	-2.126847982774	-2.824105530315
N	-2.249307402577	1.027564763575	-0.255241141389
N	-1.073820170121	-1.418011513589	-1.035927251780
N	-0.121875256525	-1.677303410396	2.048012755111
Rh	-0.371053573222	0.519045050311	-0.791164746799
C	0.209656132162	2.301595523596	-0.553141526841
N	0.559645066766	3.404819757355	-0.380549157943
C	1.015903510453	4.703813262758	-0.100311414527
H	0.661927132894	5.407261556808	-0.863323816429
H	0.647825763783	5.030227667670	0.879526030089
H	2.112036845115	4.721787714975	-0.087495417899
H	0.810904146375	0.841334836440	3.973174729094
H	-1.675372285330	-4.407228430067	-2.246320660705
H	-5.078591275382	2.645523796764	0.105575786637

C	3.071371470350	0.785397442218	-1.179198703594
C	3.841678674090	1.078816980589	0.107755392043
C	4.747325104082	-0.049302890066	0.591237592012
C	1.943666937432	-0.230019572705	-0.963386557105
C	4.083441799418	-1.419317794825	0.732780194103
C	2.309808719738	-1.708504606516	-1.124856587799
C	3.705372605273	-2.060622765857	-0.606256846518
H	3.756192271626	0.431373036003	-1.965863456590
H	3.106581063525	1.320818779624	0.894336056924
H	5.595269977532	-0.149897107779	-0.106328066800
H	3.193687623554	-1.345562696445	1.376815849975
H	1.552775901644	-0.092715094164	0.065934600609
H	1.558292202690	-2.301965724315	-0.585425535226
H	2.642697455041	1.723061645885	-1.555702607897
H	4.453838441330	1.982230962096	-0.030634333375
H	5.184461400075	0.244733074877	1.556289842960
H	1.155228299394	-0.003778907971	-1.758231441535
H	4.784457242158	-2.081620349460	1.258863146467
H	2.244759964754	-2.006463802976	-2.182104993872
H	3.760904364223	-3.154337951985	-0.522995731076
H	4.465945552332	-1.784267465971	-1.353118560479

TpRh(CNMe)-Cycloheptane σ-complex-(3)

G = -1219.214003

B	-2.613313121940	-1.230832020711	0.542877737555
H	-3.592671246991	-1.869248941407	0.812681486741
N	-1.785684577190	-0.793996455330	1.755719894586
C	-1.914788848329	0.324681091050	2.498161313917
C	-0.293743261427	-0.930037178168	3.271308216820
C	-0.964261980792	0.284705890658	3.496430838681
H	-2.660760473715	1.072003604744	2.254227188697
H	0.527921337070	-1.366588079353	3.828783039806
N	-3.062179074516	0.036020626657	-0.225184216286
C	-4.304996102924	0.480141617292	-0.465911835975
C	-2.855035284869	1.843020436281	-1.392520626593
C	-4.225312240651	1.642510159858	-1.209307017058
H	-5.157021379645	-0.070130213468	-0.088003373022
H	-2.329228599654	2.624174139591	-1.926982009311
N	-1.714419135179	-2.049344901437	-0.388221085407
C	-1.817170970316	-3.322700373064	-0.783555156919
C	-0.047254803837	-2.409973011036	-1.703175922744
C	-0.763163082294	-3.605812630297	-1.633867620789
H	-2.631646015196	-3.938506831745	-0.424938110002

H	0.846788603698	-2.170292178585	-2.265479628903
N	-2.166920073011	0.872055593883	-0.798506238776
N	-0.623922174011	-1.481897500274	-0.942620227414
N	-0.789814188831	-1.576216558062	2.224581135886
Rh	-0.193544837860	0.516755619953	-0.562109724011
C	0.129727850100	2.354017509839	-0.265010540449
N	0.309881488572	3.494564889458	-0.075754423286
C	0.551676483813	4.843172513088	0.233526122580
H	-0.191271511659	5.205249411990	0.953977739934
H	1.550151747638	4.953640917082	0.673185046728
H	0.496216894729	5.460211625721	-0.671231952455
H	-0.787096282070	1.019163929817	4.269243205438
H	-0.547372751298	-4.538869451553	-2.132274355097
H	-5.039145768549	2.251418018475	-1.573580524286
C	2.543664705275	-1.447881429813	0.372293309996
C	3.430215698868	-1.872681087059	-0.798071357902
C	4.874664422625	-1.394403611239	-0.721140739920
C	2.024221915782	-0.012728365784	0.305417570209
C	5.052954969557	0.119566623168	-0.670391860195
C	3.019147671360	1.143917799807	0.542514791551
C	4.499634360213	0.777501202903	0.596065075956
H	3.084900316389	-1.589543432262	1.320825549039
H	2.983168177746	-1.507478971298	-1.738329252646
H	5.347375664069	-1.832090757497	0.173490079175
H	4.585843616311	0.580286614185	-1.557152522841
H	1.632692161498	0.111483291623	-0.764655655694
H	2.886235144144	1.899847418568	-0.245306429130
H	1.666890023089	-2.105649270409	0.434734320430
H	3.426983263903	-2.969925202271	-0.868837687163
H	5.428939750885	-1.793724217745	-1.582684000440
H	1.215312022151	0.063316178290	1.056059374470
H	6.126602671463	0.341212201339	-0.747847656149
H	2.751525943864	1.648572770382	1.482365970604
H	5.054387588086	1.706106415995	0.792397740969
H	4.702409293860	0.126819558172	1.460494001097

TpRh(CNMe)-Cycloheptane σ-complex-(4)

G = -1219.212998

B	-2.908310071667	-0.547527640796	0.481443477866
H	-4.043860460960	-0.865327964334	0.702595277717
N	-2.100951586645	-0.166962739223	1.725713959534
C	-1.948967553888	1.050626398290	2.286679232722
C	-0.861880456237	-0.466865425548	3.433058361316

C	-1.148843709566	0.908513892726	3.400585972722
H	-2.406096486036	1.928782811255	1.845903681889
H	-0.265028855798	-1.019920037418	4.150156189221
N	-2.924617727641	0.671737331282	-0.470771789959
C	-3.969853713634	1.393845181962	-0.900770685536
C	-2.122895637431	2.203112556039	-1.768168717768
C	-3.506211506035	2.393264569496	-1.735535495238
H	-4.970868165962	1.139328284572	-0.577060912770
H	-1.355817950174	2.746301148105	-2.305583807877
N	-2.194965758234	-1.698252294894	-0.237630051960
C	-2.614225159708	-2.943642577656	-0.486117915345
C	-0.600497774333	-2.671086397281	-1.310654956937
C	-1.620438175808	-3.613998210764	-1.176758304892
H	-3.590051687149	-3.265615421381	-0.146553333112
H	0.360295784955	-2.754958970310	-1.803813448616
N	-1.785536146630	1.166905819093	-1.005361275775
N	-0.953359256788	-1.523730639118	-0.734989854660
N	-1.436591620258	-1.110723694075	2.425711983311
Rh	-0.012261721101	0.321382497311	-0.542294400505
C	0.796200271432	2.018627164857	-0.383297575388
N	1.289826261184	3.074686204608	-0.277114913969
C	1.911817561429	4.313854890470	-0.051442040991
H	2.970204305809	4.160691447045	0.192013490953
H	1.845606908088	4.944500827136	-0.945899485199
H	1.429924775406	4.834865129090	0.784546753583
H	-0.825805007097	1.680473659261	4.084494173757
H	-1.634299249282	-4.633054733196	-1.532998522645
H	-4.084513370209	3.144888345498	-2.251644163713
C	1.869687296429	-0.811745551696	0.580328005033
C	2.813362217542	0.140945522686	1.313986568636
C	3.995351304470	0.658992099665	0.504356876352
C	2.472452554820	-2.197194649035	0.317266995609
C	4.860000277657	-0.412825068889	-0.161151297280
C	3.306581729102	-2.331150422071	-0.959514548660
C	4.162794211177	-1.116508359266	-1.329279766610
H	1.671883479304	-0.388813317147	-0.471385474922
H	3.188677269262	-0.396582899861	2.199682746735
H	3.622344085189	1.333232082655	-0.285620019568
H	5.193056045782	-1.149759355982	0.587686974062
H	3.093501665887	-2.441615559865	1.191938779016
H	3.951801981042	-3.215598519388	-0.855981703969
H	0.957713407968	-0.930225844077	1.184892873426
H	2.233382249349	0.990545494690	1.700353383047
H	4.622406232923	1.277146251192	1.163417962356
H	1.674650043962	-2.950786089121	0.305051681594
H	5.774529435817	0.069469513130	-0.532841020945

H	2.644305768277	-2.549022583405	-1.811138677486
H	4.909698564470	-1.441197306855	-2.066422447669
H	3.541768119538	-0.373927849461	-1.854893790494

TpRh(CNMe)-Cycloheptane σ-complex-(5)

G = -1219.213215

B	-2.340527121734	-1.098044654488	1.090929684794
H	-3.202541279730	-1.670572126336	1.697744997771
N	-1.077487846623	-0.810379886931	1.908080892473
C	-0.779095802267	0.290169811328	2.629074537204
C	0.816015179737	-1.200581010534	2.802506995502
C	0.446291272643	0.086970290820	3.228202114415
H	-1.450401199093	1.140602886078	2.652137018714
H	1.707935777057	-1.766766189242	3.049628342156
N	-2.911919144993	0.251907194297	0.596236636049
C	-4.093090013722	0.822624875008	0.877218161375
C	-2.963335851092	2.123892833113	-0.482818257299
C	-4.172547662902	2.030505377709	0.210388070461
H	-4.791557527671	0.320872192469	1.534432166366
H	-2.597106454824	2.896768282336	-1.146769329694
N	-1.958433775908	-1.926230483345	-0.141265802548
C	-2.351926598154	-3.150166325663	-0.509525490993
C	-1.002129998630	-2.326786419107	-2.029801200957
C	-1.760534177201	-3.456884279009	-1.722318047657
H	-3.021364911274	-3.718227410349	0.123171885930
H	-0.383115996965	-2.121866424820	-2.895322989248
N	-2.215135014143	1.050326551811	-0.244070680161
N	-1.122172881296	-1.414944290639	-1.067099691352
N	-0.100514974918	-1.736698078872	2.007722937432
Rh	-0.363486181728	0.501143315779	-0.824560198343
C	0.275646724075	2.264232077569	-0.588953036277
N	0.678567004699	3.349597191727	-0.418720144974
C	1.229749228194	4.612035978114	-0.141760233585
H	0.931034166180	5.337631106365	-0.907560209494
H	0.885954545645	4.968455420682	0.836420953492
H	2.324490593472	4.546201705899	-0.127248550367
H	0.984520704240	0.762709766854	3.877734573797
H	-1.865642925343	-4.363395885049	-2.299181945024
H	-4.989213210480	2.736776636895	0.216862345476
C	1.946024011655	-0.271345273848	-1.013769015988
C	2.407858357186	-1.716931059754	-1.196993102103
C	3.322140116631	-2.211542559281	-0.078566975912
C	3.060813911607	0.757685241292	-1.231269540247

C	4.520346974969	-1.327013502390	0.275279943027
C	3.794968650497	1.152196837539	0.048343742086
C	4.134812248615	-0.019321142358	0.976601014857
H	1.529353902706	-0.173772442467	0.012160412678
H	2.922833603203	-1.799128359899	-2.168157232326
H	2.710843614185	-2.340469854010	0.828220612316
H	5.129543557085	-1.121852571742	-0.620095215699
H	3.775396564541	0.337219212223	-1.954571981837
H	4.715714405854	1.685785331962	-0.230854281620
H	1.162396423201	-0.075345189861	-1.817980617857
H	1.536913425732	-2.382075447314	-1.239933452356
H	3.680185216735	-3.214817052912	-0.350203338872
H	2.660158929745	1.662041575140	-1.707291026618
H	5.170515503576	-1.903883388089	0.947496652831
H	3.179644802791	1.874208008496	0.608934431117
H	4.946698289479	0.296731259948	1.645736772145
H	3.275045844754	-0.224022653143	1.632390694940

TpRh(CNMe)-Cycloheptane σ-complex-(6)

G = -1219.212153

B	-2.369446519063	-1.497712034689	0.737632094663
H	-3.203251751724	-2.255661313109	1.150025457601
N	-1.303219812827	-1.106682805813	1.764927031643
C	-1.340239256724	-0.098591795125	2.660343885710
C	0.505068043497	-1.257525150369	2.881694129575
C	-0.184129716031	-0.152273640879	3.409661344058
H	-2.176764224187	0.589708528898	2.690348295429
H	1.461349274360	-1.669883198172	3.184542654838
N	-3.082658272838	-0.206550989883	0.268925165357
C	-4.373134996300	0.136785132536	0.395284935646
C	-3.293783665207	1.741431907578	-0.642785338333
C	-4.559083146489	1.383270762795	-0.172148643778
H	-5.065071615874	-0.537607596655	0.883134188371
H	-2.971376247640	2.630665858492	-1.169641116235
N	-1.675875332701	-2.119829960111	-0.477535193322
C	-1.774672356301	-3.350130397539	-0.992449299017
C	-0.366087944255	-2.166360761634	-2.187025336865
C	-0.946901013826	-3.431937544906	-2.098440646652
H	-2.423427947343	-4.082224741941	-0.529468435756
H	0.343343886708	-1.777290842410	-2.907862167712
N	-2.415608412108	0.779349303058	-0.372505011862
N	-0.806702309025	-1.387149618906	-1.201718466838
N	-0.169083416390	-1.828800863247	1.892571397407

Rh	-0.434452909141	0.594070842578	-0.701835787088
C	-0.168994042943	2.422130619522	-0.305482208799
N	-0.030438445467	3.557169076196	-0.054995535833
C	0.158488100715	4.901368075759	0.306708349912
H	-0.295986973985	5.098001354347	1.285028100537
H	1.229652689441	5.127744939916	0.365505874012
H	-0.299313120042	5.565947357011	-0.435734426059
H	0.111591400469	0.504375096883	4.215508345335
H	-0.790130325390	-4.281748271292	-2.745629036040
H	-5.476951920742	1.947478452934	-0.242706948534
C	2.522047463069	-1.244534100793	-0.516442537144
C	2.016627494588	0.198600782472	-0.526363194781
C	3.030467480935	1.297032273479	-0.845984342306
C	3.481345731951	-1.511618493340	0.647052283575
C	4.328398409408	1.256285275373	-0.039555423116
C	4.956111060520	-1.216319088568	0.374992546121
C	5.228333599365	0.072449315931	-0.403798427250
H	2.994593393393	-1.501474523190	-1.478888115643
H	1.564228276447	0.386497258629	0.464169177294
H	3.295252014526	1.244886363443	-1.914456063954
H	4.110607687594	1.258670561078	1.040234492698
H	3.136364407224	-0.921575313043	1.509276740116
H	5.484620677472	-1.177982727514	1.339045916083
H	1.650617030824	-1.899221271685	-0.401266909875
H	1.261041745169	0.287242274376	-1.383829576421
H	2.537627146363	2.269607934970	-0.705732069620
H	3.386566882990	-2.560207831897	0.959691970131
H	4.869987023313	2.191620905774	-0.238312814602
H	5.403845150630	-2.056735368618	-0.175611550254
H	6.282447308936	0.347666616012	-0.263202624902
H	5.118442314659	-0.117604624712	-1.482886127519

TpRh(CNMe)-Cycloheptane σ-complex-(7)

G = -1219.212248

B	-2.786455531319	-0.896186788413	0.292930442522
H	-3.853332359319	-1.427649560343	0.429890402978
N	-2.008798000074	-0.684907833028	1.595602980224
C	-2.070021393839	0.360293216434	2.446210142106
C	-0.664760593289	-1.150645360193	3.182306465625
C	-1.211391768978	0.106154141073	3.494787375806
H	-2.705850200272	1.212575578244	2.236805608699
H	0.057009263439	-1.736116423763	3.741671950665
N	-3.019337889736	0.486144446903	-0.364644127100

C	-4.178188141708	1.103425478933	-0.639310580702
C	-2.509534846146	2.361091327605	-1.310997530326
C	-3.903959046347	2.315244947970	-1.244718022313
H	-5.116175184590	0.628719502197	-0.381653380701
H	-1.854976302020	3.119990944807	-1.720777434257
N	-1.921404067885	-1.728041394877	-0.658155735444
C	-2.136041283573	-2.936639013464	-1.189040464148
C	-0.201717320802	-2.165291583513	-1.878965675236
C	-1.053328462121	-3.265698176433	-1.985518821104
H	-3.042909022982	-3.479152230628	-0.955670533432
H	0.759833731873	-1.984036175052	-2.344466345066
N	-1.989387488593	1.257782437906	-0.780350087930
N	-0.731053390343	-1.249541561886	-1.070648190614
N	-1.145906152199	-1.623545262038	2.040622690572
Rh	-0.094553325997	0.634617897810	-0.471175803024
C	0.439070394824	2.389091468937	-0.019049548142
N	0.744074684719	3.486323914986	0.251882713992
C	1.114438516087	4.784860086668	0.638794675288
H	0.376264531214	5.196665936935	1.337130213628
H	2.092534033057	4.765243294207	1.134101839273
H	1.178231747454	5.442433048296	-0.236495179869
H	-1.014558087806	0.732154153103	4.353534649820
H	-0.904870056967	-4.167531033442	-2.560198523982
H	-4.609243780594	3.053967783135	-1.594911444272
C	3.233717493069	0.603039460169	0.659540151417
C	1.986879033809	-0.271538218348	0.514908953694
C	2.213136756033	-1.777010336286	0.561006530183
C	4.146911371669	0.569269685700	-0.568759921339
C	3.247516478638	-2.316275230590	-0.425561153627
C	5.164481639129	-0.575468340491	-0.612746186433
C	4.685519961131	-1.925334030864	-0.071166519595
H	3.785337985274	0.294995028288	1.561950086573
H	1.619011634976	-0.036478309539	-0.550569751454
H	2.544003738546	-2.031206322272	1.581250430093
H	3.008215905060	-1.986794802439	-1.450922688492
H	3.507264409046	0.533686314624	-1.464728891679
H	5.495061003622	-0.699307303278	-1.654469290465
H	2.909694433512	1.636639103279	0.839769488645
H	1.250472791429	-0.015665976436	1.294605131339
H	1.245452811812	-2.277216818671	0.431037948831
H	4.696313496669	1.517554601474	-0.647051562978
H	3.166258933354	-3.411761295553	-0.438225829519
H	6.063881941454	-0.282354591358	-0.051417755117
H	5.380587580364	-2.697850512550	-0.427612173351
H	4.778291396238	-1.935970313936	1.025934279736

TpRh(CNMe)-Cycloheptane TS_2-(1)-κ^3

G = -1219.195501

B	-2.586022809736	-1.414931501466	0.137166443196
H	-3.539993075287	-2.137912073682	0.112846392367
N	-1.986655175273	-1.391828675016	1.538339863501
C	-2.254683146154	-2.183708082618	2.593838715366
C	-0.621115424841	-0.800415866188	3.072110955979
C	-1.394449458997	-1.837772272652	3.616216988318
H	-3.036627688818	-2.930900886551	2.539568070392
H	0.177339612899	-0.229129262856	3.533464207534
N	-3.010561032058	0.004154365532	-0.292081162932
C	-4.255315050221	0.478914094655	-0.448056877371
C	-2.808205260164	2.059211577786	-0.907962753189
C	-4.178707579929	1.801015500278	-0.843115974923
H	-5.107608693050	-0.164094623768	-0.270128508311
H	-2.284789056331	2.964872475742	-1.188536006439
N	-1.554492570391	-1.917967036467	-0.890923378843
C	-1.663868130471	-2.972239750702	-1.712277061167
C	0.149297270795	-1.846649808712	-2.206022559683
C	-0.584492464124	-2.974145383501	-2.575478611581
H	-2.508307700131	-3.643320387145	-1.623379241211
H	1.060290402860	-1.445386287867	-2.632228381383
N	-2.114365888374	0.974276488743	-0.576420549795
N	-0.433282170674	-1.222941828875	-1.185000481220
N	-0.984284280048	-0.538425072941	1.824328053552
Rh	-0.042004992684	0.651546261380	-0.312460348819
C	0.215901414086	2.454269147681	0.170648381216
N	0.354145883096	3.578678885786	0.460743659416
C	0.534760546179	4.929305543232	0.801757941568
H	-0.142362359891	5.207847857055	1.617696867677
H	1.567294295174	5.098329523070	1.129255796000
H	0.331226860339	5.573296749244	-0.062420665600
H	-1.341419434584	-2.264891485925	4.607217223564
H	-0.365850571059	-3.681863843716	-3.360978051938
H	-4.994243462186	2.473581629172	-1.063176048399
C	4.141025321167	0.732380272220	-1.053798300493
C	5.264283685837	-0.182044967635	-0.563392594699
C	4.837698916999	-1.576039788375	-0.114148426297
C	3.197508167167	1.176450598566	0.068297715561
C	3.683020468934	-1.629970182345	0.886821142906
C	1.998193674177	0.248572887213	0.333068841183
C	2.332470105600	-1.240378579927	0.271014553002
H	3.570122792880	0.242277471912	-1.860433038899
H	5.769855148985	0.326675333541	0.273864326008

H	4.543322594322	-2.164181572227	-0.998865167714
H	3.905881916802	-1.005598745590	1.766951528790
H	3.790418176185	1.267181544228	0.992705535575
H	1.649348076860	0.470973969246	1.355207018599
H	4.599146288942	1.619774513832	-1.511987548054
H	6.023045693978	-0.286327587683	-1.352544079997
H	5.714917445682	-2.088079119312	0.307461953172
H	2.822073325297	2.187206029155	-0.138488741747
H	3.608344284113	-2.659176268484	1.264193100368
H	1.384459799724	0.635799934717	-0.974641596083
H	1.515325973909	-1.784437443096	0.764423230652
H	2.334034116583	-1.595053941745	-0.768154724808

TpRh(CNMe)-Cycloheptane TS_2-(1)-κ^2

G = -1219.196049

B	-2.316927315968	-1.536272211887	0.573983914953
H	-3.157722381137	-2.328357496249	0.895159315794
N	-1.446678740249	-1.034160906206	1.729833432359
C	-1.588405970871	0.085499520992	2.475524002342
C	0.045004621376	-1.155461066873	3.247505795376
C	-0.637374738871	0.053525155970	3.472198943356
H	-2.347357433003	0.822118396449	2.239607887260
H	0.874451973423	-1.580845974137	3.801965174626
N	-3.011096911974	-0.305476447200	-0.051288786631
C	-4.313572497469	0.000067460422	-0.114137996911
C	-3.139199419817	1.620612413871	-1.012764699205
C	-4.449638407494	1.232941134432	-0.727862246333
H	-5.050769676874	-0.684346976061	0.286132905154
H	-2.770162682262	2.513879581734	-1.502320009293
N	-1.417899381545	-2.167502518903	-0.496907035717
C	-1.484334883942	-3.387268137053	-1.042803777310
C	0.068980685829	-2.217478161423	-2.056483908901
C	-0.542700163923	-3.470916108473	-2.052870536235
H	-2.196230377577	-4.110572679276	-0.666998702467
H	0.860365745382	-1.833867999939	-2.688472397605
N	-2.281703605153	0.689217090311	-0.602981001106
N	-0.457624343570	-1.443207851910	-1.111409806580
N	-0.446840137528	-1.807390420456	2.203675661274
Rh	-0.159559643471	0.553646332147	-0.619415551774
C	-0.019287930433	2.419841304912	-0.328901894449
N	0.014273862107	3.575261070834	-0.162834917541
C	0.123058371471	4.954738092643	0.085187353054
H	-0.567921559393	5.249437454160	0.883216379355

H	1.145938293365	5.198968767316	0.395280888002
H	-0.117112678888	5.524278121226	-0.820108978138
H	-0.464528314580	0.790870423539	4.243174933309
H	-0.330829348175	-4.315242677830	-2.691500227472
H	-5.363270800927	1.767016085682	-0.942341128872
C	3.971634341802	1.052071359201	-0.922526137190
C	5.155047098339	0.253445631209	-0.375909910573
C	4.863117373573	-1.203263671160	-0.032022761572
C	2.887891834947	1.314903079691	0.128611805403
C	3.634140738705	-1.444927235866	0.844570350669
C	1.788194560150	0.251487999961	0.238668735590
C	2.306415278560	-1.181549385799	0.119251056785
H	3.537478553145	0.543794244557	-1.799576245127
H	5.521346747462	0.770460346842	0.526200139629
H	4.726387886012	-1.772204069037	-0.966277002863
H	3.696426326931	-0.852582560984	1.771385548962
H	3.383010965289	1.400649443191	1.109804144226
H	1.303186986502	0.363139440148	1.226570944899
H	4.351877637926	2.013553550089	-1.294844561253
H	5.984423093188	0.285034700499	-1.097391257077
H	5.752684633722	-1.631761505222	0.452307932434
H	2.432712535027	2.295994639852	-0.046861332640
H	3.645895445105	-2.495816790822	1.164717812935
H	1.248682859010	0.525644277654	-1.276515076852
H	1.532486530086	-1.854264576444	0.505523596476
H	2.448363620713	-1.455247326087	-0.936751525329

TpRh(CNMe)-Cycloheptane TS_2-(2)-κ^3

G = -1219.196300

B	2.688308219152	1.040104601290	0.554183742914
H	3.719244831468	1.598837396554	0.795787882850
N	1.732416145135	1.173902787131	1.734694633088
C	1.796990055766	1.998211554405	2.797379709709
C	-0.093076608041	0.885061507610	2.808244857573
C	0.635383853155	1.845579556077	3.527263789925
H	2.663022112919	2.628795131063	2.955717583321
H	-1.066979539232	0.459464661342	3.027559510025
N	2.968614803371	-0.444557503972	0.250067620003
C	4.113063938065	-1.121163358607	0.429430835025
C	2.601444016458	-2.456672338454	-0.428320516912
C	3.927197367381	-2.424372420078	0.009131938120
H	4.980745692677	-0.620780377158	0.839597084001
H	2.029764550871	-3.272047809634	-0.854105011153

N	2.071029462366	1.662049431835	-0.713938513757
C	2.567484010448	2.655947397174	-1.464659488124
C	0.786513550902	1.827602546002	-2.434798230265
C	1.769982767779	2.805923504658	-2.583299076470
H	3.458293865234	3.182108312698	-1.146874726657
H	-0.032411086397	1.567584535105	-3.092715040876
N	2.034245026326	-1.263282185320	-0.280933448456
N	0.967139993995	1.150716622682	-1.303433265936
N	0.574170700149	0.486971032890	1.733971277239
Rh	0.049836847562	-0.593220077517	-0.572013804539
C	-0.634330395989	-2.297093864202	-0.141015628213
N	-1.042902387899	-3.357948900870	0.131361152841
C	-1.550187291696	-4.629436562487	0.447045011889
H	-2.635670700703	-4.574450512725	0.590351695369
H	-1.337815947602	-5.338210613394	-0.362516716986
H	-1.092006468527	-5.000198603381	1.371283739095
H	0.362529488670	2.345339226871	4.445489419871
H	1.887658880872	3.512925397427	-3.390763989674
H	4.648592927726	-3.227779022576	0.007957094211
C	-3.213724532062	-0.659690504872	-0.964815561694
C	-4.250208767045	-0.803124026745	0.150895265673
C	-5.014568313680	0.466193628687	0.515834098014
C	-1.985526974569	0.159618912596	-0.525093172890
C	-4.168138077894	1.710438138307	0.788444925754
C	-2.107050572882	1.656275632876	-0.796051373970
C	-3.479633668462	2.257665121705	-0.465179077835
H	-3.672751185786	-0.206146019631	-1.858807174165
H	-3.728499139173	-1.183697019193	1.045476821608
H	-5.710420281484	0.708421809974	-0.304297389879
H	-3.425313428494	1.509548054485	1.577187524940
H	-1.903109766686	0.030915365601	0.567421674888
H	-1.329661340528	2.169379961687	-0.211424141179
H	-2.904750376393	-1.666374984402	-1.275246640945
H	-4.981130456536	-1.578169311445	-0.125475005067
H	-5.645799691676	0.253329777660	1.390940132197
H	-1.118917755884	-0.393662693898	-1.608736641436
H	-4.832777075242	2.485584164552	1.194703363517
H	-1.889179556359	1.879951413553	-1.849426536449
H	-3.353480863049	3.345269998134	-0.373469394051
H	-4.163156310626	2.114658635101	-1.316769173925

TpRh(CNMe)-Cycloheptane TS_2-(2)-κ^2

G = -1219.196583

B	-2.304439048457	-1.256707887162	0.883551635442
H	-3.143575254311	-1.922793150145	1.421298330010
N	-1.105492674838	-0.913776291771	1.773660271933
C	-0.874146748229	0.204928131239	2.498445373684
C	0.669286305644	-1.301410167384	2.887989205532
C	0.273179642305	0.002629171893	3.234931796390
H	-1.536680995694	1.060083754817	2.434239356309
H	1.521448124564	-1.869955494364	3.244173110212
N	-2.942631413430	0.075908918441	0.433968601184
C	-4.157335711727	0.574489375693	0.697606642153
C	-3.015557791815	2.022283487926	-0.491711060014
C	-4.255241218948	1.828414113647	0.120195534162
H	-4.864823493673	-0.001252762481	1.280762035470
H	-2.651152144681	2.862083225229	-1.071152286832
N	-1.806605379138	-1.992045731936	-0.367300022495
C	-2.180636039535	-3.180950749236	-0.853835590220
C	-0.765701952783	-2.238016398769	-2.238826607872
C	-1.535117035540	-3.387444876068	-2.059804803863
H	-2.876821806365	-3.797611295670	-0.300422095635
H	-0.103916632603	-1.966533175953	-3.051745611868
N	-2.233834992895	0.962835633180	-0.298420833319
N	-0.928847290272	-1.408022374535	-1.212019940458
N	-0.161587840487	-1.848564074155	2.012458487095
Rh	-0.227260981704	0.509572152182	-0.836545704082
C	0.281657636762	2.317570848483	-0.579711755181
N	0.566417741444	3.436138492117	-0.405599778141
C	0.986283292980	4.757839991907	-0.173341432998
H	0.613384237707	5.419649016444	-0.963565423641
H	0.605930132471	5.109113122022	0.792571011271
H	2.081480055101	4.803629678693	-0.160330365289
H	0.747271188786	0.690779297419	3.920335633436
H	-1.610026456652	-4.244588738449	-2.711911856053
H	-5.101834828256	2.498546536349	0.135229908881
C	2.975588358493	0.845462495690	-0.950119414370
C	3.924911827402	1.131720717884	0.215870704026
C	4.808938110886	-0.035362240055	0.643532343951
C	1.812897326755	-0.075125975732	-0.543009037675
C	4.086065598212	-1.356851258184	0.902929571904
C	2.102107603098	-1.557595332186	-0.770465360976
C	3.518540610487	-1.995527994241	-0.368475759157
H	3.530160832073	0.402034867789	-1.793424422562
H	3.314895201270	1.460989962921	1.074096132291
H	5.566364616770	-0.211288655866	-0.138214971211
H	3.288004802166	-1.216357729451	1.647905349215
H	1.626396879815	0.073794171096	0.537997483655
H	1.367894865713	-2.141796870738	-0.201006429438

H	2.599487573046	1.803787081504	-1.326678560290
H	4.574460645815	1.982117247999	-0.041739524540
H	5.368086416149	0.260602401567	1.543101500570
H	0.919914939021	0.299586133862	-1.859035798134
H	4.806558246701	-2.051311795785	1.357177627751
H	1.957600814040	-1.821483949222	-1.828301769733
H	3.502295035605	-3.088226471051	-0.255542363981
H	4.222277871798	-1.797660992474	-1.192315941600

TpRh(CNMe)-Cycloheptane TS_2-(3)-κ^3

G = -1219.195641

B	-2.844835499387	-1.035969408037	0.170870680276
H	-3.903695614122	-1.594548518151	0.168834529849
N	-2.408526214723	-0.748812520076	1.601995407422
C	-2.937352439067	-1.184759458620	2.760748789292
C	-1.149100607477	0.025605198212	3.144975405468
C	-2.155449663724	-0.707288848892	3.792951839206
H	-3.829733479855	-1.798188123986	2.764520566647
H	-0.320208586665	0.576637045099	3.575933965208
N	-2.955978806823	0.277520510502	-0.626427293224
C	-4.063541328734	0.873005612564	-1.093500433437
C	-2.305049256239	2.057408857147	-1.650097167626
C	-3.696926209454	2.026955363420	-1.759495667097
H	-5.034178420161	0.426521248723	-0.920230233097
H	-1.593907511232	2.776180656096	-2.037922844196
N	-1.813578514019	-1.924628276869	-0.553644316541
C	-2.027472831037	-3.113427903595	-1.135675226297
C	0.006115719793	-2.435935198534	-1.588320903306
C	-0.880918303247	-3.489539709881	-1.809621517635
H	-2.986307202039	-3.604004994318	-1.029187828200
H	1.018450950677	-2.297595648192	-1.947422629776
N	-1.869190474044	1.002319324350	-0.968126908034
N	-0.557501467821	-1.503377563351	-0.823138724821
N	-1.309379191514	-0.003634317847	1.829330481852
Rh	0.071378404698	0.440250688147	-0.331263571666
C	0.553417558038	2.258927059161	-0.210317024530
N	0.796338682850	3.401885006111	-0.178840373486
C	1.149145861753	4.758803260584	-0.100042268740
H	1.205609958558	5.199173493968	-1.102843694892
H	0.405106997997	5.310348703774	0.486389166906
H	2.127474368912	4.863533833088	0.384526234699
H	-2.296905654919	-0.859651816551	4.853150355341
H	-0.714043688686	-4.389668306148	-2.381999395557

H	-4.340907449439	2.734208161654	-2.260477043541
C	2.498292951195	-1.561534266691	0.406472713360
C	3.450251481044	-1.840931238015	-0.760658327405
C	4.919688742381	-1.662486004348	-0.385738828991
C	2.003258384597	-0.121078919868	0.529880226489
C	5.338641350065	-0.231451629185	-0.067486336858
C	3.124417844779	0.938458145169	0.506882746620
C	4.507283959076	0.493491891719	0.993504937030
H	3.016634138801	-1.832643179277	1.340213210673
H	3.201951242451	-1.191367571918	-1.618456532099
H	5.128324122250	-2.301258448089	0.487981391273
H	5.305824947490	0.367775547991	-0.992514912561
H	1.517790226522	0.098608352740	-0.850431075394
H	3.249713333635	1.343810604338	-0.510872583659
H	1.628549807709	-2.224903685143	0.368350030836
H	3.307522785590	-2.873390831506	-1.111837236870
H	5.557633326198	-2.042128613877	-1.196981550705
H	1.489095149557	-0.051385025297	1.502762179253
H	6.392741112710	-0.241920872029	0.245714636812
H	2.790746894376	1.790423086886	1.115560078008
H	5.061432482811	1.394555004748	1.293595110650
H	4.425287875985	-0.119496342168	1.904411903117

TpRh(CNMe)-Cycloheptane TS_2-(3)-κ^2

G = -1219.196496

B	-2.489815698853	-1.327655353148	0.533939206212
H	-3.429204547287	-2.011523620147	0.830433898851
N	-1.605159828432	-0.917387774687	1.715278466036
C	-1.663070669547	0.201773105058	2.471077022105
C	-0.167538318185	-1.190369893070	3.264675104485
C	-0.743258767384	0.072854414904	3.489649559561
H	-2.346242867131	1.006643662482	2.226163907038
H	0.607568435882	-1.694288279942	3.831753612697
N	-3.015052298517	-0.035752441139	-0.131634101026
C	-4.273297825671	0.408382509278	-0.245153163248
C	-2.900965199532	1.871998137045	-1.131036404379
C	-4.254059925141	1.635637463273	-0.884556373882
H	-5.093503255391	-0.183600522755	0.140858758106
H	-2.421043705332	2.710016591649	-1.622150144800
N	-1.621878885283	-2.074761525978	-0.483587040213
C	-1.755355830074	-3.310647378473	-0.977684004605
C	-0.001226406829	-2.348786899714	-1.877832776561
C	-0.732930937147	-3.536343079921	-1.882421218425
H	-2.565509358217	-3.944422499086	-0.641257101951

H	0.886783909446	-2.075848885666	-2.435562492140
N	-2.163483875305	0.861966832871	-0.675534896518
N	-0.540461834485	-1.478726810851	-1.026492226406
N	-0.688428041308	-1.782714991957	2.199689370755
Rh	-0.072010415687	0.504391127654	-0.619045370583
C	0.277773273272	2.361615670427	-0.501742107636
N	0.455133013142	3.515772108098	-0.477594155953
C	0.766967626328	4.883256310531	-0.387055206414
H	0.033804535768	5.396589711437	0.245454227523
H	1.763610418131	5.009680969857	0.052731592028
H	0.759251901979	5.342573267174	-1.382407423892
H	-0.523073381657	0.783429418241	4.273626074518
H	-0.545317660183	-4.430000388828	-2.458449014514
H	-5.096300217084	2.261643629329	-1.138945718251
C	2.325026177526	-1.334877941558	0.307408985892
C	3.322487974671	-1.628670025238	-0.815531079707
C	4.772970224130	-1.390544142909	-0.401165664471
C	1.790073893901	0.090295916252	0.371332086152
C	5.137439604483	0.063637394653	-0.121314857798
C	2.872103584940	1.185596014991	0.336972261169
C	4.250867247861	0.801077399723	0.885077174152
H	2.820523902227	-1.543857374763	1.270112967461
H	3.085357563407	-1.019403044471	-1.705792145419
H	4.972315479136	-1.991094277500	0.501175422020
H	5.118064792487	0.628564089046	-1.068247885347
H	1.352298808298	0.241783746829	-1.178227167925
H	3.021945472140	1.553353869349	-0.690702666133
H	1.477231570938	-2.025467920907	0.284606235343
H	3.218069210989	-2.676367199727	-1.132022081478
H	5.449652841451	-1.777175257209	-1.177036758260
H	1.224118790336	0.179345977146	1.316185907994
H	6.180281821136	0.097717806571	0.226073633787
H	2.492926489756	2.048730862716	0.902149210288
H	4.766889305195	1.729985217305	1.167778849413
H	4.155576880709	0.220874375753	1.815480514350

TpRh(CNMe)-Cycloheptane TS_2-(4)-κ^3

G = -1219.194392

B	-2.969892847297	-0.528113346575	0.045307954959
H	-4.121837101411	-0.848337788085	-0.014834977664
N	-2.634117479619	-0.058353035629	1.455280370035
C	-3.381466055956	-0.093072544157	2.574327108484
C	-1.387039837516	0.708727907388	3.012274014408
C	-2.616020475835	0.396177811305	3.613651528551

H	-4.399719088415	-0.460588875618	2.547742538400
H	-0.491050797921	1.122832576946	3.461808648649
N	-2.698318010279	0.595871753664	-0.971415295287
C	-3.585999879461	1.302230364662	-1.687770589141
C	-1.555757222012	1.981380119669	-2.160877601689
C	-2.898518467490	2.210996216176	-2.469490483627
H	-4.645171452734	1.101558432807	-1.590789838692
H	-0.662207619636	2.453512962968	-2.550169669820
N	-2.099146203012	-1.737533312064	-0.354202627195
C	-2.532411222954	-2.959057576744	-0.697175106034
C	-0.368950454912	-2.840164388200	-1.009744578718
C	-1.453642858590	-3.709979170471	-1.121456338581
H	-3.584144509671	-3.201736216539	-0.617962472814
H	0.668113638364	-3.002968077342	-1.265967750717
N	-1.446264859520	1.009323689536	-1.260519737941
N	-0.759733535722	-1.658285158915	-0.538469539062
N	-1.407733729706	0.433755050852	1.715411008558
Rh	0.233088919317	0.179988344197	-0.274625443245
C	1.030836352179	1.885835918942	-0.248945035410
N	1.462615095672	2.971655141247	-0.260760341776
C	2.053008092798	4.245476451850	-0.220213085843
H	3.127141050451	4.150908557279	-0.018801974235
H	1.918753112918	4.759430994665	-1.179292475982
H	1.596424128086	4.851858412360	0.570903009554
H	-2.905435233189	0.513798774748	4.647895787935
H	-1.452209950638	-4.732466376904	-1.468040418984
H	-3.308268712492	2.924766552047	-3.168444938274
C	1.842635795455	-0.734673439467	0.887541553135
C	2.825403298779	0.249057637801	1.528701646159
C	4.001407682223	0.739129779732	0.688801862851
C	2.515533291718	-2.094427670575	0.626180027811
C	4.904663523541	-0.348972091004	0.107687776236
C	3.336917234947	-2.269931062131	-0.654571992421
C	4.255732866952	-1.108245277238	-1.049449355328
H	1.660420751368	-0.423243924290	-0.561816407676
H	3.240454337665	-0.250743956093	2.422643424481
H	3.633858028549	1.350805676962	-0.150218248431
H	5.222780168663	-1.045308903822	0.900467896255
H	3.169982912284	-2.288185292529	1.492066789069
H	3.938580059376	-3.183556826339	-0.536573953046
H	1.061945853003	-0.927835139430	1.641467348781
H	2.272204650350	1.119285302602	1.908988599367
H	4.604736172563	1.411678208997	1.317253995258
H	1.760035929747	-2.889658972769	0.663197454793
H	5.824519655164	0.129500861077	-0.257081195511
H	2.668228368539	-2.466135548364	-1.506025283355

H	5.033230219305	-1.502963978741	-1.718113211532
H	3.690890194216	-0.382451305980	-1.654586305048

TpRh(CNMe)-Cycloheptane TS_2-(4)-κ^2

G = -1219.196089

B	-2.809150669271	-0.646856695072	0.399686609229
H	-3.929894100440	-1.001989175187	0.631874726227
N	-1.998830609254	-0.269803497878	1.643013047907
C	-1.686527858807	0.952455030472	2.131880597023
C	-0.946609196506	-0.624571629221	3.462220168754
C	-0.996778939409	0.772233825335	3.311815289317
H	-1.973241279901	1.855694719227	1.606382509653
H	-0.496350214618	-1.206202576906	4.259071854599
N	-2.862608871839	0.588756880900	-0.524437548343
C	-3.916844814417	1.320114003843	-0.909536863666
C	-2.085481121567	2.170129687894	-1.768455135527
C	-3.468732717923	2.351742901894	-1.715291964413
H	-4.912312786329	1.051099018815	-0.579897163597
H	-1.329471016070	2.740043713057	-2.295089658173
N	-2.075351235730	-1.769660630427	-0.348433141142
C	-2.529795329356	-2.976109115348	-0.704191481801
C	-0.490428773582	-2.712647948827	-1.462959636389
C	-1.544059200766	-3.625401107998	-1.425093122595
H	-3.523080113639	-3.288419634945	-0.409047729581
H	0.479287145812	-2.796660370375	-1.935977288938
N	-1.731172236833	1.106996722499	-1.051214127247
N	-0.814075116250	-1.601209395045	-0.805374012247
N	-1.551300837398	-1.246625332901	2.459572822585
Rh	0.143465137796	0.237752446001	-0.561777846020
C	0.925375931403	1.955736580939	-0.468984801729
N	1.362230996371	3.037951192486	-0.430422694198
C	1.996242193946	4.286513841342	-0.305486961933
H	3.047662945589	4.140682913493	-0.029271400215
H	1.951579753091	4.833660377352	-1.254200775285
H	1.505062377952	4.884013226074	0.471034220110
H	-0.596982300903	1.534630314082	3.965214120226
H	-1.581777545395	-4.614240365153	-1.856705490773
H	-4.058283464705	3.116684216778	-2.198242681675
C	1.622381455784	-0.684198897436	0.681413332904
C	2.569869179161	0.273349001084	1.399092233172
C	3.808128882110	0.764691913853	0.657163831609
C	2.277976122186	-2.040288210009	0.392289121192
C	4.734499781141	-0.323450269940	0.113414569461

C	3.186847818961	-2.180598688413	-0.832152943478
C	4.164394089829	-1.033379349481	-1.114043714034
H	1.540359391807	-0.326934072066	-0.922498001257
H	2.912857898203	-0.258565463496	2.305419087879
H	3.510233439431	1.403123348277	-0.190201859018
H	4.975267087532	-1.049779912621	0.906218157827
H	2.859085606851	-2.296055258843	1.294036404154
H	3.753236123833	-3.116187798755	-0.713306668326
H	0.791409506904	-0.887270885727	1.379628590518
H	1.997416122706	1.135134528599	1.770469122951
H	4.374935061368	1.412067278800	1.343354728207
H	1.498124910494	-2.809931242909	0.328800245176
H	5.689171672095	0.145777879273	-0.163207318109
H	2.572151739041	-2.324869498815	-1.733419345538
H	4.984607203384	-1.429641343225	-1.728604413104
H	3.672993375271	-0.274088284158	-1.742098303444

TpRh(CNMe)-Cycloheptane TS_2-(5)-κ^3

G = -1219.195360

B	-2.771468671213	-0.980509147416	0.474668973648
H	-3.827120716283	-1.507477831702	0.676787007536
N	-1.905351804464	-1.047028803146	1.728334148423
C	-2.100213445481	-1.737834661793	2.867313022129
C	-0.167556653214	-0.702004019782	2.924489115067
C	-0.999545468158	-1.544880214890	3.677622535963
H	-3.005834541159	-2.312410816681	3.016861217000
H	0.803457300562	-0.291875248473	3.181063266276
N	-2.999261211393	0.484956314482	0.059873537289
C	-4.137940495972	1.192926389521	0.103918163936
C	-2.525354630980	2.448132399459	-0.689625279203
C	-3.884007584030	2.467008345149	-0.367073898114
H	-5.049379266074	0.733764066240	0.464385351562
H	-1.899810478795	3.227011897885	-1.107836585267
N	-2.074968488444	-1.691328376254	-0.702493819340
C	-2.519959977982	-2.739614470463	-1.410222286662
C	-0.647636094207	-2.010879151027	-2.284461255022
C	-1.630471178664	-2.988811769966	-2.438576938104
H	-3.442359361034	-3.231127089468	-1.129202918278
H	0.239056116985	-1.820475406586	-2.875910320086
N	-2.002893127548	1.253227869225	-0.430190000923
N	-0.917269222597	-1.239879653042	-1.233710498145
N	-0.720084709181	-0.407257165849	1.756136287470
Rh	-0.019709080928	0.530121795160	-0.549006960163

C	0.664289619431	2.242572482399	-0.152913522461
N	1.076970808407	3.306620339325	0.100052181435
C	1.589392594971	4.581449959604	0.393285306099
H	1.235677374504	4.915483538610	1.375704386954
H	2.685159056493	4.549894523562	0.405507166446
H	1.267560567400	5.306539713475	-0.363920732919
H	-0.829332321887	-1.946494632633	4.666073950878
H	-1.688793172700	-3.759813039401	-3.192138218705
H	-4.582067386234	3.283968620134	-0.472789011787
C	2.036359793444	-0.200427076356	-0.441630775363
C	2.248936107488	-1.688675585443	-0.715239406787
C	3.344899477654	-2.346117221711	0.124943704321
C	3.229776759521	0.640781031137	-0.936932246431
C	4.721939440193	-1.681319766510	0.132645634754
C	4.331400123453	0.874598150304	0.096100733731
C	4.752681792696	-0.358439639339	0.901654862668
H	1.940968516646	-0.063299276771	0.651190962695
H	2.479612280944	-1.826986546856	-1.785500235514
H	2.994026064812	-2.404528729758	1.168419039892
H	5.088919166881	-1.538098945272	-0.896456092343
H	3.655166946221	0.140954376815	-1.821522979186
H	5.207797204149	1.285747068020	-0.427721806701
H	1.175550692862	0.276026791680	-1.545290673611
H	1.320853054941	-2.239562072565	-0.524719526736
H	3.448809857044	-3.387588938545	-0.213831425707
H	2.894307988128	1.620505305492	-1.301235926974
H	5.428115908457	-2.378397854775	0.605136107770
H	4.006131679042	1.659526555278	0.797370101319
H	5.760412196814	-0.182236835483	1.302697776265
H	4.102089795620	-0.466158470422	1.783084840776

TpRh(CNMe)-Cycloheptane TS_2-(5)-κ^2

G = -1219.195563

B	-2.312769289739	-1.179600554833	0.990992523669
H	-3.149426660783	-1.811257412714	1.572600365642
N	-1.069358815962	-0.854620921063	1.827206047782
C	-0.810083012145	0.255785146195	2.554795290530
C	0.750642434797	-1.250538008240	2.862981010394
C	0.366451743394	0.047896413144	3.241608652922
H	-1.476153059543	1.110212137986	2.527487799306
H	1.619093870404	-1.818647731287	3.178316110106
N	-2.928155414142	0.165343208817	0.544259266709
C	-4.119863605920	0.701153165973	0.837956278106

C	-2.973728824836	2.103452872845	-0.400644196761
C	-4.199575768839	1.951386040213	0.249755724913
H	-4.825441682010	0.152119636810	1.448575679798
H	-2.602941090820	2.926751601120	-0.999393191211
N	-1.885161214927	-1.947388968308	-0.265527480884
C	-2.290346016002	-3.141162640572	-0.714209669668
C	-0.898653043041	-2.251774934672	-2.158267188909
C	-1.680497382588	-3.384648779025	-1.932074621767
H	-2.980498393198	-3.734487963611	-0.128676876655
H	-0.245241408950	-2.011483671899	-2.988074124913
N	-2.216686257890	1.024421006611	-0.218570178747
N	-1.024415269477	-1.396206362113	-1.147226886743
N	-0.113189472026	-1.790002491680	2.014288326398
Rh	-0.247522367458	0.498939134809	-0.818170038188
C	0.338772808507	2.290912633756	-0.617150311433
N	0.686203678642	3.396542026310	-0.477175457114
C	1.180993704525	4.699729287398	-0.293202327663
H	0.780028702744	5.370869084122	-1.061515190392
H	0.890748249894	5.076864943755	0.694045299207
H	2.275049749308	4.695164040305	-0.363007304805
H	0.867194343875	0.729103135465	3.914873410380
H	-1.785961166994	-4.255285383082	-2.561728905761
H	-5.025880310010	2.645753124024	0.282846140906
C	1.790515645672	-0.122004680026	-0.555172357803
C	2.079521489663	-1.608021688610	-0.758519115032
C	3.221462578163	-2.162098696035	0.100188626540
C	2.944627920473	0.746946083052	-1.083686604982
C	4.545049289814	-1.397410503007	0.133228998831
C	3.986039177663	1.112939627058	-0.026942753836
C	4.443403497103	-0.051731359450	0.855625326560
H	1.647191505399	0.067603177809	0.526743209455
H	2.298363377547	-1.786480506631	-1.825234596841
H	2.855984716995	-2.240009276027	1.135595721977
H	4.946448765772	-1.260058442062	-0.883725498270
H	3.432146692685	0.204890288954	-1.908937050929
H	4.857047122965	1.549363322855	-0.539541570548
H	0.866409150507	0.198228383474	-1.857220700341
H	1.193720749144	-2.200391098163	-0.509374299819
H	3.408652528133	-3.195002797839	-0.228410163400
H	2.578825677723	1.675988925481	-1.536580016561
H	5.278360752642	-2.025758378377	0.658049344849
H	3.581728639764	1.910227598042	0.617201941118
H	5.411102896173	0.210448300616	1.305093718552
H	3.746355515045	-0.171704500720	1.699807886243

TpRh(CNMe)-Cycloheptane TS_2-(6)-κ^3

G = -1219.195370

B	-2.607868293347	-1.349477488650	0.236572503189
H	-3.574758808473	-2.052091482344	0.305769862188
N	-1.811413843971	-1.426617326043	1.535604918298
C	-1.908131942962	-2.317917824920	2.540352737281
C	-0.200372548909	-0.981110691193	2.868237488951
C	-0.885349087517	-2.068418927777	3.432922142821
H	-2.696622609039	-3.060189299178	2.546364506495
H	0.670171317278	-0.452367881846	3.241972993668
N	-3.046391950386	0.099828558802	-0.046313398179
C	-4.288620106512	0.604883782214	-0.011155237900
C	-2.875149236111	2.181262653359	-0.576890866327
C	-4.231248975740	1.944869567102	-0.343820518503
H	-5.125899292856	-0.031552270580	0.244510730754
H	-2.370558409659	3.091123797650	-0.877466998684
N	-1.737225124201	-1.813442006792	-0.947219127910
C	-1.936890279753	-2.855643444121	-1.766952110704
C	-0.152890703921	-1.754054695115	-2.405498353105
C	-0.937543238674	-2.863564294259	-2.722153157788
H	-2.780091662109	-3.515814546421	-1.610141599610
H	0.730827333738	-1.366819958423	-2.897081281810
N	-2.171231186816	1.067643451955	-0.396704854738
N	-0.636539441494	-1.132685389809	-1.332834202226
N	-0.763555514811	-0.601455032846	1.729641026533
Rh	-0.094039190616	0.690822919166	-0.438861573905
C	0.275538499840	2.467762284764	0.068363995754
N	0.473810458685	3.578250308837	0.377741251284
C	0.721608177696	4.917280696684	0.722118700222
H	1.783745337270	5.054210220189	0.956765408842
H	0.457863387688	5.582296092358	-0.109362235370
H	0.129733382183	5.198092047397	1.601117771065
H	-0.674526450330	-2.587441905776	4.356770638655
H	-0.802510809870	-3.564069200759	-3.532601213026
H	-5.051341192937	2.643279347415	-0.418030061699
C	2.296856467760	-1.282259318107	-0.209094798803
C	2.013721354415	0.219629008246	-0.127921856045
C	3.158683787516	1.120182799201	-0.612769360014
C	3.353451341931	-1.746669801877	0.802755023860
C	4.529413468959	0.866540713200	0.017732129560
C	4.809070168382	-1.681097686290	0.339552675403
C	5.184983439789	-0.431467540936	-0.458719057464
H	2.591595662408	-1.575266073308	-1.230575419197
H	1.854112171513	0.452816880818	0.940158156424
H	3.273452582630	1.024975988863	-1.706086173015

