

Supporting Information

Mechanistic studies of Glycine Betaine Catalysed CO₂ Reduction Using Density Functional Theory

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Chapter 8 Supporting information

8.1. Supporting information for chapter 3.4.1, 3.4.2, 3.4.3 and 3.4.4

Table S8.1.1. Energy of species involved in section 3.4.1 to section 3.4.4

Optimised product	Calculation method	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)
glycine betaine	SMD(CH ₃ CN) ω B97XD/6-31+G(d,p)	-402.276	0.167840	-402.098	-402.141
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-402.211	0.167364	-402.034	-402.077
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-402.429	0.166194	-402.253	-402.296
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-402.399	0.165843	-402.223	-402.266
N-methylaniline	SMD(CH ₃ CN) ω B97XD/6-31+G(d,p)	-326.838	0.146589	-326.683	-326.722
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-326.793	0.146105	-326.639	-326.679
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-326.980	0.145055	-326.827	-326.866
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-326.952	0.144866	-326.799	-326.839
CO ₂	SMD(CH ₃ CN) ω B97XD/6-31+G(d,p)	-188.528	0.011659	-188.512	-188.537
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-188.517	0.011789	-188.501	-188.526
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-188.593	0.011447	-188.578	-188.602
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-188.591	0.011446	-188.576	-188.600
PhSiH ₃	SMD(CH ₃ CN) ω B97XD/6-31+G(d,p)	-522.862	0.115923	-522.739	-522.779
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-522.808	0.115567	-522.685	-522.723
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-522.998	0.115059	-522.875	-522.916
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-522.971	0.114956	-522.848	-522.889
complex A2	SMD(CH ₃ CN) ω B97XD/6-31+G(d,p)	-729.125	0.316377	-728.790	-728.855
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-729.013	0.315586	-728.679	-728.745
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-729.418	0.312693	-729.087	-729.154
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-729.356	0.311789	-729.025	-729.095

complex B2	SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)	-925.145	0.285773	-924.841	-924.907
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-925.018	0.286713	-924.714	-924.777
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-925.434	0.282277	-925.133	-925.201
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-925.370	0.281294	-925.069	-925.146
cyclic complex C	SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)	-925.144	0.285636	-924.840	-924.907
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-925.027	0.285168	-924.724	-924.788
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-925.434	0.282601	-925.133	-925.200
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-925.370	0.281687	-925.069	-925.142
complex D	SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)	-1252.001	0.433612	-1251.540	-1251.626
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-1251.832	0.433342	-1251.372	-1251.456
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-1252.431	0.429620	-1251.974	-1252.061
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-1252.328	0.427252	-1251.873	-1251.969
cyclic complex E	SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)	-1251.999	0.434536	-1251.537	-1251.623
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-1251.828	0.430847	-1251.370	-1251.457
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-1252.430	0.429650	-1251.973	-1252.060
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-1252.328	0.427434	-1251.872	-1251.970
complex F	SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)	-590.805	0.180337	-590.610	-590.668
	SMD(CH ₃ CN) M06-2X/6-31+G(d,p)	-590.728	0.179998	-590.534	-590.592
	SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)	-591.027	0.178522	-590.834	-590.891
	SMD(CH ₃ CN) B3LYP/6-31+G(d,p)	-590.990	0.177995	-590.797	-590.858

Table S8.1.2. Cartesian coordinates in section 3.4.1 to section 3.4.4

glycine betaine - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)				C	-1.08069400	0.79966600	-1.22548800
C	0.30692900	-0.83320400	0.00031400	H	-0.26563900	1.51998300	-1.20813700
H	0.27797400	-1.47158500	0.88591300	H	-1.00548700	0.14857600	-2.09783700
H	0.27803200	-1.47218600	-0.88484900	H	-2.05059100	1.29888600	-1.20872500
C	1.64765300	-0.05357800	0.00007600	C	-1.08119500	0.80200900	1.22388200
O	2.63213700	-0.82741100	-0.00000500	H	-2.05133600	1.30071600	1.20604600
O	1.64283700	1.19842200	-0.00000600	H	-1.00590200	0.15263000	2.09751400
N	-0.98319700	-0.04935500	-0.00000400	H	-0.26638200	1.52254900	1.20524800
C	-2.11354900	-1.02815500	0.00011300	glycine betaine - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)			
H	-2.04335800	-1.64742200	0.89466500	C	0.31127800	-0.83909200	0.00019400
H	-3.05251800	-0.47393800	-0.00014300	H	0.27800400	-1.47586100	0.88604500
H	-2.04314900	-1.64791300	-0.89408300	H	0.27803300	-1.47628000	-0.88535200
C	-1.08980000	0.80126500	-1.22498900	C	1.65088400	-0.05444300	0.00004100
H	-0.27668000	1.52361400	-1.21192300	O	2.64260300	-0.82831300	0.00003900
H	-1.01490200	0.15380400	-2.09950700	O	1.64089000	1.20301100	-0.00002600
H	-2.05835500	1.30204500	-1.20987100	N	-0.98674800	-0.05020400	-0.00000100
C	-1.09011800	0.80188200	1.22454000	C	-2.12327300	-1.03256200	0.00010600
H	-2.05843700	1.30310000	1.20858400	H	-2.05082900	-1.65088800	0.89488600
H	-1.01606300	0.15477900	2.09939700	H	-3.06031100	-0.47532100	0.00000300
H	-0.27664800	1.52384100	1.21160600	H	-2.05080500	-1.65118100	-0.89447200
glycine betaine - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)				C	-1.09081600	0.80528200	-1.23057700
C	0.30598600	-0.84091300	0.00068300	H	-0.27121400	1.51948900	-1.21502200
H	0.27664700	-1.47756000	0.88816600	H	-1.02017400	0.15565200	-2.10358700
H	0.27660400	-1.47883400	-0.88588000	H	-2.05667500	1.31080300	-1.21233600
C	1.64319900	-0.05409200	0.00015100	C	-1.09104800	0.80578100	1.23023700
O	2.63145000	-0.81985700	0.00015400	H	-2.05685500	1.31137500	1.21155500
O	1.62283100	1.19690500	-0.00007700	H	-1.02073900	0.15645400	2.10351200
N	-0.97770800	-0.05148200	-0.00000700	H	-0.27129300	1.51980000	1.21466700
C	-2.11418900	-1.02332900	0.00077700	glycine betaine - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)			
H	-2.04437700	-1.64124700	0.89667000	C	0.31431700	-0.83603600	0.00004100
H	-3.04766400	-0.45944000	0.00073800	H	0.28188700	-1.47398100	0.88564900
H	-2.04480600	-1.64231000	-0.89440100	H	0.28192500	-1.47413600	-0.88546200

C	1.65848700	-0.05322600	0.00000500	H	2.83180300	-1.14224100	-0.66497900
O	2.64742800	-0.83092700	0.00000700	N-methylaniline - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)			
O	1.65308900	1.20425900	0.00001200	N	1.78695000	0.61763500	-0.15288200
N	-0.99035000	-0.04969700	-0.00002100	H	2.00279100	1.55092100	0.17380500
C	-2.12481500	-1.03836400	0.00000300	C	0.44640400	0.28165200	-0.06116500
H	-2.05117900	-1.65736000	0.89467000	C	0.01349300	-1.05599400	-0.05703900
H	-3.06503600	-0.48569200	-0.00003300	C	-0.52552800	1.30182200	-0.00589000
H	-2.05117800	-1.65746100	-0.89459600	C	-1.35023000	-1.35294000	-0.01175400
C	-1.09968400	0.80709900	-1.23218400	H	0.73551500	-1.86505600	-0.09167300
H	-0.28268700	1.52505900	-1.21992800	C	-1.87790100	0.99034400	0.04420200
H	-1.02980500	0.15914600	-2.10702300	H	-0.19988700	2.33949400	-0.00414700
H	-2.06699100	1.31070600	-1.21278700	C	-2.30714900	-0.34169100	0.03914300
C	-1.09977200	0.80716900	1.23213100	H	-1.66096200	-2.39437700	-0.01178700
H	-2.06699400	1.31092700	1.21254100	H	-2.60560700	1.79635600	0.08892500
H	-1.03018500	0.15920400	2.10698600	H	-3.36509500	-0.58096000	0.07719500
H	-0.28263400	1.52496100	1.21999500	C	2.81606700	-0.37155000	0.10827400
N-methylaniline - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)				H	3.78568500	0.12806200	0.09241200
N	1.78725900	0.61159200	-0.15212500	H	2.68927500	-0.86740600	1.08158700
H	2.00254700	1.54691400	0.16462800	H	2.81869200	-1.14033400	-0.67077100
C	0.44605200	0.27812900	-0.06204200	N-methylaniline - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)			
C	0.00770500	-1.05798100	-0.05837600	N	1.79000200	0.60932300	-0.15394000
C	-0.52349700	1.30016100	-0.00620800	H	2.00545300	1.55144700	0.14655100
C	-1.35593800	-1.35140200	-0.01171300	C	0.44717300	0.27645400	-0.06143900
H	0.72660500	-1.86972100	-0.09305800	C	0.00524900	-1.06296200	-0.05747700
C	-1.87660400	0.99243100	0.04449000	C	-0.52352500	1.30273400	-0.00423200
H	-0.19883300	2.33805600	-0.00478200	C	-1.36191100	-1.35436600	-0.01204400
C	-2.30973900	-0.33764700	0.04026500	H	0.72305400	-1.87475300	-0.09268200
H	-1.66924600	-2.39204600	-0.01161200	C	-1.88042600	0.99685000	0.04488700
H	-2.60257400	1.79982800	0.08827800	H	-0.19505900	2.33935400	-0.00077500
H	-3.36860600	-0.57331500	0.08044800	C	-2.31704300	-0.33600300	0.03927600
C	2.82363100	-0.36817400	0.10912500	H	-1.67716400	-2.39456900	-0.01203800
H	3.79010000	0.13810000	0.08631700	H	-2.60453000	1.80616200	0.08987300
H	2.70773100	-0.85981600	1.08638600	H	-3.37630500	-0.57078200	0.07757000

C	2.83514500	-0.36695900	0.11033200
H	3.79979100	0.14315900	0.07328500
H	2.72912200	-0.84892000	1.09438300
H	2.83765900	-1.15085200	-0.65441200

N-methylaniline - SMD(CH₃CN) B3LYP/6-31+G(d,p)

N	1.79139200	0.60515100	-0.15101200
H	2.00733400	1.55109600	0.13740000
C	0.44732500	0.27346800	-0.05914900
C	0.00053100	-1.06552600	-0.05562200
C	-0.52290000	1.30209800	-0.00363000
C	-1.36814700	-1.35373400	-0.01162300
H	0.71577200	-1.88032400	-0.09039800
C	-1.88123900	0.99922200	0.04376300
H	-0.19336800	2.33883500	-0.00034700
C	-2.32156600	-0.33296500	0.03821300
H	-1.68571600	-2.39365700	-0.01195100
H	-2.60347500	1.81082300	0.08727600
H	-3.38180300	-0.56532600	0.07517500
C	2.84503700	-0.36484500	0.10782400
H	3.80607500	0.15190700	0.06077800
H	2.75293800	-0.84407600	1.09480900
H	2.84825200	-1.15163700	-0.65431600

CO₂ - SMD(CH₃CN) ωB97XD/6-31+G(d,p)

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16458900
O	0.00000000	0.00000000	-1.16458900

CO₂ - SMD(CH₃CN) M06-2X/6-31+G(d,p)

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16293300
O	0.00000000	0.00000000	-1.16293300

CO₂ - SMD(CH₃CN) B3LYP-D3(BJ)/6-31+G(d,p)

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16923700
O	0.00000000	0.00000000	-1.16923700

CO₂ - SMD(CH₃CN) B3LYP/6-31+G(d,p)

C	0.00000000	0.00000000	0.00000000
O	0.00000000	0.00000000	1.16926300
O	0.00000000	0.00000000	-1.16926300

PhSiH₃ - SMD(CH₃CN) ωB97XD/6-31+G(d,p)

C	1.64944200	-1.20662300	0.00298500
C	0.25477200	-1.20453400	-0.00977400
C	-0.46680200	0.00000000	-0.01305000
C	0.25477200	1.20453400	-0.00977400
C	1.64944200	1.20662300	0.00298500
C	2.34865600	0.00000000	0.01028600
H	2.18905600	-2.14929300	0.00428000
H	-0.27152200	-2.15644500	-0.02036300
H	-0.27152200	2.15644500	-0.02036300
H	2.18905600	2.14929300	0.00428000
H	3.43494000	0.00000000	0.01816200
Si	-2.34526700	0.00000000	0.00555400
H	-2.87011200	0.00000000	1.39638800
H	-2.85392700	1.21370400	-0.68104000
H	-2.85392700	-1.21370400	-0.68104000

PhSiH₃ - SMD(CH₃CN) M06-2X/6-31+G(d,p)

C	1.64917200	-1.20744400	0.00307900
C	0.25392400	-1.20490000	-0.00982400
C	-0.46669100	0.00000000	-0.01340100
C	0.25392400	1.20490000	-0.00982400
C	1.64917200	1.20744400	0.00308000
C	2.34823500	0.00000000	0.01028700
H	2.19001600	-2.14958000	0.00444100
H	-0.27492900	-2.15599500	-0.02036300
H	-0.27492900	2.15599500	-0.02036300
H	2.19001600	2.14958000	0.00444100
H	3.43456200	0.00000000	0.01792200
Si	-2.34507300	0.00000000	0.00554200
H	-2.86356300	0.00000000	1.39493700

H	-2.84828400	1.21267100	-0.67949000	complex A2 - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)			
H	-2.84828400	-1.21267100	-0.67949000	C	2.65952300	-1.71789700	-0.94311600
PhSiH ₃ - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)				C	2.55939600	-0.32540300	-0.93338200
C	1.65231100	-1.20971600	0.00318600	C	2.04924600	0.34311000	0.19342500
C	0.25444700	-1.20766800	-0.01004000	C	1.65141300	-0.43158300	1.30301500
C	-0.46899200	0.00000000	-0.01411300	C	1.74991300	-1.81585100	1.27750800
C	0.25444700	1.20766800	-0.01004000	C	2.25543400	-2.47691400	0.15264800
C	1.65231100	1.20971600	0.00318600	H	3.05474800	-2.20995700	-1.82793700
C	2.35357600	0.00000000	0.01061600	H	2.87266200	0.23494000	-1.80787800
H	2.19252000	-2.15236200	0.00452900	H	1.25488000	0.07267900	2.18022500
H	-0.27325700	-2.15849600	-0.02064500	H	1.42800700	-2.38642700	2.14469400
H	-0.27325700	2.15849600	-0.02064500	H	2.33210300	-3.55965700	0.13545100
H	2.19252000	2.15236200	0.00452900	N	1.94395600	1.72456100	0.26293100
H	3.43999000	0.00000000	0.01822500	H	1.16071400	2.02420100	0.84236100
Si	-2.34801900	0.00000000	0.00571500	C	2.09555800	2.52347800	-0.93783300
H	-2.87529300	0.00000000	1.39723200	H	1.42701300	2.20422900	-1.75107200
H	-2.85978000	1.21403700	-0.68000200	H	1.86345200	3.56137700	-0.69113500
H	-2.85978000	-1.21403700	-0.68000200	H	3.12734800	2.48658600	-1.30349800
PhSiH ₃ - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)				O	-0.75815500	2.11664500	1.52388200
C	1.65506700	-1.20984900	0.00310200	C	-1.30077600	1.56254800	0.53357900
C	0.25637000	-1.20775100	-0.00974500	O	-1.42506500	2.01361800	-0.62417500
C	-0.46923800	0.00000000	-0.01367900	C	-1.86612000	0.16593100	0.88464500
C	0.25637000	1.20775100	-0.00974500	H	-1.10803200	-0.38297400	1.44425600
C	1.65506700	1.20984900	0.00310200	H	-2.74462100	0.29449500	1.52202800
C	2.35702800	0.00000000	0.01034400	C	-1.14811400	-0.95959500	-1.19520600
H	2.19500500	-2.15311900	0.00435600	H	-1.47282700	-1.66932100	-1.95660100
H	-0.26945200	-2.16010500	-0.02016400	H	-0.87805800	-0.00638500	-1.64416900
H	-0.26945200	2.16010500	-0.02016400	H	-0.31096500	-1.36957600	-0.62865800
H	2.19500500	2.15311900	0.00435600	C	-2.68471300	-2.05019200	0.33546800
H	3.44384000	0.00000000	0.01774000	H	-3.50046800	-1.88875700	1.04046200
Si	-2.35298900	0.00000000	0.00557300	H	-3.00941800	-2.70679400	-0.47228800
H	-2.88282400	0.00000000	1.39666600	H	-1.82344500	-2.48099700	0.84675600
H	-2.86712800	1.21337100	-0.68054200	C	-3.45796500	-0.16509900	-0.98670500
H	-2.86712800	-1.21337100	-0.68054200	H	-3.74280000	-0.86810200	-1.76997300

H -4.27822400 -0.03614800 -0.27942700
H -3.16214400 0.79294300 -1.40831500
N -2.28694900 -0.73365500 -0.25110400

complex **A2** - SMD(CH₃CN) M06-2X/6-31+G(d,p)

C -4.96499200 -0.73629200 -0.33813000
C -3.65083900 -1.15638800 -0.12416100
C -2.67751700 -0.24543000 0.32826000
C -3.06776900 1.09473700 0.54351200
C -4.37752600 1.49809700 0.32193000
C -5.34443600 0.58662800 -0.11945800
H -5.69737800 -1.45967400 -0.68735500
H -3.38445700 -2.19231200 -0.30743500
H -2.32365000 1.80836300 0.89021800
H -4.64818500 2.53644700 0.49535200
H -6.36770200 0.90558800 -0.29077900
N -1.37745900 -0.62497100 0.59650800
H -0.68931600 0.12923500 0.55857100
C -0.86509400 -1.88244300 0.09083200
H -1.03266300 -2.00631400 -0.98962500
H 0.21087300 -1.91225300 0.28008800
H -1.32308500 -2.73343200 0.60685200
O 1.07389000 0.90135100 0.41694400
C 1.40670200 0.58776900 -0.75446400
O 0.71058500 0.62711100 -1.78752400
C 2.83928800 0.06814200 -1.02229200
H 2.77043700 -0.94077100 -1.43719500
H 3.31337600 0.71765100 -1.76211900
C 3.28282500 -0.97009400 1.17914800
H 4.03508200 -1.04351000 1.96607800
H 2.34227300 -0.58727800 1.56927700
H 3.14199700 -1.94093500 0.70111400
C 5.09867100 -0.51951100 -0.36819500
H 5.47476600 0.18318100 -1.11233100
H 5.79039200 -0.59013100 0.47198400

H 4.94108900 -1.50150000 -0.81538800
C 4.00625600 1.33381900 0.75620100
H 4.76169700 1.23071900 1.53613100
H 4.36107500 2.00659000 -0.02614500
H 3.06114600 1.68184800 1.16622000
N 3.78789200 -0.01409000 0.14521000

complex **A2** - SMD(CH₃CN) B3LYP-D3(BJ)/6-31+G(d,p)

C -4.86645200 0.05405400 -0.74431800
C -3.57239500 0.51985400 -0.99591300
C -2.49423100 0.11706100 -0.17528200
C -2.77146500 -0.75612100 0.90580900
C -4.06576400 -1.20715000 1.14406400
C -5.13124300 -0.81044500 0.32142500
H -5.67625600 0.37914200 -1.39277700
H -3.40014100 1.19300400 -1.82847900
H -1.95504400 -1.07271300 1.54984300
H -4.24670600 -1.87539900 1.98219700
H -6.13952900 -1.16543500 0.51112300
N -1.19925200 0.52043300 -0.41031600
H -0.52797900 0.38687100 0.34667500
C -0.87562400 1.58080500 -1.34386900
H -1.40376200 2.52084400 -1.12024700
H 0.19824600 1.77029800 -1.29034600
H -1.11820700 1.29484500 -2.37462000
O 1.08974000 0.22623300 1.33520600
C 1.99483600 1.07965800 1.11678800
O 2.06040300 2.26006300 1.53338900
C 3.21316300 0.69545300 0.24021400
H 3.28408900 1.40110800 -0.58931700
H 4.11878600 0.77842700 0.84418300
C 2.08706400 -0.88396800 -1.31829700
H 2.19540900 -1.85955700 -1.79266300
H 1.16686000 -0.83127600 -0.74343700

H	2.11897500	-0.09346900	-2.06842500	C	3.94699000	1.59660700	-0.76137900
C	4.52108300	-0.80362900	-1.17187200	H	4.84150000	1.81363000	-1.34630900
H	5.36359400	-0.66452400	-0.49459000	H	3.07144700	1.51343300	-1.40128200
H	4.55765100	-1.79522900	-1.62356500	H	3.79750600	2.36551900	-0.00209900
H	4.52305700	-0.03416100	-1.94405300	C	5.37014500	0.38168500	0.81150600
C	3.24010800	-1.75895700	0.67218400	H	5.52379200	-0.57452600	1.31283800
H	3.31638800	-2.72546900	0.17364500	H	6.22780900	0.62019000	0.18135100
H	4.10042300	-1.60034400	1.32316900	H	5.20926800	1.17189000	1.54529700
H	2.31258500	-1.67592100	1.23271200	C	4.38064700	-0.80844100	-1.08018200
N	3.24724300	-0.68916100	-0.38331000	H	5.27247100	-0.55319400	-1.65408300
complex A2 - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)				H	4.53148100	-1.74850400	-0.54800800
C	-5.30762400	0.30138300	-0.51403000	H	3.50492300	-0.86664100	-1.72233300
C	-4.32720300	-0.67856600	-0.32538900	N	4.15043000	0.27792700	-0.06439700
C	-3.05284400	-0.33303200	0.18519300	complex B2 - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)			
C	-2.80871300	1.03324200	0.48187600	C	2.18900300	1.40902900	1.37635500
C	-3.79452000	1.99581500	0.28404800	C	1.99361600	0.03894600	1.20288300
C	-5.05907300	1.64419700	-0.21432800	C	2.22173600	-0.57223800	-0.03841900
H	-6.27796000	0.00351000	-0.90483500	C	2.66329400	0.23148600	-1.10160900
H	-4.55348500	-1.71077700	-0.57102400	C	2.85734000	1.60218700	-0.93448300
H	-1.83577200	1.32200500	0.87121700	C	2.61818300	2.19355200	0.30625800
H	-3.57397900	3.03402600	0.52127500	H	2.00248300	1.86466000	2.34469000
H	-5.82532100	2.39889200	-0.36556500	H	1.64026800	-0.55507700	2.04093000
N	-2.07233400	-1.27037100	0.42202400	H	2.85042200	-0.21043200	-2.07821300
H	-1.11870600	-0.92411000	0.57286600	H	3.19318500	2.20822500	-1.77112400
C	-2.18073200	-2.63969400	-0.04403900	H	2.76722900	3.26126700	0.43888900
H	-2.33037100	-2.71182900	-1.13318200	C	-2.06375700	-1.53004200	0.23377300
H	-1.25545700	-3.16294800	0.20878300	O	-2.68972100	-2.58602000	-0.01422700
H	-3.00995600	-3.16817400	0.44322400	O	-0.98084200	-1.39368900	0.84626900
O	0.68733500	-0.52522300	1.02440500	C	-2.80449100	-0.27935300	-0.30841500
C	1.57036300	-0.23326400	0.16880400	H	-3.00142000	-0.42538800	-1.37234900
O	1.42853600	-0.08696500	-1.06806000	H	-3.76177500	-0.19223700	0.21100900
C	2.96305300	-0.05280200	0.82858400	C	-0.83831500	1.07043900	-0.93954700
H	2.90035300	0.75442900	1.56178000	H	-0.18344900	0.32643400	-0.49274000
H	3.22388000	-0.97499900	1.35196300	H	-1.04655200	0.82701500	-1.98233000

H	-0.40228600	2.06713900	-0.86585500	H	-1.58526800	2.00825800	0.55181600
C	-3.03727700	2.09242600	-0.78245100	H	-2.80630500	1.80408000	1.84939500
H	-3.97957500	2.09112500	-0.23404600	C	-4.04927500	1.79297300	-0.45764900
H	-2.55628700	3.06771100	-0.70153400	H	-4.73190400	1.35404000	-1.18565400
H	-3.20952600	1.84456000	-1.83014400	H	-4.60562800	2.23695100	0.36825700
C	-1.88171900	1.41968700	1.24564700	H	-3.40902800	2.53787800	-0.93098400
H	-1.43896600	2.41571200	1.27862900	C	-4.05229400	-0.29691600	0.78681900
H	-2.83854300	1.41400100	1.76959900	H	-4.60131400	0.22513800	1.57088500
H	-1.20799100	0.67673000	1.66672900	H	-4.73986000	-0.71923300	0.05319300
N	-2.12941400	1.06556800	-0.18658900	H	-3.42386500	-1.07854300	1.20959900
Si	1.88929900	-2.40252600	-0.29845000	N	-3.18275700	0.70507600	0.09360500
H	3.09431700	-3.02482800	-0.91838800	Si	1.19949900	-1.82654600	0.32275300
H	1.63388900	-3.07225400	0.99737700	H	2.25068000	-2.77574800	0.94204500
H	0.75911600	-2.62701000	-1.23298700	H	0.28187700	-1.82983700	1.49893800
complex B2 - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)				H	0.92022800	-2.67799100	-0.86836800
C	2.99870600	2.00166100	-0.04048300	complex B2 - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)			
C	2.04646800	0.98621000	0.07284900	C	2.80798900	-1.60796100	-0.55957400
C	2.41793600	-0.36874300	0.12235500	C	2.43865900	-0.34751600	-1.03565100
C	3.79153400	-0.65628500	0.04718600	C	2.20152600	0.72186300	-0.15151700
C	4.75024500	0.34951200	-0.09152700	C	2.34654400	0.48646300	1.22736500
C	4.35507600	1.68635000	-0.13064900	C	2.71444100	-0.77393200	1.70890900
H	2.67997000	3.04055300	-0.06473900	C	2.94659700	-1.82336900	0.81559600
H	0.99444100	1.24968100	0.11875400	H	2.98229900	-2.42095300	-1.25882200
H	4.12432800	-1.69100600	0.09859800	H	2.32917400	-0.20247400	-2.10789000
H	5.80329600	0.08977000	-0.16020300	H	2.16233800	1.28898400	1.93696500
H	5.09622100	2.47473200	-0.22932400	H	2.81601700	-0.93594900	2.77835000
C	-1.44750000	-1.00303100	-0.58669300	H	3.22973300	-2.80389400	1.18769000
O	-1.87558200	-2.13543100	-0.34485600	C	-2.70978500	1.15130100	0.57292000
O	-0.23869700	-0.59475500	-0.49142700	O	-3.74839800	1.73238800	0.98183300
C	-2.43872100	0.07724300	-1.05758700	O	-1.54440300	1.61242200	0.47510700
H	-1.91139900	0.88624800	-1.56431100	C	-2.99684000	-0.31635300	0.15537100
H	-3.19227300	-0.36204200	-1.71408000	H	-3.40917900	-0.85149600	1.01283000
C	-2.22489000	1.29843800	1.07770100	H	-3.74045500	-0.31569000	-0.64396200
H	-1.62737200	0.50018900	1.51874500				

C	-0.77946500	-1.28966500	0.71158100	H	-2.78996600	-0.02423500	-1.35683600
H	-0.40424800	-0.29687000	0.93934900	C	-4.84193500	0.85645100	1.21514000
H	-1.23666100	-1.74463000	1.59082400	H	-4.68114900	-0.02349500	1.83380300
H	0.01297700	-1.92732000	0.32300800	H	-4.20835200	1.68085200	1.54547100
C	-2.36013700	-2.52254400	-0.68107800	H	-5.88972700	1.15945500	1.22528800
H	-3.12428100	-2.42603100	-1.45249100	C	-4.69787700	1.72100000	-1.06587900
H	-1.53050000	-3.12995100	-1.04416600	H	-4.43222500	1.47261000	-2.09391500
H	-2.78524200	-2.96301900	0.22081700	H	-5.75246700	1.99253900	-1.00246200
C	-1.24510400	-0.55337600	-1.59073200	H	-4.07496400	2.53811600	-0.70037100
H	-0.44861900	-1.20965400	-1.94027500	C	-5.33007700	-0.61202400	-0.70447900
H	-2.03459600	-0.48168900	-2.33983900	H	-6.37041300	-0.28739700	-0.66148100
H	-0.86064600	0.43096800	-1.33903100	H	-5.04450800	-0.82610200	-1.73539900
N	-1.83655100	-1.15578400	-0.34821600	H	-5.16380300	-1.48038100	-0.07098600
Si	1.72876500	2.42157400	-0.79820400	N	-4.46526000	0.51164200	-0.20045700
H	2.90343700	3.06882500	-1.44680600	Si	4.09572200	-2.18192400	-0.55736800
H	0.66111000	2.31949700	-1.82354400	H	5.38490800	-2.63076000	-1.15137200
H	1.28635200	3.28184000	0.32468800	H	3.87862800	-2.96354100	0.68796300
complex B2 - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)				H	3.00868900	-2.47888600	-1.52435700
C	4.89025000	1.54498900	1.17422700	cyclic complex C - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)			
C	4.85129900	0.17308200	0.90780000	Si	-1.56394600	-1.89266100	1.23438900
C	4.12218700	-0.33532300	-0.18598100	H	-0.34264500	-2.31527600	0.50226800
C	3.43172700	0.58000900	-1.00355200	H	-2.47648700	-3.06087500	1.33727800
C	3.46893000	1.95406900	-0.74066400	H	-1.16456100	-1.46750500	2.59853300
C	4.19889100	2.43887400	0.34878000	C	-2.46498200	-0.51559500	0.32741300
H	5.45703000	1.91496600	2.02453300	C	-3.69975200	-0.75318400	-0.29625700
H	5.39423700	-0.50389600	1.56408900	C	-1.91673600	0.77621200	0.24886800
H	2.85480000	0.22294300	-1.85353100	C	-4.36602000	0.26421800	-0.98119800
H	2.92731900	2.64244200	-1.38403400	H	-4.15432200	-1.74000000	-0.24777800
H	4.22716400	3.50529000	0.55580000	C	-2.58026600	1.79306400	-0.43641800
C	-2.47567300	-1.08812000	0.50512100	H	-0.95865900	0.98371300	0.72322000
O	-3.26699200	-1.73581500	1.23707200	C	-3.80595500	1.53882500	-1.05337900
O	-1.25024700	-1.29205600	0.30703300	H	-5.32144100	0.06138000	-1.45658100
C	-2.99013100	0.14222700	-0.29629600	H	-2.13999900	2.78485800	-0.48890500
H	-2.43612600	1.02647800	0.02601900				

H	-4.32332800	2.33227900	-1.58516400	H	-2.88068900	-2.90894000	1.05703600
N	2.68564200	-0.47414500	-0.79528900	H	-1.26849700	-1.42653000	-2.64486200
C	2.71939700	-1.61761100	0.16761900	H	-2.06231300	-3.32784200	-1.25201500
H	1.96427900	-1.44334100	0.93062300	N	2.25911000	-0.61707300	0.49473600
H	2.51438100	-2.53564400	-0.38406100	C	3.12501400	0.30229700	1.29387100
H	3.71409500	-1.65977000	0.61311100	H	2.60577800	1.25282600	1.39804200
C	3.71291400	-0.71404600	-1.85447400	H	3.29976900	-0.15912300	2.26687800
H	3.69146600	0.11667100	-2.56015300	H	4.06836500	0.43048600	0.76082700
H	4.69322700	-0.78486000	-1.38275500	C	2.96262600	-1.92710100	0.34123600
H	3.47275300	-1.64755400	-2.36459500	H	2.31945800	-2.60112600	-0.22631200
C	1.34194200	-0.38889700	-1.44403700	H	3.90058600	-1.75929900	-0.18941700
H	0.59912100	-0.21274700	-0.67045300	H	3.15460700	-2.33302400	1.33524700
H	1.35681200	0.43616000	-2.15732100	C	0.96887900	-0.85161400	1.21527000
H	1.14977100	-1.33027700	-1.95970000	H	0.49878700	0.11348600	1.38953800
C	3.02744900	0.82303700	-0.10261800	H	0.33647600	-1.47942600	0.58369800
H	4.04523900	0.70882100	0.27689300	H	1.19661400	-1.36045600	2.15343000
H	3.03167600	1.59276000	-0.87743600	C	2.01998700	-0.06060600	-0.88539900
C	2.12209100	1.29998900	1.06176800	H	3.00252100	0.02479100	-1.35587700
O	2.51194700	2.38867200	1.53933100	H	1.43765600	-0.81345000	-1.42437800
O	1.13853800	0.60650400	1.41252300	C	1.29116900	1.30188000	-1.00804000
cyclic complex C - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)				O	1.19962000	1.67561100	-2.19771100
Si	-2.06157700	2.03392900	0.91257400	O	0.87281900	1.87409100	0.02431200
H	-1.07291000	2.16580800	2.00689000	cyclic complex C - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)			
H	-3.39927700	2.28497300	1.51628700	Si	1.72565900	2.47487400	-0.71835900
H	-1.83344100	3.04284900	-0.14328800	H	0.70740100	2.36390600	-1.79249000
C	-2.08352900	0.29980600	0.18804400	H	2.89116600	3.21096900	-1.28123600
C	-2.53883200	-0.78383000	0.95585900	H	1.18473800	3.25768900	0.41903000
C	-1.63250100	0.04616900	-1.11502000	C	2.24335100	0.77033600	-0.12159900
C	-2.52945200	-2.08256600	0.44528800	C	2.49521700	-0.27109000	-1.03427300
H	-2.90224200	-0.61986200	1.96913000	C	2.40332600	0.50383700	1.25007900
C	-1.62469800	-1.25055900	-1.63316500	C	2.89382300	-1.53535300	-0.59242000
H	-1.26524000	0.86470400	-1.73001100	H	2.37367700	-0.10126800	-2.10149900
C	-2.06986700	-2.31786800	-0.85175100	C	2.80053900	-0.76004600	1.69717100