H	4.455437983471	0.881127303443	1.117115387437
H	3.228858123489	-1.151898187838	1.720994957653
H	5.457279890616	-1.756615103159	1.225324251172
H	1.365920399182	-1.817815499884	0.007902919143
H	1.213071897901	0.658908147299	-1.304715852926
H	2.866616470325	2.166039563847	-0.439246930881
H	3.134959355753	-2.781567527789	1.100266436792
H	5.179276850207	1.711771388184	-0.250450893914
H	5.038135820619	-2.566964831715	-0.271037946862
H	6.278554580564	-0.326367770536	-0.445045629633
H	4.919524711684	-0.575648630992	-1.517647756650

TpRh(CNMe)-Cycloheptane TS_2-(6)-κ^2

G = -1219.195179

B	-2.259579047905	-1.537587532683	0.699660855614
H	-3.065052895743	-2.328347901248	1.104084496881
N	-1.198164405017	-1.129946649815	1.726078459097
C	-1.190866100529	-0.066854809527	2.561758824751
C	0.522153791417	-1.374213636562	2.960441858833
C	-0.088396947647	-0.179360875862	3.381014116559
H	-1.963600734676	0.691070488735	2.509154874341
H	1.422097444122	-1.847058657772	3.338460761084
N	-3.001608581375	-0.253495021252	0.267231908884
C	-4.288036923468	0.082955570725	0.424974033009
C	-3.215915847584	1.732644311494	-0.544934885562
C	-4.478352075475	1.355546444116	-0.084726051279
H	-4.975998123363	-0.610266939496	0.892252440825
H	-2.899252337289	2.648181963054	-1.029961042628
N	-1.557502637971	-2.119350028907	-0.532935660047
C	-1.710243741980	-3.313895136763	-1.115772075560
C	-0.268785758702	-2.121081553229	-2.260766675765
C	-0.898529970165	-3.365355190115	-2.235171696234
H	-2.382317032259	-4.044926838680	-0.685510376473
H	0.454840795057	-1.721929525376	-2.960899218220
N	-2.334498267589	0.758861740909	-0.329474039415
N	-0.667362111191	-1.381236071019	-1.228937363739
N	-0.147665218438	-1.943342905642	1.968611183510
Rh	-0.249645792370	0.583763762759	-0.695559723753
C	-0.029308974416	2.440974449611	-0.395963784388
N	0.036884260693	3.594651785939	-0.226494033626
C	0.202159394547	4.972580127253	-0.002686517660
H	-0.357319246405	5.279619184430	0.888288222977
H	1.263508370067	5.201534769598	0.150092082151

H	-0.161729601745	5.544339429498	-0.864336197334
H	0.224579395129	0.498244375478	4.162616928312
H	-0.779678827832	-4.184380313186	-2.928476641591
H	-5.396933550236	1.921907089465	-0.122103765380
C	2.308700845845	-1.178759938110	-0.355724972926
C	1.825204120368	0.263454185829	-0.201113450266
C	2.862649051770	1.326946222244	-0.576601480932
C	3.387220171540	-1.552172963615	0.672205246160
C	4.240186746460	1.200337855535	0.082084216851
C	4.833523632127	-1.302535798449	0.250303714323
C	5.071675003894	0.033816084888	-0.454897186155
H	2.671245582729	-1.364878048984	-1.381376644789
H	1.547531663078	0.401169136632	0.862487739840
H	3.020348366478	1.325943835464	-1.668152048800
H	4.140132249240	1.133750422043	1.177004675867
H	3.172270631874	-1.005916738895	1.602889804050
H	5.471533978808	-1.362778949390	1.144698258567
H	1.460292582175	-1.847481288118	-0.192427799538
H	1.017173010780	0.522547496511	-1.585733728797
H	2.453716397282	2.317573806338	-0.338405567456
H	3.277848309675	-2.614299076020	0.931774317573
H	4.779739193681	2.138534899716	-0.111927254388
H	5.170388666979	-2.114987446880	-0.410368320116
H	6.141408108988	0.277284828789	-0.395750103609
H	4.854679239605	-0.070209493700	-1.529428900671

TpRh(CNMe)-Cycloheptane TS_2-(7)-κ^3

G = -1219.194741

B	-2.950328667872	-0.730812183813	-0.030287650789
H	-4.069203495254	-1.139692135321	-0.150067357952
N	-2.636752320839	-0.495593476211	1.441251064055
C	-3.347978142336	-0.837636646354	2.532052056258
C	-1.462368880213	0.117273045304	3.117711541735
C	-2.627328272900	-0.459761043908	3.646765237054
H	-4.312205185030	-1.320583438402	2.433879657372
H	-0.618164779907	0.553685829429	3.640494899606
N	-2.797567660322	0.580799880982	-0.824647605428
C	-3.760971290623	1.322577012324	-1.391114087478
C	-1.810755717892	2.254680782301	-1.754317424393
C	-3.175558334683	2.415174289612	-2.002002585350
H	-4.795919341261	1.013536172352	-1.321145880505
H	-0.973233954723	2.869661640004	-2.059508446537
N	-1.980196438511	-1.756707240914	-0.650785953270

C	-2.300639614738	-2.899226474541	-1.275059814574
C	-0.159151832610	-2.511283098315	-1.520495704878
C	-1.158711326703	-3.428043808975	-1.846027519091
H	-3.324468766047	-3.250079446983	-1.270149685912
H	0.891063305553	-2.514248914958	-1.783981699752
N	-1.593302316084	1.149853333336	-1.046804349769
N	-0.656929039498	-1.514355434989	-0.791455666453
N	-1.476862972032	0.092927169626	1.792228403333
Rh	0.179138156157	0.330812279158	-0.223877724308
C	0.901570155119	2.062083682490	-0.055197572603
N	1.326189366385	3.150260193274	-0.006387883741
C	1.896958439511	4.429019193759	0.100868080935
H	2.291200460996	4.755074453014	-0.869233761728
H	1.144857333831	5.151771434249	0.437762483004
H	2.718963931805	4.413170171087	0.826925014200
H	-2.906174711794	-0.576970217574	4.683957550725
H	-1.064482362321	-4.338582890886	-2.418510039583
H	-3.663607539670	3.203953789218	-2.554742781980
C	3.057236413073	0.411511116817	1.176322005905
C	1.880389316142	-0.519494921214	0.856440390605
C	2.328826746197	-1.961402940386	0.629828247514
C	3.954186767817	0.770701586404	-0.013416882763
C	3.372723599595	-2.175585111738	-0.468860746793
C	5.083934568563	-0.220923811214	-0.321446706601
C	4.775799789878	-1.701139524088	-0.076457972247
H	3.668467837640	-0.061000286106	1.965290478559
H	1.617851002503	-0.185714778671	-0.583382518644
H	2.762613262818	-2.329700292722	1.575710888717
H	3.056381427774	-1.681256116283	-1.403704118907
H	3.319261571245	0.893576687234	-0.902907030898
H	5.384135162936	-0.083616040745	-1.370715958526
H	2.663715092121	1.331615220041	1.626330285027
H	1.208597615447	-0.528119676122	1.730416220821
H	1.449558193619	-2.589155634085	0.450313465159
H	4.408278013846	1.758527918086	0.154915116493
H	3.416809106850	-3.250366017771	-0.696663933446
H	5.970922077618	0.040921237684	0.274213107645
H	5.529642852868	-2.294163971352	-0.612744779351
H	4.925510552324	-1.936961592176	0.988391927350

TpRh(CNMe)-Cycloheptane TS_2-(7)-κ^2

G = -1219.195776

B	-2.748723539812	-0.961049884633	0.334992964969

H	-3.822016835322	-1.471089423477	0.495588384370
N	-1.938847011392	-0.775154645046	1.621044454647
C	-1.846689935556	0.310719458221	2.420755903515
C	-0.782778829326	-1.391232653493	3.301968980629
C	-1.100018951542	-0.039519752160	3.525404018256
H	-2.310740038007	1.249931476043	2.143222383163
H	-0.203683225428	-2.064859986262	3.924061241913
N	-2.959752337429	0.431591128997	-0.300181983292
C	-4.099258499716	1.106555772278	-0.498836309794
C	-2.405166806944	2.320037608835	-1.182186258647
C	-3.795835923188	2.331177845125	-1.067508957474
H	-5.046644999099	0.663890082861	-0.218425045851
H	-1.735683399613	3.070959618334	-1.584230167493
N	-1.926274354906	-1.812722491801	-0.637204880388
C	-2.238484797669	-2.970445080593	-1.229601562995
C	-0.248804978433	-2.325358369375	-1.888387181602
C	-1.187178836200	-3.344625057849	-2.047816355526
H	-3.185084147191	-3.449958854378	-1.016923591631
H	0.728371608172	-2.203568700062	-2.340243971916
N	-1.910960521794	1.174167659883	-0.719104218316
N	-0.699583777709	-1.412109958677	-1.030478449115
N	-1.288932926305	-1.830005824707	2.158211094368
Rh	0.068654764509	0.445048502367	-0.489180821851
C	0.735490484912	2.201449713247	-0.271624340294
N	1.137012781411	3.295795696823	-0.195451972242
C	1.711156951864	4.568446480989	-0.032130549836
H	0.962409161783	5.274891036570	0.343684058172
H	2.538393692299	4.515755721895	0.686056343458
H	2.096986266033	4.937199242494	-0.989742156588
H	-0.826867820485	0.586991055753	4.362540993284
H	-1.111143089216	-4.226868630464	-2.665424670626
H	-4.481694706298	3.112064329716	-1.360372302794
C	2.849081922404	0.561729988648	1.018254730540
C	1.683708738079	-0.367494722626	0.673683285949
C	2.116755381003	-1.810047518064	0.450875897378
C	3.793143726108	0.913522492634	-0.135653401734
C	3.199029620681	-2.039925041164	-0.604565089856
C	4.916814955887	-0.094335754560	-0.416529872356
C	4.589939566939	-1.569389820084	-0.167316560808
H	3.426968280722	0.085285310211	1.829710476435
H	1.484436958974	-0.028678485784	-0.913831279423
H	2.508453945537	-2.178111675766	1.415721649557
H	2.920143927225	-1.555394185807	-1.556403066708
H	3.191210916175	1.057631735978	-1.044649287090
H	5.237574310870	0.032303248664	-1.461064678308
H	2.445206388456	1.483273062124	1.456245066054

H	0.972482095385	-0.362484526482	1.518683536596
H	1.234368389235	-2.424672021681	0.246746286208
H	4.257708529264	1.891439183370	0.059990460051
H	3.243059628502	-3.116939499893	-0.819660892112
H	5.795781069014	0.162565670696	0.192865827117
H	5.359441453766	-2.171280508430	-0.670566355134
H	4.701040678208	-1.794997239320	0.904463516639

TpRh(CNMe)-Cycloheptane IM-(1)

G = -1219.211285

B	-2.263319379591	-1.426769580840	0.556639136391
H	-3.071659357078	-2.177905661726	1.019370680274
N	-1.380125804174	-0.705057548027	1.603906643195
C	-1.677675753092	0.445292893351	2.282867852069
C	-0.173314599209	-0.725196481305	3.368009014467
C	-0.906028258744	0.481402528231	3.415042523320
H	-2.413254525278	1.139778540504	1.893025956102
H	0.563064313608	-1.095650487354	4.073261810236
N	-2.969790159488	-0.316281102361	-0.243088443570
C	-4.265463897476	-0.091495300687	-0.508878855419
C	-3.026838338719	1.435583138459	-1.491606768705
C	-4.355114188857	1.031181239216	-1.311081465277
H	-5.028312534674	-0.747556577894	-0.109071348989
H	-2.627038810371	2.267939018649	-2.058607810262
N	-1.320547053523	-2.170348434035	-0.396393899159
C	-1.429588034585	-3.378894885411	-0.961942784328
C	0.217315354499	-2.272618724379	-1.905077515932
C	-0.456926482361	-3.495268163099	-1.938224211480
H	-2.189570272078	-4.071455280270	-0.624020993609
H	1.053052133316	-1.924811096616	-2.499586310969
N	-2.203923490109	0.616685374959	-0.848679275132
N	-0.304206333681	-1.487360242518	-0.970243924221
N	-0.468912483421	-1.439667478545	2.301457108943
Rh	-0.081648777705	0.470282771042	-0.321059223329
C	0.004743760980	2.284521618726	0.239238761250
N	0.036560511374	3.393549943770	0.589680628560
C	0.160669441412	4.723583055179	1.030414782649
H	-0.171691439206	4.804887365457	2.071212630720
H	1.207928471101	5.040033232370	0.964745882760
H	-0.452316889899	5.385145810274	0.408459419834
H	-0.869705613088	1.258938587140	4.164818686566
H	-0.258819360864	-4.343802759008	-2.575770994660
H	-5.249236025577	1.485839521770	-1.711557564201
C	3.718247070973	0.840531119623	-1.260276372406

C	5.008173677568	0.111900730149	-0.877506906926
C	4.835769924144	-1.270949157437	-0.254188458953
C	2.891231786407	1.273571190533	-0.043388610993
C	3.812951451319	-1.365738855577	0.878328420614
C	1.840149777851	0.259895383020	0.446892892874
C	2.368079868967	-1.174021004529	0.387489991271
H	3.105433859315	0.221295743566	-1.935476306678
H	5.556459323819	0.756972686557	-0.171145155308
H	4.529305024123	-1.981892349422	-1.039265692731
H	4.053772257293	-0.646128428440	1.677372320216
H	3.604065045668	1.485988502310	0.773113348296
H	1.649541998073	0.484807768537	1.517810030985
H	3.996403503917	1.729972176871	-1.843717604503
H	5.656235294608	0.018564538373	-1.761703958106
H	5.818508900203	-1.619103149556	0.097303187345
H	2.417018324167	2.238730759369	-0.260819121699
H	3.905496871710	-2.361115834363	1.335834457535
H	0.555554082295	0.909469646494	-1.633801022057
H	1.683908513080	-1.818130640103	0.954019701798
H	2.336117321060	-1.548229660997	-0.644077268667

TpRh(CNMe)-Cycloheptane IM-(2)

G = -1219.211923

B	-2.290162307579	-1.135581100639	0.993085067156
H	-3.023297923133	-1.755087668783	1.707433607066
N	-1.015343278611	-0.598918750974	1.690664440501
C	-0.876078266468	0.572098981684	2.384111735914
C	0.672709737120	-0.864507488208	2.974391594393
C	0.213575512427	0.450366045088	3.207591659009
H	-1.567513782826	1.391802373600	2.224817696324
H	1.520603456190	-1.373121352851	3.421348947828
N	-3.021697433373	0.094901950077	0.425329563572
C	-4.281103840364	0.531914504666	0.577607031309
C	-3.191362543651	1.862094588606	-0.791605531735
C	-4.440050316998	1.672635481959	-0.187261811998
H	-4.971968661295	-0.001834719502	1.217856653033
H	-2.864599249972	2.632761408785	-1.479586131095
N	-1.826077891610	-2.001402805685	-0.183506457964
C	-2.267957488983	-3.183258425214	-0.630343803783
C	-0.845047279810	-2.336733682899	-2.074886294400
C	-1.662350786958	-3.445899061513	-1.845738399046
H	-2.978039077298	-3.754936879526	-0.046952017497
H	-0.187939654597	-2.119132685133	-2.907166828778

N	-2.349014581857	0.906814667768	-0.419065383570
N	-0.946215952371	-1.478638137781	-1.067019229185
N	-0.068640405278	-1.494804204540	2.085679389117
Rh	-0.228426141879	0.403715360400	-0.587319762110
C	0.377897122154	2.152128393142	-0.144831720965
N	0.782947622474	3.205340124253	0.137772116007
C	1.382438562790	4.436075319251	0.463256415099
H	1.027299814060	5.218819604093	-0.216058449593
H	1.129485232876	4.715848667730	1.491766384379
H	2.471440730132	4.349400334836	0.373280852358
H	0.622143703564	1.194884531598	3.876055123969
H	-1.787880790070	-4.316622947856	-2.471683045021
H	-5.329957138234	2.274909864889	-0.296118005492
C	2.811144458935	0.723370679654	-1.158407272921
C	3.968951053924	1.134754124526	-0.244588423073
C	4.921269702424	0.008292648124	0.151028097704
C	1.766197751642	-0.143305978704	-0.425926398198
C	4.280076139825	-1.280263805739	0.671692750078
C	2.042300912437	-1.630857423948	-0.626221223923
C	3.507926909068	-2.051536235050	-0.402938583512
H	3.203169297694	0.178238080813	-2.033485727628
H	3.534712955409	1.580360514379	0.668274490897
H	5.530612771021	-0.257951630500	-0.728710009694
H	3.631489695984	-1.068605740954	1.536463061751
H	1.892569678529	0.056596889326	0.658222727117
H	1.392971367112	-2.203896254066	0.049181302465
H	2.364477837768	1.634717779637	-1.575938120304
H	4.561477008914	1.932015134325	-0.721063367849
H	5.629664494741	0.393232107332	0.899768253242
H	0.017652630412	0.757129900400	-2.048053175904
H	5.088416838483	-1.921016568311	1.052391343512
H	1.766038295637	-1.932386448392	-1.646881930802
H	3.518785151725	-3.124028447132	-0.161953780483
H	4.071128347744	-1.960903617043	-1.345396417276

TpRh(CNMe)-Cycloheptane IM-(3)

G = -1219.212564

B	-2.367175077658	-1.224860095381	0.584624104615
H	-3.236682443055	-1.888221259883	1.070078489533
N	-1.412780638363	-0.565730830526	1.610504662493
C	-1.595606883624	0.617664276908	2.272240621045
C	-0.206595839261	-0.676112799005	3.371189962989
C	-0.819636102033	0.595954500268	3.402112836081

H	-2.264430392321	1.372643139278	1.874405792004
H	0.494497815286	-1.104482883873	4.079570286546
N	-2.978242851152	-0.076327879851	-0.239671902765
C	-4.251809569829	0.256576009977	-0.499149775537
C	-2.893905175118	1.634011837789	-1.543291690908
C	-4.250679527295	1.357371043940	-1.335869536463
H	-5.065308703823	-0.315179083870	-0.070838854913
H	-2.428260212838	2.409048400061	-2.140538458847
N	-1.498274438312	-2.072817346209	-0.349075770400
C	-1.694382107548	-3.296155534715	-0.855810199937
C	0.039911116060	-2.364887818504	-1.832414190415
C	-0.725860225693	-3.533187752610	-1.813686077187
H	-2.507985325573	-3.911176479026	-0.493574032914
H	0.902041420886	-2.111965940968	-2.434516318855
N	-2.139637787749	0.764144539171	-0.883431507064
N	-0.428407321107	-1.496816857996	-0.942762213584
N	-0.571394186714	-1.373898174464	2.315202367020
Rh	-0.037531066462	0.454442933882	-0.348609444221
C	0.190042028173	2.283976010709	0.112802402557
N	0.272792841422	3.413643373807	0.380490544500
C	0.492395546852	4.759958096907	0.723102205699
H	-0.037253045018	5.002083971779	1.651031759578
H	1.564823311440	4.935563009241	0.867932195831
H	0.128132393135	5.415867804748	-0.075284661856
H	-0.704541886453	1.378076466553	4.139069436830
H	-0.589009579069	-4.423825284275	-2.408504761883
H	-5.105414317263	1.878510648079	-1.741280112547
C	2.315699116971	-1.352382616565	0.435025711742
C	3.125622305505	-1.742783044398	-0.807789247750
C	4.633086026947	-1.580099032790	-0.614403584334
C	1.837581659744	0.102160072207	0.478873458081
C	5.116876979507	-0.137091320152	-0.522040766089
C	2.935451900526	1.088236515730	0.044582076064
C	4.372109373459	0.751913858403	0.474287107899
H	2.956710170204	-1.539362459230	1.314863041881
H	2.801042758897	-1.144868993750	-1.676529311258
H	4.919130146868	-2.118530646924	0.303695713668
H	5.033548412480	0.331791359204	-1.516761888103
H	0.623525672250	0.783302807818	-1.680503982191
H	2.935243333724	1.202953463468	-1.050868219518
H	1.461494368214	-2.023353910839	0.575453875682
H	2.921180034314	-2.792256439838	-1.065302195870
H	5.170917609523	-2.076663452529	-1.435726665044
H	1.607707206268	0.318647997489	1.542835935721
H	6.190234452602	-0.140663704309	-0.280910566982
H	2.681792680872	2.083889482742	0.436216699001

H	4.937571329823	1.690656656934	0.570476810980
H	4.378038691378	0.296198365388	1.477186839394

TpRh(CNMe)-Cycloheptane IM-(4)

G = -1219.211388

B	-2.737455738707	-0.552102066085	0.533643849682
H	-3.839164449330	-0.812248125153	0.920902578466
N	-1.767663770074	-0.090933245508	1.640505130833
C	-1.409472090773	1.173836142898	2.005515512678
C	-0.789900908806	-0.278120331374	3.527619638239
C	-0.758905664708	1.094001887967	3.215158550611
H	-1.665158465913	2.024052476859	1.383732978016
H	-0.385454044942	-0.782854695291	4.398135440148
N	-2.808493285123	0.575642996850	-0.513289363472
C	-3.853550717404	1.262680080468	-0.998584636766
C	-2.010399151614	1.903629184859	-2.008526310746
C	-3.389848673594	2.135347453096	-1.965710691704
H	-4.851485077165	1.077253226461	-0.621974031227
H	-1.249295304939	2.361237643017	-2.629496087802
N	-2.108751922367	-1.782186039408	-0.134232953866
C	-2.665875364229	-2.943672416759	-0.493889180932
C	-0.611260555577	-2.849275036734	-1.260324837002
C	-1.739890866692	-3.669099643224	-1.220700550086
H	-3.681180119384	-3.173119171787	-0.197284341457
H	0.346339577720	-3.018547153174	-1.734469269657
N	-1.673565700379	0.962084967501	-1.135347753050
N	-0.837905404146	-1.719157362080	-0.596726771648
N	-1.403123735004	-0.982355894597	2.591662154746
Rh	0.145520545237	0.095574703048	-0.311819913143
C	0.931191432269	1.813531457384	-0.128090629215
N	1.328057184474	2.904206336440	-0.036729744250
C	1.976216657898	4.139945403146	0.143841419792
H	3.044794346971	3.970443277201	0.325081063454
H	1.857296140060	4.762899756475	-0.749364581991
H	1.546731767029	4.666074949777	1.003428465795
H	-0.328704952875	1.903833758517	3.787078715615
H	-1.859152397162	-4.651926456208	-1.651321986134
H	-3.966338044614	2.830560265380	-2.557929918384
C	1.650893231180	-0.820729813851	0.782432565523
C	2.681455003577	0.054524567184	1.510910774925
C	3.840179935404	0.669418207389	0.725381547525
C	2.315294700156	-2.075895454960	0.209551465940
C	4.662359448634	-0.285948467221	-0.139494688948

C	2.996928525119	-1.980915584387	-1.156303471684
C	3.898331798303	-0.763348351738	-1.374614745730
H	0.934051736005	-0.046274374375	-1.601189102670
H	3.132269208846	-0.574146338682	2.302432123214
H	3.474043871267	1.465068030640	0.058692175860
H	5.013198449838	-1.142273053007	0.457741235640
H	3.069009671927	-2.414901556349	0.943595257990
H	3.590374150434	-2.897618407954	-1.298440102733
H	0.982803742358	-1.183853404952	1.588837064969
H	2.157178958830	0.858765922619	2.053065018573
H	4.506396047116	1.166062315020	1.448074405387
H	1.584590389917	-2.893875271952	0.172028699896
H	5.569480860770	0.244169127770	-0.463823166100
H	2.239985682865	-1.988131233804	-1.955253766951
H	4.602870969438	-0.993069300189	-2.186446041035
H	3.291227371879	0.079833112839	-1.738494195134

TpRh(CNMe)-Cycloheptane IM-(5)

G = -1219.212565

B	-2.337154283124	-1.101003407661	0.961986479666
H	-3.096282323362	-1.723240564728	1.646019374137
N	-1.077649340596	-0.584505314397	1.703373267048
C	-0.949148948435	0.575162574669	2.417902638824
C	0.576210177132	-0.879401355132	3.025287419884
C	0.118379552083	0.434313337118	3.266854681039
H	-1.631379884543	1.401490136705	2.253557881123
H	1.410124154358	-1.399135034665	3.485274508942
N	-3.039388062763	0.144025585062	0.389320332513
C	-4.301553948621	0.585432571869	0.500746741421
C	-3.154746972335	1.930223392737	-0.806156516549
C	-4.426139631485	1.738396604625	-0.251958417455
H	-5.018693817723	0.045802909347	1.106241964911
H	-2.798711947762	2.709497296519	-1.469455997147
N	-1.843959522837	-1.955994550868	-0.211347691989
C	-2.249489496257	-3.145690550949	-0.672079879484
C	-0.778084645168	-2.282952961621	-2.058846184711
C	-1.589317260063	-3.402705951088	-1.860312279388
H	-2.975204430803	-3.726354200592	-0.117529828329
H	-0.082356411226	-2.059301292830	-2.857728038678
N	-2.331497869451	0.965184254812	-0.416756007967
N	-0.937105458069	-1.423505917165	-1.060142357085
N	-0.145678569650	-1.492072799911	2.108747709500
Rh	-0.214033980165	0.438084234922	-0.528146363018

C	0.423176015623	2.171694192173	-0.066881419004
N	0.859593806289	3.213227278993	0.212236788130
C	1.459137955863	4.444062311332	0.536968274907
H	0.898776858608	5.267667219719	0.080948423566
H	1.469835866385	4.579117626835	1.624116735216
H	2.489795841694	4.462492533762	0.164874377420
H	0.514106034830	1.166410743293	3.956391592486
H	-1.676804644013	-4.276910519339	-2.487889744239
H	-5.308225602248	2.347383867726	-0.384389326571
C	1.773505926806	-0.135859852798	-0.332596045319
C	2.019552749436	-1.642982476208	-0.449542954984
C	3.305475522403	-2.144781277231	0.211944058837
C	2.782599998201	0.637339168183	-1.204745629072
C	4.614340650609	-1.453742173132	-0.171900086067
C	4.077093749817	1.051688298013	-0.499513509786
C	4.730833689327	-0.027115452692	0.369190271669
H	1.951279649525	0.138137621481	0.730528892285
H	2.033470308952	-1.919131179619	-1.517717828719
H	3.186077419819	-2.055137231186	1.305387718829
H	4.747131525205	-1.460581647316	-1.266068769458
H	3.029831028638	0.012536943480	-2.077834625127
H	4.795579566638	1.391752442996	-1.261972507394
H	0.060586220544	0.802406226513	-1.980050142055
H	1.193802610229	-2.202147020486	0.005586525327
H	3.395375475756	-3.222928326063	0.009124205701
H	2.340960138560	1.545397142354	-1.636109147946
H	5.444280408706	-2.051167096874	0.232093621417
H	3.875113150222	1.932757324516	0.132992935706
H	5.789054691407	0.234754906563	0.510594432549
H	4.286659307034	-0.011863591767	1.376374444486

TpRh(CNMe)-Cycloheptane IM-(6)

G = -1219.213488

B	-2.216994191738	-1.436676818889	0.682648552927
H	-2.945636268810	-2.219539868484	1.218912073350
N	-1.188121919437	-0.764607506065	1.626222735462
C	-1.360983281048	0.362837678219	2.381489560663
C	0.286106504946	-0.851246000670	3.171960997203
C	-0.417265113018	0.355658042305	3.376426428725
H	-2.141439919516	1.074842976199	2.138429732126
H	1.121839780829	-1.250519659916	3.736788300481
N	-3.036372446130	-0.291291808519	0.060010761440
C	-4.358289830192	-0.069317617050	0.002196970673

C	-3.286877287555	1.531887246887	-1.056025031992
C	-4.571602683202	1.098092173969	-0.707247420216
H	-5.050064178774	-0.758918093466	0.469102810368
H	-2.979856067182	2.402574301346	-1.623244108866
N	-1.423688132614	-2.122743317240	-0.437225945257
C	-1.553524312512	-3.332769270271	-0.995266780430
C	-0.086754386408	-2.154012523991	-2.131116755815
C	-0.710244413203	-3.403316054018	-2.089598864195
H	-2.234255008943	-4.058689316546	-0.569802315017
H	0.656643803315	-1.768687401674	-2.817716770019
N	-2.373565210677	0.688275869546	-0.592256985259
N	-0.519836954484	-1.395888404818	-1.131732879076
N	-0.185091063134	-1.526883155281	2.143203467130
Rh	-0.199415828256	0.520245737527	-0.427596603661
C	0.026406255683	2.303475024615	0.195670081182
N	0.157643109746	3.392064429258	0.585046942010
C	0.389519814701	4.697731467081	1.054327678912
H	0.260799182347	4.732405672538	2.141768984785
H	1.411622828439	5.005694119630	0.806332613575
H	-0.316196205840	5.395395360683	0.590063568930
H	-0.253525714305	1.106962415600	4.135875606229
H	-0.563338233987	-4.239594130084	-2.756536700852
H	-5.517475846675	1.563443739030	-0.942335034239
C	2.291296954032	-1.213044377516	-0.067469793163
C	1.823313671930	0.247574720261	-0.022241612619
C	2.748126606717	1.186274678756	-0.802276411375
C	3.558237951892	-1.474087652158	0.762613456756
C	4.243706908661	1.138951724177	-0.460869826831
C	4.886270826121	-1.315072829816	0.020554599940
C	4.949009148423	-0.129631893632	-0.944593434061
H	2.459081444983	-1.530394958486	-1.110457812441
H	1.871478940150	0.544115881693	1.048870236595
H	2.648527411447	0.974547242831	-1.880559560111
H	4.391074665236	1.268250540505	0.624135740096
H	3.540521056995	-0.800387216911	1.633586745771
H	5.694275729032	-1.223862748470	0.762367386611
H	1.496917558626	-1.856847785168	0.323556214615
H	0.181992227721	1.032082602099	-1.807762223854
H	2.403135861935	2.223953947675	-0.679120778818
H	3.519115424425	-2.489921422033	1.181691035211
H	4.722434057246	2.009370143503	-0.934134774626
H	5.103863876355	-2.235258148145	-0.542213630662
H	6.004673538512	0.086688939396	-1.161430402789
H	4.505059357195	-0.415364696010	-1.911009825521

TpRh(CNMe)-Cycloheptane IM-(7)

G = -1219.210899

B	-2.694874260850	-0.873090859742	0.409770698135
H	-3.759338303328	-1.318170618558	0.726367244659
N	-1.785802019870	-0.489278407243	1.597029820659
C	-1.643415402376	0.723300597776	2.208006018182
C	-0.852555073978	-0.881593822766	3.475904222797
C	-1.027666668932	0.515100012848	3.419134362260
H	-2.005642189802	1.628337097548	1.733829682052
H	-0.400019429928	-1.474439756068	4.263338582733
N	-2.891834971922	0.398092265499	-0.437282056716
C	-4.003682109644	1.037365845121	-0.830356108562
C	-2.235411273366	2.039726495327	-1.665404534158
C	-3.632715643855	2.107013287449	-1.624343985016
H	-4.977612792452	0.681974653327	-0.518506347081
H	-1.525330323067	2.677498683627	-2.178589246958
N	-1.920883439562	-1.888332141698	-0.439498427934
C	-2.330904233620	-3.011669064202	-1.039466937416
C	-0.288299023237	-2.536090575000	-1.691354004503
C	-1.312314690390	-3.470381765132	-1.855423595704
H	-3.316685845712	-3.408664545484	-0.834342761921
H	0.698341561253	-2.501621084214	-2.136826681435
N	-1.802303444780	1.006731652378	-0.952758962779
N	-0.661344766069	-1.593300301094	-0.831431423148
N	-1.314999658468	-1.480760952826	2.393225865889
Rh	0.098868807372	0.238306230597	-0.210293973666
C	0.698178026796	1.990379377573	0.215258259271
N	1.033478048043	3.085137974003	0.423428419890
C	1.588394519104	4.338140132173	0.741795920141
H	0.820719445601	4.993681681705	1.167029581886
H	2.395121389171	4.209132678097	1.473236786994
H	1.996918641941	4.806443824116	-0.160622928060
H	-0.745939401390	1.257855660488	4.151777737064
H	-1.307223733695	-4.357452426671	-2.470896539605
H	-4.278893557922	2.824346004118	-2.108423544734
C	2.904132839793	0.370536325211	1.124723779588
C	1.726849907510	-0.565168784129	0.813052561040
C	2.236711737616	-1.923176074173	0.341409885857
C	3.650476608991	0.922947789868	-0.097163382632
C	3.132883563368	-1.914766255440	-0.901826550807
C	4.805547601935	0.061498221384	-0.616250648333
C	4.566322040504	-1.453134665212	-0.616568101237
H	3.627683799376	-0.164989406014	1.768080900003
H	0.914395713052	0.368409939084	-1.485504111492
H	2.831577317732	-2.369712128607	1.160568110252

H	2.683928151400	-1.291034902339	-1.693163981433
H	2.925054304402	1.073728776821	-0.907632610203
H	5.043189036070	0.392268487676	-1.638432362678
H	2.544178475321	1.204796118265	1.744108068228
H	1.202781470498	-0.745555306885	1.773461356178
H	1.395007565457	-2.608507699579	0.200864953288
H	4.054349184299	1.922316365904	0.130153297309
H	3.176732738322	-2.937645188677	-1.305351939052
H	5.709989477183	0.265700623394	-0.023782155182
H	5.253805794953	-1.904714226719	-1.345711459803
H	4.861788491154	-1.870766842903	0.357949247892

TpRh(CNMe)-Cycloheptane TS_3-(1)

G = -1219.208854

B	-2.325837904146	-1.321464709268	0.859440275098
H	-3.154084062069	-1.969385437253	1.433243985727
N	-1.731429436662	-0.164278738443	1.689437888073
C	-2.368897436621	0.978500041917	2.037408537799
C	-0.455203079651	0.815474430436	3.098040063287
C	-1.578494131041	1.647430771357	2.944855701293
H	-3.330973461653	1.228739364236	1.605837942447
H	0.426004049571	0.966570832546	3.711785454824
N	-2.948093100909	-0.645924600102	-0.377813976758
C	-4.175387318538	-0.689942531236	-0.917141589405
C	-2.865477406442	0.579589187100	-2.142796518687
C	-4.174629926446	0.090278410715	-2.059095839888
H	-4.959276513824	-1.271851826124	-0.448857264181
H	-2.413211749864	1.223380887533	-2.887914134585
N	-1.199399251669	-2.243575358729	0.371956548811
C	-1.192171179352	-3.582695688050	0.314064752516
C	0.474005168289	-2.792781461383	-0.875749369223
C	-0.130514653891	-3.985654855233	-0.473571723969
H	-1.948300286017	-4.152277611589	0.838687896759
H	1.342108992450	-2.632578372391	-1.503488648501
N	-2.139234366923	0.130276698155	-1.126915938709
N	-0.168702454640	-1.753753474952	-0.357744854793
N	-0.549842327841	-0.276170334686	2.353174421279
Rh	-0.059885048880	0.314191335753	-0.446969380997
C	-0.098815284514	2.214382573453	-0.503030813913
N	-0.135482766389	3.376506506690	-0.510989744530
C	-0.147519929922	4.782775265437	-0.485294997831
H	-0.463998419392	5.133217063121	0.503269936875
H	0.856577793045	5.167295164746	-0.696336301804

H	-0.843469519428	5.166514385107	-1.239356471073
H	-1.784273206929	2.592817483206	3.426701139321
H	0.166266937777	-4.994544393787	-0.717762857759
H	-4.998268138484	0.274508222881	-2.733045475247
C	3.667667067828	0.342418354281	-1.580990076550
C	5.001538420673	-0.100507499710	-0.975941045013
C	4.915736432714	-1.057601568241	0.210324200456
C	2.861293985226	1.250748609810	-0.645244182776
C	3.937871873617	-0.662913447725	1.318321934413
C	1.876867367769	0.529134630929	0.293646373567
C	2.470050121458	-0.757191922238	0.869272099807
H	3.063055344506	-0.531911310340	-1.874525769798
H	5.541684822365	0.808612351777	-0.663956484170
H	4.618061595462	-2.054493738864	-0.155129512389
H	4.169223254728	0.346108331852	1.696259648293
H	3.589359451551	1.825690313760	-0.045609501664
H	1.707260699170	1.205128454434	1.156041969468
H	3.884383622311	0.880461022198	-2.514948495728
H	5.624549690560	-0.565397533324	-1.754586099396
H	5.925628595629	-1.182604245270	0.628711270199
H	2.329277230037	2.003220175294	-1.241893545408
H	4.097157607902	-1.343257757243	2.167226583401
H	0.519934972547	0.333431741140	-1.850280744637
H	1.830769199099	-1.086875787263	1.698159651825
H	2.425971885853	-1.567114296417	0.131340903843

TpRh(CNMe)-Cycloheptane TS_3-(2)

G = -1219.208216

B	-2.517021917609	-0.714708118982	1.097415869434
H	-3.389744363845	-1.108361694287	1.817483613653
N	-1.386953771815	0.046158886849	1.822348601742
C	-1.481011106681	1.273844691523	2.383582271170
C	0.432560772850	0.337486408066	2.907147746064
C	-0.324150113919	1.507502302694	3.093468724554
H	-2.360530232369	1.887594547710	2.227941836230
H	1.422358730330	0.098724875724	3.281063318648
N	-3.088573407260	0.288937070103	0.077851258646
C	-4.330847306768	0.737573430863	-0.156057537662
C	-2.930176390615	1.633684585899	-1.592873304529
C	-4.280800012461	1.613728429734	-1.224926918765
H	-5.158854530507	0.401841576473	0.455547638582
H	-2.437648000522	2.177392670266	-2.390296309984
N	-1.924289747472	-1.895036546676	0.316118776411
C	-2.392517723844	-3.146946968523	0.219277840029

C	-0.835207310694	-2.831619344022	-1.294572089140
C	-1.720104381091	-3.792460977172	-0.800965661894
H	-3.174773653288	-3.486435448739	0.885736645261
H	-0.115390512015	-2.902752102093	-2.099663735663
N	-2.224966851572	0.834379641310	-0.802263050373
N	-0.959495039779	-1.698957127811	-0.614207738439
N	-0.207008879856	-0.543806463375	2.151597217737
Rh	-0.134889821343	0.202133867291	-0.640914026788
C	0.557588830107	1.973958743409	-0.604888539660
N	1.022000102491	3.038581171197	-0.555023238814
C	1.654904931959	4.292435175477	-0.473186086162
H	1.327596365169	4.933549468912	-1.299025440157
H	1.401269140123	4.776228557124	0.476373322869
H	2.741480178726	4.160555591165	-0.530075196150
H	-0.067934318038	2.389276747587	3.663624762793
H	-1.848193268410	-4.810436177950	-1.136958073650
H	-5.100546346626	2.155416517438	-1.673311934176
C	2.871177772510	0.184452097853	-1.384107272787
C	4.102221152817	0.800547548782	-0.713782362446
C	5.041596811146	-0.187038416322	-0.026088901220
C	1.850200105018	-0.354950476133	-0.361097763079
C	4.397393737941	-1.195044465322	0.928430830052
C	2.068478339415	-1.836564104715	-0.072649239731
C	3.529080331338	-2.236228824902	0.216581940994
H	3.183177410267	-0.623659329134	-2.067494351319
H	3.745817305168	1.537080099047	0.028664900261
H	5.575085711586	-0.760537151490	-0.802332428627
H	3.819388520931	-0.674764078225	1.708506791783
H	2.051498607022	0.176345790975	0.589580824840
H	1.430628845858	-2.121954662719	0.775562945456
H	2.425163887757	0.947149344136	-2.035742518131
H	4.686834364697	1.372068287706	-1.452060080599
H	5.816250765487	0.380902604372	0.510677575612
H	0.095451940584	0.199182954507	-2.140688422379
H	5.208933621079	-1.716582310381	1.456017263390
H	1.731997629031	-2.443160983454	-0.924322433751
H	3.516650897518	-3.165145741541	0.804417408475
H	4.035624789479	-2.497744320226	-0.726195638615

TpRh(CNMe)-Cycloheptane TS_3-(3)

G = -1219.208767

B	-2.356583019593	-1.223764560796	0.930375064371
H	-3.199300819819	-1.849210313553	1.508124958624

N	-1.595732668663	-0.212995005241	1.813784429006
C	-2.096410643949	0.932612851285	2.332283951738
C	-0.130063731440	0.493749716616	3.201072422113
C	-1.180081641271	1.428433781402	3.232627735457
H	-3.062715753319	1.307118622194	2.015263138756
H	0.805986612709	0.502174132626	3.748463398959
N	-2.999288196860	-0.381784674065	-0.187614214191
C	-4.260526828826	-0.270754337813	-0.630574963428
C	-2.928611728440	0.987493947727	-1.844124881730
C	-4.268302897727	0.607412884820	-1.698952362089
H	-5.059730069520	-0.823709468457	-0.153192188327
H	-2.472383514078	1.655152431214	-2.565442885676
N	-1.356630066561	-2.188569869588	0.280707570252
C	-1.446786353419	-3.519814152470	0.157161533126
C	0.192794510501	-2.779559069634	-1.100269156986
C	-0.468072905526	-3.949159391107	-0.718323958165
H	-2.207179250429	-4.064308037019	0.701850603775
H	1.026119188037	-2.647364496407	-1.776145633605
N	-2.177161561468	0.386358873103	-0.930247009129
N	-0.342146731894	-1.728164525230	-0.491030724224
N	-0.380982459973	-0.496127923723	2.356947680929
Rh	-0.049201509074	0.328143856552	-0.400587296198
C	0.056443667939	2.221237625655	-0.280023353057
N	0.076139170673	3.379379020250	-0.176312276877
C	0.147595350712	4.775121177434	-0.019493944129
H	-0.129258415679	5.048341032375	1.004696438299
H	1.168515975555	5.120507838135	-0.218077144083
H	-0.538462615242	5.267501747764	-0.717434457247
H	-1.260313336501	2.327791432651	3.826809145186
H	-0.260342919006	-4.960495888085	-1.034025087016
H	-5.116995430492	0.922830673229	-2.287807521362
C	2.496335383857	-1.068543156331	0.624942664734
C	3.283649167055	-1.808627097157	-0.464209884644
C	4.780908411167	-1.499746081106	-0.442273169747
C	1.936325433334	0.306681287735	0.233493706963
C	5.153333287282	-0.099469126957	-0.917626668494
C	2.898002335926	1.096685391161	-0.665515672812
C	4.381483893317	1.046596586448	-0.264422368068
H	3.180444637024	-0.939645106584	1.482638627599
H	2.881647804780	-1.567794132338	-1.461963562086
H	5.145736361061	-1.643912637477	0.587647794244
H	4.989872122015	-0.037371135682	-2.006479838269
H	0.420350333733	0.445620365107	-1.838569773608
H	2.818979829593	0.756435647403	-1.709867559846
H	1.685225077435	-1.694004589964	1.014273993131
H	3.150526863187	-2.892840110750	-0.335995455725

H	5.321429524906	-2.232584582621	-1.059644554676
H	1.850851304318	0.876721891795	1.179909637632
H	6.232880486482	0.049197240381	-0.766959861497
H	2.572566108015	2.147020127688	-0.686493472047
H	4.863862177790	1.989089623383	-0.562942232354
H	4.476430430368	0.995407324025	0.832545356501

TpRh(CNMe)-Cycloheptane TS_3-(4)

G = -1219.207626

B	-2.778193490965	-0.262177619926	0.661531103454
H	-3.891373184400	-0.384387517097	1.087262468159
N	-1.881078219271	0.684433681334	1.483191985092
C	-1.957879596713	2.035616804594	1.518173399391
C	-0.537298572956	1.308326410797	3.023655050469
C	-1.102268776014	2.484673334613	2.499226376345
H	-2.607542192123	2.571422150989	0.836015085074
H	0.201072850030	1.198918318242	3.810382643678
N	-2.819615256238	0.350703869559	-0.750746225446
C	-3.830223167295	0.719581551427	-1.551535807616
C	-1.910378503864	1.073217145568	-2.561093115462
C	-3.294004397772	1.197279627605	-2.733633303490
H	-4.856248107360	0.616241247331	-1.221434649808
H	-1.102597114672	1.316957108658	-3.241031184225
N	-2.122756010716	-1.648383225314	0.555821028461
C	-2.710846434040	-2.843469748448	0.699800269015
C	-0.718267335133	-3.115497450827	-0.176691690117
C	-1.846479252876	-3.820836972333	0.246011121553
H	-3.708365418246	-2.909261220888	1.114518219473
H	0.199111203941	-3.483566971492	-0.616503748945
N	-1.639149151125	0.564412703545	-1.365489758702
N	-0.887301197959	-1.812487311444	0.019269637898
N	-1.011932417400	0.227705838799	2.420941983091
Rh	0.157145272171	-0.039558204423	-0.277970125142
C	0.917420896702	1.682192597557	-0.522326770017
N	1.280239006518	2.777130907659	-0.672078143453
C	1.862010982917	4.054475697605	-0.756759154202
H	2.952801872479	3.967374364376	-0.681064617972
H	1.604173889588	4.524860482680	-1.711854292576
H	1.495102590011	4.684564948329	0.060980185276
H	-0.917354261065	3.507846417014	2.794648326174
H	-2.006067458709	-4.888377251094	0.225697678052
H	-3.825918476129	1.575616466799	-3.594081988484
C	1.755206556378	-0.693053580833	0.889784441067
C	2.848865015960	0.318262999468	1.259953735161

C	3.895484631803	0.703374216900	0.212886752773
C	2.380774736584	-2.055596242469	0.571318691758
C	4.640889706167	-0.447315839674	-0.465190850518
C	2.893821655150	-2.318827637839	-0.844260673079
C	3.768087352618	-1.218965004614	-1.455658608607
H	0.877648417465	-0.477309408911	-1.535277736087
H	3.401570927152	-0.101772805774	2.122157347619
H	3.435693675847	1.301196798720	-0.588935905844
H	5.070891097279	-1.125768162899	0.288330644630
H	3.224686338438	-2.200587910781	1.270350615540
H	3.465603081218	-3.259789141593	-0.822236852140
H	1.185515536282	-0.844371310745	1.823324092780
H	2.381596216644	1.240386361682	1.644469416516
H	4.627587632536	1.366330016923	0.700209475629
H	1.676180318313	-2.854111607685	0.835012657174
H	5.497897852811	-0.022222662832	-1.007506763015
H	2.045317611269	-2.501004775009	-1.522340268333
H	4.398316480282	-1.668734877703	-2.235919220701
H	3.131147558486	-0.487753516127	-1.976035827321

TpRh(CNMe)-Cycloheptane TS_3-(5)

G = -1219.209582

B	-2.443334777047	-0.930925720586	1.128702731450
H	-3.282001710784	-1.448930353273	1.809374367871
N	-1.303954832395	-0.255451816513	1.922547973301
C	-1.401730097004	0.880172161602	2.652842547209
C	0.535381062106	-0.089062671521	3.000880956584
C	-0.232732388952	1.031117329617	3.364599182608
H	-2.292825084701	1.494985456357	2.602893886293
H	1.536223213676	-0.360954946126	3.317964108419
N	-3.069813003296	0.196861060347	0.287030539855
C	-4.330127334866	0.637327710586	0.156975583591
C	-2.999673468425	1.778971265008	-1.168024661738
C	-4.336958216094	1.663428617601	-0.770127109846
H	-5.129248598318	0.189580645220	0.734300844161
H	-2.547224908862	2.449818596390	-1.888664723969
N	-1.849465306506	-1.967278287528	0.165698314442
C	-2.253719142305	-3.221327206487	-0.077651515256
C	-0.754017042124	-2.635234572286	-1.570477435862
C	-1.575026642439	-3.696778316508	-1.184151045580
H	-2.999029249079	-3.684071677641	0.556181417009
H	-0.044586359375	-2.565998260600	-2.385146474548
N	-2.248930545506	0.893318239552	-0.525297324178

N	-0.922901275731	-1.604448116538	-0.752038146486
N	-0.108732890039	-0.866554645689	2.142733373476
Rh	-0.143035317034	0.296785415918	-0.519595345109
C	0.528313726836	2.060008925794	-0.269425033871
N	0.983890096516	3.117593570462	-0.108710177823
C	1.576511795030	4.376298921976	0.101021165415
H	0.987406640079	5.156424659200	-0.393501071565
H	1.623449446225	4.590734281502	1.174305474897
H	2.592525489370	4.380023443188	-0.309193517713
H	0.024961467293	1.829511352570	4.046096629410
H	-1.659300744725	-4.670576208224	-1.642626336219
H	-5.184278843932	2.240797339190	-1.109463087936
C	1.859765524932	-0.260795028039	-0.388797270211
C	2.093382637974	-1.768314967322	-0.258588610881
C	3.434828688744	-2.172739420536	0.356710939933
C	2.771873366311	0.337250757790	-1.477742864483
C	4.697363434769	-1.595442692106	-0.283621663497
C	4.142631479523	0.825978501088	-0.998188781349
C	4.879878934567	-0.098538839208	-0.024898424861
H	2.145031708308	0.191298398940	0.584403015951
H	2.014176247683	-2.228376451539	-1.257792387651
H	3.433388126513	-1.881860411823	1.421041630808
H	4.706046634517	-1.800571488401	-1.366673307036
H	2.910503872887	-0.421783244837	-2.264656986811
H	4.775848151891	1.005072228005	-1.881373715402
H	0.026844265037	0.510889939663	-2.011045807552
H	1.305485778076	-2.219788280520	0.357037103418
H	3.497418839244	-3.271734272401	0.348506930650
H	2.291937231400	1.180977103790	-1.991591357395
H	5.564291035497	-2.131842890770	0.128179705331
H	4.021884862862	1.810912271424	-0.516403819742
H	5.948698907947	0.157578557345	-0.046649507132
H	4.549813193726	0.107416336896	1.004895629621

TpRh(CNMe)-Cycloheptane TS_3-(6)

G = -1219.210816

B	-2.359158888516	-1.195617587210	0.947907787143
H	-3.162681529472	-1.802846331343	1.596268800123
N	-1.551516372466	-0.147674158130	1.745047747095
C	-2.014064224516	1.038931373059	2.206599023970
C	-0.025455531597	0.618164765047	3.033089279918
C	-1.058292654277	1.572932420897	3.041107936587
H	-2.982171713769	1.414009504140	1.895858516745

H	0.929483606465	0.642295698500	3.546536499920
N	-3.068564330779	-0.389389154160	-0.156046604929
C	-4.354305131477	-0.293498172983	-0.526190586362
C	-3.104787739277	0.952854416761	-1.835829167146
C	-4.430845689140	0.566212897768	-1.606708639650
H	-5.120362397552	-0.842462894687	0.006891353599
H	-2.696597260915	1.611703178765	-2.593105095675
N	-1.394961002128	-2.181247133788	0.271716753830
C	-1.464973055577	-3.517732950388	0.205184951706
C	0.094035876376	-2.800291024448	-1.164588833430
C	-0.524006134801	-3.964719548421	-0.703713929192
H	-2.183873078736	-4.054444079876	0.810559787761
H	0.895337920248	-2.674776236050	-1.881954895146
N	-2.296755761202	0.372947452235	-0.957325597290
N	-0.432451275535	-1.737109034369	-0.570714643696
N	-0.324697738853	-0.418778585023	2.265092845509
Rh	-0.139414204067	0.307487000123	-0.568976225787
C	0.048424888007	2.199630671568	-0.520262581214
N	0.162850881041	3.355436597538	-0.461982512721
C	0.327572671003	4.748512620475	-0.358583153748
H	0.435383237263	5.032203233930	0.694125959411
H	1.224356509626	5.059649943853	-0.905830204500
H	-0.544060862143	5.262155147155	-0.778908884522
H	-1.101426680472	2.510669558478	3.576874521784
H	-0.313647552772	-4.984524699933	-0.988921074491
H	-5.314782226380	0.866592268556	-2.149785243681
C	2.376083162927	-1.116071612058	0.443106503645
C	1.890637599973	0.232631643871	-0.104395672775
C	2.785169775960	0.779303797901	-1.220086040994
C	3.655963917096	-1.005257132910	1.286731314098
C	4.285909931325	0.887874795967	-0.918874576906
C	4.971885304002	-1.146490621529	0.519253811782
C	5.002057255794	-0.462593532204	-0.849322451146
H	2.543462492160	-1.829103459689	-0.380667813823
H	1.961869786545	0.939069623244	0.749750234522
H	2.672863135339	0.146627441743	-2.117467533506
H	4.446029343637	1.453716373855	0.013899058840
H	3.638995181805	-0.036664057828	1.810499205156
H	5.786696206154	-0.748123667138	1.142843590142
H	1.587584292710	-1.549123291554	1.068486443966
H	0.225507732755	0.371288035087	-2.038811790005
H	2.421040368558	1.773893230050	-1.520571049764
H	3.640704762231	-1.764637864067	2.081826086784
H	4.746036285660	1.489484901415	-1.717009926806
H	5.201218741739	-2.213664794608	0.379920775243
H	6.051317529474	-0.347494681735	-1.156013268548

H	4.548808570600	-1.124549603385	-1.603739459330

TpRh(CNMe)-Cycloheptane TS_3-(7)

G = -1219.205909

B	-2.766021419748	-0.738655235504	0.523591864442
H	-3.854989315051	-1.112540527298	0.855749914168
N	-2.095109628838	0.227536289094	1.516365607958
C	-2.458529048594	1.508827005556	1.753749375333
C	-0.944696066209	0.860270307521	3.201619250487
C	-1.737413364522	1.961939829745	2.836113174605
H	-3.197801990141	1.999215901933	1.131277576645
H	-0.214888593191	0.782139380850	3.999814063849
N	-2.864230598857	0.039383817720	-0.802797439574
C	-3.895814831688	0.336685262133	-1.606330987935
C	-2.031858679130	1.123713662751	-2.462851160671
C	-3.409924958028	1.041701096988	-2.692772816751
H	-4.899701774318	0.025293897514	-1.346256539931
H	-1.254876614689	1.579920014967	-3.064975745004
N	-1.861780118022	-1.954950430834	0.283158716393
C	-2.228378203824	-3.240806320936	0.197585731735
C	-0.176102439014	-3.018995134268	-0.544445732527
C	-1.176069161138	-3.967804095572	-0.325184263848
H	-3.217559731842	-3.543714973530	0.515594649770
H	0.821657704557	-3.146904983189	-0.944608005915
N	-1.717717739856	0.517873123227	-1.323975297648
N	-0.591670237000	-1.814364013364	-0.168035831932
N	-1.163811621877	-0.183637639190	2.414419711193
Rh	0.138858085418	0.132956524216	-0.234558641931
C	0.635280330948	1.959689956225	-0.392270475856
N	0.888106466581	3.085223044123	-0.539850231390
C	1.310774273206	4.423789490696	-0.626721685017
H	0.532366880052	5.088408982011	-0.236492319258
H	2.227030620775	4.560340067340	-0.040108455154
H	1.513126156205	4.686227799102	-1.670967565398
H	-1.779833259765	2.940138545319	3.293811403407
H	-1.134906348952	-5.029676001020	-0.515620030289
H	-3.969545058018	1.433967950092	-3.529061707578
C	3.001762497194	0.798623000481	0.795716064420
C	1.850063220601	-0.212140907639	0.921183571658
C	2.395359369215	-1.636290028909	0.918330475673
C	3.645391759076	0.914636388024	-0.591985817476
C	3.205213561816	-2.047110439404	-0.316038123832
C	4.792470707006	-0.060070457497	-0.879954982056

C	4.628921127118	-1.479825379131	-0.325127537035
H	3.788833186612	0.534768011189	1.527529343267
H	0.920368738163	-0.107989677959	-1.509128457678
H	3.065655210734	-1.750542251604	1.791343678732
H	2.674735191679	-1.752708155171	-1.237489609195
H	2.862325697901	0.781448294860	-1.349871531678
H	4.930734196618	-0.110514963415	-1.970393594771
H	2.646482452443	1.788830344051	1.115148547307
H	1.403210671756	-0.055924970675	1.919988999422
H	1.580611001510	-2.344855769480	1.098201836882
H	4.029751378185	1.935916127720	-0.741049073509
H	3.274871761784	-3.145433312825	-0.339251631631
H	5.732057219800	0.353803725974	-0.484248232731
H	5.289664439264	-2.144990858071	-0.898924162317
H	5.007499746098	-1.515226524937	0.707749710171

TpRh(CNMe)-Cycloheptane product-(1)

G = -1219.236972

B	-2.417271165438	-1.448735457057	0.491763935674
H	-3.287230117374	-2.208157750222	0.800772415814
N	-1.843800611185	-0.765432548677	1.738487347119
C	-2.187209650637	-0.900143190754	3.029390558423
C	-0.558393575814	0.559685497291	2.841254359411
C	-1.384872143667	-0.064141195170	3.782020581005
H	-2.976916446515	-1.582328507977	3.317046252683
H	0.230678165609	1.288032400388	2.987154280713
N	-2.962123858513	-0.379573883069	-0.471273817692
C	-4.207487062055	-0.187970345302	-0.935223926254
C	-2.841452753894	1.267237497287	-1.849131718338
C	-4.182453400757	0.867800660774	-1.826322689126
H	-5.019388665381	-0.821129394528	-0.600840462365
H	-2.360357993636	2.053482568333	-2.418567430277
N	-1.294871473559	-2.199441112319	-0.243976990261
C	-1.296001552248	-3.461150060046	-0.700516747000
C	0.456564774935	-2.399762558878	-1.483310072943
C	-0.182476165995	-3.641474010029	-1.497949444686
H	-2.094401865011	-4.137843846223	-0.424556876340
H	1.364874320068	-2.080529031686	-1.978999447874
N	-2.119307253814	0.510620511490	-1.033014418229
N	-0.212928899502	-1.542892933188	-0.721323695448
N	-0.843495264954	0.129889782562	1.618438867400
Rh	-0.046597830444	0.516014310152	-0.369587367689
C	0.048073203528	2.397144595879	-0.205394576554

N	0.123582685350	3.555092502796	-0.108921246561
C	0.247596691455	4.953055964074	-0.019379637908
H	-0.328248714366	5.328312802804	0.833941975859
H	1.300493085622	5.226081184733	0.113788028457
H	-0.127721243041	5.423584086904	-0.935169864596
H	-1.395372177722	0.072740636829	4.853163853197
H	0.122712630004	-4.538703958652	-2.015205080279
H	-5.010209598633	1.280976926574	-2.383451145032
C	3.678890057456	0.246637639258	-1.462010341535
C	4.939823869904	-0.384812456328	-0.869410285625
C	4.718086435821	-1.398079512581	0.250264906277
C	2.963031001832	1.182561071306	-0.483502339951
C	3.795590662608	-0.951293138862	1.385880853999
C	1.895145647251	0.526835921435	0.408782481349
C	2.327371296982	-0.840588609367	0.944887336751
H	2.983690098468	-0.531195075970	-1.815608430507
H	5.576482894492	0.432229351910	-0.491498104057
H	4.293411141221	-2.320369052993	-0.180279795189
H	4.148083562646	-0.000234088087	1.817220688679
H	3.742764965084	1.645818106033	0.148234995619
H	1.809048070656	1.181696556017	1.298990587309
H	3.972465406950	0.810222743952	-2.359070091774
H	5.520037490138	-0.871060771410	-1.667919718104
H	5.699146722392	-1.683362836728	0.658668393082
H	2.512002513528	2.014808185506	-1.039308638255
H	3.871926210090	-1.693289804532	2.193969296222
H	0.530437319907	0.695953946137	-1.802299954525
H	1.661621784600	-1.105024593170	1.779753254023
H	2.166885831671	-1.624689051267	0.195153341300

TpRh(CNMe)-Cycloheptane product-(2)

G = -1219.237773

B	-2.645906873668	-0.694754350215	1.007708585345
H	-3.595459057197	-1.111574651698	1.602332104980
N	-1.609913117415	-0.135135786959	1.989882982635
C	-1.647652461409	-0.058870943394	3.329814965186
C	0.230935452708	0.801603616535	2.588308342158
C	-0.480105912026	0.538733153461	3.764184572699
H	-2.502977530317	-0.436570986453	3.875266868336
H	1.205508807144	1.256898179888	2.455633951529
N	-3.074456503091	0.416668343486	0.033064722715
C	-4.284905021853	0.957249634368	-0.180359121971
C	-2.823594798883	1.838968137810	-1.560892299801

C	-4.174483756829	1.884598095622	-1.198662162958
H	-5.137411360938	0.638370400194	0.405685676081
H	-2.290249612341	2.391387255295	-2.325195181239
N	-2.007329307059	-1.817702469191	0.173685611393
C	-2.476746069920	-3.049283461519	-0.077419943150
C	-0.737904018462	-2.652595245035	-1.355811929498
C	-1.687336763045	-3.630693083999	-1.051102250933
H	-3.342676402440	-3.420096624847	0.455660052834
H	0.076112508112	-2.669294298738	-2.069940598967
N	-2.174235225656	0.954364768291	-0.815510137065
N	-0.933133148539	-1.572099585154	-0.609741097871
N	-0.457844518573	0.392561081904	1.530170089020
Rh	-0.100045085867	0.341722346800	-0.617417617304
C	0.632307067585	2.079976786031	-0.777734607779
N	1.135642578415	3.124109620697	-0.888793531989
C	1.781511645364	4.361839936832	-1.059396742146
H	1.470579667538	4.821480324603	-2.004374140050
H	1.526296385518	5.037047286039	-0.235089932937
H	2.867282943942	4.213853930656	-1.076663275152
H	-0.186578494988	0.752282622749	4.781260691311
H	-1.784446942799	-4.617353329395	-1.478600533880
H	-4.957285719999	2.496547871296	-1.621778219244
C	2.871502244130	-0.012125752836	-1.425282824581
C	4.204596363078	0.590771742579	-0.971464736952
C	5.108059381201	-0.315920628862	-0.140954706348
C	1.880729283826	-0.226218055614	-0.265623126542
C	4.458674134105	-1.009963301839	1.057371254122
C	2.009128400849	-1.610494287144	0.368863976035
C	3.446067766559	-2.084669057888	0.654839017615
H	3.047354215457	-0.963814411651	-1.956267995077
H	3.974839985389	1.500055250325	-0.387250549595
H	5.518978995091	-1.101186018406	-0.797141420659
H	3.993639975228	-0.269459687503	1.727610381648
H	2.187027984991	0.490756685894	0.520920872178
H	1.429935273698	-1.615727411272	1.305736291933
H	2.443580873249	0.660254857387	-2.179755509623
H	4.776077809649	0.933611292967	-1.848370137362
H	5.974178445546	0.270560979874	0.200904162156
H	0.121589825954	0.208576786258	-2.148988076971
H	5.259447982397	-1.482371489854	1.644428962236
H	1.542159189053	-2.372974778949	-0.265964935195
H	3.400312482865	-2.857732354384	1.435529023039
H	3.845761034675	-2.596890935037	-0.234949814344

TpRh(CNMe)-Cycloheptane product-(3)

G = -1219.237918

B	-2.387022081859	-1.278846763320	0.722685834747
H	-3.213581121293	-1.993461434018	1.207336114419
N	-1.764953069603	-0.380653775556	1.800945729411
C	-2.004250339166	-0.319124108495	3.120826526883
C	-0.449302417687	1.133168583294	2.578585678324
C	-1.179070843654	0.645067636410	3.667958825263
H	-2.744787100893	-0.965915222659	3.573692546821
H	0.325142007719	1.890996907553	2.543359916230
N	-3.018499903827	-0.396654181130	-0.368888828346
C	-4.294284004849	-0.326399674884	-0.782636238467
C	-3.048666687517	1.022961373063	-1.984885691686
C	-4.366212652743	0.579772944603	-1.822903002646
H	-5.056990143127	-0.930444853789	-0.308020332065
H	-2.636438443190	1.730865258828	-2.693937788939
N	-1.280193568644	-2.120652467830	0.062772670230
C	-1.205265734482	-3.449994808384	-0.107013715704
C	0.434361397477	-2.477950778428	-1.196809318564
C	-0.112987098652	-3.730605460980	-0.905569620558
H	-1.941176682175	-4.099168338024	0.349716674052
H	1.290986732924	-2.210404490712	-1.802870243217
N	-2.249365551486	0.430783023571	-1.107744795981
N	-0.269409733932	-1.522231341126	-0.604594330449
N	-0.811357885499	0.510495858805	1.464789071434
Rh	-0.137674192566	0.549676567678	-0.600292417155
C	0.000318315830	2.431552804668	-0.757321061493
N	0.118250110336	3.585461002455	-0.864637410677
C	0.269658594187	4.974507415168	-1.023714471427
H	-0.559936462656	5.501456260596	-0.539088454372
H	1.211737334313	5.302733783195	-0.570520371832
H	0.281010751456	5.232149590914	-2.088912328694
H	-1.114909689395	0.948417275964	4.702397869936
H	0.233600541988	-4.699043055962	-1.233788224931
H	-5.240881714165	0.870456884829	-2.385665564567
C	2.164752981376	-0.544906155260	1.079282043070
C	3.208911257366	-1.603921634593	0.713069694998
C	4.662136091612	-1.134528552035	0.779522970918
C	1.849612184554	0.579754002064	0.054200009686
C	5.123163175089	-0.312883812766	-0.416365687987
C	2.857202552376	0.714883712029	-1.089322583333
C	4.316562372903	0.954014621056	-0.674156291446
H	2.503117435377	-0.086411394523	2.024850586547
H	3.011512414329	-2.027665168930	-0.282815985760
H	4.803855651517	-0.549124002665	1.703436265909

H	5.077511807515	-0.944230205383	-1.319773409380
H	0.332895366423	0.493214051757	-2.079481263129
H	2.813036807703	-0.163099227755	-1.756108817887
H	1.240177875321	-1.070532928982	1.350697164644
H	3.085099684198	-2.441247177080	1.415790275461
H	5.320827859184	-2.010656069566	0.873418598259
H	1.931757618104	1.528596420524	0.619303337753
H	6.183712963533	-0.051355075490	-0.284011099488
H	2.530499944098	1.556975414387	-1.716528889906
H	4.824084550669	1.526075123354	-1.465610271823
H	4.338105743580	1.595913643564	0.223366106908

TpRh(CNMe)-Cycloheptane product-(4)

G = -1219.232571

B	2.897254846721	0.179728314739	0.535222933311
H	4.046678809189	0.314803733407	0.834736500487
N	2.170496985598	-0.663863801134	1.585054682080
C	2.632490635435	-1.243058631897	2.704525997716
C	0.478818479096	-1.619055544557	2.504275721156
C	1.576748840671	-1.875154661435	3.333052871989
H	3.677723646527	-1.159066631277	2.973291073597
H	-0.557757907410	-1.914215018367	2.616942601947
N	2.785496680876	-0.502819648837	-0.838775886143
C	3.743905672961	-0.961146610869	-1.659490466000
C	1.776600072140	-1.215121301184	-2.600074405248
C	3.142246436177	-1.435653531013	-2.809565586091
H	4.784874059712	-0.911008128495	-1.366623165026
H	0.931647113287	-1.422236125786	-3.245947521435
N	2.218261526336	1.556066298887	0.424218635704
C	2.809115815339	2.759986754826	0.450733341332
C	0.718519823331	2.985600380799	-0.168836922843
C	1.882495728758	3.714614781338	0.082716843579
H	3.852114290836	2.845546388120	0.727173994285
H	-0.248356538673	3.333052356606	-0.504402012506
N	1.575967538126	-0.653975272287	-1.414478531405
N	0.922451196702	1.690240512359	0.047395453078
N	0.849050379036	-0.891651397569	1.457581380011
Rh	-0.181836078797	-0.068625675936	-0.291218464045
C	-1.046250422263	-1.688175610711	-0.735082639104
N	-1.484951003122	-2.724293186082	-1.036222516270
C	-2.175822586733	-3.907627669687	-1.351729431736
H	-3.247564868625	-3.770203298005	-1.161307880897
H	-2.030230781849	-4.160101868121	-2.407978149115

H	-1.806270555814	-4.735211314594	-0.736219296829
H	1.597509624684	-2.434464904797	4.256608739747
H	2.024977906354	4.782074778651	0.006151414261
H	3.621959854122	-1.868379467996	-3.674931304469
C	-1.761458316170	0.543717653820	0.945215897299
C	-2.899685634083	-0.449955915415	1.236648539467
C	-3.980171492697	-0.700582850905	0.183002572664
C	-2.341778269540	1.950416997765	0.746826172886
C	-4.696984816622	0.530746692929	-0.369607210248
C	-2.884195266657	2.355651878975	-0.624694634952
C	-3.813283481516	1.349904503842	-1.309142688200
H	-0.873693297156	0.564395762380	-1.524204071261
H	-3.422623117433	-0.090228221561	2.143731517198
H	-3.559934457252	-1.238017198893	-0.680000844348
H	-5.081051599530	1.155611685989	0.452203466336
H	-3.160033258643	2.072624542991	1.481107531723
H	-3.420018345083	3.309671444409	-0.496908137642
H	-1.211759978842	0.605462747475	1.902487263020
H	-2.477683151559	-1.428383648125	1.520965154688
H	-4.724024233126	-1.379962747066	0.628578279424
H	-1.597495763075	2.697058113695	1.052973900529
H	-5.582824709248	0.187338184631	-0.923494510906
H	-2.053971137118	2.566299479273	-1.314243664416
H	-4.438151373077	1.890713892254	-2.034099232780
H	-3.210122520301	0.644856002437	-1.900613305598

TpRh(CNMe)-Cycloheptane product-(5)

G = -1219.238942

B	-2.591505638419	-0.816320314397	0.937628369837
H	-3.522256630271	-1.309143733897	1.503023565051
N	-1.604776200139	-0.228762224881	1.955233189122
C	-1.653928851202	-0.219048468562	3.297015751873
C	0.179247845399	0.776785710788	2.612859525151
C	-0.523458313663	0.420068611154	3.768932140745
H	-2.490157746684	-0.668568855004	3.817068355593
H	1.128670817512	1.289093584074	2.509100877435
N	-3.072140924263	0.299168246097	-0.007206185120
C	-4.311400632702	0.768954016867	-0.223530714351
C	-2.887777273708	1.793768177389	-1.543138985611
C	-4.244581565756	1.739139489021	-1.204914365433
H	-5.150908581502	0.374053696847	0.334261731851
H	-2.379023894380	2.407736858053	-2.276652488492
N	-1.870490913529	-1.872203100516	0.082412720787

C	-2.230962539474	-3.136823176870	-0.184652403502
C	-0.508295276805	-2.586691410901	-1.428782924991
C	-1.378848497905	-3.642612416194	-1.147869138693
H	-3.072561767646	-3.582644359965	0.329651160906
H	0.317974086345	-2.528836220217	-2.126502926191
N	-2.194727619613	0.925330018171	-0.818589160956
N	-0.807676707010	-1.532715965423	-0.680122941621
N	-0.480591551351	0.382470366029	1.531024742839
Rh	-0.092499921498	0.422779818925	-0.610227245725
C	0.548589386664	2.201072982522	-0.708165408546
N	0.984332342755	3.278390858345	-0.785584934091
C	1.516707137394	4.574111681754	-0.911029038629
H	1.514525757604	4.881037095548	-1.963116533067
H	0.917042922624	5.284878541606	-0.331476728201
H	2.547229038824	4.592488353355	-0.539350760997
H	-0.248421208155	0.600837178942	4.797473209971
H	-1.387177569946	-4.630124728941	-1.584345740434
H	-5.058204641517	2.315376872597	-1.619885512144
C	1.899137541830	-0.089449203368	-0.237824790773
C	2.025465718270	-1.473394740057	0.412142265875
C	3.316368677980	-1.734611475570	1.188103515031
C	2.845328126715	0.045897361606	-1.442205144019
C	4.619079870511	-1.536898482429	0.414567102250
C	4.277854599475	0.506379324360	-1.135989195010
C	4.932471674468	-0.068835742413	0.122478351982
H	2.223346351955	0.649145163510	0.524598027063
H	1.933684948390	-2.243341867130	-0.369899860278
H	3.341838543373	-1.077055349290	2.074039699059
H	4.594024032215	-2.115445105146	-0.523708444024
H	2.875027479356	-0.925750975306	-1.963387278163
H	4.908330666929	0.274775184101	-2.008820116872
H	0.148836227127	0.353999458405	-2.142476891202
H	1.184631153644	-1.647658058208	1.099974505911
H	3.280833700968	-2.763220256466	1.578971135593
H	2.435940682794	0.745475846545	-2.182299335428
H	5.440541086613	-1.963504021463	1.007925177469
H	4.287352047258	1.605294759001	-1.052903911144
H	6.019716526203	0.071430185449	0.038520498431
H	4.629327475943	0.521021811555	1.001527483887

TpRh(CNMe)-Cycloheptane product-(6)

G = -1219.240086

B	-2.410123235085	-1.233120570400	0.830055648738

H	-3.243945679327	-1.910560449158	1.354092339281
N	-1.661911018085	-0.403747804731	1.882718291531
C	-1.812217574988	-0.361190140892	3.216442862379
C	-0.211063934239	1.010928898971	2.604458482282
C	-0.897106055387	0.538704634565	3.728739828159
H	-2.559627955745	-0.974849639512	3.702833456349
H	0.603353952926	1.723056138510	2.535673147590
N	-3.059516327600	-0.285040450245	-0.193210874269
C	-4.353412342715	-0.122876118765	-0.514076754380
C	-3.107896701895	1.174738961603	-1.772246815645
C	-4.437294730627	0.812753429056	-1.527142249678
H	-5.119360129754	-0.689271045879	0.000090992059
H	-2.699799408532	1.872531267008	-2.493603294946
N	-1.404967759213	-2.120052531081	0.074235709345
C	-1.437862122119	-3.442713813589	-0.149183208603
C	0.205117072616	-2.545932686161	-1.296253912419
C	-0.415642970495	-3.766923826394	-1.021164193175
H	-2.191098455577	-4.056458598033	0.327794386222
H	1.051478211911	-2.318406387045	-1.933389682104
N	-2.290700826284	0.509848278245	-0.966385471132
N	-0.392349086802	-1.567173895303	-0.628880115502
N	-0.680138779652	0.438122439605	1.503438790054
Rh	-0.147829270321	0.496305556393	-0.603455114805
C	0.083980325703	2.371143057229	-0.728969426494
N	0.258160999171	3.519471964698	-0.817324386245
C	0.482522731404	4.900501224251	-0.959159984549
H	0.651188115305	5.357507367428	0.022328606625
H	1.363223902432	5.074036328409	-1.587775908094
H	-0.386992453665	5.376778068435	-1.426023472445
H	-0.748465225844	0.812064034531	4.762854416567
H	-0.158601186332	-4.743463808250	-1.403302750469
H	-5.327690530302	1.173236649462	-2.020579723031
C	2.242865206927	-0.834557424907	0.718784615399
C	1.876443521706	0.409176504376	-0.106436276049
C	2.804858398106	0.633753958299	-1.299766731683
C	3.528105040901	-0.670219412333	1.544106293555
C	4.311533688982	0.660905107148	-1.012176149377
C	4.821131608390	-1.077633379174	0.832774255478
C	4.894151234542	-0.707057107832	-0.650147169497
H	2.340041931747	-1.717310695391	0.068297246570
H	2.032983218188	1.267514135812	0.580450925133
H	2.621754086341	-0.150895558259	-2.054598205253
H	4.533280535091	1.391503921435	-0.216219882829
H	3.600194715366	0.381217156870	1.863950571238
H	5.672093364992	-0.623556438604	1.362963828095
H	1.415975826325	-1.067693290801	1.403558726491

H	0.213008575510	0.452823823121	-2.113239134345
H	2.521777594750	1.576604382351	-1.792933154636
H	3.451399272495	-1.252297064431	2.474015622670
H	4.821518892990	1.034750078357	-1.912567175742
H	4.961222281495	-2.165130085303	0.925670000080
H	5.944871837494	-0.765136412865	-0.967818196426
H	4.367071616778	-1.468085730831	-1.247029628069

TpRh(CNMe)-Cycloheptane product-(7)

G = -1219.232637

B	-2.865692153105	-0.665056737224	0.444173768747
H	-3.976848685473	-1.024568691359	0.699312945783
N	-2.302094527524	0.175608140085	1.592836536221
C	-2.877623728770	0.570476622532	2.739819231960
C	-0.837405349031	1.371585518776	2.615842398468
C	-1.970745455757	1.346578078530	3.435974349590
H	-3.889195654645	0.267099048447	2.977457469802
H	0.120475180917	1.855554677758	2.769734344934
N	-2.862512109251	0.175374186349	-0.846000493126
C	-3.879263983361	0.559916913559	-1.633610668343
C	-1.976161415066	1.235334547246	-2.494528275334
C	-3.358457315858	1.251937413963	-2.710568369833
H	-4.899162150671	0.308087467993	-1.372188817779
H	-1.174038158349	1.649761152226	-3.093592584707
N	-1.960917271444	-1.883457522844	0.191705927394
C	-2.339207751090	-3.156841916489	0.001654189325
C	-0.237328116764	-2.924866199978	-0.580026097068
C	-1.261741779338	-3.869348260017	-0.486587892904
H	-3.353736319899	-3.460314935856	0.225843869773
H	0.781419713294	-3.041165698773	-0.927572773409
N	-1.691333882863	0.585313008119	-1.373343218540
N	-0.660902876346	-1.737406129337	-0.160542925740
N	-1.049611369872	0.665032726359	1.512729029336
Rh	0.134905261628	0.201816125515	-0.260393651981
C	0.753781602265	1.962433462945	-0.562535433957
N	1.097747262196	3.048568961043	-0.802752906117
C	1.663750704497	4.313173809697	-1.041918839422
H	0.928802714335	5.100518861664	-0.841531652246
H	2.532160088360	4.459484541497	-0.388169149060
H	1.989556757621	4.387641335319	-2.085666164752
H	-2.107928230519	1.820406824036	4.396645385193
H	-1.220802482516	-4.918651390060	-0.737604892423
H	-3.898512891697	1.694267986165	-3.534553364379

C	2.980737653457	0.820766939461	0.865135244731
C	1.813548970280	-0.177141710298	0.957296178064
C	2.350166794350	-1.608205241461	0.949259726993
C	3.675351290095	0.906774807154	-0.500893392305
C	3.209887951996	-2.022440088820	-0.250098641261
C	4.850067873956	-0.052424140599	-0.705513109283
C	4.642080382721	-1.480194427913	-0.184816886663
H	3.738061478072	0.560081641030	1.629476673057
H	0.939849693130	-0.205118837917	-1.522701092052
H	2.980311999178	-1.741510290561	1.849640978724
H	2.728182662634	-1.716641727204	-1.192904007609
H	2.927793286906	0.724928229903	-1.283321857189
H	5.075500031738	-0.087116369720	-1.782003244850
H	2.622405072304	1.819992343947	1.156308462297
H	1.377151458811	-0.040313473672	1.962568794865
H	1.522835519972	-2.312685746734	1.084777403472
H	4.045191621387	1.930618202355	-0.671216882087
H	3.263962378982	-3.121777201867	-0.274177507932
H	5.751486908142	0.361438113513	-0.228736342147
H	5.316938864014	-2.147390220835	-0.739573037541
H	4.972369481972	-1.539665727650	0.863508263311

TpRh(CNMe)-Cycloheptane 1,2-migration-(1/2-ie)

G = -1219.202871

B	-2.819212190968	-1.008873383321	0.004139424518
H	-3.890793669345	-1.540580364323	0.096808337235
N	-2.039359619689	-0.915790707689	1.318212837264
C	-2.062000283079	0.068242481267	2.240668275276
C	-0.711017388463	-1.540484979316	2.861969017833
C	-1.211483051822	-0.290325657595	3.265015585747
H	-2.666987252541	0.955557682286	2.094928513000
H	-0.013390880207	-2.191631212823	3.377663596174
N	-3.041344509214	0.426122280369	-0.531047844428
C	-4.196912870213	1.080276403256	-0.723154525626
C	-2.524352766875	2.386259557746	-1.285821005493
C	-3.917947112976	2.345680105770	-1.203164822545
H	-5.136039189473	0.590168143427	-0.501180196881
H	-1.867106409598	3.176575810407	-1.625454106167
N	-1.963292360775	-1.770275035049	-1.013662600152
C	-2.155739527831	-2.967815217518	-1.576820444303
C	-0.225866828865	-2.154222842661	-2.228411309927
C	-1.062413611915	-3.261636559267	-2.372211982858
H	-3.055483839304	-3.529931641733	-1.363096058428

H	0.736273444465	-1.948675392087	-2.683618911224
N	-2.010074671415	1.228160707815	-0.879455663263
N	-0.776369096774	-1.265726974374	-1.403146791958
N	-1.210174729307	-1.913574590664	1.691645893812
Rh	-0.133885870399	0.570972026489	-0.696067224298
C	0.436690301930	2.256922689766	-0.056834601018
N	0.783410062745	3.301058941035	0.342599952237
C	1.191367687727	4.518930388481	0.912324339489
H	1.797040064446	4.334899208027	1.807764026716
H	1.786680069046	5.096523677591	0.195275319044
H	0.314223076235	5.110804455765	1.198555963752
H	-0.990800997543	0.265824455676	4.165050377409
H	-0.897233244282	-4.145699279189	-2.969429650213
H	-4.619855742106	3.123298285002	-1.464671012678
C	4.141643600011	-0.781082029055	-1.269015432950
C	5.319022052877	-0.210307581494	-0.478367040012
C	5.410034509729	-0.639292052935	0.982548944127
C	2.793230021937	-0.209168069242	-0.819581330106
C	4.149556595462	-0.433468484437	1.824566946711
C	2.106724268236	-0.972884475222	0.316121381945
C	3.018611530476	-1.401489859357	1.470566521222
H	4.128704365861	-1.880734456958	-1.199120979550
H	5.258330600945	0.889356054653	-0.528711186103
H	5.674880026222	-1.708324764555	1.027275130321
H	3.802492547821	0.610049766234	1.748126404308
H	2.950169517807	0.840708771143	-0.525540294693
H	1.293748060588	-0.351257687809	0.755021769731
H	4.296841860284	-0.547231794758	-2.331142624906
H	6.259328612405	-0.481932811328	-0.979493197678
H	6.250531824215	-0.103262075672	1.446776021406
H	2.107344700647	-0.161924975005	-1.686499821137
H	4.419834816906	-0.579592018075	2.879509640017
H	1.600750330503	-1.864960810870	-0.077544391547
H	2.383530523241	-1.578285427026	2.348584148393
H	3.468121172212	-2.378012890795	1.232140232455

TpRh(CNMe)-Cycloheptane 1,2-migration-(1/2-ii)

G = -1219.202927

B	-2.919441296663	-0.720552361272	0.207324191635
H	-4.044165108536	-1.085046800787	0.412574472461
N	-2.087418873088	-0.482735404315	1.471183330208
C	-2.023915722415	0.633481716499	2.225609952272
C	-0.715402038951	-0.922686180810	3.040722235484

C	-1.143071821753	0.398194282011	3.260128622104
H	-2.597270491561	1.515698900705	1.965461933871
H	-0.019967700781	-1.517766561810	3.622875930121
N	-2.985407639194	0.611512303973	-0.579472310303
C	-4.056941156586	1.361308298241	-0.878250179849
C	-2.252142869930	2.333977870323	-1.664205960728
C	-3.637843505882	2.481074611043	-1.571470328056
H	-5.042927050031	1.037716565302	-0.570654737493
H	-1.511641868048	2.966835608704	-2.136459374810
N	-2.204125940122	-1.754941710271	-0.667340741284
C	-2.564981309604	-3.000392163461	-0.995267230922
C	-0.597656067228	-2.557747839632	-1.858775712017
C	-1.562046514706	-3.561922835555	-1.765078750365
H	-3.509845081624	-3.400235426695	-0.650926285273
H	0.350568231770	-2.552524624167	-2.382923386830
N	-1.873516829557	1.208018388477	-1.064558400452
N	-0.992884511910	-1.477123040363	-1.189394941018
N	-1.285266037444	-1.449496633505	1.965410338942
Rh	-0.095494350902	0.347935817386	-0.803341756314
C	0.685373472564	2.020584215103	-0.392255431821
N	1.145685084961	3.062610340621	-0.123665172582
C	1.710336039578	4.264070221552	0.336206521627
H	0.988113517786	4.805616167588	0.958346887573
H	2.602674495579	4.052639159803	0.937785871679
H	1.997634203721	4.901624323779	-0.508220494920
H	-0.858577694546	1.076384137939	4.052210192691
H	-1.535485121196	-4.550862673874	-2.197304188954
H	-4.245913430537	3.283656483284	-1.961093673278
C	5.130853171041	-1.360678366388	-0.099625276147
C	5.289679967426	-0.524973311598	1.171773956139
C	4.052172216469	-0.413994688489	2.056695939814
C	4.240558956573	-0.701154159611	-1.158187710183
C	2.778181074105	0.041253001406	1.346739208797
C	2.744219397590	-1.000468832043	-1.036558536698
C	2.211315154706	-1.022865086626	0.402993941872
H	4.751575492910	-2.365238592125	0.148384917145
H	5.609106068177	0.487048961588	0.872146602419
H	3.851693627972	-1.391546466404	2.524286680043
H	2.966797237410	0.978756133237	0.798369725914
H	4.401731352314	0.387051405934	-1.112082840437
H	2.203774654235	-0.258761181533	-1.652502692088
H	6.129873381366	-1.518049178212	-0.528928126820
H	6.114177302408	-0.933412534649	1.773735128520
H	4.277080418317	0.273905249363	2.884710438815
H	4.567787627286	-1.001868499363	-2.162741407413
H	2.012656289168	0.280622792147	2.098528051036

H	2.529827358845	-1.976227049586	-1.496687836144
H	1.102380685545	-0.990628267048	0.432683984437
H	2.414892092974	-2.012215855819	0.841901827578

TpRh(CNMe)-Cycloheptane 1,2-migration-(1/3-ii)

G = -1219.201277

B	-2.931909505818	-0.574969505312	0.036562119284
H	-4.093293539885	-0.868594729600	0.107839739009
N	-2.300270669510	-0.151766175612	1.363619366216
C	-2.263773010735	1.078749145247	1.915249701216
C	-1.287708512398	-0.382294968048	3.223599406242
C	-1.612451167358	0.981783198804	3.126719158702
H	-2.689174609656	1.933166190727	1.401797649166
H	-0.770264732213	-0.902300010112	4.022325774294
N	-2.798522679850	0.604719035059	-0.958419846265
C	-3.763612419225	1.321222616289	-1.553887594537
C	-1.803464245738	2.075873447450	-2.194909669250
C	-3.175443178721	2.281490846625	-2.355324002700
H	-4.802998600198	1.090806329219	-1.358781657257
H	-0.961823917346	2.587595184760	-2.643849074914
N	-2.148398541392	-1.760626373966	-0.536367892818
C	-2.551291616408	-3.010844059278	-0.785809630455
C	-0.451315233667	-2.787745175256	-1.377515775233
C	-1.491627169290	-3.715661408701	-1.328544596337
H	-3.564817265169	-3.310817153257	-0.553405296609
H	0.560261701386	-2.902498793851	-1.747274753309
N	-1.591484547866	1.066310370801	-1.354348924741
N	-0.854703184050	-1.615495028384	-0.890142211743
N	-1.702503284194	-1.061069613768	2.163129310347
Rh	0.068645144250	0.227188664925	-0.642663440271
C	0.853554512800	1.928166851191	-0.382396962827
N	1.330345284353	2.979810839032	-0.194212595567
C	1.939367708361	4.199004135772	0.146382354961
H	2.783977489390	4.016334323318	0.822416195336
H	2.311250296312	4.706252484542	-0.751714272532
H	1.219573079710	4.854180431206	0.650961574601
H	-1.407628430309	1.775109816282	3.831541410303
H	-1.475877589894	-4.748067315833	-1.643838575159
H	-3.666492264902	3.018548617292	-2.972854465837
C	3.800916486531	-2.336541037698	0.343248576436
C	4.769291873504	-1.545916781221	-0.533519557960
C	5.124600674245	-0.151300820883	-0.030802884455
C	2.384148103183	-1.756989882417	0.372574894780

C	3.933924131425	0.770435792642	0.239729242593
C	2.145149003885	-0.698279260048	1.448983042237
C	3.175116598167	0.439338569799	1.528231754278
H	4.190325846984	-2.406310711346	1.372614202237
H	4.327751974915	-1.460155206529	-1.540131463921
H	5.716192959763	-0.236811885009	0.895418563538
H	3.256728975003	0.766351113883	-0.629085687534
H	2.167516596435	-1.347769709328	-0.634726270317
H	1.124777412022	-0.277991751764	1.338919245229
H	3.760205771708	-3.367918545571	-0.033427151938
H	5.698100697589	-2.120518338709	-0.659619007575
H	5.787633273068	0.322141531471	-0.769194062137
H	1.648192865476	-2.556439790139	0.528977806098
H	4.310791253358	1.801588503478	0.317336288914
H	2.097219630390	-1.204691358764	2.424187750503
H	2.659262867553	1.338893244218	1.894220781812
H	3.923795164027	0.201758796373	2.299558895867

TpRh(CNMe)-Cycloheptane 1,2-migration-(1/3-ie)

G = -1219.203883

B	-2.896978864946	-0.872190635733	0.061755244116
H	-4.006180813938	-1.320232234301	0.155382590892
N	-2.097754834287	-0.869575885126	1.367711317978
C	-2.055268117179	0.085665264044	2.319251785993
C	-0.775364331652	-1.605492515462	2.867083257070
C	-1.206545477536	-0.345451621035	3.316537365978
H	-2.617087934081	1.006085691703	2.210979599010
H	-0.099922558460	-2.303908778854	3.349117717785
N	-3.011900477692	0.589287515324	-0.435587150013
C	-4.114410703010	1.336237063071	-0.598477884863
C	-2.349154290285	2.525671890385	-1.135650480953
C	-3.741157711993	2.590422403431	-1.042788832102
H	-5.087326082945	0.913877172329	-0.382886950229
H	-1.634654848391	3.273080630006	-1.456144955112
N	-2.114443288959	-1.671944776812	-0.985100779970
C	-2.403692910258	-2.837353026856	-1.573968636157
C	-0.425857376975	-2.155057059752	-2.233364334191
C	-1.345494959847	-3.192555322835	-2.391613498817
H	-3.340645617603	-3.335367049149	-1.361252156489
H	0.543808539934	-2.009812544349	-2.695991164417
N	-1.923650584407	1.319586207804	-0.768178084568
N	-0.897998044185	-1.248896035583	-1.379808431431
N	-1.313010491579	-1.918068371621	1.696030070206

Rh	-0.103945915365	0.508429530575	-0.631219074553
C	0.606642114323	2.119112829422	0.060544786264
N	1.040297072145	3.115913356358	0.494011392827
C	1.580464197573	4.261932254738	1.100708418085
H	1.417377165848	5.142492355404	0.468228989271
H	1.108569355101	4.434079901357	2.075499139537
H	2.659218018766	4.133125154404	1.249280694869
H	-0.942719668641	0.171598012417	4.228187637756
H	-1.255199106447	-4.071424793825	-3.012093257834
H	-4.382109492188	3.427831605151	-1.274459874494
C	2.722664860177	-0.480443667769	-1.025611051604
C	3.681256584119	0.655985768582	-0.656203441696
C	5.117840860136	0.178841906031	-0.442972013672
C	2.062538400480	-1.197520065043	0.160352445009
C	5.355101507392	-0.657159483295	0.810429980031
C	2.986673867594	-1.457904535195	1.353184238092
C	4.423635369609	-1.855182632568	1.002017529423
H	3.279644963696	-1.220175336028	-1.622840231233
H	3.316892574293	1.181016302741	0.242027608208
H	5.417173316294	-0.404263293520	-1.329109259536
H	5.258945750649	-0.009817802692	1.697604684733
H	1.200923384763	-0.630327557545	0.583752410850
H	3.024933969298	-0.560833377871	1.990476852485
H	1.950910764123	-0.097523283571	-1.719626408376
H	3.677914725779	1.402699893599	-1.462417759916
H	5.791340873314	1.047780947964	-0.414987789632
H	1.624435102422	-2.142615122838	-0.188290752429
H	6.398662511606	-1.003462988707	0.803563030442
H	2.518463580435	-2.234105572914	1.972414973991
H	4.826619580832	-2.470883126427	1.817780563970
H	4.439386822659	-2.499492383345	0.108157458954

TpRh(CNMe)-Cycloheptane 1,2-migration-(2/5-ii)

G = -1219.203495

B	-2.446618026881	-1.274164037298	0.096256914577
H	-3.379908013407	-2.027977438579	0.128811746310
N	-1.845277082375	-0.951387140909	1.464652852096
C	-2.206209925276	0.021289823325	2.326571940890
C	-0.554378165341	-1.161327480001	3.146289959948
C	-1.394059050509	-0.072521533849	3.436798675257
H	-3.000791457586	0.716679188990	2.082345110592
H	0.238663349342	-1.588607902696	3.750450022334
N	-2.925677046626	0.052147028252	-0.542040822190

C	-4.170753125473	0.429697326624	-0.869044983133
C	-2.773791170203	2.056403559221	-1.342642328703
C	-4.126522445361	1.711510414054	-1.383983922347
H	-4.998793212194	-0.248299864099	-0.707422301413
H	-2.272654646073	2.961861488989	-1.660226574943
N	-1.358185763826	-1.867372912719	-0.806764866074
C	-1.267800297082	-3.091089090493	-1.338019352795
C	0.447283106112	-1.886417941015	-1.982790228787
C	-0.117208138648	-3.155965913765	-2.103870015041
H	-2.030025524497	-3.830515466771	-1.129373071844
H	1.346436789696	-1.487877736769	-2.436049632867
N	-2.064232628656	1.051621905477	-0.835054530023
N	-0.301698200855	-1.120275686410	-1.190492694714
N	-0.829604924041	-1.688350218091	1.961140369959
Rh	-0.118263593103	0.820690197850	-0.476564257851
C	-0.007237895043	2.577842316958	0.212652735693
N	0.038025890041	3.661789122095	0.651160560244
C	0.083228152513	4.916767985716	1.281705034451
H	0.526037858956	5.665068975300	0.613872108410
H	-0.930338920710	5.238269334760	1.548004955825
H	0.684606858151	4.859058928026	2.196762592663
H	-1.409009390894	0.549866457915	4.320209586371
H	0.253370981193	-3.995636784107	-2.672343563282
H	-4.950978586136	2.307633056393	-1.745418532021
C	2.933821578719	0.533859175888	-0.450488653742
C	4.455303925207	0.701797728088	-0.491030933374
C	5.257461379504	-0.576241305378	-0.704463704350
C	2.422031883548	-0.109696808040	0.846554178004
C	4.982418387836	-1.703411437469	0.288533324425
C	2.478901230479	-1.640711543022	0.937011094238
C	3.589272149957	-2.320029051167	0.140327695516
H	2.603644565598	-0.034417784034	-1.334602976735
H	4.768542481588	1.175269522360	0.454010201168
H	5.059758410069	-0.957645544303	-1.719967764853
H	5.125594938906	-1.340861835402	1.320131824011
H	2.990328963050	0.344008416208	1.674377041426
H	2.581924201426	-1.913051306276	1.997830163279
H	2.494347144675	1.539189306459	-0.554835061409
H	4.716912528097	1.413453385214	-1.287433510071
H	6.326867906035	-0.320505616588	-0.682461505736
H	1.374964646755	0.188048061435	1.073482209183
H	5.741840925385	-2.483007816092	0.136608463479
H	1.511427583326	-2.057847539864	0.628875400069
H	3.616060169598	-3.376245520134	0.441735200112
H	3.324800453874	-2.332878593551	-0.930007766891

TpRh(CNMe)-Cycloheptane 1,2-migration-(5/7-ie)

G = -1219.201660

B	-2.404585463844	-1.337860784759	0.452676822323
H	-3.262139629748	-2.152931417349	0.648044895254
N	-1.639985753064	-0.945341827762	1.716644575582
C	-1.753109870280	0.164794997394	2.475860465657
C	-0.372179171588	-1.263124547699	3.399970294477
C	-0.942968120699	0.008005567632	3.580680554017
H	-2.391183073190	0.986495496745	2.173217460226
H	0.323370786385	-1.790563827146	4.043500321789
N	-3.073704029796	-0.074611397747	-0.141283140245
C	-4.383627245801	0.199616809943	-0.238521430672
C	-3.233497932085	1.875049168761	-1.069527149821
C	-4.537924751353	1.441422589460	-0.824368647357
H	-5.110774993750	-0.517523101567	0.119584179525
H	-2.873593164237	2.785959052704	-1.530473770429
N	-1.430642604313	-1.894709270436	-0.596597085825
C	-1.367316911587	-3.116582511795	-1.136051276453
C	0.125242174291	-1.821891769015	-2.087919124806
C	-0.375316172272	-3.123029880313	-2.101289614565
H	-2.031675390754	-3.896959664441	-0.788253970919
H	0.904230773731	-1.373626497533	-2.693325454158
N	-2.364272735129	0.956460552420	-0.655524384790
N	-0.508662658376	-1.093027565390	-1.170183439450
N	-0.791296220453	-1.833724785079	2.278272625598
Rh	-0.376852344073	0.897126374329	-0.618963566948
C	-0.288691354858	2.720624973411	-0.116230832606
N	-0.248804440245	3.844611498375	0.206704418954
C	-0.179331703285	5.174016696160	0.656873819030
H	0.606930519416	5.276130666249	1.414162348643
H	0.043394405248	5.849477735098	-0.177609551575
H	-1.136118459813	5.468641381401	1.103300432329
H	-0.793723074295	0.703961179083	4.393943404044
H	-0.063697446254	-3.947967144414	-2.724188936219
H	-5.459901268488	1.955216262892	-1.051592327627
C	2.813773548585	-0.502116404544	-0.141505454720
C	2.166582684888	0.217974664563	1.044324892158
C	2.898094597628	0.114223355501	2.379407984258
C	2.733513173894	-2.026597406980	-0.028737064600
C	3.262679526785	-1.303900332008	2.819082866812
C	3.890044192761	-2.682882288300	0.729605308383
C	4.372574390335	-1.933071825226	1.973241046184
H	3.858034498830	-0.173152349179	-0.272468915148
H	1.150701283287	-0.193795161972	1.185386115400

H	3.825378405375	0.709830758677	2.336429091249
H	2.366463617005	-1.942935834148	2.803788015870
H	1.772615664136	-2.282223797646	0.447320900703
H	3.577774086469	-3.697801277235	1.015814119213
H	2.295656416985	-0.184562278958	-1.063244245748
H	2.051746882588	1.289732715427	0.807881715294
H	2.264110145463	0.582103630531	3.146574074737
H	2.687963311178	-2.474313901155	-1.030940510170
H	3.589126348233	-1.259636543952	3.867640602883
H	4.745090115161	-2.814537731927	0.049537396444
H	4.963113203313	-2.628026000851	2.586024400199
H	5.074819691662	-1.137526710227	1.677838567619

TpRh(CNMe)-Cycloheptane 1,2-migration-(5/6-ii)

G = -1219.202808

B	-2.413055686572	-1.441692575266	-0.085678254052
H	-3.306554384514	-2.242414580677	-0.079514537990
N	-1.723065526136	-1.246265407210	1.267454323888
C	-2.032859895666	-0.375999945506	2.250287468729
C	-0.305825031689	-1.597979366946	2.818899280475
C	-1.137828618250	-0.564146167926	3.282276005498
H	-2.853612854964	0.322767970726	2.138025354512
H	0.533748821069	-2.070562751761	3.317708606470
N	-2.994103139455	-0.079917517623	-0.538196695666
C	-4.275935016303	0.255225466749	-0.750488450657
C	-2.997888838502	1.994602155981	-1.151754640700
C	-4.331456405890	1.579292543039	-1.141717496214
H	-5.055838571262	-0.481079400659	-0.605368930138
H	-2.566130001244	2.952804900410	-1.411284626522
N	-1.354257353617	-1.870424621940	-1.107259291362
C	-1.196433063142	-3.029832700513	-1.754863718969
C	0.464109390106	-1.683568621765	-2.248240239012
C	-0.037132246923	-2.960032462654	-2.507076714861
H	-1.917940561496	-3.826182399599	-1.626727457683
H	1.349500904735	-1.192820980745	-2.636406731365
N	-2.205141437541	0.989908507240	-0.787913015483
N	-0.334400285686	-1.040146829914	-1.398926050447
N	-0.659728779845	-2.005706366411	1.607892843451
Rh	-0.230223676745	0.837292158561	-0.534730199487
C	-0.156583627211	2.559717757153	0.243456420819
N	-0.126604814387	3.624262485116	0.728582114610
C	-0.084351729725	4.860115499454	1.395550810520
H	0.541445894642	4.785239235793	2.292904685070

H	0.329478653138	5.635247694314	0.739698346419
H	-1.095265700306	5.157651879012	1.697489321694
H	-1.096627910586	-0.036792560737	4.224729013059
H	0.380488049545	-3.719823012481	-3.150416432260
H	-5.207445371221	2.158503758890	-1.392548355105
C	2.261270312297	-0.171007763580	0.464736983494
C	2.836617886949	0.679836660117	-0.673323711560
C	4.026386674002	0.070078930609	-1.409611844059
C	3.184315045439	-0.246672691354	1.684634796784
C	5.183325452128	-0.408603144740	-0.530917291082
C	4.200467088399	-1.389979828661	1.653586497514
C	4.844446154582	-1.655602876578	0.291047739163
H	1.995409399143	-1.180602934030	0.117612461145
H	3.126002060362	1.658263062431	-0.256279299252
H	3.677876949842	-0.792438011870	-2.001548340806
H	5.524405073078	0.406182130139	0.128124190422
H	3.707820186065	0.717388662189	1.780875659857
H	4.985218228645	-1.173892006793	2.393718071919
H	1.306366541269	0.265602606482	0.836951743546
H	2.060418398722	0.909209562623	-1.429419990527
H	4.397371326586	0.806067500347	-2.137411753616
H	2.576848473287	-0.346136005188	2.594300776073
H	6.032818861214	-0.634808277020	-1.190030181659
H	3.713622339019	-2.315257341191	1.993692505315
H	5.751713649998	-2.254136200832	0.450170729966
H	4.177992304619	-2.291298985206	-0.312267749878

TpRh(CNMe)-Cycloheptane 1,2-migration-(6/7-ie)

G = -1219.203945

B	-2.829444114029	-0.746423145946	0.216462357158
H	-3.941942365533	-1.141991784083	0.429118984276
N	-1.886520467333	-0.819503048910	1.420830624095
C	-1.658154027666	0.117953162193	2.363757812939
C	-0.464214850238	-1.676286864149	2.755431539946
C	-0.736744695144	-0.390863842365	3.254407039431
H	-2.153233166183	1.081198339144	2.324109669005
H	0.201020539032	-2.433190659136	3.156836704210
N	-2.923142034862	0.732044031511	-0.232245139727
C	-3.994981277259	1.538786258018	-0.250589575650
C	-2.241466139097	2.649593489591	-0.966253637866
C	-3.608011443393	2.783193513779	-0.710403557046
H	-4.958033267070	1.161629670371	0.068349931648
H	-1.529183486352	3.367266133409	-1.352833766884

N	-2.217669088809	-1.553977961248	-0.933946263792
C	-2.641297099299	-2.680364402980	-1.517152658758
C	-0.726497504658	-2.074789448153	-2.399997735088
C	-1.713697881850	-3.058253877834	-2.471844035177
H	-3.570869205935	-3.137465466166	-1.203873572694
H	0.185038273963	-1.962659721610	-2.975888652752
N	-1.842730280608	1.413954539796	-0.675303509991
N	-1.038206188452	-1.178097763870	-1.466164534616
N	-1.156270567967	-1.931045907058	1.653301457433
Rh	-0.067471817113	0.505060764376	-0.753105133785
C	0.787769969337	2.047690921045	-0.070407040947
N	1.303488570980	3.001285449084	0.370558883593
C	1.944551305459	4.091826364280	0.981608075319
H	3.015542300406	3.883155275080	1.090202686887
H	1.823938930775	4.996356156996	0.373884667991
H	1.518786570807	4.273636921510	1.975614453052
H	-0.329350796054	0.092107932383	4.131206410871
H	-1.749223353650	-3.917130113701	-3.125021571395
H	-4.225302336090	3.658055244774	-0.849467989024
C	2.937226710675	-1.988789137415	0.967413509867
C	1.995651896572	-1.454203193482	-0.111001438284
C	2.665727264860	-0.803492085214	-1.323225659767
C	3.661039264923	-0.881461437757	1.736740042654
C	3.726455044236	0.258871184619	-1.029229144763
C	4.984950541596	-0.418241714386	1.123872964400
C	4.999583149928	-0.316015751522	-0.403158506754
H	3.661473172596	-2.692247793727	0.524428747521
H	1.328767302130	-0.735546548060	0.419061459627
H	3.136956748599	-1.593198401439	-1.932380168764
H	3.307981853730	1.046804385100	-0.383137342049
H	2.969989598165	-0.027681385868	1.827414451158
H	5.246767010618	0.559172632283	1.556466566106
H	2.330044696019	-2.577873785447	1.666932890574
H	1.332193308852	-2.259700144799	-0.452079597792
H	1.894431425775	-0.360103524908	-1.984206376544
H	3.854185449078	-1.206905485098	2.767963829633
H	3.980250022840	0.752856515807	-1.977286502635
H	5.789141801691	-1.102364119895	1.432363365765
H	5.867094616915	0.289204246645	-0.700247294726
H	5.177144844086	-1.311232375572	-0.839024257893