H	2.20742400	1.28444900	1.98084100	C	-4.94051600	-0.78508700	-1.33144600
C	3.04701700	-1.78191000	0.77595000	H	-4.36700100	1.21344300	-1.86185100
H	3.07898100	-2.32717700	-1.31281200	C	-4.88541900	-1.79661400	-0.36599300
H	2.91306200	-0.94686300	2.76144800	H	-4.15108900	-2.35742200	1.58541400
H	3.35217300	-2.76558300	1.12136900	H	-5.46927900	-0.95225000	-2.26610600
N	-1.75041400	-1.14998800	-0.35586900	H	-5.37171800	-2.75117600	-0.54838200
C	-1.21551400	-0.47514900	-1.58712600	N	3.04877700	-1.13555900	0.09546600
H	-0.97228100	0.55235700	-1.33117400	C	2.88445500	-0.92197200	1.57603400
H	-0.33037600	-1.01986800	-1.91439600	H	2.72470900	0.13964800	1.75029400
H	-1.98947500	-0.50974500	-2.35481800	H	2.02902500	-1.50911900	1.91231500
C	-2.06960200	-2.57743000	-0.69358100	H	3.79385000	-1.26218700	2.07338800
H	-2.45109900	-3.07044300	0.20050400	C	3.26061600	-2.60404200	-0.15667700
H	-2.82038200	-2.59017600	-1.48381400	H	3.37762200	-2.76223300	-1.22931800
H	-1.15459400	-3.06405600	-1.03242800	H	4.15763900	-2.92517900	0.37359100
C	-0.71293300	-1.13215400	0.73108000	H	2.38906200	-3.14621500	0.21227100
H	-0.48975600	-0.09593300	0.96536500	C	1.80306200	-0.70037300	-0.62850000
H	-1.12390200	-1.64761200	1.59978500	H	1.64847300	0.35835600	-0.43324800
H	0.17233100	-1.64942700	0.36517000	H	1.94847100	-0.87876300	-1.69492300
C	-3.02996400	-0.48252600	0.11491600	H	0.96726800	-1.29497100	-0.25773000
H	-3.74540000	-0.58635600	-0.70315100	C	4.26887100	-0.38698700	-0.42755000
H	-3.38420000	-1.07160200	0.96305700	H	5.12805700	-0.80155200	0.10412600
C	-2.96442700	1.01060100	0.53458800	H	4.35526800	-0.65150800	-1.48342000
O	-4.08121300	1.43378900	0.93101900	C	4.30342800	1.16274200	-0.29658300
O	-1.87764000	1.63667800	0.44781500	O	5.36110700	1.64660600	-0.77616600
cyclic complex C - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)				O	3.34128000	1.76774200	0.24153200
Si	-2.80432700	2.35179700	0.43736700	complex D - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)			
H	-2.07566900	2.82562900	-0.76812100	C	-0.82960700	3.99171100	0.48982300
H	-1.85341800	2.22006500	1.57015700	C	-0.66707000	2.99939100	1.45691000
H	-3.81381700	3.38682600	0.79033600	C	0.32808300	2.01865000	1.32427900
C	-3.61980100	0.68603100	0.10625300	C	1.16231900	2.06781900	0.19626100
C	-3.57347500	-0.34549500	1.06411300	C	1.00310100	3.05720900	-0.77268900
C	-4.31342500	0.44226100	-1.09623800	C	0.00451600	4.02052700	-0.62751200
C	-4.20016800	-1.57519900	0.83249300	H	-1.60685300	4.74113300	0.60835600
H	-3.04317600	-0.19401900	2.00145000	H	-1.32910700	2.99140900	2.31974600

H	1.94659000	1.32604100	0.06617100	H	-2.95144900	1.90905700	-1.49378500
H	1.65834300	3.07380400	-1.63910700	C	-3.24350200	0.34987500	0.61042500
H	-0.12194400	4.79158600	-1.38205200	H	-3.93588300	1.18763500	0.52377600
Si	0.53005200	0.64453700	2.58821900	H	-3.71427300	-0.49685100	1.10456200
H	-0.07601900	-0.61860000	2.08647500	H	-2.34717000	0.65896500	1.14698300
H	1.96911900	0.39414300	2.84857600	C	-4.04334800	-0.50426100	-1.53972800
H	-0.15103000	1.02789700	3.84978700	H	-3.72139800	-0.79425800	-2.54078700
N	-2.84017400	-0.07056900	-0.76588900	H	-4.49902200	-1.34733700	-1.02510200
C	-1.80621300	-1.16609500	-0.71195800	H	-4.73380400	0.33786800	-1.59559400
H	-0.92506800	-0.73598000	-0.23029800	complex D - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)			
H	-1.54993200	-1.39735100	-1.74841400	C	-1.93503700	3.66056900	0.09574000
C	-2.16967900	-2.48540800	0.00796100	C	-1.74045100	2.77440300	1.15694900
O	-3.32040200	-2.66354100	0.45579300	C	-0.61357100	1.93772000	1.20644100
O	-1.19606800	-3.28127000	0.04365800	C	0.31726500	2.01884600	0.15721100
N	1.59096300	-2.59237100	0.34140200	C	0.12627000	2.90060400	-0.90734000
H	0.61049700	-2.75220500	0.09954100	C	-1.00148800	3.72414700	-0.93898500
C	1.99040800	-3.01412400	1.66376900	H	-2.81308600	4.29993900	0.07857300
H	2.04248400	-2.18346100	2.38279200	H	-2.47780500	2.73987500	1.95661900
H	1.25733400	-3.73549600	2.02972400	H	1.20419500	1.38895900	0.17172600
H	2.97081400	-3.50603100	1.64788900	H	0.85896500	2.94776500	-1.70873200
C	2.27060800	-1.62205900	-0.35166600	H	-1.14936600	4.41446700	-1.76461400
C	3.48521900	-1.07710200	0.11240300	Si	-0.37082300	0.76296800	2.65632800
C	1.76874400	-1.15928000	-1.59007900	H	-0.71085500	-0.63660500	2.29540900
C	4.16380500	-0.11746600	-0.63981900	H	1.01826000	0.82495200	3.16038500
H	3.90265900	-1.40074500	1.06010300	H	-1.29848300	1.19988600	3.72889100
C	2.45385200	-0.20046800	-2.32274900	N	-2.85243100	-0.81652400	-1.00655500
H	0.83849300	-1.57273500	-1.96948100	C	-1.47889900	-1.38192700	-0.76204900
C	3.66157600	0.33338800	-1.85881000	H	-0.90931100	-0.59939000	-0.25063200
H	5.09646700	0.28670400	-0.25483000	H	-1.03285700	-1.54797600	-1.74660400
H	2.03846400	0.13782200	-3.26854600	C	-1.37424600	-2.69122400	0.05641600
H	4.19276000	1.08493000	-2.43449000	O	-2.40863800	-3.30075700	0.39060400
C	-2.22067100	1.10046600	-1.46016000	O	-0.17863500	-3.00638200	0.28216300
H	-1.33819700	1.40889400	-0.90044700	N	1.90076800	-1.12296700	0.98139800
H	-1.94022200	0.80207400	-2.47076500	H	1.13825500	-1.69340700	0.60425800

C	2.37266800	-1.59262300	2.27014000	C	-0.15163900	4.00997100	-0.60812400
H	2.80407300	-0.77374300	2.85535100	H	-1.77764700	4.72441700	0.61850500
H	1.52010200	-1.99009500	2.82552700	H	-1.50764300	2.96779900	2.33061300
H	3.13108800	-2.38472500	2.17879300	H	1.78724000	1.30898900	0.09407300
C	2.81182700	-0.68726000	0.03608600	H	1.51204700	3.06286100	-1.60925400
C	4.13177800	-0.32894900	0.36876800	H	-0.27285700	4.78253100	-1.36219400
C	2.40221900	-0.54738500	-1.30792800	Si	0.35284800	0.64226600	2.63186500
C	4.99870700	0.15799900	-0.61154800	H	-0.03569100	-0.67851500	2.07742700
H	4.48458100	-0.42865700	1.38988600	H	1.76182000	0.54941000	3.09042400
C	3.27774500	-0.06665100	-2.27306200	H	-0.52232000	0.94942100	3.79139200
H	1.38326800	-0.81906800	-1.57669700	N	-2.84992900	-0.21790300	-0.82197200
C	4.58736500	0.29498600	-1.93573300	C	-1.70815800	-1.20635600	-0.67783600
H	6.01274100	0.42835800	-0.32847500	H	-0.91535300	-0.68049900	-0.14513000
H	2.93449500	0.02731300	-3.30006600	H	-1.36038100	-1.41653900	-1.69048500
H	5.26941700	0.67172500	-2.69128900	C	-1.99254200	-2.54857400	0.03860500
C	-2.68363500	0.47470300	-1.74235700	O	-3.14723900	-2.81295000	0.44781100
H	-2.09930000	1.15128200	-1.11687100	O	-0.95790500	-3.26938300	0.12112100
H	-2.16223700	0.27542600	-2.67972400	N	1.81074500	-2.50817500	0.39470000
H	-3.67270000	0.89289900	-1.93531400	H	0.82974200	-2.71515200	0.18491200
C	-3.55344100	-0.53740800	0.28435900	C	2.25036800	-2.84351700	1.73442100
H	-4.49927800	-0.04477600	0.05438800	H	2.24210500	-1.98221800	2.41849800
H	-3.71422500	-1.48078000	0.80124000	H	1.57893300	-3.60560600	2.13549400
H	-2.91838300	0.12625000	0.87366400	H	3.26754600	-3.25503300	1.72842700
C	-3.67371200	-1.74250700	-1.84519700	C	2.40895300	-1.50824000	-0.33775700
H	-3.14833300	-1.90051000	-2.78837200	C	3.58059000	-0.84730600	0.09702400
H	-3.79126900	-2.67925800	-1.30513700	C	1.85879200	-1.12835100	-1.58764400
H	-4.63876800	-1.26638000	-2.02429100	C	4.16804000	0.14710500	-0.69137800
complex D - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)				H	4.02756100	-1.10496300	1.05047700
C	-0.99726000	3.97728300	0.50445100	C	2.45201200	-0.13297500	-2.35624300
C	-0.84056300	2.98032700	1.47249100	H	0.96288500	-1.62903100	-1.94109000
C	0.15920900	1.99848200	1.34594000	C	3.61559800	0.51877400	-1.91988600
C	1.00444900	2.05002300	0.22117800	H	5.06569700	0.64165400	-0.32891600
C	0.85140500	3.04481500	-0.74739000	H	2.00029600	0.14076900	-3.30636800
				H	4.07339000	1.29758100	-2.52183500

C	-2.30843400	0.99889100	-1.51756700	O	1.67592800	-1.14669400	-0.16334000
H	-1.49692300	1.40517000	-0.91818700	N	4.43375900	-0.44438100	0.52787000
H	-1.94259400	0.70343200	-2.50078700	H	3.47747600	-0.72671300	0.29149800
H	-3.11342200	1.72761400	-1.61388000	C	5.36821300	-1.52116900	0.79621400
C	-3.37265100	0.19393400	0.52413000	H	6.03787600	-1.27579700	1.63005700
H	-4.15233000	0.94049500	0.37240400	H	4.79739100	-2.41000600	1.07504400
H	-3.76392700	-0.68935600	1.02206500	H	5.99427900	-1.77260200	-0.07484000
H	-2.54798900	0.62477800	1.08950800	C	4.84478000	0.79014700	0.07446000
C	-3.96050600	-0.79568600	-1.65162200	C	6.20486800	1.18174200	0.06220000
H	-3.54915700	-1.07630500	-2.62196700	C	3.88185400	1.72945500	-0.37760100
H	-4.35479300	-1.66661000	-1.13399900	C	6.57295400	2.45975300	-0.37208100
H	-4.72664300	-0.02921700	-1.77355000	H	6.97320500	0.49153100	0.39443200
complex D - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)							
C	-6.27993200	1.03296900	-0.44728100	C	4.26639700	2.99568800	-0.80901200
C	-5.46306400	1.17654100	0.67810300	H	2.83265300	1.44595800	-0.38010800
C	-4.34132400	2.03004500	0.65900200	C	5.61671400	3.38029500	-0.81114900
C	-4.06868300	2.73745500	-0.52775300	H	7.62599300	2.73179400	-0.36774200
C	-4.88415200	2.59637100	-1.65650500	H	3.50333500	3.69182700	-1.14956400
C	-5.99105200	1.74346400	-1.61808500	H	5.91115200	4.36976900	-1.14855900
H	-7.14061300	0.37037900	-0.41031300	C	-2.75939000	-2.77412300	-0.81615000
H	-5.70885700	0.61736900	1.57867100	H	-3.09820000	-1.93132400	-0.21330100
H	-3.21397600	3.40794500	-0.57723900	H	-2.66644900	-2.47923500	-1.86176500
H	-4.65531300	3.15292400	-2.56149100	H	-3.45189000	-3.61109000	-0.72031900
H	-6.62655700	1.63422100	-2.49276500	C	-1.54213200	-3.62569200	1.12475000
Si	-3.23378400	2.21446800	2.17187700	H	-2.27350700	-4.43309600	1.18114500
H	-2.45240900	0.97367300	2.42330200	H	-0.56751100	-3.95542400	1.47752000
H	-2.28561900	3.33557600	1.95203000	H	-1.88806800	-2.76339700	1.69627100
H	-4.04447300	2.48812300	3.38765300	C	-0.94832200	-4.38288500	-1.14450300
N	-1.40935800	-3.21355800	-0.31662700	H	-0.87322900	-4.05755400	-2.18297500
C	-0.45705200	-2.03496600	-0.46061300	H	0.02109300	-4.70526800	-0.77128800
H	-0.90132100	-1.21454200	0.10665300	H	-1.68873900	-5.17850400	-1.05162100
H	-0.46412100	-1.76637400	-1.51908000	cyclic complex E - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)			
C	1.01491900	-2.21166200	-0.00416700	H	-0.99148600	-0.90330300	-1.02967500
O	1.41344600	-3.30927200	0.45143200	C	-1.23125000	0.61298400	-2.44761300

H	-0.17903000	0.45386100	-2.69277400	H	4.72122000	-1.17907400	-0.55759100
H	-1.84612100	0.22861200	-3.27587300	C	2.22478800	-0.75491000	-1.28590200
H	-1.39543200	1.69327900	-2.37758800	H	3.00437500	-0.59679200	-2.03204400
C	-2.79513500	-0.06287000	-0.67113500	H	1.31381600	-1.12868700	-1.74560900
C	-3.10570500	-0.96640000	0.36828800	H	2.02866800	0.16870900	-0.74080000
C	-3.79934700	0.81922100	-1.10969300	C	2.93463900	-3.08245800	-1.01495300
C	-4.36774800	-0.97121500	0.94694600	H	3.28924500	-3.81127600	-0.28523300
H	-2.33895600	-1.65590400	0.71607100	H	1.99174300	-3.40527500	-1.45171800
C	-5.06169300	0.80412600	-0.51364900	H	3.68673600	-2.92956400	-1.78950000
H	-3.59884400	1.52333600	-1.91050300	C	1.74743700	-1.95864600	0.83471200
C	-5.36111100	-0.08433400	0.51633200	H	1.62728800	-0.97242300	1.29192200
H	-4.58022200	-1.67821100	1.74482400	H	2.24102300	-2.61565000	1.55223700
H	-5.81798300	1.49993700	-0.86766900	C	0.34143300	-2.52402800	0.52833800
H	-6.34535000	-0.09165100	0.97439200	O	-0.27679300	-2.87061700	1.55555400
N	-1.51275400	-0.04116100	-1.18678200	O	-0.06459000	-2.55537700	-0.66256200
Si	-0.59634600	1.53441300	1.80663100	cyclic complex E - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)			
H	-0.66892500	0.05319400	1.81417700	H	-1.49629300	-0.67345100	-1.40666800
H	-0.52190600	1.99200300	3.22070600	C	-0.79461600	1.19011100	-2.10101900
H	-1.81440500	2.09824600	1.17796600	H	0.01822800	0.60889100	-2.54189100
C	0.92968000	2.13156200	0.88715600	H	-1.39751400	1.62102500	-2.91430100
C	0.82280500	2.72892000	-0.37761500	H	-0.35167500	2.02268900	-1.53991500
C	2.21199600	1.96867600	1.43571200	C	-2.68305200	0.77448600	-0.57422500
C	1.95712400	3.13574200	-1.08070400	C	-3.51458400	-0.14712600	0.10157900
H	-0.15598000	2.87672600	-0.82580000	C	-3.01596700	2.14239200	-0.51508800
C	3.34850000	2.37830100	0.73939800	C	-4.62251400	0.29246400	0.81365500
H	2.33318600	1.51074100	2.41522100	H	-3.27496100	-1.20872000	0.06095900
C	3.22262000	2.95833600	-0.52309000	C	-4.13270600	2.56493500	0.20837600
H	1.85105800	3.59226200	-2.06055900	H	-2.40378400	2.87576700	-1.03028200
H	4.33159900	2.24132300	1.18054900	C	-4.94528500	1.65343200	0.87975800
H	4.10796800	3.27367500	-1.06755800	H	-5.24477900	-0.43831400	1.32410200
N	2.71164500	-1.78245900	-0.31282400	H	-4.36602900	3.62616500	0.24024800
C	4.01232800	-1.31696300	0.25930100	H	-5.81284300	1.98913300	1.43898200
H	3.84537100	-0.37242100	0.77635200	N	-1.56378300	0.32746600	-1.23492300
H	4.38086100	-2.07042600	0.95556700				

Si	0.80772400	2.63944700	1.18179600	cyclic complex E - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-			
H	-0.26226700	1.61147300	1.08804500	31+G(d,p)			
H	1.01716300	2.97862300	2.60774600	H	-0.59039600	-1.59403100	-1.32609000
H	0.36930300	3.83907300	0.43034700	C	-1.04026400	-0.24811300	-2.88560100
C	2.40455500	1.97532300	0.44765500	H	-0.05488800	-0.52934600	-3.26302100
C	2.68269000	2.10791300	-0.92234200	H	-1.80016000	-0.61011700	-3.59579400
C	3.32335200	1.27804800	1.24695700	H	-1.09343500	0.84633900	-2.86510200
C	3.83416000	1.54999100	-1.47924100	C	-2.36189900	-0.68881000	-0.83756500
H	1.99693500	2.65434000	-1.56693600	C	-2.54073500	-1.45426900	0.34131500
C	4.47730700	0.71923000	0.69508900	C	-3.38667800	0.21064800	-1.20977400
H	3.14074600	1.16379700	2.31390500	C	-3.69122400	-1.31386900	1.10945400
C	4.73227600	0.85201300	-0.67030700	H	-1.75994000	-2.14587400	0.64750600
H	4.03189700	1.66381400	-2.54139300	C	-4.53404600	0.34164800	-0.42177800
H	5.17618600	0.18209800	1.33044400	H	-3.28435500	0.80845300	-2.10860700
H	5.63017400	0.41853200	-1.10140100	C	-4.70258800	-0.41309300	0.74218700
N	1.16686200	-2.37680300	0.38882900	H	-3.79830400	-1.91101700	2.01168100
C	2.00563500	-2.13896700	1.60406500	H	-5.30406200	1.04501700	-0.72891700
H	1.64559100	-1.23479900	2.09776400	H	-5.59703700	-0.30629900	1.34828000
H	1.91213900	-2.99888000	2.26796100	N	-1.19976500	-0.81256300	-1.56236500
H	3.04197500	-2.01229400	1.28736200	Si	-1.00117200	1.48505500	2.15876100
C	1.32010300	-1.19660200	-0.52086500	H	-0.60086500	0.07926400	2.42186700
H	2.38870000	-1.02743400	-0.67110600	H	-0.87700400	2.23534100	3.43711200
H	0.81639700	-1.41713300	-1.45821100	H	-2.40735700	1.51821200	1.69833300
H	0.86090800	-0.33481100	-0.03459700	C	0.11516200	2.27379700	0.86868600
C	1.65103200	-3.61128500	-0.29959100	C	-0.30909100	2.42222400	-0.46414000
H	1.54767500	-4.45064900	0.38983600	C	1.40808700	2.71660600	1.20773400
H	1.04618800	-3.76622000	-1.19177600	C	0.53046900	2.98836800	-1.42798700
H	2.69902500	-3.46420700	-0.56442000	H	-1.29937900	2.08635000	-0.75612600
C	-0.25685400	-2.56136000	0.84989200	C	2.25100000	3.28124300	0.24706200
H	-0.56148800	-1.61390600	1.30946600	H	1.76612900	2.61808200	2.22983800
H	-0.23203100	-3.33474200	1.61942200	C	1.81272700	3.41761300	-1.07401900
C	-1.31138300	-2.94263800	-0.21605100	H	0.18483000	3.09037800	-2.45267100
O	-2.32757300	-3.47573900	0.27231000	H	3.24721500	3.61132200	0.52768800
O	-1.09619600	-2.63687700	-1.41680700	H	2.46738900	3.85500900	-1.82248400

N	2.98303500	-1.12019400	0.03072000	H	-3.37684800	5.67288700	-0.39764500
C	3.89083600	-0.23516200	0.83655000	H	-4.56937500	4.97859600	1.68286300
H	3.28843900	0.54108700	1.30677500	N	-1.55082400	1.49788700	-0.95188400
H	4.38967500	-0.84226900	1.59197000	Si	2.72361200	2.15290800	0.99680600
H	4.62297500	0.21061700	0.16317500	H	1.53600700	1.98144400	0.12215600
C	2.29903200	-0.27740100	-1.01067400	H	2.38729100	1.73354800	2.38160000
H	3.06943300	0.23921700	-1.58289500	H	3.06826500	3.60072700	1.02520200
H	1.71188500	-0.93349500	-1.64487500	C	4.16044600	1.11921000	0.35103500
H	1.65798400	0.43919800	-0.50225400	C	4.34962900	0.92454000	-1.03163900
C	3.80552700	-2.18446100	-0.63547900	C	5.09014700	0.53670200	1.23461500
H	4.30550600	-2.76727600	0.13880500	C	5.42969200	0.17877300	-1.51459700
H	3.13848800	-2.81322400	-1.22096300	H	3.64805700	1.35397500	-1.74348400
H	4.54119500	-1.69553900	-1.27449100	C	6.17165200	-0.21031000	0.75553500
C	1.98429000	-1.74127400	0.99047000	H	4.97213800	0.66087900	2.30877400
H	1.44899500	-0.91010200	1.45396900	C	6.34357900	-0.38979800	-0.62080400
H	2.57373300	-2.24442800	1.75760500	H	5.55580000	0.04000700	-2.58509700
C	0.94150500	-2.73555100	0.42764700	H	6.87608100	-0.65207500	1.45534900
O	0.29648900	-3.31691000	1.33268900	H	7.18216100	-0.97123400	-0.99446400
O	0.79778400	-2.85099000	-0.82218700	N	-1.31641100	-4.17268000	0.42131800
cyclic complex E - SMD(CH ₃ CN) B3LYP/6-31+G(d,p)				C	-1.50974600	-5.65413800	0.60793100
H	-1.67918500	0.50952300	-0.71176300	H	-2.46109200	-5.82145900	1.11386200
C	-0.99686200	1.75592200	-2.26744300	H	-1.51198400	-6.13253500	-0.37191200
H	-0.46382600	0.86108800	-2.59732900	H	-0.68700200	-6.03655600	1.21315600
H	-1.76750200	1.99373300	-3.01810300	C	-1.30879400	-3.51593400	1.77554400
H	-0.28057400	2.58686600	-2.24856800	H	-0.50197700	-3.95610100	2.36262800
C	-2.34685900	2.41222100	-0.29822700	H	-1.15492100	-2.44824000	1.63755500
C	-3.03346000	2.03160700	0.88389400	H	-2.27039600	-3.70828300	2.25359500
C	-2.49425800	3.74738400	-0.74479100	C	0.00137600	-3.94252700	-0.26804500
C	-3.81924300	2.94510700	1.58070600	H	-0.02842400	-4.43953400	-1.23860600
H	-2.93688900	1.01031600	1.24339600	H	0.14070600	-2.87073300	-0.38878300
C	-3.28488200	4.65346300	-0.02989900	H	0.78926200	-4.37282500	0.35127400
H	-1.98981700	4.07802000	-1.64652600	C	-2.47154500	-3.65796500	-0.42695500
C	-3.95517700	4.26963500	1.13540900	H	-3.38364500	-3.92063500	0.11332800
H	-4.33330500	2.62008100	2.48231500	H	-2.44405900	-4.23113900	-1.35602800

C	-2.52639200	-2.14806000	-0.78021400	H	0.91720600	-0.94644600	-2.10100100
O	-3.52137000	-1.86159200	-1.48804100	C	0.22852400	-0.66448100	1.20253200
O	-1.62496600	-1.37246900	-0.35475900	H	0.81474700	-0.90343600	2.09130400
complex F - SMD(CH ₃ CN) ωB97XD/6-31+G(d,p)				H	-0.00114300	0.39803100	1.16444100
C	-2.00864300	-2.28320600	-0.08889100	H	-0.67989500	-1.26769500	1.17743000
H	-2.67641600	-2.33600000	0.77132400	N	1.04831000	-1.01047900	0.00059700
H	-2.58429400	-2.29907900	-1.01459400	C	2.37068600	-0.28743800	0.02569100
H	-1.30326200	-3.11471400	-0.06965100	H	2.93014000	-0.63804900	-0.84512400
C	-0.44254000	-0.99229800	1.24425700	H	2.88648500	-0.62138900	0.92928800
H	0.21629900	-1.86087000	1.24200100	C	2.35167700	1.26357100	0.00967300
H	0.12839300	-0.06739500	1.28105500	O	3.50715600	1.74079300	0.04147600
H	-1.13653400	-1.04932600	2.08390700	O	1.25617100	1.86662700	-0.03235600
C	-0.32302400	-0.93545100	-1.20252400	C	-4.33391800	0.39732800	-0.00766100
H	-0.93161000	-0.94282300	-2.10760100	O	-5.49190400	0.34851200	0.08730900
H	0.25257300	-0.01508000	-1.13640700	O	-3.17590200	0.44485300	-0.10257700
H	0.32875100	-1.80902900	-1.18138700	complex F - SMD(CH ₃ CN) B3LYP-D3(BJ)/6-31+G(d,p)			
N	-1.23801200	-1.00360200	-0.02194000	C	3.08155200	-0.52898800	-0.84881500
C	-2.22916800	0.13506700	-0.04402400	H	2.73640800	-1.04335400	-1.74571000
H	-2.89673200	-0.02271400	0.80564800	H	3.56671900	0.41058000	-1.11355100
H	-2.80810800	0.01967300	-0.96295800	H	3.76725900	-1.16472600	-0.28778400
C	-1.68907400	1.58744700	0.01730900	C	1.23155300	-1.52692300	0.39057900
O	-2.61719500	2.42776900	-0.00365800	H	1.96093600	-2.13790500	0.92296200
O	-0.45541100	1.79299700	0.07783600	H	0.37266100	-1.30026300	1.01682100
C	3.94543700	0.07713900	0.01319300	H	0.92034000	-2.02424800	-0.52831600
O	4.73039100	0.92253300	-0.14759000	C	2.36723800	0.47845900	1.25646400
O	3.16210200	-0.76950200	0.17420200	H	2.84703800	1.40933500	0.95234600
complex F - SMD(CH ₃ CN) M06-2X/6-31+G(d,p)				H	1.50273000	0.67849300	1.88461700
C	1.33062300	-2.47863500	0.02312400	H	3.08371200	-0.16796600	1.76388800
H	1.92465100	-2.73205600	-0.85551400	N	1.89306700	-0.22965000	0.01917200
H	1.88025600	-2.71328100	0.93522300	C	0.94563800	0.65235400	-0.77568300
H	0.37919100	-3.01228000	0.00504800	H	0.70237300	0.09516300	-1.68227400
C	0.28776300	-0.69178900	-1.24685900	H	1.51977800	1.53796100	-1.05509000
H	-0.61902600	-1.29782300	-1.25346900	C	-0.37602300	1.10315900	-0.09995700
H	0.05292500	0.37015900	-1.24162100				

O	-1.07245600	1.81994100	-0.86296000
O	-0.63643100	0.73361500	1.07400200
C	-2.98647200	-0.72032200	-0.06216400
O	-3.78087200	-0.11428300	0.54426600
O	-2.23678300	-1.36826600	-0.68338900

complex **F** - SMD(CH₃CN) B3LYP/6-31+G(d,p)

C	3.08179700	-1.66585100	-0.76696500
H	2.83764100	-1.65543400	-1.82962000
H	4.07671200	-1.25060200	-0.60296800
H	3.02808000	-2.68300200	-0.37676100
C	0.70748300	-1.40174200	-0.24739900
H	0.71066800	-2.42700500	0.12434100
H	-0.01115600	-0.78983300	0.29308600
H	0.49565600	-1.39012000	-1.31751500
C	2.41853000	-0.83809100	1.43376800
H	3.41848900	-0.42012400	1.55812700
H	1.68207700	-0.23770400	1.96302300
H	2.39947300	-1.87371500	1.77469000
N	2.07825800	-0.81931000	-0.03187300
C	2.16240700	0.59591300	-0.59091700
H	1.95589800	0.50992800	-1.65997500
H	3.20083700	0.90790900	-0.46443600
C	1.23662200	1.69214000	0.00927600
O	1.43965000	2.81356800	-0.52376700
O	0.41435800	1.39351900	0.91244500
C	-5.03692700	-0.31366500	-0.06240600
O	-6.09201500	0.19012900	-0.04923800
O	-3.98220000	-0.81813500	-0.07581600

8.2. Supporting information for chapter 4

Table S8.2.1. Energy of species involved in figure 4.2

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-31++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
CO ₂	-188.5269446	0.011787	-188.511588	-188.535860		-188.581469
PhSiH ₃	-522.8548462	0.116246	-522.730677	-522.770631		-522.924458
I'	-711.3835857	0.128945	-711.242421	-711.297028		-711.508452
TS' ₁₋₂	-711.3183607	0.129347	-711.178519	-711.225950	-505.55	-711.444471
II'	-711.4030962	0.133423	-711.259535	-711.306272		-711.528722
III'	-1234.2714120	0.251438	-1234.000462	-1234.070126		-1234.462797
TS' ₃₋₅	-1234.1976836	0.251970	-1233.927959	-1233.995236	-831.79	-1234.390204
V'_A	-1234.3086414	0.257668	-1234.033307	-1234.097675		-1234.495161

Table S8.2.2. Energy of species involved in figure 4.3

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
A	-326.8235558	0.146988	-326.668492	-326.707709		-326.896965
X'	-515.3575242	0.159920	-515.185305	-515.237874		-515.483915
TS' ₁₀₋₁₁	-515.2926030	0.157636	-515.124486	-515.170916	-1704.02	-515.420342
XI'	-515.3499623	0.161773	-515.177097	-515.225731		-515.478139
XII'	-1038.2257247	0.281061	-1037.925616	-1037.992168		-1038.416990
TS' ₁₂₋₁₃	-1038.1596857	0.280504	-1037.861731	-1037.923696	-739.98	-1038.352689
XIII'	-1038.2377356	0.285042	-1037.934786	-1037.997780		-1038.428444
TS' ₁₂₋₁₄	-1038.1337090	0.279320	-1037.836476	-1037.901113	-690.51	-1038.327660
XIV'_A	-1038.2555947	0.282360	-1037.953830	-1038.021377		-1038.449485

Table S8.2.3. Energy of species involved in figure 4.4

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XXII'	-1038.2443916	0.282697	-1037.942163	-1038.011263		-1038.437070
TS' ₂₂₋₁₄	-1038.1886695	0.282244	-1037.888457	-1037.953688	-286.83	-1038.388659
XIV'_B	-1038.2545625	0.282311	-1037.952830	-1038.021332		-1038.448282

Table S8.2.4. Energy of species involved in figure 4.5

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	<i>ZPE</i> (hartree)	<i>H</i> (hartree)	<i>G</i> (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
I' ₂	-711.3864533	0.128742	-711.245529	-711.298261		-711.510582
TS' _{1-2_2}	-711.3204977	0.130023	-711.180265	-711.226126	-602.68	-711.444481
II' ₂	-711.4031678	0.133779	-711.258527	-711.306820		-711.528773

Table S8.2.5. Cartesian coordinates in chapter 4

CO ₂				H	2.60478600	-1.79507800	0.07532700
C	0.00000000	0.00000000	0.00000000	H	3.36489300	0.57666200	0.07195900
O	0.00000000	0.00000000	1.16477100	C	-2.82292500	0.36807600	0.09460000
O	0.00000000	0.00000000	-1.16477100	H	-3.79294000	-0.13153400	0.06862700
PhSiH ₃				H	-2.71938400	0.88463200	1.06108600
C	-0.01202400	-1.64827400	1.20494600	H	-2.82046000	1.12211200	-0.69933700
C	-0.01202400	-0.25495700	1.20207400	I'			
C	-0.00815600	0.46679700	0.00000000	Si	0.67221300	1.49613500	-0.08248200
C	-0.01202400	-0.25495700	-1.20207400	H	0.44906300	2.95905200	-0.21008600
C	-0.01202400	-1.64827400	-1.20494600	H	1.43715800	1.25092900	1.16816900
C	-0.01092400	-2.34707700	0.00000000	H	1.48183600	1.04737800	-1.24537600
H	-0.01661400	-2.18744700	2.14733200	C	-0.94277700	0.54536800	-0.03414500
H	-0.02018600	0.27286900	2.15262500	C	-1.60076100	0.30351600	1.18036300
H	-0.02018600	0.27286900	-2.15262500	C	-1.53614500	0.07162800	-1.21303400
H	-0.01661400	-2.18744700	-2.14733200	C	-2.81272000	-0.38233500	1.21673100
H	-0.01363100	-3.43281700	0.00000000	H	-1.16196400	0.64804500	2.11371900
Si	0.02717000	2.34364900	0.00000000	C	-2.74793200	-0.61504500	-1.18209300
H	1.42206200	2.85764400	0.00000000	H	-1.04649500	0.23238800	-2.17052000
H	-0.65608000	2.85684700	-1.21469300	C	-3.38855500	-0.84142000	0.03410700
H	-0.65608000	2.85684700	1.21469300	H	-3.30520200	-0.56088000	2.16767500
A (N-methylaniline)				H	-3.18981900	-0.97652700	-2.10555100
N	-1.78776600	-0.61484500	-0.13461000	H	-4.33237400	-1.37736800	0.06077200
H	-2.00365900	-1.54582300	0.18515200	C	3.56416800	-0.84728400	0.06189900
C	-0.44268600	-0.27920300	-0.05426800	O	4.40059700	-0.04172500	-0.02995700
C	-0.00847300	1.05472700	-0.05078900	O	2.73004700	-1.65520900	0.15408000
C	0.52582600	-1.29807100	-0.00715800	TS' ₁₋₂			
C	1.35336500	1.35032800	-0.00994200	Si	-1.04320200	0.16196000	0.92563900
H	-0.72785400	1.86542200	-0.08122600	H	-1.25439000	-0.99474000	1.81322700
C	1.87740800	-0.98949100	0.03900100	H	-1.24781900	1.55041700	1.37424600
H	0.20647500	-2.33749600	-0.01535800	H	-1.53968300	-0.12182000	-0.66314500
C	2.30702100	0.33934800	0.03628100	C	0.74211100	0.06146700	0.35469000
H	1.66528000	2.39074000	-0.01031000	C	1.43464000	1.21301100	-0.04900000

C	1.41764600	-1.16779600	0.31897800	C	-1.60779700	0.80422400	0.34235800
C	2.75982600	1.14070300	-0.47117200	C	-3.39427000	-0.81593700	0.35984200
H	0.93829000	2.18085600	-0.02807100	C	-2.49242700	1.77726100	-0.11132600
C	2.74234400	-1.24541000	-0.10283700	H	-0.56739000	1.07085600	0.50673000
H	0.90802900	-2.07731700	0.63003100	C	-4.28371100	0.15830300	-0.08916300
C	3.41340300	-0.08985500	-0.49947700	H	-3.75916100	-1.82485700	0.53710300
H	3.28231500	2.04199700	-0.77624000	C	-3.83177700	1.45496500	-0.32592700
H	3.25140500	-2.20395300	-0.12107200	H	-2.13349900	2.78512400	-0.29551300
H	4.44632200	-0.14866400	-0.82848700	H	-5.32646500	-0.09299900	-0.25569800
C	-2.87859400	-0.09856300	-0.57249100	H	-4.52418700	2.21378000	-0.67740500
O	-3.14885600	0.11610800	0.61754700	C	0.08347400	-1.97179700	-1.43933900
O	-3.34713000	-0.28805200	-1.64649500	O	0.88851100	-2.32373400	-2.25827300
II'				Si	-0.82768000	-1.80041500	1.14156200
Si	-1.07064500	1.42058800	-0.02213700	H	-1.53841900	-3.03949600	1.52781900
H	-1.24214500	2.25102700	1.18745300	O	0.23528000	-2.20391800	-0.12898100
H	-1.24805200	2.20095700	-1.26410900	H	-0.83653700	-1.42239100	-1.69733800
H	-1.27136400	-1.46282400	-0.00128600	H	0.05896700	-1.31849700	2.21756400
C	0.59053400	0.57325600	-0.00973700	H	2.60428500	-1.68304700	1.80044800
C	1.22167000	0.20824500	-1.20912700	C	2.35998500	0.57623700	0.20978200
C	1.22952500	0.26054400	1.20017800	H	3.30884100	-1.90719300	-0.52507100
C	2.44693100	-0.45357100	-1.20092000	C	2.09589700	1.55292900	1.18292700
H	0.75462100	0.44327700	-2.16266500	C	1.49472000	2.76420900	0.84583800
C	2.45494400	-0.40089200	1.21257900	C	1.98672400	0.84993800	-1.11442000
H	0.76862800	0.53688500	2.14557200	C	1.13881000	3.01983700	-0.47812900
C	3.06334000	-0.75861200	0.01105400	C	1.37853000	2.05777400	-1.45639300
H	2.92199300	-0.72709900	-2.13769500	H	4.65391800	-0.67922500	1.07416900
H	2.93625600	-0.63311500	2.15727300	H	2.36640700	1.37237600	2.22090300
H	4.01962400	-1.27225900	0.01912600	H	1.30500200	3.50772900	1.61409800
C	-2.29297700	-1.04781900	0.01120900	H	0.67398900	3.96469800	-0.74378600
O	-2.33829300	0.29207400	0.00638100	H	1.09881300	2.24725000	-2.48819300
O	-3.27849900	-1.73107200	0.02797300	H	2.17203900	0.11186300	-1.89031900
III'				TS' ₃₋₅			
Si	3.26711600	-1.01434300	0.65220300	Si	-2.13813500	-1.11723900	0.73574200
C	-2.04466400	-0.50763300	0.58391900	C	3.80292100	-0.16047200	-0.35625200

C	4.08944700	1.21153700	-0.42836100	C	-2.07772300	1.29920800	-0.52175000
C	4.79063000	-1.02517800	0.13527100	C	-2.64110000	-0.49025200	0.98728800
C	5.32447300	1.70382400	-0.01880800	C	-3.13272600	0.92937500	-1.35394300
H	3.34073500	1.90684400	-0.79956900	H	-1.43800100	2.13103900	-0.80319800
C	6.02965100	-0.53526900	0.54400800	C	-3.69791700	-0.86169500	0.16030200
H	4.59354400	-2.09180000	0.20815800	H	-2.45052800	-1.06777600	1.88947500
C	6.29599900	0.82908100	0.46673600	C	-3.94242200	-0.15287500	-1.01502900
H	5.52983400	2.76794700	-0.07819700	H	-3.31879700	1.48191600	-2.26990800
H	6.78310200	-1.21789900	0.92410500	H	-4.32626800	-1.70599900	0.42773500
H	7.25951800	1.21352300	0.78691700	H	-4.76109300	-0.44443200	-1.66602600
C	-0.31931400	0.02679500	-0.20433100	C	2.04791500	2.02201700	0.85153300
O	-1.07399400	0.60666500	0.65284300	O	2.59247300	1.88976700	-0.42491100
Si	2.15970600	-0.82372900	-0.90495400	Si	-0.35281800	1.02701000	1.73389000
H	2.12533700	-2.29851100	-0.77953200	H	0.38359800	-0.19197700	2.15988600
O	0.97156500	-0.16618200	0.11529900	O	0.64539400	1.98619900	0.79614400
H	-0.48361400	0.19750900	-1.28245900	H	2.36854800	2.99177400	1.24409300
H	1.79512900	-0.41155700	-2.28471200	H	-0.76547700	1.77651500	2.94856000
H	-0.86000700	-1.34502100	-0.25390200	H	2.42098100	1.21354400	1.50073600
C	-3.71369300	-0.22301100	0.23952600	C	1.56598200	-0.81035300	-0.78149800
H	-1.64267400	-1.23102500	2.12196300	H	3.02351600	0.75383200	-2.58447800
C	-4.80454100	-1.00055400	-0.17902600	C	0.32397000	-1.43297000	-0.96301900
C	-6.03171000	-0.41568800	-0.48691400	C	0.02717900	-2.63972200	-0.33180600
C	-3.88924600	1.16686800	0.33335600	C	2.50579500	-1.43680200	0.05266000
C	-6.18858100	0.96350700	-0.37795500	C	0.96991700	-3.24145000	0.49743400
C	-5.11521400	1.75354500	0.03281200	C	2.21309200	-2.63886800	0.68995300
H	-2.56280000	-2.53489800	0.39753300	H	0.71067500	1.36518900	-2.19162700
H	-4.69324800	-2.07827800	-0.26679700	H	-0.43502400	-0.96208900	-1.58275100
H	-6.86163800	-1.03602300	-0.81161100	H	-0.94522400	-3.09942800	-0.47880400
H	-7.14345100	1.42366900	-0.61427000	H	0.73832400	-4.17874400	0.99445100
H	-5.23480600	2.82939100	0.11821900	H	2.95028900	-3.10591100	1.33593200
H	-3.05244800	1.78590900	0.63759200	H	3.47831100	-0.97593500	0.21271500
V'_A				X'			
Si	1.95100300	0.84350400	-1.56879900	C	-0.41170000	0.46513200	-0.47707300
C	-1.81385400	0.59164700	0.65822000	C	-1.00355500	-0.63939700	-1.11329300

C	-1.05903600	1.02857600	0.63061900	N	-1.04727000	-0.54042600	0.32960500
C	-2.20517600	-1.15911200	-0.65276900	C	-2.02985700	0.30636500	-0.51308100
H	-0.50431100	-1.09499000	-1.96467600	O	-2.24707200	1.47564500	-0.35394900
C	-2.26326000	0.49368900	1.08570200	O	-2.46202200	-0.62817100	-1.28114700
H	-0.62691000	1.87882900	1.14577000	H	-1.64785800	-1.26405800	-0.54850700
C	-2.84730500	-0.59811100	0.45264700	XI'			
H	-2.64258400	-2.01372300	-1.16011700	C	-0.32475900	0.23469600	-0.02024000
H	-2.74625600	0.94379400	1.94784700	C	-1.05737600	0.23112800	-1.20908100
H	-3.78456400	-1.00911000	0.81228800	C	-0.97384300	0.03682400	1.20104700
C	1.32023800	2.22694600	-0.50161400	C	-2.43184900	0.00714000	-1.17704100
H	1.56882500	2.20304400	0.56416200	H	-0.53913500	0.39602900	-2.14872400
H	2.23914100	2.44630500	-1.04835800	C	-2.34788200	-0.18732500	1.22856500
H	0.60192000	3.04212000	-0.67458300	H	-0.39305400	0.05099900	2.11850100
N	0.82310900	0.93440300	-0.92794400	C	-3.07701500	-0.20113200	0.04053500
C	2.25827400	-1.10352900	0.54602100	H	-2.99752800	-0.00233600	-2.10310600
O	2.30159400	-0.40452100	1.47743600	H	-2.84872100	-0.34798400	2.17768400
O	2.24784300	-1.83773000	-0.35897700	H	-4.14794200	-0.37517600	0.06413300
H	1.00660100	0.71575500	-1.89582900	C	1.51797400	1.86910700	0.11577200
TS' ₁₀₋₁₁				H	1.32011100	2.22418500	1.13386400
C	0.35350400	-0.22978500	0.13182300	H	2.58905600	1.91651900	-0.07635000
C	1.21874600	-1.26445100	-0.21118700	H	0.98571100	2.50993500	-0.59228500
C	0.82378200	1.07194200	0.29640300	N	1.08134200	0.48959500	-0.05282400
C	2.57308500	-0.99549300	-0.39184200	C	2.02053900	-0.51969300	-0.04062400
H	0.82718700	-2.26895800	-0.33995700	O	3.21317100	-0.33093500	0.04025500
C	2.17864200	1.33167100	0.11004900	O	1.52951800	-1.77505400	-0.14453600
H	0.13062300	1.86847400	0.54568100	H	0.56585700	-1.77588100	-0.20329000
C	3.05406100	0.30196200	-0.23105400	XII'			
H	3.25004500	-1.79867400	-0.66383900	H	-0.64332200	-3.70298900	-1.33860300
H	2.55044700	2.34417200	0.22908100	Si	0.74691400	1.25556500	-2.34381400
H	4.10882200	0.51114400	-0.37650200	C	-1.53171200	-0.03648100	0.63953200
C	-1.43917800	-0.60717200	1.74855400	C	-0.71618400	0.83612300	1.35727000
H	-1.34001800	0.37856300	2.21281400	C	-2.66346000	0.44695000	-0.01803700
H	-2.47862800	-0.93571900	1.81519800	C	-1.02950800	2.19115300	1.41471500
H	-0.79369400	-1.32199000	2.26155700	H	0.18154100	0.46476200	1.84126400

C	-2.96537600	1.80318200	0.03708000	C	1.13711200	2.20174400	0.71307200
H	-3.28713900	-0.23385800	-0.58474400	H	-0.08036300	1.03884600	2.05044400
C	-2.15258400	2.68024500	0.75395600	C	0.22835700	2.56564300	-1.48992700
H	-0.38204100	2.86400900	1.96819400	H	-1.72192800	1.71535600	-1.85464200
H	-3.84266600	2.17578900	-0.48196600	C	1.25768400	2.73575300	-0.56667700
H	-2.39234600	3.73796400	0.79471600	H	1.94566500	2.30447400	1.42877300
C	-0.75950600	-2.06019400	1.84968100	H	0.31910500	2.97831300	-2.48939600
H	-1.26858000	-1.57708600	2.68475800	H	2.15745800	3.27330400	-0.84765000
H	-1.01865400	-3.11775700	1.83821300	C	-2.78508000	0.80355700	1.82486300
H	0.32354000	-1.96079000	1.98231400	H	-2.60008200	1.84148900	2.09831700
N	-1.20944800	-1.42729000	0.61198400	H	-3.85939200	0.62693800	1.78377500
C	-1.09046500	-2.06065900	-0.58712100	H	-2.34292700	0.13840500	2.57595400
O	-1.32503000	-1.58396200	-1.68340200	N	-2.19609300	0.57171400	0.50703400
O	-0.66197700	-3.34077400	-0.44421800	C	-2.40554000	-0.61828400	-0.08757100
H	0.68569500	0.21125100	-3.39288200	O	-1.94411900	-0.89335900	-1.27589500
C	1.76074000	0.63071800	-0.88687100	O	-3.49548400	-1.25525800	0.34463300
H	-0.61944400	1.62985200	-1.90914000	H	-1.14156200	-1.61603800	0.60709800
H	1.41093000	2.46987100	-2.89247900	C	1.22705900	-1.39113600	-0.21641000
C	2.33256200	1.52886800	0.02570000	H	-0.12502500	-1.84997800	-2.37158000
C	3.01583900	1.07737300	1.15206700	H	-0.81808500	-3.37480500	-0.73553900
C	3.14405400	-0.29141700	1.38652100	C	2.18352300	-0.84960700	-1.08246400
C	2.60011800	-1.20033400	0.48128100	C	3.42731800	-0.42454000	-0.61264600
C	1.91966300	-0.73978200	-0.64506400	C	3.74100300	-0.55383800	0.73708200
H	2.23323400	2.59960200	-0.13640000	C	2.80496700	-1.10223700	1.61596700
H	3.44775000	1.79120900	1.84739600	C	1.56007600	-1.50213700	1.14084300
H	3.67533500	-0.64711200	2.26433100	H	1.94824100	-0.74804600	-2.13924100
H	2.70934200	-2.26810800	0.64778700	H	4.14982600	0.00415200	-1.30136900
H	1.50714000	-1.46007800	-1.34653800	H	4.70979400	-0.22928300	1.10633700
TS' ₁₂₋₁₃				H	3.04664000	-1.21164700	2.66960000
H	-3.59707900	-2.04574300	-0.20010600	H	0.82280000	-1.89745600	1.83717400
Si	-0.46035000	-1.93149700	-0.89883000	XIII'			
C	-1.02964400	1.32412900	0.13941400	H	-3.95139400	0.58107100	-0.72058400
C	-0.00490700	1.49267100	1.06832400	Si	-1.12760700	-2.11312000	-0.95774000
C	-0.92171200	1.86488400	-1.13945000	C	-0.44761600	1.25900200	0.46927200

C	0.70058900	1.62477500	1.18932800	C	-2.37778200	-0.37536900	-1.42716700
C	-0.61820300	1.79893900	-0.81858000	C	-3.17547700	-0.34818000	0.85114300
C	1.64573800	2.48405500	0.63603900	C	-2.96890800	-1.62075600	-1.61862800
H	0.88332300	1.22694500	2.17932900	H	-1.82511000	0.09391800	-2.23479500
C	0.33263100	2.65603600	-1.35571300	C	-3.75668100	-1.59842000	0.65977900
H	-1.49656500	1.54708500	-1.39539300	H	-3.24505200	0.16010700	1.80616800
C	1.47635600	3.00748400	-0.64003100	C	-3.65391200	-2.23771100	-0.57411100
H	2.52736100	2.73768700	1.21742500	H	-2.88217700	-2.11454200	-2.58120900
H	0.17008300	3.05936100	-2.35116100	H	-4.29247600	-2.07224200	1.47613500
H	2.21317700	3.68049300	-1.06624600	H	-4.10858500	-3.21200900	-0.72192400
C	-1.21552500	-0.02973600	2.41439600	C	-2.09858100	2.57192000	-0.96599300
H	-1.22969000	0.84342300	3.07818400	H	-3.16415200	2.56905000	-1.19971800
H	-2.04290500	-0.68088300	2.69952000	H	-1.81866700	3.53568000	-0.54149300
H	-0.27994200	-0.57965400	2.57902300	H	-1.52558600	2.42273200	-1.89094200
N	-1.36549700	0.35787300	1.02615500	N	-1.84904400	1.53028800	0.02797800
C	-2.49068800	-0.13972400	0.29886100	C	-0.55952100	1.55782400	0.55962300
O	-2.15216500	-0.77989500	-0.91051900	O	0.13745700	2.55250400	0.62522200
O	-3.37686600	0.89618400	-0.01465500	O	-0.49359300	0.62164300	1.76287200
H	-2.98746900	-0.87264800	0.95064300	H	-0.13368900	1.13588400	2.50235600
C	0.63504400	-1.71402700	-0.50186000	Si	0.68057100	-0.68863700	0.90539000
H	-1.25050100	-2.58458200	-2.35306800	H	0.11589200	0.45366700	-0.19037700
H	-1.63100600	-3.12696100	0.01021800	H	1.00690200	-1.15356900	2.29787700
C	1.42597200	-0.88629100	-1.31264700	H	-0.15832100	-1.77051800	0.33542900
C	2.72167200	-0.54528200	-0.93940000	C	2.41142500	-0.47341500	0.19524400
C	3.25337100	-1.03394900	0.25270400	C	3.50490800	-1.02909300	0.87515000
C	2.48671400	-1.86117700	1.06915600	C	2.65072200	0.17991600	-1.02088700
C	1.18733900	-2.19664400	0.69221700	C	3.93408800	0.25744900	-1.55441800
H	1.02008700	-0.48149400	-2.23585000	C	5.00650000	-0.31524900	-0.87214400
H	3.31172400	0.11102600	-1.57071100	C	4.79197800	-0.95700700	0.34568500
H	4.26409000	-0.76652700	0.54604500	H	1.82311200	0.64655800	-1.54963400
H	2.89975800	-2.24579400	1.99695700	H	4.09981100	0.76897100	-2.49764100
H	0.59672100	-2.84105800	1.33988600	H	6.00867500	-0.25207100	-1.28547400
TS' ₁₂₋₁₄				H	5.62650600	-1.39647700	0.88370300
C	-2.47755700	0.26205100	-0.18931000	H	3.35010300	-1.52317100	1.83166700

XIV'A

C	1.53892700	0.46480900	0.70522000
C	0.94527000	-0.49743800	1.52704500
C	2.73515400	0.16283900	0.04657400
C	1.53993400	-1.74545200	1.68121800
H	0.00442200	-0.28203700	2.02236100
C	3.31162000	-1.09543500	0.19021000
H	3.22484200	0.91628000	-0.56116000
C	2.72123100	-2.05390100	1.01031900
H	1.06546300	-2.48418000	2.31969700
H	4.23848900	-1.31789000	-0.32878300
H	3.18058500	-3.02963500	1.12969600
C	0.26076700	2.35723900	1.68679300
H	0.84850800	2.19578500	2.59286100
H	0.16949700	3.42441200	1.48518500
H	-0.74382200	1.94244900	1.82560400
N	0.93679100	1.73954200	0.55573900
C	0.83670400	2.32834800	-0.67509700
O	0.27699000	3.39337800	-0.88156400
O	0.26581700	-0.06707900	-2.81939600
H	-0.28373100	0.32645900	-3.49982500
Si	-0.32478600	-1.39062600	-1.98619200
H	1.28728100	1.72977400	-1.47959700
H	-0.97275100	-2.34015200	-2.93189500
H	0.84274400	-2.03778800	-1.35221800
C	-1.56378900	-0.85354200	-0.68681300
C	-2.06911600	-1.78074000	0.23654400
C	-1.98037000	0.47871500	-0.58044900
C	-2.86502100	0.87724100	0.42138500
C	-3.34765400	-0.05545100	1.33588800
C	-2.95023200	-1.38965100	1.24042500
H	-1.60343600	1.22685400	-1.27267400
H	-3.16902700	1.91755700	0.48764700
H	-4.03505900	0.25324100	2.11769900

H	-3.32620000	-2.12152000	1.94910500
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H	-1.76135700	-2.82351400	0.18491300
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XXII'

H	0.30734300	0.74914900	-1.17534400
C	2.08893300	0.01229000	0.73712400
C	2.69044800	-0.53904000	-0.40369400
C	2.27748400	1.37594900	0.99853100
C	3.45236500	0.25223100	-1.25968000
H	2.54077600	-1.58984100	-0.63643000
C	3.04124100	2.17087600	0.14506800
H	1.81367300	1.83404500	1.86978600
C	3.62755300	1.60864800	-0.98703700
H	3.90757200	-0.18809400	-2.14148100
H	3.17376200	3.22680400	0.35915200
H	4.21971300	2.22611000	-1.65524500
C	-0.74984300	-2.43805100	0.34322800
O	-0.99794900	-3.26586600	-0.49047000
Si	1.01259700	-1.03503400	1.84503900
H	-0.13964700	-0.24632900	2.34215100
O	0.45031500	-2.35030900	0.94003300
H	-1.48770700	-1.70144300	0.70087000
H	1.76188100	-1.63373800	2.96877600
N	-0.50261000	0.15388100	-1.27008800
C	-0.56923600	-0.56880200	-2.52580000
C	-1.64379700	0.65002800	-0.65480000
C	-1.52637400	1.67092600	0.30560400
C	-2.64231200	2.12587700	0.99415800
C	-3.90392300	1.58182600	0.74700600
C	-2.91430700	0.11138400	-0.90864100
C	-4.02577000	0.57772800	-0.20881700
H	-1.04600400	-1.54363000	-2.38915500
H	-1.11135900	-0.01357600	-3.30507900
H	0.45142100	-0.75069000	-2.86775600
H	-0.54839800	2.10361900	0.50213500

H	-2.52631400	2.91555600	1.73077900	H	-2.58177000	-2.77780300	-1.18344000
H	-4.77446300	1.93996300	1.28593400	H	0.16212800	0.74760000	-0.97807200
H	-3.03565900	-0.67846400	-1.64187600	H	0.03741500	3.19107400	-0.67026400
H	-4.99837400	0.14204500	-0.41715600	H	-2.05729300	4.23890600	0.17798500
TS' ₂₂₋₁₄				H	-3.88767000	0.36515400	0.43348700
H	-0.87637500	-1.31205100	-0.99945200	H	-4.01106700	2.81385900	0.72919300
C	2.38731400	-0.52738200	0.03134200	XIV'_B			
C	2.80779900	0.24005600	-1.06555500	H	-0.04118100	-1.58505300	-1.11270000
C	2.25436700	0.12658700	1.26585000	C	2.36970500	0.03132500	-0.40039700
C	3.06608500	1.60548700	-0.94237900	C	2.29215800	1.28580300	-1.02673300
H	2.93380900	-0.23543500	-2.03614400	C	2.48310300	-0.00286800	0.99746100
C	2.50623700	1.49090100	1.39979500	C	2.31169200	2.46335100	-0.28343300
H	1.95072600	-0.44005600	2.14467300	H	2.20053300	1.34594600	-2.10858900
C	2.90876100	2.23458600	0.29164300	C	2.49863800	1.17287400	1.74736700
H	3.39410500	2.17668000	-1.80633900	H	2.54454300	-0.95922900	1.51166000
H	2.39118000	1.97330000	2.36602500	C	2.40864500	2.40689300	1.10714300
H	3.10889100	3.29737500	0.39295000	H	2.24898000	3.42401800	-0.78576400
C	-1.17508000	-1.67749900	0.86720600	H	2.58193000	1.12395700	2.82887100
O	-1.80635700	-2.53689500	1.40807300	H	2.41904100	3.32396300	1.68850400
Si	1.81657600	-2.32143300	-0.18137200	C	-0.56149600	-1.37285400	1.57935100
H	2.19579400	-3.03838400	1.07287400	O	-0.09280200	-2.40629500	2.01625800
O	0.21186300	-2.34878800	-0.45219300	Si	2.19787200	-1.55651500	-1.38273200
H	-0.46782600	-0.97567900	1.31982800	H	2.72109700	-2.66513600	-0.54563200
H	2.58666200	-2.88874500	-1.32627100	O	0.60116800	-1.80089400	-1.79882900
N	-1.73670600	-1.02271500	-0.45082000	H	-0.29449900	-0.38287800	1.97842900
C	-2.90910700	-1.76378100	-0.95784400	H	2.93289600	-1.47295100	-2.66465400
C	-1.86391100	0.41811100	-0.31701200	N	-1.45974100	-1.31108200	0.53739800
C	-0.75597200	1.20389400	-0.62025500	C	-2.07931800	-2.55716900	0.09133800
C	-0.82999400	2.58211900	-0.43959700	C	-2.01790300	-0.05614000	0.15674500
C	-2.00069100	3.16432700	0.03885900	C	-1.18548900	1.05894800	0.02192600
C	-3.03538900	0.98497000	0.17737100	C	-1.72541800	2.28964200	-0.33519200
C	-3.10026000	2.36501000	0.34715100	C	-3.08900500	2.41717800	-0.58839200
H	-3.68374300	-1.81036700	-0.19320000	C	-3.38525600	0.06700100	-0.09928400
H	-3.27508600	-1.26521300	-1.85536300	C	-3.91239300	1.29947400	-0.47605400

H	-2.95397000	-2.81075900	0.70014200	H	0.18433700	-1.66541400	-0.84231500
H	-2.37617200	-2.45778800	-0.95423800	C	3.20150500	-0.60742300	0.29661600
H	-1.34564200	-3.35689000	0.19003800	H	3.64082100	1.38522800	0.98661300
H	-0.11534800	0.96457000	0.17008400	H	2.46987200	-2.49690600	-0.43524600
H	-1.06418800	3.14455700	-0.43532300	H	4.20410900	-0.97970500	0.48351700
H	-3.50585600	3.37543200	-0.88007900	C	-2.70999400	-0.36639100	0.34618700
H	-4.04102500	-0.79124000	-0.00075600	O	-3.61311000	-0.60477600	1.07610800
H	-4.97607300	1.38504800	-0.67402700	Si	-1.05157100	1.09872800	-0.55491900
I' ₂				H	-1.58109100	1.21845100	-1.92441300
C	0.28161000	1.00701400	0.07765800	O	-1.99303400	-0.82786800	-0.55234900
C	-0.58757800	1.25573900	-0.99530300	H	-2.28739700	0.89775300	0.56387500
C	-0.26075700	0.46943500	1.25425400	H	-0.93557400	2.49977100	-0.03509400
C	-1.94716300	0.97057000	-0.90129200	II' ₂			
H	-0.20131700	1.67801600	-1.92004900	C	0.59122600	-0.57391300	0.04895200
C	-1.62093200	0.18016500	1.35268700	C	1.26425600	-0.38950300	-1.16845500
H	0.38469100	0.26728600	2.10518300	C	1.18647300	-0.07961600	1.22039300
C	-2.46567900	0.43043500	0.27372400	C	2.48871900	0.27274000	-1.21656200
H	-2.60182200	1.16831900	-1.74437800	H	0.83122600	-0.76904200	-2.09093400
H	-2.02063300	-0.23672700	2.27214500	C	2.40995300	0.58327300	1.17640000
H	-3.52548100	0.20761600	0.34944800	H	0.69331600	-0.21458400	2.18023600
C	0.45262000	-2.37026700	-0.27676500	C	3.06061500	0.76026700	-0.04350400
O	-0.28228400	-2.30690000	-1.17726800	H	2.99562900	0.40677500	-2.16688600
Si	2.12066200	1.35689700	-0.06905000	H	2.85668000	0.95965000	2.09117000
H	2.72067900	1.41973700	1.28653000	H	4.01547400	1.27539500	-0.07923900
O	1.19479000	-2.45411400	0.61838500	C	-2.29217900	1.03881800	-0.13298600
H	2.80223900	0.28555700	-0.84258000	O	-3.27596300	1.72424100	-0.15990200
H	2.33961100	2.64320000	-0.77832500	Si	-1.07089400	-1.41759700	0.10035800
TS' _{1-2_2}				H	-1.25025400	-2.17495600	1.35513700
C	0.60720200	0.34592100	-0.18284500	O	-2.33447500	-0.28404900	0.08131000
C	1.59824800	1.19134100	0.34101400	H	-1.27450600	1.43893400	-0.27642100
C	0.94013100	-0.98984300	-0.45658100	H	-1.24592400	-2.26974700	-1.09477700
C	2.88702700	0.71910000	0.57910800				
H	1.36499700	2.22856200	0.56719600				
C	2.22772700	-1.46083500	-0.22105600				

8.3. Supporting information for chapter 5

Table S8.3.1. Energy of species involved in figure 5.1.1 to figure 5.1.3

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-31++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
A	-326.8235558	0.146988	-326.668492	-326.707709		-326.896965
B	-402.2270179	0.167234	-402.050167	-402.092700		-402.359810
CO ₂	-188.5269446	0.011787	-188.511588	-188.535860		-188.581469
PhSiH ₃	-522.8548462	0.116246	-522.730677	-522.770631		-522.924458
I	-1113.6323641	0.298275	-1113.311732	-1113.388560		-1113.879403
TS ₁₋₂	-1113.5911617	0.301944	-1113.268932	-1113.337940	-229.88	-1113.869532
II	-1113.6567417	0.304102	-1113.331927	-1113.402029		-1113.908890
III	-1636.5401604	0.422965	-1636.088312	-1636.176426		-1636.845900
TS ₃₋₄	-1636.4779843	0.423897	-1636.026885	-1636.113110	-39.85	-1636.801064
IV	-1636.5172515	0.428363	-1636.061728	-1636.146056		-1636.828617
TS ₄₋₅	-1636.5169993	0.427988	-1636.062661	-1636.144686	-58.92	-1636.827284
V_A	-1636.5621860	0.427802	-1636.106722	-1636.192670		-1636.865087
V'_B	-1234.3072065	0.257289	-1234.032110	-1234.097465		-1234.495756
TS' ₅₋₆	-1234.2601704	0.255420	-1233.987394	-1234.050178	-386.56	-1234.451049
VI'	-1234.2976613	0.252613	-1234.025199	-1234.096264		-1234.489369
VII'	-441.3022128	0.176244	-441.113849	-441.164519		-441.407768
TS' ₇₋₈	-441.2547303	0.175601	-441.069172	-441.114199	-1552.82	-441.364656
VIII'	-441.3189717	0.180854	-441.127818	-441.172805		-441.420857

Table S8.3.2. Energy of species involved in figure 5.1.4 to figure 5.1.6

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-31++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
IM2	-1113.6644969	0.304251	-1113.339705	-1113.409141		-1113.908140
TS _{IM}	-1113.6287974	0.303957	-1113.305168	-1113.372760	-160.54	-1113.877867
IM3	-1113.6379844	0.303728	-1113.313689	-1113.383188		-1113.886260
IX	-1365.6895193	0.464755	-1365.197353	-1365.282652		-1366.024703
TS ₉₋₁₅	-1365.6703099	0.461198	-1365.181656	-1365.266659	-35.82	-1366.004111
XV	-1365.6723316	0.461374	-1365.182816	-1365.270347		-1366.005123
XVIII	-1152.6902455	0.315635	-1152.353330	-1152.426442		-1152.938229
TS ₁₈₋₁₉	-1152.6884667	0.314559	-1152.353091	-1152.425078	-64.05	-1152.935803
XIX	-1152.8083181	0.318460	-1152.468169	-1152.541905		-1153.026237
XX	-1365.6925048	0.461634	-1365.202765	-1365.291590		-1366.020123
TS ₂₀₋₂₁	-1365.6569084	0.460335	-1365.168691	-1365.256600	-47.76	-1366.002387
XXI	-1365.7517715	0.467230	-1365.257565	-1365.340076		-1366.081631
XVI	-1478.9755683	0.471447	-1478.474138	-1478.565385		-1479.347054
TS ₁₆₋₁₇	-1478.9739402	0.471511	-1478.473183	-1478.562571	-51.02	-1479.345019
XVII	-1478.9914118	0.474632	-1478.487846	-1478.576294		-1479.352093
XXIII	-881.4667811	0.339538	-881.106314	-881.178433		-881.665340
TS ₂₃₋₂₄	-881.4285371	0.336929	-881.070577	-881.142039	-78.88	-881.639229
XXIV	-881.4750235	0.340751	-881.114402	-881.182014		-881.673717

Table S8.3.3. Energy of species involved in figure 5.1.8

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
III₄	-1636.5331676	0.421307	-1636.082373	-1636.173996		-1636.834062
TS _{3-5_4}	-1636.4698762	0.422787	-1636.019698	-1636.105611	-138.65	-1636.791214
V₄	-1636.5329445	0.427274	-1636.078008	-1636.166652		-1636.842269

Table S8.3.4. Energy of species involved in figure 5.1.9 and figure 5.1.10

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
TS _{3-5_2}	-1636.4559095	0.422733	-1636.006515	-1636.089722	-471.12	-1636.770402
TS _{3-5_3}	-1636.4785996	0.422265	-1636.028884	-1636.113828	-518.63	-1636.785151
TS _{3-5_5}	-1636.4660978	0.422788	-1636.015777	-1636.104123	-182.60	-1636.785400
TS _{3-5_7}	-1636.4553988	0.422855	-1636.005114	-1636.092833	-849.85	-1636.775220
TS _{3-4_6}	-1636.4823843	0.423092	-1636.032244	-1636.117450	-736.83	-1636.781772
TS _{4-5_6}	-1636.5295891	0.426212	-1636.076535	-1636.161337	-53.47	-1636.821766

Table S8.3.5. Energy of species involved in figure 5.1.11

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
V_B	-1636.5540470	0.427027	-1636.099013	-1636.187227		-1636.866245
TS ₅₋₆	-1636.5146957	0.424638	-1636.062398	-1636.149035	-349.70	-1636.831270
VI	-1636.5465749	0.422289	-1636.094394	-1636.187351		-1636.859194

Table S8.3.6. Energy of species involved in figure 5.1.12

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
IM ₂	-1113.6630535	0.303763	-1113.338595	-1113.408550		-1113.908191
TS _{IM_2}	-1113.6296867	0.303988	-1113.306006	-1113.372784	-175.41	-1113.873541
IM ₃	-1113.6397791	0.303242	-1113.315763	-1113.386515		-1113.888409

Table S8.3.7. Energy of species involved in figure 5.2.1

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XII_A	-1440.4704901	0.450590	-1439.990572	-1440.081971		-1440.784570
TS ₁₂₋₁₃	-1440.4111774	0.451807	-1439.931378	-1440.017674	-157.84	-1440.745528
XIII	-1440.4887949	0.455673	-1440.005040	-1440.091839		-1440.799482

Table S8.3.8. Energy of species involved in figure 5.2.3

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
X	-917.6086629	0.330461	-917.256122	-917.329892		-917.852059
TS ₁₀₋₁₁	-917.5532732	0.327855	-917.205017	-917.273148	-1679.71	-917.789817
XI	-917.6177640	0.332912	-917.264663	-917.332468		-917.852766

Table S8.3.9. Energy of species involved in figure 5.2.4

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XII_B	-1440.4824074	0.449810	-1440.003250	-1440.095198		-1440.790135
TS ₁₂₋₁₄	-1440.3829452	0.449969	-1439.905693	-1439.990189	-837.10	-1440.703905
XIV_B	-1440.5105992	0.452329	-1440.028693	-1440.119738		-1440.818781
XII_{2A}	-1440.4719754	0.449172	-1439.993103	-1440.085106		-1440.784010
TS _{12-14_2}	-1440.3798525	0.448391	-1439.903129	-1439.993199	-703.03	-1440.695205
XIV_{2A}	-1440.5088744	0.453121	-1440.026731	-1440.116810		-1440.816267

Table S8.3.10. Energy of species involved in figure 5.2.5

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XII_{2B}	-1440.4817404	0.451178	-1440.001342	-1440.091309		-1440.784302
TS _{12-13_2}	-1440.4092794	0.449987	-1439.931364	-1440.018486	-249.43	-1440.727742
XIII₂	-1440.4835022	0.453497	-1440.001155	-1440.091719		-1440.793601

Table S8.3.11. Energy of species involved in figure 5.2.6

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
TS _{12-13_3}	-1440.4293674	0.447382	-1439.954921	-1440.038898	-843.86	-1440.740085
TS _{12-13_4}	-1440.4094884	0.450608	-1439.931317	-1440.017138	-753.08	-1440.721761

Table S8.3.12. Energy of species involved in figure 5.3.1 and figure 5.3.2

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XXII_A	-1440.5064474	0.452740	-1440.024202	-1440.115714		-1440.812208
TS ₂₂₋₂₅	-1440.4912954	0.454540	-1440.009061	-1440.096621	-101.39	-1440.790822
XXV_A	-1440.4916616	0.455674	-1440.008018	-1440.096553		-1440.788977
XXV_B	-1440.4932520	0.456844	-1440.009240	-1440.094404		-1440.791646
TS ₂₅₋₂₆	-1440.4715629	0.455138	-1439.989782	-1440.073927	-220.93	-1440.779771
XXVI_A	-1440.4942507	0.456654	-1440.010868	-1440.091962		-1440.792648
XXVI_B	-1440.4968084	0.454717	-1440.013908	-1440.103523		-1440.802054
TS ₂₆₋₁₄	-1440.4692567	0.453058	-1439.988816	-1440.074470	-326.68	-1440.778620
XIV_A	-1440.5139925	0.452567	-1440.032336	-1440.121500		-1440.825396

Table S8.3.13. Energy of species involved in figure 5.3.3 and figure 5.3.4

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XXVII	-1227.4430594	0.304259	-1227.114865	-1227.196436		-1227.745861
TS ₂₇₋₂₈	-1227.4189550	0.305463	-1227.091794	-1227.166018	-193.18	-1227.723109
XXVIII	-1227.4350060	0.308313	-1227.105556	-1227.176898		-1227.729490
TS ₂₈₋₂₉	-1227.4270777	0.307665	-1227.098569	-1227.171120	-271.72	-1227.722708
XXIX	-1227.4361550	0.307933	-1227.106931	-1227.180493		-1227.728811
TS ₂₉₋₃₀	-1227.4231041	0.305088	-1227.096322	-1227.171206	-315.52	-1227.719731
XXX	-1227.4623201	0.304126	-1227.134678	-1227.214877		-1227.763562

Table S8.3.14. Energy of species involved in figure 5.3.6

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XXVIII₂	-1227.4326560	0.306525	-1227.104945	-1227.177420		-1227.727612
TS _{28-29_2}	-1227.4248721	0.307839	-1227.096283	-1227.167626	-218.12	-1227.722113
XXIX_{2A}	-1227.4325159	0.308208	-1227.103158	-1227.175760		-1227.727922