TpRh(CNMe)-Cycloheptane 1,2-migration-(7/7-ii)

G = -1219.203123

B	-2.628500696160	-1.267534194704	0.264792191387
H	-3.598148424963	-1.947942556401	0.456475194941
N	-1.785623153688	-1.000207534018	1.513516093281
C	-1.906820865247	0.002607774668	2.407459431876
C	-0.281106991799	-1.349180716033	2.980912156787
C	-0.947814653626	-0.178531524226	3.381626341401
H	-2.653796909337	0.777237465742	2.278912206980
H	0.543023691871	-1.862182898098	3.464871234532
N	-3.105468582511	0.093188761107	-0.301588303835
C	-4.357292534080	0.557835226061	-0.432182235760
C	-2.944995616742	2.067081263753	-1.173120379374
C	-4.307278888341	1.824180201774	-0.983300403220
H	-5.193791351506	-0.054157414656	-0.120419262432
H	-2.439750909102	2.927479838351	-1.593087397147
N	-1.747675872969	-1.935250749970	-0.796504817960
C	-1.846434456673	-3.146320495026	-1.354607785045
C	-0.137752104582	-2.078424959363	-2.221395133860
C	-0.828840852846	-3.288941488579	-2.280966551781
H	-2.632873710841	-3.823012259262	-1.046741869204
H	0.718010388313	-1.741350357142	-2.793150733685
N	-2.234839129924	1.020420238881	-0.760411725525
N	-0.694301974448	-1.273786140712	-1.317554818598
N	-0.787038511576	-1.840821413205	1.858022856064
Rh	-0.276510875847	0.653373540139	-0.674736044812
C	0.062016609983	2.410137330792	-0.062750925286
N	0.258895127355	3.494804750415	0.330177968231
C	0.495904611594	4.755171828594	0.904376146058
H	1.347788595833	5.241119356053	0.414597302947
H	-0.386813571774	5.394060688456	0.785533645203
H	0.713736468211	4.651585839449	1.974282263336
H	-0.763229672891	0.439122250037	4.249106908920
H	-0.620379960702	-4.142154347374	-2.908754298849
H	-5.135352269272	2.474422776173	-1.222554319148
C	3.217061816789	-0.752159294986	1.444465128391
C	2.383926524692	0.003575505751	0.408640881217
C	2.745985985578	-0.250386691097	-1.052080765240
C	4.652996538882	-0.232167138081	1.551818214918
C	4.215572579297	-0.037131886964	-1.417577170550
C	5.658217959715	-0.851016599379	0.577233439734
C	5.136212973717	-1.115125298179	-0.837151331215
H	3.204900073486	-1.831326543906	1.224685396698
H	2.468189264493	1.080096918547	0.627679823393
H	2.477506144796	-1.287839800687	-1.304880768195
H	4.546696219188	0.965220447123	-1.101094900671
H	4.630200486309	0.860234483581	1.413239348415
H	6.537512626668	-0.192169514433	0.523243498398

H	2.717384761627	-0.639245604949	2.415991308116
H	1.323646422339	-0.277618035959	0.592133565691
H	2.118781641154	0.393345560437	-1.698415829523
H	5.027453332120	-0.386174343335	2.573185089105
H	4.299344717429	-0.048404886289	-2.513025863851
H	6.026080043911	-1.801814971892	0.989828183879
H	6.000675414622	-1.260304458160	-1.499428427224
H	4.591767031477	-2.071766408820	-0.855721557911

TpRh(CNMe)-Cycloheptane 1,3-migration-(1/4)

G = -1219.203506

B	-2.672257679392	-0.619087075801	1.034253974247
H	-3.728067609907	-0.938764656670	1.505852300917
N	-1.576122420191	-0.348022651642	2.066790241805
C	-1.211945385331	0.825071356914	2.624989419313
C	-0.017558942236	-0.820874414039	3.439674484212
C	-0.197890870774	0.570436362006	3.524264442733
H	-1.687283161475	1.754139551029	2.333015964396
H	0.679782923994	-1.450063432643	3.982790124026
N	-2.887639541927	0.669855969806	0.205887217111
C	-3.978921217036	1.447170702801	0.136144439617
C	-2.399646474160	2.303636816523	-1.125759201458
C	-3.714669796750	2.511977059261	-0.704162372196
H	-4.866322536586	1.180510439706	0.695506803223
H	-1.782792291160	2.880880521591	-1.802682488543
N	-2.196125941902	-1.724777388737	0.082545653699
C	-2.666267896527	-2.963730456633	-0.095834276610
C	-0.940556786435	-2.641434668164	-1.411098855105
C	-1.889989060214	-3.597678012330	-1.050056998854
H	-3.517406161769	-3.308494883261	0.476778442095
H	-0.145075477698	-2.694859806855	-2.145312410829
N	-1.914439993051	1.194961983259	-0.572585557703
N	-1.129410461915	-1.521009870706	-0.716063133888
N	-0.847435270194	-1.369652503080	2.563430176100
Rh	-0.133454954114	0.288592882422	-0.682725791043
C	0.762906546262	1.952071810323	-0.609997408708
N	1.316807964882	2.981527852681	-0.548759438750
C	2.051087262138	4.164120321924	-0.357134238044
H	3.073439493834	3.921042040777	-0.041901760895
H	2.096985147314	4.742482454613	-1.287365087106
H	1.580656567524	4.779059484684	0.419081136795
H	0.326115523636	1.281563513935	4.147048380333
H	-1.998745116365	-4.602226565256	-1.430303284229

H	-4.378755611216	3.317431956893	-0.979754820428
C	4.614452147715	0.037790563462	-0.660010916800
C	4.000351190302	0.353589598061	0.706271781391
C	3.307022025547	-0.811102333536	1.401785419016
C	3.611513826011	0.004587117750	-1.814002605425
C	2.172893112457	-1.450342714005	0.613045474674
C	2.667697841067	-1.214864173493	-1.900004190791
C	2.600332740528	-2.131277326227	-0.683455107886
H	5.184453234555	-0.903072159513	-0.607043431728
H	3.276282044933	1.177866769570	0.584403147498
H	4.053522967875	-1.590826845640	1.627570047401
H	1.415742203379	-0.653522383620	0.416296072410
H	3.014486247430	0.926651909513	-1.756643914215
H	1.641605358614	-0.854651066915	-2.117599234789
H	5.355375910501	0.816068789419	-0.893629904186
H	4.786047460531	0.735674030319	1.373972852591
H	2.914646320946	-0.467537286540	2.369516852461
H	4.165066099664	0.081180689219	-2.759674409835
H	1.633636372293	-2.158841430848	1.255109372801
H	2.938709451352	-1.823622342252	-2.774634193549
H	1.898280843303	-2.944322980713	-0.912369174397
H	3.572994847304	-2.622083494714	-0.524895481036

TpRh(CNMe)-Cycloheptane 1,3-migration-(3/7)

G = -1219.205021

B	-2.823134592787	-0.595259709878	0.299614208075
H	-3.959602978911	-0.913699345409	0.516163549971
N	-1.956409399956	-0.461702899230	1.552035684200
C	-1.712898868021	0.634915732420	2.298880933192
C	-0.731967795947	-1.122176731443	3.164982431685
C	-0.917152744630	0.257380386616	3.360009425150
H	-2.109750060192	1.602743520968	2.015580793148
H	-0.170431092766	-1.825025427252	3.771302064604
N	-2.840509613558	0.769198741692	-0.430487164121
C	-3.880643827504	1.589119124286	-0.643776853419
C	-2.065683035677	2.490689101970	-1.487395842192
C	-3.433894280239	2.710721130931	-1.316263933642
H	-4.866699212767	1.308576210276	-0.296715315239
H	-1.315342717346	3.100177748902	-1.974631455490
N	-2.185136629730	-1.628886806537	-0.636139078111
C	-2.638199580126	-2.823517675736	-1.030174868581
C	-0.676053945334	-2.450581620791	-1.936662964798
C	-1.700076534984	-3.395815352949	-1.871108418739

H	-3.595578622556	-3.183989575668	-0.677076409118
H	0.246359630335	-2.465820227242	-2.504512006620
N	-1.721670300815	1.322185047730	-0.951290505008
N	-0.974657732324	-1.395188850210	-1.180896755161
N	-1.357561183894	-1.551183503866	2.077826749380
Rh	0.029912112400	0.371070655819	-0.793573984328
C	0.932467186592	1.997620107748	-0.457996762318
N	1.493214134288	3.005407582464	-0.257162606444
C	2.222803072995	4.146685342840	0.116710921864
H	3.153498714923	3.846725490208	0.614066450693
H	2.471827238033	4.749033817688	-0.764830940669
H	1.635115301845	4.760299916853	0.809540717091
H	-0.533517218453	0.883730116872	4.152871885817
H	-1.752792996046	-4.353360608175	-2.366987965837
H	-4.014030848980	3.560540500042	-1.643368335934
C	4.050165460751	0.430096214310	0.654368892735
C	4.292132622058	-0.022241991364	-0.787892292383
C	3.217617330301	-0.899740324304	-1.425591921125
C	4.100758629584	-0.710524424505	1.675312874886
C	2.756516864010	-2.094392824835	-0.593688835112
C	2.770392073804	-1.431333369570	1.902715720526
C	1.950985008945	-1.683017289903	0.637996994161
H	3.090500697219	0.963638900352	0.737720083820
H	5.248240682309	-0.570958371109	-0.807667960820
H	2.327259736937	-0.279902317648	-1.658149807757
H	3.624405508339	-2.702182235203	-0.291930457824
H	4.867619026251	-1.430247467376	1.348846977177
H	2.967902866479	-2.392399396698	2.400504284677
H	4.828671145830	1.165271951869	0.904356402868
H	4.441818755724	0.860506481219	-1.427168413877
H	3.587374517576	-1.243415887240	-2.402840037244
H	4.454416854450	-0.328076942931	2.642499494796
H	2.144178603489	-2.748164886366	-1.227646561047
H	2.148942288803	-0.851683756738	2.599968333356
H	1.149128826967	-2.399994598371	0.856040670428
H	1.407062472305	-0.734969045524	0.417505448659

TpRh(CNMe)-Cycloheptane 1,3-migration-(4/7)

G = -1219.202378

B	-2.696193635875	-0.918020624746	0.360099238677
H	-3.770048655342	-1.419778183720	0.547667813210
N	-1.876015952205	-0.703306314771	1.630616220347
C	-1.822991040518	0.383244169242	2.428112853592

C	-0.646353651705	-1.256953674155	3.279082008355
C	-1.030872878491	0.074121329304	3.513884710689
H	-2.340815280563	1.297080644878	2.161076695473
H	-0.018651337609	-1.899910744709	3.886691797235
N	-2.925050724533	0.455332940779	-0.316084995893
C	-4.079350689192	1.109011775819	-0.515422439285
C	-2.422976571490	2.309222715918	-1.313176239384
C	-3.809628628945	2.307196832022	-1.149194976412
H	-5.011315053215	0.666912137346	-0.187679640393
H	-1.774122330575	3.042368429144	-1.774937398310
N	-1.902491791142	-1.797071347314	-0.613024088025
C	-2.193727544501	-3.011086341142	-1.090541851887
C	-0.320945646310	-2.304216305788	-1.986127898533
C	-1.201703390518	-3.385194517172	-1.979574326779
H	-3.086281829130	-3.524437299381	-0.757358205919
H	0.584288093431	-2.156334428240	-2.560442797450
N	-1.904537738878	1.191960758676	-0.809018679671
N	-0.745611412742	-1.356338391208	-1.150416250606
N	-1.154078298033	-1.721266479220	2.146091541052
Rh	-0.031025422281	0.527973064736	-0.653395963639
C	0.569956768286	2.261139637364	-0.186323424125
N	0.929709625140	3.331681535353	0.118783499725
C	1.375174678679	4.587185581747	0.565354732583
H	0.809131132383	4.896005728468	1.452186391585
H	2.438523454407	4.535460310617	0.826446957329
H	1.242895218238	5.341168417486	-0.219569739719
H	-0.773711810606	0.712890894177	4.346868634391
H	-1.129565271770	-4.303357790015	-2.542885789297
H	-4.513667467244	3.065716349729	-1.456886428785
C	3.585429800414	0.180121030477	1.371962274322
C	2.332602616528	-0.694324342607	1.371052785298
C	2.381216719354	-1.974047155261	0.549082983100
C	3.890491828212	0.832232362149	0.020953037686
C	2.868047428637	-1.808227043125	-0.889519919992
C	4.726300693471	-0.007974551635	-0.945490924034
C	4.363127385350	-1.494292272594	-0.997238799063
H	4.455136410791	-0.405251033501	1.713669571293
H	1.478095500115	-0.070906814643	1.026946501669
H	3.044074010120	-2.701154762295	1.045488304539
H	2.280781838011	-1.023043245039	-1.406063896637
H	2.933883789233	1.093471306777	-0.459623367795
H	4.630750507901	0.426997085610	-1.951356869957
H	3.442974342655	0.967935403327	2.125100311235
H	2.059029759934	-0.950599865586	2.403343372882
H	1.374380484720	-2.417952100695	0.557756519964
H	4.405840446079	1.791240235934	0.174605685498

H	2.654974296329	-2.738779748222	-1.433633703096
H	5.790390224365	0.082367818513	-0.682084320442
H	4.769439635128	-1.915682870312	-1.926765647147
H	4.878592725972	-2.028834485777	-0.184793818602

TpRh(CNMe)-Cycloheptane 1,4-migration-(3/4)

G = -1219.201915

B	-2.624048149889	-1.028860834340	0.572060907435
H	-3.667035701571	-1.566547040449	0.823454967011
N	-1.758007488587	-0.730388569571	1.796176214856
C	-1.747157633470	0.375445648476	2.568530489671
C	-0.360260107914	-1.127442163283	3.353557133781
C	-0.850310162982	0.167527432593	3.595152795630
H	-2.366598178730	1.231033252384	2.326175332855
H	0.367957826900	-1.695359457576	3.922805561912
N	-2.938470787185	0.307259455086	-0.145372783169
C	-4.127099911812	0.897181820619	-0.341813919282
C	-2.550063008333	2.132656769567	-1.240783575356
C	-3.930491762591	2.075334399026	-1.037207249649
H	-5.028627378341	0.428644719652	0.031245423443
H	-1.948433939209	2.872828921619	-1.752684706774
N	-1.831409057451	-1.907832377700	-0.401229293315
C	-2.089751269293	-3.145862461473	-0.834242100650
C	-0.270891910208	-2.396871009845	-1.803795327643
C	-1.109447251741	-3.509497887344	-1.740231428488
H	-2.952838734179	-3.681614658981	-0.461060811888
H	0.614995216750	-2.235538807302	-2.405392209096
N	-1.966843934926	1.065218749516	-0.701439105954
N	-0.708122999271	-1.440532972884	-0.985181460440
N	-0.906469795394	-1.664299134777	2.271615826802
Rh	-0.062523480939	0.487242502354	-0.550838055073
C	0.474185365737	2.253881736559	-0.145236028170
N	0.797534808368	3.348579501485	0.112832005729
C	1.218576950497	4.626988553762	0.515222312819
H	1.280925408560	5.299804699174	-0.348280389874
H	0.511787067899	5.046637923397	1.240710691808
H	2.208036543950	4.564668835250	0.984237236608
H	-0.594236403882	0.846907093400	4.395743637568
H	-1.017794308590	-4.440995384013	-2.278257996923
H	-4.677117461898	2.785854677612	-1.358859472376
C	2.506756492957	-0.343680945111	1.221023970209
C	3.409826882823	0.824253867267	0.833778936447
C	3.734230231747	0.968730296163	-0.648896254534

C	3.163182461978	-1.715012806005	1.073946476887
C	4.259477689542	-0.289040884923	-1.340866154351
C	3.052973898783	-2.343321544356	-0.317301602939
C	3.187499383299	-1.371585952837	-1.491228644991
H	1.551866216097	-0.340295610232	0.649095266026
H	4.349648833293	0.712434296720	1.398992647006
H	2.824904320800	1.290423115933	-1.186722356406
H	5.133838064982	-0.687098213375	-0.801215796017
H	4.222497460764	-1.615127461645	1.358282803739
H	3.819428004315	-3.126761225111	-0.407971564312
H	2.171267128749	-0.201285323497	2.256579696280
H	2.958523538142	1.763348150376	1.186928211969
H	4.459991272398	1.786556148458	-0.769713607976
H	2.721973865701	-2.410378505999	1.799759199105
H	4.624758085414	-0.003103396400	-2.336630802652
H	2.085140308464	-2.858433348263	-0.399396393108
H	3.367218045019	-1.957253559131	-2.404145357718
H	2.225492826609	-0.858101410474	-1.667210460335

TpRh(CNMe)-Cyclooctane σ-complex-(1)

G = -1258.463379

B	-3.001725778028	-0.572826980463	0.207058163297
H	-4.147777355846	-0.921566864805	0.274686146173
N	-2.359851317368	-0.239908466190	1.555380350559
C	-2.309140447807	0.949836699168	2.189706962370
C	-1.351217513215	-0.608251433514	3.395631531294
C	-1.659394155836	0.763100346330	3.391399033776
H	-2.724348828722	1.841853069734	1.735553186978
H	-0.841926097406	-1.188183026430	4.157597441956
N	-2.934844372945	0.686585643892	-0.690474917110
C	-3.938847484361	1.399957604732	-1.221584130395
C	-2.022040404695	2.256700610769	-1.862571244390
C	-3.403718902188	2.424048325148	-1.980140938302
H	-4.964740807777	1.120738088877	-1.018806612016
H	-1.210059419792	2.823191732838	-2.300789099806
N	-2.181807476815	-1.671849421534	-0.477403587542
C	-2.559433811092	-2.888598075534	-0.883353479702
C	-0.467478874962	-2.546038290545	-1.443596381210
C	-1.486882341062	-3.495999552363	-1.511467013405
H	-3.565670478969	-3.236872812950	-0.689985739096
H	0.545757947021	-2.594594266056	-1.823482212078
N	-1.752768603665	1.210010884043	-1.086904927816
N	-0.892288705611	-1.453919995204	-0.810406217335

N	-1.774313804410	-1.208547516898	2.291090514445
Rh	-0.033915688411	0.405992731355	-0.409590809179
C	0.674900957770	2.132097979559	-0.131485739123
N	1.090845253222	3.215488552503	0.022529743329
C	1.588807499745	4.500251026584	0.296091642217
H	2.348674429878	4.449273642718	1.085213614102
H	2.043628038949	4.934936521489	-0.602049886943
H	0.777064072879	5.155522652381	0.633161381642
H	-1.444604453652	1.504264440035	4.148055771480
H	-1.449431977768	-4.479800558430	-1.954563051834
H	-3.934810071494	3.176682560428	-2.543410324910
C	3.260909621087	-2.568534690597	-0.004715757200
C	3.412880422693	-1.822561178528	-1.341264621164
C	2.791296383955	0.254617019652	1.645420487452
C	4.448759288467	-0.695625207458	-1.359759114659
C	4.178393298438	0.338512366035	1.003775881539
C	4.186216168864	0.555344742763	-0.518041361213
H	4.214272063374	-2.509591793303	0.537916430420
H	5.418808532179	-1.118842993804	-1.048943475705
H	2.895784848192	-0.081782435116	2.688214693040
H	4.766767104863	-0.556853604843	1.246057074347
H	3.120971648864	-3.639178772167	-0.208930001610
H	2.365352883475	1.266384139373	1.701613013875
H	4.583098420541	-0.378387486232	-2.404302548871
H	4.710934546437	1.166541126549	1.492209216203
C	2.097640487878	-2.134586563154	0.901807412100
H	2.293799613911	-2.479039125351	1.928430274070
H	1.185862686308	-2.658891242119	0.590525655847
C	1.766357221785	-0.647323975453	0.965465026266
H	1.678704453901	-0.299944157588	-0.117784743107
H	0.810097514749	-0.541125675121	1.506896295690
H	3.721438826805	-2.546647295628	-2.108354322524
H	4.976933381776	1.276599505367	-0.767966191324
H	3.246705714838	1.032789533468	-0.839656358783
H	2.443590841053	-1.432232088408	-1.688210136113

TpRh(CNMe)-Cyclooctane σ-complex-(2)

G = -1258.463631

B	-2.708222853174	-1.122882018745	0.816235142028
H	-3.682790708077	-1.693165290833	1.222461539755
N	-1.508043381258	-1.178422865313	1.761994370105
C	-1.146943613710	-0.304154405239	2.723253380488
C	0.182857841626	-2.045088803894	2.724553762710

C	-0.047835473539	-0.821446784042	3.376415530954
H	-1.688710825873	0.623478735880	2.866369906887
H	0.953643310496	-2.783216852041	2.918574980692
N	-3.079446106184	0.359284899995	0.588933269386
C	-4.203544433682	1.001868830730	0.939125593002
C	-2.836897092869	2.413148353822	-0.038169016743
C	-4.095344700107	2.326395796339	0.560025602185
H	-4.999423878257	0.462201561487	1.435893340763
H	-2.338237131854	3.258982570309	-0.494177457398
N	-2.298790671507	-1.731319312412	-0.528949755792
C	-2.724087300297	-2.851391029695	-1.122376252333
C	-1.146236433522	-1.934592413803	-2.337224689661
C	-2.011967040880	-3.027041754553	-2.295619928066
H	-3.497895994397	-3.449681871794	-0.659351206546
H	-0.412803280418	-1.661417010320	-3.086837949753
N	-2.235438406485	1.225699755370	-0.013997010196
N	-1.321809045846	-1.164151907094	-1.264619328355
N	-0.694653632751	-2.256065090841	1.753721733224
Rh	-0.441084187851	0.626457686203	-0.693600839783
C	0.350291122353	2.268656932039	-0.191936932760
N	0.870290063814	3.266657159345	0.130453827432
C	1.542186138475	4.411595947275	0.591971305253
H	1.131415515262	4.726173648466	1.558504937429
H	2.609376953721	4.192415923027	0.718313287521
H	1.433541315166	5.235208594855	-0.123623959490
H	0.499281397002	-0.381544152276	4.198189873507
H	-2.107054583609	-3.827143545609	-3.014114991895
H	-4.823229229088	3.113184431639	0.689773809822
C	4.278981024429	0.772223713881	-1.124069526225
C	4.218004387662	0.890628933081	0.406124343500
C	2.094578890433	-1.720005677123	-1.166755595157
C	4.457723793855	-0.413122084055	1.171727255407
C	3.306899756173	-2.182964963444	-0.351562140023
C	3.433283518008	-1.541813947889	1.040544523649
H	4.911253177267	-0.083400793100	-1.394115680123
H	5.444026638915	-0.803219469678	0.868357922078
H	2.176727146878	-2.101815158831	-2.196316596491
H	4.237755208194	-2.032625931909	-0.915150480617
H	4.797027051464	1.648647851669	-1.538005953946
H	1.195361038827	-2.180286637197	-0.730452918492
H	4.552166880250	-0.166400206446	2.239506987531
H	3.214459801329	-3.271562963117	-0.239151321655
C	2.920456140079	0.685915581110	-1.826825712379
H	3.068896941519	0.379335115271	-2.873643724571
H	2.494062946103	1.699501964841	-1.872089245286
C	1.867385854913	-0.213033460516	-1.179995809507

H	1.705092229872	0.105129892714	-0.137388805679
H	0.944511059369	-0.019338534866	-1.815385630742
H	4.989839918463	1.600598163347	0.735763250684
H	3.730656890397	-2.319759339587	1.757616172991
H	2.446914084168	-1.199231695820	1.387862892999
H	3.258103968757	1.338940929390	0.714305917680

TpRh(CNMe)-Cyclooctane σ-complex-(3)

G = -1258.463693

B	-2.612807972316	-1.442803533450	0.786155161626
H	-3.470012101314	-2.177176410893	1.192969805255
N	-1.705021879962	-0.857989720905	1.873004305374
C	-1.897725097606	0.255474263371	2.609710223007
C	-0.020387675281	-0.723958878481	3.171068853259
C	-0.827386415271	0.387726581330	3.468825381006
H	-2.770928822320	0.879336473946	2.458736093874
H	0.923718440730	-1.017722728854	3.617251587674
N	-3.296771487916	-0.266839858395	0.047549025347
C	-4.602822448907	0.023365630200	-0.049027835014
C	-3.442307813309	1.525482428899	-1.151108514893
C	-4.748510401965	1.169733633810	-0.807263105623
H	-5.333651698208	-0.612964551658	0.433202426751
H	-3.078695520010	2.350346876273	-1.750817419510
N	-1.739658679561	-2.191125835812	-0.225671702065
C	-1.711805680105	-3.487757403755	-0.552710033461
C	-0.192745570932	-2.406956230106	-1.709782966725
C	-0.728594891826	-3.679650237247	-1.507560789695
H	-2.390941582531	-4.182959495657	-0.076596237830
H	0.598973746734	-2.084330273498	-2.376401512363
N	-2.579526723403	0.655872343019	-0.632567768137
N	-0.804186914154	-1.520667772167	-0.926846572170
N	-0.550630961335	-1.470811260877	2.212207635631
Rh	-0.566822759506	0.525496304476	-0.666913846853
C	-0.406787248498	2.399993702613	-0.495900083165
N	-0.326419294698	3.562825503735	-0.386857255887
C	-0.224824796883	4.950097555419	-0.190559685022
H	-0.885702075659	5.266102567613	0.625314656305
H	0.805855198935	5.218958573010	0.069149578192
H	-0.507708496761	5.488350053902	-1.103176920439
H	-0.659458888381	1.166173184922	4.199504974396
H	-0.445986230871	-4.603818618018	-1.988900546007
H	-5.665600789009	1.670883287092	-1.078513187855
C	2.362881579400	-1.137184066444	0.164173145838

C	3.296862416762	-1.690200137965	-0.921591572886
C	3.977427437388	1.623435544090	0.532339155757
C	4.788442706337	-1.660218455089	-0.583209770450
C	5.008942297605	0.520184317110	0.814465152859
C	5.470572602605	-0.301591289582	-0.399380382523
H	2.872506165614	-1.150318948622	1.136139200346
H	4.938233348121	-2.242606869028	0.341176081528
H	3.520140077308	1.939813922114	1.482454587215
H	4.642292513491	-0.164165042499	1.590309886047
H	1.492546703348	-1.788475131436	0.301456046357
H	4.523364949981	2.503504152883	0.158833921855
H	5.329522552911	-2.207419990782	-1.369285429153
H	5.882502050690	1.011406778641	1.264914224301
C	1.846617436051	0.275707603309	-0.096956529056
H	1.274266336275	0.607698374646	0.785289270084
H	1.206278410550	0.208290474056	-1.050062739213
C	2.879374660216	1.331238580718	-0.486096075976
H	3.337879454373	1.052791928789	-1.445843362528
H	2.343072191941	2.269124592945	-0.688445782368
H	3.028863969432	-2.738162440539	-1.118267869392
H	6.545970008520	-0.501505482991	-0.293519118464
H	5.380501415700	0.294566744646	-1.320920545714
H	3.123129247478	-1.163193312825	-1.874869219450

TpRh(CNMe)-Cyclooctane σ-complex-(4)

G = -1258.463872

B	-2.773759902450	-1.064613975654	0.658024396297
H	-3.736783952856	-1.677123971847	1.027917012318
N	-1.808497559174	-0.665100217904	1.777998956961
C	-1.818279233487	0.451706334303	2.534474432093
C	-0.183516036988	-0.875118834492	3.140516261450
C	-0.777836799042	0.364209857913	3.435257069796
H	-2.552365209748	1.231276582122	2.367705134298
H	0.669661275522	-1.349789245872	3.613285903772
N	-3.265957586657	0.222478999782	-0.048704526452
C	-4.514940455794	0.701960937034	-0.148190945555
C	-3.139977332847	2.031104298507	-1.225432618109
C	-4.486323872168	1.866648841948	-0.891599177912
H	-5.334566484684	0.172142806099	0.319860191995
H	-2.655728705193	2.801418292147	-1.812311234113
N	-2.006857821093	-1.897816711972	-0.372845081715
C	-2.198534653436	-3.157137552826	-0.780137957876
C	-0.518545489844	-2.277132254187	-1.882618452800

C	-1.260787252160	-3.451805188417	-1.754046778436
H	-2.986598390341	-3.755505963579	-0.341872708740
H	0.308556000490	-2.048774241790	-2.543255779384
N	-2.417021687376	1.038048576933	-0.715222897459
N	-0.970357958467	-1.351346067894	-1.039431932723
N	-0.805404557732	-1.491520275406	2.144289583942
Rh	-0.440602361515	0.628820418280	-0.694421603516
C	-0.045329420303	2.462206852803	-0.472906934522
N	0.161033116154	3.607125767051	-0.344130031512
C	0.438240613884	4.968131996240	-0.135066022532
H	1.469777544128	5.092269663109	0.215667044577
H	0.314824415100	5.532404978764	-1.067252152676
H	-0.240945033298	5.380921589841	0.620171178735
H	-0.495964082954	1.084299596976	4.190303805362
H	-1.136123297104	-4.378647119087	-2.293516806862
H	-5.318516479569	2.499564974032	-1.161199683593
C	2.947675842406	1.046935989953	0.093175485396
C	4.013728382580	0.769728842770	1.164520025958
C	3.083705930256	-2.043457578594	-1.033314868371
C	5.316915387055	0.143307329398	0.664151056569
C	4.488223790456	-1.454980047244	-1.203553113277
C	5.285448787411	-1.277351931339	0.097763973732
H	3.436588180441	1.184997377285	-0.880630795512
H	5.737302459707	0.807876992582	-0.109544625924
H	2.544056481657	-1.951083986429	-1.988597694035
H	4.441145390273	-0.493511073851	-1.733272473506
H	2.462784571982	2.007579795760	0.311337134638
H	3.184103839172	-3.125015535693	-0.854149679754
H	6.038999328157	0.162376277560	1.493831745995
H	5.041764127044	-2.121971682458	-1.878792626532
C	1.835669818926	-0.007158571631	0.006230842753
H	1.345565095888	0.148561266244	-1.020334044987
H	1.133927073707	0.173291610177	0.842094192633
C	2.230774763954	-1.477375755953	0.094317479765
H	2.746630861645	-1.627845371162	1.053167492155
H	1.307440383498	-2.064334012986	0.182830530241
H	4.283996165185	1.725429213706	1.635139913392
H	6.329466021291	-1.567662411541	-0.084597947663
H	4.920721251986	-1.980399676652	0.862635874372
H	3.584183716329	0.162842197139	1.975933476851

TpRh(CNMe)-Cyclooctane σ-complex-(5)

G = -1258.463412

B	-2.265657386875	-1.531709679552	0.963320301170
H	-3.031881398637	-2.311283853489	1.457784253813
N	-1.046252674735	-1.217587346860	1.828784005591
C	-0.854687708620	-0.193289801771	2.685657159369
C	0.855376523173	-1.561871407848	2.724241403932
C	0.372057172478	-0.369769218071	3.290711009902
H	-1.595270451985	0.590444860342	2.792938800519
H	1.791310967689	-2.075757642648	2.918002997300
N	-3.027758656364	-0.213324972607	0.693649387694
C	-4.268415238221	0.131035917042	1.069500516201
C	-3.378400474790	1.772423937910	-0.083833507043
C	-4.539635746366	1.401238492355	0.597167657853
H	-4.867798120987	-0.560595302883	1.647354117757
H	-3.147203273607	2.681216469617	-0.624955589382
N	-1.799458223301	-2.085221863509	-0.389269343023
C	-2.082623546549	-3.256631065430	-0.968546836207
C	-0.911499542231	-2.021981008506	-2.350456693408
C	-1.528048950814	-3.267815619560	-2.236085385601
H	-2.655342042447	-4.001900018830	-0.432155540327
H	-0.379560899789	-1.589321494857	-3.189002133075
N	-2.477430984772	0.795191743909	-0.019444042126
N	-1.069318157469	-1.321417144925	-1.228432095475
N	0.001214495003	-2.068179099091	1.845822243067
Rh	-0.588030455922	0.636116816993	-0.708930656517
C	-0.274511900843	2.446286146026	-0.271695132818
N	-0.127754086320	3.573612018235	0.006079136586
C	0.115913659103	4.903485699473	0.387502566064
H	-0.302164882919	5.093874786309	1.382956945704
H	1.195564178327	5.093463034024	0.417815124467
H	-0.342593437361	5.597606150591	-0.326909444601
H	0.841114619895	0.263835310467	4.030065693725
H	-1.567822418829	-4.059128153087	-2.969440524779
H	-5.448051355087	1.971957052052	0.718788345657
C	1.842237024267	0.259182791714	-1.043710642093
C	2.432349378229	-1.035316179956	-1.624285591420
C	4.595380934399	0.894666551446	0.652972792915
C	2.960581433891	-2.019717066163	-0.579116743614
C	4.021863831358	-0.422774983629	1.177338166128
C	4.194202119587	-1.625877470330	0.235703307171
H	1.495923901175	0.055582695916	-0.015484884681
H	2.133761819170	-2.243973751972	0.114093706592
H	4.293432446594	1.711309993845	1.327415246913
H	2.961267179831	-0.303555612276	1.433618107573
H	0.971649681637	0.539216946954	-1.732640672786
H	5.693718183590	0.844673666618	0.715617649032
H	3.184409699000	-2.964200863796	-1.096518161077

H	4.519745127633	-0.636766508602	2.133606356655
C	2.755148361049	1.496214672221	-1.076747472297
H	2.361012252718	2.248525599994	-0.377791305573
H	2.682906499977	1.948445074280	-2.077656747402
C	4.235147341525	1.269356226170	-0.780106644725
H	4.641085498107	0.516448564133	-1.469675112745
H	4.766372477616	2.198923843598	-1.031401623207
H	1.651656223492	-1.563120790390	-2.181520965337
H	4.468905775959	-2.505642637196	0.834119235793
H	5.052179439588	-1.456357910438	-0.435293688972
H	3.209218769778	-0.792719593961	-2.365077054835

TpRh(CNMe)-Cyclooctane σ-complex-(6)

G = -1258.464469

B	-2.787454175039	-1.202442794609	0.188014608143
H	-3.810068303976	-1.825808270965	0.258611715161
N	-2.203269028839	-0.781433588402	1.539897252471
C	-2.450864032609	0.341122649533	2.245843697975
C	-1.043216455667	-0.949574389579	3.319453674520
C	-1.717253078462	0.280576805716	3.411816773228
H	-3.115474968063	1.105897355347	1.861423807315
H	-0.358472872210	-1.404334467165	4.027221481841
N	-3.060305746198	0.075219128826	-0.644231171532
C	-4.228566919921	0.537857123256	-1.114316420534
C	-2.613536478606	1.892155775580	-1.726725278166
C	-3.995260420270	1.706728019756	-1.813791505833
H	-5.143234030546	-0.005061000065	-0.913871157139
H	-1.986783949264	2.672416877677	-2.139826831078
N	-1.735877803749	-2.030892631562	-0.556294870044
C	-1.768494503897	-3.299140114965	-0.979561682630
C	0.153599267487	-2.392888635751	-1.525449012194
C	-0.570295270107	-3.583110926514	-1.611305479510
H	-2.641510061315	-3.911510011811	-0.794988680075
H	1.141695785642	-2.150271882181	-1.899361127421
N	-2.062677871060	0.906796315229	-1.023371602467
N	-0.554964212027	-1.469338514026	-0.880315822026
N	-1.336881513040	-1.585480474984	2.193328963890
Rh	-0.176961283556	0.517316006422	-0.421269530303
C	0.150307477818	2.352585510934	-0.109777869324
N	0.346729280508	3.492440666038	0.069671202300
C	0.599194177423	4.844756402254	0.353363955849
H	0.734644244668	5.412696848271	-0.574877915842
H	-0.238510883807	5.277212801254	0.913174126732

H	1.510003822092	4.937639479088	0.957009355125
H	-1.679068935826	1.012071568234	4.206460474012
H	-0.268365105322	-4.513043328254	-2.069208018439
H	-4.717439158221	2.329758929890	-2.319830872583
C	1.822268361958	-0.059759165660	0.902964092515
C	2.865083343386	1.039444387685	1.148083362761
C	3.957000669682	-1.979561291819	-0.675400600105
C	3.620810624199	1.519785632747	-0.092401700581
C	3.895569574632	-0.670573241268	-1.473055751337
C	4.562017312257	0.541819284420	-0.801190029533
H	1.595920071201	-0.020640184157	-0.213739074761
H	2.875103653579	1.870304658649	-0.826610723550
H	3.293069820432	-2.722726071346	-1.143558656430
H	2.859390678266	-0.413388516007	-1.737516914733
H	0.922897204922	0.139088820126	1.510635131425
H	4.973733767784	-2.388308859399	-0.782887273399
H	4.206204551398	2.407583858317	0.190292701590
H	4.387996301041	-0.858467249118	-2.437273689797
C	2.250820682354	-1.492333133667	1.236866567397
H	1.502198416782	-2.192028056143	0.840875675296
H	2.185423039329	-1.590814983675	2.331322250365
C	3.656861132151	-1.907266632040	0.818935161645
H	4.392049965316	-1.247636947740	1.303049259146
H	3.848005998500	-2.902295017479	1.245662457182
H	2.355904013198	1.913024250024	1.579690192846
H	5.092923259491	1.119484850797	-1.570477872367
H	5.344409479093	0.202047991266	-0.104515503572
H	3.574183085008	0.701224383013	1.918602696574

TpRh(CNMe)-Cyclooctane σ-complex-(7)

G = -1258.465979

B	-2.865022570603	-1.159857683907	0.265456842934
H	-3.895173734912	-1.764304665012	0.378513255287
N	-2.197347021666	-0.787124229707	1.592788293793
C	-2.383164306557	0.318477156852	2.342955974098
C	-0.941952104989	-1.027252809693	3.297964751194
C	-1.586315687523	0.211085472772	3.463198575423
H	-3.053848186561	1.105511306830	2.018625712793
H	-0.226219815382	-1.513890187344	3.951746293020
N	-3.156153585813	0.143960972321	-0.517113877471
C	-4.338133913182	0.644219805718	-0.907505671694
C	-2.729133878563	1.977867006523	-1.578117821588
C	-4.117532503954	1.825456184481	-1.590156569631

H	-5.252359011023	0.116422678892	-0.668385589673
H	-2.108532954141	2.754203228782	-2.007585551985
N	-1.874751064049	-1.990926473341	-0.555721744689
C	-1.955565066696	-3.253029294431	-0.990573232083
C	-0.042750312638	-2.382111866313	-1.618831822406
C	-0.796179916832	-3.554991647468	-1.683089294973
H	-2.831572241292	-3.848757792134	-0.769407824688
H	0.930387403982	-2.157846999364	-2.039171912068
N	-2.162501926760	0.962692357278	-0.931936581074
N	-0.698500438643	-1.450507358469	-0.930419463102
N	-1.311252490599	-1.624875150123	2.173102222662
Rh	-0.251429131675	0.519020798248	-0.453208325832
C	0.126787065292	2.336857109783	-0.103508918004
N	0.353330160309	3.465679930728	0.107017740972
C	0.655537824816	4.797875173199	0.434313066448
H	0.477449108669	5.453395122601	-0.426376359974
H	0.031461282711	5.135236735657	1.270483095969
H	1.709588459505	4.881148588925	0.725502547070
H	-1.489206983603	0.918391949290	4.274570287842
H	-0.537242495894	-4.485456867936	-2.165540133732
H	-4.852386402318	2.477112843042	-2.038592657846
C	2.856067559910	0.935944829221	1.006529800651
C	1.800833018638	-0.136288102116	0.703945980542
C	5.129256713869	-0.520375700150	-0.818856471388
C	2.213353459509	-1.595090408607	0.910728750142
C	4.716480254035	-1.554271822778	0.235896804964
C	3.326612810485	-2.180529283752	0.042129316254
H	3.566807497519	0.526625690617	1.735710747004
H	2.523219267613	-1.684086557485	1.965397712754
H	6.027313519404	0.011364500386	-0.467683067572
H	4.779346444599	-1.124469402890	1.244555740694
H	2.368871186799	1.778257868759	1.518355864175
H	5.444096348667	-1.067055297551	-1.721206297174
H	1.309660559664	-2.212740229259	0.817430848279
H	5.475230179237	-2.348791706466	0.221385924855
C	3.593545442718	1.498619569944	-0.212820261763
H	4.444341953369	2.105160610675	0.134643810299
H	2.912105179442	2.196337130864	-0.725637921781
C	4.078960793321	0.496483535782	-1.255886551271
H	3.214372143650	-0.031094154268	-1.685284729977
H	4.496757937516	1.069425695203	-2.096342995788
H	0.931671354689	0.019848280686	1.368384259324
H	3.381714697611	-3.251065017863	0.282999359497
H	3.043755383769	-2.141405117328	-1.021507968480
H	1.528418734551	-0.018202308306	-0.404026961231

TpRh(CNMe)-Cyclooctane σ-complex-(8)

G = -1258.463995

B	-1.897798534783	-1.687243254606	1.101304170316
H	-2.468283952554	-2.558644213166	1.696927826262
N	-0.874914862281	-0.919930356831	1.942559501913
C	-1.065024445237	0.203994756133	2.664302179790
C	0.984168791728	-0.528324094141	2.906313233152
C	0.117509854597	0.501656487611	3.307860046036
H	-2.019797173977	0.716511519535	2.657515267890
H	2.019085287491	-0.692748566819	3.188253217521
N	-2.956095827603	-0.677780893634	0.594493782964
C	-4.269525064505	-0.626540509754	0.862183171197
C	-3.738562829227	1.024355422455	-0.484164054984
C	-4.817323733755	0.452741006090	0.194811878939
H	-4.716742737169	-1.367832277473	1.511862543853
H	-3.703831298814	1.882520670632	-1.143470609591
N	-1.208126548045	-2.295195569402	-0.126493595626
C	-1.130371780693	-3.574713568208	-0.508846235963
C	-0.269036499325	-2.292337470447	-2.065531247416
C	-0.527353012253	-3.627509085792	-1.752755815956
H	-1.509701310644	-4.357114085645	0.135531690015
H	0.172194258674	-1.866137826324	-2.957542006405
N	-2.627023302501	0.337053530168	-0.237107059015
N	-0.671659030685	-1.498651276761	-1.075669903987
N	0.385070575514	-1.381790462842	2.085095772248
Rh	-0.703662908465	0.567036568282	-0.795685579731
C	-0.829886383629	2.430626997516	-0.529978425103
N	-0.939888560282	3.582075078481	-0.351625856853
C	-1.023425692209	4.958443107506	-0.083643087927
H	-1.686708790170	5.136529725133	0.770860166824
H	-0.030020070913	5.356834826850	0.154839427855
H	-1.417816910457	5.495646971842	-0.954526028962
H	0.319311544542	1.332831066640	3.968420275119
H	-0.312103345014	-4.502391649428	-2.347667269257
H	-5.848039161820	0.774303450305	0.191935610254
C	2.630250444063	-0.391397070314	-1.761214731980
C	1.780320197532	0.550117539749	-0.888992784518
C	4.991769438070	-0.591237118347	0.453855029810
C	2.491154860672	1.811803908531	-0.395371712085
C	4.877112983379	0.896956700982	0.097813970515
C	3.620758290521	1.612507955504	0.618588403560
H	3.465326412688	0.181558837921	-2.185241247409
H	2.891078482564	2.358440208113	-1.265907661127
H	5.793792588239	-1.040842118606	-0.152402721666

H	4.951743243212	1.043307583341	-0.988219338783
H	2.045546586349	-0.715575562766	-2.631246776605
H	5.338387262128	-0.659550254874	1.496850726278
H	1.740004232576	2.467260661853	0.065457147446
H	5.766288207019	1.395968046554	0.507707741976
C	3.134954359813	-1.645344043324	-1.042672664395
H	3.867052107894	-2.151464993832	-1.691441971853
H	2.287152296365	-2.338843292241	-0.934613280298
C	3.730756752210	-1.443011640131	0.345451198484
H	2.953449183706	-1.046759700740	1.011877505420
H	3.962007114801	-2.437303527335	0.753483800729
H	0.954968117365	0.919241983214	-1.589286339856
H	3.905977221599	2.614981382081	0.967306847196
H	3.224157610955	1.096858638514	1.507009335250
H	1.380993460745	0.001389852248	-0.018699461461

TpRh(CNMe)-Cyclooctane σ-complex-(9)

G = -1258.463321

B	-2.545181827418	-1.487135535961	0.773639005176
H	-3.374125159391	-2.234251358595	1.214369344036
N	-1.484114052203	-1.046232888207	1.786812371486
C	-1.528082453085	0.000115322822	2.636931756859
C	0.335266781448	-1.122422919072	2.893859361087
C	-0.365493930552	-0.004486552561	3.378271023304
H	-2.373265885438	0.678415681343	2.642332187116
H	1.301029922209	-1.506424630547	3.204361010859
N	-3.267245627085	-0.221938822281	0.249941443543
C	-4.561647895263	0.114328637557	0.354052004903
C	-3.491496092337	1.681400082801	-0.749193449273
C	-4.756016604959	1.332440313265	-0.269362102594
H	-5.250130812788	-0.544392491906	0.867493828305
H	-3.174307037163	2.549312065676	-1.313445979573
N	-1.843085030563	-2.151779581465	-0.414169708084
C	-1.930726111820	-3.402015723967	-0.881063203212
C	-0.528029852596	-2.254386122527	-2.117415063579
C	-1.099186300303	-3.520156349607	-1.980941691216
H	-2.575135761712	-4.120654631345	-0.391685263738
H	0.180525039903	-1.888004865518	-2.850852794132
N	-2.606092289232	0.740685272175	-0.431916606309
N	-0.977830159076	-1.440962147641	-1.164611382131
N	-0.339203629991	-1.746509154964	1.937392929669
Rh	-0.621073134490	0.558915621135	-0.732299502713
C	-0.373670350178	2.399734428020	-0.386795580801

N	-0.245094695136	3.541831756356	-0.164443170882
C	-0.073697752449	4.894809728403	0.172848736946
H	-0.516140372000	5.099478891311	1.155073835706
H	0.994074748908	5.140387339380	0.210809997117
H	-0.554596923221	5.539262502561	-0.572677889279
H	-0.072940253729	0.691104424076	4.151978743429
H	-0.934035841696	-4.393226098973	-2.594194772611
H	-5.678701862881	1.884136259220	-0.369770959571
C	3.917444671786	1.537786131947	0.249434423619
C	2.838749928688	1.298229664296	-0.817550753904
C	4.771130471199	-1.615094983147	0.349842332299
C	1.837865186526	0.182967418609	-0.494251439486
C	3.292935435245	-1.549810749475	0.744416325083
C	2.311541346149	-1.269823284061	-0.404368536341
H	3.538838305081	1.211922312565	1.226674113156
H	1.350163714479	0.419514557222	0.469982849348
H	5.386737913363	-1.635914419201	1.262585448599
H	3.134361752952	-0.813135365729	1.542523912064
H	4.078346023516	2.619949534681	0.354591583107
H	4.947155031142	-2.581068220158	-0.148434856784
H	1.105556569017	0.228531391990	-1.374034174900
H	3.028016408959	-2.514739554020	1.198119088393
C	5.282156943751	0.904823556121	-0.046155137600
H	5.904371773614	0.956229529363	0.860657635178
H	5.791629471450	1.535368062684	-0.791427637013
C	5.285043707621	-0.523311709006	-0.581847762909
H	4.723468371155	-0.558874314199	-1.526780945717
H	6.319230106213	-0.773954298405	-0.859088374410
H	2.255106362486	2.218989347743	-0.948782883320
H	1.415194305338	-1.878487047706	-0.240964547138
H	2.741425418881	-1.598055246635	-1.364125988075
H	3.307436987677	1.111643233558	-1.796060133091

TpRh(CNMe)-Cyclooctane σ-complex-(10)

G = -1258.463484

B	-2.811974985366	-1.195562077701	0.384433232517
H	-3.793606070644	-1.860975965676	0.566704614729
N	-2.031076725630	-0.853142275274	1.656497461190
C	-2.208309218820	0.193485496310	2.488689341755
C	-0.591841975451	-1.097895106159	3.208870485827
C	-1.293554259171	0.080972297065	3.514361862095
H	-2.959262685142	0.947448135772	2.283538000508
H	0.218034594243	-1.568306494811	3.756020753330

N	-3.247775901687	0.129642880316	-0.287496599722
C	-4.486371718258	0.584921548259	-0.528419336204
C	-3.021198562773	2.040583674388	-1.271490791280
C	-4.394460607862	1.812795014294	-1.156213813056
H	-5.344461667503	-0.004842024905	-0.232735615420
H	-2.486318827765	2.872631661852	-1.711825170500
N	-1.876538572596	-1.925429273776	-0.583740426715
C	-1.954155748549	-3.159540614631	-1.093304150212
C	-0.177418088723	-2.147972290959	-1.889110130501
C	-0.878360157828	-3.353617907838	-1.941741015649
H	-2.768680119890	-3.813579704220	-0.810487129137
H	0.725074349098	-1.847225387086	-2.407113333236
N	-2.342906212526	1.023470201876	-0.747292596885
N	-0.782485631342	-1.299024396563	-1.061247529902
N	-1.037582665726	-1.657229860625	2.091956605943
Rh	-0.373695570104	0.658675664849	-0.499165235754
C	-0.068676169807	2.470906427833	-0.064052045272
N	0.089005527268	3.600051091445	0.201519739453
C	0.288662558612	4.934302877005	0.592875390904
H	-0.488897194197	5.240715548988	1.302552070097
H	1.266796161834	5.041885788636	1.076740645833
H	0.253777075956	5.599165461015	-0.278486800158
H	-1.158118478276	0.747522395281	4.354244404968
H	-0.640487778739	-4.235826618002	-2.516866882023
H	-5.202142936074	2.447034995629	-1.489609451027
C	3.079225519136	-1.948885031169	-0.724774164910
C	2.216375979271	-1.451992692999	0.444851499333
C	5.306932425377	0.401032383385	-0.323600620022
C	1.847624021464	0.031409177733	0.417391464025
C	3.979406699276	1.124871530475	-0.581274131775
C	2.961128795668	1.071171042633	0.568476227005
H	2.933688577699	-1.290299662938	-1.592958974671
H	1.429972698764	0.233489338211	-0.636276444284
H	5.856314866527	0.315316792531	-1.273902922246
H	3.505982711332	0.751447891579	-1.499186177676
H	2.707887333745	-2.931421662674	-1.048868165669
H	5.924793498952	1.049209553870	0.317169205666
H	1.098945762939	0.198963100935	1.210830137582
H	4.220001885555	2.174852752352	-0.798382166573
C	4.574129530784	-2.099178472804	-0.423418877965
H	5.115713957063	-2.266500790539	-1.367373992109
H	4.709786776966	-3.020371604690	0.163968366310
C	5.243380489857	-0.967061390996	0.349238686022
H	4.765632456920	-0.866845828975	1.334386135231
H	6.275384206414	-1.276943898713	0.568722787827
H	1.274577965495	-2.012995529647	0.487012284784

H	2.477148175140	2.051691130353	0.665575129407
H	3.475001358424	0.902403632581	1.527016618876
H	2.717899570671	-1.662155923085	1.402182539331

TpRh(CNMe)-Cyclooctane TS_2-(1)-κ^3

G = -1258.437526

B	-3.013148224164	-0.746649250602	-0.111482478919
H	-4.117890424045	-1.182825692282	-0.260053307315
N	-2.856585468545	-0.188799555770	1.297114742494
C	-3.695333605562	-0.248761153632	2.347876632341
C	-1.838059824139	0.774494815635	2.911042966796
C	-3.079537435381	0.364485400015	3.420557828830
H	-4.665373900291	-0.720826395467	2.254429256666
H	-1.032040744213	1.299841484280	3.411781143406
N	-2.752001913279	0.356863386447	-1.152610283202
C	-3.621377848613	0.935537943493	-1.994789779323
C	-1.622117797333	1.778902044625	-2.308858942029
C	-2.941308101932	1.863266387864	-2.760552167182
H	-4.662260118682	0.638723329940	-1.990188677739
H	-0.739999811238	2.314129486565	-2.638060534811
N	-1.994902143445	-1.874836291234	-0.375914827298
C	-2.276524183502	-3.129107808219	-0.756632477684
C	-0.112172104618	-2.812951575885	-0.836764417612
C	-1.094938920145	-3.777047399812	-1.058883912438
H	-3.304273995189	-3.466823982270	-0.788060855565
H	0.958531641360	-2.889753449980	-0.967981902608
N	-1.518866908063	0.870834742201	-1.343173125195
N	-0.655727700831	-1.672222172819	-0.416005667558
N	-1.714152278197	0.438786478548	1.634351270124
Rh	0.125753629901	0.275500291056	-0.131591986386
C	0.752694346898	2.048743468621	-0.179279242072
N	1.095731614060	3.161938217453	-0.274952130788
C	1.537156383585	4.494668911909	-0.322674202354
H	1.988132517021	4.713454251006	-1.297964610752
H	0.694529387853	5.176992887946	-0.161715494001
H	2.286765345026	4.670102573434	0.458405308719
H	-3.472182014262	0.499208232978	4.417989714812
H	-0.962927882918	-4.794590845808	-1.394787520357
H	-3.339324186132	2.496786031709	-3.539144395662
C	3.293030344176	-2.345567403719	0.312848510014
C	3.445573966989	-1.770264566659	-1.106631429209
C	2.800750797873	0.658913739681	1.650787476302
C	4.458577893160	-0.635241876053	-1.266887022450

C	4.164124650931	0.644387976948	0.954255287129
C	4.165666719933	0.699396140789	-0.581601967661
H	4.280298121411	-2.295519575941	0.793794581875
H	5.437096966291	-0.995798174599	-0.906183370220
H	2.991044561613	0.477023714236	2.722970474664
H	4.736135777550	-0.235533649117	1.280856692245
H	3.093728218055	-3.423824675378	0.220085343302
H	2.388408425903	1.675180893125	1.604691143651
H	4.587560507827	-0.449577520226	-2.343516050536
H	4.727127345966	1.502944595093	1.347748783532
C	2.214787436321	-1.796377926498	1.280487079112
H	2.597689532631	-1.952787486180	2.303784445429
H	1.328919667061	-2.437600680159	1.218990312522
C	1.728546132011	-0.345045107313	1.216333448886
H	1.606063350599	-0.183703951000	-0.318227195723
H	0.938343459752	-0.281807027792	1.984630063148
H	3.794086436647	-2.589111605895	-1.753543841724
H	4.943124818425	1.404101659430	-0.909977284492
H	3.217820957783	1.112592377790	-0.954760039027
H	2.480720730340	-1.461361406673	-1.530247759638

TpRh(CNMe)-Cyclooctane TS_2-(1)-κ^2

G = -1258.437906

B	-2.980037734468	-0.637792958030	0.226719069522
H	-4.117664431701	-1.000179882600	0.332396878081
N	-2.269675507649	-0.397859086715	1.561410368581
C	-2.039749193904	0.763946099588	2.215421455556
C	-1.387504124645	-0.945779455119	3.422497292592
C	-1.461354933870	0.458491014666	3.428814813993
H	-2.299036407707	1.717546860178	1.770835043732
H	-0.997911285454	-1.608852131877	4.187086278854
N	-2.957168029897	0.686864796479	-0.567755858994
C	-3.977271151487	1.467276662856	-0.947311031164
C	-2.085664876526	2.380603150640	-1.579142201586
C	-3.467779407637	2.572701463699	-1.605866291901
H	-4.995144034927	1.177587568966	-0.719012329737
H	-1.291291442560	2.993651577672	-1.987778225294
N	-2.193309104315	-1.684957587255	-0.572769059879
C	-2.624230445046	-2.828848957044	-1.115650082730
C	-0.525990110217	-2.507018660021	-1.662176082931
C	-1.584534049649	-3.399300028991	-1.828119769872
H	-3.641033159362	-3.158686503383	-0.946677160355
H	0.483413173543	-2.549002682665	-2.053394544866

N	-1.787844252966	1.243825880793	-0.954417603123
N	-0.897936171951	-1.482891859873	-0.896660352987
N	-1.875362206696	-1.456313480967	2.300635560854
Rh	0.054514954604	0.309664290688	-0.425650738770
C	0.898062399646	1.990678687488	-0.218617253044
N	1.428253700070	3.026797777884	-0.127313316760
C	2.180822030648	4.203099595292	0.037001427368
H	2.291110660280	4.435227566788	1.103065739786
H	3.176885025418	4.069981433796	-0.402782588175
H	1.683594088488	5.044655718776	-0.458201763223
H	-1.144563950100	1.146050594696	4.200081472705
H	-1.591537821706	-4.325877781257	-2.382119849790
H	-4.017614448055	3.391449259726	-2.045534383187
C	3.280503736883	-2.350839899874	0.308656556160
C	3.595584946867	-1.889161978882	-1.121948711529
C	2.474528271171	0.294849169976	1.581311906743
C	4.486903797322	-0.653357527938	-1.210884238381
C	3.753127192785	0.785652589118	0.840855167559
C	3.925964331029	0.666541193677	-0.682134141795
H	4.023833749613	-1.920790760178	0.997706001053
H	5.429434488642	-0.869273085389	-0.679729346384
H	2.809991252275	-0.247901565590	2.482377524915
H	4.633462657019	0.308475615853	1.297496343372
H	3.427108270700	-3.437617100019	0.377842179934
H	1.946901419699	1.174201539020	1.972624222305
H	4.765589279066	-0.501271063340	-2.264211414165
H	3.861922259124	1.851614002096	1.093416270880
C	1.873465034011	-2.061525634937	0.827304099603
H	1.818910548862	-2.466436770262	1.852165580230
H	1.141444276178	-2.642900650809	0.256302135095
C	1.424044576807	-0.603574385832	0.931099992426
H	1.421517405404	-0.311532495685	-0.765958673870
H	0.558953649620	-0.605102891633	1.618936143153
H	4.108087445730	-2.700658813764	-1.657285080705
H	4.648944780324	1.445365698852	-0.970966029183
H	3.003953842273	0.916662953111	-1.220047709378
H	2.665235237842	-1.715337307035	-1.684360363572

TpRh(CNMe)-Cyclooctane TS_2-(2)-κ^3

G = -1258.445646

B	-2.710113186872	-1.172893513043	0.675520578465
H	-3.687648239057	-1.796396854198	0.973420035814
N	-1.655412383313	-1.300676391940	1.770461035678

C	-1.615775515821	-2.131441634084	2.829112103360
C	0.205846887307	-0.912474030398	2.747735464910
C	-0.426401787101	-1.917157965715	3.496346874111
H	-2.435977771755	-2.809260537892	3.030467632546
H	1.162525971705	-0.429936355417	2.919609320629
N	-3.086018443268	0.306847174285	0.467959476968
C	-4.246023525030	0.915418132277	0.757674927637
C	-2.859466826280	2.365490081133	-0.125715674805
C	-4.149589477455	2.245469154468	0.395659043014
H	-5.059366735224	0.352709146596	1.197363059390
H	-2.357068943406	3.228782539727	-0.544282003268
N	-2.171360900873	-1.702848363500	-0.667462291328
C	-2.671548184731	-2.692662022988	-1.421439226295
C	-1.024133289385	-1.720885658951	-2.490725765838
C	-1.960529375807	-2.748926599604	-2.605294646137
H	-3.503259442064	-3.282929510207	-1.059213254542
H	-0.270727001296	-1.389962088015	-3.193873571694
N	-2.228766396079	1.196075263686	-0.078822256049
N	-1.151431606923	-1.102190127613	-1.319784905412
N	-0.539390623168	-0.548456557570	1.713340271549
Rh	-0.246808079113	0.633947239658	-0.559100193647
C	0.376347726097	2.344782614798	-0.068368366830
N	0.718447011075	3.415569885600	0.253360547241
C	1.138270029838	4.704317395220	0.622326545404
H	0.824957473757	5.439072320037	-0.129305900091
H	0.703246350253	4.980570739997	1.589844522491
H	2.230896869683	4.733485342962	0.707631554437
H	-0.075774072214	-2.406196246843	4.393650370298
H	-2.104305474195	-3.427955727307	-3.432312459921
H	-4.905749140139	3.011137145136	0.484383496039
C	4.346494312546	0.768680142094	-0.912768352085
C	4.513816168808	0.549198517999	0.597987450947
C	1.964985355745	-1.492598561694	-1.131163822878
C	4.748561216548	-0.901343918829	1.025152318201
C	3.252242550881	-2.186175615223	-0.664919012333
C	3.634005887815	-1.924392759621	0.800307244994
H	4.879587726148	-0.026238602184	-1.449415029068
H	5.651037635843	-1.261377827263	0.502690231938
H	1.853801875183	-1.651679205769	-2.215055410625
H	4.096723894646	-1.936264556352	-1.320215597173
H	4.865420968734	1.694721037374	-1.199322587955
H	1.124449613508	-2.017234989048	-0.656691220076
H	5.005781908194	-0.905727627845	2.095076029675
H	3.093958275138	-3.264577413546	-0.806315582230
C	2.901763840719	0.901581908642	-1.422453754976
H	2.899126639889	0.778539826777	-2.517773828997

H	2.587704979715	1.940842997436	-1.251459779299
C	1.835679870067	-0.010698954297	-0.799548237869
H	1.899889946112	0.096885410968	0.294161961849
H	0.813603601229	0.557069407562	-1.721269652948
H	5.385057327524	1.125176730179	0.941343354995
H	3.975401473387	-2.866595928462	1.251550040745
H	2.735532850646	-1.641997618453	1.370815537093
H	3.654649224351	0.972286353623	1.142460758541

TpRh(CNMe)-Cyclooctane TS_2-(2)-κ^2

G = -1258.445438

B	-2.588415824088	-1.223905062237	0.726697441265
H	-3.511892671684	-1.879984263002	1.118090260390
N	-1.388256857361	-1.212834439894	1.675101098706
C	-0.963429155046	-0.251941865320	2.525929132809
C	0.247230837679	-2.066372744352	2.741596302097
C	0.103765249495	-0.758480512389	3.237164007983
H	-1.447458286333	0.716657794372	2.565238924374
H	0.969591478537	-2.824386634243	3.024772222986
N	-3.063156118123	0.232488132845	0.541715997906
C	-4.214258676437	0.799824355753	0.923162244597
C	-2.928460410087	2.314585960642	-0.004960233958
C	-4.177958120815	2.142953759405	0.590931598877
H	-4.977738977569	0.203334393267	1.406215028671
H	-2.477918591000	3.203798713568	-0.429099158743
N	-2.141781245704	-1.762940186724	-0.639669048369
C	-2.591802685879	-2.830221127326	-1.308872859652
C	-1.052298446596	-1.820160755157	-2.498330607967
C	-1.919834245272	-2.911398771185	-2.515409535344
H	-3.353451781435	-3.461526526420	-0.870112177365
H	-0.340093812261	-1.489045530405	-3.243974390793
N	-2.264704661690	1.160246393343	-0.030321697199
N	-1.186463692702	-1.138997103678	-1.362230434741
N	-0.649841452238	-2.335501247628	1.804857709933
Rh	-0.336914557897	0.654439488617	-0.740373099185
C	0.312200055627	2.382395215994	-0.309704285213
N	0.694427884040	3.451580218321	-0.037842056807
C	1.209497814474	4.718770179521	0.288531161436
H	0.976579746085	4.962807238747	1.331269511024
H	2.297943783318	4.723009242675	0.158973310660
H	0.772757679567	5.485510652915	-0.361820802602
H	0.683776166454	-0.259869304834	4.000862995026
H	-2.039868441542	-3.652566146423	-3.291171866611

H	-4.946462292613	2.884337054039	0.751008163385
C	4.255061819845	0.674967640859	-1.012879380645
C	4.465985660916	0.701956061429	0.507716121845
C	1.821171582335	-1.521777372277	-0.834604818361
C	4.679294679907	-0.667434463552	1.154365561887
C	3.093618916007	-2.165336955260	-0.258268951658
C	3.519420212370	-1.663111656134	1.131255316270
H	4.735887347209	-0.220880520559	-1.425119182557
H	5.550835161188	-1.137744401868	0.668178037506
H	1.713102919583	-1.835716030968	-1.884265110495
H	3.934866928905	-2.074437431351	-0.958174667368
H	4.796209364242	1.517369445717	-1.467303635118
H	0.968473879245	-1.952497056745	-0.293429024742
H	4.973701433796	-0.509498298444	2.202696801872
H	2.888750210233	-3.243294616052	-0.199623774521
C	2.800186154077	0.783102067879	-1.494902568437
H	2.763931608526	0.511109449761	-2.562408235910
H	2.522071290125	1.846609938306	-1.460745053902
C	1.729773860316	-0.006196028781	-0.728920775108
H	1.783149017944	0.271086398727	0.336328564592
H	0.692836876136	0.489474047329	-1.879502960965
H	5.357328843572	1.305899115493	0.729668190564
H	3.829888682618	-2.526198148696	1.737138503268
H	2.651541450983	-1.238740968292	1.656721443074
H	3.629468420771	1.224254727111	0.999439865669

TpRh(CNMe)-Cyclooctane TS_2-(3)-κ^3

G = -1258.446047

B	-2.801321934382	-1.318866629710	0.276176581200
H	-3.773076705838	-2.013011395078	0.361021780543
N	-2.237557767327	-1.041485845553	1.664695808578
C	-2.560983177053	-1.602562080865	2.845096554572
C	-0.897578612356	-0.195799232427	3.098508119376
C	-1.719610212453	-1.084478062784	3.808727720976
H	-3.365006115458	-2.324926820045	2.911605071047
H	-0.094127984236	0.433491090089	3.465978761962
N	-3.174865100837	0.000701317775	-0.426896249253
C	-4.399818894844	0.461253610777	-0.721340290203
C	-2.893486979234	1.892568369209	-1.418522716371
C	-4.272279823369	1.680126502281	-1.359952670338
H	-5.275273211510	-0.117901560777	-0.457439363891
H	-2.335383734995	2.714950831570	-1.848639952650
N	-1.757129428738	-2.029754543959	-0.606982737082

C	-1.862872644091	-3.228852899890	-1.198376348358
C	-0.013173571147	-2.252986528518	-1.852449588510
C	-0.758631492775	-3.422584973905	-2.006510377468
H	-2.723075768554	-3.855769187887	-1.002421719926
H	0.918894510473	-1.959365453817	-2.317126011941
N	-2.242416276807	0.878517195130	-0.856210118248
N	-0.614965660042	-1.425146724619	-1.001816914931
N	-1.216116463390	-0.175293901023	1.811899138733
Rh	-0.184199648277	0.562965118918	-0.476096046943
C	0.071418042757	2.422452988311	-0.301676699737
N	0.169824605859	3.583613610464	-0.204668376887
C	0.306526934457	4.976593757368	-0.086404841047
H	1.328260547076	5.228763670477	0.221092021165
H	0.099035432408	5.464639847053	-1.046407891779
H	-0.392002769249	5.363136074941	0.664920579918
H	-1.708249661097	-1.309719670776	4.865334999321
H	-0.531990397723	-4.279055832947	-2.623671403650
H	-5.060337465504	2.314165539174	-1.737915760003
C	2.277808339553	-1.217336261752	0.357182248315
C	3.164394207106	-1.766790010192	-0.772619251834
C	4.143038321210	1.352048631731	0.856236034275
C	4.650748667483	-1.905302791801	-0.437000951061
C	5.067871080956	0.150619239302	1.091244452639
C	5.463233861010	-0.637131009606	-0.166138968270
H	2.802989705727	-1.352251934528	1.313210522529
H	4.739562200025	-2.560322536462	0.445908977704
H	3.734014885188	1.686064714121	1.822703184144
H	4.632875321774	-0.539755840710	1.825755466338
H	1.372019335677	-1.825033506597	0.454739624141
H	4.768493354688	2.184448834452	0.496019069210
H	5.136999742448	-2.449971982705	-1.260071768193
H	5.977465535912	0.536668689090	1.572411556908
C	1.861153560868	0.251479279235	0.236375364620
H	1.482891543807	0.573267174730	1.222321240380
H	1.241340100121	0.404375382456	-1.127144752061
C	3.001558653229	1.200588085673	-0.148743595233
H	3.416400627490	0.914574846663	-1.126625453697
H	2.579153053125	2.200517693795	-0.312092094400
H	2.805934314060	-2.769301132366	-1.046752185427
H	6.512681559049	-0.948827766348	-0.068479675112
H	5.439785298654	0.021709225595	-1.048465034178
H	3.046241002316	-1.156860919307	-1.683341795052

TpRh(CNMe)-Cyclooctane TS_2-(3)-κ^2

G = -1258.446173

B	-2.445508648204	-1.487074696484	0.795500113460
H	-3.269461749776	-2.245600478036	1.223910805661
N	-1.533332610494	-0.873176321054	1.861415100818
C	-1.661308874525	0.305379344902	2.511928130109
C	0.033719273883	-0.835424089242	3.305248229428
C	-0.661872616214	0.377216450815	3.458166027298
H	-2.445696345059	1.005859238736	2.250453077468
H	0.898502318263	-1.196094177976	3.851519373067
N	-3.169822370457	-0.324919139745	0.079694716224
C	-4.476287993314	-0.034561948880	0.032513932224
C	-3.348618526628	1.496384931135	-1.061238233830
C	-4.644726216538	1.131253585406	-0.694001779846
H	-5.193073955763	-0.680560503762	0.523482313613
H	-3.005200198134	2.339516657343	-1.648554730173
N	-1.580770544709	-2.217298719195	-0.239543381285
C	-1.632492496468	-3.492083365400	-0.643150199612
C	-0.120199389061	-2.416398262155	-1.813213950283
C	-0.707357937578	-3.672354906672	-1.655854856485
H	-2.322877835711	-4.181139969461	-0.174305612389
H	0.651756079466	-2.089627789449	-2.498828418022
N	-2.468718810402	0.615109079199	-0.591849636135
N	-0.646629306621	-1.550564559709	-0.950326149181
N	-0.494535798637	-1.584651871796	2.348314357097
Rh	-0.350581972725	0.487900038292	-0.683551670008
C	-0.227182120089	2.377271359484	-0.642761242003
N	-0.219184294483	3.545371576584	-0.638673984414
C	-0.131268649952	4.947760485378	-0.598227662802
H	-0.804835681393	5.345820527358	0.169271271975
H	0.894921543223	5.251242124442	-0.359394390475
H	-0.408426565653	5.374773052286	-1.569107573400
H	-0.466698086435	1.182886486328	4.151594191475
H	-0.491931630871	-4.579331235200	-2.200491559793
H	-5.569992939919	1.636677894285	-0.927262151725
C	2.191548661550	-1.085789811316	0.240812014180
C	3.052746464531	-1.550816152496	-0.943658135849
C	3.844018151387	1.555138877865	0.780597326955
C	4.561226248875	-1.581762413438	-0.690156816336
C	4.904144164647	0.447694216434	0.890856251539
C	5.283147805136	-0.259938797237	-0.417823110759
H	2.788372505881	-1.140930550397	1.163014310146
H	4.748729019170	-2.252264199857	0.165127103906
H	3.432012035227	1.760926570104	1.780792073990
H	4.606485865285	-0.307678015932	1.629730581897
H	1.364632028376	-1.778273058689	0.420374319298
H	4.365080901298	2.478188542609	0.481482423556

H	5.044919816752	-2.061125775686	-1.554373072681
H	5.804542595087	0.913619128154	1.315449387915
C	1.636343869575	0.332302811360	0.146015932232
H	1.188807669053	0.594225974543	1.123469977394
H	1.036899148603	0.357153945281	-1.372165696846
C	2.691762793412	1.378506803670	-0.211902615841
H	3.103702861635	1.172662702479	-1.210804233212
H	2.203898232373	2.356210147468	-0.306949042828
H	2.752534915741	-2.571693395135	-1.219931834862
H	6.358263405568	-0.486975072477	-0.389614648064
H	5.156523259327	0.423820658784	-1.271823973737
H	2.841455153145	-0.935576111440	-1.834471219331

TpRh(CNMe)-Cyclooctane TS_2-(4)-κ^3

G = -1258.446007

B	-3.057611275260	-0.836252467132	0.376205685964
H	-4.146660095301	-1.310356854357	0.526226748254
N	-2.594702995832	-0.175472492462	1.667934193776
C	-3.137127938434	-0.223696957000	2.899021876986
C	-1.268708293170	0.925193246578	2.931877798293
C	-2.313223800101	0.478108626741	3.755766237637
H	-4.067123160230	-0.750504346552	3.072931498557
H	-0.399532391832	1.519891347764	3.191435759260
N	-3.101616813425	0.194986096177	-0.767288536034
C	-4.177135030259	0.691447893737	-1.397010046124
C	-2.357863737400	1.558087686661	-2.260263518757
C	-3.750262891218	1.577821341048	-2.367408007332
H	-5.170420661442	0.371641584563	-1.109602881615
H	-1.609219023230	2.089449700986	-2.834738405142
N	-2.086779555729	-1.955357116185	-0.053913872410
C	-2.393360910174	-3.241383738756	-0.277169789588
C	-0.333796472059	-2.862687980258	-0.916039139561
C	-1.293339764899	-3.870968405663	-0.826363600135
H	-3.379856370160	-3.612898247736	-0.031898240517
H	0.670376866999	-2.906966013980	-1.315254195841
N	-1.978004567596	0.724144159759	-1.296914540138
N	-0.811175268541	-1.714670532655	-0.439553955300
N	-1.446937923688	0.529015575870	1.679235408770
Rh	-0.071170752332	0.259608915881	-0.500543934406
C	0.474936117140	2.029741482707	-0.841744420224
N	0.750530205169	3.136358832634	-1.097161007601
C	1.132142257052	4.466909944905	-1.334093678281
H	0.346157632883	5.151482440505	-0.994621494452

H	2.056593891389	4.694485407965	-0.789533174766
H	1.305321945448	4.631434587356	-2.404389389565
H	-2.451691527613	0.646677936469	4.813919462861
H	-1.200579582488	-4.904484558491	-1.124511935550
H	-4.356866045835	2.144198198570	-3.058179868553
C	2.774449324784	0.975105373278	0.638005548630
C	4.028344216080	0.769009380451	1.505940348800
C	3.238387559622	-1.959444122115	-0.828355198681
C	5.320740031968	0.440064102974	0.756352496656
C	4.464670728054	-1.101277625127	-1.143509818938
C	5.431040223771	-0.902622005656	0.033749156163
H	3.087362318295	1.335791665889	-0.353620453518
H	5.495981753551	1.239453082453	0.016355378425
H	2.562021893070	-1.928597363425	-1.697163873105
H	4.151551171132	-0.121904792143	-1.531767718925
H	2.192419768771	1.801021030340	1.069060791071
H	3.566746393919	-3.007043275764	-0.735005200008
H	6.154275841466	0.511224589152	1.471061788097
H	4.997672377720	-1.581061236595	-1.976006915682
C	1.810428917261	-0.218248428234	0.514239343975
H	1.380473960952	-0.208254711473	-0.902971380860
H	1.205937662002	-0.237043234796	1.437183152479
C	2.470964536997	-1.598563728258	0.439116191831
H	3.144424335661	-1.706496034118	1.301965807909
H	1.693632414289	-2.353235056469	0.607533460351
H	4.215205404164	1.704353383573	2.052987115929
H	6.463301126942	-0.982931982548	-0.334666969233
H	5.316891950325	-1.727189920289	0.755146985665
H	3.837407071370	0.017901673254	2.286840114502

TpRh(CNMe)-Cyclooctane TS_2-(4)-κ^2

G = -1258.448196

B	-2.741171401094	-1.154185301126	0.604052464033
H	-3.730367398366	-1.735270849480	0.951148025833
N	-1.842173476165	-0.701716464376	1.757810378245
C	-1.715522293454	0.520465311887	2.322927546253
C	-0.500614953269	-0.956622359524	3.394094440123
C	-0.848087203151	0.405872548841	3.388352400592
H	-2.244496339088	1.378506609596	1.925322179668
H	0.162699259178	-1.485574452548	4.069561567068
N	-3.161701768728	0.099125669283	-0.194521174994
C	-4.380857070219	0.628325723619	-0.361196887324
C	-2.899055822817	1.869564766634	-1.398153908275

C	-4.265756948909	1.771451255908	-1.132312919352
H	-5.244224308077	0.150149221183	0.083786752279
H	-2.355327994294	2.606203517530	-1.977370225612
N	-1.928732303827	-2.061933393698	-0.328826084921
C	-2.196848737138	-3.306686804111	-0.737798035209
C	-0.370940434453	-2.593610312517	-1.719477880870
C	-1.219436507184	-3.696961092580	-1.635764361032
H	-3.062137905102	-3.828879836963	-0.350732078750
H	0.525066954837	-2.452477178011	-2.311081729145
N	-2.243581987849	0.859309751218	-0.831731302750
N	-0.799710207554	-1.616986996272	-0.922213052341
N	-1.100572703231	-1.618594093938	2.414574876430
Rh	-0.182999767132	0.362034361464	-0.693312408267
C	0.277183256586	2.196117929162	-0.687953720747
N	0.520697101440	3.337632864014	-0.725494223047
C	0.912059618963	4.687052926368	-0.684808568062
H	1.856489597656	4.784875528801	-0.135886881825
H	1.051448547818	5.074152709560	-1.700867823690
H	0.146106093492	5.286645178714	-0.180035639121
H	-0.521451496537	1.187053649325	4.059937054442
H	-1.132894669218	-4.641828073090	-2.150830400760
H	-5.056214783213	2.430630193945	-1.458849827643
C	2.500030880947	0.962691755532	0.744362256855
C	3.711746949836	0.626251324596	1.632319043624
C	3.173875701275	-1.610018447363	-1.241396494152
C	5.055150382450	0.494506749746	0.912270391899
C	4.371181377388	-0.661311363952	-1.307666927085
C	5.263205342219	-0.670042003868	-0.056773309153
H	2.853817422867	1.519611142958	-0.135932721139
H	5.236685031301	1.432382294746	0.359958221808
H	2.543889003405	-1.444690848532	-2.130115141967
H	4.032742490554	0.364447308982	-1.511466492749
H	1.855546913537	1.662078276245	1.294485987363
H	3.548120328950	-2.642582972213	-1.326274180256
H	5.844874782947	0.444735996241	1.676766605751
H	4.970126414622	-0.943929884044	-2.184484370870
C	1.606940889925	-0.218297456514	0.339326060244
H	1.241771977258	0.050408901496	-1.227322102153
H	0.948854465547	-0.439267919088	1.199008821731
C	2.319842688868	-1.530543702537	0.018034738644
H	2.946546119319	-1.787122838538	0.885277473002
H	1.565527191889	-2.324828466112	-0.015062071410
H	3.826669078773	1.439218022722	2.363447419168
H	6.316248532133	-0.639439367533	-0.369597241919
H	5.148265608823	-1.626584433458	0.477077797555
H	3.508119755268	-0.270525828327	2.235732873978

TpRh(CNMe)-Cyclooctane TS_2-(5)-κ^3

G = -1258.444733

B	-2.701343290794	-1.197766068877	0.564966974698
H	-3.681392054123	-1.834402570318	0.824480530525
N	-1.669115708857	-1.348675037600	1.677009654259
C	-1.629580995887	-2.233367920045	2.691071818415
C	0.160119119560	-0.965885424210	2.714329466415
C	-0.460342222996	-2.024857867772	3.394658288080
H	-2.435898007131	-2.941021209297	2.838594198877
H	1.101961872536	-0.472490084703	2.930813961416
N	-3.081022121426	0.284573611110	0.386400369665
C	-4.250372399457	0.880323729827	0.664399739435
C	-2.858574304770	2.353531371716	-0.170623323179
C	-4.156919439538	2.216649428707	0.325358305730
H	-5.067941384913	0.304961086247	1.079239555286
H	-2.355156631520	3.227360650734	-0.565392887097
N	-2.135593043830	-1.685758517312	-0.783474935837
C	-2.652593983247	-2.615404362583	-1.599916029634
C	-0.974418711879	-1.620786476699	-2.596525767114
C	-1.932905299543	-2.617532341542	-2.779948613611
H	-3.500584474299	-3.206858259676	-1.279798841667
H	-0.205834956279	-1.266938170193	-3.272607087310
N	-2.220208185282	1.187912947873	-0.131053658646
N	-1.095418537263	-1.071733276093	-1.389577656385
N	-0.572741098467	-0.565899913225	1.684152595133
Rh	-0.213903211271	0.655133183119	-0.567852372276
C	0.353949007181	2.377627787144	-0.053257047468
N	0.637551737590	3.463439091674	0.274033186783
C	1.018884775754	4.760490895079	0.654700179643
H	0.686044630835	4.968270241311	1.678316150107
H	2.110353918624	4.857421377134	0.612954633221
H	0.575043759540	5.503310862677	-0.019054732743
H	-0.115892818863	-2.551069222200	4.273128599247
H	-2.083580960886	-3.243367466551	-3.646748039204
H	-4.919959513280	2.975668668564	0.412473101066
C	1.881380835443	0.053790428191	-0.727949435456
C	2.159325225784	-1.388543369767	-1.178696558458
C	4.848435252709	0.428423175845	0.513362431665
C	2.678571080196	-2.305596698113	-0.066598286071
C	4.249880314486	-0.746093054197	1.301168869439
C	4.071123493263	-2.054756370312	0.518509253996
H	1.857060265670	0.066362003770	0.371104745761

H	1.945260492277	-2.275509739492	0.757266461911
H	4.672551898227	1.362393821564	1.070556600344
H	3.286728387920	-0.465786631253	1.748425532317
H	0.877457606332	0.622311216678	-1.698992611423
H	5.941477767794	0.296856679269	0.499717924587
H	2.657527072449	-3.338616729383	-0.445305592607
H	4.915497881373	-0.929788882011	2.156619680080
C	2.964422169459	1.043878850268	-1.185412934230
H	2.796005658443	2.016369044973	-0.699560657147
H	2.857639123788	1.231747843280	-2.266181374589
C	4.408899941866	0.615244670000	-0.936789641295
H	4.626352227369	-0.301118460449	-1.502560626655
H	5.059202526449	1.382085936144	-1.383750681141
H	1.243347485486	-1.854416322270	-1.547336558411
H	4.281294152249	-2.893903505734	1.196654982549
H	4.833741556476	-2.128142341080	-0.273133377135
H	2.853890867003	-1.393841901098	-2.033980451021

TpRh(CNMe)-Cyclooctane TS_2-(5)-κ^2

G = -1258.445528

B	-2.186929000242	-1.551817452330	0.887337702375
H	-2.929458178261	-2.346685244145	1.391141504117
N	-0.977794898907	-1.197885846326	1.753012432048
C	-0.754703670555	-0.107519984229	2.520459877153
C	0.832265602093	-1.592086844886	2.805605114349
C	0.416270694336	-0.313774200899	3.218673968468
H	-1.439420119241	0.732280151857	2.512723908299
H	1.709756018525	-2.152238442825	3.110677888839
N	-2.977333950583	-0.254601435020	0.608665291949
C	-4.206998604647	0.087178572793	1.014010724032
C	-3.334746941027	1.737080207490	-0.137829504882
C	-4.485926434534	1.363017174523	0.556127030118
H	-4.795357690710	-0.605784525463	1.601978069964
H	-3.113030957906	2.653731566709	-0.671022028914
N	-1.702596291037	-2.109925244156	-0.457119621846
C	-2.045444606073	-3.256481000124	-1.054346078651
C	-0.799094011948	-2.071702108822	-2.412033035937
C	-1.484673018434	-3.281826860275	-2.318422223493
H	-2.659316196051	-3.976724720314	-0.529319212749
H	-0.233011286593	-1.662395884660	-3.239589357718
N	-2.433177474265	0.757883961511	-0.102085693314
N	-0.923861843178	-1.376106017892	-1.282363996889
N	-0.005673960935	-2.118895516462	1.924888325485

Rh	-0.441655639747	0.608388450121	-0.832062648178
C	-0.209056239131	2.469393748921	-0.591270804023
N	-0.130532769580	3.628121602640	-0.469859142426
C	0.101066955346	5.002388307129	-0.285134155663
H	-0.486798265497	5.373000585067	0.562195785515
H	1.164523470621	5.176993529880	-0.081582745895
H	-0.183825171421	5.560581129381	-1.184461850528
H	0.891851551091	0.354884786973	3.922111895873
H	-1.559034443930	-4.061929412384	-3.061031589700
H	-5.392039998850	1.932841690877	0.698247318054
C	1.668134597189	0.218488035076	-0.638575995089
C	2.327972681429	-0.916069850453	-1.438170080350
C	4.555030042141	0.790541451499	0.948767980922
C	2.993538516209	-2.000646802047	-0.583309858120
C	4.106697571725	-0.623329266817	1.314049166428
C	4.267718113567	-1.659283865778	0.191731446797
H	1.410874781076	-0.170771300625	0.362597258196
H	2.236133120840	-2.369126726218	0.128209215473
H	4.266544711117	1.480052179264	1.757847668575
H	3.062234511731	-0.609663368882	1.649507703938
H	0.690093229777	0.632896826725	-1.892365540820
H	5.655782237909	0.811599945003	0.913652573321
H	3.221254307160	-2.848705213598	-1.246723552085
H	4.688634756155	-0.939537617934	2.191385902002
C	2.522660398955	1.490685157902	-0.515534270660
H	2.156492251156	2.079100624688	0.340187309074
H	2.349998057151	2.113916645796	-1.406912883082
C	4.039051834118	1.332031894662	-0.378081024094
H	4.429225526192	0.721017706751	-1.202990568371
H	4.482538483428	2.327450211255	-0.530238570479
H	1.571364174933	-1.432692143779	-2.031984127322
H	4.632888942722	-2.599847476960	0.627420557644
H	5.059625499543	-1.339126248752	-0.505066033285
H	3.037602615047	-0.504254361436	-2.172588764444

TpRh(CNMe)-Cyclooctane TS_2-(6)-κ^3

G = -1258.440921

B	-2.915656983471	-0.975498880120	-0.295791098819
H	-3.960143096453	-1.506490063286	-0.540666543767
N	-2.784566074316	-0.744051037530	1.204353982941
C	-3.556676878093	-1.191722167275	2.211971703803
C	-1.860029408215	-0.047195461312	3.001148129632
C	-2.998333361899	-0.764472555881	3.399821583850

H	-4.444563707797	-1.777532254752	2.009236577333
H	-1.126706976349	0.466802877075	3.613192948949
N	-2.830599420200	0.365553359769	-1.049348801888
C	-3.799918387537	1.005771384160	-1.720390729816
C	-1.939231886067	2.158263490132	-1.842987382037
C	-3.275579966523	2.169899021188	-2.249035601955
H	-4.793800785336	0.580765979463	-1.776430469386
H	-1.146929948486	2.869190849663	-2.042490729208
N	-1.769503486442	-1.864417847149	-0.819784279031
C	-1.876467201791	-3.013130787128	-1.503546544292
C	0.216460900323	-2.367931573551	-1.485740421835
C	-0.621121727691	-3.383464990140	-1.947549892425
H	-2.844209346915	-3.481622069920	-1.627465116996
H	1.282893835333	-2.235372877205	-1.617289660006
N	-1.681221540533	1.070449907843	-1.123405805213
N	-0.478300762408	-1.464396713105	-0.799096324600
N	-1.740517765244	-0.038858970960	1.680905556490
Rh	0.066256818268	0.436998462756	-0.091389826395
C	0.537213788308	2.236856332967	0.211909782223
N	0.792845876351	3.369223823333	0.348343122436
C	1.157005126308	4.709228834350	0.559496704502
H	0.336013643369	5.253930080162	1.040030283845
H	2.040207723941	4.758416269603	1.207914656432
H	1.394369914887	5.196432475679	-0.393839093706
H	-3.363858200331	-0.939232663813	4.401350472958
H	-0.353246613858	-4.255575356888	-2.524940476632
H	-3.782707981615	2.910230912918	-2.849587397456
C	1.748662364219	-0.176833570558	1.153926796945
C	2.925044553908	0.791448010076	1.381828224877
C	3.955385185367	-2.220926796724	-0.488991386001
C	3.773130449808	1.247420315264	0.188772200393
C	4.002955342680	-0.900187844282	-1.257616276451
C	4.697433881605	0.246777553623	-0.508816305869
H	1.571011272784	0.101378599724	-0.349779691982
H	3.100433327818	1.676383283736	-0.571457620295
H	3.316129657580	-2.939092749379	-1.025536303600
H	2.993447758391	-0.581521980253	-1.553434615437
H	1.045820969449	0.022020779210	1.978848459512
H	4.965184210378	-2.660784380515	-0.510080241971
H	4.399084467306	2.082789999018	0.539603627525
H	4.529310633841	-1.086794709336	-2.204224571716
C	2.107998521820	-1.672831941707	1.297036775201
H	1.380632642625	-2.294097954431	0.762909215515
H	1.950886440485	-1.919948616185	2.359130756345
C	3.524804633443	-2.148833344493	0.971458127341
H	4.253927527088	-1.546793720817	1.531623664954

H	3.622153850424	-3.161850169352	1.389074810335
H	2.512943788034	1.705711020696	1.833068802408
H	5.298331518870	0.822898497679	-1.226502784210
H	5.423171187970	-0.161890936489	0.212332800010
H	3.585635594587	0.371362264450	2.158083296243

TpRh(CNMe)-Cyclooctane TS_2-(6)-κ^2

G = -1258.441760

B	-2.681651389747	-1.264908270023	0.220454759152
H	-3.674099843994	-1.929336511624	0.327160540476
N	-2.052353160935	-0.843398040454	1.551498455421
C	-2.250755699217	0.291157894100	2.260369936545
C	-0.981960643731	-1.105730649331	3.375209937085
C	-1.569873769424	0.169603835931	3.452467131250
H	-2.853683126683	1.099789445668	1.864037414209
H	-0.354283082089	-1.609191419948	4.102605280092
N	-3.033632627241	0.024857808932	-0.555143010441
C	-4.230345750780	0.490687571575	-0.934864594823
C	-2.672351613552	1.920776352169	-1.516879543381
C	-4.051550871619	1.711451677128	-1.562052876365
H	-5.125477688829	-0.082168350534	-0.728019464662
H	-2.082587708945	2.744970145082	-1.899973665980
N	-1.639846089318	-2.041011882855	-0.593523569905
C	-1.715137348487	-3.264223711684	-1.130553016481
C	0.191634346219	-2.336087997185	-1.690783655812
C	-0.555669023135	-3.503607435125	-1.846977432465
H	-2.588579677640	-3.879342465853	-0.957543122762
H	1.167826939209	-2.074985220424	-2.081954084431
N	-2.068419838623	0.901779984246	-0.910228901503
N	-0.466103935800	-1.466679288675	-0.927641830067
N	-1.275421200614	-1.711737325719	2.234082735383
Rh	-0.033738886873	0.496536061548	-0.410674844608
C	0.320867333742	2.346145956696	-0.201219347483
N	0.510620524224	3.495563591396	-0.122187768468
C	0.829762519702	4.854708014340	0.042629640148
H	1.012904447947	5.323075216227	-0.931402662783
H	0.004799090766	5.378616550484	0.538545569738
H	1.732391559227	4.953116892693	0.657567418989
H	-1.508827599933	0.891977934141	4.254014081274
H	-0.291821619870	-4.392587965872	-2.399921581670
H	-4.808186343468	2.350246526359	-1.992696289345
C	1.562435663884	0.049638475139	0.944616000178
C	2.688969073798	1.074024158060	1.138255071136

C	3.858440360302	-1.982588528096	-0.593565742101
C	3.560269961227	1.497355691356	-0.051278339414
C	3.931637240059	-0.691552514754	-1.412015528370
C	4.546937028662	0.506970116743	-0.676613811186
H	1.440944256539	0.227798248020	-0.755105078922
H	2.898593691826	1.866702979329	-0.851682166518
H	3.215851686242	-2.711733535783	-1.110501419200
H	2.939178793251	-0.411106197038	-1.790483535105
H	0.811429696394	0.255042696202	1.729190468414
H	4.863833376943	-2.432518077408	-0.586387918763
H	4.143982201285	2.371240262311	0.278266728271
H	4.525765770114	-0.904159873025	-2.312036959950
C	1.983326185606	-1.415303328511	1.162047473987
H	1.269650891768	-2.097171737739	0.688539193470
H	1.838398485737	-1.592467447010	2.240551960651
C	3.414395932374	-1.856534425289	0.858979847089
H	4.123992576198	-1.211597824925	1.396900291018
H	3.537433858694	-2.847616733113	1.320082072250
H	2.234568154466	1.995647817261	1.530466827259
H	5.149880721200	1.083510874518	-1.392475847573
H	5.261980736273	0.155245957188	0.083510568307
H	3.341181311997	0.716698786798	1.952874841391

TpRh(CNMe)-Cyclooctane TS_2-(7)-κ^3

G = -1258.444169

B	-3.002404578201	-0.914367504661	-0.106456260313
H	-4.078691450148	-1.419017555125	-0.247911528271
N	-2.793346466055	-0.534851760694	1.354572247074
C	-3.541235120098	-0.831982650697	2.433591678446
C	-1.755137338836	0.293333566042	3.029194437642
C	-2.909382858141	-0.314473281690	3.546413554090
H	-4.465495417120	-1.386546583044	2.329462924543
H	-0.969111297617	0.825635478662	3.553955753238
N	-2.897084231378	0.333427594617	-1.001160804283
C	-3.868004275787	0.951798598296	-1.690137403370
C	-1.962860811493	1.986786124883	-2.016311164014
C	-3.316192556265	2.027160542043	-2.360022019357
H	-4.882479479648	0.575967606480	-1.656361118411
H	-1.148494691481	2.630671891912	-2.324886371290
N	-1.923297256622	-1.910397033271	-0.578479835205
C	-2.125830125109	-3.136372156185	-1.081854934735
C	-0.004087460947	-2.622956484343	-1.248525690188
C	-0.917328310872	-3.640889133162	-1.521869156111

H	-3.122256348266	-3.558659870751	-1.092961190505
H	1.058135553712	-2.582125647418	-1.445504344044
N	-1.721187957044	0.965229658027	-1.200237528003
N	-0.611664552003	-1.588253881221	-0.672273796103
N	-1.694440415315	0.157148520833	1.711794961767
Rh	0.044533031813	0.351778930276	-0.192379702991
C	0.520429377065	2.164237303820	0.016706587246
N	0.735510969715	3.307400602303	0.125341458988
C	1.077925236951	4.659345992852	0.292463109634
H	0.623402594079	5.057409090412	1.207341611474
H	2.167822610044	4.761063445062	0.364463661334
H	0.724849122350	5.249673156842	-0.561078017126
H	-3.237870666893	-0.363625440570	4.574478234294
H	-0.725825121263	-4.600233680984	-1.978610195947
H	-3.817269327973	2.728054589410	-3.010888320214
C	2.921492983634	0.773591049794	1.226063189536
C	1.791113823487	-0.240328791717	0.972954107325
C	5.214141446481	-0.666547349940	-0.653792298609
C	2.236454498781	-1.706103187316	1.045319542166
C	4.730500353927	-1.726233957820	0.341216725551
C	3.306012260067	-2.250425854443	0.093849629569
H	3.617744758540	0.320774095216	1.948129957423
H	2.619750731763	-1.864201494431	2.069579646967
H	6.123382938804	-0.187855335761	-0.257906734131
H	4.799924306413	-1.346412663173	1.369174411983
H	2.492274983016	1.636546828418	1.757071172764
H	5.527053597568	-1.179443934863	-1.576557258282
H	1.341271583279	-2.336130676742	0.976589997022
H	5.439589489259	-2.564502757432	0.300750756779
C	3.713593907180	1.347994819834	0.041348483166
H	4.575814521010	1.898305316232	0.451926973287
H	3.088206290283	2.103844791740	-0.455736299394
C	4.206252592597	0.405033901878	-1.051476800089
H	3.343065989534	-0.062501047681	-1.544425960662
H	4.668580504550	1.025252994115	-1.833743665368
H	1.097870328932	-0.132745378844	1.825163165726
H	3.304741972315	-3.343339764221	0.212303593821
H	3.027657745707	-2.073474919603	-0.955593724441
H	1.541755942958	-0.028743601788	-0.503411873058

TpRh(CNMe)-Cyclooctane TS_2-(7)-κ^2

G = -1258.445987

B	-2.723087208161	-1.223135492014	0.296870725682

H	-3.724802163342	-1.863402820837	0.452945542268
N	-2.020200693301	-0.824706093677	1.597641373668
C	-2.129291142910	0.321064379038	2.307548263037
C	-0.889833580006	-1.136629087852	3.377249349503
C	-1.406802824000	0.167970796916	3.471297608756
H	-2.704106949658	1.159213166901	1.931301599043
H	-0.259175765488	-1.669723415380	4.080313799951
N	-3.082725122250	0.075525721803	-0.458969958402
C	-4.286484265114	0.572463331321	-0.771597054232
C	-2.726708836264	1.959079755869	-1.447245129086
C	-4.111371094842	1.786439744027	-1.412575891878
H	-5.183155557765	0.024014265001	-0.512100168891
H	-2.137879587827	2.765975657782	-1.866770484719
N	-1.745928831899	-2.025730925118	-0.570458667024
C	-1.885091113668	-3.251890897603	-1.087318101396
C	0.002875050291	-2.377486226258	-1.779850150500
C	-0.781207787622	-3.527163283552	-1.874178302080
H	-2.760341205265	-3.842856515438	-0.850899140637
H	0.951364885875	-2.145495261212	-2.246500138577
N	-2.116725107327	0.925416849254	-0.872491503515
N	-0.581339682244	-1.483035847154	-0.985768824720
N	-1.262571100076	-1.730220859054	2.252519188054
Rh	-0.074630948672	0.467500313288	-0.477676539096
C	0.305596178606	2.303316416005	-0.209832245419
N	0.488966305951	3.447825526281	-0.069267375406
C	0.827079739335	4.793278357980	0.158317272467
H	0.714037004044	5.375514999477	-0.763476620562
H	0.176829619737	5.221302919863	0.929740058066
H	1.868937712155	4.861397261873	0.494277261878
H	-1.274731602789	0.888907136910	4.265540837574
H	-0.575560391721	-4.427242322041	-2.433747276870
H	-4.874063461077	2.444110598659	-1.802151992606
C	2.684289529653	0.952303374694	1.059401015153
C	1.560338025926	-0.059368075734	0.796715031673
C	5.046170354569	-0.520444633256	-0.696618354865
C	1.982164672042	-1.527325991770	0.874638237076
C	4.501916922665	-1.576536019829	0.271714742213
C	3.081692378807	-2.084169297098	-0.031039546137
H	3.356525580491	0.502930828966	1.806112277233
H	2.322569013267	-1.677060232316	1.916358872732
H	5.932641647154	-0.043316988120	-0.250275225799
H	4.533969202755	-1.200814833938	1.303176226693
H	2.245262913567	1.823529764065	1.568976868330
H	5.411047912051	-1.036177448901	-1.598373032108
H	1.081923535088	-2.146226765477	0.785889292638
H	5.201861117202	-2.423363473916	0.259034919307

C	3.514669725743	1.508463173409	-0.106865713848
H	4.351928647770	2.079602700649	0.326094698513
H	2.898776261002	2.245712229090	-0.643931063484
C	4.068113391154	0.552589351454	-1.159074967189
H	3.237239086703	0.079939584055	-1.699654718631
H	4.576731553559	1.165759674064	-1.917934258130
H	0.828889781470	0.063384241141	1.617375672135
H	3.062715003292	-3.175918732007	0.092244217028
H	2.838767661277	-1.913457838513	-1.089760973010
H	1.396865093275	0.169514490326	-0.856583830986

TpRh(CNMe)-Cyclooctane TS_2-(8)-κ^3

G = -1258.444694

B	-2.678330099448	-1.337080636722	0.445230631490
H	-3.627310431038	-2.038422565968	0.646725606811
N	-1.693572872662	-1.439999132116	1.605732987764
C	-1.631879519242	-2.349532687269	2.596469039047
C	0.065308243612	-0.965741983407	2.724929156345
C	-0.507167745525	-2.083272302991	3.351624958939
H	-2.392595402472	-3.114264581355	2.692759189110
H	0.965767111144	-0.419880131426	2.988011496533
N	-3.141833094212	0.121009036401	0.264932036027
C	-4.357927713711	0.638596828517	0.494708067655
C	-3.025785419888	2.207121126696	-0.260197983088
C	-4.334020861898	1.982462414729	0.173930258036
H	-5.155489022385	0.007600374707	0.865256369043
H	-2.561069941951	3.115793228461	-0.622493971759
N	-2.013113374416	-1.768014642106	-0.877323279499
C	-2.418445622579	-2.721179517521	-1.728943567214
C	-0.746768166627	-1.614822273903	-2.613117830646
C	-1.627373653523	-2.667867981265	-2.861335261881
H	-3.245047078087	-3.368092208797	-1.465145338600
H	0.040812566885	-1.208544002794	-3.235901794278
N	-2.317434237666	1.083406765343	-0.203355563519
N	-0.978592915919	-1.084622852169	-1.414100435564
N	-0.653992887799	-0.586200911006	1.677761111704
Rh	-0.260142415339	0.685534459697	-0.527658812760
C	0.173945167328	2.430306784832	0.038523546038
N	0.391830248655	3.521254604609	0.397723710033
C	0.669959967562	4.834201005133	0.812671870393
H	0.186085123840	5.037092964112	1.775146064137
H	1.751746740996	4.970061928901	0.927745730703
H	0.302447363093	5.555514417983	0.072723317402

H	-0.161654307380	-2.610371892529	4.229178922231
H	-1.684072807475	-3.294431858679	-3.738785172189
H	-5.146831551874	2.690782949449	0.233320818466
C	2.233590130620	-1.230508210733	-0.915455647922
C	1.872529855623	0.216146130872	-0.546096371990
C	5.125758330204	-1.135840024455	0.559692947543
C	2.936624913190	1.228741200482	-0.999422016741
C	5.161535643228	-0.060053381325	-0.534697653975
C	4.294110700383	1.184097352956	-0.286612793688
H	2.981476398894	-1.226260823790	-1.719795079406
H	3.111682343722	1.103801436828	-2.081875014260
H	5.581793219365	-2.057202387095	0.165075762138
H	4.901541576807	-0.491379897110	-1.509916821169
H	1.370021028128	-1.752134909412	-1.332555551569
H	5.786560290702	-0.806898264718	1.376950413905
H	2.536737775659	2.245412741747	-0.884911752695
H	6.209551988249	0.254423408170	-0.638648288704
C	2.715980410161	-2.079846093478	0.266977152117
H	3.085502331206	-3.042452529514	-0.120552329653
H	1.837073962659	-2.320254314347	0.885602649583
C	3.772750183078	-1.470026337469	1.181439888074
H	3.365707318056	-0.570245064281	1.665771858614
H	3.949637559075	-2.175563138298	2.006634965496
H	0.906827876444	0.729698005342	-1.585466164216
H	4.852410002741	2.068362143527	-0.626786959055
H	4.147852476156	1.332976266784	0.795219934471
H	1.796786290784	0.292987117209	0.551354562264

TpRh(CNMe)-Cyclooctane TS_2-(8)-κ^2

G = -1258.445598

B	-1.858894483240	-1.729266968593	1.063350636863
H	-2.412015989100	-2.613832206431	1.652821812879
N	-0.793393103775	-1.007989378526	1.893840318172
C	-0.830267654947	0.211665908529	2.476522668868
C	1.035342644196	-0.824847171185	2.973407933329
C	0.341184363451	0.378691122618	3.184539116552
H	-1.680706698969	0.870033686593	2.345818216441
H	2.004372934343	-1.126118739456	3.357332758160
N	-2.917708042953	-0.691439244856	0.629448724828
C	-4.205987369343	-0.603266212624	0.987473848177
C	-3.700169044356	1.073398589003	-0.333553347547
C	-4.756139474207	0.516777985634	0.390469903488
H	-4.637233839150	-1.347656405705	1.644650622053

H	-3.677732724770	1.955479468843	-0.962275156080
N	-1.211402306024	-2.311131349623	-0.202975651934
C	-1.205623640837	-3.579651044359	-0.627955188518
C	-0.276313460428	-2.298399564538	-2.144589801640
C	-0.610534661680	-3.625502051742	-1.875374689729
H	-1.622339662769	-4.360142932066	-0.004683768050
H	0.186783466297	-1.871421133913	-3.024677605302
N	-2.600273205443	0.339810932501	-0.185363228721
N	-0.631120221633	-1.514212589486	-1.128880824122
N	0.351515558476	-1.655561038835	2.197905742534
Rh	-0.592586295680	0.558242840561	-0.847528105569
C	-0.692259030708	2.440847248079	-0.707460807292
N	-0.789281192321	3.602962359721	-0.646450409595
C	-0.810362440356	5.004769967570	-0.544320777093
H	-1.565034982885	5.317845355656	0.185983850123
H	0.170324742817	5.371231821753	-0.218236035671
H	-1.050710287740	5.452994819616	-1.515437437698
H	0.641893527575	1.236056861749	3.769971687521
H	-0.444190930510	-4.491142542367	-2.498749056936
H	-5.773150641408	0.872177547327	0.463366845275
C	2.435871174827	-0.341767589975	-1.578011451335
C	1.531733405379	0.413789555190	-0.580146379710
C	5.012646290085	-0.421430933255	0.357469627044
C	2.149063486661	1.702410984384	-0.043476691418
C	4.692881271458	1.063500023533	0.130456238510
C	3.418740412665	1.578804768272	0.814933993054
H	3.172793942704	0.357390460314	-1.995278337991
H	2.358300837889	2.383724615614	-0.887259502346
H	5.776395047496	-0.738545633544	-0.369962605309
H	4.651774555159	1.295908754574	-0.941545797918
H	1.860174630051	-0.679620383384	-2.446278509359
H	5.491243011478	-0.512533661691	1.344934824350
H	1.406379169156	2.203210619115	0.590845157381
H	5.551317540511	1.638010776365	0.506315222904
C	3.120661782095	-1.580676381280	-0.995487785990
H	3.821271906535	-1.979891523994	-1.746444536850
H	2.347781700593	-2.353027670650	-0.853512297817
C	3.845326773383	-1.403517699631	0.332652976280
H	3.114902561072	-1.131904418054	1.106434940196
H	4.226828057322	-2.387952414896	0.639904376146
H	0.568412348151	0.819219104380	-1.837396466147
H	3.616041341066	2.589041522671	1.202300111222
H	3.190032374256	0.969611527776	1.703075455308
H	1.304594302291	-0.255067576925	0.267405023700