Table S8.3.15. Energy of species involved in figure 5.3.7

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XXIX_{2B}	-1227.4333816	0.307252	-1227.104799	-1227.178487		-1227.728001
TS _{29-30_2}	-1227.4211255	0.304903	-1227.094841	-1227.168141	-267.42	-1227.717800
XXX₂	-1227.4634175	0.305385	-1227.135161	-1227.212479		-1227.761119

Table S8.3.16. Energy of species involved in figure 5.3.9

	ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)
	ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
XXII_B	-1440.4897064	0.452230	-1440.007678	-1440.100417		-1440.805295
TS ₂₂₋₁₄	-1440.4357477	0.451617	-1439.955616	-1440.046105	-254.99	-1440.757694
XIV_c	-1440.4977170	0.451065	-1440.016605	-1440.111120		-1440.815989
XXII₂	-1440.5032661	0.452684	-1440.021091	-1440.112085		-1440.817935
TS _{22-14_2}	-1440.4278791	0.451035	-1439.948580	-1440.037810	-351.18	-1440.752060
XIV_{2B}	-1440.5047823	0.451859	-1440.023314	-1440.114962		-1440.819744

Table S8.3.17. Energy of species involved in figure 5.4.1.2

		ω B97XD/6-31+G(d,p)					SMD(CH ₃ CN) ω B97XD/6-31++G(d,p)
		ϵ (hartree)	ZPE (hartree)	H (hartree)	G (hartree)	Imaginary frequency (cm ⁻¹)	ϵ_{sol} (hartree)
Black line	CO ₂	-188.5903926	0.011565	-188.575246	-188.599542		-188.574656
	PhSiH ₃	-522.9532567	0.115425	-522.829803	-522.873465		-522.878449
	CH ₃ COO ⁻	-228.5393157	0.048149	-228.485760	-228.519168		-228.596054
	(IM1a+Si-1a) ₂	-1463.0834374	0.299598	-1462.758804	-1462.845914		-1462.967685
	TS _{2a}	-1463.0661253	0.298866	-1462.743538	-1462.826386	-423.10	-1462.952361
	IM3a	-1463.1055725	0.304259	-1462.777571	-1462.860484		-1462.993062
	TS _{2a_2}	-1463.1027463	0.304360	-1462.775577	-1462.854030	-37.46	-1462.994829
	IM2a_2	-1463.1163977	0.305362	-1462.787645	-1462.868120		-1463.011838
Red line	PhSiH ₃	-522.9532567	0.115425	-522.829803	-522.873463		-522.878449
	CO ₂	-188.5903926	0.011565	-188.575246	-188.599542		-188.574656
	CH ₃ COO ⁻	-228.5393156	0.048146	-228.485760	-228.519218		-228.596051
	(IM1a+Si-1a) ₃	-1463.0833234	0.299474	-1462.758771	-1462.846215		-1462.966751
	TS _{2a}	-1463.0661253	0.298867	-1462.743537	-1462.826383	-423.13	-1462.952360
	IM3a_2	-1463.1033283	0.304122	-1462.775347	-1462.858720		-1462.994124
	TS _{2a_3}	-1463.1032034	0.303845	-1462.776249	-1462.857818	-23.87	-1462.994212
	IM2a_3	-1463.1318890	0.305614	-1462.802811	-1462.883906		-1463.024480

Table S8.3.18. Cartesian coordinates in chapter 5

CO ₂				H	3.36489300	0.57666200	0.07195900
C	0.00000000	0.00000000	0.00000000	C	-2.82292500	0.36807600	0.09460000
O	0.00000000	0.00000000	1.16477100	H	-3.79294000	-0.13153400	0.06862700
O	0.00000000	0.00000000	-1.16477100	H	-2.71938400	0.88463200	1.06108600
PhSiH ₃				H	-2.82046000	1.12211200	-0.69933700
C	-0.01202400	-1.64827400	1.20494600	B (glycine betaine)			
C	-0.01202400	-0.25495700	1.20207400	C	-0.30785100	-0.86611500	-0.00017500
C	-0.00815600	0.46679700	0.00000000	H	-0.27875300	-1.50191000	-0.88815900
C	-0.01202400	-0.25495700	-1.20207400	H	-0.27889900	-1.50221900	0.88759100
C	-0.01202400	-1.64827400	-1.20494600	C	-1.65769600	-0.05074200	-0.00014900
C	-0.01092400	-2.34707700	0.00000000	O	-2.62396600	-0.81812400	-0.00036600
H	-0.01661400	-2.18744700	2.14733200	O	-1.57042300	1.19749000	0.00007600
H	-0.02018600	0.27286900	2.15262500	N	0.98521400	-0.06100300	0.00007100
H	-0.02018600	0.27286900	-2.15262500	C	2.14208900	-0.99770000	0.00002100
H	-0.01661400	-2.18744700	-2.14733200	H	2.09426800	-1.62462100	-0.89116200
H	-0.01363100	-3.43281700	0.00000000	H	3.07143200	-0.42440400	0.00018400
Si	0.02717000	2.34364900	0.00000000	H	2.09412400	-1.62488900	0.89100900
H	1.42206200	2.85764400	0.00000000	C	1.04636900	0.80078400	1.22353200
H	-0.65608000	2.85684700	-1.21469300	H	0.18038400	1.46344800	1.19425300
H	-0.65608000	2.85684700	1.21469300	H	1.00244600	0.15325300	2.10063400
A (N-methylaniline)				H	1.98653900	1.35532800	1.21298900
N	-1.78776600	-0.61484500	-0.13461000	C	1.04657700	0.80119800	-1.22309000
H	-2.00365900	-1.54582300	0.18515200	H	1.98672400	1.35577300	-1.21217500
C	-0.44268600	-0.27920300	-0.05426800	H	1.00285700	0.15395700	-2.10041700
C	-0.00847300	1.05472700	-0.05078900	H	0.18056000	1.46382600	-1.19376200
C	0.52582600	-1.29807100	-0.00715800	I			
C	1.35336500	1.35032800	-0.00994200	C	-1.20543500	-0.29925100	-0.15383900
H	-0.72785400	1.86542200	-0.08122600	C	-1.56925000	0.76916700	-0.98805300
C	1.87740800	-0.98949100	0.03900100	C	-0.81760400	-0.00326300	1.16074200
H	0.20647500	-2.33749600	-0.01535800	C	-1.54638300	2.08705500	-0.53186500
C	2.30702100	0.33934800	0.03628100	H	-1.88507100	0.57438300	-2.01078200
H	1.66528000	2.39074000	-0.01031000	C	-0.78912700	1.31315100	1.62216900
H	2.60478600	-1.79507800	0.07532700	H	-0.51443300	-0.80564200	1.82771400

C	-1.15471500	2.36171300	0.77862900	C	0.30350900	2.70443400	0.98277000
H	-1.84263200	2.89502600	-1.19483800	H	0.54486400	0.99808400	2.26240800
H	-0.49604200	1.51573200	2.64848200	C	0.88658000	2.37179600	-1.33430300
H	-1.14751700	3.38505500	1.14325200	H	1.63505800	0.41403800	-1.84675000
C	-4.62687900	0.07830400	-0.00087800	C	0.42458000	3.20346000	-0.31257500
O	-4.84013000	0.26220300	-1.13215900	H	-0.01543800	3.35572000	1.79180000
Si	-1.28473700	-2.08031900	-0.77656900	H	1.01382400	2.76617600	-2.33795400
H	-0.82755400	-3.02352100	0.25920500	H	0.19113500	4.24387400	-0.51970000
O	-4.43639600	-0.10309600	1.13307900	C	4.08707000	-0.73198700	0.14066600
H	-2.72655200	-2.35188400	-1.07076400	O	5.24886200	-0.48087600	0.44582600
H	-0.56081300	-2.21510400	-2.06249100	Si	1.30265500	-1.29496900	0.64474900
C	2.01940200	-1.45208800	0.77185300	H	1.76796800	-2.41215200	-0.16719800
O	1.78761200	-1.94127500	1.88310200	O	3.46806400	-0.76544100	-0.94710300
O	1.73702900	-1.84826700	-0.38307300	H	3.41471700	-0.99293800	1.06667500
C	2.77277600	-0.08473200	0.90733700	H	1.40414000	-1.45764300	2.11199600
H	2.14375500	0.59346200	1.48843100	C	-1.18341900	-1.67902300	-0.48143800
H	3.71176700	-0.24585700	1.44229600	O	-0.74040800	-1.73436400	-1.61020200
C	1.87753800	0.97640100	-1.14232400	O	-0.51860400	-1.66000800	0.63623300
H	1.39128900	0.03508200	-1.39218800	C	-2.70188200	-1.55667800	-0.27574800
H	1.22606300	1.57490000	-0.50375700	H	-3.19691700	-1.79763900	-1.21645900
H	2.15788300	1.53899700	-2.03496300	H	-3.05459800	-2.21283400	0.52249400
C	3.82750900	1.91187000	-0.02981400	C	-2.42630100	0.84713800	-0.81386200
H	4.73340300	1.67639400	0.53025500	H	-1.35957000	0.86770700	-0.59097700
H	4.08649400	2.44207800	-0.94826000	H	-2.57910200	0.54134000	-1.84880900
H	3.16660800	2.52864300	0.58027100	H	-2.85868400	1.83057400	-0.63066400
C	4.01952300	-0.20448400	-1.22152900	C	-4.58846200	-0.02733400	-0.08667500
H	4.26910500	0.34580600	-2.13054300	H	-5.07913400	-0.80263600	0.50298400
H	4.92595100	-0.42155300	-0.65391300	H	-4.90888100	0.95782300	0.25412100
H	3.47794400	-1.12472800	-1.44279200	H	-4.83057400	-0.15240000	-1.14228600
N	3.12394500	0.64680500	-0.37783000	C	-2.76188900	0.16327400	1.51637600
TS ₁₋₂				H	-3.00142600	1.20924100	1.70886000
C	1.08131200	0.52171900	0.22422100	H	-3.34812300	-0.49016100	2.16348600
C	0.62681100	1.37176600	1.24292000	H	-1.69943100	-0.01725400	1.66210600
C	1.22283400	1.04591400	-1.06836300	N	-3.10925400	-0.14296000	0.08934600

II

C	-1.07933000	0.56055100	0.20429500
C	-0.89104300	1.30850400	-0.96771700
C	-0.84201300	1.19762800	1.43035900
C	-0.47537500	2.63937000	-0.92374500
H	-1.07881000	0.84770200	-1.93602800
C	-0.42838000	2.52925700	1.48293600
H	-0.96926900	0.64486300	2.35636100
C	-0.24104600	3.25355000	0.30604600
H	-0.35071600	3.19958200	-1.84647500
H	-0.25840300	3.00315700	2.44535500
H	0.06907000	4.29371300	0.34801300
C	-4.19327900	-0.72943000	-0.78502100
O	-5.36067500	-0.42701700	-0.68772100
Si	-1.63602000	-1.24237800	0.10968900
H	-1.56262200	-2.06799200	1.32030400
O	-3.39079600	-0.96824400	0.22908700
H	-3.71222500	-0.84039300	-1.77903200
H	-1.62131900	-1.79579500	-1.26701700
C	1.32156700	-1.55693200	0.80666100
O	1.16906400	-1.42668200	2.01664200
O	0.45189800	-1.67898700	-0.11784500
C	2.77827900	-1.52294600	0.27156800
H	3.47263000	-1.54256100	1.11234500
H	2.97348200	-2.35575300	-0.40785500
C	2.59249700	0.93872500	0.28657300
H	1.50514000	0.92122400	0.34231500
H	3.01016900	0.87854900	1.29157600
H	2.92328100	1.84540800	-0.22034800
C	4.53754600	-0.14319200	-0.71098100
H	4.89038300	-1.04496500	-1.21261000
H	4.74790900	0.73202300	-1.32745200
H	5.02816800	-0.04149000	0.25743200
C	2.37961700	-0.26257700	-1.83529400

H	2.54871600	0.70130400	-2.31689400
H	2.80648800	-1.06926100	-2.43266300
H	1.31932200	-0.44636400	-1.66986600
N	3.06467300	-0.24818100	-0.50121200

III

Si	2.91111400	-2.41302400	-0.96465800
C	-2.43297100	0.07176800	-0.04602100
C	-2.27058700	-0.20559100	1.31788800
C	-3.03595700	1.28901000	-0.39766500
C	-2.66040900	0.71430400	2.29261600
H	-1.82817700	-1.15104900	1.61635000
C	-3.43919100	2.20624400	0.56964100
H	-3.18019400	1.52838900	-1.44872600
C	-3.24060000	1.92494400	1.92212000
H	-2.51521800	0.48088400	3.34380500
H	-3.91394200	3.13731200	0.27173900
H	-3.55190900	2.63827400	2.67987000
C	-2.51105200	-3.41247400	-0.11702200
O	-1.65349000	-3.30116800	0.74474200
Si	-1.77803700	-1.08601500	-1.38948200
H	-0.47390900	-1.73865800	-1.20894600
O	-2.78817700	-2.54735600	-1.05508100
H	-3.15758100	-4.30301400	-0.17072400
H	-2.35594700	-0.85663500	-2.72236600
H	3.71611700	-3.58565100	-0.51917200
C	2.49811500	-1.40503800	0.57878200
H	1.68576800	-2.89950600	-1.62642300
C	3.44025800	-0.51272700	1.11771600
C	3.22357300	0.12088000	2.34153100
C	1.31175400	-1.62180600	1.29672100
C	2.04862100	-0.12748900	3.05235700
C	1.09299300	-0.99204900	2.52289700
H	3.76942200	-1.60166400	-1.86052100
H	4.37397600	-0.32967200	0.58850100

H	3.97702000	0.78991400	2.74870000	H	8.04086700	-1.00854400	0.58417900
H	1.88088000	0.35051200	4.01308000	H	7.65493300	0.69759600	2.34881500
H	0.17309200	-1.18622200	3.06536400	C	1.78463700	0.75312000	-1.43144700
H	0.54673700	-2.29443600	0.91463500	O	1.78652100	0.57150600	-0.15185200
C	0.72055500	0.52544000	-2.11206500	Si	3.30555600	-1.20758800	-0.96706400
O	1.30838000	-0.32847500	-2.76544200	H	2.36895100	-2.06241000	-0.19153400
O	-0.51582500	0.62750000	-1.83314400	O	2.59225700	-0.18133100	-2.11054300
C	1.65875700	1.62126700	-1.54518000	H	1.98308900	1.76844700	-1.82308700
H	2.45765200	1.11396300	-0.99947900	H	4.02722500	-2.14456100	-1.88215400
H	2.09845900	2.17411300	-2.37903100	H	0.67457400	0.57157600	-1.95286200
C	0.48279600	1.96992500	0.60952400	C	-1.48099000	1.21648000	-0.74602200
H	-0.35163300	1.35292300	0.28942500	H	0.15484400	-1.20011900	-0.88732400
H	1.25619300	1.35592900	1.06876600	C	-2.53385500	1.93239900	-1.33845200
H	0.14365300	2.73976700	1.30425300	C	-3.09336700	3.04261700	-0.70541800
C	2.17417300	3.53954800	-0.14769800	C	-0.98386500	1.66229900	0.49123800
H	2.62757900	4.01683600	-1.01746400	C	-2.60819900	3.45604600	0.53458900
H	1.76685600	4.29724400	0.52345700	C	-1.54805500	2.76858000	1.12607200
H	2.91712100	2.93997900	0.37998600	H	-1.14402200	-0.46863600	-3.00218700
C	0.01541300	3.45696900	-1.27996200	H	-2.93497800	1.61140100	-2.29552200
H	-0.36848600	4.19067100	-0.56967700	H	-3.90351600	3.58543700	-1.18353100
H	0.46537000	3.95919300	-2.13813700	H	-3.03879900	4.32374700	1.02634500
H	-0.77084200	2.77513300	-1.59998200	H	-1.14142500	3.10858000	2.07430200
N	1.06918600	2.64418100	-0.59642900	H	-0.11247200	1.16800600	0.91405200
TS ₃₋₄				C	-3.47963500	-1.34002900	-1.01427300
Si	-0.83586100	-0.35137200	-1.56139100	O	-4.11339700	-0.80023500	-1.90011500
C	4.68822600	-0.51512900	0.11309700	O	-2.19738200	-1.44981600	-0.88394100
C	4.49326000	0.45100200	1.11306000	C	-4.23429100	-1.99087100	0.16129800
C	5.98437300	-1.02569500	-0.05737700	H	-5.30260000	-1.97558500	-0.05579400
C	5.55128000	0.88254000	1.91038400	H	-3.89241300	-3.01591400	0.32030200
H	3.49899900	0.86849800	1.23843600	C	-4.31671900	0.21571100	1.27147500
C	7.04677700	-0.59839900	0.73906500	H	-3.54961700	0.64373300	0.62648500
H	6.17126700	-1.76852900	-0.82960900	H	-5.29607500	0.32816800	0.80598100
C	6.83059600	0.35833500	1.72750700	H	-4.29182600	0.70611900	2.24451800
H	5.37866400	1.63466500	2.67563700	C	-5.01760800	-1.80154900	2.45609100

H	-4.84877100	-2.87398000	2.55959200	C	-3.06707300	-0.51960200	3.11621100
H	-4.86695000	-1.30815700	3.41680400	C	-1.81588600	0.06541200	2.92142300
H	-6.03095500	-1.61611000	2.09898500	H	-3.56200700	2.05383500	-1.48407400
C	-2.65339700	-1.42332800	2.01795200	H	-4.60056000	0.51261300	0.27143500
H	-2.59536100	-0.88457800	2.96403600	H	-5.04624600	-0.80056200	2.31160100
H	-2.47215200	-2.48735600	2.17159500	H	-3.26348700	-1.09847400	4.01405900
H	-1.93381900	-1.02818300	1.30664700	H	-1.03558800	-0.05780500	3.66685300
N	-4.04176900	-1.24766400	1.46911900	H	-0.57869300	1.24568900	1.59615900
IV				C	-1.91621200	-0.50637500	-2.09474800
Si	-2.24765300	1.84343400	-0.83440500	O	-3.09230500	-0.79202200	-2.16864900
C	3.07069400	0.32541400	0.10493700	O	-1.40868700	0.66521800	-1.79617100
C	2.66166500	0.17816100	1.43876700	C	-0.83594000	-1.56737100	-2.30693900
C	4.05076500	-0.56323000	-0.36273000	H	-1.23056300	-2.33489700	-2.97350500
C	3.18534100	-0.81894000	2.26206600	H	0.07626500	-1.11785500	-2.70640800
H	1.90000800	0.85050800	1.82432600	C	-1.66830600	-2.57056000	-0.17759100
C	4.56201200	-1.58353500	0.44015500	H	-2.08510300	-1.64967000	0.23112700
H	4.41970500	-0.45137100	-1.38118100	H	-2.41138900	-3.06904300	-0.79997400
C	4.12747900	-1.71586100	1.75930100	H	-1.34732400	-3.21806700	0.63837000
H	2.85915500	-0.89884500	3.29623900	C	0.25224300	-3.51504500	-1.34830000
H	5.31325100	-2.26323700	0.04603500	H	1.06882700	-3.28356400	-2.03265700
H	4.53419500	-2.49758500	2.39494000	H	0.65696600	-3.94427100	-0.43145300
C	1.08989900	3.14916300	0.17231400	H	-0.44956700	-4.20836000	-1.81395300
O	0.67660900	1.84156300	-0.04295100	C	0.47601800	-1.37895600	-0.21088700
Si	2.28309000	1.58383500	-1.10688800	H	0.61857100	-1.83570700	0.76864500
H	1.45557100	0.77009500	-2.09092700	H	1.42556300	-1.32883900	-0.73884300
O	2.22798200	3.24651800	-0.65061000	H	0.07263800	-0.37052900	-0.11508200
H	1.36212000	3.33768000	1.22876800	N	-0.46155000	-2.24736700	-1.00646500
H	3.47865800	1.77094100	-2.02362700	TS ₄₋₅			
H	0.32984500	3.89231700	-0.13126000	Si	2.04901900	-1.77733000	-0.97385000
C	-2.55913700	0.98922100	0.80004200	C	-3.01115500	-0.35802700	0.08064200
H	-1.45613700	3.07246800	-0.86736600	C	-2.60155900	-0.29579400	1.42035700
C	-3.81597400	0.39964000	1.01504600	C	-3.99058900	0.55909800	-0.33011900
C	-4.06936900	-0.35078400	2.16238600	C	-3.12224000	0.64953200	2.30454400
C	-1.56134200	0.81360200	1.77390700	H	-1.84479300	-0.99288400	1.76862700

C	-4.49897500	1.52835700	0.53500400	H	2.05455900	1.56447200	0.33105900
H	-4.36215900	0.51250300	-1.35262800	H	2.44603400	3.07268700	-0.53782900
C	-4.06250700	1.57799000	1.85916400	H	1.38230200	3.10726200	0.90910500
H	-2.79483400	0.66294600	3.34116500	C	-0.18739200	3.69071400	-1.04423400
H	-5.24947200	2.23204400	0.18437000	H	-1.00979100	3.57095200	-1.75005500
H	-4.46644000	2.31966700	2.54267100	H	-0.57577600	4.04339200	-0.08833700
C	-0.96825900	-3.10021800	0.03962700	H	0.54840400	4.39464500	-1.43563900
O	-0.53040800	-1.80960300	-0.20522100	C	-0.51397000	1.45704000	-0.13836200
Si	-2.25572900	-1.54997100	-1.20951700	H	-0.66626600	1.83162800	0.87397400
H	-1.46655400	-0.70397600	-2.18387600	H	-1.45333300	1.48051100	-0.68726300
O	-2.13228600	-3.19709700	-0.74903500	H	-0.13687000	0.43426300	-0.11969700
H	-1.21814600	-3.26839900	1.10574000	N	0.46456000	2.36309800	-0.83527100
H	-3.47723400	-1.75388200	-2.08079600	V_A			
H	-0.23587400	-3.86768700	-0.26943200	Si	-1.62881500	-2.31388300	0.30024500
C	2.43341000	-1.07490600	0.72553300	C	3.07421000	-0.67220900	0.10210700
H	1.37282600	-3.05513100	-1.19624200	C	3.52348000	-0.72849200	-1.22584500
C	3.72737100	-0.56118500	0.91968400	C	3.25970700	0.52284600	0.81276500
C	4.07234900	0.10128700	2.09757700	C	4.11433900	0.37602500	-1.83710600
C	1.49717400	-0.91413100	1.76030200	H	3.41730300	-1.65043300	-1.79262700
C	3.12656600	0.25710300	3.10888800	C	3.86873800	1.62468400	0.21107700
C	1.84096600	-0.25634200	2.93908900	H	2.89529800	0.61087800	1.83471100
H	3.38044900	-1.87925900	-1.62768300	C	4.28871000	1.55748800	-1.11693000
H	4.47061900	-0.66198700	0.13336200	H	4.45113800	0.31082300	-2.86760500
H	5.07682000	0.49384300	2.22423900	H	4.01644300	2.53697700	0.78300700
H	3.39212200	0.76935300	4.02917500	H	4.76221000	2.41608600	-1.58462100
H	1.10183600	-0.14628700	3.72744900	C	0.63078000	-2.72685000	-1.16647900
H	0.49018400	-1.28757300	1.60456800	O	-0.31320500	-1.84061300	-0.64143400
C	1.84792400	0.67518900	-2.08343000	Si	2.27296400	-2.15590500	0.93512600
O	3.03410800	0.90861200	-2.17215900	H	1.31304000	-1.68438100	1.95101000
O	1.27473700	-0.47777500	-1.84122500	O	1.56117400	-3.15505800	-0.21650500
C	0.82371700	1.80679000	-2.19753100	H	1.13704900	-2.18981000	-1.97936000
H	1.26593800	2.61986800	-2.77388600	H	3.30116700	-3.03299300	1.54063600
H	-0.10296200	1.45066400	-2.65268000	H	0.14714300	-3.62833100	-1.56433400
C	1.67903900	2.54146500	0.02588200	C	-3.00607100	-1.10151700	-0.06003400

H	-1.99562900	-3.65970600	-0.23342900	C	1.49060500	-1.47796900	0.08952100
C	-3.71620600	-0.47910500	0.97455900	C	1.77225800	-0.70787600	1.22827300
C	-4.73567900	0.43028300	0.69780500	C	2.28834000	-1.28732800	-1.04819100
C	-3.34567800	-0.78417700	-1.38247400	C	2.81068800	0.21870700	1.23088400
C	-5.05578800	0.73930300	-0.62363500	H	1.18213600	-0.83520700	2.13305400
C	-4.35823400	0.13064000	-1.66627900	C	3.33554800	-0.36842000	-1.04815900
H	-1.34637700	-2.42099700	1.74155300	H	2.09654200	-1.86839200	-1.94723600
H	-3.44326600	-0.67759100	2.00683300	C	3.59819700	0.38424900	0.09356600
H	-5.27228200	0.90516200	1.51375200	H	3.00771100	0.80837100	2.12074600
H	-5.84851300	1.44947500	-0.84067100	H	3.94614500	-0.24224800	-1.93718600
H	-4.60765500	0.36196000	-2.69802500	H	4.41255700	1.10257600	0.09683900
H	-2.80867700	-1.25135300	-2.20496500	O	-1.39897100	-2.08485800	-0.07631300
C	0.11443900	1.10863800	1.92955600	H	0.16657100	-3.51659300	1.35770300
O	0.83385000	1.12624800	2.93789400	C	-2.08255900	-1.43654900	0.97030200
O	-0.71740700	0.26625900	1.52698400	H	-1.39259000	-0.76988700	1.51457700
C	0.31907100	2.40019700	1.06665300	H	-2.50301500	-2.17899400	1.65840700
H	-0.10851600	3.25089000	1.60413400	O	-3.13918700	-0.70206500	0.44985400
H	1.38890800	2.56597500	0.93814800	Si	-2.88577900	0.40077900	-0.79271400
C	-1.77655600	2.34457300	-0.24715200	H	-2.67473900	-0.25333500	-2.10481100
H	-2.02925300	1.42516900	0.27874800	H	-4.13609900	1.19199200	-0.80763300
H	-2.13693000	3.21437300	0.30485300	C	-1.39184800	1.45615200	-0.39992700
H	-2.18482500	2.34270500	-1.25882400	C	-1.35566500	2.23912600	0.76435700
C	0.11040200	3.69288400	-0.98957100	C	-0.27318900	1.47559000	-1.24369100
H	1.19722900	3.72464800	-1.07848500	C	-0.24270200	3.01719100	1.07288200
H	-0.34443500	3.73418400	-1.98098100	H	-2.20698900	2.24262700	1.44180000
H	-0.23700400	4.53380000	-0.38775100	C	0.83851600	2.25951800	-0.94546100
C	0.24076700	1.27182700	-1.13377900	H	-0.26474500	0.86511100	-2.14335700
H	-0.18749300	1.33882200	-2.13583200	C	0.85468100	3.03013200	0.21362900
H	1.32846900	1.35222900	-1.17911400	H	-0.23261200	3.61543300	1.97919700
H	-0.05165100	0.33950300	-0.65194700	H	1.69742400	2.25433400	-1.60857100
N	-0.28412300	2.42029400	-0.32585000	H	1.72487600	3.63462200	0.45186800
V_B				TS' ₅₋₆			
Si	0.12394100	-2.75324300	0.08068800	Si	-1.03611100	2.45016100	-0.04669600
H	0.29061300	-3.63566200	-1.09327300	H	-1.20096500	3.29731100	1.15230100

C	0.72447400	1.87678100	-0.21896000	C	1.35558700	-1.50593900	0.40735800
C	1.11151500	1.09801800	-1.32030600	C	1.50935500	-0.55826200	1.43002300
C	1.67756000	2.15234200	0.77006900	C	2.37472800	-1.61979100	-0.54931300
C	2.40684600	0.60550700	-1.42911600	C	2.63824900	0.25261000	1.49286400
H	0.39070800	0.85494900	-2.09765200	H	0.73302900	-0.44038000	2.18248500
C	2.97972900	1.66800700	0.66113000	C	3.50622200	-0.80843400	-0.49330400
H	1.40111400	2.74090200	1.64156700	H	2.28756400	-2.35015700	-1.35064800
C	3.34274800	0.89280100	-0.43702000	C	3.63657700	0.12964700	0.52821800
H	2.68379800	-0.01104200	-2.27806000	H	2.73352900	0.98853500	2.28495300
H	3.70724200	1.88974600	1.43578200	H	4.28454500	-0.90847800	-1.24368800
H	4.35335600	0.50436500	-0.51804900	H	4.51623500	0.76478300	0.57344700
O	-2.08027300	1.10286400	0.07446400	O	-1.38183100	-1.66383300	-0.57244500
H	-1.52677200	3.13045900	-1.26800800	H	-0.77062600	-2.80341800	1.59231700
C	-2.86875800	0.21373800	-1.19019800	C	-3.27802800	-0.88133400	1.41646300
H	-2.05437200	0.21685700	-1.93573500	H	-2.30988400	-0.50105800	1.79556300
H	-3.69529100	0.89560300	-1.43463100	H	-3.44510200	-1.96977200	1.50447500
O	-3.10557300	-0.84747000	-0.52462300	O	-4.10553900	-0.14235400	0.94124500
Si	-1.88576500	-0.33751100	1.13614000	Si	-1.41058700	-0.40442400	-1.67207400
H	-1.16723000	0.48784200	2.17629000	H	-0.53830900	-0.75413700	-2.82402300
H	-3.04429200	-0.84439300	1.89408800	H	-2.81882700	-0.25690900	-2.09374800
C	-0.50088000	-1.48462100	0.59462400	C	-0.75729200	1.16439000	-0.89730800
C	-0.63088500	-2.44998200	-0.41504600	C	-1.54249800	1.92812200	-0.01822700
C	0.74530100	-1.35840300	1.22741400	C	0.55695400	1.58236700	-1.14914800
C	0.44760700	-3.25249300	-0.78148900	C	-1.02251200	3.06614400	0.59468500
H	-1.58793900	-2.56290500	-0.91394100	H	-2.56990200	1.63607800	0.19031800
C	1.82488000	-2.16038900	0.86737900	C	1.07803800	2.72134800	-0.54123500
H	0.88078200	-0.60834800	2.00201700	H	1.19277000	1.00113300	-1.81261500
C	1.67769400	-3.10885000	-0.14169400	C	0.28841400	3.46329900	0.33391100
H	0.32688800	-3.99529900	-1.56470200	H	-1.64343800	3.64763000	1.26956500
H	2.78143700	-2.03599800	1.36593000	H	2.10195400	3.02122800	-0.74197700
H	2.51759000	-3.73504300	-0.42886100	H	0.69217000	4.35169100	0.81060400
VI'				VII'			
Si	-0.21027100	-2.51093900	0.24821300	N	-0.96117400	0.60603200	-0.89241100
H	0.08251200	-3.76719100	-0.48330400	H	-1.12579200	0.36626200	-1.85827300

C	-2.26268100	-1.30551100	0.58871200	H	0.34523600	2.05732300	0.75262500
H	-1.52010200	-0.90595800	1.30443200	C	2.22003900	-1.09998900	-0.48124000
H	-1.86463900	-1.99433500	-0.17995100	H	0.28009300	-2.03926900	-0.51916200
O	-3.43868700	-1.03915600	0.66582700	C	2.93299400	0.06713600	-0.20998200
C	-1.68899700	1.76756600	-0.42550700	H	2.81081800	2.11601200	0.44179000
H	-1.14390700	2.70875100	-0.58564500	H	2.73765900	-1.98524200	-0.83609500
H	-2.64294500	1.81367400	-0.95240300	H	4.00844500	0.09186700	-0.35215200
H	-1.91628500	1.67143500	0.64104000	VIII'			
C	0.32499600	0.32041400	-0.44531000	N	-1.17831300	0.33103600	-0.03804700
C	1.07670300	-0.66868300	-1.10341600	H	-3.17051300	-0.06696700	-1.44967600
C	0.87585100	0.94214500	0.68419300	C	-2.02839600	-0.83927800	-0.10455000
C	2.33840600	-1.01991500	-0.64482300	H	-2.21998600	-1.29127900	0.88127100
H	0.65983600	-1.16148700	-1.97857400	H	-1.53247800	-1.57835300	-0.74486600
C	2.14288300	0.57563200	1.13679500	O	-3.30050400	-0.50560600	-0.60175600
H	0.32439800	1.71374000	1.21007500	C	-1.64988200	1.32150400	0.92893700
C	2.88373500	-0.40268500	0.48227200	H	-1.12719400	2.26873900	0.78928200
H	2.90094400	-1.78479100	-1.17170000	H	-2.71635700	1.48925200	0.77094600
H	2.55143900	1.06961500	2.01326700	H	-1.49122500	0.98426400	1.96625900
H	3.86939200	-0.67965600	0.84049500	C	0.22232700	0.11031700	-0.03008300
TS' ₇₋₈				C	1.07293300	1.15892500	-0.41009600
N	-1.25541900	-0.00541200	0.32273800	C	0.79433700	-1.11368900	0.33717200
H	-1.87631300	0.99806100	0.15968800	C	2.45039500	0.98646800	-0.42324800
C	-2.14985400	-0.20729900	-0.95033200	H	0.63937600	2.10512200	-0.71891200
H	-2.72499000	-1.14277900	-0.81829200	C	2.17830600	-1.28758200	0.30140500
H	-1.45958800	-0.31466400	-1.80615000	H	0.16830100	-1.93640700	0.66648300
O	-2.82680700	0.95063400	-0.84919100	C	3.01372200	-0.24185300	-0.07330600
C	-1.70490100	-0.76382200	1.50336000	H	3.08925000	1.81042900	-0.72649500
H	-1.22416000	-0.36028500	2.39644100	H	2.60070500	-2.24719000	0.58372100
H	-2.78760400	-0.64726900	1.58572500	H	4.08989500	-0.37888400	-0.09501900
H	-1.45096800	-1.82264100	1.40328300	IM2			
C	0.17610400	0.00685900	0.14430200	N	-2.96095000	0.16930500	-0.73317800
C	0.88050500	1.17549000	0.41499200	C	-1.88495300	-0.78112500	-1.16977700
C	0.84035300	-1.13418800	-0.30310000	H	-0.93852600	-0.24769500	-1.15959700
C	2.26205300	1.20276200	0.23644300	H	-2.12827200	-1.14325000	-2.16981700