TpRh(CNMe)-Cyclooctane TS_2-(9)-κ^3

G = -1258.445872

B	-2.748852848202	-1.407852673244	0.227379475595
H	-3.693262661572	-2.140848707053	0.292300154539
N	-2.000521041998	-1.399909848456	1.556738929630
C	-2.090070798561	-2.262078336754	2.587186509349
C	-0.462624392458	-0.831720681993	2.928480720961
C	-1.113863327552	-1.932937212774	3.505790875379
H	-2.841424167019	-3.041937358766	2.591149507699
H	0.367391760619	-0.249030973812	3.313800380987
N	-3.224394227013	0.011507332060	-0.135778497693
C	-4.483062271257	0.474130343979	-0.172237258105
C	-3.100989228096	2.069858403875	-0.761348248769
C	-4.456775289366	1.797855300920	-0.567990110097
H	-5.308451710500	-0.178075792158	0.082385645566
H	-2.614873758594	2.980904891422	-1.087713032502
N	-1.820486828087	-1.890904055585	-0.904365434799
C	-1.967273563313	-2.963708780865	-1.695246139750
C	-0.204250395880	-1.825373097945	-2.326718925175
C	-0.945250327134	-2.969112833211	-2.626042176736
H	-2.793597112565	-3.644778497505	-1.538015119991
H	0.676219552982	-1.423908391256	-2.812414277868
N	-2.368597535929	0.991332721401	-0.500218355126
N	-0.732349370415	-1.187193297433	-1.285354211159
N	-1.001840579482	-0.517706622372	1.758630638207
Rh	-0.279509556217	0.684084408110	-0.440326137488
C	0.004162137484	2.488244997371	0.025037422998
N	0.147172002652	3.613506739711	0.310323302110
C	0.319815880320	4.969518667128	0.633994613982
H	1.352833670186	5.151251806035	0.952731754565
H	0.104879038965	5.601860441482	-0.236116941610
H	-0.353842888231	5.251767594711	1.451493293254
H	-0.912145972891	-2.410126048111	4.453931959651
H	-0.768268656950	-3.689676863264	-3.410393281957
H	-5.295893728405	2.462945166877	-0.707188320067
C	4.228892490648	1.285767253609	0.344806560965
C	2.957062859677	1.243201608529	-0.518336551656
C	4.600402792363	-1.941232863969	0.284853859842
C	1.836667140804	0.303399076976	-0.029634005664
C	3.238616527628	-1.661472653155	0.928861797622
C	2.124908024793	-1.200479741789	-0.030383375247
H	3.984366030577	0.981032167511	1.370125146113
H	1.633674604903	0.587492365066	1.019002081387
H	5.352170755535	-2.078406912409	1.077981032711
H	3.336258523050	-0.939927284978	1.749993009944

H	4.562595184816	2.329700658962	0.432650204075
H	4.536313950947	-2.910667393302	-0.233376306719
H	1.063325499296	0.661793918966	-1.253476645887
H	2.912911022729	-2.592281977363	1.413508074799
C	5.414436491746	0.477844220800	-0.194474353178
H	6.189750228013	0.412931421540	0.584796567015
H	5.868537823114	1.051119332919	-1.017764054503
C	5.111967081209	-0.919527253925	-0.723871905245
H	4.400885871921	-0.847104126374	-1.559767276076
H	6.034622853456	-1.317238588502	-1.171104561866
H	2.528642151124	2.253383047595	-0.559819127766
H	1.197037065394	-1.702308153115	0.267740775311
H	2.340053712417	-1.557067011176	-1.049569822573
H	3.222001361208	1.009316872915	-1.562190408519

TpRh(CNMe)-Cyclooctane TS_2-(9)-κ^2

G = -1258.446028

B	-2.382454931012	-1.553854059419	0.743891005389
H	-3.173257301468	-2.350252859149	1.165498639653
N	-1.357081348674	-1.071644894369	1.775288078867
C	-1.382462576841	0.041338420024	2.543547485039
C	0.346321954010	-1.207041675080	3.049883164531
C	-0.292328965440	-0.000112655470	3.385701399190
H	-2.166902861309	0.780556202170	2.431555235437
H	1.249189342807	-1.638046410176	3.469121757328
N	-3.150405903948	-0.311492007810	0.241341147162
C	-4.447754824901	-0.002952769752	0.363168305725
C	-3.400932282044	1.633207003517	-0.656318331678
C	-4.661466652955	1.242023140552	-0.202336307822
H	-5.125942822868	-0.694095230427	0.847486807121
H	-3.099258336512	2.535801256947	-1.174074932160
N	-1.640508842231	-2.168532051741	-0.450347535840
C	-1.747451382685	-3.394274294463	-0.976390680590
C	-0.340342008048	-2.207851483601	-2.169850060473
C	-0.926636153983	-3.470846271648	-2.087554015684
H	-2.397724068624	-4.126580747714	-0.515855741686
H	0.373356047598	-1.817548791490	-2.884914431839
N	-2.498930896531	0.692775435707	-0.385572381856
N	-0.771432265491	-1.433884870286	-1.177247613843
N	-0.298278500114	-1.849337575926	2.086323873065
Rh	-0.402864048863	0.555694261990	-0.706027260700
C	-0.230066743142	2.422887264532	-0.434889985323
N	-0.187358502586	3.578385687790	-0.270911684600

C	-0.069066080968	4.961863627371	-0.050668562970
H	-0.547369333001	5.234861609401	0.896944501511
H	0.989319599694	5.244115317118	-0.006708011365
H	-0.549221718683	5.518783482532	-0.863647364159
H	-0.004664429407	0.730136646058	4.128694202311
H	-0.775466269288	-4.317192158178	-2.740598707740
H	-5.593578330198	1.781697529362	-0.279272552215
C	3.918991955662	1.515673013161	0.348373160715
C	2.708633876528	1.348977289782	-0.589290027787
C	4.643718665863	-1.647435655854	0.267900539719
C	1.670460085584	0.303876817938	-0.149937388366
C	3.224537766481	-1.517963711952	0.829781460937
C	2.124323175067	-1.156269346364	-0.188324420547
H	3.650811597733	1.168093829888	1.353568999653
H	1.376293986298	0.531755461325	0.893842648372
H	5.355602114739	-1.724969607306	1.104802669831
H	3.198641845307	-0.805397781699	1.663829090665
H	4.128012568091	2.588408857564	0.468641772799
H	4.711327780473	-2.606960388153	-0.268035675379
H	0.884987803261	0.496707360225	-1.569550453474
H	2.961649762927	-2.483920750993	1.283646555825
C	5.217950945267	0.854767961876	-0.127015757485
H	5.946047274024	0.862952499718	0.699067878430
H	5.654525566717	1.490591608011	-0.913191577487
C	5.108847192628	-0.557675579131	-0.690756661197
H	4.452972335349	-0.547883606064	-1.573258454327
H	6.098323816921	-0.843054008059	-1.076890561138
H	2.202887325198	2.317704478950	-0.670106178860
H	1.258277413246	-1.778716355171	0.044991281058
H	2.440821648621	-1.435501085697	-1.206613170203
H	3.054306255720	1.126926019630	-1.611458131538

TpRh(CNMe)-Cyclooctane TS_2-(10)-κ^3

G = -1258.445379

B	3.099824609320	0.841198936129	0.005500892925
H	4.200557517860	1.305694957182	-0.071395055659
N	2.782272021466	0.488801545955	1.452483100275
C	3.469023929022	0.772742847247	2.575068177491
C	1.615146802020	-0.293561853672	3.062440868427
C	2.751957920150	0.284343713482	3.648554156570
H	4.414976547968	1.297526369953	2.526461080473
H	0.782571460333	-0.799656973114	3.539045135812
N	3.013196484907	-0.417318901333	-0.880542527664

C	4.013691881514	-1.068467487901	-1.492674252024
C	2.112735169471	-2.066214822115	-1.934654328153
C	3.484653675013	-2.141465299719	-2.184293435564
H	5.032022831696	-0.715320220308	-1.393640884544
H	1.307001441050	-2.697117698315	-2.289056912122
N	2.090416986378	1.864483124208	-0.554314396502
C	2.366158302437	3.058268908832	-1.099320867944
C	0.250842438603	2.585390249596	-1.414087762228
C	1.210509820731	3.567571075888	-1.660099975905
H	3.371585971717	3.456014453534	-1.051653100196
H	-0.790996603402	2.550565473362	-1.705532389187
N	1.839057619187	-1.027550501458	-1.150996237716
N	0.782879417242	1.569783930017	-0.737553721906
N	1.642449593888	-0.167454034251	1.742920484475
Rh	0.025986343592	-0.341974556393	-0.296120412689
C	-0.621606453064	-2.109640441167	-0.246609277295
N	-1.000558614870	-3.215441608254	-0.271607827177
C	-1.522227990607	-4.519300376681	-0.261772473116
H	-2.242369371527	-4.630661169849	0.558248110059
H	-2.031446201425	-4.734779327841	-1.209097760514
H	-0.715563179614	-5.247849104894	-0.120520963492
H	3.015703751094	0.332476880831	4.695167666557
H	1.082861166076	4.506870479567	-2.176957071256
H	4.012732313376	-2.863323275484	-2.789250904646
C	-3.232482885563	1.939463168314	-0.675263295822
C	-2.318391413739	1.791113152636	0.554518777999
C	-5.138799731569	-0.557441619349	0.244111945490
C	-1.710824026395	0.403481465069	0.812408855702
C	-3.715471727433	-1.118107877123	0.128971374531
C	-2.735152727892	-0.659359561651	1.223446014292
H	-2.986712275161	1.164072371055	-1.414422866933
H	-1.440001839473	0.105102264405	-0.633745124643
H	-5.679520633389	-0.763292640991	-0.692875978840
H	-3.293431375461	-0.889837777462	-0.858587935578
H	-3.004856601253	2.889862940185	-1.180662468026
H	-5.669137724848	-1.127273045264	1.023075375881
H	-1.013795075479	0.528648658148	1.657203513894
H	-3.796392671495	-2.215459948805	0.148674326122
C	-4.741715799830	1.943784634362	-0.398472066543
H	-5.275688144954	1.839349181522	-1.355850036017
H	-5.014127552405	2.939627461138	-0.015929079568
C	-5.283784136722	0.920993947117	0.595501563731
H	-4.840219467437	1.106642274704	1.583620321502
H	-6.356220608137	1.125823797437	0.728253322921
H	-1.491871811850	2.506985687782	0.486974038567
H	-2.187931488584	-1.524087822254	1.617396009951

H	-3.304049357894	-0.272226677380	2.084815892829
H	-2.873269443835	2.087932894740	1.459738601894

TpRh(CNMe)-Cyclooctane TS_2-(10)-κ^2

G = -1258.447381

B	-2.729884108418	-1.270636345169	0.419758340676
H	-3.711499593378	-1.928466464169	0.624269326961
N	-1.901780372755	-0.972671309310	1.672564822877
C	-1.935772894009	0.111205682265	2.479197886269
C	-0.613678356573	-1.428330965278	3.308226770478
C	-1.109945041226	-0.135880967333	3.555095495811
H	-2.535915001281	0.977425783280	2.226401283136
H	0.075677495737	-2.016541896244	3.904022101771
N	-3.167413719387	0.077658847699	-0.196512488846
C	-4.400986104011	0.583001114799	-0.326296294394
C	-2.937974823743	2.030022172535	-1.084043664576
C	-4.307626403529	1.840733111608	-0.895689971494
H	-5.258446047764	0.007857427571	-0.000584110076
H	-2.406397094698	2.871759026263	-1.511512447864
N	-1.840557148082	-1.996909545987	-0.594232157180
C	-2.013554705829	-3.187685090273	-1.178584055052
C	-0.189652367223	-2.249836943447	-1.956184625539
C	-0.973232898951	-3.398599937947	-2.066033688479
H	-2.863301390263	-3.803013495504	-0.913055416863
H	0.720873532557	-1.977224785155	-2.474664409843
N	-2.259958319853	0.965339884359	-0.661692028334
N	-0.715135313756	-1.416756362395	-1.060248002718
N	-1.092438986216	-1.928361007805	2.177769097537
Rh	-0.186828518883	0.525082610263	-0.537236328873
C	0.240194278958	2.358565055627	-0.353351181795
N	0.483809153764	3.500317827297	-0.305871422308
C	0.861295912217	4.848998567074	-0.186430015244
H	0.014045557131	5.448024157045	0.166203979017
H	1.684159326963	4.945750273749	0.532187523777
H	1.191160869152	5.238789497475	-1.156570074876
H	-0.898460056188	0.518999745896	4.388407495207
H	-0.807525908777	-4.257842751787	-2.698409321208
H	-5.113200669356	2.515999901183	-1.142692134963
C	2.991869235825	-1.739821168060	-0.813360120053
C	2.083757212060	-1.486822871585	0.401860711926
C	4.989515039592	0.735927908600	-0.068024430746
C	1.541041025974	-0.070453613878	0.598897279972
C	3.586975104935	1.339953068931	-0.220588275165

C	2.595992501035	0.992993610983	0.903107142259
H	2.781336187307	-0.996858978479	-1.595487705608
H	1.275506234765	0.253362638366	-0.985208754485
H	5.533007273607	0.852559335706	-1.018591190089
H	3.155568061306	1.060720700579	-1.190180518663
H	2.720944797962	-2.706045413125	-1.262531061722
H	5.544193485838	1.341060473605	0.665942878517
H	0.852913371908	-0.110156025122	1.462223215211
H	3.706498901632	2.432293791923	-0.274245235928
C	4.498683862230	-1.786816918760	-0.530926879118
H	5.039038022193	-1.772456841479	-1.490464735712
H	4.728675152398	-2.763194947560	-0.077160818629
C	5.079074949150	-0.717710900702	0.389801186234
H	4.627585107129	-0.815483401265	1.387124219593
H	6.143082648954	-0.951598173766	0.540877790028
H	1.227487976207	-2.169742498835	0.384198818279
H	2.080102322680	1.899952784008	1.238481656944
H	3.154790306553	0.651441270421	1.789945735801
H	2.629984089306	-1.748443263798	1.324303053435

TpRh(CNMe)-Cyclooctane IM-(1)

G = -1258.451320

B	-2.908289006637	-0.592166525747	0.269943066153
H	-4.039484276745	-0.909826045057	0.495587417546
N	-2.098148226205	-0.210860959613	1.523578404377
C	-1.799313323102	1.023455937469	2.018337517387
C	-1.335629361337	-0.535667478247	3.488969947484
C	-1.289058306289	0.855818722762	3.285762150794
H	-1.993493930802	1.917752875108	1.437626588182
H	-1.025861300124	-1.103571354583	4.359319003357
N	-2.891626166712	0.622514215041	-0.677918101597
C	-3.895463923335	1.342241429958	-1.201168383010
C	-1.973749206279	2.089494010649	-1.959609255738
C	-3.354369209181	2.304038610982	-2.034264176124
H	-4.922199764631	1.114119510113	-0.944541829601
H	-1.163236465014	2.608633636989	-2.457493201890
N	-2.169491669932	-1.741467065020	-0.430448931524
C	-2.650524783774	-2.866017414233	-0.972408033300
C	-0.531571021098	-2.648129930192	-1.501541736671
C	-1.632120256770	-3.488956025378	-1.671084243181
H	-3.683755556752	-3.146112817828	-0.812884741815
H	0.479027927302	-2.745510573384	-1.878760947748
N	-1.708089173471	1.074791913810	-1.145425491780

N	-0.861348405040	-1.604705571560	-0.745790600475
N	-1.828132910735	-1.170026980244	2.437114312434
Rh	0.049854468337	0.191243368536	-0.231781719805
C	0.826275563281	1.892650393993	0.112034186140
N	1.301061094370	2.941249307913	0.281707511640
C	2.033439371485	4.113913310326	0.544733098217
H	2.272316581355	4.169798445088	1.613156649638
H	2.967560142123	4.099534871415	-0.029406678734
H	1.450411560221	4.997020189739	0.262082760368
H	-0.939626096010	1.622846444556	3.962070147473
H	-1.676519094934	-4.420315414995	-2.215346840734
H	-3.881960753198	3.045405620348	-2.615952165957
C	3.285535190599	-2.343552952531	0.120895062561
C	3.407532534355	-1.748036657400	-1.288378845326
C	2.560367480407	0.168955702675	1.663633841723
C	4.305909587231	-0.517960590287	-1.371552119370
C	3.773999265183	0.728735515344	0.863166191551
C	3.803589264533	0.744628986674	-0.672938229619
H	4.096487547161	-1.947731858320	0.751257199672
H	5.298882312745	-0.778435992820	-0.967174000256
H	2.978639257925	-0.418857778548	2.500897258905
H	4.689354076863	0.215580052331	1.195039357604
H	3.465854294016	-3.427147860703	0.078758021701
H	2.061853866113	1.016739624706	2.156134293261
H	4.468714966980	-0.271732765417	-2.431766443994
H	3.914780944288	1.769078338928	1.197881996772
C	1.945443575186	-2.132018496384	0.823029841313
H	2.045905625743	-2.577631898634	1.829231151109
H	1.176231319002	-2.733961890374	0.328202143542
C	1.460616460718	-0.691747271326	1.021924432635
H	0.889429066252	0.152243098307	-1.492640784371
H	0.694706567304	-0.772778155723	1.824378702090
H	3.809911829417	-2.505194232548	-1.976144925478
H	4.484982200557	1.558415362632	-0.967285290094
H	2.826515777407	1.011248290996	-1.088285200611
H	2.410087469649	-1.488809230293	-1.672967336827

TpRh(CNMe)-Cyclooctane IM-(2)

G = -1258.463202

B	-2.507193533252	-1.079198458893	0.760462847001
H	-3.295697385551	-1.757000298734	1.352268813888
N	-1.236817003486	-0.717272024743	1.570200027898
C	-1.072608221422	0.339240815169	2.423716254702

C	0.367369344095	-1.251147227193	2.878501645861
C	-0.034051376300	0.044816386106	3.269145492410
H	-1.711019877926	1.212213792056	2.350298741395
H	1.160248604361	-1.865746429838	3.291427863172
N	-3.152185275078	0.261401338617	0.364411726159
C	-4.390714969177	0.745178000766	0.542543784798
C	-3.170447971040	2.206929304328	-0.555990249833
C	-4.452815012118	2.000765683873	-0.033265686648
H	-5.137073609337	0.160248297557	1.064976221526
H	-2.771927764877	3.055222120154	-1.099683972008
N	-2.050483877635	-1.786704523062	-0.521684726646
C	-2.531143319447	-2.871911050209	-1.141448657576
C	-1.045859652060	-1.889038250811	-2.428688599854
C	-1.912349635291	-2.983201378186	-2.373406631516
H	-3.276739009351	-3.489602389734	-0.657758986774
H	-0.359555811614	-1.583720054250	-3.208515147603
N	-2.399363117312	1.154473138070	-0.313230795674
N	-1.133724928551	-1.180834810860	-1.309798768734
N	-0.358910976669	-1.711419184117	1.879835250688
Rh	-0.313185502277	0.550657387680	-0.532276585272
C	0.376050851287	2.170617541509	0.190213049867
N	0.806667903417	3.149619372283	0.647950603604
C	1.402717066910	4.304305324825	1.187153730412
H	1.380691543737	4.259633593923	2.281584592924
H	2.444494435973	4.373496323131	0.854083224257
H	0.860876694104	5.197102712871	0.856146423689
H	0.376769445928	0.666862087758	4.051677064494
H	-2.061200851284	-3.748640814130	-3.120180275487
H	-5.302460123909	2.666304496581	-0.073748271230
C	4.109297529870	0.543262835966	-1.234316499467
C	4.597902376288	0.534157963617	0.222092022134
C	1.790983932368	-1.628625374728	-0.759029669660
C	4.905630983459	-0.846684152689	0.803687631696
C	3.114400212568	-2.316392226791	-0.361011997538
C	3.758480623262	-1.848010541357	0.952182192955
H	4.464005913358	-0.362043602880	-1.742878437359
H	5.682422902649	-1.311652703909	0.172962355494
H	1.602362685499	-1.853186421259	-1.820317671204
H	3.856490648067	-2.242860371558	-1.167346705511
H	4.591317543360	1.374145023354	-1.770689551122
H	0.992269583840	-2.129843955852	-0.197649452708
H	5.371152732569	-0.707059513444	1.791429501165
H	2.893664310000	-3.390597017373	-0.281255537825
C	2.591736783126	0.714860143257	-1.410796307246
H	2.337260155333	0.532257519545	-2.467470093854
H	2.374981123912	1.781878559740	-1.247909894183

C	1.665813046455	-0.123715227019	-0.523903261717
H	1.933449417955	0.064467735232	0.534102089271
H	-0.056018054995	1.129700272567	-1.914168029186
H	5.523713355701	1.123481106412	0.293431232681
H	4.170334936550	-2.723424865705	1.474865245570
H	2.988379051558	-1.441797179104	1.624619068321
H	3.868173122402	1.055058171483	0.863517765403

TpRh(CNMe)-Cyclooctane IM-(3)

G = -1258.462158

B	-2.367662601579	-1.386085746314	0.762507733326
H	-3.136404885350	-2.094801738986	1.344352935355
N	-1.446223603882	-0.546690653864	1.680729116035
C	-1.729598004058	0.664529354369	2.251227008905
C	-0.161015744948	-0.373157731425	3.379831120566
C	-0.908260038368	0.824885303263	3.336583945641
H	-2.491741547973	1.308014832508	1.826402612006
H	0.611879343416	-0.661466019290	4.084383364026
N	-3.136451827925	-0.376398536161	-0.110683553554
C	-4.448580893031	-0.196542985473	-0.325032364464
C	-3.293251256692	1.231563166466	-1.532403927931
C	-4.602190347712	0.832968044763	-1.235248590701
H	-5.176585254781	-0.815109616610	0.184428925981
H	-2.940439757737	2.003184966197	-2.206420019867
N	-1.463242093344	-2.214922782668	-0.156797241096
C	-1.588038091618	-3.477738998628	-0.584417510909
C	-0.034763324137	-2.456383024753	-1.755607754726
C	-0.685484477682	-3.684490535508	-1.610728277236
H	-2.310536198004	-4.138877653435	-0.123591275405
H	0.743619817776	-2.162730950453	-2.446610164515
N	-2.421709288915	0.495938402137	-0.853863359892
N	-0.502695217847	-1.583176329211	-0.871398964858
N	-0.493736349191	-1.196491009124	2.407263409194
Rh	-0.271007590626	0.429716534754	-0.424063577145
C	-0.203497307904	2.294377856839	-0.059692550029
N	-0.195277049383	3.434823548880	0.171089600591
C	-0.102564989472	4.808202219847	0.460969845259
H	-0.410919802215	4.993439435457	1.495828922988
H	0.931860453403	5.146256856986	0.331310540932
H	-0.752108534993	5.379450537146	-0.211384473806
H	-0.848828463546	1.676245703150	3.999706673979
H	-0.517392147408	-4.592570184962	-2.170114287164
H	-5.524990307076	1.231530449468	-1.630401412228

C	2.231257431626	-1.096806661627	0.450232212530
C	2.957403598355	-1.684689259762	-0.771953717576
C	3.967264180366	1.613339319076	0.361754257887
C	4.484520078950	-1.718031323643	-0.686004899240
C	5.000933082372	0.498608676450	0.554481356651
C	5.241801570757	-0.389386394615	-0.674182526662
H	2.922362291782	-1.128635213942	1.307438769064
H	4.763491525445	-2.277100638311	0.223067447391
H	3.718964328722	2.043900608475	1.345302049933
H	4.736354582779	-0.135172228087	1.410873850435
H	1.410711807863	-1.758053775342	0.749511690175
H	4.459857113432	2.423800345900	-0.201006100827
H	4.862999817106	-2.315698271922	-1.529383517470
H	5.946776068023	0.981248242069	0.839894506864
C	1.681650266193	0.331511322707	0.300293568657
H	1.512771854067	0.710985519655	1.331087042917
H	0.294443406183	0.740597519444	-1.804690650310
C	2.667622054813	1.285556352803	-0.381372342120
H	2.910606970125	0.912106010268	-1.386641350524
H	2.175875953637	2.249592476255	-0.569271713350
H	2.626467626239	-2.723799914873	-0.912827434600
H	6.312899826945	-0.630798383604	-0.730888147236
H	5.022983470032	0.175684521519	-1.594405377385
H	2.654125476987	-1.154843564254	-1.688889424462

TpRh(CNMe)-Cyclooctane IM-(4)

G = -1258.462816

B	-2.771832778965	-0.963075746191	0.748026562859
H	-3.758381802804	-1.426268372930	1.241232873537
N	-1.758742278438	-0.394759808775	1.763230724650
C	-1.580886302555	0.893565394620	2.177833306496
C	-0.552088941142	-0.502699131110	3.519739061973
C	-0.789671490031	0.867950622156	3.302775745603
H	-2.049030870267	1.715940801437	1.649237152548
H	0.030004769133	-0.971864643726	4.305385698363
N	-3.156713971267	0.185337067207	-0.204537175660
C	-4.351516976719	0.707167112836	-0.520411649571
C	-2.775901706070	1.699131017581	-1.687340387464
C	-4.158881381510	1.690876341712	-1.472866253290
H	-5.251900463868	0.337545298790	-0.046296737304
H	-2.182047539144	2.308743555010	-2.358184703796
N	-2.035785227268	-2.029264269961	-0.073632936641
C	-2.446714906430	-3.231106583752	-0.493514803816

C	-0.536928361391	-2.732978518005	-1.455323582407
C	-1.512754098746	-3.728367453570	-1.384153499995
H	-3.372341603654	-3.649607379803	-0.119904908516
H	0.375466870139	-2.699549969737	-2.037457881863
N	-2.185095398419	0.787784829705	-0.923959099701
N	-0.854667355847	-1.718815884714	-0.655925724528
N	-1.140411046023	-1.255458127041	2.606317144951
Rh	-0.159415672486	0.218355862275	-0.343822889509
C	0.342914196159	2.042500320932	-0.180088349931
N	0.589055988452	3.178766907434	-0.125582612458
C	1.043325123600	4.501734350899	0.024660446848
H	2.008803736973	4.502882334179	0.544580150704
H	1.165494750697	4.971497776480	-0.957517901375
H	0.321445002488	5.083232024085	0.608415272226
H	-0.440190077107	1.710734710440	3.882006909548
H	-1.529135323455	-4.677159237839	-1.899132032138
H	-4.909490226251	2.305144385203	-1.947947387762
C	2.584819991483	0.713661804028	0.931137630620
C	3.935027414720	0.298879527330	1.545837029258
C	2.907610648911	-1.483200521586	-1.505811728046
C	5.128670499662	0.332200136576	0.588043337369
C	4.066124687797	-0.492997809960	-1.640760866006
C	5.170443569476	-0.651963098209	-0.583333956893
H	2.797386052842	1.383339168798	0.084043253880
H	5.198423874101	1.352886355573	0.173525034511
H	2.123812850849	-1.211004505593	-2.229132455306
H	3.687907938444	0.538626947083	-1.628722139149
H	2.047851457477	1.335006500161	1.665502397774
H	3.277368403551	-2.475734711990	-1.813482556952
H	6.046503455107	0.191397924805	1.178955788101
H	4.503001809032	-0.627102794711	-2.640576765279
C	1.620635525951	-0.416294026478	0.523022980238
H	0.518122135057	0.264638281886	-1.703296295859
H	1.192435728154	-0.798589443284	1.472096046441
C	2.307007820065	-1.624895718906	-0.111554188337
H	3.108466645498	-1.970487262318	0.561843576908
H	1.598107051966	-2.460252870424	-0.118203697801
H	4.172116328821	0.994943188343	2.364026316394
H	6.147837661475	-0.521319657231	-1.069411252541
H	5.173227147267	-1.685692804557	-0.203157842626
H	3.853895664513	-0.687871195163	2.025218820720

TpRh(CNMe)-Cyclooctane IM-(5)

G = -1258.464905

B	-2.056167074392	-1.292812935102	1.200160411553
H	-2.637379484524	-2.017220442122	1.954713512117
N	-0.850313797719	-0.556008454585	1.826671290782
C	-0.814268598318	0.673041748424	2.421154002784
C	0.951432228448	-0.505530069894	2.971767182408
C	0.342650524194	0.752148437873	3.157948594603
H	-1.622352685177	1.380915955047	2.276176013275
H	1.889340516766	-0.870487611365	3.377693442965
N	-3.019799563825	-0.215260023980	0.669493080978
C	-4.319880097106	0.003596995832	0.919055145679
C	-3.590048491005	1.461382506967	-0.554324697198
C	-4.734868418130	1.077694237848	0.153901785640
H	-4.854709175689	-0.623224898432	1.621315987673
H	-3.457045252917	2.257003556941	-1.277855137181
N	-1.512167470711	-2.090404878308	0.009968814877
C	-1.730016952271	-3.356625975082	-0.362127696725
C	-0.520519965902	-2.340560713629	-1.887611120817
C	-1.109559958133	-3.568294842700	-1.579490373020
H	-2.304725136592	-4.018510874418	0.272766738093
H	0.062844422008	-2.056761320584	-2.753418717712
N	-2.567568144292	0.675855659220	-0.239750092051
N	-0.762028236246	-1.459156402728	-0.922354218522
N	0.232007154740	-1.290138987702	2.190369364354
Rh	-0.410911291008	0.566009308859	-0.572825408481
C	-0.178188918520	2.429064723042	-0.297647467204
N	-0.084419254885	3.579077028566	-0.143786266525
C	0.187384510316	4.944711945981	0.054974559042
H	-0.377168551110	5.319246331735	0.915862318299
H	1.258756988739	5.084976916836	0.241279634341
H	-0.098882930864	5.518409623834	-0.833490622750
H	0.699402879099	1.591758786059	3.737514025082
H	-1.080130824268	-4.479717397529	-2.157509814475
H	-5.721815152346	1.514094708903	0.109979154238
C	1.630140631120	0.217741512219	-0.577250420092
C	2.239452876131	-0.366221131444	-1.865996719326
C	4.351540099618	-0.065375876197	1.098433094757
C	2.921779951502	-1.726899247258	-1.687035746699
C	4.030010603997	-1.504100742453	0.660375320775
C	4.194815226541	-1.804159781057	-0.837669769712
H	1.616193192374	-0.583439020116	0.177760553976
H	2.185176323488	-2.420214048858	-1.247728765754
H	3.898219656715	0.119285883429	2.085964582971
H	3.016733673021	-1.790131586913	0.973549539828
H	-0.363424885304	0.905025057633	-2.053517171325
H	5.439224983587	0.001068793099	1.257240663256
H	3.160139748167	-2.131074999005	-2.684056172963

H	4.700460313512	-2.166489324980	1.226808726512
C	2.478691470010	1.361553151440	-0.018076946874
H	2.069247660673	1.673006873670	0.957909730962
H	2.394311962246	2.236711155045	-0.686242949852
C	3.971348569887	1.074679887504	0.156280373732
H	4.432299687446	0.902656677309	-0.826634728666
H	4.448168189019	1.992124669593	0.534853815711
H	1.469690194984	-0.485527739847	-2.639357543847
H	4.576859654925	-2.829846707442	-0.941585603210
H	4.978057899547	-1.161850513839	-1.270710472389
H	2.951513518431	0.350731414660	-2.307444817892

TpRh(CNMe)-Cyclooctane IM-(6)

G = -1258.456588

B	-2.531184072113	-1.185445077713	0.244660984313
H	-3.501503098865	-1.825537046675	0.528960872849
N	-1.794070598656	-0.570311415053	1.456435176901
C	-2.044647757895	0.625318898059	2.068622513982
C	-0.958766930853	-0.722268660444	3.416100455231
C	-1.505177108969	0.576268072976	3.329231317900
H	-2.586516907347	1.407772313504	1.549352869583
H	-0.430441912914	-1.178294536808	4.246673490827
N	-2.927691612657	-0.014113359857	-0.673987236451
C	-4.115405069158	0.358916616201	-1.174294841791
C	-2.538932318743	1.691578812866	-1.928534421040
C	-3.917884790288	1.458275937993	-1.989245173209
H	-5.013677072553	-0.187071597628	-0.915241690139
H	-1.942063116136	2.450418904741	-2.420557089229
N	-1.516659480819	-2.054250766285	-0.506292125163
C	-1.642609046296	-3.271347647690	-1.048825825360
C	0.271699795232	-2.386632488222	-1.664481089721
C	-0.512772160278	-3.533929404932	-1.801719144263
H	-2.526979713087	-3.864363728106	-0.854934576018
H	1.240379280902	-2.156128869845	-2.087540723525
N	-1.954730605394	0.798933812790	-1.138986915612
N	-0.337483697197	-1.507241759025	-0.877063497450
N	-1.143704351182	-1.410099789243	2.306386092785
Rh	-0.005640605035	0.439228770577	-0.233203536691
C	0.206672024379	2.273980801095	0.217204116328
N	0.301622466288	3.411047130073	0.446001240198
C	0.546486215273	4.754315895312	0.784589414484
H	0.569949530911	5.371525909594	-0.120226839117
H	-0.243155181342	5.124633203598	1.447435507124

H	1.512136459606	4.835542586978	1.297566498303
H	-1.499496459079	1.357878826134	4.075595821277
H	-0.286195428589	-4.427292006416	-2.364144616230
H	-4.661053415198	2.005264862860	-2.550472714473
C	1.620018591250	0.034497340260	1.019831336294
C	2.778591933167	1.048217154424	1.075553399038
C	3.785632847923	-2.044209903221	-0.633235800249
C	3.503619034474	1.468194842493	-0.208114355603
C	3.617782199646	-0.778930750825	-1.468049974598
C	4.378295374618	0.438403881323	-0.922172685589
H	0.839882808777	0.752555030753	-1.454258069202
H	2.755141741955	1.840599181600	-0.925539274343
H	3.156188025776	-2.847544377095	-1.046885152042
H	2.554182209298	-0.518654865241	-1.534996651604
H	1.027926285816	0.258463835985	1.931758672227
H	4.824374514490	-2.397743179419	-0.736051669643
H	4.139956693633	2.332498498256	0.041211484920
H	3.944227843956	-0.994730188320	-2.495556585605
C	2.063054366323	-1.439082810663	1.232179745193
H	1.336970267584	-2.133749987135	0.793008255509
H	1.980523213441	-1.625839299811	2.316033535724
C	3.477109152077	-1.883895829574	0.849486639276
H	4.219041360601	-1.211969645416	1.303691602680
H	3.650976082870	-2.857526869667	1.331563657841
H	2.384327368041	1.975922298329	1.518497348057
H	4.882414579271	0.955643579024	-1.750814316942
H	5.187434882598	0.107294981553	-0.251755838178
H	3.533037360466	0.703939880977	1.804818380236

TpRh(CNMe)-Cyclooctane IM-(7)

G = -1258.460023

B	-2.568416107342	-1.167903745502	0.307766855940
H	-3.538232519205	-1.802086613448	0.606540530156
N	-1.798379966318	-0.575792113586	1.509006972245
C	-2.001383461870	0.626457316593	2.126096983366
C	-0.927746000923	-0.752789215816	3.451125477700
C	-1.437203639350	0.561048720644	3.375249768683
H	-2.532511690269	1.424231450325	1.619334229656
H	-0.396821545013	-1.225116495875	4.270710771151
N	-2.976280441232	0.019976615027	-0.585516096763
C	-4.174638007136	0.412730724967	-1.043676713677
C	-2.609245597908	1.747145317883	-1.817391726397
C	-3.991283334962	1.526108248426	-1.842718998838

H	-5.069865131742	-0.130490428495	-0.768740087073
H	-2.020326795059	2.510656036621	-2.311729838475
N	-1.583605252668	-2.037921210070	-0.482553319736
C	-1.760328957038	-3.226263552749	-1.073377509331
C	0.130294218293	-2.341664020601	-1.756004655050
C	-0.679651860223	-3.470524169380	-1.900296992302
H	-2.643908943555	-3.813489354297	-0.859116209260
H	1.066698161068	-2.095667506749	-2.238183554495
N	-2.009967920708	0.834676566084	-1.062548389436
N	-0.415708493736	-1.492610225978	-0.892969273369
N	-1.156858225103	-1.434294631895	2.345462672845
Rh	-0.037263873905	0.432046442599	-0.224276853237
C	0.219048292384	2.248714469876	0.275689785177
N	0.342515340570	3.372786882570	0.550281918015
C	0.630897994937	4.695286971313	0.933548655541
H	0.578068695506	5.358839194142	0.063447605597
H	-0.091161608891	5.034791535952	1.684150910579
H	1.640159213204	4.743874745463	1.359413847372
H	-1.394177738690	1.341427633640	4.121634811735
H	-0.500091242418	-4.339977541539	-2.514691939258
H	-4.745567532611	2.089937594106	-2.371523428941
C	2.793903425956	0.959505903740	0.996098119073
C	1.620742878717	-0.033511143271	0.944961347758
C	4.820696994900	-0.634705501674	-1.001839761271
C	2.055241992182	-1.505661301324	1.063454398093
C	4.491252272642	-1.605134690771	0.138096171792
C	3.060917083267	-2.163167529987	0.111044187209
H	3.585486598105	0.538262741408	1.636081336828
H	2.501227428548	-1.607097377178	2.072833401708
H	5.759221647793	-0.104621143443	-0.775012516319
H	4.683542505878	-1.140601745559	1.113960411397
H	2.465628354846	1.863622489793	1.533507649575
H	5.028488865033	-1.231604118654	-1.903965731712
H	1.150347393754	-2.127609683841	1.096809953400
H	5.206288141545	-2.437752248072	0.075010246775
C	3.409016255419	1.436056661001	-0.324616885977
H	4.320569521433	2.014500295941	-0.099715485808
H	2.710005966335	2.147535320161	-0.792236377264
C	3.738852952757	0.375436445137	-1.366743042145
H	2.814844339130	-0.157412084296	-1.630985163156
H	4.051855336939	0.890052576163	-2.287572061925
H	1.076400723559	0.128677850361	1.900254563644
H	3.095466522136	-3.223750908904	0.399824201412
H	2.694916656772	-2.165940312957	-0.922552754713
H	0.801136114266	0.747057865971	-1.451005418496

TpRh(CNMe)-Cyclooctane IM-(8)

G = -1258.465287

B	-2.103365357685	-1.541754064368	1.223951348166
H	-2.666270512926	-2.264975989024	1.993619794919
N	-1.074590850822	-0.583751529984	1.878082007729
C	-1.346353628391	0.611412255793	2.486420789038
C	0.517763510352	-0.243998060794	3.263917973622
C	-0.337369062252	0.875626763055	3.374945318157
H	-2.239566373056	1.169068913546	2.228484203377
H	1.447665711218	-0.437024293919	3.788624507149
N	-3.124411124499	-0.642748408433	0.503291596026
C	-4.463716398406	-0.591402146266	0.565381526978
C	-3.728682224422	0.884386280959	-0.888111180799
C	-4.902256542867	0.380982207141	-0.314174459789
H	-5.006273815764	-1.250998687448	1.230722443333
H	-3.599503817782	1.657105457939	-1.636681272848
N	-1.341548367168	-2.361888658391	0.177830006715
C	-1.311199213473	-3.676582956287	-0.071493011058
C	-0.097304224808	-2.616222658551	-1.566081843093
C	-0.521846223196	-3.892175476328	-1.186613050854
H	-1.847285413845	-4.365157120633	0.568643756556
H	0.534829509109	-2.309230939141	-2.389911174506
N	-2.668175542724	0.260804282426	-0.390872550807
N	-0.595395787072	-1.706749650788	-0.737040829592
N	0.072031941089	-1.119610034770	2.387026539300
Rh	-0.491567562346	0.344528275182	-0.506585981072
C	-0.434387253932	2.238706074692	-0.347189856661
N	-0.443521285705	3.400358994843	-0.271474663197
C	-0.307609822013	4.794450322636	-0.145452762042
H	-0.994557963623	5.171650336251	0.620069997540
H	0.720513920782	5.041479907625	0.144503131718
H	-0.536690316926	5.282737141098	-1.099168219007
H	-0.221624034169	1.747946696788	4.002575023507
H	-0.283404657601	-4.835718038653	-1.654128987368
H	-5.921098362346	0.678724423425	-0.513675897455
C	2.320286035380	-0.057796356948	-1.704413309463
C	1.577709934957	0.167328526730	-0.373423514462
C	5.296728042891	-0.263196479279	-0.268268067114
C	2.175405111469	1.302317692650	0.467111348749
C	4.736985456390	1.124364670950	0.054112399153
C	3.580238825448	1.141680046904	1.065000033845
H	2.784995241859	0.888247089175	-2.020559433674
H	2.184487731048	2.224015519406	-0.143888282256
H	5.973116021179	-0.187055842364	-1.134263629828

H	4.417652063331	1.630032935224	-0.867445347536
H	1.606442584227	-0.284745833615	-2.508415422574
H	5.928440925899	-0.581707269068	0.575964279925
H	1.495491004463	1.505048392724	1.309893533391
H	5.567908327862	1.732416585874	0.439398437562
C	3.355125379925	-1.198202253734	-1.723650954706
H	3.966072870062	-1.109524621991	-2.637181656479
H	2.804098729862	-2.146118428694	-1.827598016911
C	4.274827028581	-1.365411920915	-0.518432216397
H	3.664678966928	-1.513542238359	0.383269716830
H	4.825213576667	-2.309105391999	-0.647500108223
H	-0.376849935045	0.600856494347	-1.999191469264
H	3.728447504062	1.985021653492	1.756101833042
H	3.612275777578	0.240630964099	1.697522620548
H	1.636611942250	-0.758193554230	0.226877002161

TpRh(CNMe)-Cyclooctane IM-(9)

G = -1258.462492

B	-2.396299232507	-1.438010721905	0.693229142896
H	-3.139617674043	-2.209829813554	1.225382819766
N	-1.421608237229	-0.715838696914	1.656744405361
C	-1.646445326594	0.438352742480	2.356120744255
C	-0.027549380067	-0.719768649505	3.277571778564
C	-0.754756493787	0.484421288525	3.396768612830
H	-2.422450275069	1.128723290092	2.045834206106
H	0.782827201732	-1.084260520197	3.899846414025
N	-3.199048742295	-0.327435375850	-0.009007175294
C	-4.518935224861	-0.120663985473	-0.131809589865
C	-3.415593900905	1.449623051520	-1.203598869183
C	-4.710687965203	1.016888084582	-0.894046772865
H	-5.224659850617	-0.798792979310	0.331038178477
H	-3.091278225211	2.301002875485	-1.790175044135
N	-1.547099480123	-2.155338081742	-0.364154099986
C	-1.655153874966	-3.381660410468	-0.890670616309
C	-0.155254935027	-2.231242457362	-2.011519931889
C	-0.775820236012	-3.481314636611	-1.953703779541
H	-2.348105716043	-4.096982698823	-0.466995897941
H	0.608442540865	-1.863907462650	-2.685535892754
N	-2.516490908802	0.632980765445	-0.669031971620
N	-0.622452011415	-1.445491434739	-1.049444992150
N	-0.437811079836	-1.442798981481	2.255012843898
Rh	-0.348802326255	0.499145994134	-0.400780359528
C	-0.183981982887	2.304884589238	0.175608358041

N	-0.089648429883	3.406435713622	0.537992747202
C	0.088759495990	4.728950708055	0.983189312501
H	-0.041373243521	4.777779079446	2.069927668971
H	1.097371920639	5.073883892907	0.729229453689
H	-0.644921872518	5.388486948208	0.506723327196
H	-0.639297140832	1.267599430228	4.132548409796
H	-0.604019717560	-4.336287998340	-2.590300018257
H	-5.649194361492	1.463578871856	-1.187582595193
C	4.000577860875	1.464755110397	-0.069072041784
C	2.599465591001	1.233387717824	-0.673964681120
C	4.677393644577	-1.700167553356	0.096992868576
C	1.664681984754	0.285370123727	0.097733740961
C	3.410975423017	-1.462939645603	0.928125293414
C	2.125184466713	-1.177950734578	0.123399062316
H	3.970656920932	1.243331270725	1.005322331102
H	1.663737773202	0.622703747752	1.158456489570
H	5.555276552481	-1.690132769343	0.762803237722
H	3.573406033150	-0.658712440772	1.657089600398
H	4.241591565220	2.536818808179	-0.128261850850
H	4.628760269554	-2.721465226661	-0.312443354032
H	0.095977849392	0.965644020489	-1.778638301090
H	3.251915005944	-2.364478272045	1.537422699161
C	5.156052894900	0.713767032479	-0.739365994907
H	6.056192434607	0.805906624917	-0.110815363299
H	5.398304673757	1.231580142952	-1.681028468487
C	4.923930352438	-0.755221314648	-1.074499371491
H	4.090561133905	-0.835258863784	-1.786911213697
H	5.804562971451	-1.118807188296	-1.624627641259
H	2.111372972979	2.212810872431	-0.762059426511
H	1.321364087588	-1.779755521442	0.559382407328
H	2.248712105282	-1.551217708038	-0.904707576004
H	2.694757118613	0.881983345796	-1.714460263082

TpRh(CNMe)-Cyclooctane IM-(10)

G = -1258.462307

B	-2.792925294491	-1.121525978206	0.547752699860
H	-3.805501692124	-1.639652809545	0.918400250232
N	-1.878528446609	-0.626610264564	1.686984216602
C	-1.753342451224	0.626570719607	2.212276635549
C	-0.818194337172	-0.861537185389	3.523495869854
C	-1.057116275033	0.519537556989	3.394069400017
H	-2.189033893033	1.484064346056	1.712640197632
H	-0.295406494415	-1.386078626572	4.315749519287

N	-3.125678232175	0.097494298550	-0.333982729558
C	-4.303650632129	0.629161731788	-0.693652978740
C	-2.665683904912	1.737769675242	-1.650558217533
C	-4.060233191654	1.693340452080	-1.542299235506
H	-5.229254018461	0.208513097211	-0.321576946596
H	-2.035648423876	2.410060035333	-2.221053115448
N	-1.971403919844	-2.102963621983	-0.298579419328
C	-2.319107320923	-3.272502352867	-0.847329493967
C	-0.355978311722	-2.658551408545	-1.615531119355
C	-1.308671685550	-3.674898674359	-1.702017369557
H	-3.259264972153	-3.738569456160	-0.582049378981
H	0.595971320597	-2.553973435545	-2.120816446292
N	-2.115380505634	0.771988527259	-0.924668601431
N	-0.758730890074	-1.722920597335	-0.760996851059
N	-1.318014093198	-1.545274138906	2.508170229637
Rh	-0.124137717404	0.188792193140	-0.249942049970
C	0.336778600459	2.001741286891	0.081320194440
N	0.565128133009	3.131801906753	0.239701106805
C	1.005910820025	4.444645903227	0.488003489252
H	0.149230702185	5.122355262946	0.569676547411
H	1.575433567351	4.473123723184	1.424521723654
H	1.651543622327	4.781011770779	-0.331351361648
H	-0.768514652118	1.317397795592	4.063350509043
H	-1.263248123884	-4.576817779277	-2.293771732763
H	-4.785521844070	2.336239970295	-2.018797005723
C	3.049529375934	-1.464625666462	-1.223426529674
C	2.315849268226	-1.689787814845	0.111660717752
C	4.814484790336	0.988165986088	0.002119241371
C	1.588655792715	-0.486611836451	0.723134963391
C	3.338014612666	1.373296029481	0.158367780970
C	2.553743995394	0.593792548975	1.231991000439
H	2.628903419711	-0.585831097748	-1.726770970682
H	0.626454918299	0.346023605381	-1.561349561908
H	5.207739235141	1.454359550227	-0.915371727938
H	2.817340722253	1.282228957944	-0.803840223527
H	2.842352273648	-2.306670105650	-1.901641984501
H	5.377576626982	1.444981766037	0.831264475936
H	1.071655953603	-0.876631924882	1.623257490525
H	3.315751283106	2.449378245046	0.393589423025
C	4.577268231354	-1.347748075644	-1.135041328758
H	4.962495074726	-0.978388496094	-2.098786124730
H	4.992445082318	-2.361194077495	-1.020056455842
C	5.152616974569	-0.499656783230	-0.004560799101
H	4.866508611721	-0.940269469711	0.960218378956
H	6.248172816667	-0.591528185007	-0.042729387602
H	1.593797496577	-2.505390196622	0.002705817190

H	1.981552527976	1.294357892866	1.858115101248
H	3.272579529510	0.130632671671	1.931345501714
H	3.040612944495	-2.069370447542	0.854077665921

TpRh(CNMe)-Cyclooctane TS_3-(1)

G = -1258.446550

B	-2.899414776488	-0.560228547715	0.208651170538
H	-4.038674486618	-0.904698678624	0.350582504340
N	-2.350700612857	0.296461599516	1.361111867813
C	-2.678318261821	1.578240018579	1.635425128212
C	-1.384430358552	0.763931072870	3.206786509416
C	-2.073733793608	1.926799245840	2.823804949931
H	-3.312390468009	2.144715666658	0.963393998287
H	-0.762860449356	0.597363116984	4.079570336432
N	-2.777539297450	0.311051767605	-1.054426424344
C	-3.676779113159	0.723040071658	-1.959624941497
C	-1.681055876154	1.464959207083	-2.500127867217
C	-3.017538852300	1.477192367668	-2.913747667182
H	-4.719550099985	0.449741329272	-1.858247748809
H	-0.809530855282	1.918341817998	-2.957710759421
N	-2.021945796457	-1.803469834644	0.010068692064
C	-2.435914289829	-3.069499098057	-0.126779116040
C	-0.296035946731	-2.952182190902	-0.585724188164
C	-1.360961927800	-3.849342574166	-0.507114445942
H	-3.472208046782	-3.321721518407	0.056894154026
H	0.737160518969	-3.139432534937	-0.845636645477
N	-1.551819926063	0.761736597322	-1.380736347333
N	-0.696116809671	-1.724395155607	-0.267473138679
N	-1.554909081577	-0.216981181827	2.330198103965
Rh	0.150085079594	0.187473146161	-0.150031008132
C	0.724295762074	1.995612154433	-0.122808556706
N	1.007952644352	3.122615268109	-0.170347947168
C	1.423231022982	4.465523523030	-0.118217693661
H	0.588050266509	5.102628325900	0.192516648255
H	2.243102592789	4.571706294053	0.601784552984
H	1.770899977190	4.789150600473	-1.105393684269
H	-2.126499301087	2.876425420674	3.337169360669
H	-1.346772027448	-4.912162929729	-0.695960553393
H	-3.441030381173	1.959905169063	-3.782072924425
C	3.098860924977	-2.435940708840	0.275799255318
C	3.106198603765	-1.934233961544	-1.175612121481
C	2.841102294921	0.607808569210	1.498626039346
C	4.133210070500	-0.851752266266	-1.509596887425

C	4.127009323397	0.534473042293	0.666072088386
C	3.971411952417	0.522135028365	-0.860104519799
H	4.128205759165	-2.374735218036	0.656496958210
H	5.134557482169	-1.236050048453	-1.249717021886
H	3.144048118547	0.421472868311	2.545628624114
H	4.714864144853	-0.342665509625	0.970408167249
H	2.882017298863	-3.515282402099	0.264503849788
H	2.484845500220	1.647823022366	1.499198821172
H	4.140913939371	-0.718198063343	-2.602205160104
H	4.745350212871	1.395726274420	0.959401060005
C	2.121161888834	-1.806118824794	1.297451168947
H	2.592977628171	-1.925349603314	2.290464993210
H	1.220476757767	-2.427249095869	1.352344945518
C	1.674462064265	-0.343772098282	1.190407329518
H	0.976640635242	0.061908466292	-1.405836668508
H	0.994769737639	-0.218261818287	2.057157486655
H	3.331342632194	-2.790160076042	-1.829866259596
H	4.735735345377	1.177176910997	-1.303431501380
H	3.004642702995	0.957676133931	-1.145429455385
H	2.108315093280	-1.590840487726	-1.471611390947

TpRh(CNMe)-Cyclooctane TS_3-(2)

G = -1258.460584

B	-2.507508618592	-0.953581820741	1.174600522674
H	-3.297510908114	-1.485615059378	1.900930384020
N	-1.341841662254	-0.250020870112	1.903789691190
C	-1.426560930353	0.901754508249	2.611528686300
C	0.527943208958	-0.045145108248	2.920984553789
C	-0.237862099695	1.077475421026	3.282948147937
H	-2.322852766943	1.509785601579	2.573450050217
H	1.537963187635	-0.304393899354	3.218725707231
N	-3.195870032147	0.164005614137	0.368480162384
C	-4.465913210888	0.591191094815	0.307230480921
C	-3.216457639300	1.761823582223	-1.070804560828
C	-4.530723277477	1.626509438803	-0.607374432486
H	-5.229682138611	0.128818891467	0.919818447284
H	-2.808348512635	2.444921904058	-1.806275665327
N	-1.954142370550	-1.982274616290	0.177941721009
C	-2.375768110317	-3.233052627457	-0.054394016178
C	-0.991590546718	-2.622922476646	-1.645527238373
C	-1.781220584216	-3.691293913085	-1.215010286951
H	-3.073510155114	-3.705306158206	0.624924647324
H	-0.346924339101	-2.540694195546	-2.511370604610