H	-1.83620600	-1.61111500	-0.46281800	TS _{IM}			
C	-2.95945100	1.37191200	-1.62586400	N	-2.62386000	-0.18793000	-0.70485600
H	-1.99136200	1.86023700	-1.51688300	C	-1.37338500	-0.66916300	-1.38793600
H	-3.76284700	2.03905600	-1.30936700	H	-0.53355900	-0.06034600	-1.06184200
H	-3.12764500	1.04193900	-2.65216900	H	-1.51242800	-0.55909000	-2.46387500
C	-4.28151400	-0.51524200	-0.83362500	H	-1.20533200	-1.71598200	-1.13046700
H	-5.06485200	0.16645600	-0.50030300	C	-2.72662700	1.30385400	-0.86349600
H	-4.27027800	-1.40368800	-0.20124500	H	-1.83389500	1.76510200	-0.44416100
H	-4.45660800	-0.80200600	-1.87175800	H	-3.62845900	1.64322300	-0.35147600
C	-2.74888900	0.58524200	0.70991900	H	-2.79533400	1.51996800	-1.93030200
H	-2.78689400	-0.32890200	1.30681800	C	-3.80821600	-0.82441000	-1.35578600
H	-3.59402300	1.22032100	0.98603600	H	-4.71407400	-0.52067000	-0.82942300
C	-1.42537200	1.32171400	1.06855500	H	-3.69851000	-1.90859900	-1.31349900
O	-0.61698600	1.54684200	0.12019200	H	-3.85839300	-0.49915900	-2.39534300
O	-1.33612600	1.56704000	2.26835800	C	-2.63786800	-0.60722500	0.75020400
Si	1.69962700	1.28557400	0.25979500	H	-2.76572700	-1.69032900	0.77056600
H	1.50382000	1.94293200	-1.04235500	H	-3.51489400	-0.14302200	1.20962300
H	1.51757300	2.02949000	1.51093400	C	-1.39590100	-0.27379400	1.59821900
O	3.47960700	1.25067400	0.31730900	O	-0.75805400	0.76803900	1.17828000
C	4.22702100	0.87445700	-0.69404000	O	-1.18429800	-0.97813300	2.56080200
H	5.29808800	1.02502700	-0.48697600	Si	0.99387200	1.24562200	1.18688500
O	3.83248000	0.41334000	-1.74774800	H	0.81826900	2.66533400	1.57984600
C	1.24798900	-0.54355500	0.36885200	H	1.43225100	0.73471600	2.54049700
C	1.46909300	-1.42676500	-0.69832600	O	2.57525000	2.59620900	-0.19832600
C	0.63281800	-1.04848800	1.52542100	C	1.56465800	2.71620200	-0.90045400
C	1.06608600	-2.76098500	-0.62286500	H	1.55684800	3.40435700	-1.76324600
H	1.97081700	-1.06653500	-1.59208000	O	0.48420000	2.06422100	-0.67111700
C	0.23282200	-2.38155900	1.60613900	C	1.68087800	-0.29978000	0.25286400
H	0.44693500	-0.38736200	2.36784100	C	2.06646400	-0.41566300	-1.09170000
C	0.44381400	-3.24173600	0.52801200	C	1.68309000	-1.48054400	1.01252600
H	1.25317200	-3.42895400	-1.45913600	C	2.40560100	-1.64374000	-1.65602400
H	-0.23241700	-2.75181400	2.51559900	H	2.10693700	0.46523100	-1.72157000
H	0.14280800	-4.28369000	0.59309300	C	2.00113900	-2.71963000	0.45409300
				H	1.41935000	-1.43224500	2.06604400

C	2.36154500	-2.80691800	-0.88748100	C	3.07668800	-1.02207100	-1.48826400
H	2.71210500	-1.69215200	-2.69768100	H	2.64925100	1.01947700	-0.96889700
H	1.97973700	-3.61197900	1.07367900	C	2.18519500	-2.70316000	-0.00991900
H	2.62285300	-3.76538900	-1.32704800	H	1.09282800	-1.97045500	1.68917600
IM3				C	2.90663500	-2.36530300	-1.15311000
N	-2.53786400	-0.24201400	-0.90205000	H	3.65992900	-0.75063500	-2.36388200
C	-1.19703300	-0.61101100	-1.47729500	H	2.06330100	-3.74581300	0.27044500
H	-0.42690400	-0.00631200	-1.00190400	H	3.34797800	-3.14269200	-1.77062300
H	-1.21990300	-0.40112600	-2.54726400	IX			
H	-1.01571800	-1.67256500	-1.30312100	N	-3.65939600	-0.27998400	-0.55361100
C	-2.68025700	1.25542900	-0.90626700	H	-2.41991300	-1.86398800	-3.01042700
H	-1.84018500	1.68766000	-0.35896400	C	-4.02124100	-1.21913000	0.49654500
H	-3.63827800	1.50986400	-0.45012300	H	-4.97634600	-0.95736100	0.96705700
H	-2.65992500	1.58599500	-1.94590700	H	-4.11351200	-2.21559900	0.06289300
C	-3.61090900	-0.83212900	-1.75820700	H	-3.24425400	-1.26399600	1.26597900
H	-4.58310100	-0.62071700	-1.31110600	C	-3.18585700	0.99116700	-0.21139200
H	-3.46009700	-1.90985500	-1.83036600	C	-3.39835600	1.49565000	1.08146800
H	-3.55528300	-0.38527900	-2.75103100	C	-2.47002300	1.78649900	-1.12128100
C	-2.71138300	-0.82288500	0.48478800	C	-2.90072500	2.74084700	1.44884100
H	-2.80526400	-1.90353400	0.36999200	H	-3.95243500	0.91614600	1.80985900
H	-3.65231500	-0.43115400	0.88132400	C	-1.98268400	3.03300100	-0.74314600
C	-1.59506200	-0.56434400	1.51635800	H	-2.26072000	1.42909600	-2.12267500
O	-0.95464200	0.54213400	1.29860300	C	-2.18393400	3.52126100	0.54536600
O	-1.47315000	-1.38021400	2.40234500	H	-3.08493400	3.10506100	2.45504700
Si	0.82470800	0.89588700	1.52906400	H	-1.42844800	3.62185000	-1.46764500
H	1.32092700	2.19524900	2.03672000	H	-1.79964500	4.49315400	0.83529700
H	0.85669400	0.11067300	2.81561100	C	-3.62208900	-0.74790100	-1.87769000
O	2.16969900	3.19273200	-0.40868300	H	-3.76437100	0.07426900	-2.58356000
C	0.97712000	2.98241100	-0.56589500	H	-4.41107000	-1.49062500	-2.02888900
H	0.36632800	3.67362600	-1.18382300	O	-2.34999100	-1.40064000	-2.16804200
O	0.28167500	1.99340300	-0.09249900	Si	0.03510900	-1.09571400	-1.56300000
C	1.76430900	-0.34157800	0.44605200	H	-0.22399000	0.18749100	-2.22231700
C	2.50471200	-0.02293800	-0.70230400	H	-0.02956300	-2.32047500	-2.37301300
C	1.63502200	-1.69828400	0.78623900	C	-0.42110100	-1.29176000	0.22876700

C	-0.46082100	-0.19147900	1.09750900	H	-4.21938100	-1.23505900	-0.26928000
C	-0.63698400	-2.57345500	0.75778600	H	-3.42859000	-0.29167100	1.01690000
C	-0.70320700	-0.37151000	2.45792300	C	-2.55159300	1.70411000	-0.47516900
H	-0.32273700	0.81426000	0.71065200	C	-3.28931900	2.67753100	0.19445400
C	-0.87474000	-2.75457300	2.11797000	C	-1.19220400	1.85536400	-0.72123000
H	-0.62662400	-3.44106100	0.10247400	C	-2.64577900	3.83811800	0.60905800
C	-0.90306400	-1.65136400	2.97088600	H	-4.35043900	2.54819300	0.37756400
H	-0.75279700	0.49330600	3.11220800	C	-0.56133000	3.01960900	-0.29299100
H	-1.04230200	-3.75189500	2.51221000	H	-0.61026800	1.06892100	-1.19079100
H	-1.09274200	-1.79014900	4.03073200	C	-1.28341200	4.01031300	0.36606800
C	3.95659500	-0.52861700	-0.69062100	H	-3.21173600	4.60914400	1.12020900
H	4.43512200	-0.63170100	-1.66801800	H	0.50353500	3.12604800	-0.46562100
H	3.97255900	-1.50499700	-0.20170800	H	-0.78754700	4.91620400	0.69815700
C	2.49594300	-0.11093000	-0.88851000	C	-3.11540800	0.05528600	-2.10517100
O	1.84022600	-1.07748000	-1.45406800	H	-2.51954100	0.61195200	-2.81989200
O	2.05962100	0.97088800	-0.54482900	H	-3.61123100	-0.86125100	-2.38888200
N	4.79243000	0.41040300	0.13841400	O	-1.83263400	-2.23964700	-2.16783700
C	6.15332900	-0.20097300	0.28566500	Si	-0.27571300	-1.94767900	-1.40417600
H	6.59332900	-0.33989600	-0.70224100	H	0.05308300	-0.67725100	-2.10048500
H	6.77722500	0.46898200	0.87746200	H	0.40976200	-3.18984000	-1.81656900
H	6.06085400	-1.16269100	0.79078800	C	-0.94034600	-1.80858600	0.36047200
C	4.19209500	0.58801700	1.50607700	C	-0.58977400	-0.77960300	1.24642400
H	3.22469600	1.07440800	1.40327700	C	-1.85437200	-2.77267900	0.81348800
H	4.07611300	-0.39454200	1.96509600	C	-1.14329100	-0.70341400	2.52424200
H	4.87049300	1.19966500	2.10099800	H	0.12020600	-0.02015900	0.93311200
C	4.93356400	1.74760500	-0.53410500	C	-2.38755500	-2.72206900	2.10105300
H	5.57964400	2.37300900	0.08231500	H	-2.15965700	-3.57375200	0.14564800
H	5.38834700	1.59635200	-1.51376700	C	-2.03897000	-1.67986400	2.95895100
H	3.94620700	2.19273000	-0.63454300	H	-0.86720700	0.11306000	3.18552400
TS ₉₋₁₅				H	-3.07726200	-3.49224100	2.43322300
N	-3.22565400	0.49609900	-0.90691700	H	-2.45927200	-1.63116400	3.95889100
H	-1.79848900	-2.85492000	-2.90402200	C	3.84423900	-0.83679600	-0.19188900
C	-4.01726700	-0.23180200	0.10088900	H	4.26975300	-1.27999000	-1.09535000
H	-4.94983300	0.30449500	0.28385000	H	3.92305700	-1.56739900	0.61560300

C	2.34339100	-0.54634500	-0.44320100	C	-2.08568100	0.14520000	-2.43615300
O	1.72212300	-1.62775300	-0.60075700	H	-1.39630600	0.84276300	-2.89844400
O	1.92268500	0.62122500	-0.46509700	H	-2.26485500	-0.84581700	-2.84796500
N	4.71638200	0.34063000	0.18115300	O	-1.66507800	-2.69740600	-2.01228400
C	6.10198700	-0.16446000	0.42996200	Si	-0.22661100	-2.25055500	-1.12173100
H	6.47540900	-0.64396000	-0.47520400	H	0.04568100	-1.00397800	-1.89487000
H	6.74436700	0.67615600	0.69543500	H	0.57367200	-3.47300700	-1.33110800
H	6.07866400	-0.88611800	1.24685900	C	-1.01198400	-1.91990300	0.56280100
C	4.20348000	0.99111800	1.43113400	C	-0.75287200	-0.76063700	1.30601200
H	3.20756500	1.37957800	1.22703600	C	-1.98508900	-2.80300000	1.05426600
H	4.16420800	0.23903700	2.22005800	C	-1.46051000	-0.47320700	2.47283000
H	4.88924300	1.79101400	1.71284700	H	0.00115900	-0.06008500	0.96168300
C	4.75658400	1.34327400	-0.93394200	C	-2.67361400	-2.54131600	2.23730100
H	5.41053500	2.16417900	-0.63712600	H	-2.22480400	-3.70564900	0.49808200
H	5.15479500	0.85395800	-1.82364800	C	-2.42229100	-1.36538200	2.94363000
H	3.73940900	1.68801900	-1.11130500	H	-1.25804300	0.44587200	3.01536900
XV				H	-3.41090800	-3.24925800	2.60345800
N	-2.68169700	0.49295600	-1.35509500	H	-2.96603100	-1.15111400	3.85859400
H	-1.71084900	-3.60626200	-2.31375300	C	3.80246100	-0.80199900	0.12222200
C	-3.66936300	-0.39447200	-0.70966200	H	4.24282100	-1.48344900	-0.60892500
H	-4.67069100	-0.01098700	-0.91441800	H	3.85196400	-1.27854700	1.10374000
H	-3.54358800	-1.39872800	-1.11490200	C	2.31163900	-0.58901300	-0.24314900
H	-3.47623400	-0.39890200	0.36354600	O	1.71570400	-1.69367000	-0.25241000
C	-2.36561700	1.74348200	-0.70317400	O	1.87463100	0.55295200	-0.46713100
C	-3.39875100	2.55137700	-0.23677200	N	4.68299000	0.42608600	0.17608400
C	-1.02739100	2.09098700	-0.54172700	C	6.06829600	-0.00738800	0.53810200
C	-3.07891300	3.75208800	0.38777400	H	6.43401400	-0.70293300	-0.21763900
H	-4.43657600	2.26596100	-0.36929700	H	6.71560800	0.86955000	0.57915500
C	-0.72682100	3.29477200	0.08850400	H	6.04629400	-0.49801500	1.51145300
H	-0.22558700	1.42045800	-0.84538500	C	4.18533200	1.38381700	1.21717400
C	-1.74530500	4.12489000	0.54967200	H	3.17897600	1.69055500	0.93844000
H	-3.87360800	4.39795200	0.74433700	H	4.17475200	0.87254800	2.18055600
H	0.31273100	3.56939800	0.23000400	H	4.86410400	2.23669600	1.25576000
H	-1.50375200	5.06092500	1.04179500	C	4.71880100	1.10427200	-1.16140300

H	5.40188100	1.95240500	-1.10243000	H	-0.39312900	1.58090800	-2.92413100
H	5.07822400	0.38804300	-1.90130900	H	0.10624700	3.35538400	0.95689200
H	3.70743000	1.42566500	-1.40311600	H	-0.84969200	3.43554800	-1.33778700
XVIII				O	3.68124700	-1.60604600	-0.79254400
N	-1.68494600	-1.36173300	0.10015300	H	4.51695700	-1.10625800	-0.69898300
C	-1.44490100	-2.09940300	-1.15141400	C	4.86059200	0.55132900	0.90153700
H	-1.61488900	-1.40873100	-1.97834100	H	5.22924300	1.32011100	1.60458900
H	-0.41029600	-2.44911000	-1.15935700	O	3.65824300	0.16590500	1.16205400
H	-2.14465700	-2.93411800	-1.21375400	O	5.59282700	0.15460000	-0.00469200
C	-2.94499800	-0.66483000	0.22956400	TS ₁₈₋₁₉			
C	-4.13295200	-1.38671000	0.16197200	N	1.77026300	-1.67840000	-0.44126700
C	-2.93008800	0.71368600	0.40656100	C	1.68799100	-2.94279000	0.31027300
C	-5.33795100	-0.70355900	0.28958800	H	2.21742700	-2.81967500	1.25330600
H	-4.12201100	-2.46379700	0.03100000	H	0.62857900	-3.13531000	0.50687200
C	-4.14445700	1.38316200	0.53142500	H	2.13718200	-3.74866600	-0.27270200
H	-1.98624700	1.25129300	0.41461100	C	2.86895600	-0.78169700	-0.17315500
C	-5.34428400	0.67863700	0.47387700	C	4.16280300	-1.29353400	-0.11292400
H	-6.27221100	-1.25291100	0.24917700	C	2.60341600	0.56859400	0.02708400
H	-4.14704600	2.45958600	0.66457600	C	5.21639600	-0.42094600	0.13749400
H	-6.28778500	1.20524100	0.56995800	H	4.34975100	-2.35038500	-0.27277500
C	-0.77546700	-1.26654000	1.00058300	C	3.66878400	1.42843800	0.27651500
H	-0.98434800	-0.69189300	1.89644300	H	1.58420200	0.94291100	0.02868300
H	0.17382400	-1.78195000	0.84677100	C	4.97097600	0.93813900	0.33099600
H	1.48382800	-2.12865000	-0.38731200	H	6.22973400	-0.80532400	0.18010900
Si	2.48323800	-1.09332200	0.23889200	H	3.46738600	2.48100300	0.44304400
H	2.18449400	-1.54998100	1.64419900	H	5.79608100	1.61316600	0.53209000
C	1.36003700	0.39641000	-0.22838700	C	0.82877600	-1.34820900	-1.24990900
C	0.79238600	0.46253000	-1.51175600	H	0.89405500	-0.40372600	-1.77873100
C	1.08549100	1.46040500	0.64776000	H	-0.01626800	-2.00861900	-1.41090800
C	0.00641300	1.54185700	-1.91413700	H	-0.90838500	-1.80463800	0.48613700
H	1.00186900	-0.33875400	-2.21834800	Si	-2.19268100	-1.06546100	-0.05092500
C	0.28805500	2.53996500	0.26161300	H	-2.07674600	-1.73784500	-1.40061200
H	1.54377900	1.45708700	1.63282900	C	-1.33067800	0.63933700	-0.02724900
C	-0.24740600	2.58705700	-1.02497700	C	-0.82627000	1.14118300	1.18264700

C	-1.15704100	1.42887300	-1.17480600	H	1.14331000	-3.01010500	2.38458300
C	-0.19338200	2.38274200	1.25207100	H	0.35777500	-2.85752500	0.81417800
H	-0.94979000	0.55409800	2.09015900	Si	-1.73734500	-0.44948900	-0.95892400
C	-0.48421800	2.65123200	-1.12553500	H	-1.34612100	-0.53282600	-2.37078700
H	-1.58107700	1.09139200	-2.11813100	C	-0.86593600	0.89571300	-0.02818600
C	-0.00848600	3.13703300	0.09283500	C	-0.67056800	0.82037100	1.35775900
H	0.16047900	2.76002300	2.20777000	C	-0.40863100	2.03149100	-0.70855400
H	-0.35924100	3.23896700	-2.03094900	C	-0.03948000	1.85366800	2.04308800
H	0.48715400	4.10260100	0.14069800	H	-1.00372500	-0.05599400	1.90550800
O	-3.04648600	-1.57123000	1.28367700	C	0.21976300	3.06942400	-0.02555000
H	-3.95601000	-1.21073000	1.31454600	H	-0.52621300	2.10476200	-1.78704700
C	-4.89608700	0.06095000	-0.39868500	C	0.40431700	2.98017100	1.35164300
H	-5.52829300	0.63161300	-1.10190100	H	0.10380900	1.78171000	3.11715300
O	-3.73460000	-0.22462900	-0.88046700	H	0.57484000	3.93985800	-0.56829100
O	-5.33668200	-0.23684900	0.71169100	H	0.89629400	3.78724200	1.88656200
XIX				O	-1.65701500	-1.93931500	-0.24891700
N	1.79982200	-1.39470600	1.25499700	H	-2.24341300	-2.01578700	0.51488400
C	2.51707400	-0.86674400	2.39542900	C	-4.20827900	-0.12734000	-0.00886400
H	2.26869200	0.18774100	2.55668400	H	-5.20334800	0.29686600	-0.19505300
H	2.21653200	-1.41324100	3.29068500	O	-3.41028100	-0.00007700	-1.05565900
H	3.60985600	-0.95313400	2.28735500	O	-3.89957400	-0.65392800	1.04065700
C	2.02366200	-0.83248800	0.00842400	XX			
C	2.70916500	0.39149300	-0.12960200	N	3.02071700	-0.70145800	1.08954000
C	1.55128800	-1.44908800	-1.16927800	C	3.11336800	0.11756500	2.31108900
C	2.87326400	0.98003800	-1.37679500	H	3.26834400	1.15616500	2.01964800
H	3.09872000	0.90507700	0.74007200	H	2.18225100	0.03058200	2.87062100
C	1.72999800	-0.84711300	-2.41049200	H	3.96200000	-0.22713800	2.90485300
H	1.03481400	-2.39965400	-1.12175400	C	3.89557600	-0.36834700	-0.01191900
C	2.38365900	0.37577700	-2.53233200	C	5.25317400	-0.16648700	0.22060400
H	3.39192300	1.93234700	-1.44071400	C	3.33762600	-0.23535900	-1.28061300
H	1.34627700	-1.34919700	-3.29418800	C	6.07337200	0.15969400	-0.85450500
H	2.51892700	0.84047200	-3.50323300	H	5.67379300	-0.27602800	1.21451100
C	1.31327400	-2.75849300	1.33629400	C	4.17338200	0.09190900	-2.34510100
H	2.02468700	-3.48755200	0.91681100	H	2.26824100	-0.36594600	-1.41894700

C	5.53565900	0.28864300	-2.13446100	H	-4.06721600	-2.81209200	-2.13085500
H	7.13457500	0.31065100	-0.69066500	H	-5.34633600	-2.18219900	-1.05608300
H	3.75228500	0.20513000	-3.33810300	H	-4.34268200	-1.05005500	-2.00318400
H	6.18115900	0.54842100	-2.96654400	C	-3.42445800	-3.19620000	0.44953400
C	2.16510100	-1.65412600	0.97366300	H	-4.43280000	-3.31894300	0.84635900
H	2.20550000	-2.29440300	0.10406100	H	-3.18482400	-4.02412000	-0.21930200
H	1.45519300	-1.84583300	1.77037100	H	-2.69400100	-3.12703400	1.25337900
H	0.39486600	3.07516700	2.05058700	N	-3.37336000	-1.91999800	-0.33487300
Si	0.12328200	1.85230000	1.26370100	TS ₂₀₋₂₁			
H	1.24389300	1.60790800	0.31164900	N	3.82114900	-1.62667100	-0.36477500
C	-1.43188700	2.07984100	0.23618800	C	4.77877600	-2.60640000	0.17145100
C	-2.59586600	2.63041200	0.79712500	H	4.91081700	-2.40383600	1.23553300
C	-1.44417400	1.76747800	-1.13122400	H	4.39387300	-3.61383600	0.02103100
C	-3.73168200	2.85930900	0.02286400	H	5.73453300	-2.49208500	-0.33981600
H	-2.61545000	2.89711400	1.85112800	C	4.16422400	-0.22325700	-0.23727400
C	-2.57815900	1.99413400	-1.91310900	C	5.34917700	0.24537300	-0.79894400
H	-0.55396400	1.34569900	-1.59197400	C	3.28996600	0.61131000	0.45012600
C	-3.72339200	2.54205000	-1.33624600	C	5.65166200	1.59709800	-0.67520100
H	-4.61577600	3.30020800	0.47260400	H	6.01218400	-0.41540800	-1.34761000
H	-2.55826100	1.77058300	-2.97624300	C	3.60978000	1.96073600	0.56663200
H	-4.59971700	2.74126100	-1.94565800	H	2.38236200	0.21917100	0.89630200
O	0.01244500	0.62634400	2.38015900	C	4.78540300	2.45230800	0.00621400
H	-0.37868600	-0.21977500	2.08094200	H	6.56319100	1.98312100	-1.11765300
C	-0.83304300	-1.49688900	0.05669000	H	2.93202600	2.61819200	1.09941400
O	0.22987200	-1.17238300	-0.51203000	H	5.03073400	3.50451400	0.10078800
O	-1.02694900	-1.65254500	1.28640200	C	2.67839200	-1.97991900	-0.82659300
C	-2.00057000	-1.70979600	-0.92887800	H	2.00464700	-1.22015400	-1.21125000
H	-2.06352200	-0.82687500	-1.56710700	H	2.41090500	-3.02931400	-0.87425100
H	-1.78117700	-2.57841900	-1.55493400	H	1.24334500	-2.07284200	1.06798000
C	-3.75488000	-0.76303700	0.54401900	Si	-0.20808000	-1.82589700	0.67435100
H	-3.07209000	-0.73349100	1.38946600	H	-0.31766800	-2.52148200	-0.62427300
H	-3.67657700	0.15494700	-0.03889600	C	-0.22208300	0.04211100	0.45443700
H	-4.78304200	-0.91238300	0.87574100	C	-0.17892600	0.89060700	1.57155500
C	-4.35187600	-1.99786600	-1.46374400	C	-0.20745400	0.62765100	-0.82071200

C	-0.12778500	2.27630800	1.42228300	H	3.63229900	1.18320600	-2.33298800
H	-0.19317800	0.46323800	2.57185400	C	3.04371800	0.28742100	0.14508600
C	-0.14266300	2.01317200	-0.97569700	C	3.45224400	-0.88909200	-0.48564800
H	-0.28686100	-0.00249400	-1.70436600	C	3.18248200	0.39247600	1.53330800
C	-0.10406500	2.84030300	0.14603100	C	3.98049400	-1.94032700	0.25935400
H	-0.10314800	2.91601700	2.30001000	H	3.35300100	-1.01888100	-1.55454200
H	-0.12627600	2.44681800	-1.97128300	C	3.70918500	-0.66308600	2.27067600
H	-0.05351100	3.91848800	0.02665500	H	2.87930700	1.28812000	2.06006400
O	-0.98338100	-2.42821500	2.00402700	C	4.10918100	-1.83714900	1.63956700
H	-1.93422000	-2.46011500	1.84514600	H	4.29091500	-2.84515200	-0.25254700
C	-2.91637600	-1.16038900	-1.05948300	H	3.80991200	-0.55743900	3.34566600
O	-2.34115800	-1.50978200	-2.08943000	H	4.52411700	-2.65702400	2.21581400
O	-2.69346300	-1.49286300	0.14214700	C	2.96230100	2.69987500	-0.20698200
C	-4.05398800	-0.13732100	-1.33493300	H	4.04604900	2.71324600	-0.35626800
H	-3.64619200	0.64817000	-1.97433300	H	2.48737900	3.46444200	-0.82079400
H	-4.85650100	-0.64192000	-1.87873200	H	2.74207300	2.91505200	0.83738400
C	-3.64930700	1.27146000	0.65838300	Si	0.30472300	1.37983200	-0.07603900
H	-2.97209000	0.52858900	1.07326300	H	0.76875100	1.70827200	1.27611300
H	-3.09545900	1.94289000	-0.00009100	C	0.06424000	-0.39603100	-0.62395400
H	-4.14813600	1.83843700	1.44555000	C	-0.43125900	-0.66805400	-1.90826300
C	-5.67969100	1.55093500	-0.65990000	C	0.28438600	-1.47441700	0.24492700
H	-6.42182900	1.03689800	-1.27133100	C	-0.70272900	-1.97475800	-2.31379000
H	-6.16814000	2.03595700	0.18634300	H	-0.59581300	0.14942300	-2.60795500
H	-5.15627700	2.29434600	-1.26167500	C	0.01631500	-2.78189700	-0.15672300
C	-5.40493700	-0.43940100	0.71795700	H	0.67089500	-1.29558500	1.24401400
H	-5.85058000	0.08876900	1.56194000	C	-0.47986100	-3.03430100	-1.43498400
H	-6.18452800	-0.91882300	0.12446000	H	-1.07329100	-2.16631500	-3.31635000
H	-4.67391800	-1.17413800	1.05009900	H	0.20444100	-3.60314200	0.52771400
N	-4.69166300	0.55469100	-0.14702100	H	-0.67923500	-4.05394800	-1.74979200
XXI				O	0.14713800	2.54863400	-1.25484900
N	2.40955200	1.37522000	-0.60089600	H	-0.69043600	3.01730500	-1.23425400
C	2.57134100	1.24069100	-2.06905800	C	-2.04979400	0.93750000	1.35648300
H	2.05540900	0.35053500	-2.42771100	O	-1.46668500	0.34421400	2.24256700
H	2.11774600	2.11085700	-2.53849600	O	-1.51841000	1.58382400	0.35945300

C	-3.58588600	0.91603700	1.32237400	H	-2.98169200	0.63064200	-2.39281000
H	-3.94734000	0.61050100	2.30440300	H	-2.86799100	2.53393100	-2.51574800
H	-3.99660900	1.89091800	1.05306900	N	4.83044600	0.48012600	-0.33667400
C	-3.43280900	-1.41449800	0.48695000	C	3.83119100	1.44449500	0.23236800
H	-2.39198500	-1.32329900	0.17647400	H	2.82520700	1.08210000	0.02035600
H	-3.47795300	-1.70676300	1.53597400	H	3.98667900	2.41856500	-0.23235300
H	-3.94392000	-2.14476200	-0.14027000	H	3.98262100	1.51029600	1.31024600
C	-5.58665700	-0.25973600	0.57837300	C	4.56867900	0.28898700	-1.80237700
H	-6.07446200	0.71368400	0.51979300	H	3.59736200	-0.18904900	-1.91402500
H	-6.00042700	-0.92891100	-0.17652500	H	5.35045400	-0.35242600	-2.21091200
H	-5.72626700	-0.68917900	1.57060900	H	4.59678300	1.26649800	-2.28517000
C	-3.92632600	0.39519200	-1.08483000	C	6.20623600	1.04032900	-0.16156400
H	-4.31500400	-0.36307700	-1.76497800	H	6.93432800	0.30772000	-0.51096700
H	-4.46973800	1.33192800	-1.21178300	H	6.37358000	1.25365400	0.89436900
H	-2.86382000	0.55214900	-1.25653600	H	6.29321300	1.95776100	-0.74482200
N	-4.12124300	-0.08840000	0.32156200	C	4.75872500	-0.83650700	0.41180100
XVI				H	5.21777700	-0.67610000	1.38745800
N	-3.45425100	1.73534100	-0.73609700	H	5.34599100	-1.56213000	-0.15649800
C	-3.51056900	3.02036000	-0.02659200	C	3.32218600	-1.35594000	0.63592300
H	-2.75972800	3.00497700	0.76557500	O	2.60883100	-1.39741700	-0.43336600
H	-3.29733000	3.83153700	-0.72179900	O	3.01015600	-1.65951400	1.77634300
H	-4.50378300	3.13447700	0.40879800	Si	0.64532000	-1.82005100	-0.47747900
C	-3.80881200	0.55517800	0.02822200	H	0.86412400	-1.91374000	-1.93279400
C	-3.04053900	0.22052600	1.13647500	H	0.88586600	-2.91239200	0.47269900
C	-4.89618800	-0.20744000	-0.38266500	O	-1.13701000	-2.34065300	-0.58440800
C	-3.36466700	-0.93356800	1.84064300	C	-2.01324900	-1.89137200	-1.41283000
H	-2.17654700	0.81345700	1.41701100	H	-2.96456000	-2.44673300	-1.37603300
C	-5.21640100	-1.35132700	0.34317000	O	-1.87594800	-0.93960700	-2.18351700
H	-5.48199000	0.08655900	-1.24802500	C	0.34978000	-0.07957900	0.21418400
C	-4.45029600	-1.71457800	1.44898500	C	0.09167100	1.00394800	-0.64029900
H	-2.75280100	-1.23061200	2.68484300	C	0.47584100	0.18683000	1.58646600
H	-6.06212300	-1.95848500	0.03973800	C	-0.02483200	2.30446100	-0.14611800
H	-4.69505500	-2.61478700	2.00198300	H	-0.02072300	0.82196700	-1.70624400
C	-3.09680000	1.62903100	-1.96086000	C	0.34969100	1.48360400	2.08833200

H	0.70407400	-0.62444200	2.27149100	C	6.28034400	0.94615500	-0.02827700
C	0.10286600	2.54937300	1.22242000	H	6.94800600	0.29947100	-0.59832200
H	-0.19719300	3.13216500	-0.83124300	H	6.53276200	0.89998600	1.03131200
H	0.45732600	1.66247000	3.15408900	H	6.36320800	1.97279500	-0.38719000
H	0.02300000	3.56123100	1.61034000	C	4.80499700	-0.98508700	0.18593100
TS ₁₆₋₁₇				H	5.34056200	-1.08099900	1.13049400
N	-3.63022700	1.61164700	-0.80909200	H	5.31003700	-1.55807300	-0.59501900
C	-3.22641900	2.87992500	-0.18608100	C	3.35684500	-1.47640100	0.39265700
H	-2.29835800	2.71978200	0.36502600	O	2.64154300	-1.42459500	-0.67560900
H	-3.06831700	3.63074100	-0.95926400	O	3.02832100	-1.82739700	1.51537500
H	-4.01580900	3.19353600	0.49755700	Si	0.67328500	-1.75418100	-0.70751600
C	-3.98121900	0.52248300	0.07669200	H	0.83903500	-1.69942200	-2.17175800
C	-3.06449200	0.12379600	1.04340000	H	0.87905200	-2.95855800	0.10652600
C	-5.20127900	-0.12190100	-0.09862200	O	-1.14098800	-2.18085300	-0.80640500
C	-3.37779100	-0.97169000	1.84002800	C	-2.03055400	-1.58312800	-1.51626800
H	-2.09991400	0.61046600	1.13951700	H	-3.01092100	-2.09114200	-1.48334200
C	-5.50359400	-1.21043900	0.71414300	O	-1.88300100	-0.55016800	-2.17322300
H	-5.90955600	0.22682000	-0.84402200	C	0.45896200	-0.08650700	0.16512200
C	-4.59147900	-1.63701700	1.67729800	C	0.32472100	1.09409600	-0.58309200
H	-2.65724600	-1.31574700	2.57328700	C	0.51908800	0.02704300	1.56234900
H	-6.45284900	-1.72058600	0.59438400	C	0.27422900	2.34275300	0.03797000
H	-4.82675000	-2.49211200	2.30152100	H	0.25392400	1.03024200	-1.66581100
C	-3.64082300	1.43865100	-2.07801700	C	0.44782400	1.27199200	2.19100800
H	-3.90213200	0.47299800	-2.48847200	H	0.65250100	-0.86571500	2.16609400
H	-3.36908500	2.26210100	-2.72968600	C	0.33322100	2.43583200	1.43033900
N	4.87342800	0.47582300	-0.21619400	H	0.19563700	3.24572400	-0.56307100
C	3.96019900	1.28772700	0.65502000	H	0.49874700	1.33468400	3.27403900
H	2.92564600	1.03237900	0.42436600	H	0.29609200	3.40593200	1.91772100
H	4.13786000	2.34424300	0.45244800	XVII			
H	4.17219900	1.05743600	1.69932100	N	3.78895700	-0.39748000	1.71550400
C	4.48505200	0.66102500	-1.65408600	C	3.01268200	0.31927500	2.72145300
H	3.49823300	0.22454100	-1.79881300	H	1.94964600	0.41599300	2.46605000
H	5.21431400	0.14380100	-2.27855500	H	3.09785600	-0.20949200	3.67440500
H	4.49072900	1.72917600	-1.87426100	H	3.43656000	1.31707200	2.84678700

C	4.07416900	0.29316000	0.49320000	H	-0.71630800	-2.78371500	0.37182200
C	3.14893700	1.16503500	-0.08414100	H	-0.98985900	-2.22407700	-2.10836400
C	5.28839700	0.04586100	-0.15311700	O	1.20666300	-2.05968600	-1.14521800
C	3.44009600	1.78421200	-1.29816900	C	2.21157900	-2.03775600	-0.45057400
H	2.19838500	1.35652200	0.40243800	H	3.20675800	-2.09634000	-0.91135100
C	5.56572700	0.65420500	-1.37320100	O	2.17120200	-1.96316800	0.85559100
H	6.01697300	-0.60936300	0.31549800	C	-0.56065800	-0.01896900	-0.27088500
C	4.64267600	1.52725200	-1.94929600	C	-0.51375900	0.37322100	1.07565500
H	2.71424600	2.46153800	-1.73672500	C	-0.45209700	0.97428700	-1.25409800
H	6.51335600	0.46180000	-1.86554200	C	-0.37913200	1.71535100	1.43179800
H	4.86464000	2.00740000	-2.89634300	H	-0.57093900	-0.37929100	1.86007300
C	3.47512500	-1.75611000	1.55682300	C	-0.31402600	2.31706900	-0.90321900
H	4.23379200	-2.28102800	0.97180700	H	-0.49252800	0.70120600	-2.30422100
H	3.32148200	-2.24579100	2.51675200	C	-0.28214300	2.69125000	0.43995100
N	-4.82856800	0.40120300	0.50918900	H	-0.33464100	1.99804900	2.47970300
C	-4.02885800	1.57752900	0.02229100	H	-0.23340600	3.07212600	-1.67915100
H	-2.97962900	1.29343700	-0.06379400	H	-0.16895800	3.73617100	0.71149500
H	-4.13519300	2.38427200	0.74749100	XXIII			
H	-4.40742300	1.88226200	-0.95329100	N	-0.56656500	-0.84720400	1.17826100
C	-4.22125000	-0.12000900	1.77827800	C	-0.39932400	-0.27000900	2.49966600
H	-3.22280800	-0.49343800	1.56177300	H	-1.24509500	-0.53433100	3.14086200
H	-4.84637900	-0.92881000	2.15746300	H	0.50012500	-0.68779800	2.95452200
H	-4.18109100	0.69655800	2.49946500	H	-0.29945800	0.82323900	2.46119800
C	-6.23268600	0.84195100	0.78700400	C	-1.76028800	-0.64974900	0.47502500
H	-6.82611300	-0.02581200	1.07686000	C	-2.72747500	0.25520400	0.93593100
H	-6.64821200	1.29449700	-0.11355200	C	-2.01503500	-1.34772500	-0.71706600
H	-6.21971400	1.57162100	1.59699600	C	-3.89190500	0.47646400	0.20762400
C	-4.88066500	-0.68239400	-0.54952800	H	-2.56156500	0.81840300	1.84618400
H	-5.53424300	-0.32247500	-1.34405500	C	-3.17559200	-1.10627700	-1.44300300
H	-5.30281300	-1.57371600	-0.08203800	H	-1.31595700	-2.09811900	-1.07031000
C	-3.49615500	-0.95792500	-1.14929100	C	-4.12397700	-0.19039700	-0.99198000
O	-2.73541500	-1.68377800	-0.37644800	H	-4.61876500	1.19172300	0.58098200
O	-3.19973800	-0.47121800	-2.22145400	H	-3.34403800	-1.65397500	-2.36544600
Si	-0.92825800	-1.80852900	-0.70690400	H	-5.03192700	-0.01053700	-1.55775200

C	0.58639000	-1.26748100	0.49488400	H	2.21888600	0.07354000	1.80442800
H	0.52555200	-1.04741900	-0.56998600	C	1.48139500	2.71719400	-0.92995600
H	1.48190800	-0.79502600	0.90285800	H	-0.58852800	2.56932600	-0.30069500
N	2.93810500	0.67767300	-0.98724100	C	2.78601700	2.27511500	-0.71684300
H	2.71836100	-0.17239500	-1.48796900	H	4.06004800	0.97514300	0.43545000
C	1.83150500	1.44858200	-0.65991300	H	1.27072700	3.44880700	-1.70270600
C	1.81376600	2.29778800	0.45691700	H	3.59600000	2.65791500	-1.32931500
C	0.67573800	1.37824400	-1.46206300	C	-1.49426000	0.47528300	1.05758700
C	0.66979400	3.03788100	0.75980400	H	-1.63158500	0.55580700	-0.01682800
H	2.68682700	2.38584300	1.09398800	H	-2.33593700	0.19062900	1.67752200
C	-0.46166000	2.09897400	-1.13542000	N	-1.63997900	-1.84771400	-0.11001400
H	0.67696800	0.73317300	-2.33768300	H	-2.18354600	-1.33542200	-0.80308600
C	-0.47669800	2.93885300	-0.01909800	C	-0.28745400	-1.95972600	-0.41571400
H	0.68166000	3.69213800	1.62726000	C	0.57155900	-2.79685400	0.31020300
H	-1.35249300	1.99266200	-1.74722000	C	0.24912600	-1.15763600	-1.44038300
H	-1.37075900	3.49854100	0.23406600	C	1.93517100	-2.82587500	0.01409700
C	4.03138800	0.52431400	-0.05459600	H	0.18236500	-3.43641000	1.09586700
H	4.73200200	-0.20843100	-0.45648100	C	1.60566400	-1.19964100	-1.72209400
H	4.56566800	1.47151000	0.07330900	H	-0.41638000	-0.50121700	-1.99583100
H	3.70618100	0.17840000	0.94090400	C	2.46309800	-2.03118800	-0.99734200
C	1.77524200	-3.22211100	-0.07351500	H	2.58448400	-3.48594500	0.58242300
H	1.84982900	-4.30639500	0.08540400	H	1.99994500	-0.56788400	-2.51225700
O	2.51673300	-2.59229100	-0.79622400	H	3.52409900	-2.06054600	-1.22332900
O	0.77114200	-2.72018800	0.63059800	C	-2.34122200	-2.90528100	0.58446200
TS ₂₃₋₂₄				H	-3.40869500	-2.67740000	0.57635500
N	-0.37347200	0.77671200	1.62599100	H	-2.19101200	-3.88978300	0.11842300
C	-0.17461900	0.66031600	3.07263800	H	-2.02207800	-2.97510800	1.63158700
H	0.26195400	1.58604800	3.45030600	C	-3.21754700	1.61743900	-1.24736100
H	-1.13704800	0.48214000	3.55125300	H	-4.01497900	2.00529800	-1.91865300
H	0.49539300	-0.17384000	3.28960300	O	-2.68940100	0.51800400	-1.58042600
C	0.72070700	1.28881600	0.83345400	O	-2.93133400	2.31357200	-0.24263300
C	2.01550800	0.83799200	1.06284300	XXIV			
C	0.43616500	2.23262100	-0.15097300	N	-0.32032300	-0.53568500	1.88019600
C	3.05001200	1.33864300	0.27906800	C	-0.52116800	0.45004300	2.92216000

H	-1.45100900	0.23530300	3.45599000	C	3.50539400	-1.68034700	-1.17425400
H	0.30473700	0.38201200	3.63671800	H	4.39758200	-2.06613400	-1.68712800
H	-0.57117900	1.48574100	2.55121300	O	3.72859300	-0.48520500	-0.66392800
C	-1.40363700	-0.81108700	1.01351300	O	2.46491600	-2.30110200	-1.10241900
C	-2.47506100	0.07776400	0.87099300	III₄			
C	-1.42735100	-2.00956400	0.28324800	Si	0.03057600	-3.00135400	0.02509100
C	-3.52165800	-0.20975100	-0.00261100	C	-3.65013200	0.49183100	-0.07074100
H	-2.47947600	1.02112900	1.40490200	C	-3.02333600	-0.23700800	-1.09334500
C	-2.46642000	-2.28077700	-0.59634700	C	-4.80560400	-0.04367600	0.52267400
H	-0.62685900	-2.73272300	0.40162200	C	-3.53321700	-1.46664300	-1.50241700
C	-3.52265200	-1.38203200	-0.75000100	H	-2.11077800	0.13496200	-1.54799600
H	-4.33176100	0.50566000	-0.10843400	C	-5.31817900	-1.27132300	0.11032300
H	-2.45662600	-3.21135900	-1.15589400	H	-5.31278100	0.50167400	1.31556900
H	-4.33434200	-1.59894900	-1.43670400	C	-4.67978000	-1.98393300	-0.90413200
C	1.01958900	-0.65968200	1.36538600	H	-3.02148500	-2.01986600	-2.28386700
H	1.05304000	-1.48137100	0.65096100	H	-6.21179900	-1.67200700	0.57930800
H	1.70460500	-0.90359400	2.18390500	H	-5.07712500	-2.94275700	-1.22454900
N	1.60184100	0.53559000	0.68660300	C	-0.94311200	0.87403500	1.80183900
H	2.89986000	-0.13260600	-0.20098600	O	0.01694300	0.86378600	2.53773000
C	0.71795400	1.12379700	-0.28060800	Si	-2.98602300	2.13065200	0.51865800
C	0.23400800	2.42674300	-0.15993800	H	-4.03612900	2.80755900	1.31650600
C	0.31292000	0.34233400	-1.36881500	O	-1.71791300	1.94272000	1.65643100
C	-0.66686600	2.92945900	-1.09902000	H	-1.24937000	-0.00327200	1.21371900
H	0.53965900	3.05741700	0.66757500	H	-2.50319000	3.01603800	-0.55488300
C	-0.59386600	0.84406900	-2.29129700	H	-0.17334300	-4.23744800	0.83580500
H	0.69434000	-0.66870600	-1.47435400	C	1.77041500	-2.36713900	0.37879900
C	-1.09434500	2.13915300	-2.15936400	H	-0.98857200	-2.02161000	0.45831900
H	-1.04118100	3.94261400	-0.98760500	C	2.83712700	-2.68028700	-0.47635300
H	-0.91541300	0.21520500	-3.11513500	C	4.13437800	-2.24674000	-0.20620400
H	-1.80745900	2.52633900	-2.87987200	C	2.04518300	-1.59059100	1.51392900
C	2.30024700	1.46735400	1.57165300	C	4.39138300	-1.48538600	0.93418400
H	3.03399300	0.90614700	2.15537000	C	3.34196800	-1.15464100	1.79099700
H	2.84099400	2.19867000	0.96533400	H	-0.10886500	-3.36647600	-1.40111900
H	1.64526800	2.00546200	2.26752500	H	2.65148700	-3.25793000	-1.37803900

H	4.94366600	-2.50791800	-0.88205700	H	-4.32684500	-1.58988800	2.97800100
H	5.40466500	-1.16215100	1.15796000	H	-3.72943200	-3.62617500	1.69238500
H	3.52897300	-0.56433100	2.68403500	C	-1.38086000	1.92062500	-1.32367400
H	1.24354500	-1.29035500	2.18373100	O	-0.40660600	1.65697800	-2.09547100
C	0.49531300	0.57485700	-1.33907400	Si	-4.04808600	1.48475800	-0.98989700
O	0.18454600	-0.52988100	-1.80932000	H	-4.22900800	2.51791900	0.07241800
O	-0.23488000	1.50318500	-0.91426900	O	-2.69050900	1.73209000	-1.90095800
C	2.03686200	0.76486400	-1.29389600	H	-1.38384700	2.89923900	-0.79537400
H	2.46302600	-0.02833900	-0.67894300	H	-5.18733400	1.54099700	-1.93650300
H	2.43350900	0.66613600	-2.30725900	H	-1.43351800	1.15985500	-0.32100100
C	2.11094000	2.28001300	0.67258900	C	0.81526200	0.99732200	0.91629300
H	1.03401300	2.42281000	0.66347600	H	-0.65551200	-0.46543200	-1.29321800
H	2.35375700	1.38843800	1.25019600	C	1.18646300	0.75094500	2.24959400
H	2.62602100	3.15392200	1.07511500	C	2.06164700	1.59827300	2.92770100
C	4.05761200	2.00129800	-0.75700700	C	1.33749100	2.14362800	0.29118500
H	4.39714600	1.83425500	-1.78007300	C	2.57910300	2.72251300	2.28751200
H	4.46547400	2.93991600	-0.37749200	C	2.20797400	2.99448300	0.97119600
H	4.37189800	1.16950800	-0.12475400	H	-1.17143500	-0.90237400	1.16995000
C	2.10994300	3.21612100	-1.58745000	H	0.80520100	-0.12654500	2.76413200
H	2.51074000	4.14180200	-1.17072400	H	2.33335400	1.38067700	3.95622800
H	2.48376800	3.06900900	-2.60207800	H	3.25446800	3.38906400	2.81630000
H	1.02000100	3.21476100	-1.57594000	H	2.59049900	3.87989100	0.47073300
N	2.56883600	2.07301500	-0.74133300	H	1.04525700	2.35474500	-0.73636300
TS _{3-5_4}				C	2.07332700	-1.96056800	0.49070800
Si	-0.32204200	-0.29444900	0.12311700	O	2.28789100	-2.13278100	1.67416700
C	-3.98344000	-0.17802200	-0.11374900	O	0.98155900	-1.60110400	-0.09814200
C	-3.65105600	-1.34269400	-0.82255100	C	3.20823200	-2.19562200	-0.52690300
C	-4.22696700	-0.29268300	1.26090000	H	4.06068800	-2.64176100	-0.01352800
C	-3.56062300	-2.57478800	-0.18086900	H	2.86464500	-2.84867600	-1.33189600
H	-3.43702400	-1.27972300	-1.88674800	C	4.11787300	0.05436200	-0.10500600
C	-4.14214700	-1.52406800	1.90978900	H	3.25061600	0.31377800	0.50079600
H	-4.47198900	0.59517200	1.83964500	H	4.88093700	-0.41256500	0.51835500
C	-3.80660300	-2.66713700	1.18875900	H	4.50561200	0.95245700	-0.58552600
H	-3.29296400	-3.46313200	-0.74571700	C	4.90803900	-1.27360400	-1.99200700

H	4.60871600	-1.97838500	-2.76837200	C	1.52022900	5.14549500	-1.01347800
H	5.30474700	-0.36643200	-2.44842900	C	1.60517100	3.96983600	-1.75700400
H	5.66332400	-1.72510000	-1.34816000	H	1.21619900	1.49468500	2.55411600
C	2.69208000	-0.28080900	-2.08569700	H	0.95748000	3.79152400	2.04707900
H	3.18974700	0.52688700	-2.62280900	H	1.21624500	5.98781100	0.94547700
H	2.32465600	-1.03466000	-2.78115800	H	1.65086500	6.10923500	-1.49759000
H	1.85757100	0.12323400	-1.52181500	H	1.80833100	4.01605600	-2.82345300
N	3.70960300	-0.91882700	-1.17189300	H	1.50847000	1.82311200	-1.71806000
V₄				C	3.17840000	-0.57493900	0.58403900
Si	0.89248700	1.00718400	1.15333700	O	3.75962900	0.07022000	-0.26517300
C	-3.76316000	-0.87299900	-0.29731900	O	2.27629100	-0.18421900	1.42687400
C	-3.45247500	-0.54715800	1.03124600	C	3.53083600	-2.06587800	0.75366800
C	-4.99632200	-0.45105600	-0.81300200	H	4.47716800	-2.26427800	0.24911400
C	-4.34598300	0.17176300	1.82030700	H	3.59639700	-2.33341500	1.81028900
H	-2.48873400	-0.82952400	1.44784100	C	2.26722100	-2.58454400	-1.30540300
C	-5.89746800	0.26267000	-0.02514800	H	1.82379200	-1.58628700	-1.31144400
H	-5.25468900	-0.66884700	-1.84706600	H	3.22517900	-2.59222200	-1.82627900
C	-5.57228400	0.57363600	1.29340800	H	1.57452800	-3.30305400	-1.74455400
H	-4.08161700	0.42628200	2.84194200	C	3.03638000	-4.37143700	0.17743500
H	-6.84615200	0.58554000	-0.44314200	H	3.21214800	-4.64461000	1.21879200
H	-6.26759400	1.13935500	1.90618100	H	2.30481800	-5.04866700	-0.26453800
C	-0.47839000	-0.07589100	-1.04025600	H	3.97075900	-4.41776500	-0.38303000
O	0.70559800	-0.03163300	-0.37563300	C	1.19358800	-2.93296900	0.86593000
Si	-2.55245100	-1.83938100	-1.34493500	H	0.54221700	-3.69802200	0.44197700
H	-2.88786600	-1.60153300	-2.77755000	H	1.38634800	-3.12709100	1.92138200
O	-0.98344100	-1.42655100	-0.98664400	H	0.74304600	-1.95333900	0.71659100
H	-0.34013400	0.17909400	-2.10322100	N	2.50099300	-2.98026700	0.12536200
H	-2.60870900	-3.29954300	-1.07642300	TS _{3-5_2}			
H	-1.23058400	0.60122900	-0.60016400	C	-1.09532600	2.12545800	0.88303500
C	1.18144200	2.64083600	0.24138400	Si	0.74461500	0.77822300	1.84316800
H	-0.55649200	0.69377600	1.46161100	H	-0.26246900	0.56795500	0.46242500
C	1.12235900	3.83596200	0.97266900	H	1.61241200	1.10035900	3.04032100
C	1.27640200	5.07651200	0.35690500	H	-0.49756500	0.39202600	2.60562900
C	1.43013800	2.73525900	-1.13478000	C	2.08301700	1.38244900	0.55552500

C	3.40658600	1.48789500	1.00089100	H	-1.19735000	0.97723500	-2.19389600
C	1.85285400	1.61617300	-0.80524700	C	-3.46084000	0.42575300	-0.69039600
C	2.88915600	1.91002300	-1.69025500	C	-3.01883800	-0.62970100	0.12585800
C	4.20462000	1.97293200	-1.22859700	C	-4.83517200	0.53282800	-0.95481700
C	4.45879100	1.76735000	0.12620800	C	-3.92236800	-1.54380400	0.65981800
H	0.83541400	1.56965700	-1.18559100	H	-1.96504400	-0.74019300	0.37246700
H	2.67170000	2.10146400	-2.73839200	C	-5.74029100	-0.38517600	-0.42568700
H	5.01657400	2.20302000	-1.91289500	H	-5.20781900	1.34244300	-1.57811100
H	5.47507200	1.83746800	0.50554600	C	-5.28338800	-1.42382700	0.38290200
H	3.61787700	1.33499600	2.05749800	H	-3.55268400	-2.33841000	1.29994800
C	0.68911200	-2.03487100	1.31525200	H	-6.80032600	-0.28407600	-0.63771900
O	-0.48785800	-2.27770500	1.52428000	H	-5.98914500	-2.13553600	0.80112000
O	1.39098200	-1.01117700	1.65326100	TS _{3-5_3}			
C	1.49555900	-3.06547200	0.49192100	Si	1.14250300	1.02123800	1.21546000
H	2.36602300	-3.42510900	1.04546100	C	-3.20377100	0.93581700	0.14879200
H	0.83644500	-3.89705500	0.24132800	C	-3.03784000	0.60474000	-1.20347100
C	3.23210500	-1.65102600	-0.59774000	C	-4.03532700	0.11644700	0.92854300
H	3.01199000	-0.90259100	0.15970300	C	-3.68700500	-0.50055900	-1.75470300
H	4.03721300	-2.30828200	-0.26630500	H	-2.36786400	1.20377300	-1.81180200
H	3.49300200	-1.16336100	-1.53760100	C	-4.68781000	-0.98904600	0.38249500
C	2.35775600	-3.62551900	-1.72028200	H	-4.18298200	0.33896800	1.98404500
H	1.45327200	-4.18254100	-1.96708000	C	-4.51689000	-1.29827100	-0.96632500
H	2.80811700	-3.22380700	-2.62882000	H	-3.55540100	-0.72842100	-2.80937000
H	3.06868800	-4.27683200	-1.21044200	H	-5.33129700	-1.60251500	1.00636300
C	0.92892900	-1.66829500	-1.46293800	H	-5.03306000	-2.14974600	-1.40095600
H	1.28372700	-1.34630600	-2.44248500	C	-0.16220900	2.83971200	-0.49958400
H	0.03114400	-2.28111700	-1.55633400	O	-0.30412300	1.85040300	-1.25645300
H	0.71735600	-0.79327900	-0.84516100	Si	-2.48973000	2.47586700	0.97979300
N	2.00512600	-2.49161400	-0.81684300	H	-2.07327700	2.06372000	2.34656300
H	-1.81732300	1.47008000	1.39040800	O	-1.27822500	3.31266300	0.20538700
O	-1.50831300	2.63949800	-0.28342400	H	0.42956200	3.71280100	-0.81080900
O	-0.15368100	2.64526600	1.51254100	H	-3.58355300	3.46855600	1.11286200
Si	-2.27719000	1.65858400	-1.43613100	H	0.69538400	2.53934100	0.57965400
H	-3.00874800	2.60171100	-2.30760700	C	2.65134700	0.91512000	0.08630500

H	-0.27797800	0.74993900	0.90411400	C	-5.26718400	-1.11553700	-0.54288600
C	3.87940900	0.64617100	0.71169700	C	-6.34174900	0.63807700	0.70687800
C	5.06026600	0.55845600	-0.02207200	C	-6.47860400	-1.80064100	-0.62026600
C	2.64668400	1.09161200	-1.30637100	H	-4.37860000	-1.52934100	-1.01161800
C	5.03668300	0.73107200	-1.40353200	C	-7.55396500	-0.04460500	0.63448500
C	3.82692600	0.99580300	-2.04206700	H	-6.30761400	1.59613400	1.22215700
H	1.47474500	1.48475100	2.57988400	C	-7.62299700	-1.26756800	-0.03063700
H	3.91819100	0.48026400	1.78464700	H	-6.52998000	-2.75129500	-1.14300400
H	5.99583500	0.34723500	0.48666900	H	-8.44383200	0.37856200	1.09117300
H	5.95612600	0.66169900	-1.97769300	H	-8.56757300	-1.80002800	-0.09298200
H	3.79985700	1.14069700	-3.11859700	C	-1.17707100	0.66688300	-1.07703700
H	1.71099200	1.32007900	-1.80854100	O	-0.46090700	-0.23563000	-1.60660200
C	1.84413300	-1.90565700	1.31556100	Si	-3.54605000	1.01944600	0.24678000
O	2.97226500	-2.22226400	1.63836300	H	-2.96176000	0.89181000	1.61252100
O	1.17145000	-0.86084200	1.64631700	O	-2.54845000	0.31991200	-0.87212900
C	1.10186100	-2.95708100	0.45393000	H	-1.12976700	1.69421800	-1.49647700
H	1.80666700	-3.31999700	-0.29619300	H	-3.76261900	2.47533400	0.00244800
H	0.83570500	-3.79156200	1.10850200	H	-0.81090700	0.95413900	0.12306800
C	0.08304800	-1.43898000	-1.24843600	C	1.70828000	1.36771500	0.17657100
H	0.12024200	-0.48696600	-0.72532500	H	-0.26309200	-0.98333700	0.57438800
H	1.02034600	-1.62465200	-1.77391200	C	2.52568400	2.13272100	1.02750900
H	-0.75315400	-1.40397900	-1.94668300	C	3.46036700	3.03491700	0.52050500
C	-0.60589500	-3.75791900	-1.06681400	C	1.84837900	1.56006800	-1.20926700
H	-0.73012000	-4.60608700	-0.39249200	C	3.59160300	3.20342200	-0.85637200
H	-1.55691700	-3.52438100	-1.54718700	C	2.77693400	2.46829300	-1.71641100
H	0.14691300	-3.98889900	-1.82141400	H	0.26991500	0.67340300	2.40303400
C	-1.26260900	-2.18866500	0.66573700	H	2.44965000	2.01094400	2.10413600
H	-2.13350500	-1.89493500	0.07976400	H	4.08119500	3.60756300	1.20295100
H	-1.49453400	-3.05754500	1.28437700	H	4.31266000	3.91219000	-1.25366800
H	-0.91723800	-1.36304700	1.28148600	H	2.85826400	2.60617700	-2.79119700
N	-0.16220700	-2.56584000	-0.28264700	H	1.21407900	0.98310400	-1.87938900
TS _{3-5_5}				C	3.14000700	-1.08648900	1.73543300
Si	0.55182500	0.13843900	1.04843400	O	3.72218300	-0.36425400	2.52075600
C	-5.17982300	0.11454700	0.12320300	O	1.88830700	-1.11062900	1.42022500

C	3.93274300	-2.16403100	0.96747700	H	1.97820200	-0.68234100	1.06841500
H	4.94353500	-2.21903900	1.37320300	H	-0.27882300	-1.13083800	1.18861000
H	3.43543700	-3.13259000	1.05107500	H	2.51016400	-1.37007300	-0.68090000
C	4.64573300	-0.48452500	-0.68920300	C	5.68567600	-0.36525100	-0.25556200
H	3.94997200	0.25315100	-0.29173700	H	3.72203800	-0.16319900	-2.35916200
H	5.59323400	-0.43030600	-0.15259300	C	6.72813100	-1.29315900	-0.38420700
H	4.79271000	-0.30716700	-1.75443900	C	8.00789700	-1.02815300	0.10373400
C	5.01966300	-2.86119300	-1.08795100	C	5.97170000	0.84642200	0.39409300
H	4.60773800	-3.86075500	-0.94502600	C	8.26969100	0.18318700	0.73832100
H	5.14139700	-2.66058200	-2.15277800	C	7.24735100	1.12104400	0.88193200
H	5.98226000	-2.77697400	-0.58285900	H	4.36277500	-2.22411300	-1.38316100
C	2.76447000	-1.96996500	-1.25485500	H	6.53355500	-2.24565700	-0.87269000
H	2.97532200	-1.84712000	-2.31739500	H	8.79556900	-1.76847600	-0.00585700
H	2.33445700	-2.95217300	-1.06082500	H	9.26271200	0.39386300	1.12555500
H	2.06662200	-1.20443600	-0.93093500	H	7.44404100	2.06698500	1.37906600
N	4.07179600	-1.85995700	-0.51104000	H	5.17895400	1.57605000	0.52322800
TS _{3-5_7}				C	-3.20112400	-1.50711700	1.06190000
Si	3.99719700	-0.78162400	-1.03890300	O	-2.96936500	-1.14241900	2.20647900
C	-1.65579500	1.08311500	-0.11875300	O	-2.43235500	-1.51202600	0.03764700
C	-1.97367200	1.76172600	1.06617500	C	-4.63219800	-2.00398700	0.74309400
C	-2.14169200	1.60776200	-1.32565100	H	-4.61236400	-2.97272300	0.23888500
C	-2.75477600	2.91749700	1.04753600	H	-5.20048300	-2.06766000	1.67158300
H	-1.62188600	1.37408400	2.01774400	C	-4.86067900	-1.10953900	-1.57028400
C	-2.92612400	2.76091700	-1.35100800	H	-3.79061200	-0.91247400	-1.54754600
H	-1.89416900	1.11733600	-2.26474800	H	-5.04406600	-2.11053500	-1.96255900
C	-3.23729100	3.41822900	-0.16100100	H	-5.39175800	-0.36428400	-2.16350700
H	-2.98148500	3.42939000	1.97826300	C	-6.82330200	-1.42817500	-0.16216800
H	-3.27909600	3.15699400	-2.29922500	H	-7.22632300	-1.29570000	0.84231800
H	-3.83617800	4.32425500	-0.17730000	H	-7.36153300	-0.78968700	-0.86400200
C	2.05624200	-0.07278600	0.15532500	H	-6.91545900	-2.47217700	-0.46383200
O	3.15321200	0.59889400	-0.05077700	C	-5.23884100	0.35682400	0.35100700
Si	-0.65210800	-0.51270700	-0.10148300	H	-5.89160700	1.00693600	-0.23175400
H	-0.56768300	-1.24030600	-1.38308900	H	-5.51251600	0.37340500	1.40601700
O	0.93969400	0.33899500	-0.34181100	H	-4.20334200	0.67436900	0.23617800

N	-5.38093400	-1.04595600	-0.16433100	H	-1.11174400	2.41164800	1.40260900
TS _{3-4_6}				C	-2.48800700	-1.29299500	-1.69463600
Si	-0.76050800	0.92569700	-1.26843300	O	-3.57801300	-1.71947200	-2.05057200
C	4.67100900	0.40317400	-0.07692400	O	-1.90660300	-0.25238900	-2.19301700
C	5.79654800	0.97458100	-0.68778500	C	-1.69591900	-2.07015600	-0.61706200
C	4.81946100	-0.83233100	0.56730100	H	-1.32955200	-2.99542000	-1.07045200
C	7.03365300	0.33658800	-0.65330300	H	-0.85039500	-1.50083700	-0.23211000
H	5.71390400	1.93209400	-1.19846400	C	-3.52418500	-3.50162700	0.29220300
C	6.05592200	-1.47480100	0.60288200	H	-4.19826400	-3.10966700	-0.46718300
H	3.95813700	-1.29108800	1.04453000	H	-3.01411000	-4.38678200	-0.09087400
C	7.16420900	-0.89142500	-0.00674600	H	-4.05275900	-3.74577600	1.21500900
H	7.89462200	0.79533200	-1.12992100	C	-1.52536600	-2.99618500	1.60856700
H	6.15444800	-2.43185400	1.10643200	H	-0.80496800	-2.20820300	1.84195300
H	8.12777900	-1.39112900	0.02204900	H	-2.07959100	-3.29605700	2.49936900
C	0.72388700	0.71581700	1.15031300	H	-1.02197400	-3.86188500	1.17573500
O	-0.13312300	-0.15375300	1.42051700	C	-3.16127300	-1.24740600	1.19264800
Si	3.02201800	1.27970000	-0.12656400	H	-3.66907600	-1.55306800	2.10857400
H	2.57592800	1.51415100	-1.52164800	H	-2.38653900	-0.50882000	1.40877200
O	1.94734600	0.27233100	0.67111100	H	-3.88082200	-0.85334800	0.47587000
H	0.84180800	1.60250500	1.79641300	N	-2.49899900	-2.45907600	0.60269500
H	3.08802500	2.59312700	0.57040900	TS _{4-5_6}			
H	0.27980600	1.53628700	-0.01732500	Si	-1.57655900	-1.12026100	1.40794500
C	-2.23146600	1.66568000	-0.28399300	C	3.12363200	-1.20216200	0.31302400
H	0.22260600	-0.17617300	-1.14678200	C	2.43667900	-1.25714500	1.53382900
C	-3.52088600	1.63536200	-0.84549400	C	4.11040300	-0.21627500	0.16246700
C	-4.61312100	2.21277200	-0.19933300	C	2.70312500	-0.35049400	2.55813600
C	-2.08739300	2.33407500	0.93960200	H	1.66634300	-2.00985300	1.68265100
C	-4.44737400	2.83871000	1.03318100	C	4.38423000	0.69703300	1.18011400
C	-3.17566400	2.90312800	1.59775300	H	4.67825400	-0.16179700	-0.76464600
H	-0.42728900	1.80835500	-2.40899800	C	3.67563400	0.63239300	2.38065600
H	-3.68148800	1.14722800	-1.80068800	H	2.14765000	-0.40546600	3.48903800
H	-5.59358300	2.17082300	-0.66477300	H	5.15760200	1.44839700	1.04564900
H	-5.29744500	3.28420000	1.54166300	H	3.88792000	1.33956200	3.17701000
H	-3.02668800	3.40083700	2.55155600	C	0.06652100	-1.89246600	-1.87042700

O	-0.45042600	-0.84082100	-1.25680000	C	-0.49480700	2.08376500	-1.90315000
Si	2.68469500	-2.36466500	-1.10485100	H	-0.35759700	2.60444500	-2.85227700
H	2.22384500	-3.64441400	-0.50058800	H	-0.69665200	1.01249400	-2.04187200
O	1.53902800	-1.74713300	-2.11685700	H	-1.28190500	2.55498500	-1.31793800
H	-0.31771800	-2.05810600	-2.89402800	N	0.79832300	2.18081300	-1.13715000
H	3.92445600	-2.55780300	-1.89980500	V_B			
H	-0.03796700	-2.84477800	-1.30163900	Si	0.13676800	1.75591000	0.36107700
C	-3.21257700	-0.71157200	0.60588400	H	0.47113100	2.19556100	1.72322800
H	-0.76951800	-2.22354000	0.85983600	C	0.20223700	-0.12550600	0.18386600
C	-4.31391900	-0.51062100	1.45428300	C	-0.06574500	-0.75777400	-1.03745200
C	-5.56966500	-0.19380800	0.94112300	C	0.55377000	-0.93883700	1.27090500
C	-3.40714900	-0.58664300	-0.77876300	C	0.03083800	-2.14291300	-1.17746400
C	-5.74508500	-0.07372500	-0.43536400	H	-0.34333300	-0.16465900	-1.90588700
C	-4.66322600	-0.27092100	-1.29190600	C	0.65867100	-2.32193400	1.14084500
H	-1.88540900	-1.44999200	2.82448300	H	0.76591900	-0.47763600	2.23281500
H	-4.19223500	-0.60130400	2.53084900	C	0.40181900	-2.92865000	-0.08899500
H	-6.40752700	-0.04160000	1.61486400	H	-0.19131200	-2.60772900	-2.13357400
H	-6.72308500	0.17023100	-0.84016600	H	0.93151100	-2.92909000	2.00046400
H	-4.79921800	-0.18014100	-2.36577800	H	0.47369600	-4.00762700	-0.19346900
H	-2.55142900	-0.73437900	-1.43265700	O	-1.52184800	2.15381400	0.29844900
C	-0.44322700	1.39278500	0.94184500	H	0.69135000	2.45151100	-0.82046600
O	-1.13359600	2.38341600	1.03032300	C	-2.22049700	2.32482500	-0.89602100
O	-0.62947700	0.29241300	1.65284100	H	-2.14209600	1.41984400	-1.52400000
C	0.77900200	1.26576100	0.05852300	H	-1.83995100	3.19119100	-1.45256900
H	1.68739200	1.44000600	0.64194900	O	-3.56980500	2.56731000	-0.61774400
H	0.74679200	0.24647800	-0.34764400	Si	-4.34577900	1.62754900	0.53193200
C	1.06328100	3.59280400	-0.73891700	H	-3.96945900	1.96643200	1.92321400
H	0.27306400	3.91155900	-0.06047500	H	-5.78035200	1.92647200	0.30736700
H	2.03333400	3.63880100	-0.24084100	C	-4.00743800	-0.19212200	0.23448400
H	1.07576900	4.21303300	-1.63687400	C	-4.55219700	-0.84492100	-0.88151600
C	1.89834000	1.67984800	-2.02189800	C	-3.19431700	-0.93526500	1.10081200
H	1.67383000	0.64499000	-2.29767600	C	-4.29647000	-2.19267800	-1.12408000
H	1.95480700	2.32136900	-2.90286000	H	-5.18689300	-0.29380900	-1.57204400
H	2.83563900	1.71574600	-1.46465000	C	-2.94310000	-2.28539000	0.87007300

H	-2.74081600	-0.44974200	1.96109100	C	-0.12819500	2.95307300	0.06936200
C	-3.49295300	-2.91499300	-0.24372000	H	-0.84981600	2.49037700	2.04451500
H	-4.72782900	-2.67958500	-1.99385600	H	0.54801100	3.09181600	-1.97175800
H	-2.30351300	-2.84101800	1.54823600	H	-0.23977300	4.02622400	0.19280100
H	-3.29304700	-3.96675700	-0.42739600	O	-1.38314000	-2.19411900	-0.32756700
C	3.53688400	1.84190400	-0.09685700	H	0.72958400	-2.44837700	0.76071000
O	3.68857900	2.97816900	-0.53952300	C	-2.13290000	-2.82308200	1.08572300
O	2.57840700	1.31489000	0.53027300	H	-1.69406700	-2.12704100	1.82772300
C	4.77916300	0.92749200	-0.36461600	H	-1.66189400	-3.81906100	1.11364800
H	5.06945700	1.04076400	-1.41084600	O	-3.36314100	-2.71384100	0.78158900
H	5.60625400	1.26416500	0.26581100	Si	-2.79785300	-1.55466000	-1.11178900
C	3.49869200	-1.10206700	-0.95432000	H	-2.08621600	-1.03756000	-2.33223300
H	2.57922600	-0.60457200	-0.65340100	H	-3.76552000	-2.52138200	-1.66006300
H	3.72167100	-0.89425500	-2.00182100	C	-3.44506700	0.04969800	-0.36420700
H	3.41913200	-2.17703600	-0.78775800	C	-4.10654400	0.13392400	0.87025700
C	5.88478400	-1.24872000	-0.49421300	C	-3.22715600	1.24136200	-1.07212900
H	6.70244800	-0.84834000	0.10624100	C	-4.52240000	1.36260800	1.37953600
H	5.77818200	-2.31928800	-0.31112600	H	-4.28312600	-0.78293300	1.42417200
H	6.08416500	-1.07237100	-1.55180200	C	-3.64864100	2.47122900	-0.57175300
C	4.33021600	-0.82988300	1.33082900	H	-2.70055700	1.21146600	-2.02267200
H	4.21632200	-1.90645900	1.46685100	C	-4.29479300	2.53497900	0.66022500
H	5.16948200	-0.45871100	1.92134900	H	-5.03110900	1.40474200	2.33865500
H	3.41454200	-0.29553500	1.58266100	H	-3.46134500	3.37977100	-1.13724700
N	4.61735000	-0.56271800	-0.11549100	H	-4.62208200	3.49191000	1.05761500
TS ₅₋₆				C	3.39556700	-1.65634000	0.15434900
Si	0.33548600	-1.70188400	-0.44835900	O	3.55476300	-2.78549700	0.59549800
H	0.60126600	-2.18686700	-1.81248700	O	2.42482900	-1.15247000	-0.49513600
C	0.11595500	0.16442600	-0.26289000	C	4.59374600	-0.70128200	0.42849500
C	-0.34773400	0.71303900	0.93960600	H	4.88623300	-0.82387300	1.47291900
C	0.43117100	1.04757100	-1.30380100	H	5.43259400	-1.00328200	-0.20395900
C	-0.46614000	2.09165400	1.11042800	C	3.24153800	1.28401200	1.03622700
H	-0.63753800	0.05635500	1.75657800	H	2.33034400	0.78788500	0.70966800
C	0.31321600	2.42688600	-1.14461800	H	3.45123300	1.05441200	2.08179800
H	0.77025600	0.64925200	-2.25780000	H	3.15000600	2.36146500	0.89460100