N	-2.424571300519	0.878580427836	-0.475971888556
N	-1.097969782715	-1.604904424458	-0.801440156260
N	-0.136165857151	-0.847060638176	2.101459725773
Rh	-0.315513627763	0.297007847782	-0.585955018809
C	0.329083699715	2.064641957536	-0.303910346236
N	0.737147432953	3.133612297793	-0.097092819865
C	1.275855812253	4.405089314438	0.171069037895
H	1.332343872954	4.563176955636	1.253657786968
H	2.283138046375	4.478799493808	-0.253925155088
H	0.642783133708	5.182493839699	-0.270589425157
H	0.033642725480	1.891958980518	3.939578064984
H	-1.899300965765	-4.658168781938	-1.680647604722
H	-5.400635161487	2.196947443092	-0.897754622384
C	4.008559419506	0.280355640832	-1.727515500582
C	4.624731130459	0.715307885471	-0.388802119408
C	1.914193418314	-1.766698003112	-0.417015513434
C	5.080635740364	-0.421124505124	0.528804700942
C	3.311877813779	-2.249162236483	0.026177004705
C	4.029600385207	-1.388958699655	1.076038071053
H	4.378191118788	-0.718712265244	-1.991276786862
H	5.832139188473	-1.014324987822	-0.019530552398
H	1.660293310514	-2.295777075135	-1.348128920150
H	3.976914984104	-2.381593393379	-0.837762237414
H	4.381598216268	0.938762627262	-2.526053696745
H	1.198457194145	-2.118473247748	0.337416697189
H	5.618457128840	0.021457875779	1.381287220036
H	3.177440072632	-3.261798780526	0.433107965857
C	2.473028227883	0.330654166016	-1.781839034983
H	2.136892366844	-0.149091273655	-2.715573652984
H	2.195250325320	1.390910416578	-1.890813744597
C	1.699644018041	-0.265317730229	-0.602169173812
H	2.056391188105	0.225739671132	0.321747320001
H	-0.220449066589	0.553899658645	-2.077153512630
H	5.509506360347	1.337744413644	-0.586824936195
H	4.550749348780	-2.053303548099	1.780335857072
H	3.292260144172	-0.842534065467	1.683209405164
H	3.920183664100	1.370279461463	0.149743424105

TpRh(CNMe)-Cyclooctane TS_3-(3)

G = -1258.458767

B	-2.474933139440	-1.213042814182	1.056139211781
H	-3.282863131853	-1.823266503067	1.696446176506
N	-1.698183325486	-0.148562320079	1.858527929698

C	-2.196381184413	1.016438422879	2.334610021164
C	-0.190874997064	0.652069448117	3.146818227583
C	-1.253662262937	1.572370437593	3.170424512801
H	-3.179358623294	1.361042346617	2.035488254351
H	0.765571362473	0.702295673818	3.655387020984
N	-3.175515245262	-0.432937076680	-0.072141626465
C	-4.454367687118	-0.361214220269	-0.470439234699
C	-3.191217379964	0.863570102652	-1.787514733134
C	-4.517741851738	0.469213174674	-1.574559493066
H	-5.225311061297	-0.905088011099	0.060838380524
H	-2.774248221663	1.506176769263	-2.553927705437
N	-1.488827360046	-2.194422967099	0.406958779321
C	-1.585941227450	-3.528720679100	0.323273081279
C	-0.027375253615	-2.823894951821	-1.052134228922
C	-0.662845982306	-3.982454116206	-0.598817863158
H	-2.312530526206	-4.057849020927	0.926165146448
H	0.759464530599	-2.708947458423	-1.784563717460
N	-2.395447208850	0.315171407915	-0.878043806470
N	-0.522661917965	-1.756737008101	-0.437750319119
N	-0.459459386011	-0.385183470027	2.367315110445
Rh	-0.243606243687	0.300264863245	-0.434313046168
C	-0.150619080944	2.198385880496	-0.380371192730
N	-0.115154425262	3.358644440350	-0.313119439518
C	-0.041353735946	4.758670658370	-0.199227548876
H	-0.068487129999	5.046665407625	0.857460998282
H	0.892435586914	5.120039996236	-0.644190699493
H	-0.887808392835	5.222756324091	-0.717265753138
H	-1.325199784346	2.501097444894	3.718785016053
H	-0.474941533620	-5.002111718798	-0.899893819033
H	-5.393541198266	0.745467105817	-2.143064952173
C	2.323371899819	-1.017791967390	0.604695241669
C	3.022969447039	-1.908624582266	-0.436551670782
C	4.013650536673	1.593058150301	-0.373273470481
C	4.552305991638	-1.901793550764	-0.400674800107
C	5.054783645834	0.586437565664	0.121061337267
C	5.278795245033	-0.618287985694	-0.803720881157
H	3.032543753475	-0.846695813815	1.430478246806
H	4.872783308190	-2.171262105033	0.619792823586
H	3.813402738353	2.321167049829	0.429613595883
H	4.801033092893	0.229919956350	1.128024985302
H	1.501846844573	-1.572180403503	1.072486177114
H	4.472569462005	2.171247955151	-1.192793821353
H	4.914288010033	-2.713791716901	-1.049768805631
H	6.002535439058	1.130678764780	0.241526059821
C	1.773111796001	0.336009937721	0.115792112601
H	1.719640650826	0.984890039359	1.013557176391

H	0.178971146363	0.365256232232	-1.891245341340
C	2.679071056937	1.051057872996	-0.893299581344
H	2.863352112316	0.401068529853	-1.761109187348
H	2.144229913372	1.912399134713	-1.317309827753
H	2.707352161300	-2.949935414619	-0.276070890048
H	6.352845954525	-0.851023316120	-0.831509576186
H	5.013014597622	-0.348450454353	-1.838530921672
H	2.684342255020	-1.654593157268	-1.452937969400

TpRh(CNMe)-Cyclooctane TS_3-(4)

G = -1258.458313

B	-2.848773985354	-0.657022867505	0.882085441564
H	-3.885142198222	-0.996904740586	1.377938725268
N	-1.963293036969	0.217646939711	1.790195939057
C	-2.187931888507	1.510580264845	2.123125326795
C	-0.521102338809	0.695106597123	3.293238706855
C	-1.275639253305	1.864543570891	3.091729345641
H	-2.973664621541	2.078597147670	1.638865297158
H	0.315610781702	0.531452625400	3.963372253270
N	-3.121350669240	0.205207261592	-0.364851683036
C	-4.251025022078	0.596255518058	-0.972720207082
C	-2.507989066503	1.356273743113	-2.074575724344
C	-3.907807175261	1.347336831403	-2.082412978089
H	-5.215742186233	0.312367652426	-0.571337970920
H	-1.814054637864	1.816761725251	-2.767918786555
N	-2.071018633680	-1.901663413761	0.429823342379
C	-2.531693276437	-3.156667408579	0.340728829721
C	-0.625759637442	-3.004067155862	-0.733845943921
C	-1.635295705874	-3.906697343618	-0.395253892522
H	-3.470629645859	-3.422722134025	0.808708785485
H	0.273186166005	-3.165216869308	-1.314283105497
N	-2.048784515843	0.666742007502	-1.037447602599
N	-0.888128404501	-1.803601946966	-0.228068307919
N	-0.939458381147	-0.296225140059	2.519389018098
Rh	-0.076728266442	0.118210070497	-0.255729579201
C	0.435977793730	1.945721248339	-0.275364748416
N	0.661090610852	3.086019778206	-0.313073526154
C	1.049522262512	4.436283210076	-0.258544546745
H	2.051559696809	4.515329955711	0.179423675676
H	1.065109845385	4.864604336313	-1.266771293269
H	0.343076463752	5.003106107968	0.357687700776
H	-1.172890199795	2.822428227892	3.581837983762
H	-1.698393313832	-4.954492641665	-0.647616269926
H	-4.572266613104	1.815023605883	-2.793901645346

C	2.794450213291	0.690641230279	0.652881476321
C	4.209530905238	0.328172248898	1.141573094993
C	2.737128658679	-1.918229118395	-1.375160501620
C	5.257626228072	0.143340901986	0.041435360496
C	3.879616875520	-1.013033018300	-1.838546936720
C	5.118499301380	-1.031609744738	-0.928881144668
H	2.898677109801	1.208226925717	-0.312982414487
H	5.285699055663	1.071726783493	-0.554872646921
H	1.867827583278	-1.749977041613	-2.029121460284
H	3.520950279178	0.019204100537	-1.955579941567
H	2.380445222643	1.445868596814	1.339675640068
H	3.047991254346	-2.963797149480	-1.540408855227
H	6.246590114338	0.070381146070	0.519061130318
H	4.169366260862	-1.333343652788	-2.849427541012
C	1.755886136992	-0.446179753844	0.571468162729
H	0.552645459150	0.016394950967	-1.631741242729
H	1.438346055045	-0.638310297039	1.612543529117
C	2.329339467029	-1.777763442588	0.087325365547
H	3.208453113283	-2.029756244705	0.702826825930
H	1.611904489164	-2.568864524710	0.332374970293
H	4.573287846427	1.144967188486	1.782633539024
H	6.020366881076	-1.029771598905	-1.557579780745
H	5.155970365097	-1.981922788991	-0.373205979778
H	4.178803487541	-0.555526451090	1.796103310959

TpRh(CNMe)-Cyclooctane TS_3-(5)

G = -1258.460992

B	-2.214530487123	-1.229792031919	1.263863280095
H	-2.880351096358	-1.820817276553	2.065691092673
N	-1.390303028377	-0.066195836750	1.853911140932
C	-1.875766160883	1.114570741789	2.301995573684
C	0.249804323785	0.919842973024	2.807554980941
C	-0.848961538318	1.789469981011	2.923926263211
H	-2.912226112723	1.384770693604	2.136677231120
H	1.269544694163	1.060291651368	3.149719744827
N	-3.124003841441	-0.585273565130	0.201741994936
C	-4.451457483859	-0.613814377180	0.010997619031
C	-3.495182566658	0.573946237875	-1.571236089886
C	-4.742445077972	0.124715817806	-1.121454826239
H	-5.091536320830	-1.156233277297	0.695410479633
H	-3.247042013624	1.178499802980	-2.435655470113
N	-1.270791554381	-2.215048483545	0.561510127048
C	-1.219447874754	-3.548677438106	0.675028733037
C	0.108693163090	-2.903103303206	-0.948610203631

C	-0.343484190167	-4.039271770996	-0.274268072546
H	-1.813957827774	-4.051963743957	1.426452916810
H	0.804482256650	-2.822725363402	-1.773123310203
N	-2.531831542756	0.141558857399	-0.767272468427
N	-0.450064961323	-1.811961817248	-0.438007095565
N	-0.074615085030	-0.196753612081	2.171975609298
Rh	-0.345561539313	0.246054356332	-0.706594179463
C	-0.369005904239	2.136379427969	-0.881217841445
N	-0.451056333062	3.292568616175	-0.980377585944
C	-0.421817672397	4.696971698192	-1.042756641129
H	-1.085451737434	5.118587348976	-0.279902360560
H	0.599453784495	5.054385048174	-0.865972984088
H	-0.753627304858	5.037054902388	-2.029976991376
H	-0.888679257030	2.761991767155	3.393868107517
H	-0.069721502974	-5.068200677318	-0.452905076760
H	-5.712965098005	0.308360797327	-1.558316698836
C	1.725418416182	0.171754714266	-0.520549743312
C	2.483242668022	-0.552541991689	-1.651416484605
C	4.415279655368	0.720613068672	1.196432745997
C	3.417730431023	-1.683356817068	-1.200233297574
C	4.374195655481	-0.807983430895	1.050500547238
C	4.653593313874	-1.351179324552	-0.358596282398
H	1.778716116816	-0.455641465761	0.382110933520
H	2.818916856078	-2.406910819744	-0.622634972411
H	3.900373302438	1.007582113828	2.127523650007
H	3.411872590639	-1.204533608072	1.399396527592
H	-0.205755165344	0.213078750510	-2.215573298743
H	5.466323637584	1.016554767282	1.339361512407
H	3.759615352865	-2.223809404431	-2.097719538550
H	5.121267792165	-1.218370833233	1.744785804099
C	2.359977901084	1.527196563779	-0.196106988262
H	1.856484154496	1.961229254396	0.684814783079
H	2.165310679621	2.220676878930	-1.032401383493
C	3.870694826933	1.555421129304	0.041446380172
H	4.391186796529	1.275656561427	-0.885511048806
H	4.160194545837	2.602519968287	0.221255223006
H	1.775986348375	-0.995495894530	-2.366540868385
H	5.223477221854	-2.286414913840	-0.261202698548
H	5.318874804678	-0.667413642186	-0.908437211002
H	3.048830668880	0.177727160465	-2.254626619612

TpRh(CNMe)-Cyclooctane TS_3-(6)

G = -1258.452462

B	-2.535822029799	-1.360998349196	0.488446218274
H	-3.468021723253	-2.042602060160	0.808753689270
N	-2.111400805389	-0.332376123015	1.552494367389
C	-2.817717950735	0.749239595014	1.949644375397
C	-1.075686506479	0.453043688001	3.248325216489
C	-2.183187154784	1.293681488247	3.044878870062
H	-3.715304181914	1.049009026987	1.421397085140
H	-0.296817776588	0.522927437399	3.999749702508
N	-2.898426074345	-0.545457310948	-0.767565961862
C	-4.005389590324	-0.493525997683	-1.522969148031
C	-2.463884903286	0.824396409737	-2.367436514833
C	-3.776589126606	0.382737884879	-2.568374905213
H	-4.874466640640	-1.084007366709	-1.261416995514
H	-1.866288222756	1.511339472291	-2.955142620060
N	-1.343193034671	-2.257422208634	0.136862647383
C	-1.325305767714	-3.590485004297	0.004152395476
C	0.552873410502	-2.755990372003	-0.761667148795
C	-0.122821158214	-3.961710570602	-0.565979580239
H	-2.175854404085	-4.177829475417	0.324883981095
H	1.531855330724	-2.575220277561	-1.183268211227
N	-1.948359636648	0.259145062450	-1.282382346422
N	-0.182547470794	-1.738000810316	-0.329963548547
N	-1.033698267012	-0.526741009504	2.356127749141
Rh	-0.019741388343	0.339447753509	-0.262909438784
C	-0.047994158677	2.238877113386	-0.301188509613
N	-0.125761680486	3.397579226467	-0.364584003636
C	-0.133621549341	4.803982488595	-0.378278995833
H	-0.245257646436	5.168641740522	-1.405280774631
H	-0.967211953625	5.178631239414	0.225704959477
H	0.808022903636	5.183718675724	0.035076733205
H	-2.479359558772	2.163928083770	3.613347291448
H	0.217314674712	-4.958250842782	-0.804191426257
H	-4.457188705841	0.657063060475	-3.360803500407
C	1.712856731570	0.495022652765	0.908941207552
C	2.745703228994	1.577750592153	0.536390876469
C	4.053654160933	-1.767122320981	-0.190130537674
C	3.350744589836	1.643115202849	-0.869486024694
C	3.678633591734	-0.863202686009	-1.359885299869
C	4.311147398025	0.534219158884	-1.293579111937
H	0.725179004740	0.418560762181	-1.578056261532
H	2.530482158864	1.692162400932	-1.603143345601
H	3.534336908859	-2.733621201387	-0.283985374960
H	2.587979440956	-0.745442109697	-1.405809831031
H	1.174875301622	0.944631912178	1.765020161871
H	5.128013144679	-2.002321708573	-0.260063258642
H	3.886664238896	2.602105925781	-0.952592610741

H	3.969893184329	-1.364135038659	-2.294218116778
C	2.326467771930	-0.801043989350	1.508430635329
H	1.677773916800	-1.664435334088	1.318162031053
H	2.287817282435	-0.681322825362	2.603900079066
C	3.774942235062	-1.185442490663	1.190245043101
H	4.440736344595	-0.328604474236	1.364903224438
H	4.084381212714	-1.935258346514	1.933615815429
H	2.266287474763	2.554687339976	0.702682506300
H	4.712242286181	0.802748647302	-2.281069113130
H	5.182545606561	0.519868871873	-0.619385427301
H	3.573151022904	1.561005220607	1.267609641431

TpRh(CNMe)-Cyclooctane TS_3-(7)

G = -1258.455632

B	-2.538403268508	-1.309793109647	0.628594855469
H	-3.467419783947	-1.988317221404	0.964230065781
N	-2.000828795078	-0.383695118216	1.732855086705
C	-2.633324866162	0.688701286601	2.258391852161
C	-0.809240127742	0.243569804478	3.391581649116
C	-1.896857862410	1.131333249241	3.335699310276
H	-3.555817862275	1.055688507333	1.823844168674
H	0.027049992796	0.233169456748	4.081923333375
N	-2.967523201225	-0.377858226239	-0.522894861689
C	-4.129279859004	-0.228439741429	-1.176255451986
C	-2.622770952930	1.133390332127	-2.013991322226
C	-3.959480620224	0.740885539533	-2.148117864278
H	-4.991929478874	-0.822196928990	-0.901177530379
H	-2.054674424456	1.862019752808	-2.580314341132
N	-1.412056833408	-2.211306960905	0.103949117616
C	-1.488562693260	-3.513668107477	-0.205456746048
C	0.315205061992	-2.656134801500	-1.111134516388
C	-0.396348072705	-3.850825158786	-0.980569324379
H	-2.324346347828	-4.104893216055	0.145723449551
H	1.221541486809	-2.448782075198	-1.663057196242
N	-2.038562583906	0.454744411380	-1.033946580590
N	-0.292372909320	-1.681346838974	-0.446177488938
N	-0.873648614127	-0.669925475345	2.432530116703
Rh	-0.025506809352	0.358405013938	-0.186696950935
C	0.066437403640	2.250766435892	-0.021745664273
N	0.074714826555	3.411062811621	0.056910926670
C	0.169507076038	4.806472119133	0.205807997607
H	-0.090415038087	5.303241780791	-0.735350494102
H	-0.517035582803	5.145412890136	0.989269547710

H	1.193975152597	5.080407297168	0.483491578215
H	-2.116072750972	1.966728450391	3.985502926533
H	-0.149391065205	-4.817832102428	-1.392155561108
H	-4.692958815030	1.105924237429	-2.851806872692
C	2.882921940587	1.316713966953	0.436605403802
C	1.799351043213	0.298315281101	0.828288877947
C	4.763643745212	-0.695399103736	-1.300120112684
C	2.356132598909	-1.065524149435	1.282983105827
C	4.681410759938	-1.292133908352	0.109195721373
C	3.323752694084	-1.919577141032	0.452726115234
H	3.777822348795	1.135343827553	1.052802282093
H	2.897385213723	-0.864551175365	2.228882588129
H	5.673472306171	-0.080917147811	-1.388792851925
H	4.945291631366	-0.544476545826	0.868231053174
H	2.546674833731	2.320966720483	0.739793856509
H	4.897814314553	-1.527366407865	-2.009654172404
H	1.503484294620	-1.695026630994	1.575204830072
H	5.463755009546	-2.060924246490	0.183867505936
C	3.289257189932	1.419987373772	-1.036500407143
H	4.178242219499	2.067250143591	-1.116882858503
H	2.485393111917	1.945387694999	-1.576240551385
C	3.557478596557	0.111776691763	-1.767863969875
H	2.653486788515	-0.511745433132	-1.712013754695
H	3.692362341902	0.336466375577	-2.836433480243
H	1.383084754512	0.698069435686	1.774173579871
H	3.501385614368	-2.825157066438	1.051182332772
H	2.857561786804	-2.284348950823	-0.469306163256
H	0.631488469962	0.531305161669	-1.539820055401

TpRh(CNMe)-Cyclooctane TS_3-(8)

G = -1258.462028

B	-2.495223064796	-1.156580527613	1.096940296148
H	-3.289152369394	-1.722970585942	1.793207645057
N	-1.650454924656	-0.093197693658	1.829850362011
C	-2.095262647406	1.091852163027	2.306446415063
C	-0.058741235962	0.697438133703	3.017719878424
C	-1.097359735901	1.642960700770	3.079225121332
H	-3.085896614661	1.452320172599	2.054695698638
H	0.924618190418	0.736094007066	3.473763831576
N	-3.232466849857	-0.394325266291	-0.019807966898
C	-4.531562003260	-0.305616732199	-0.341715688805
C	-3.331123879304	0.871119359402	-1.756199147009
C	-4.648232551346	0.504775610969	-1.456236594992

H	-5.277735046571	-0.824207707933	0.247033896272
H	-2.950487276825	1.492211433930	-2.558518807671
N	-1.556036288946	-2.182747781851	0.453111188696
C	-1.567211421129	-3.519253832907	0.540985704205
C	-0.012679271788	-2.893428808236	-0.877317731231
C	-0.591457999127	-4.024553079993	-0.297714988201
H	-2.270948556717	-4.014122581676	1.197630977957
H	0.789220726989	-2.815571538010	-1.599961000215
N	-2.490721116728	0.326097137772	-0.885260863458
N	-0.598587460162	-1.794266619453	-0.418623307584
N	-0.389302138423	-0.346789792432	2.272090713355
Rh	-0.322794478516	0.242235513592	-0.635419394151
C	-0.144765296292	2.125359089513	-0.835811678199
N	-0.093671555362	3.279478994378	-0.974177527595
C	0.084950936698	4.670791257447	-1.074012046755
H	-0.646484794646	5.188078207787	-0.443508123758
H	1.095278719080	4.939174054968	-0.743700100420
H	-0.049000106691	4.993810990200	-2.112308563012
H	-1.117550997522	2.584872490684	3.608877398100
H	-0.334582345784	-5.059851408792	-0.464190264607
H	-5.552177515546	0.786929571089	-1.975575850480
C	2.528560280126	-0.548834939497	-1.472892758419
C	1.714284127390	-0.019390352010	-0.275597501893
C	5.404830686927	-0.564677886934	0.205011518864
C	2.328712238509	1.239133698845	0.352640225464
C	4.897659929972	0.877680235690	0.176228741648
C	3.681514593277	1.152889796792	1.073568299053
H	3.043676589649	0.297191608575	-1.952592734435
H	2.432822996489	2.005998938645	-0.436998267583
H	6.150360622808	-0.702117863124	-0.593992658149
H	4.660987307526	1.176573443271	-0.854297914625
H	1.855496064830	-0.926521163899	-2.255709023190
H	5.947894422256	-0.719750921267	1.150663440938
H	1.610106035996	1.651392518057	1.078242573549
H	5.730987626600	1.527829287001	0.478313001298
C	3.525003566079	-1.691077722317	-1.189891420579
H	4.208391264709	-1.786717036754	-2.049800117566
H	2.956572977636	-2.633532767372	-1.163386644519
C	4.341805694499	-1.650294737474	0.097627070831
H	3.659222430072	-1.585270247449	0.956202449078
H	4.843710065972	-2.623189791100	0.205317178352
H	-0.082232132119	0.185916928418	-2.128898715156
H	3.829905668563	2.117139178124	1.582368052917
H	3.627570834887	0.405774056872	1.880985356739
H	1.667250807479	-0.800042583000	0.504612685589

TpRh(CNMe)-Cyclooctane TS_3-(9)

G = -1258.461095

B	-2.478929944960	-1.334239974634	0.930952209924
H	-3.267385648818	-2.016603952821	1.520390021078
N	-1.688908713941	-0.351502161977	1.822475233355
C	-2.173787033484	0.775675024986	2.396504315392
C	-0.173992334376	0.318506043227	3.175366451879
C	-1.225882896451	1.246772249437	3.276637918751
H	-3.150884476714	1.158263954050	2.125546077677
H	0.782154393164	0.312884765893	3.687081317105
N	-3.209076342822	-0.440406573278	-0.088975902075
C	-4.497383691047	-0.334555753701	-0.447169437552
C	-3.274412147723	1.050185874752	-1.637621692382
C	-4.592605073535	0.619897171862	-1.443434368743
H	-5.251791420106	-0.944496171683	0.033659451943
H	-2.880366721475	1.783330896974	-2.331451641024
N	-1.501544801902	-2.231950887569	0.157743600013
C	-1.566643613842	-3.553902750178	-0.052378103626
C	-0.033531701805	-2.682789248457	-1.360243749083
C	-0.638353826131	-3.894204700634	-1.018396491617
H	-2.273938732372	-4.157241289675	0.501788919870
H	0.754284254074	-2.476660921821	-2.073797699939
N	-2.453554101824	0.406335864972	-0.817430604609
N	-0.553899934585	-1.692939653096	-0.646216022444
N	-0.455150772686	-0.645950698372	2.311992143323
Rh	-0.293318535160	0.348120545821	-0.438910641246
C	-0.163579213897	2.229733714683	-0.191415035784
N	-0.089850752696	3.375785191044	-0.009021475004
C	0.025041231228	4.754650074721	0.244347114745
H	0.102384035826	4.928286502341	1.323298396486
H	0.921253089109	5.150439561159	-0.246122406604
H	-0.855320339805	5.281709984849	-0.139609010989
H	-1.286338043945	2.127424308683	3.900424179900
H	-0.427537755996	-4.875813205846	-1.415386982273
H	-5.483423532042	0.952801333404	-1.955398134965
C	4.034052388931	1.423095993256	-0.593692003876
C	2.608850827012	1.026097037932	-1.032995877450
C	4.801494932175	-1.587313640229	0.343436749945
C	1.746189906600	0.290703818909	0.008146419152
C	3.578010060644	-1.160026413716	1.163180644507
C	2.242977928075	-1.109286558820	0.390665385694
H	4.067321889234	1.491407903605	0.501268990458
H	1.797201779549	0.890699859161	0.942372238143
H	5.715338031614	-1.396193945941	0.928564451466

H	3.758998919877	-0.191922548809	1.647928203627
H	4.243265719774	2.444575935243	-0.945378127588
H	4.757499126166	-2.680095246167	0.212813578736
H	0.072698483565	0.562487282576	-1.894782130756
H	3.480821491616	-1.875221618625	1.992804947945
C	5.170533505065	0.535101393292	-1.111274059862
H	6.099985048450	0.794286769945	-0.579531370765
H	5.351228969383	0.794089388767	-2.166592813297
C	4.954883611496	-0.972400052914	-1.043740825452
H	4.082982221942	-1.239243327415	-1.657724829124
H	5.809925993633	-1.457989478143	-1.537125303623
H	2.085346423852	1.946053375979	-1.326544830910
H	1.471371956887	-1.577612403465	1.011754536416
H	2.324598813500	-1.741167899579	-0.505913771745
H	2.655310651702	0.430769406040	-1.959864533120

TpRh(CNMe)-Cyclooctane TS_3-(10)

G = -1258.458053

B	-2.914208474563	-0.703830767089	0.726350992870
H	-3.988079415284	-1.060331610489	1.120508544870
N	-2.103093014648	0.122813321144	1.740909578052
C	-2.345520777316	1.403099308417	2.106659873900
C	-0.768920907726	0.532816880700	3.358585486218
C	-1.502816361315	1.713726669236	3.150520745554
H	-3.092103668587	1.994955496290	1.590201331525
H	0.017807718564	0.337984148399	4.079013764204
N	-3.084702064465	0.217675904205	-0.497073152245
C	-4.163852530666	0.646149199476	-1.168024104703
C	-2.341018113882	1.452516404286	-2.092980568422
C	-3.735994223386	1.451763650771	-2.207903832443
H	-5.156797218542	0.347507729786	-0.856126115504
H	-1.595513135209	1.944325664597	-2.706768634352
N	-2.107045180506	-1.930748561607	0.274641034086
C	-2.565421949458	-3.173448532107	0.070628945518
C	-0.588449205987	-2.967630644875	-0.857001425331
C	-1.622644574398	-3.882017822599	-0.648867007665
H	-3.536244844456	-3.461495332599	0.452625298827
H	0.347451733078	-3.091318851427	-1.386633787616
N	-1.963122378867	0.708045943543	-1.060831940322
N	-0.881348598106	-1.802018023908	-0.291140902880
N	-1.135130172901	-0.425156328550	2.518628840958
Rh	-0.050033884806	0.099677983398	-0.185388675706
C	0.515553172002	1.911892004949	-0.124931927266

N	0.791234971747	3.041537036504	-0.115888923715
C	1.253867249317	4.366292261014	-0.024219670515
H	0.418484522391	5.042649685789	0.186928972395
H	1.991873090087	4.445116760601	0.782904570630
H	1.724819199549	4.663459266877	-0.968051840654
H	-1.430474759780	2.651893196963	3.682309584713
H	-1.672606848603	-4.910685315964	-0.972748345356
H	-4.343412209852	1.959258192554	-2.942735035994
C	2.917337613987	-1.880144919499	-1.129342955411
C	2.316457518571	-1.853173406334	0.287967164839
C	4.905843401106	0.614615502167	-0.473956435740
C	1.702325056694	-0.533175495754	0.770009170009
C	3.473052376716	1.110567809175	-0.239412899780
C	2.765586917629	0.550008614600	1.010013548834
H	2.495988736198	-1.059033398427	-1.720847442941
H	0.632371310569	0.021729205153	-1.535455642798
H	5.222258745265	0.912051140253	-1.486492437217
H	2.853406769583	0.911661993045	-1.123201630253
H	2.597388452008	-2.796169353210	-1.650053273411
H	5.573014179081	1.156041587760	0.215273126574
H	1.268613251932	-0.756546597931	1.760905867099
H	3.526468634046	2.208909235926	-0.172482456593
C	4.449890692632	-1.851014667432	-1.201690485107
H	4.753635201668	-1.661088839488	-2.243447225843
H	4.825289834924	-2.858550356381	-0.963449888197
C	5.175699451301	-0.874907487306	-0.279826535779
H	4.974601358766	-1.145573772171	0.765657705261
H	6.256293901499	-1.035769346515	-0.409100797534
H	1.559202982437	-2.637104277621	0.387065004914
H	2.296919164311	1.372478874736	1.570474140296
H	3.529751778870	0.152429877091	1.701812775719
H	3.100123466779	-2.149354340120	1.008344109431

TpRh(CNMe)-Cyclooctane product-(1)

G = -1258.471472

B	2.967293276143	0.725843985851	0.274610612481
H	4.084731798478	1.118106009626	0.437016375572
N	2.538888375766	-0.161146240308	1.446246301254
C	3.232608145221	-0.576715305088	2.518177372918
C	1.206255055855	-1.419973425325	2.568467392903
C	2.414098373927	-1.393699243126	3.274604509560
H	4.256250711806	-0.257015114019	2.665913003194
H	0.277188446009	-1.929294110947	2.799661855461

N	2.874343684055	-0.083780776163	-1.030935183977
C	3.825089768562	-0.412875690210	-1.919447752396
C	1.874956477816	-1.143928869417	-2.613651738611
C	3.230002904340	-1.102624387441	-2.958805883414
H	4.855264128831	-0.127327940584	-1.748892327659
H	1.034955886354	-1.576019500778	-3.144399918833
N	2.004927697285	1.918633575200	0.140690836181
C	2.325474269829	3.214244928538	0.004735365188
C	0.185943811084	2.945662950925	-0.392266188970
C	1.186109663764	3.917905807244	-0.331938045042
H	3.347005414455	3.538647960368	0.155792657203
H	-0.864952331095	3.054040208963	-0.627518457847
N	1.674883483729	-0.528464753608	-1.454958019965
N	0.681944725137	1.748045919464	-0.098924937104
N	1.294779544017	-0.676212330311	1.472881962196
Rh	-0.059212080823	-0.217259549402	-0.200137956140
C	-0.638706214455	-1.992498046133	-0.488725828459
N	-0.955747603879	-3.086342184750	-0.732047802497
C	-1.469424199201	-4.375990504923	-0.956329757509
H	-0.658847198302	-5.112883641506	-0.942577581480
H	-2.194737144971	-4.627905396072	-0.173421184079
H	-1.970723037482	-4.415817122432	-1.930058147107
H	2.654671733941	-1.892223289595	4.201899408526
H	1.090100568543	4.979013646899	-0.506593287083
H	3.705304337622	-1.507471971767	-3.839952537991
C	-3.317895008073	2.100441012193	0.488526819643
C	-3.327614534823	1.781787656296	-1.012901118652
C	-2.708318147531	-0.975561343397	1.414309471295
C	-4.227403963005	0.621616599367	-1.438427371599
C	-3.987910225610	-0.995922261831	0.561796252465
C	-3.862111931717	-0.781232481848	-0.954001255615
H	-4.307220007522	1.844441700053	0.894465309953
H	-5.257345142026	0.843265332729	-1.108658433296
H	-3.051653664310	-0.887258361527	2.462432441119
H	-4.700429099378	-0.258752566271	0.958055520680
H	-3.254858441228	3.193285870349	0.607805835423
H	-2.239417836771	-1.970540834614	1.367267365577
H	-4.263954523780	0.606301884077	-2.538460821683
H	-4.471969566966	-1.967043138497	0.746019713123
C	-2.213679288150	1.510374890358	1.393140002854
H	-2.625941146742	1.538723437702	2.419724856424
H	-1.376294625913	2.216144293510	1.427273770655
C	-1.630995497618	0.101675900423	1.197167395291
H	-0.939989622418	0.150675851507	-1.409607778116
H	-0.990245698273	-0.005284252589	2.089232298822
H	-3.689853083214	2.672038405280	-1.548948856910

H	-4.539150601748	-1.481486937464	-1.465858053786
H	-2.852498826503	-1.031249193296	-1.297549366637
H	-2.310574989042	1.603118938318	-1.378242113505

TpRh(CNMe)-Cyclooctane product-(2)

G = -1258.489227

B	-2.691370069662	-0.688832520400	1.155796972592
H	-3.591665152176	-1.142001623905	1.798448992608
N	-1.556352166449	-0.231508456329	2.081706908158
C	-1.457280697308	-0.284324682368	3.419805573137
C	0.350716399316	0.631672776266	2.575731070509
C	-0.242071096344	0.261241665727	3.787767471418
H	-2.259455484724	-0.705963764978	4.011834837680
H	1.314636999217	1.089997853049	2.385376792018
N	-3.180877356642	0.510847256248	0.324856643671
C	-4.396212569273	1.079408633287	0.269473408634
C	-3.047690326579	2.069917785661	-1.151312858116
C	-4.360454599641	2.094404839044	-0.667162386837
H	-5.198848988051	0.716269256328	0.898572087790
H	-2.574772339569	2.684847169639	-1.907606563927
N	-2.156225672072	-1.745817763179	0.174553522936
C	-2.648618673582	-2.960202093851	-0.114007328604
C	-1.036432536328	-2.469389729576	-1.520423924779
C	-1.954834838737	-3.470451301332	-1.194882980819
H	-3.461689994259	-3.370477127047	0.470894654712
H	-0.290442761081	-2.432824212519	-2.304946770261
N	-2.349891911462	1.115989462107	-0.549247574248
N	-1.161070131220	-1.443408826910	-0.688311273536
N	-0.448222353535	0.330505323989	1.560091253091
Rh	-0.286533684462	0.442866059193	-0.604891555944
C	0.481100181688	2.172509286247	-0.671375451754
N	0.988343853960	3.219654191059	-0.723273063539
C	1.612433442773	4.475687952646	-0.828556443801
H	1.520371945168	5.022426526430	0.116527153925
H	2.675064540517	4.345633622206	-1.062482877917
H	1.143103909108	5.063342126333	-1.625663310500
H	0.155432282883	0.374371563745	4.785461190233
H	-2.094261766760	-4.425996959808	-1.677802914422
H	-5.166907315354	2.749455778574	-0.961789980468
C	3.963999768396	-0.327659448577	-1.793955251681
C	4.699554355338	0.413915857465	-0.666576267404
C	1.769877603469	-1.652798870805	0.121871175633
C	5.092840170615	-0.435860822627	0.543591405859

C	3.131010738731	-2.125186393847	0.677045723580
C	3.989411838255	-1.072354161016	1.391913017760
H	4.207946001301	-1.397057784023	-1.747712439488
H	5.748202273669	-1.247500591993	0.184316022480
H	1.427470051759	-2.407609680693	-0.600399870312
H	3.734125387869	-2.590195950748	-0.114470152312
H	4.358226040082	0.010756426990	-2.763607088088
H	1.048750219481	-1.699647785388	0.952034041103
H	5.722022679025	0.180128393736	1.204460788589
H	2.917144564881	-2.942299189125	1.381278386205
C	2.443042021975	-0.111999862316	-1.820532300751
H	1.999384440451	-0.785136256500	-2.572463759449
H	2.266784558877	0.903614750369	-2.209734244778
C	1.685377727704	-0.257523987787	-0.501156406380
H	2.151848860105	0.436711221749	0.220636443138
H	-0.211216456854	0.447855208725	-2.156155729424
H	5.630169947614	0.842228081721	-1.066527994411
H	4.488669077791	-1.548679377090	2.248138788080
H	3.347724263190	-0.292700548930	1.830677356735
H	4.098550747183	1.277743372348	-0.337982971468

TpRh(CNMe)-Cyclooctane product-(3)

G = -1258.486722

B	-2.585046393217	-1.335513323691	0.685901394320
H	-3.446744723244	-2.053821150181	1.099046556852
N	-1.861801943682	-0.653570503386	1.851805819982
C	-2.069886580515	-0.754916497024	3.174187042204
C	-0.419036301834	0.638915133952	2.784751706725
C	-1.162254761525	0.062241681313	3.820266267282
H	-2.848037451215	-1.402388416053	3.557654495142
H	0.406557785652	1.339066847530	2.832394512166
N	-3.187252612146	-0.261814303969	-0.239030643405
C	-4.467378986081	-0.035477961180	-0.575718768840
C	-3.158619022266	1.360623985996	-1.651045735586
C	-4.501936738143	1.005972629896	-1.483036070193
H	-5.259734860526	-0.636394669964	-0.147962766796
H	-2.714954687863	2.122639707423	-2.280642512900
N	-1.575807158782	-2.145564595338	-0.145566528913
C	-1.681898722245	-3.412254875603	-0.576831103273
C	-0.018900667196	-2.423579417500	-1.611134633485
C	-0.695594788468	-3.642453333769	-1.515344054869
H	-2.459946988064	-4.055375985607	-0.186075168364
H	0.811443191495	-2.138951396969	-2.242653551585

N	-2.379536869174	0.592882980478	-0.900608210923
N	-0.546389629218	-1.534846788299	-0.778283938179
N	-0.849298961021	0.201572196538	1.607759405971
Rh	-0.246828168737	0.510758978642	-0.464187321781
C	-0.034407014015	2.386414029195	-0.338656020686
N	0.117237124543	3.538758280089	-0.266225649898
C	0.313720140725	4.930195675965	-0.208360438757
H	-0.446687028266	5.390937333172	0.432061596238
H	1.305443527013	5.150850527539	0.201969316542
H	0.242228022694	5.362105774795	-1.213042855167
H	-1.053140026077	0.216545469989	4.883505901755
H	-0.495817915404	-4.556132498578	-2.054734787762
H	-5.369671909017	1.438151579234	-1.959013839956
C	2.114887812459	-0.971135138806	0.754625864466
C	2.865918498361	-1.982362738508	-0.129709128441
C	4.096493719239	1.441666337064	-0.338111385329
C	4.375267137211	-2.069469256514	0.097593232388
C	4.972461431190	0.433465490550	0.404310959198
C	5.222036666755	-0.879434597111	-0.352760526877
H	2.710845763491	-0.828661374124	1.670914896813
H	4.559592595027	-2.242303758159	1.171277421487
H	3.908553210636	2.300280615183	0.327763339236
H	4.544634647610	0.212264100109	1.391795183634
H	1.188412878515	-1.440004699201	1.111905579287
H	4.679741151988	1.841546024836	-1.184615288921
H	4.749727379867	-2.966997436608	-0.417890594310
H	5.935291231282	0.922084050846	0.611645553066
C	1.755071409942	0.405776363757	0.143818927646
H	1.782389097658	1.120717993852	0.990562973423
H	0.186006228438	0.645526032151	-1.950782188421
C	2.754356272427	0.946688237615	-0.883687149598
H	2.925339464902	0.204847521815	-1.677475535401
H	2.297958912355	1.796986454195	-1.409259142944
H	2.447752338824	-2.983213031490	0.052000841044
H	6.277114515527	-1.165781632038	-0.237854330735
H	5.079784505422	-0.715537062820	-1.433474126833
H	2.682414958118	-1.783729902777	-1.193735018223

TpRh(CNMe)-Cyclooctane product-(4)

G = -1258.485588

B	-2.998021966723	-0.566768520661	0.757366845830
H	-4.072749325262	-0.874399512769	1.180896927877
N	-2.296739361796	0.386829039317	1.727443171273

C	-2.712516887305	0.904299298820	2.894469934802
C	-0.688348309011	1.623462182039	2.438945708455
C	-1.708126652286	1.712110640538	3.393073805656
H	-3.690958096719	0.656817004222	3.285881940161
H	0.292656311074	2.085285360251	2.423956363332
N	-3.145380702506	0.117433929076	-0.613997249480
C	-4.248759856118	0.425955876032	-1.313705189472
C	-2.461666547774	0.955824849433	-2.473225810698
C	-3.859929727355	0.974493043237	-2.521101953527
H	-5.230389258207	0.227096773146	-0.902892239568
H	-1.736368982929	1.279317371072	-3.210378019198
N	-2.134539482853	-1.823200497342	0.548685743130
C	-2.542241903882	-3.101262715897	0.571718345502
C	-0.523159386727	-2.994125562001	-0.275969441369
C	-1.536404641936	-3.895009482496	0.058004448707
H	-3.525293871236	-3.349677792299	0.950582702812
H	0.441998546371	-3.181999519874	-0.727113798570
N	-2.045318901214	0.437957660866	-1.324688736863
N	-0.883022050382	-1.752191371806	0.031536827541
N	-1.055700765186	0.825568025137	1.444443785946
Rh	-0.101794143490	0.154710207212	-0.394350075375
C	0.449550219710	1.868758550367	-0.970034122962
N	0.715119695920	2.926682427256	-1.377464907458
C	1.163583015239	4.187844835239	-1.806756142326
H	2.131714835762	4.414381264238	-1.344071842444
H	1.280416807276	4.196251200280	-2.896320721943
H	0.442108518273	4.961548582590	-1.521687820736
H	-1.712065339032	2.277838928557	4.312948851978
H	-1.533361350765	-4.968343285011	-0.058770018861
H	-4.494493315901	1.326203185816	-3.321036337850
C	2.708040856459	1.014868190545	0.513461130808
C	4.069052993914	0.847656768448	1.216761450980
C	2.897160154479	-1.979422977866	-0.815661252046
C	5.233183493608	0.446187945001	0.308124408734
C	4.087503320024	-1.187064472047	-1.361415521482
C	5.216584825234	-0.935043998977	-0.349858571289
H	2.899975299729	1.249872072455	-0.544092629638
H	5.310924401697	1.201154012681	-0.493304582865
H	2.103683896428	-1.982748631079	-1.576463234888
H	3.746164655655	-0.230528059570	-1.780739539702
H	2.224113862340	1.918672583210	0.918743777772
H	3.220295931786	-3.028037802162	-0.699733468594
H	6.165677054115	0.533663788250	0.886465761522
H	4.491017429932	-1.746814079289	-2.217306509644
C	1.696559531213	-0.139194293980	0.649996650078
H	0.567453746037	-0.378627802775	-1.690070066903

H	1.348671323937	-0.097891412094	1.700135448521
C	2.338430873775	-1.522781939060	0.528236044537
H	3.153454901655	-1.598944935902	1.267623527696
H	1.612257453769	-2.267116823502	0.875413377346
H	4.346977133504	1.809612759847	1.672810242811
H	6.182879845797	-1.051673104985	-0.861309935117
H	5.203567690946	-1.718154112811	0.424654149296
H	3.982417200937	0.145995351077	2.059963367767

TpRh(CNMe)-Cyclooctane product-(5)

G = -1258.486603

B	-2.435329102308	-1.013143362730	1.246665136585
H	-3.225249234445	-1.562564514747	1.956320806005
N	-1.529828705253	-0.096504208360	2.074066387117
C	-1.524920272839	0.137930746026	3.395713318702
C	0.110935928757	1.242065226711	2.436597023716
C	-0.483564808628	0.999644050618	3.679582699391
H	-2.261199070559	-0.329841813063	4.036690811328
H	0.968117271182	1.857045927682	2.193558703359
N	-3.169824641671	-0.187728130333	0.179044299641
C	-4.484499096172	0.001160414175	-0.017368318792
C	-3.342773633739	1.029652134699	-1.585286172683
C	-4.647773385674	0.784855828094	-1.143754926890
H	-5.207392018529	-0.440366648255	0.656668664006
H	-2.992931832272	1.591096755188	-2.443422830138
N	-1.564488774592	-2.055537112035	0.525982701851
C	-1.693469502864	-3.390253716258	0.541500074468
C	-0.143549629526	-2.820227882771	-0.900807944987
C	-0.795247251241	-3.929274249363	-0.357643793074
H	-2.421001593318	-3.857195947914	1.192836746134
H	0.628415803371	-2.785064897266	-1.656283325409
N	-2.465560553115	0.440297375395	-0.783067156112
N	-0.604798754554	-1.696906642225	-0.360664780439
N	-0.526053015746	0.578845811684	1.478462088962
Rh	-0.299368917364	0.361357233550	-0.696726667632
C	-0.147649684408	2.199411678701	-1.104093018160
N	-0.114942536527	3.331797889470	-1.374189786047
C	0.046631171683	4.691328566465	-1.692349441107
H	-0.603640053556	5.306389085065	-1.060394713895
H	1.088888280237	4.990000023081	-1.528183800619
H	-0.211310010096	4.866556261582	-2.742945882869
H	-0.194577399455	1.392583816039	4.643043855335
H	-0.634425359404	-4.971244440507	-0.590205137334

H	-5.574208807117	1.121788299876	-1.584716546148
C	1.769749797834	0.154562199752	-0.483124557290
C	2.465619369804	-0.771858327288	-1.503230031391
C	4.476334210781	0.649817266095	1.178661629754
C	3.253019282846	-1.938346223596	-0.896179055044
C	4.309726009362	-0.878963047502	1.231889722462
C	4.519260858182	-1.633789454439	-0.088826057643
H	1.804905225488	-0.341428183669	0.500478226589
H	2.572355601214	-2.507939836661	-0.241025875263
H	3.965161648182	1.096155760388	2.047168338617
H	3.325875286122	-1.147943906426	1.637472372463
H	-0.160809594241	0.136532758068	-2.224868436272
H	5.544625935630	0.873633016844	1.323085077943
H	3.534495102349	-2.627817814180	-1.708687799977
H	5.033366143321	-1.253510893115	1.970107379636
C	2.539661753004	1.474623038137	-0.366979259477
H	2.087508203859	2.111600889441	0.410839691735
H	2.424598136691	2.035425457373	-1.310677067359
C	4.041800474912	1.376992638483	-0.091916797180
H	4.545324569462	0.923404402482	-0.956771903036
H	4.440537662631	2.402211682449	-0.041211157708
H	1.732167409017	-1.192637191046	-2.201218979100
H	4.984808500946	-2.602892581519	0.141829182859
H	5.253087647740	-1.106741604434	-0.718501510868
H	3.133066212050	-0.181083747344	-2.152703706833

TpRh(CNMe)-Cyclooctane product-(6)

G = -1258.477078

B	-2.684724873460	-1.141331942940	0.536426764031
H	-3.671072251075	-1.752519677007	0.824000577121
N	-2.299510677509	-0.194049473709	1.675560384530
C	-2.939768060719	0.061731268990	2.827421889469
C	-1.150567486839	1.322520736739	2.673176209161
C	-2.235495188217	1.035475433426	3.508277217996
H	-3.848254599496	-0.470880763831	3.078117759534
H	-0.340933343684	2.028028378041	2.815966641300
N	-2.923581342966	-0.323125429853	-0.745020253439
C	-4.028333769782	-0.182898449310	-1.494539753915
C	-2.364419368035	0.918406910567	-2.409800985706
C	-3.719351271229	0.614260630624	-2.580425174985
H	-4.952318307572	-0.665486253667	-1.202563341402
H	-1.700884294050	1.508610311803	-3.030651297955
N	-1.527647246990	-2.109702839161	0.249074083377

C	-1.586655545290	-3.443289094485	0.113980929760
C	0.382990851918	-2.728104708104	-0.530815887926
C	-0.376398408449	-3.889888220101	-0.378449479030
H	-2.491732628116	-3.975536367986	0.376835635622
H	1.394705335333	-2.608903213324	-0.893473052262
N	-1.898731486319	0.348899388074	-1.305280585413
N	-0.311183332821	-1.663608821137	-0.144074696834
N	-1.197590120534	0.576464223243	1.575655448165
Rh	0.004272038592	0.416015125756	-0.264902950379
C	0.180584091223	2.268990485765	-0.588096119426
N	0.244659649235	3.403693143944	-0.842044615611
C	0.445875393219	4.767653293880	-1.117632934660
H	0.425553479563	4.940242543581	-2.199553547901
H	-0.341288550054	5.367622130933	-0.647755455237
H	1.419703485865	5.085247784486	-0.726028467312
H	-2.469342442558	1.470844709216	4.468467786039
H	-0.084434660132	-4.906172184851	-0.596605107393
H	-4.375110990679	0.921185912125	-3.381689067494
C	1.768398705902	0.557497757609	0.896512839109
C	2.874427143526	1.521490221191	0.410661003126
C	4.012551607377	-1.932761824881	0.030152002293
C	3.480417364215	1.419921489198	-0.991970179400
C	3.693359840214	-1.129303693441	-1.225247630317
C	4.395583433328	0.234059588536	-1.288348116145
H	0.807461691273	0.217878404096	-1.570232392460
H	2.666528613844	1.425436881901	-1.732802783220
H	3.447393133470	-2.878721980608	0.017144258109
H	2.611447888817	-0.956725259923	-1.293615654711
H	1.332792457529	1.119255844765	1.738859623277
H	5.075341850181	-2.222929842370	0.004144316070
H	4.057768507015	2.342344551832	-1.165683334522
H	3.961589893799	-1.733939659035	-2.103331043184
C	2.292022693154	-0.746736191529	1.573453216819
H	1.629146707330	-1.594258064075	1.363817439714
H	2.194757496465	-0.596339078905	2.660559917160
C	3.735131397680	-1.212142710746	1.344030222882
H	4.433470762664	-0.371945226858	1.457816227414
H	3.992341759940	-1.903300415178	2.160640621726
H	2.460420338143	2.538971995896	0.486471994329
H	4.821236927746	0.382380933633	-2.290856996454
H	5.256658284974	0.247263886130	-0.600456545557
H	3.702634311767	1.523250745044	1.141496120086

TpRh(CNMe)-Cyclooctane product-(7)

G = -1258.480360

B	-2.601863303065	-1.079069379569	0.660422821015
H	-3.559051206323	-1.704457397003	1.009682599890
N	-2.115732373737	-0.180011534547	1.796871981746
C	-2.634621234850	0.012449204271	3.019626357066
C	-0.879992858132	1.300541326128	2.741851210899
C	-1.869848593264	0.961072392410	3.669931014070
H	-3.508865514759	-0.541863881708	3.336273252293
H	-0.065342453156	2.008029599266	2.836156203503
N	-2.957748990224	-0.208699889137	-0.560659371143
C	-4.132534049824	-0.045832659751	-1.190049288118
C	-2.574895053581	1.111864616263	-2.215313794432
C	-3.938411004908	0.801751039686	-2.263998746556
H	-5.020314545377	-0.549695028245	-0.829664483235
H	-1.980568857025	1.736387023062	-2.871623968094
N	-1.478985663843	-2.034634501036	0.224925031386
C	-1.591176454852	-3.347486565899	-0.032022142042
C	0.269317957243	-2.588122862499	-0.905779733891
C	-0.484204053913	-3.753758952174	-0.748537743241
H	-2.461362349397	-3.893649261718	0.308844767491
H	1.198019973273	-2.439462179927	-1.438506168000
N	-1.997201032443	0.499267491104	-1.189946724348
N	-0.323570534148	-1.562798637718	-0.305225562256
N	-1.036182631071	0.607119324728	1.619699798171
Rh	-0.003678735658	0.515394110087	-0.326284657690
C	0.211408499601	2.378774301533	-0.554046704955
N	0.328964913336	3.525274814901	-0.720630856357
C	0.563392489610	4.896991533555	-0.921866763839
H	0.392273370828	5.158140296994	-1.972238336423
H	-0.110375953993	5.490747918493	-0.294230529407
H	1.600443686303	5.138624760351	-0.660683076628
H	-2.005521330400	1.348328675251	4.668833382716
H	-0.254442762436	-4.745235625896	-1.108827994938
H	-4.672726686011	1.137308489838	-2.981226083448
C	3.006686773274	1.354438736926	0.116916546307
C	1.815001364294	0.591360195892	0.724227861314
C	4.687358312695	-1.221270839441	-0.947795848615
C	2.206247608020	-0.663978565057	1.532367186547
C	4.501539660112	-1.425784261463	0.559617318945
C	3.074559401920	-1.802328400023	0.982041910614
H	3.865474494667	1.262194446575	0.802073476848
H	2.750977127019	-0.297894062123	2.425069764031
H	5.665769310306	-0.751969760156	-1.137467862562
H	4.827385636581	-0.538459809472	1.117912855975
H	2.766422336694	2.429990657224	0.131473973607
H	4.741097356744	-2.216777174062	-1.417038300253