C	5.62964400	1.49808200	0.61212600	C	-3.33238100	-1.15038700	1.28807100
H	6.46746000	1.12611500	0.02131900	C	-4.33477300	-1.31537500	-1.30030300
H	5.49828800	2.56716500	0.43907300	H	-4.12626700	0.81525500	-1.36643600
H	5.81474400	1.31518200	1.67109800	C	-3.65765900	-2.39230600	0.74856100
C	4.11526100	1.07314800	-1.24392600	H	-2.92727200	-1.10162600	2.29619600
H	3.97836700	2.14892100	-1.36105800	C	-4.16102800	-2.47546600	-0.54775200
H	4.97252800	0.73383700	-1.82762300	H	-4.72413700	-1.37575600	-2.31232800
H	3.21616400	0.52957400	-1.52731200	H	-3.51030900	-3.29465000	1.33446200
N	4.38478000	0.78471800	0.20232000	H	-4.41309100	-3.44265800	-0.97306200
VI				C	3.46370000	1.58351600	0.35996000
Si	0.10160000	1.64970700	0.83788100	O	3.68657800	2.78121400	0.19286800
H	0.42599800	1.87469400	2.25979900	O	2.52244000	0.99076200	0.95294100
C	0.00666500	-0.18587800	0.41563600	C	4.57074200	0.67995700	-0.27900000
C	-0.50068600	-0.60529500	-0.82243300	H	4.76648800	1.04388900	-1.28945900
C	0.41642800	-1.16976100	1.32434600	H	5.48726800	0.77554600	0.30909200
C	-0.57248900	-1.95839600	-1.15047000	C	3.03888300	-1.02259900	-1.20929800
H	-0.86307700	0.12859900	-1.53927300	H	2.20569800	-0.56151800	-0.68382600
C	0.34059500	-2.52479500	1.00738100	H	3.17907200	-0.55854100	-2.18659000
H	0.81253000	-0.86866200	2.29133900	H	2.86942700	-2.09480400	-1.31732600
C	-0.14926300	-2.92170900	-0.23672300	C	5.43084400	-1.45760900	-1.09051000
H	-0.98479500	-2.25926200	-2.10882800	H	6.33929300	-1.29213600	-0.51005000
H	0.65154300	-3.27135300	1.73360300	H	5.23557600	-2.52769300	-1.17831800
H	-0.22504500	-3.97730500	-0.48229900	H	5.54556600	-1.02010500	-2.08290800
O	-1.51187700	2.17789100	0.66357700	C	4.11115200	-1.42507200	0.95392800
H	0.77251100	2.49016300	-0.16913000	H	3.89973000	-2.48737500	0.82270400
C	-1.86370300	3.06791600	-1.92211400	H	5.03909900	-1.28752700	1.51146100
H	-0.80433900	3.32598800	-1.75423700	H	3.28533100	-0.90977900	1.44339500
H	-2.60867900	3.70097300	-1.40786700	N	4.28206600	-0.80667800	-0.40011000
O	-2.19298600	2.15037900	-2.63870300	IM2 ₂			
Si	-2.97771300	1.68394900	1.24969100	C	-1.64642300	1.73877500	-0.83035300
H	-2.92285300	1.55575800	2.73186400	O	-1.69600400	2.96091500	-0.86853700
H	-3.96315700	2.72243500	0.85523300	O	-0.69284400	0.94658000	-1.11929200
C	-3.49785200	0.02798600	0.54697700	C	-2.95098900	1.02567800	-0.37058100
C	-4.00654600	-0.07622200	-0.75591100	H	-3.56355400	1.74359000	0.17641400

H	-3.50538000	0.66328400	-1.24056800	O	-2.45664100	1.61953000	-1.33949200
C	-1.79883600	0.20158500	1.64918000	O	-0.56217400	0.38207200	-1.50268800
H	-0.81338900	0.36753400	1.22076400	C	-2.55443300	-0.73051600	-0.94475300
H	-2.16084700	1.11209700	2.12824200	H	-3.62519600	-0.59240500	-1.09876500
H	-1.76126300	-0.61991400	2.36521300	H	-2.17834000	-1.53787700	-1.57633300
C	-4.06389300	-0.52909300	1.14531300	C	-2.86059800	-0.09753900	1.42435600
H	-4.78084000	-0.71052700	0.34373300	H	-2.18214700	0.75936700	1.36521000
H	-3.94377600	-1.43219800	1.74551000	H	-3.87843100	0.17302500	1.14111200
H	-4.41217200	0.29151300	1.77346800	H	-2.84030200	-0.50592700	2.43565100
C	-2.21249800	-1.35314500	-0.20357700	C	-3.18601100	-2.40596300	0.68204200
H	-1.99010400	-2.14510700	0.51270400	H	-2.82114300	-3.18027700	0.00599400
H	-2.97591600	-1.67948600	-0.91144000	H	-3.08087300	-2.73895800	1.71485300
H	-1.31061400	-1.04185600	-0.72640100	H	-4.23304000	-2.18591400	0.46978500
N	-2.74650200	-0.16661800	0.54737100	C	-0.93118700	-1.47840200	0.80453200
Si	1.40950400	1.23274200	-0.64632000	H	-0.90561100	-1.97105300	1.77729400
H	1.53197300	1.71236000	-2.03009600	H	-0.52878600	-2.13206700	0.03049700
H	0.83210300	2.06034900	0.43032700	H	-0.36890800	-0.54608700	0.84951200
O	3.13865400	1.53387900	-0.25115600	N	-2.37241100	-1.16974300	0.48947700
C	3.60912800	1.50546000	0.97000300	Si	0.78928300	1.49540800	-1.10526700
H	4.66033200	1.83299000	1.01334700	H	1.42575400	1.68738700	-2.44866600
O	3.00308100	1.16669500	1.97134500	H	0.05205700	2.73818100	-0.89052700
C	1.33165600	-0.64753700	-0.45609600	O	1.53052400	2.76604200	0.97580200
C	1.13135900	-1.45523600	-1.58586100	C	0.50808700	2.43308400	1.60924400
C	1.38994200	-1.27733100	0.79542900	H	0.25652200	2.99726300	2.52898000
C	0.97633200	-2.83545200	-1.47318600	O	-0.27593600	1.49394400	1.27631300
H	1.07497600	-0.99523100	-2.56921700	C	1.89653300	0.09849600	-0.43453100
C	1.22310600	-2.65834900	0.91612000	C	2.07868000	-0.95297900	-1.34961600
H	1.58760600	-0.68093100	1.68242000	C	2.49780200	-0.03171700	0.82128300
C	1.01130000	-3.44125600	-0.21692400	C	2.79417400	-2.10071500	-1.01590300
H	0.82899500	-3.43817000	-2.36498400	H	1.65042900	-0.87778200	-2.34695200
H	1.27883600	-3.12461100	1.89613300	C	3.22119600	-1.17566800	1.16177300
H	0.89128600	-4.51691000	-0.12436200	H	2.41260400	0.77640200	1.53586900
TS _{IM_2}				C	3.36478400	-2.21873200	0.25035400
C	-1.83105400	0.58465300	-1.28179200	H	2.91717300	-2.89432000	-1.74788200

H	3.68114300	-1.24579800	2.14348000	C	3.63599500	-0.16867100	1.35953500
H	3.92997900	-3.10736500	0.51688100	H	2.28204700	1.45254700	0.90281500
IM3 ₂				C	4.11726100	-1.41943600	0.97631500
C	-1.80408100	0.05438700	-1.45234500	H	4.01628900	-2.99189000	-0.49484500
O	-2.26329300	1.03185500	-1.99431900	H	4.01917600	0.30891300	2.25653000
O	-0.55305600	-0.32410400	-1.40215500	H	4.87348500	-1.91934000	1.57514000
C	-2.72344100	-0.97713300	-0.78336400	XII_A			
H	-3.74996100	-0.77185200	-1.08805200	C	0.33950700	-0.40385900	0.15846900
H	-2.43147400	-1.98258300	-1.09496900	C	-0.04690700	0.94441700	0.13759400
C	-3.12456200	0.39791100	1.22309600	C	0.93754800	-0.89737300	1.32778700
H	-2.33235100	1.10937200	0.95182700	C	0.14426600	1.77071300	1.24425900
H	-4.08336400	0.64824800	0.76754700	H	-0.52292000	1.36171900	-0.74650100
H	-3.21979500	0.33973600	2.30818600	C	1.13345100	-0.07502900	2.43813600
C	-3.67349200	-1.98749300	1.19611600	H	1.27480300	-1.92994400	1.36570200
H	-3.34976000	-2.96987400	0.84919900	C	0.73336600	1.26128500	2.40130600
H	-3.70118100	-1.97147200	2.28580800	H	-0.18319800	2.80552800	1.20449000
H	-4.66293400	-1.75738200	0.79883500	H	1.58929300	-0.48371800	3.33580400
C	-1.33496600	-1.28580500	1.27314400	H	0.87132000	1.89806100	3.27070200
H	-1.44212100	-1.41753900	2.35073600	Si	0.00035300	-1.54424100	-1.30732900
H	-0.98677800	-2.20842000	0.80819000	H	0.68756400	-2.83623700	-1.13670800
H	-0.65963300	-0.45350500	1.06008300	H	-1.47333200	-1.79077200	-1.32423900
N	-2.70122800	-0.95746300	0.72521000	H	0.33473200	-0.85795500	-2.57875200
Si	0.87115000	0.66125500	-1.66067000	C	3.54128900	-1.69794700	-0.40977600
H	1.20108200	0.24453200	-3.05339500	O	3.43392100	-2.76276400	0.20917200
H	0.64015400	2.10575900	-1.63290700	O	3.06935300	-1.32808300	-1.51013200
O	0.99850400	3.18626300	1.05456100	C	4.40829600	-0.66819100	0.39294300
C	-0.10362200	2.63329800	1.09140600	H	3.92297900	-0.49193900	1.35559400
H	-0.94410300	3.18102900	1.58648600	H	5.39904100	-1.09526600	0.56575700
O	-0.41519100	1.48622700	0.62276900	C	3.30475500	1.38296200	-0.43625700
C	2.16748000	-0.11756500	-0.56964800	H	2.71161200	0.76236600	-1.10610400
C	2.67505900	-1.36966200	-0.95269000	H	2.80734700	1.46557400	0.53125200
C	2.66414600	0.47984800	0.59836100	H	3.48883100	2.37394200	-0.85561700
C	3.63523900	-2.02341200	-0.18381300	C	5.46378200	1.51992700	0.67455800
H	2.32190400	-1.84115100	-1.86781500	H	6.42155600	1.02096200	0.82745000

H	5.62418000	2.50196200	0.22547800	H	0.55342800	-2.23916300	1.55493800
H	4.94830500	1.62927100	1.62939200	C	0.61297000	0.84326100	2.99959800
C	5.31702600	0.54890100	-1.55500200	H	0.10312800	2.68009800	1.99165200
H	5.46839100	1.54111300	-1.98394900	H	0.96453100	-1.14823300	3.74654700
H	6.27922000	0.06284800	-1.38549400	H	0.75464800	1.31697900	3.96684500
H	4.68094000	-0.07151300	-2.18720500	Si	0.15872700	-1.13580300	-1.20219500
N	4.62285300	0.69752100	-0.23785600	H	0.07518600	-2.57018500	-1.46245300
N	-3.53044100	-0.69450300	0.54426400	H	-2.04294200	-1.44924500	-1.25076900
C	-2.77029100	-0.98324800	1.76037700	H	-0.43003200	-0.19990900	-2.17848800
H	-1.96695200	-0.25295700	1.85106000	C	2.91227100	-1.25979200	-1.07250400
H	-3.40956100	-0.94810200	2.64860800	O	2.95192800	-2.28153600	-0.42154300
H	-2.33654900	-1.98118400	1.68507500	O	1.88045900	-0.73062200	-1.66780300
C	-3.41408200	0.58476900	-0.06798700	C	4.18032800	-0.40472800	-1.22418800
C	-3.22404400	0.71840300	-1.44548900	H	5.03541600	-0.99538300	-0.89504200
C	-3.42636700	1.72497900	0.73736500	H	4.31717900	-0.07636900	-2.25655500
C	-3.05126200	1.98028200	-2.00361800	C	3.71736900	0.48714200	1.04109500
H	-3.20204700	-0.16470100	-2.07158600	H	2.67221900	0.17761300	1.03928800
C	-3.23654700	2.98379400	0.17474500	H	4.34318500	-0.32947700	1.40116700
H	-3.57632000	1.62456800	1.80740500	H	3.83434000	1.37236400	1.66573500
C	-3.04798700	3.11865900	-1.19819600	C	5.51826600	1.41741500	-0.32307300
H	-2.90218000	2.07175200	-3.07494500	H	5.85471100	1.59969000	-1.34437500
H	-3.24550200	3.86137000	0.81420500	H	5.49141100	2.35578600	0.23165200
H	-2.90506300	4.10013200	-1.63897400	H	6.18819800	0.71326400	0.17091500
C	-4.38909500	-1.67006000	0.13298300	C	3.19971800	1.86475300	-0.92099200
O	-4.51133900	-2.74897800	0.68498000	H	3.17876800	2.71523300	-0.23934100
O	-5.12358400	-1.32838900	-0.95026100	H	3.56405300	2.16853700	-1.90297900
H	-5.68533700	-2.09321000	-1.12541000	H	2.20945700	1.42566900	-1.00847100
TS ₁₂₋₁₃				N	4.14086600	0.83860900	-0.35874800
C	0.21201700	-0.39269300	0.51005000	N	-2.92228500	-0.72481600	0.47789600
C	0.06868000	0.99380700	0.65337600	C	-2.92519000	-0.87309900	1.91098100
C	0.52009600	-1.15891000	1.64396600	H	-2.14638500	-0.26408700	2.39408300
C	0.26093400	1.61024300	1.89106300	H	-3.89781800	-0.59603700	2.33842100
H	-0.24564800	1.59940400	-0.19466300	H	-2.70697100	-1.92057100	2.12222300
C	0.73278200	-0.54319300	2.87508400	C	-3.18316600	0.48558000	-0.10002700

C	-3.40374400	0.61392900	-1.49547700	H	5.39772400	-0.47352400	-0.35213100
C	-3.21932600	1.67673900	0.66585500	H	4.69401500	-0.50026700	-2.00214800
C	-3.55948600	1.86267100	-2.08077500	C	3.56398600	1.34512500	0.60152100
H	-3.49447700	-0.27731700	-2.10512100	H	2.62649100	0.80521500	0.72197500
C	-3.39244300	2.91680100	0.06086700	H	4.29672400	0.96959200	1.31594400
H	-3.09462200	1.62792700	1.74126500	H	3.39691000	2.41370200	0.73911800
C	-3.54265600	3.03415900	-1.31970900	C	5.28324800	1.96979700	-1.01039800
H	-3.72687700	1.91890500	-3.15353600	H	5.70148800	1.74674200	-1.99261000
H	-3.41174100	3.80674100	0.68599000	H	4.98790500	3.01910500	-0.96205500
H	-3.68206300	4.00417600	-1.78639200	H	6.02164600	1.75652900	-0.23690100
C	-2.50357800	-1.92112300	-0.32482100	C	3.02258800	1.48998300	-1.77961500
O	-1.72068500	-2.74101600	0.30562400	H	2.70910700	2.51433800	-1.57450900
O	-3.70030500	-2.54156700	-0.83818700	H	3.44926400	1.41301600	-2.78060700
H	-3.53875600	-3.47156900	-0.64276700	H	2.19830600	0.78589700	-1.67512200
XIII				N	4.08277400	1.11498600	-0.78653900
C	0.41666800	-0.50490800	0.73064300	N	-2.85660500	-0.84337100	0.30868300
C	-0.07435700	0.76191100	0.38403100	C	-2.80459600	-1.10693400	1.73297900
C	0.96053200	-0.66773200	2.01307300	H	-2.00680400	-0.53720200	2.22730000
C	-0.03141500	1.82865200	1.28064500	H	-3.76416500	-0.86651100	2.20390500
H	-0.53197500	0.91753100	-0.59065900	H	-2.59838000	-2.16667500	1.87945300
C	1.01036300	0.39556500	2.91550800	C	-3.38654000	0.34459100	-0.16514300
H	1.36710100	-1.63204000	2.30408800	C	-3.86265500	0.48293700	-1.48513000
C	0.51356900	1.64736300	2.55188900	C	-3.46130300	1.47203300	0.67698600
H	-0.45008500	2.78931300	0.99440300	C	-4.33955200	1.70563300	-1.94382000
H	1.43382800	0.24466200	3.90448100	H	-3.90489300	-0.37725700	-2.14311900
H	0.53696100	2.47087100	3.26006800	C	-3.95551900	2.68362300	0.20684000
Si	0.28316600	-1.95245000	-0.47354800	H	-3.10989000	1.40431000	1.69985700
H	0.99788600	-3.18156600	-0.10427500	C	-4.38800900	2.82169400	-1.11000000
H	-2.27039300	-1.44544500	-1.56572600	H	-4.70430800	1.77578100	-2.96482100
H	0.07153500	-1.51837200	-1.87796900	H	-3.99666400	3.53173200	0.88512100
C	3.38942300	-1.31377000	-0.42771800	H	-4.77531600	3.76823900	-1.47263500
O	3.65990400	-1.96811400	0.57715800	C	-2.45252200	-1.90045000	-0.58029200
O	2.32479400	-1.27432500	-1.11829800	O	-1.31956100	-2.55520100	-0.14298200
C	4.48944800	-0.33957900	-0.94100500	O	-3.49242700	-2.85101300	-0.68242700

H	-3.06334300	-3.69868100	-0.83932700	N	1.84989200	1.23719900	-0.80739000
X				C	0.94749400	1.33305100	0.41139900
C	-1.21173200	-1.57056200	0.05546500	H	0.01287900	0.83428800	0.14639900
C	-1.26568200	-2.08434300	-1.25286300	H	0.74061300	2.39540700	0.56148700
C	-0.18193700	-2.00141400	0.90453700	C	1.48778500	0.72302100	1.74799200
C	-0.33169400	-3.01717700	-1.68831700	O	0.63950000	0.82214400	2.65044800
H	-2.05631400	-1.75543800	-1.92394100	O	2.63479300	0.23003200	1.74919200
C	0.75249400	-2.93094200	0.45264100	TS ₁₀₋₁₁			
H	-0.08814300	-1.59687700	1.90611900	C	1.91035000	0.50060100	0.14265400
C	0.68721500	-3.45054900	-0.83758100	C	2.37810800	0.83811100	-1.13165000
H	-0.40502000	-3.41262000	-2.69737200	C	1.16176600	1.41023500	0.88152500
H	1.54537100	-3.23797200	1.12741600	C	2.08059600	2.08454900	-1.66746300
H	1.41447100	-4.18103600	-1.17630300	H	2.97005300	0.12833600	-1.70314100
C	-2.32828200	-0.33520100	1.87787100	C	0.87092800	2.66043500	0.33386900
H	-1.43253000	0.14913200	2.27893300	H	0.75156100	1.15497600	1.85218100
H	-3.17125400	0.34984500	1.98896200	C	1.32359000	3.00130600	-0.93517200
H	-2.53467100	-1.24450400	2.46057200	H	2.44569700	2.34093400	-2.65696600
N	-2.15684000	-0.61757200	0.45382400	H	0.25347100	3.34351800	0.90650500
C	-2.93236400	2.13127900	-0.61464100	H	1.08916900	3.97325500	-1.35723200
O	-1.89409500	2.50506600	-0.99030500	C	1.82284000	-1.12562000	2.03277600
O	-3.98910500	1.79184200	-0.26360600	H	0.74464700	-1.01215300	2.19165500
H	-3.04190000	-0.75903800	-0.01542900	H	2.13226200	-2.14934600	2.25242800
C	1.14946600	1.85338400	-1.96778000	H	2.35756000	-0.44253000	2.69454900
H	0.21888700	1.31447900	-2.14472300	N	2.21162900	-0.82714900	0.63832400
H	0.92492400	2.89568900	-1.73984800	C	1.80872300	-1.93588000	-0.32418400
H	1.79452200	1.79176300	-2.84657800	O	0.68425900	-2.19288000	-0.67964600
C	2.13693300	-0.19861100	-1.12503000	O	2.97148500	-2.41676500	-0.58667800
H	2.77358600	-0.23429900	-2.01131800	H	3.25841100	-1.47230600	0.19064300
H	2.62767300	-0.63421100	-0.25612600	C	-2.49608900	-1.77491700	-1.56609700
H	1.19003200	-0.70402800	-1.31799100	H	-1.50047500	-2.21932900	-1.56709800
C	3.13159900	1.96466800	-0.55494600	H	-3.20774700	-2.45239600	-1.09213900
H	2.89924200	3.01021200	-0.34552300	H	-2.81706300	-1.55602700	-2.58638300
H	3.60406900	1.49711100	0.30961200	C	-1.45393200	0.41725800	-1.42754100
H	3.75569800	1.89242200	-1.44771200	H	-1.75032300	0.57935300	-2.46546200

H	-1.44854800	1.34899800	-0.86492300	C	-2.91713400	1.43352400	-1.68024600
H	-0.47566500	-0.06200800	-1.38338000	H	-2.32608300	0.88936000	-2.41815100
C	-3.80207700	0.13849400	-0.79377900	H	-3.94366600	1.06447100	-1.67648600
H	-4.51815300	-0.56514000	-0.36578100	H	-2.90591700	2.50185600	-1.90262000
H	-3.73798600	1.03910100	-0.18241400	C	-0.88334500	1.66810700	-0.37658300
H	-4.07474900	0.36615800	-1.82605000	H	-0.87086800	2.72032500	-0.66608000
N	-2.45158500	-0.50148000	-0.78909900	H	-0.45201900	1.53162000	0.61278400
C	-2.01976000	-0.82804400	0.62936900	H	-0.35026700	1.06139200	-1.11114400
H	-1.09292800	-1.39419700	0.53261200	C	-3.06253100	2.00345100	0.69183300
H	-2.79069300	-1.47960200	1.04995500	H	-4.11132200	1.70264200	0.66614300
C	-1.78433200	0.37549100	1.59424700	H	-2.62214100	1.77821200	1.66298900
O	-1.17191900	0.01468600	2.61750600	H	-2.97169700	3.06328600	0.44824100
O	-2.19796000	1.50229600	1.25188400	N	-2.31405500	1.21340900	-0.33304600
XI				C	-2.40184500	-0.26853100	-0.02650100
C	1.97703000	-0.24291000	-0.03214900	H	-2.01488900	-0.78700300	-0.90429800
C	2.63640100	0.36964100	-1.09944800	H	-3.46508600	-0.50516700	0.07220500
C	1.96704300	0.36918700	1.22399900	C	-1.67065500	-0.76567500	1.25716500
C	3.26544400	1.59704800	-0.90922400	O	-1.52603100	-2.01448700	1.25935300
H	2.63727000	-0.10831300	-2.07089600	O	-1.34305000	0.06512700	2.11811600
C	2.61121200	1.58983400	1.40781300	XII_B			
H	1.41855400	-0.08696900	2.04229600	C	4.10596300	-0.29326500	-0.39086200
C	3.25810300	2.21177300	0.34192200	C	5.05305300	0.61579900	-0.86070000
H	3.77262400	2.06938800	-1.74503100	C	4.29365000	-0.91384400	0.84444400
H	2.59160900	2.06020600	2.38595500	C	6.18325800	0.90483000	-0.09985100
H	3.75600300	3.16567700	0.48522700	H	4.89848300	1.10066400	-1.81999300
C	1.49694400	-2.50683200	0.84590500	C	5.41661200	-0.61232700	1.60842400
H	0.76004100	-2.41197800	1.64927100	H	3.54898600	-1.61527500	1.20486500
H	1.40443300	-3.49649000	0.39724200	C	6.36623400	0.29368300	1.13819200
H	2.50510300	-2.39435500	1.24731000	H	6.91587000	1.61466600	-0.47134600
N	1.30638200	-1.49056400	-0.19326700	H	5.55235500	-1.09147500	2.57286600
C	0.35782000	-1.63961600	-1.17591000	H	7.24435900	0.52176100	1.73406900
O	0.22704200	-0.86206500	-2.11444600	C	3.23262800	-1.29805400	-2.46726900
O	-0.44715100	-2.70244700	-1.03563900	H	3.75907500	-2.24122500	-2.28768400
H	-0.85137300	-2.68110000	-0.12129700	H	2.27431200	-1.50220000	-2.94244800

H	3.84226800	-0.67815100	-3.13252800	H	-2.64565100	4.47826000	-0.10632900
N	2.97985200	-0.61526200	-1.20750700	C	-1.15998800	1.66020700	-1.24518200
C	1.68687000	-0.38513700	-0.81025900	H	-1.70294400	1.63916100	-2.19091900
O	0.71571300	-0.71914900	-1.48667800	H	-0.17480500	2.10858700	-1.37764300
O	1.60824900	0.25679600	0.34493900	H	-1.04569000	0.65145700	-0.85423300
H	0.66389600	0.24260400	0.71826000	N	-1.93622200	2.49218700	-0.26975200
Si	-1.54285300	-2.57103700	1.49397500	TS ₁₂₋₁₄			
H	-0.16155300	-2.41843300	0.98684200	C	3.67098200	0.04410500	-0.41022300
H	-1.81686400	-4.04143800	1.55755600	C	3.63818100	1.27935900	-1.06070400
H	-1.74040900	-2.03661200	2.85622800	C	4.31606800	-0.06132000	0.82538100
C	-2.79580300	-1.86132900	0.27407100	C	4.21201800	2.40061300	-0.46652600
C	-4.11721300	-1.60131900	0.66728500	H	3.14074800	1.37310400	-2.02009600
C	-2.45857500	-1.65222200	-1.07157200	C	4.87329800	1.06265700	1.42072300
C	-3.41182600	-1.21819000	-1.99366500	H	4.35254000	-1.02598000	1.31675300
C	-4.72471000	-0.98241500	-1.58786400	C	4.82130900	2.30098800	0.78072600
C	-5.07419700	-1.16837500	-0.25059900	H	4.17009000	3.35823900	-0.97715500
H	-1.43341000	-1.80685600	-1.39895400	H	5.35826800	0.96991700	2.38766400
H	-3.12846200	-1.07281700	-3.03283500	H	5.26138900	3.17711800	1.24666000
H	-5.47102800	-0.65824500	-2.30791900	C	3.14587800	-1.21005700	-2.45319000
H	-6.09250500	-0.98073300	0.07790700	H	4.11771800	-0.85026600	-2.79562900
H	-4.40420800	-1.72996100	1.70773000	H	3.01516200	-2.25327800	-2.73901100
C	-1.44644000	1.14773400	1.82826800	H	2.34991300	-0.62093400	-2.93747100
O	-2.34685300	1.12455700	2.66825600	N	3.09446000	-1.11526200	-1.00263500
O	-0.68727900	0.20971700	1.44670200	C	1.92495800	-1.70719400	-0.47896600
C	-1.25094800	2.50326200	1.08348500	O	1.43471900	-2.71294500	-0.98980300
H	-1.71432700	3.30304800	1.66257500	O	1.87507100	-1.61779900	0.96487300
H	-0.19592800	2.72066400	0.89917600	H	1.47440200	-2.46251400	1.21538000
C	-3.32111100	1.93311300	-0.14228400	Si	0.37634400	-0.05473300	0.96684300
H	-3.25450200	0.87656600	0.111136400	H	0.91665500	-0.51318100	-0.62853400
H	-3.84352800	2.46252100	0.65428200	H	0.22789500	-0.12702700	2.46896300
H	-3.82794600	2.05282500	-1.10009900	H	1.51381700	0.90507300	0.90910900
C	-2.01399800	3.89159900	-0.77427900	C	-1.06076900	-1.33678300	0.63143100
H	-1.00916800	4.31481900	-0.80195900	C	-1.89664800	-1.69503000	1.69814800
H	-2.44152800	3.88399200	-1.77810800	C	-1.38329500	-1.84589400	-0.63569100

C	-2.49384500	-2.66399800	-0.83525900	H	-1.32087100	0.49648300	-1.68518900
C	-3.31955400	-2.99630900	0.24054000	C	-4.26755300	-1.00888100	-0.93714300
C	-3.01677800	-2.51014700	1.51116700	H	-5.62312000	-0.36713200	0.60845400
H	-0.72836600	-1.62138600	-1.47433800	H	-2.70631300	-1.42639700	-2.35676100
H	-2.70092200	-3.06592600	-1.82389100	H	-4.85514500	-1.87859700	-1.21063300
H	-4.17938500	-3.64409500	0.09229400	C	-1.69763600	2.54610400	1.61662500
H	-3.64724600	-2.76904200	2.35778100	H	-1.36137300	1.62601900	2.10259100
H	-1.67681000	-1.30918200	2.69138900	H	-0.93812600	3.32198300	1.71292100
C	-1.81767900	1.80812500	1.07450000	H	-2.61362700	2.89820900	2.09878800
O	-2.14496400	1.68669300	2.24060700	N	-1.91562600	2.30169300	0.19610300
O	-0.78821600	1.34111400	0.45640300	C	-1.29264500	3.07383900	-0.73019600
C	-2.74050800	2.61185000	0.13224900	O	-0.44881900	3.92832700	-0.47953300
H	-3.51538800	3.09631500	0.72689700	O	-1.28129300	-3.62708600	-1.27311300
H	-2.17472900	3.35244100	-0.43735400	H	-1.32190700	-4.39629700	-0.70134600
C	-4.04431700	0.53731800	-0.16498600	Si	0.12868700	-2.69121700	-1.18598700
H	-3.24337100	-0.09604700	0.21512300	H	-1.61414300	2.85353400	-1.75927300
H	-4.65601800	0.89784900	0.66220900	H	1.29335300	-3.52229200	-1.54933600
H	-4.64574700	-0.02442100	-0.87945100	H	-0.20749800	-1.62861600	-2.14955400
C	-4.53892600	2.51281500	-1.51016300	C	0.28268700	-2.11813200	0.60607200
H	-4.11112800	3.40968800	-1.95982500	C	1.49701200	-2.23620700	1.29908500
H	-5.01446500	1.90248800	-2.27895800	C	-0.81453000	-1.57472100	1.29110500
H	-5.27092300	2.78961800	-0.75108000	C	-0.69538600	-1.12763300	2.60750800
C	-2.50382500	1.24740600	-1.93815100	C	0.52493900	-1.23501600	3.27300700
H	-3.04657800	0.56271900	-2.59034200	C	1.61937400	-1.79953900	2.61745000
H	-2.15465200	2.11666200	-2.49704100	H	-1.77869600	-1.49871200	0.79488400
H	-1.66221700	0.74617000	-1.46536000	H	-1.56204000	-0.71481100	3.11759600
N	-3.44755000	1.72163700	-0.87067400	H	0.61818400	-0.89814800	4.30185300
XIV_B				H	2.56969500	-1.90627600	3.13305500
C	-2.72508800	1.19776300	-0.20362400	H	2.36639100	-2.65099300	0.79519700
C	-3.92859800	0.93852800	0.45405000	C	3.22959600	-0.75207700	-0.91410800
C	-2.29105800	0.34617800	-1.22155200	O	4.08675800	-1.61941000	-0.71889400
C	-4.69123000	-0.16730300	0.08920800	O	2.10840600	-0.81847300	-1.47774200
H	-4.27288600	1.59615900	1.24499700	C	3.66066600	0.63253200	-0.32996400
C	-3.06890400	-0.74624500	-1.59418200	H	3.99437700	0.47764700	0.69827500

H	4.49873200	1.02177300	-0.91391700	H	3.13046200	-0.20813100	2.36722400
C	1.42219000	1.26292200	0.50523200	Si	3.12744100	1.63849400	-1.90307300
H	0.94429400	0.44938300	-0.03644000	H	2.27170900	2.49404900	-1.04366900
H	1.76690600	0.89461000	1.47301000	H	2.33795700	1.20488200	-3.08238500
H	0.75946300	2.11660400	0.62916500	H	4.28929600	2.44908500	-2.34844900
C	3.18163700	2.92658500	0.37954700	C	3.73179200	0.12595500	-0.96991000
H	4.07044400	3.24707600	-0.16546900	C	3.11103400	-1.11929700	-1.13333900
H	2.43036200	3.71838800	0.37383100	C	4.81376500	0.21386500	-0.08091000
H	3.45002600	2.67143600	1.40559700	C	5.25940000	-0.90412300	0.62147600
C	2.18062800	2.10033800	-1.67208200	C	4.62752100	-2.13525000	0.44429500
H	1.43123900	2.88966900	-1.59272400	C	3.55205000	-2.23999700	-0.43356700
H	3.05826900	2.46195500	-2.21086200	H	5.31766600	1.16571500	0.06894500
H	1.78935200	1.20035300	-2.14590400	H	6.10425400	-0.81745600	1.29884600
N	2.60934400	1.72158700	-0.28624000	H	4.97704200	-3.00926900	0.98596700
XII_{2A}				H	3.05172400	-3.19353700	-0.57261700
C	0.16514900	0.08449700	0.27194500	H	2.26369300	-1.21814400	-1.80766200
C	-0.22470600	0.46422100	-1.01736500	O	-2.81174300	2.36724500	-0.52587300
C	0.06438100	-1.26263300	0.64257800	C	-3.66694700	1.47256200	-0.61445900
C	-0.66998500	-0.48849200	-1.92869500	O	-4.62821900	1.32183700	-1.39665300
H	-0.21072300	1.50812000	-1.30563600	C	-3.43395000	0.37472800	0.47909500
C	-0.36452600	-2.21172200	-0.28048300	H	-2.43754200	-0.05049500	0.34868000
H	0.34649400	-1.56741500	1.64181300	H	-3.49031400	0.83842600	1.46716700
C	-0.72709500	-1.83432800	-1.57372000	C	-4.35363700	-1.52245600	-0.81448500
H	-0.97285300	-0.16727700	-2.91990100	H	-5.03242100	-2.37590600	-0.76175900
H	-0.40984800	-3.25635100	0.01524900	H	-4.65329900	-0.80988600	-1.58282200
H	-1.05344400	-2.57886800	-2.29361700	H	-3.32936700	-1.85701800	-0.98338400
C	0.03723300	2.43015300	1.09250200	C	-3.96745300	-1.73773000	1.57641400
H	-0.97350500	2.36973000	0.68194300	H	-3.99587800	-1.21580500	2.53371700
H	0.01139500	2.86297600	2.09257400	H	-4.64611300	-2.59275900	1.59892800
H	0.64952700	3.08007400	0.45876600	H	-2.94874400	-2.06915700	1.36871300
N	0.61003000	1.08199500	1.18138000	C	-5.78519000	-0.32332700	0.76670700
C	1.76098100	0.97551400	1.91877500	H	-6.45597600	-1.18431500	0.78655400
O	2.29908300	1.91377200	2.47692800	H	-5.79514400	0.18115500	1.73417500
O	2.24436700	-0.28113800	1.99124700	H	-6.04660100	0.37363100	-0.03012400