H	1.278784444844	-1.107431654315	1.928931098491
H	5.191648471777	-2.224343349374	0.867720054045
C	3.456577708068	1.035319489135	-1.310541547899
H	4.411393430762	1.551598424599	-1.505036363968
H	2.725885900048	1.476565229994	-2.005308703553
C	3.597069350845	-0.436342105508	-1.668749072030
H	2.624429050273	-0.915904129736	-1.501732213864
H	3.781521584824	-0.512499233268	-2.750804655237
H	1.483884201544	1.268558824403	1.531442573338
H	3.137178475702	-2.543465396369	1.792484740334
H	2.578649936649	-2.330475094592	0.160715958912
H	0.702927784493	0.370419564333	-1.695123138988

TpRh(CNMe)-Cyclooctane product-(8)

G = -1258.486605

B	-2.623724502358	-1.138539319401	1.004441517102
H	-3.482581622208	-1.724506763735	1.594734108007
N	-1.820276112703	-0.264782886954	1.972196504466
C	-1.976594303699	-0.097940960111	3.294760174863
C	-0.247374545979	1.057207947691	2.596903472700
C	-0.984666776589	0.750341457085	3.745276975813
H	-2.780882691079	-0.599680863866	3.817396139879
H	0.627160736949	1.686501797660	2.495726708196
N	-3.243524090758	-0.258704987371	-0.091831361429
C	-4.530071421679	-0.064051026679	-0.422544707387
C	-3.232150866882	1.061490019805	-1.789334500193
C	-4.575375714251	0.784884843842	-1.511992157651
H	-5.318699208135	-0.547791579515	0.139487380913
H	-2.795232479144	1.674874193629	-2.568363392038
N	-1.671794879988	-2.140655849861	0.331788268856
C	-1.775584349285	-3.476464687758	0.272212947925
C	-0.082886929944	-2.816433039441	-0.956355283803
C	-0.770582031927	-3.959283004294	-0.542275653797
H	-2.562109248019	-3.984383555743	0.815281722041
H	0.765740698506	-2.729665123964	-1.619922825662
N	-2.443447790615	0.429305688666	-0.929770563586
N	-0.625534553639	-1.728164769828	-0.421416083129
N	-0.757202888465	0.442890496117	1.535115157871
Rh	-0.300817989463	0.336529699112	-0.623566935690
C	-0.099965972885	2.188157568350	-0.950786689515
N	-0.031809952375	3.326504728639	-1.187395441089
C	0.165236706933	4.693750363203	-1.447206980562
H	-0.543748423427	5.293962158185	-0.866103519939

H	1.186324477803	4.981411501226	-1.169750968983
H	0.015457866233	4.901288861684	-2.512791329889
H	-0.816041853929	1.093950425485	4.755052198539
H	-0.565256707553	-4.986728798279	-0.802805262357
H	-5.450528641237	1.143954847869	-2.032987389716
C	2.538524853760	-0.653371324629	-1.302418552829
C	1.739815496588	0.098886113771	-0.216565417262
C	5.408247308795	-0.563131566917	0.301721766729
C	2.436709294422	1.414422206749	0.165099032265
C	4.991977410869	0.889394320836	0.050734089287
C	3.797053147726	1.383870164616	0.879947119333
H	3.143723703087	0.071131965066	-1.866267152949
H	2.563450506969	2.014020590668	-0.755102805442
H	6.110097405569	-0.877954710802	-0.486538404326
H	4.782460973292	1.050699837621	-1.014973267310
H	1.862229952028	-1.065364986391	-2.061439062404
H	5.982991167959	-0.594934637030	1.240811678891
H	1.765688278873	2.008890360355	0.801810221141
H	5.866052067620	1.520434180972	0.266327137636
C	3.422108726958	-1.813875292276	-0.817134020453
H	4.064074900958	-2.146203868942	-1.649952382015
H	2.765811302531	-2.668272808344	-0.587923005472
C	4.285406248481	-1.586893274648	0.419339750843
H	3.638784659680	-1.323988251606	1.267958685068
H	4.738929609669	-2.550676695855	0.694463291280
H	-0.020791834529	0.182050752372	-2.138829954201
H	4.003917630873	2.415268856121	1.203500740162
H	3.715034194136	0.801177792746	1.811356491562
H	1.692608055478	-0.535144105900	0.689042789708

TpRh(CNMe)-Cyclooctane product-(9)

G = -1258.489838

B	-2.579151925960	-1.330592765085	0.739211484099
H	-3.415752516158	-2.047957462393	1.202074625376
N	-1.885103155237	-0.537636170108	1.854869880858
C	-2.089089923837	-0.555120233357	3.182019166648
C	-0.499113845835	0.877996349940	2.692956280849
C	-1.217130064808	0.342689434423	3.767923969661
H	-2.840105122552	-1.205573310992	3.611769443925
H	0.299469186928	1.611018011771	2.686911083475
N	-3.213441369775	-0.347134864325	-0.259946783424
C	-4.498442109243	-0.192895441622	-0.618075724288
C	-3.235844034327	1.185066019447	-1.769382107064

C	-4.565605407444	0.788285740850	-1.588458131615
H	-5.270468546515	-0.796756509267	-0.158517661756
H	-2.816859291232	1.923808453912	-2.442085752295
N	-1.533226925016	-2.160648958215	-0.025486510253
C	-1.546074107286	-3.467835565800	-0.328287309857
C	0.111660482789	-2.487634988307	-1.381393110156
C	-0.500657323006	-3.729169242341	-1.193699838905
H	-2.303350273370	-4.116347021216	0.093052343382
H	0.969437128133	-2.214114765348	-1.984268258291
N	-2.434103682995	0.496929435390	-0.967462806616
N	-0.511065425522	-1.556246870476	-0.670330035088
N	-0.910165427404	0.341993158209	1.550964160230
Rh	-0.304139484277	0.508903563852	-0.530341825756
C	-0.123431873146	2.393347912146	-0.549201383545
N	0.015593993438	3.549589835190	-0.567339497536
C	0.195386208283	4.943441421645	-0.620251601758
H	1.152475320805	5.214924649951	-0.161049624204
H	0.193745502284	5.283393494795	-1.662138460968
H	-0.613600987976	5.447822920704	-0.080030576383
H	-1.116230447694	0.575040232377	4.817713609641
H	-0.223466710355	-4.678471544010	-1.626957609123
H	-5.445407857208	1.155839964395	-2.095546034868
C	4.114771794844	1.185829046493	-0.739136574281
C	2.661435851538	0.835332913524	-1.120109995585
C	4.555630428110	-1.532005315023	0.979654748497
C	1.711632661351	0.459961471557	0.028164431931
C	3.365666816100	-0.797847415450	1.610002261800
C	2.062735343095	-0.830109796071	0.785093105680
H	4.141570319216	1.531016369809	0.302941313562
H	1.810200644985	1.272831331299	0.779767021613
H	5.475513667351	-1.273152252411	1.528081375656
H	3.630883432207	0.242800981462	1.837543560389
H	4.437518318997	2.055028553892	-1.331726564941
H	4.410176366810	-2.612062572394	1.139025649265
H	0.110182701572	0.541397200056	-2.026631044752
H	3.182309915785	-1.262290789065	2.589916602724
C	5.156155677744	0.085074035877	-0.965678840727
H	6.103936736788	0.381645096707	-0.488388074449
H	5.370684817778	0.037351156740	-2.045079040936
C	4.785034862811	-1.322744187337	-0.513863718785
H	3.896770389012	-1.656908588645	-1.069138155627
H	5.590507122190	-2.002021752255	-0.830435983224
H	2.230340198780	1.705840437927	-1.633011466311
H	1.230670245523	-1.058419580655	1.464716856589
H	2.100524692775	-1.683034698312	0.094446933372
H	2.654542352371	0.038520625305	-1.882971538473

TpRh(CNMe)-Cyclooctane product-(10)

G = -1258.484265

B	-3.034240222216	-0.596803175439	0.547814384155
H	-4.140669326234	-0.923932936618	0.860588846739
N	-2.416498827112	0.293235944915	1.628898892512
C	-2.932804084423	0.745192885066	2.782938355535
C	-0.881689786519	1.490801246902	2.541656185367
C	-1.979142559812	1.525080134718	3.409076377862
H	-3.939546554078	0.475419973432	3.075292301868
H	0.094560426939	1.953404903710	2.635911004698
N	-3.065900996393	0.171625274345	-0.786402878066
C	-4.106536687731	0.525020759876	-1.557427520992
C	-2.228941195764	1.124658417042	-2.523890525285
C	-3.618038446977	1.147996987329	-2.690152121445
H	-5.118922106729	0.302372903820	-1.245283966944
H	-1.444654127070	1.493284011375	-3.174355850240
N	-2.156555277853	-1.842742874069	0.332346098820
C	-2.563276251681	-3.117038977850	0.224647121994
C	-0.483736004728	-2.955099825636	-0.451974665644
C	-1.518962329576	-3.874196699744	-0.267834708843
H	-3.573010869665	-3.389267078247	0.503895734926
H	0.513919884193	-3.106195662625	-0.842827979011
N	-1.910316801788	0.535013709118	-1.378749773901
N	-0.868948625399	-1.739824516252	-0.078147928184
N	-1.158391819920	0.748832862632	1.476906191909
Rh	-0.051393679502	0.177630640158	-0.311418935746
C	0.560189701425	1.918515031647	-0.723974087005
N	0.870849662863	2.999364770576	-1.025329558463
C	1.391222920318	4.264569010087	-1.349405541469
H	0.576386358314	4.966441465947	-1.558487492277
H	1.985365329933	4.648992606632	-0.511720708859
H	2.034080297601	4.188862733577	-2.234168414849
H	-2.064420388301	2.038861935246	4.355093079749
H	-1.506217682311	-4.935490247163	-0.465838355316
H	-4.183126385736	1.550311646317	-3.517868207269
C	3.003133789540	-1.934650969258	-0.555416590167
C	2.285024994507	-1.587955389519	0.760962587122
C	4.940699435090	0.669338585158	-0.342398141815
C	1.640218064049	-0.198992629436	0.886540432032
C	3.493674134502	1.177423366259	-0.354188287050
C	2.688839418182	0.925810895650	0.935955357876
H	2.632206153370	-1.285777227216	-1.356176405836

H	0.707494871288	-0.291051406125	-1.581222859127
H	5.343520881686	0.724048427451	-1.366476376976
H	2.946775807456	0.754813016421	-1.206325787979
H	2.727679366744	-2.954011640311	-0.867881155558
H	5.546721180766	1.371298272025	0.252281905965
H	1.174167306649	-0.203824132112	1.888542796414
H	3.541829479247	2.259538243143	-0.554314908139
C	4.536655611693	-1.901455963176	-0.503579638561
H	4.928424054441	-1.955881078932	-1.531858147602
H	4.885147573012	-2.819971371067	-0.005562628677
C	5.188035126671	-0.726946944466	0.220641263614
H	4.896004150170	-0.747290187338	1.279521001375
H	6.274951060640	-0.897264396889	0.224584289859
H	1.512584585893	-2.336265211617	0.968520217628
H	2.182434209789	1.856813219381	1.235414484737
H	3.395999841235	0.723766293895	1.760849364141
H	3.000959359316	-1.709742632745	1.594382870400

TpRh(CNMe)-Cyclooctane 1,2-migration-(2/4-ii)

G = -1258.452884

B	-2.676590739348	-0.790255340891	-0.002855685355
H	-3.734265425646	-1.355191288329	0.005454921192
N	-2.210691086402	-0.344957242683	1.383952484835
C	-2.249611645637	0.877853541126	1.953921946117
C	-1.507719926888	-0.613358497195	3.377869470700
C	-1.797403608968	0.756159146249	3.251178947618
H	-2.583730346230	1.744313839278	1.395611724550
H	-1.135120081151	-1.151962009651	4.242889723565
N	-2.806760636780	0.454561302482	-0.912346014433
C	-3.920850346501	0.978340303556	-1.446366155403
C	-2.193262908745	2.192228892150	-2.048682886050
C	-3.580138294513	2.097432014169	-2.181542528715
H	-4.878134708206	0.508931218952	-1.260340083008
H	-1.497174968823	2.907127713730	-2.468373758917
N	-1.626041306417	-1.724573444031	-0.623317349963
C	-1.718802233296	-3.020897327493	-0.938525243375
C	0.258453148828	-2.269205813452	-1.519464274680
C	-0.526891196277	-3.421205995038	-1.517186514275
H	-2.627777822726	-3.567101940731	-0.722303440234
H	1.264556959425	-2.118883557637	-1.892356139166
N	-1.741474552075	1.200452136182	-1.285331222355
N	-0.408788669492	-1.255365099295	-0.968792451794
N	-1.756940020893	-1.271923720006	2.254305998212

Rh	0.071205026826	0.726163590632	-0.616077131275
C	0.483042900761	2.547571431206	-0.298098085754
N	0.724722135366	3.673599402641	-0.092145565861
C	1.013273028227	5.013271920779	0.218922217217
H	1.561260806648	5.487742685294	-0.603772803960
H	0.082878304561	5.567264669867	0.389269749987
H	1.624358609926	5.066430026778	1.127591665934
H	-1.696480145986	1.537388985913	3.991115537197
H	-0.267145271390	-4.402197321280	-1.885670011047
H	-4.237148693742	2.745530357402	-2.741878525157
C	1.695909632252	-2.942615594325	3.094572821582
C	3.115269358889	-2.905148829526	3.682947260028
C	1.888911178241	0.039480070188	1.862650070453
C	3.447206433167	-1.686031009370	4.546335500043
C	2.137433879179	0.215434325131	3.367311488222
C	3.485412319621	-0.304548164620	3.888309076231
H	1.024026066019	-2.331252625048	3.712188772471
H	2.717048343381	-1.645797504970	5.372199372548
H	0.804346295184	0.178061032954	1.688306687022
H	1.323443969134	-0.250092688392	3.937557339956
H	1.297845446004	-3.963417351381	3.172512855567
H	2.407654636401	0.862775278965	1.340677532352
H	4.423561343067	-1.861788330215	5.022565088177
H	2.053003482483	1.289546152345	3.584029649356
C	1.579119445264	-2.525246644333	1.626572246204
H	0.514563506973	-2.400984251658	1.379395834766
H	1.948181230348	-3.353940439097	1.000931076313
C	2.342940521388	-1.270130816284	1.222077567922
H	3.420406427606	-1.410655425289	1.394412078861
H	2.254451109039	-1.160552330050	0.127942381235
H	3.259372398865	-3.789614223508	4.319427144341
H	3.861162426848	0.396962575350	4.646760014612
H	4.238824684710	-0.289441926977	3.085085799666
H	3.860192591501	-3.007329090565	2.877633745728

TpRh(CNMe)-Cyclooctane 1,2-migration-(2/3-ii)

G = -1258.454429

B	-2.426844649235	-1.658395762439	-0.241360212488
H	-3.243210223178	-2.536644171018	-0.286027448474
N	-1.858390588412	-1.390804235603	1.153977687001
C	-2.306689419812	-0.535439458536	2.095752455691
C	-0.563235085811	-1.642353647333	2.826309798111
C	-1.495019972443	-0.659958104426	3.203431862330

H	-3.157398562781	0.108353988117	1.905129739152
H	0.255939272516	-2.058597715744	3.402730202671
N	-3.094247438917	-0.359193987722	-0.754012975310
C	-4.384520171807	-0.141761375610	-1.051181601557
C	-3.243389424840	1.702507629926	-1.392055637622
C	-4.532434460560	1.169347021610	-1.461717516099
H	-5.103441737273	-0.943965689921	-0.946080681714
H	-2.882640810610	2.693635189187	-1.635870966350
N	-1.266021406022	-2.001349551419	-1.181779737969
C	-0.972980563529	-3.146185832537	-1.807820125613
C	0.583321918450	-1.659994865760	-2.233546137157
C	0.212385513532	-2.978270090108	-2.501633866832
H	-1.626991974534	-4.002551775195	-1.707484403164
H	1.435003673534	-1.092519331550	-2.590161120504
N	-2.389451826190	0.775378598575	-0.965706089212
N	-0.310862755845	-1.084829337859	-1.431499166792
N	-0.783692606923	-2.079366085251	1.594030959991
Rh	-0.427439577578	0.804401015651	-0.597065597873
C	-0.552297450982	2.532233642054	0.162708605892
N	-0.640405891454	3.598448454946	0.637040770320
C	-0.745374713630	4.834436264670	1.297024700437
H	-0.236412849732	4.790848844084	2.267390362257
H	-0.290843356790	5.629583652134	0.694358062790
H	-1.800193979810	5.080503998981	1.465539440348
H	-1.568168981474	-0.124209635331	4.139187703112
H	0.728088669598	-3.701726945580	-3.115005753468
H	-5.438519436193	1.665847276991	-1.775156108661
C	4.286417083190	-0.309792640353	2.010436205167
C	4.608939961593	-1.576539660009	1.203425722021
C	2.616690724780	1.052300837433	-0.458128668439
C	5.244146084139	-1.339123165927	-0.167876188966
C	4.042283381679	0.816944340119	-0.972921516294
C	4.408916883966	-0.650192620828	-1.248754993129
H	4.951257926444	0.503364433906	1.689199758829
H	6.166106736079	-0.751265265786	-0.021922274449
H	2.526681088989	2.090723202848	-0.102447209732
H	4.772969724256	1.249922306933	-0.277085320435
H	4.539816081045	-0.480721203967	3.065951964623
H	1.940267148168	0.986738036852	-1.334046289315
H	5.572058599839	-2.311608583984	-0.563606712947
H	4.152768361115	1.399414916959	-1.898031113286
C	2.821319530126	0.139784308453	1.971628710338
H	2.742767332867	1.155709893029	2.389327426632
H	2.245024425445	-0.506992652113	2.649598887003
C	2.112618055294	0.094967110604	0.621515211479
H	2.094814674105	-0.935115972384	0.239419840139

H	1.044581754200	0.305417101699	0.862884207215
H	5.316182651121	-2.190105227496	1.778433731568
H	4.989016394567	-0.698341408826	-2.180796892661
H	3.498939287945	-1.239115767992	-1.441076861491
H	3.706182302124	-2.197789006275	1.098164872606

TpRh(CNMe)-Cyclooctane 1,2-migration-(3/5-ii)

G = -1258.453395

B	-2.985012927988	-0.917868537471	0.480652003726
H	-4.042062670677	-1.384852048748	0.804037699041
N	-2.064274636808	-0.557587085909	1.650613784639
C	-2.053286888249	0.579496658504	2.375897500347
C	-0.502358649656	-0.797930574820	3.079668546980
C	-1.053150728373	0.472968811883	3.319135889254
H	-2.746633122784	1.384473151949	2.161521002297
H	0.310817518474	-1.294953981445	3.597774479181
N	-3.260930992884	0.376065663179	-0.324692208027
C	-4.425776425535	1.008239226944	-0.532001249037
C	-2.809979742085	2.132609070952	-1.505058412441
C	-4.188585354668	2.144736052783	-1.281996384282
H	-5.340873100451	0.598030267772	-0.124785344741
H	-2.184308397963	2.822018561813	-2.057375094388
N	-2.256031490002	-1.903556840064	-0.437830199836
C	-2.516594910125	-3.189184019149	-0.699193021324
C	-0.698599368815	-2.580085273008	-1.765040742424
C	-1.540576195172	-3.672418011196	-1.552212366674
H	-3.377219436705	-3.670295111772	-0.253012719125
H	0.188562771511	-2.497117434998	-2.381445114056
N	-2.265446843210	1.066158825881	-0.924757279547
N	-1.136733031633	-1.522834319104	-1.085160060672
N	-1.112183003876	-1.414771135874	2.076648679547
Rh	-0.394603729205	0.391420794684	-0.821732221179
C	0.257372151291	2.138528850438	-0.506198925639
N	0.646437733491	3.220682732502	-0.288803294791
C	1.147268722529	4.470928078362	0.110877292600
H	0.428826973940	4.970716058332	0.771131616152
H	2.090959373876	4.339894335116	0.654256870696
H	1.328463934364	5.109195157455	-0.761963006047
H	-0.770619191170	1.200386350719	4.066977229880
H	-1.454048292787	-4.667460623931	-1.961997200623
H	-4.908259618371	2.872813521654	-1.625088711605
C	5.260612456750	-1.405382763549	0.457741253698
C	5.183699568704	-0.122788971598	1.300867272632

C	2.572153966872	-0.655044852648	-1.265218794847
C	3.837722689418	0.147090123638	1.977734215823
C	2.155330931588	-0.720021340731	0.212161145991
C	2.625086848087	0.445734465090	1.096057046839
H	4.525471275069	-2.128869919700	0.834076313513
H	3.592338935744	-0.722022047069	2.610629225547
H	2.363353670435	-1.627134405898	-1.738201622582
H	2.489366835338	-1.668695258336	0.653165870689
H	6.235558272391	-1.884751391252	0.622178073956
H	1.937572675131	0.076641273242	-1.798937763319
H	3.969542804694	0.990207571422	2.672280393876
H	1.053512230070	-0.815015149791	0.301881152410
C	5.106616601311	-1.215018959459	-1.056150498368
H	4.962504631787	-2.199226713788	-1.528251628897
H	6.064079145954	-0.837307606037	-1.447253684890
C	4.019683356990	-0.260134451488	-1.541431281900
H	4.205470461305	0.743418797520	-1.132709441477
H	4.134049897138	-0.148954353624	-2.629340874322
H	5.935254154874	-0.183106493082	2.100288181717
H	1.793486729687	0.730002761543	1.757392893506
H	2.823321851502	1.334001256010	0.474503413008
H	5.479974547485	0.746922591363	0.692971269117

TpRh(CNMe)-Cyclooctane 1,2-migration-(4/6-ii)

G = -1258.451255

B	-2.063304019971	-1.499530567619	0.709091601118
H	-2.833658501713	-2.347740823232	1.054603289041
N	-1.039291411423	-1.201644832769	1.800185704780
C	-0.692675547406	-0.041670194176	2.400271906151
C	0.385712859459	-1.727824007953	3.295821971891
C	0.235349572683	-0.332560224725	3.378421962735
H	-1.129455154646	0.900417438251	2.093161291717
H	1.018330083212	-2.378898521838	3.889660678068
N	-2.878093613619	-0.227495365055	0.375846651936
C	-4.152930406078	0.019534767856	0.713390072029
C	-3.363715904555	1.733649922219	-0.405446966390
C	-4.509949331774	1.266320551942	0.237595748124
H	-4.712914872716	-0.720411832731	1.270134892144
H	-3.188490334506	2.659159601646	-0.938490257848
N	-1.387520581008	-1.984341241885	-0.592139981612
C	-1.430173826774	-3.204487518031	-1.138952330266
C	-0.348646412316	-1.847645789051	-2.479178390954
C	-0.770096808607	-3.170257165476	-2.355355855015

H	-1.927331683492	-4.011964125700	-0.617103946595
H	0.196933547577	-1.367106490517	-3.282948925940
N	-2.390919895250	0.828224451435	-0.315460299407
N	-0.713237957920	-1.144584043549	-1.406266948827
N	-0.382823525816	-2.246385079502	2.349856778750
Rh	-0.513810734659	0.857019272635	-0.954456690556
C	-0.362666281795	2.702782116029	-0.541635747639
N	-0.273756895602	3.837886150298	-0.273602964284
C	-0.131172435189	5.189296467605	0.086063317741
H	0.926016429865	5.422599634550	0.257851232200
H	-0.511230840656	5.839411052273	-0.710839382273
H	-0.689867968142	5.393802442225	1.006714682375
H	0.717448527060	0.358068582905	4.055972879250
H	-0.619873990666	-3.982743478675	-3.050270090616
H	-5.464710663081	1.761414785685	0.331266756819
C	2.510952125702	-1.712326390748	0.625561139913
C	3.672326068943	-1.138251202706	1.451946100576
C	2.837786173846	0.359106676506	-1.805126170221
C	3.684651428081	0.378305233687	1.649082894447
C	2.673334254227	1.247258143970	-0.559870666766
C	3.854570434741	1.276486571866	0.421921102370
H	1.642234150729	-1.037276895455	0.669919129494
H	2.740564750208	0.659432831867	2.144570775231
H	1.844543941263	0.171902541929	-2.257930207778
H	1.780804150304	0.957423490101	0.018136578368
H	2.152376237557	-2.635566223852	1.097574502528
H	3.388004100299	0.938984552036	-2.561968450605
H	4.486114232505	0.622561677205	2.362528692858
H	2.472737506535	2.268791340909	-0.915445558672
C	2.863867113299	-2.053837813847	-0.820592208568
H	1.950267846005	-2.371009884481	-1.341316660901
H	3.523850074495	-2.936090794808	-0.813452956917
C	3.565500867266	-0.972193623408	-1.633296002077
H	4.559183101225	-0.777597839761	-1.204053347752
H	3.766296042609	-1.375031641524	-2.637069357281
H	3.638469764545	-1.581489765192	2.457478568427
H	3.973215492968	2.305161457040	0.790744125145
H	4.796521962625	1.047414654392	-0.099499604746
H	4.633535476556	-1.466396051281	1.021950781405

TpRh(CNMe)-Cyclooctane 1,2-migration-(5/8-ie)

G = -1258.454041

B	-2.655422740236	-1.306554278286	-0.025376084492

H	-3.586265005763	-2.064217596063	-0.013301738203
N	-2.079823526430	-0.989993618700	1.356073286187
C	-2.505928333664	-0.059774520430	2.234915413207
C	-0.814749063190	-1.180448345743	3.058744091267
C	-1.712975603782	-0.142627373034	3.359553119440
H	-3.330988996770	0.599805233922	1.992409969076
H	-0.015791660092	-1.584780135741	3.671106136531
N	-3.132431991700	0.022516087339	-0.662134067530
C	-4.373828351138	0.391708096073	-1.012022802396
C	-2.981275144975	2.032410884823	-1.448079083725
C	-4.330139486006	1.676906274047	-1.518437414433
H	-5.199300457797	-0.294045463957	-0.871135819785
H	-2.481478227077	2.943917911720	-1.750161434148
N	-1.549742819830	-1.885395289558	-0.914270646599
C	-1.443841491791	-3.098940198865	-1.466034804136
C	0.277376711174	-1.874477766174	-2.055982442897
C	-0.279088114774	-3.144390395263	-2.211404341488
H	-2.206105476580	-3.845631988971	-1.285399552325
H	1.182580027956	-1.459256502884	-2.481657552849
N	-2.273497529064	1.030705630245	-0.932033302300
N	-0.490871811502	-1.127671529910	-1.265104014886
N	-1.037926588076	-1.688561345733	1.854246005977
Rh	-0.331126493551	0.807618992230	-0.539197871649
C	-0.234456864377	2.563370255935	0.156678219419
N	-0.197284397870	3.646979751952	0.596531561213
C	-0.162933809801	4.905302326506	1.220720325648
H	0.471025726888	4.866994083431	2.114514103167
H	0.237418774525	5.661975182301	0.535630045839
H	-1.174566049106	5.201950045158	1.521134375826
H	-1.776992188634	0.453986607841	4.258423218113
H	0.105844557621	-3.972057643142	-2.787918478597
H	-5.152124606957	2.268578615588	-1.892633274825
C	4.729087884865	-1.938249478769	-0.133062539842
C	3.854145896693	-2.012938143423	1.127246537555
C	4.095789897216	1.250780264285	-0.578923555485
C	2.427372011811	-1.479448631925	0.983668174096
C	2.751240843322	0.518846195677	-0.650816644871
C	2.223854636267	0.010836702472	0.706882073205
H	4.082334760540	-1.951218340255	-1.020953400200
H	1.922707981823	-2.042860966964	0.182594758103
H	4.471799328509	1.406436163229	-1.601875150319
H	2.815435999891	-0.324733429752	-1.348711494009
H	5.329583961106	-2.855198909133	-0.210634701805
H	3.911585868524	2.257141937170	-0.171278163717
H	1.868326439669	-1.726227727699	1.896258146154
H	2.041827709235	1.222961084676	-1.118994535452

C	5.705564689904	-0.756567301843	-0.187690586696
H	6.110421806247	-0.668378624844	-1.207968525235
H	6.567151402832	-1.003653750757	0.451652620031
C	5.185215384388	0.602955742486	0.268965805028
H	4.842705657535	0.530060434831	1.311039895196
H	6.038351838117	1.296152585331	0.300147737669
H	3.760968763125	-3.065581974415	1.427998195222
H	1.129178305411	0.172313526134	0.837030653561
H	2.648857124465	0.619698781571	1.520557684473
H	4.363575035254	-1.518344902058	1.969331969431

TpRh(CNMe)-Cyclooctane 1,2-migration-(8/10-ii)

G = -1258.453259

B	-3.034240527388	-0.771198403473	0.598508210005
H	-4.112739083852	-1.144299937123	0.969791140773
N	-2.049574660153	-0.457590531643	1.727840485547
C	-1.913647541329	0.694417603105	2.416001506557
C	-0.500572200486	-0.811417888653	3.147024548276
C	-0.916696814530	0.515520568144	3.351716008236
H	-2.525289391277	1.558529302554	2.183796660025
H	0.266068376149	-1.372106430735	3.671039272481
N	-3.236589751758	0.518364149307	-0.233859267381
C	-4.354822460450	1.236463481940	-0.416376272838
C	-2.696728138118	2.195716876907	-1.489747052431
C	-4.059290858483	2.326459737928	-1.213116377797
H	-5.281806219595	0.913982833659	0.039924648161
H	-2.041712911549	2.814862317908	-2.089284981592
N	-2.420481393018	-1.836648275118	-0.315496503550
C	-2.802311691839	-3.099464587790	-0.534465755511
C	-0.988520738119	-2.673375197403	-1.691391998221
C	-1.910410725471	-3.683591449623	-1.415902137980
H	-3.681076444289	-3.493954007745	-0.041142442129
H	-0.129257104675	-2.682441189256	-2.350848677956
N	-2.215324147649	1.106696603414	-0.895461451304
N	-1.301373653422	-1.567798957695	-1.018102493397
N	-1.183568601379	-1.393544579379	2.170769403913
Rh	-0.400718964171	0.290695007363	-0.847177633938
C	0.392758553830	1.992400170276	-0.622428949492
N	0.870638168885	3.049171640378	-0.464578422672
C	1.481097150025	4.266321350097	-0.117563954012
H	0.818785228003	4.846342104270	0.535726273941
H	2.420502589804	4.075284461300	0.415445165176
H	1.698220890950	4.857091041119	-1.015175996291

H	-0.550684766433	1.233261098781	4.072250174355
H	-1.928255723453	-4.690502447589	-1.804897143585
H	-4.732287919158	3.099735430324	-1.552017992227
C	4.872238748281	0.044575102112	-1.129245516578
C	3.970038998708	-1.112181274410	-1.585110059022
C	3.819934894666	-0.127760008386	1.977387910392
C	2.487901493846	-0.979458816116	-1.224573670308
C	2.597544559582	0.173931574325	1.107118655459
C	2.100527451903	-1.006931769282	0.258146440596
H	4.266916332645	0.956206117908	-1.036765057813
H	2.120695241574	-0.037593182692	-1.676775718523
H	4.205310552388	0.815189055409	2.396068454616
H	2.798204045415	1.032191911828	0.451580100973
H	5.596480573290	0.267552752518	-1.925064630383
H	3.483522992408	-0.720972159672	2.841774352758
H	1.945286654878	-1.788586379356	-1.735779763319
H	1.780349789521	0.500506353188	1.766097656371
C	5.677417695278	-0.205927612034	0.152729615364
H	6.104307449031	0.748603186656	0.498419094960
H	6.540899998898	-0.835434923529	-0.112544114547
C	4.962491785273	-0.890009144549	1.314672234283
H	4.601281812643	-1.876013517290	0.988717400145
H	5.714882914427	-1.108121107485	2.086362250028
H	4.024863458284	-1.193539386808	-2.679477498234
H	0.997971668822	-1.068528919221	0.351392006812
H	2.425123457918	-1.960335585433	0.704235162349
H	4.357677430777	-2.069672176374	-1.203602688995

TpRh(CNMe)-Cyclooctane 1,2-migration-(7/9-ii)

G = -1258.452120

B	-1.742547298910	-1.947191975895	0.850268522322
H	-2.225261899509	-2.934423468780	1.332872901332
N	-0.935062131765	-1.098244232195	1.831787450134
C	-1.386528324404	-0.131051191821	2.656503443942
C	0.749083458359	-0.487528422824	2.984188219367
C	-0.326702252499	0.300783026060	3.425381500759
H	-2.422392082915	0.186343384146	2.629370596571
H	1.778152330973	-0.485750826925	3.326669652472
N	-2.897252945838	-1.074299771593	0.298912784991
C	-4.220899161799	-1.240224668069	0.439542381280
C	-3.841627914145	0.571318857195	-0.742297249819
C	-4.870921212835	-0.206808917206	-0.208349816480
H	-4.600766724771	-2.087508583755	0.995666721387

H	-3.883710201959	1.472167821846	-1.341007041095
N	-0.856593796260	-2.353402320799	-0.331535745066
C	-0.504071970993	-3.573356870330	-0.750148788099
C	0.279641362130	-2.069685989006	-2.140312121269
C	0.235232310843	-3.444777896977	-1.912596422079
H	-0.803445325209	-4.447466540488	-0.186596102739
H	0.742036058286	-1.520062788430	-2.951053277005
N	-2.662373532870	0.039471141042	-0.429760424808
N	-0.371080412301	-1.419443481675	-1.176629756714
N	0.380913691759	-1.327670932457	2.025783499977
Rh	-0.794801881158	0.584806869344	-0.836700508996
C	-1.222327393759	2.394670884267	-0.491652418924
N	-1.501387537844	3.506690466983	-0.257744507375
C	-1.797406488550	4.829894116052	0.111207668381
H	-1.961623145441	5.448199967974	-0.779221788911
H	-2.703107461680	4.852661045266	0.728267127570
H	-0.968727647102	5.255572866587	0.689407477220
H	-0.332827117179	1.066142088508	4.188405683496
H	0.673035048534	-4.230822414454	-2.509253445978
H	-5.934974109528	-0.043242084104	-0.290528390368
C	4.707950437980	-0.446444709509	-1.119218910835
C	3.257999456137	-0.583373498349	-1.611166319127
C	3.817088255694	1.185231380960	1.565268521327
C	2.476384665251	0.727522060651	-1.698336001135
C	3.341164976447	2.027290064350	0.377308838101
C	2.138568237031	1.458863463803	-0.395176658823
H	5.064508287512	0.573803732296	-1.314872897646
H	3.033821016283	1.424244078783	-2.347394717558
H	4.790613744882	1.570638377842	1.907076748172
H	4.162771458183	2.207318687678	-0.329435034019
H	5.355845065291	-1.092751664536	-1.727433246027
H	3.116680855115	1.359478773602	2.396675170635
H	1.532851429448	0.534891802353	-2.242369842647
H	3.078553361505	3.020857760110	0.766455960682
C	4.934633758486	-0.825655158983	0.348584903327
H	5.941976180618	-0.499145713832	0.651303572940
H	4.944752361228	-1.924344740616	0.415141735310
C	3.907736680083	-0.322973823022	1.357635716423
H	2.914288877811	-0.719892024055	1.104387816928
H	4.148830924484	-0.777839664531	2.330215373973
H	3.266776654759	-1.019651243340	-2.620703704866
H	1.483226753333	2.301359097045	-0.664278538505
H	1.549958998217	0.803237259457	0.275713195734
H	2.708975346270	-1.304206772122	-0.986645140196

TpRh(CNMe)-Cyclooctane 1,2-migration-(8/9-ie)

G = -1258.454691

B	-2.373504838286	-1.566812578221	-0.153290067025
H	-3.171197245500	-2.462681328302	-0.176333750906
N	-1.698372722893	-1.351047774925	1.204601238035
C	-2.096706808077	-0.564535461810	2.225367958509
C	-0.241608074902	-1.610715151398	2.737670955759
C	-1.180034564577	-0.696793827273	3.247035956235
H	-2.990993077566	0.042402410332	2.145341682225
H	0.649254885462	-2.006918816356	3.214199224161
N	-3.108157309069	-0.262330147752	-0.548861119845
C	-4.420972747570	-0.067857244539	-0.747355561159
C	-3.351344822820	1.818983344859	-1.087413939033
C	-4.628872569813	1.254425800378	-1.090393183926
H	-5.111215810480	-0.892975589195	-0.628386850591
H	-3.032721410849	2.828771821876	-1.312686128829
N	-1.282169380982	-1.831731548810	-1.195688954490
C	-0.999108336478	-2.939685974285	-1.889073613888
C	0.492477560657	-1.394028035252	-2.336863773351
C	0.138118325631	-2.708725559759	-2.642869815290
H	-1.624020736643	-3.817552712655	-1.789017796310
H	1.312243465849	-0.790740320953	-2.710274135448
N	-2.447563335763	0.898758986365	-0.761266096235
N	-0.366671043616	-0.879248442940	-1.458983595444
N	-0.555124677842	-2.001976799512	1.510319438628
Rh	-0.468516718403	0.961238938134	-0.513523711397
C	-0.586490302108	2.653922837738	0.321763573301
N	-0.675773669452	3.700929061859	0.836844148257
C	-0.765017964750	4.920537156324	1.528524841708
H	-0.205131785301	4.864906712765	2.469781937640
H	-0.354768126558	5.735630367069	0.920596249613
H	-1.813087963289	5.145924667855	1.757243234359
H	-1.191677121005	-0.209589964461	4.211683130639
H	0.633625512281	-3.390078702130	-3.318036767589
H	-5.566401124892	1.738570489837	-1.319291783539
C	5.172515373064	0.313654286076	-0.578383796655
C	3.875860742439	0.474411690135	-1.387757498611
C	3.713532231776	-1.462211075617	1.753119295401
C	2.670564998970	0.996595482498	-0.602380276824
C	3.007356100484	-0.102838298272	1.731377452108
C	2.095757946868	0.117095809901	0.514048711491
H	5.150496190581	0.999513240620	0.278550187250
H	2.936631161269	1.975504797025	-0.169135631746
H	4.480384457667	-1.457069846697	2.543499539817
H	3.730968348356	0.720269517776	1.803774401783

H	6.019679938266	0.653437760368	-1.190212475588
H	2.971309692231	-2.217511350293	2.054452739088
H	1.872298262604	1.222699524793	-1.337341029330
H	2.399370929604	-0.034653668889	2.644023140978
C	5.488107393660	-1.115320360572	-0.120949688515
H	6.308341894188	-1.082045841078	0.612949416066
H	5.888257389083	-1.664801934684	-0.987271177055
C	4.335114872113	-1.938696734256	0.444251304775
H	3.546839563001	-2.038500315798	-0.316305176698
H	4.702012290979	-2.963116604382	0.601887640419
H	4.054353286423	1.183838492742	-2.207878709133
H	1.173380176841	0.601344018356	0.904796645772
H	1.761682207885	-0.853669482713	0.123400665877
H	3.619187551254	-0.478944011902	-1.875938675443

TpRh(CNMe)-Cyclooctane 1,2-migration-(8/9-ie)

G = -1258.453773

B	-2.776743282372	-1.276123440331	-0.059654721065
H	-3.735934380287	-1.997139101254	-0.065076550481
N	-2.085779795137	-1.145346579289	1.300255336084
C	-2.361850332976	-0.279062597380	2.296607718068
C	-0.713935180431	-1.605695358331	2.863649067380
C	-1.494518442724	-0.536990355345	3.336791448776
H	-3.142744955240	0.464595984037	2.188310699245
H	0.089307489340	-2.134541483679	3.365399856602
N	-3.235774142690	0.133271388162	-0.506062049667
C	-4.481165367033	0.580575751814	-0.727605528726
C	-3.053044276130	2.208689317225	-1.087829325299
C	-4.417367074692	1.909944169646	-1.099448628076
H	-5.323246546403	-0.087626365480	-0.601801516051
H	-2.536919636547	3.129445584712	-1.327955154739
N	-1.752787034557	-1.787298644344	-1.078020818445
C	-1.698677385304	-2.949681793128	-1.737063319687
C	0.072778127172	-1.749952315616	-2.221951686193
C	-0.538913637222	-2.974881009151	-2.491166015716
H	-2.487767574151	-3.680223446113	-1.615287046356
H	0.999949779617	-1.339305793571	-2.605946489698
N	-2.354755182112	1.133989334854	-0.729977039072
N	-0.664833227541	-1.046031071424	-1.364930922745
N	-1.071181007819	-1.969172126123	1.639553454064
Rh	-0.401523267456	0.810710642428	-0.481329442432
C	-0.188285514362	2.510897637095	0.317874179143
N	-0.076556086111	3.563066125132	0.817941280517

C	0.053281985628	4.781862996546	1.504718484655
H	0.828011918550	4.700071651628	2.276278112716
H	0.329440320807	5.585388244253	0.811629761463
H	-0.895543739811	5.043180067404	1.987730111621
H	-1.437772621350	-0.031089404780	4.290111334475
H	-0.190290943845	-3.762509088610	-3.142091411350
H	-5.236855207402	2.566228818206	-1.351341725324
C	4.082252039856	-1.749612460097	1.311619606754
C	2.987111768437	-0.714844147115	1.614987539007
C	5.127771519993	-0.136244572948	-1.334263282519
C	2.058147897098	-0.389056198751	0.443208883256
C	3.654338354875	-0.470000082671	-1.594110585953
C	2.642285171854	0.343489800815	-0.771265256135
H	3.752437652819	-2.390400592173	0.483282809275
H	1.594280044056	-1.329938924419	0.109566473519
H	5.756790110857	-0.907870632114	-1.804370855497
H	3.464551058755	-1.540145948268	-1.435438490655
H	4.179819595187	-2.428874787731	2.169559192616
H	5.360352009262	0.800245052604	-1.864531499993
H	1.226971329599	0.207241978462	0.883733717507
H	3.468512850079	-0.302187124230	-2.664789446949
C	5.474142404588	-1.173225310198	1.030302701386
H	6.117742976903	-1.970553068258	0.627294902098
H	5.923967590074	-0.888650462165	1.994178989712
C	5.552853969897	0.047291258565	0.119075171845
H	4.978375927614	0.871990369538	0.565306383396
H	6.594928786510	0.398569151765	0.119018030270
H	2.343226495446	-1.101197101036	2.416460298848
H	1.810084005040	0.631279222066	-1.441862050545
H	3.081136643306	1.304262172547	-0.460422698996
H	3.433829678489	0.208333956619	2.016149054067

TpRh(CNMe)-Cyclooctane 1,3-migration-(3/7)

G = -1258.453530

B	-3.037277576058	-0.772191023156	0.449770486540
H	-4.144860724959	-1.172743864224	0.679159115785
N	-2.212253535626	-0.439354226839	1.693960589059
C	-2.111556873956	0.738365308295	2.344141519839
C	-0.908740463558	-0.798202418309	3.339982060902
C	-1.271544589814	0.557149002204	3.422601958814
H	-2.629969998425	1.619993760541	1.985721276374
H	-0.260240250108	-1.368895961800	3.995821541081
N	-3.160091538978	0.512391365427	-0.405483306182

C	-4.261625590633	1.207296671104	-0.726780835365
C	-2.504818703827	2.192048627889	-1.601395803570
C	-3.893051549782	2.298027569899	-1.491395129084
H	-5.230607992797	0.869476828331	-0.382632676198
H	-1.794561597273	2.820420830497	-2.123476393258
N	-2.288260129057	-1.821594030672	-0.380540105853
C	-2.634359005167	-3.075583843044	-0.689418838252
C	-0.692102626419	-2.609896810238	-1.595299223714
C	-1.636232227321	-3.629271357332	-1.471643395570
H	-3.566415909515	-3.486709072288	-0.324071286167
H	0.242619760113	-2.593284045517	-2.142625596626
N	-2.077570911682	1.116095192980	-0.945316705140
N	-1.090692162905	-1.528798099348	-0.927102615595
N	-1.476033776989	-1.394480015154	2.300676960686
Rh	-0.258919678412	0.345277638818	-0.640819637851
C	0.452435580938	2.071256211452	-0.337601391781
N	0.875617079421	3.143189460655	-0.134387435764
C	1.404133425911	4.389476440815	0.241678559965
H	0.702989380165	4.912548636968	0.902635318768
H	2.351589560188	4.248154188453	0.775470366283
H	1.587464085103	5.011395971400	-0.642423735596
H	-0.972057880459	1.291523445038	4.156810368038
H	-1.599887567132	-4.622789107339	-1.892494329307
H	-4.534970819411	3.055345166223	-1.915872719303
C	2.505481087103	-1.890789582836	-0.049481064386
C	2.793876329115	-1.221532534346	-1.399965875323
C	4.320458493361	0.213178285279	1.642251254664
C	4.269673819733	-0.960136900792	-1.715660507095
C	5.271980586197	-0.428751520146	0.623537999649
C	5.069553592649	0.005010866273	-0.836855125539
H	3.385694578070	-2.464248274072	0.269069369918
H	4.787077154742	-1.934179964725	-1.700692757991
H	4.380984372077	-0.338934637179	2.592634574925
H	5.220444156690	-1.523879769398	0.682687170746
H	1.705592203825	-2.634588484468	-0.166140962051
H	4.696744843938	1.224313785810	1.863321190255
H	4.335752724004	-0.606624915830	-2.755159717446
H	6.295988717594	-0.178300287027	0.933209948206
C	2.062297060363	-0.929485664278	1.051252965065
H	2.009822608562	-1.467515893364	2.010194147068
H	0.996804621834	-0.649443175489	0.879086672245
C	2.861492083024	0.356034863363	1.224000263955
H	2.814979172457	0.942706320212	0.295453714395
H	2.339750113174	0.969047633055	1.974228792716
H	2.416130537908	-1.862779626953	-2.209490134529
H	6.055746245418	0.109876880906	-1.310455783379

H	4.624856490211	1.011445734829	-0.877215836867
H	2.216112816087	-0.280665491634	-1.491876129608

TpRh(CNMe)-Cyclooctane 1,3-migration-(6/10)

G = -1258.453879

B	-2.952746266675	-0.770575041681	0.494222349726
H	-4.047650847531	-1.191358410849	0.746569154879
N	-2.095845666176	-0.466211458962	1.723586836556
C	-1.945429792907	0.704444359011	2.377395159008
C	-0.800619472463	-0.882533113570	3.362244375259
C	-1.107689475531	0.486019498381	3.450776419766
H	-2.430641719514	1.607299280865	2.025533370031
H	-0.172556960196	-1.480803416031	4.013724907053
N	-3.116692000084	0.537509283627	-0.316171027529
C	-4.234962210387	1.234460395662	-0.567454736890
C	-2.522390941460	2.263204385585	-1.478319824029
C	-3.905508596500	2.353794852625	-1.308090274560
H	-5.186562265283	0.877233913524	-0.195543128701
H	-1.838642833976	2.915443442687	-2.006472102886
N	-2.222699765440	-1.787569153867	-0.393223722358
C	-2.572157708284	-3.033550701311	-0.729201138800
C	-0.675238657652	-2.520085639247	-1.703136384486
C	-1.604746084585	-3.551863788579	-1.572177043355
H	-3.484376548168	-3.464889815833	-0.337973790275
H	0.235484418348	-2.476359686609	-2.288325302911
N	-2.061234672118	1.168501375701	-0.878415564029
N	-1.052202366264	-1.465854234887	-0.981499784267
N	-1.396139939915	-1.451975062771	2.323588303497
Rh	-0.225694207475	0.406118410806	-0.674000026478
C	0.471259240773	2.134216349275	-0.345899977074
N	0.874950002174	3.210131180209	-0.125746983036
C	1.413435289405	4.448946181827	0.260279236436
H	2.459943919204	4.321638633128	0.562765885127
H	1.371942212280	5.161365319225	-0.571956450701
H	0.849503351531	4.859825909302	1.106120065957
H	-0.775949360387	1.205076208389	4.186279011069
H	-1.579401115795	-4.530403400465	-2.027564898131
H	-4.569525862319	3.119965284449	-1.679320332289
C	2.828852881734	-1.411282169218	-1.356938310832
C	2.473887274993	-2.125552527199	-0.046941032968
C	4.890832710561	0.662881652037	0.228327482625
C	1.999728564303	-1.225610621185	1.090497234935
C	3.482086688767	0.885595737129	0.777631329207

C	2.961422558437	-0.215778077618	1.713260416313
H	2.229374250383	-0.486159852018	-1.440543195462
H	1.098898159580	-0.662319503013	0.752488631853
H	5.110546186705	1.437879020493	-0.522791206371
H	2.779149278483	1.020405899967	-0.053736488543
H	2.500525017855	-2.027331425923	-2.206440898575
H	5.612687846933	0.821960291451	1.044676254077
H	1.595567396816	-1.862202845438	1.889768479263
H	3.480093683556	1.846696368512	1.313261065055
C	4.321114546165	-1.114462877102	-1.582468398624
H	4.423451175286	-0.352896492508	-2.370967631544
H	4.775129775388	-2.027621513887	-1.996390261957
C	5.161701617557	-0.710312554723	-0.373459577872
H	5.067658260952	-1.476355903982	0.409356525273
H	6.218055670373	-0.743447772919	-0.676821177598
H	1.658646495956	-2.836414903411	-0.237644716586
H	2.419242391663	0.249422102666	2.548482475319
H	3.811065929442	-0.746364748777	2.172695318972
H	3.321689320744	-2.741782457970	0.289227707610

TpRh(CNMe)-Cyclooctane 1,4-migration-(1/7)

G = -1258.454411

B	-2.867103861191	-0.826671875709	0.071660719609
H	-3.974431461697	-1.284645184693	0.133227843987
N	-2.167032024628	-0.717084010946	1.425931891209
C	-2.099159486427	0.335823837738	2.266380574878
C	-1.190842109568	-1.438588893100	3.176553501696
C	-1.469103109440	-0.082485833593	3.419765858361
H	-2.492444472345	1.304388761070	1.980786873290
H	-0.698870281766	-2.157797891725	3.822448363826
N	-2.969862134226	0.584427470427	-0.550322516081
C	-4.074600525835	1.303256868983	-0.801976614588
C	-2.308232206879	2.460226857667	-1.401550088087
C	-3.702213313594	2.517596420524	-1.345755084300
H	-5.048295045439	0.890544955489	-0.571952129477
H	-1.592995666593	3.183492571908	-1.771656551930
N	-2.021567549964	-1.703964526256	-0.859537935030
C	-2.290012939074	-2.914038807665	-1.360232879187
C	-0.306823272137	-2.267323997427	-2.037117480899
C	-1.213385878868	-3.322800987721	-2.127436524017
H	-3.227440696959	-3.401349960317	-1.125897902199
H	0.666461907762	-2.151196266180	-2.497903795003
N	-1.881147260024	1.295039296315	-0.920412271537

N	-0.799285014482	-1.300514663594	-1.261975999800
N	-1.610409536844	-1.816580168689	1.976984677716
Rh	-0.050295725861	0.543063853055	-0.679451223694
C	0.622281944865	2.231704225049	-0.153532647385
N	1.046324334311	3.269728565368	0.181812467990
C	1.568828660620	4.480879187421	0.665955596037
H	1.463116216722	5.270893745364	-0.086851007902
H	1.039174576428	4.785746949228	1.576394053768
H	2.632990605579	4.360606227719	0.900823461201
H	-1.245488537184	0.503977874410	4.299583196555
H	-1.103679064681	-4.247054520450	-2.674525903898
H	-4.344864316786	3.324370691253	-1.664805386656
C	2.972152882908	-2.260696220145	-0.542821847081
C	2.988220624602	-1.068122403686	-1.511230821178
C	3.325012711005	-0.271444809211	2.079240144091
C	4.162040723394	-0.096893343149	-1.373865151377
C	4.554363052138	-0.061497654804	1.192657979736
C	4.291230622784	0.734014538995	-0.095852861165
H	4.010096798594	-2.492865772636	-0.267227353558
H	5.091629008305	-0.677629800355	-1.496696612374
H	3.577018531966	-0.972696278341	2.889792912924
H	5.012176946782	-1.026659825742	0.936745915280
H	2.617562245524	-3.150868572734	-1.081648557633
H	3.090684875343	0.684900140213	2.573427960279
H	4.127427381099	0.594875034583	-2.228369880307
H	5.310804935304	0.461516961806	1.794082177070
C	2.095582563893	-2.117353161711	0.711516735770
H	2.402902216458	-2.874053481504	1.449262525008
H	1.058143289872	-2.369939131246	0.446351423360
C	2.059639698407	-0.751480343991	1.380961809528
H	1.783120968150	0.017362230817	0.635298927577
H	1.228418898044	-0.738789632240	2.098384874012
H	3.019551409922	-1.451665816747	-2.541895634110
H	5.123312562036	1.433457245636	-0.258751352683
H	3.398620661274	1.369537999060	0.027200013159
H	2.037133498402	-0.501911543791	-1.467246874781