N	-4.39437800	-0.80221400	0.49854400	H	8.08990100	-1.26082000	0.98546400
TS _{12-14_2}				H	7.92689800	1.15519500	0.43927200
C	-0.36108100	0.19037300	-0.17357600	H	5.72786800	2.16727700	-0.04562200
C	-0.65826200	-0.16964600	1.14338800	O	-2.97016800	-2.48004700	0.65107400
C	-0.68435500	1.47534900	-0.62280500	C	-3.95097800	-1.72538100	0.73814100
C	-1.24062100	0.75450200	2.00639000	O	-4.92191000	-1.71597200	1.52296200
H	-0.46198700	-1.17712500	1.49015800	C	-3.88885500	-0.61233200	-0.36328400
C	-1.24597500	2.40284900	0.24978300	H	-2.96515100	-0.04522000	-0.24018700
H	-0.47481300	1.74145700	-1.65195100	H	-3.87906600	-1.08582900	-1.34823300
C	-1.52012000	2.04812300	1.57098600	C	-5.07181200	1.13582100	0.92392500
H	-1.47039500	0.45807800	3.02449900	H	-5.86307000	1.88583400	0.86796400
H	-1.46275000	3.40725200	-0.10302100	H	-5.26587800	0.39426300	1.69875300
H	-1.94801800	2.77436400	2.25576100	H	-4.10413100	1.61218900	1.08588800
C	-0.11474600	-2.15454100	-0.91321200	C	-4.73928400	1.38857400	-1.47120200
H	-1.16489100	-2.22718300	-0.62081900	H	-4.69554300	0.86106200	-2.42484300
H	0.05529300	-2.65771000	-1.86481400	H	-5.53732800	2.13319300	-1.49378400
H	0.49632200	-2.65203600	-0.14879900	H	-3.78007500	1.86983600	-1.27403700
N	0.25220500	-0.73951700	-1.06423500	C	-6.32007500	-0.27479800	-0.63835200
C	1.60238700	-0.57364500	-1.38501500	H	-7.11070000	0.47745400	-0.65604700
O	2.26013900	-1.36908700	-2.02648200	H	-6.26104100	-0.77973000	-1.60385800
O	1.89932000	0.89922700	-1.67479200	H	-6.46744400	-0.99902200	0.16369200
H	2.38904900	0.91476900	-2.51228000	N	-5.01400300	0.40807200	-0.38414500
Si	2.95994400	1.17747700	-0.05135500	XIV_{2A}			
H	2.20050100	-0.32044300	-0.03723100	C	-1.81529100	-1.99448600	0.07542700
H	3.39782600	2.46864600	-0.69010300	C	-3.12659800	-2.28821200	-0.29726800
H	2.16141700	1.63425700	1.11563000	C	-1.49190800	-1.86381600	1.43016400
C	4.61479700	0.34190000	0.25648200	C	-4.10235500	-2.44866200	0.67934800
C	5.78709000	1.11103400	0.20718200	H	-3.40167500	-2.34980900	-1.34326200
C	4.72826400	-1.02153500	0.56015400	C	-2.46929400	-2.06198500	2.40057600
C	5.96909800	-1.59561000	0.82305800	H	-0.48888800	-1.57432400	1.72962600
C	7.12145800	-0.81235800	0.78508500	C	-3.77958500	-2.34956700	2.02936100
C	7.03042300	0.54349300	0.47670100	H	-5.12631600	-2.63425300	0.37518600
H	3.83825400	-1.64522900	0.57291000	H	-2.20814200	-1.95762200	3.44914100
H	6.03915500	-2.65533200	1.04818500	H	-4.54832100	-2.46935200	2.78524300

C	-1.15657000	-1.20700100	-2.22117400	C	-0.55227000	3.37749000	-0.27836400
H	-2.13460200	-0.72390700	-2.17134000	H	-0.85640500	4.15899000	-0.97599300
H	-0.40073400	-0.47250100	-2.50352500	H	-0.09433100	3.82619900	0.60542900
H	-1.16940800	-1.98810000	-2.98679600	H	0.15171500	2.69241800	-0.75504800
N	-0.81298800	-1.78101700	-0.91788600	C	-2.71131600	3.52630700	0.85198000
C	0.46227000	-2.16718500	-0.70415000	H	-2.21334100	3.92326900	1.73842700
O	1.40367900	-1.88688600	-1.45004600	H	-2.97267300	4.34107800	0.17458500
O	1.51048900	0.86516100	-0.89342300	H	-3.59654900	2.94270300	1.10755500
H	1.51106500	0.04391200	-1.41639400	N	-1.76309400	2.61279900	0.14315400
Si	2.32762600	0.70086900	0.55437000	XII_{2B}			
H	0.60889500	-2.75907000	0.20960000	C	-3.65673900	2.19737900	1.69084800
H	2.21890000	2.02686400	1.21604400	C	-2.35163100	2.47305000	1.28471200
H	1.61827000	-0.30747500	1.39443900	C	-1.95518300	2.32088100	-0.05226300
C	4.12182600	0.23792400	0.35402800	C	-2.91944800	1.89806500	-0.97693100
C	5.13783800	1.07736600	0.83195200	C	-4.22904600	1.63002100	-0.58059900
C	4.48664300	-0.96159900	-0.27974500	C	-4.59988600	1.77313800	0.75579000
C	5.82758300	-1.30478100	-0.43042000	H	-3.93987000	2.32519800	2.73179000
C	6.82501200	-0.45868600	0.05263000	H	-1.63065200	2.81194200	2.02606600
C	6.48040600	0.73302200	0.68555900	H	-2.63306900	1.74980500	-2.01398600
H	3.71761900	-1.62655500	-0.66777600	H	-4.96217900	1.31117700	-1.31654600
H	6.09432200	-2.23273600	-0.92677300	H	-5.62151100	1.57015000	1.06435100
H	7.87040000	-0.72642800	-0.06779700	C	-0.20942200	-1.35692100	-1.73858400
H	7.25453100	1.39608400	1.05955900	O	0.81967300	-1.74431200	-2.31856100
H	4.88402700	2.01458000	1.32199100	O	-0.78426400	-0.24761000	-1.76012400
O	-3.92924000	0.45399200	-1.90092700	C	-0.80767300	-2.49002700	-0.84617700
C	-3.64831900	1.07760400	-0.86268800	H	-0.98598300	-3.36889100	-1.47027000
O	-4.17717200	1.07428500	0.26652800	H	-0.08333900	-2.74761200	-0.06940900
C	-2.41548600	2.02201100	-1.09166800	C	-3.17681700	-1.84779700	-1.11491300
H	-1.62842300	1.47511700	-1.61329300	H	-2.85487000	-0.94652700	-1.63521200
H	-2.72699900	2.86164300	-1.71894400	H	-3.28415000	-2.67833600	-1.81499400
C	-1.34560700	1.50242900	1.05682400	H	-4.11166400	-1.67957400	-0.57780800
H	-0.81229400	1.93186800	1.90725400	C	-2.51063400	-3.41541500	0.63121300
H	-2.24319300	0.97004300	1.36966200	H	-1.71541800	-3.66563800	1.33452400
H	-0.68558100	0.84126900	0.49385300	H	-3.43769900	-3.21040700	1.16992100

H	-2.66254400	-4.23774800	-0.06936700	C	-1.53015300	2.23635600	-1.63427100
C	-1.93131600	-1.06720100	0.84278400	C	-2.43335500	3.29195200	-1.52616200
H	-2.89891800	-0.83407800	1.29097300	C	-2.84591700	3.72933300	-0.26819400
H	-1.21376800	-1.39339900	1.59600500	H	-2.63710800	3.46162700	1.85767200
H	-1.55465100	-0.21380500	0.28373000	H	-1.02489800	1.58196200	1.65319300
N	-2.11164000	-2.19654800	-0.12672900	H	-1.23057400	1.90167100	-2.62488900
Si	-0.15810900	2.60789200	-0.55475700	H	-2.81234500	3.77413000	-2.42258200
H	0.25021200	3.92521700	0.01328700	H	-3.55081300	4.55099800	-0.18011400
H	0.70534700	1.57312100	0.05030400	C	-1.61578600	-2.08472300	-1.33384800
H	-0.03335300	2.65574200	-2.02631100	O	-0.83597400	-3.00463800	-1.47085600
N	2.56461600	-1.24819900	0.74002300	O	-1.41015600	-0.81983600	-1.52911200
C	2.87675700	-2.50279100	0.05258600	C	-3.04818700	-2.42014100	-0.86675200
H	3.95573100	-2.54342200	-0.11061300	H	-3.75605000	-2.29015000	-1.68976400
H	2.57349300	-3.33287700	0.69054300	H	-3.05598400	-3.46053000	-0.54058500
H	2.35455500	-2.55866000	-0.90840300	C	-3.97852800	-0.21693000	-0.16555500
C	3.18367700	-0.04797500	0.25006300	H	-3.14765700	0.24475800	-0.69329500
C	2.99536500	0.30777500	-1.08456400	H	-4.83951200	-0.32672100	-0.82653200
C	3.98502300	0.72597800	1.08689700	H	-4.24300200	0.37400800	0.711172800
C	3.60783600	1.45886600	-1.57374500	C	-4.75730200	-2.28127700	0.85691800
H	2.35114400	-0.29425200	-1.72253800	H	-4.44753000	-3.23284900	1.28994900
C	4.58021900	1.88247800	0.59163000	H	-5.19802300	-1.64877600	1.62829900
H	4.12451500	0.43103700	2.12143600	H	-5.48168500	-2.45271900	0.05971000
C	4.39433000	2.25054600	-0.74011900	C	-2.52012900	-1.47828900	1.37329600
H	3.45167600	1.74073300	-2.61014800	H	-2.98432800	-1.03349200	2.25338200
H	5.19528500	2.49277500	1.24556800	H	-2.15020300	-2.47862400	1.60076200
H	4.86159600	3.15149300	-1.12549600	H	-1.69179600	-0.84933800	1.05370600
C	1.59591300	-1.24214300	1.67674900	N	-3.56139200	-1.58615400	0.29160900
O	0.92349800	-2.21801400	2.01301600	Si	0.09235500	0.09000200	-0.79101500
O	1.40431500	-0.03424800	2.25160800	H	1.25494900	0.80341700	0.33553200
H	0.70905700	-0.16439100	2.90637000	H	0.32425800	-1.05338300	0.10494200
TS _{12-13_2}				H	0.91875300	0.23200700	-2.00334900
C	-2.33544900	3.11411500	0.87309900	N	2.62082500	-0.35757700	1.45388000
C	-1.42946000	2.05876500	0.76275800	C	2.44309500	-1.62229000	2.13670700
C	-1.01779000	1.59358700	-0.49544000	H	3.38815900	-1.94160000	2.58955500

H	1.70061700	-1.47506000	2.91849300	H	-1.72380500	-3.55859100	0.23058500
H	2.08767800	-2.41676800	1.46308800	C	-3.85400300	-0.92882100	-0.07038800
C	3.54315000	-0.26898500	0.41549900	H	-3.19676900	-0.34541900	-0.71386600
C	4.27949800	-1.39833500	0.00493600	H	-4.59487800	-1.46760100	-0.66354400
C	3.76606900	0.94150900	-0.27450900	H	-4.34448700	-0.29469000	0.66967200
C	5.18855700	-1.31792100	-1.04543200	C	-3.87158300	-2.78662300	1.50170100
H	4.14223700	-2.35227200	0.49855900	H	-3.25028000	-3.50335500	2.04003800
C	4.66906600	0.99951500	-1.32926800	H	-4.40578300	-2.15187700	2.21107900
H	3.25656600	1.84185400	0.04182400	H	-4.58489800	-3.31926600	0.87167900
C	5.39062800	-0.12326000	-1.72989900	C	-2.00599900	-1.22577300	1.50576500
H	5.73741300	-2.21052800	-1.33273000	H	-2.54722500	-0.60669500	2.22359000
H	4.81751800	1.94935600	-1.83556500	H	-1.40405300	-1.97279300	2.02641500
H	6.09971200	-0.06616000	-2.54949600	H	-1.36899500	-0.61133800	0.87244700
C	1.53677200	0.60516400	1.58298900	N	-3.00329400	-1.93425400	0.64382000
O	0.51156100	0.25034600	2.24580000	Si	0.15915700	1.72231000	-0.46529300
O	2.06408500	1.88168700	1.89143100	H	2.27694400	1.37955600	1.48187300
H	1.34984800	2.30992800	2.37495500	H	0.94651400	2.96565900	-0.22204700
XIII₂				H	0.58142500	1.12566600	-1.74325800
C	-3.67746600	2.70273900	0.82235500	N	2.43143800	-0.34547200	0.38683300
C	-2.31404700	2.41489900	0.78341100	C	1.76321400	-1.51932100	-0.16379700
C	-1.67297700	2.10215900	-0.42343000	H	2.46385400	-2.35739100	-0.20092100
C	-2.44056300	2.08685500	-1.59518400	H	0.94185700	-1.79414100	0.49922300
C	-3.80207500	2.38434500	-1.56504500	H	1.34299900	-1.34992800	-1.15946200
C	-4.42353400	2.69133000	-0.35552500	C	3.77295200	-0.09309500	0.09164700
H	-4.15510000	2.94647400	1.76725600	C	4.30823300	-0.52429100	-1.13345000
H	-1.74257800	2.43006000	1.70868200	C	4.62101000	0.57223600	0.99289200
H	-1.97684100	1.80707300	-2.53667100	C	5.63999100	-0.27806400	-1.44795400
H	-4.37864300	2.36850300	-2.48513800	H	3.67372400	-1.03868500	-1.84696200
H	-5.48433700	2.92357200	-0.33082300	C	5.94546100	0.83290300	0.65495800
C	-1.28874900	-2.13124100	-1.35640200	H	4.26082100	0.84917400	1.97795600
O	-0.64902500	-2.97191300	-1.99752500	C	6.46859700	0.41116700	-0.56480500
O	-1.26915800	-0.87965200	-1.38540600	H	6.02867800	-0.62151200	-2.40213700
C	-2.27973400	-2.82216800	-0.35374400	H	6.57996300	1.34974700	1.36906100
H	-3.05059500	-3.34248500	-0.92812400	H	7.50607500	0.60464500	-0.81645200

C	1.72472900	0.44287100	1.32704700	C	-1.11584000	2.03661100	0.46252500
O	0.42245500	0.74688700	0.88584200	H	-2.61796800	1.33432500	-2.48670600
O	1.58562400	-0.24807400	2.54726000	H	-4.15727500	3.08602200	-1.66955100
H	0.98130900	0.26074500	3.09769500	H	-3.73317200	4.20124100	0.50635900
TS _{12-13_3}				H	-1.77349700	3.52333800	1.87575500
H	1.96620200	-2.26196900	-0.43504200	H	-0.29216900	1.70227900	1.09142900
Si	-0.15320600	0.08036500	-1.47533800	O	3.05804300	-1.98221400	-1.14277400
C	-2.30353200	-1.61387400	0.60276900	C	3.72862000	-0.94151700	-0.87813800
C	-2.81521800	-0.67017500	1.49314600	O	4.67843900	-0.47005400	-1.50774700
C	-3.05178900	-1.99332700	-0.51248700	C	3.26465300	-0.24913600	0.43066400
C	-4.06190600	-0.09721700	1.26316300	H	2.17455300	-0.14395300	0.43182100
H	-2.22661900	-0.35575500	2.34851500	H	3.54878600	-0.87343300	1.28266400
C	-4.29209000	-1.40786100	-0.74330100	C	3.51212000	2.05110800	-0.45251600
H	-2.64597300	-2.72520000	-1.20034100	H	3.88735200	3.04523500	-0.20421700
C	-4.80126400	-0.45909700	0.14129100	H	3.99199900	1.65768100	-1.34672500
H	-4.43956000	0.65453100	1.94860300	H	2.43012200	2.07160200	-0.58577300
H	-4.86254300	-1.69716800	-1.62029400	C	3.18234300	1.66090100	1.92365200
H	-5.76625100	0.00071400	-0.04612300	H	3.38845000	0.98310500	2.75276300
C	-0.64466800	-2.50420800	2.20525000	H	3.58804500	2.65053500	2.13958400
H	-1.54018900	-2.81523900	2.74358300	H	2.10649100	1.72402400	1.75669600
H	0.08203800	-3.31533100	2.20694100	C	5.31257000	1.06984200	0.89316700
H	-0.19998200	-1.63436200	2.71003300	H	5.67785000	2.07911700	1.09029500
N	-1.01587600	-2.18957600	0.83295000	H	5.51594700	0.42449200	1.74921600
C	0.01015300	-1.92316000	-0.03782600	H	5.75254600	0.65240500	-0.01196700
O	-0.30616000	-1.65261300	-1.30832800	N	3.83055300	1.13001800	0.68861400
O	1.13865900	-2.48124900	0.25352300	TS _{12-13_4}			
H	0.30891500	-0.27563800	0.22851900	H	2.97189500	-4.03741600	-0.19432900
C	-1.32245500	1.40361200	-0.77084600	Si	3.72828500	-0.94921700	-0.69496200
H	-0.66529400	0.05384800	-2.89205800	C	0.32384100	-0.72218600	-0.22339100
H	1.24809000	0.56385700	-1.65656500	C	0.12855700	0.27639700	0.72967700
C	-2.42824100	1.80940100	-1.52748800	C	0.16608700	-0.43803800	-1.58124500
C	-3.29658600	2.80177000	-1.07086200	C	-0.19270200	1.56661900	0.32233200
C	-3.06054400	3.42635500	0.15001000	H	0.23094000	0.05394000	1.78463500
C	-1.95909300	3.04505800	0.91765800	C	-0.14348900	0.85899300	-1.98131000

H	0.32240400	-1.21919200	-2.31507600	H	-4.65436500	2.35383700	-1.16380800
C	-0.31554000	1.86574100	-1.03225800	H	-4.20572500	1.96249700	0.54347400
H	-0.31962000	2.34151500	1.07039400	H	-2.95361000	1.97941500	-0.73642800
H	-0.22877500	1.08382600	-3.04040000	C	-3.96970500	0.01754400	-2.19265900
H	-0.52596300	2.88352900	-1.34737100	H	-4.15204800	-1.04202100	-2.37626500
C	0.13811100	-2.56585100	1.44827900	H	-4.62639800	0.62306200	-2.82031200
H	-0.82787400	-2.08991700	1.63437200	H	-2.92470500	0.25173400	-2.40188800
H	0.00603600	-3.64308100	1.35185200	C	-5.67241700	-0.01128100	-0.44337000
H	0.81848100	-2.36405300	2.28360100	H	-6.32043800	0.59738800	-1.07662100
N	0.70047000	-2.03707700	0.19815400	H	-5.83523900	-1.07055400	-0.64838400
C	1.87990200	-2.52993100	-0.22697500	H	-5.82652600	0.20060700	0.61507500
O	2.45375500	-2.12670000	-1.33142800	N	-4.24811600	0.31725800	-0.75981100
O	2.14527500	-3.75861200	0.21863900	XXIIA			
H	3.03231000	-1.59747700	0.68704600	C	0.67678600	-1.10093900	-0.63778600
C	3.46504700	0.79015300	0.02587200	O	1.34930300	-1.76260500	0.13448500
H	3.96680500	-0.54099500	-2.13406700	O	-0.63493900	-1.19299000	-0.74534700
H	5.01212400	-1.63655000	-0.35273700	H	1.17933000	1.58501100	0.35143800
C	3.37766700	1.89277900	-0.83211600	H	1.09987700	-0.37373300	-1.34224100
C	3.17171300	3.18145400	-0.33704400	N	0.40273400	1.32717500	0.96559500
C	3.06110000	3.38922200	1.03485900	C	0.74955000	1.10376100	2.34827700
C	3.15246300	2.30441400	1.90845500	H	1.78486400	0.75817000	2.39885000
C	3.34078100	1.02204200	1.40292700	H	0.65827500	2.01065100	2.96649700
H	3.46704700	1.73883600	-1.90502900	H	0.12454600	0.32137000	2.79487600
H	3.09947400	4.02083600	-1.02318500	C	-3.33655600	-1.62145000	-0.04414900
H	2.90398800	4.39065900	1.42553100	C	-4.33334900	-2.59079700	0.13702000
H	3.06564300	2.46067000	2.97994300	C	-3.69707400	-0.37921800	-0.58554000
H	3.37759000	0.17793300	2.08864600	C	-5.65785600	-2.32482000	-0.20320600
O	-2.55529900	-1.03691700	2.22376800	H	-4.07899000	-3.56736300	0.54350600
C	-3.39461800	-0.32692600	1.64587700	C	-5.01947600	-0.11277100	-0.92819100
O	-4.24497300	0.47049000	2.08990800	H	-2.94382800	0.38752500	-0.74179500
C	-3.31492300	-0.52402300	0.09398100	C	-6.00072300	-1.08355500	-0.73622900
H	-2.30298800	-0.29411400	-0.24275400	H	-6.41901500	-3.08552200	-0.05872300
H	-3.53257100	-1.56872400	-0.14280600	H	-5.27799600	0.85708800	-1.34161100
C	-4.00027800	1.77379400	-0.51008000	H	-7.03272300	-0.87474800	-1.00215800

Si	-1.58258300	-1.95619900	0.46434200	TS ₂₂₋₂₅			
H	-1.31868200	-3.41311800	0.49390400	C	0.27608300	-0.34825500	-0.40258700
H	-1.20589900	-1.33796200	1.75372400	O	0.95712400	-1.33876800	-0.02183500
O	2.50496100	1.74978000	-0.98047000	O	-1.09495100	-0.50405500	-0.47186900
C	3.55979200	1.08606300	-1.06448000	H	1.43549300	1.19205600	0.82068600
O	4.37326700	0.97333800	-1.99790900	H	0.61582000	0.28758700	-1.23620300
C	3.83978600	0.30404200	0.25829600	N	0.41457400	0.98252300	0.84639900
H	4.17594200	1.00829000	1.02474700	C	0.09202800	0.43409700	2.16650400
H	2.91846700	-0.17832900	0.58527000	H	0.65351800	-0.49474900	2.28449300
C	6.23687600	-0.22299900	-0.05442200	H	0.36671600	1.14433700	2.95009000
H	6.95940800	-1.03963700	-0.10322700	H	-0.97127800	0.20445700	2.23964200
H	6.18850500	0.33066000	-0.99258100	C	-3.60683700	-1.61662900	-0.11906300
H	6.48442600	0.44540600	0.77200600	C	-4.54549500	-2.54351400	0.35701500
C	4.86481400	-1.52237400	1.49514900	C	-4.08264500	-0.43267400	-0.70092000
H	3.87841500	-1.96588000	1.63694100	C	-5.91328400	-2.30305000	0.25219000
H	5.62948500	-2.30100100	1.47916000	H	-4.20996400	-3.46970200	0.82026200
H	5.07471300	-0.81298900	2.29677400	C	-5.45069000	-0.18610300	-0.80524700
C	4.53119200	-1.76870100	-0.89880900	H	-3.37350900	0.30255300	-1.07113800
H	5.25065500	-2.58893400	-0.86748800	C	-6.36779800	-1.12102400	-0.33053100
H	3.51978600	-2.13270500	-0.71092800	H	-6.62399900	-3.03466200	0.62474400
H	4.58071200	-1.23378300	-1.84593100	H	-5.80067000	0.73584800	-1.26015200
N	4.87896000	-0.79814700	0.19168500	H	-7.43354900	-0.93098400	-0.41530700
C	-0.80524700	1.91636200	0.63256700	Si	-1.77066300	-1.96367100	0.02313900
C	-0.97793400	2.43739400	-0.66545500	H	-1.36552700	-3.08098700	-0.86221500
C	-1.88030700	1.99399700	1.53302600	H	-1.45202000	-2.31317700	1.42932600
C	-2.17728900	3.03016900	-1.03158900	O	3.10313000	1.66245200	0.66758500
H	-0.14856000	2.38646100	-1.36594300	C	3.97513200	0.90349300	0.17520800
C	-3.08088100	2.59001400	1.14779300	O	4.88487500	1.16256300	-0.62861300
H	-1.78402600	1.59369800	2.53662100	C	3.85618400	-0.55106700	0.71200200
C	-3.24190900	3.11665300	-0.12881300	H	4.44005300	-0.64817500	1.63211400
H	-2.28166200	3.43679800	-2.03343900	H	2.80900600	-0.78097900	0.90456400
H	-3.89773300	2.63610300	1.86217200	C	5.82836600	-1.62332300	-0.33847100
H	-4.17589900	3.58689500	-0.41898100	H	6.13411600	-2.39142500	-1.05112400
				H	6.12064600	-0.62585300	-0.66866800

H	6.24910800	-1.83863700	0.64529600	C	-4.27188500	-0.51674900	-0.80730800
C	3.87225400	-2.94678300	0.31042700	C	-5.86299300	-2.24332300	0.68764600
H	2.78112900	-2.93677500	0.33387600	H	-4.04066500	-3.24866300	1.19624600
H	4.23584500	-3.74626700	-0.33795800	C	-5.65108700	-0.32447100	-0.75579000
H	4.27398000	-3.07444100	1.31677600	H	-3.65715400	0.16671000	-1.38714300
C	3.72742500	-1.44502800	-1.58943200	C	-6.44951500	-1.18820200	-0.00813100
H	4.02461300	-2.28750400	-2.21678300	H	-6.47908900	-2.91563200	1.27733200
H	2.64393400	-1.42490400	-1.45341200	H	-6.10342500	0.50174800	-1.29651200
H	4.09885800	-0.50564900	-1.99547300	H	-7.52396400	-1.03704600	0.03596600
N	4.33856200	-1.63609700	-0.23150300	Si	-1.80337800	-1.84194300	-0.16568200
C	-0.29971100	2.16035800	0.43774400	H	-1.43838400	-2.82078100	-1.21674400
C	0.41100700	3.16376500	-0.22312400	H	-1.40400800	-2.36299000	1.16553200
C	-1.67896300	2.27725200	0.61648500	O	3.11566600	1.35677300	0.88896300
C	-0.26352500	4.28504000	-0.69973100	C	3.98909900	0.55096000	0.47100700
H	1.48747800	3.06469800	-0.33805400	O	5.04956800	0.78758100	-0.12695900
C	-2.34107900	3.40389500	0.13969500	C	3.64856300	-0.92768900	0.80070700
H	-2.24313400	1.48967900	1.10220400	H	4.15353300	-1.22177100	1.72568800
C	-1.63868100	4.41096500	-0.52028500	H	2.56987100	-1.04305700	0.89872800
H	0.29456100	5.06542100	-1.20731600	C	5.54356800	-2.13364500	-0.24584400
H	-3.41382500	3.49059000	0.28226200	H	5.80959600	-2.81899700	-1.05270200
H	-2.16013500	5.28802200	-0.89018000	H	6.01013100	-1.15623100	-0.37360400
XXV_A				H	5.82169600	-2.56721900	0.71643700
C	0.14963300	-0.13892700	-0.52825700	C	3.36068700	-3.21200500	0.02824800
O	0.80898700	-1.20219300	-0.24945800	H	2.28671400	-3.03529300	-0.05620100
O	-1.24565600	-0.29494200	-0.52405700	H	3.68795400	-3.96346600	-0.69278600
H	1.45532800	1.08119400	0.69856000	H	3.61661700	-3.53145600	1.03966900
H	0.43240200	0.44708000	-1.42220400	C	3.62855000	-1.45037900	-1.61751200
N	0.40780700	1.02299600	0.64122600	H	3.86035100	-2.23312800	-2.34206000
C	-0.05177300	0.54745500	1.96070600	H	2.55102700	-1.27577900	-1.56091100
H	0.34499700	-0.45895700	2.10315300	H	4.17403900	-0.53628100	-1.84597000
H	0.32828100	1.21789800	2.73302200	N	4.06467700	-1.92689900	-0.26184700
H	-1.14073400	0.51901100	1.99172900	C	-0.08581100	2.33865700	0.26850600
C	-3.66159900	-1.57240800	-0.11341300	C	0.84213800	3.33356400	-0.03142900
C	-4.48262400	-2.42746100	0.63510400	C	-1.45526500	2.58524700	0.18057400

C	0.38781100	4.59216700	-0.42119400	C	5.12834500	-0.33354400	0.34058800
H	1.90446700	3.12072600	0.05654700	H	3.31356100	-1.46138500	0.69121500
C	-1.89467300	3.84696200	-0.20717500	C	4.82367200	1.88026600	-0.57204800
H	-2.16650900	1.79350600	0.38445900	H	2.76896400	2.46787500	-0.94254000
C	-0.97682900	4.85217400	-0.50893400	C	5.66541000	0.87215500	-0.10896000
H	1.10909500	5.36918900	-0.65266500	H	5.78198100	-1.11605100	0.71208700
H	-2.96006300	4.04079300	-0.28079100	H	5.23788700	2.82203500	-0.91685600
H	-1.32667700	5.83411100	-0.81185800	H	6.73958700	1.02690000	-0.09188200
XXV_B				C	-1.82157500	2.04534000	-0.82205700
C	0.90982400	-0.10905100	1.23962100	H	-1.45555600	1.08720900	-0.45397000
O	-0.44754300	0.16854000	1.22867400	H	-2.14633200	1.94821200	-1.86212000
O	0.99689500	-1.41268100	1.48679900	C	-0.66788300	3.08259900	-0.74443700
H	1.02734500	1.19888000	-0.44343600	O	0.43993800	2.57558600	-1.07166300
H	1.47569100	0.56036300	1.90542100	O	-0.92584800	4.24804600	-0.42074600
Si	-0.96114000	-1.47237600	1.66511600	N	-3.05292300	2.35946400	0.00003200
N	1.47951400	0.27691600	-0.18147600	C	-3.95079600	1.16682000	-0.04511100
C	1.06961000	-0.68436100	-1.23375400	H	-3.44412200	0.32424500	0.43130900
H	-0.01599600	-0.78048300	-1.21852400	H	-4.87248900	1.39901900	0.49141200
H	1.39851400	-0.29041900	-2.19573600	H	-4.17575800	0.93543500	-1.08723200
H	1.51576200	-1.65657100	-1.03453800	C	-3.77326600	3.54976500	-0.54757600
C	-1.16252900	-2.85991100	0.38737700	H	-3.07002200	4.38223700	-0.56013900
C	-2.38959100	-3.04352800	-0.26451400	H	-4.10719800	3.31540500	-1.55990700
C	-0.12177900	-3.74688200	0.06827500	H	-4.63437500	3.75798300	0.08982300
C	-2.57425700	-4.05557500	-1.20742600	C	-2.65821600	2.60871400	1.42728300
H	-3.22119000	-2.38408100	-0.02481500	H	-3.56924100	2.70090800	2.02064600
C	-0.29827200	-4.76716200	-0.86277500	H	-2.05676200	1.76209400	1.76315900
H	0.84093600	-3.62111600	0.55487800	H	-2.07425400	3.52702800	1.45677600
C	-1.52564800	-4.92054800	-1.50827100	H	-0.84779300	-1.91996900	3.07719800
H	-3.53509800	-4.17265600	-1.70073600	H	-2.42274100	-1.01153400	1.65872500
H	0.52042200	-5.44479200	-1.08833300	TS ₂₅₋₂₆			
H	-1.66243200	-5.71140200	-2.24012400	C	1.25093400	-1.00968400	1.07543000
C	2.92681700	0.47731300	-0.15044000	O	0.36930700	0.02278500	1.48284400
C	3.75228000	-0.53986600	0.32194600	O	0.38934900	-2.06812300	0.98542500
C	3.44335200	1.69033700	-0.59402000	H	1.27213300	1.38316100	0.44272200

H	2.04089900	-1.16057400	1.82228400	O	0.19751700	4.15165200	-0.18725600
Si	-0.99880700	-1.11320200	1.71147700	N	-2.22391300	2.58124600	-0.39134800
N	1.90230600	-0.63445400	-0.18513700	C	-3.19622800	1.46523300	-0.63659200
C	1.16850100	-0.97948500	-1.38695600	H	-3.07851400	0.71595600	0.14587200
H	0.10507900	-0.79565500	-1.22012200	H	-4.20574000	1.87749000	-0.62325200
H	1.51219700	-0.35251200	-2.21626900	H	-2.98776600	1.01407600	-1.60730700
H	1.26805800	-2.03645600	-1.66876900	C	-2.43117000	3.64876500	-1.42089800
C	-2.30782300	-1.88210100	0.53317200	H	-1.70312700	4.43982800	-1.25427600
C	-3.67058300	-1.62920500	0.75684500	H	-2.29183000	3.20428100	-2.40745000
C	-1.98227000	-2.71042800	-0.55032700	H	-3.45094800	4.02311200	-1.32326900
C	-4.66441000	-2.16145700	-0.06225500	C	-2.46595400	3.12691000	0.98660800
H	-3.95950700	-0.99957600	1.59895300	H	-3.50908600	3.43829200	1.05072400
C	-2.96625300	-3.23217300	-1.39210100	H	-2.26401900	2.32772800	1.70389800
H	-0.93799100	-2.95351800	-0.71895800	H	-1.80336700	3.97504000	1.14776700
C	-4.31076900	-2.95733400	-1.15247700	H	-1.05507300	-1.73669100	3.06043700
H	-5.71200700	-1.96141500	0.14745700	H	-1.89772400	0.13282400	1.98181600
H	-2.68291900	-3.86653500	-2.22769100	XXVIA			
H	-5.07848200	-3.36854500	-1.80178600	C	0.16454000	-2.38352700	0.81779300
C	3.30787200	-0.62787900	-0.24261800	O	-0.00069600	-1.29593000	1.71583000
C	4.01189400	-1.15739100	-1.33314100	O	-1.10927200	-2.83441500	0.71780700
C	4.04342200	-0.03082900	0.79639400	H	0.70900600	-0.01581600	2.41060200
C	5.40381100	-1.09964000	-1.37457200	H	0.86862500	-3.11721900	1.24523400
H	3.48146400	-1.63015900	-2.15163600	Si	-1.79297000	-1.44097200	1.76351200
C	5.43102000	0.00331900	0.75451700	N	0.68881200	-1.92134000	-0.49674500
H	3.52326900	0.43413500	1.62792800	C	0.13724500	-2.57126900	-1.67564700
C	6.12530000	-0.52831400	-0.33200000	H	-0.72598600	-3.15306600	-1.36201000
H	5.92335100	-1.51908900	-2.23110000	H	-0.19651500	-1.83762500	-2.42142100
H	5.97257400	0.47086200	1.57135800	H	0.86845500	-3.24044000	-2.14838000
H	7.20902800	-0.48801200	-0.36749400	C	-2.77236900	-0.55131300	0.37391000
C	-0.84517100	1.98943100	-0.46572100	C	-3.31865400	0.72287700	0.60210600
H	-0.81731000	1.13680500	0.21790300	C	-2.97244800	-1.10718600	-0.89788400
H	-0.68851300	1.62492000	-1.48530700	C	-4.00883500	1.42021400	-0.39104400
C	0.29325900	2.94529500	-0.10839500	H	-3.20392100	1.17598200	1.58586100
O	1.40359100	2.34235200	0.24283800	C	-3.65635200	-0.42078200	-1.90175200

H	-2.58425400	-2.09982800	-1.09565900	H	0.14225400	4.05250000	0.45094100
C	-4.17284400	0.85060200	-1.65386400	H	-2.63497600	-2.37717500	2.56104700
H	-4.43173000	2.39847500	-0.17692700	H	-1.80932000	-0.25076900	2.72535400
H	-3.79651100	-0.88286700	-2.87517100	XXVI_B			
H	-4.71194000	1.38513600	-2.43085500	C	0.93831200	-0.65891700	-0.79665300
C	1.97235300	-1.40189900	-0.59314200	O	0.46559700	0.52982400	-1.34040300
C	2.54441200	-1.12244800	-1.85459800	O	2.26636800	-0.52090700	-0.38334500
C	2.73686700	-1.07676000	0.54855400	H	-0.01552600	1.06254300	-0.65907700
C	3.80103800	-0.53093500	-1.95943500	H	0.90266900	-1.41117900	-1.59514800
H	2.01143000	-1.37248000	-2.76424200	N	0.16269800	-1.15867100	0.32248800
C	3.98353900	-0.47551500	0.42578500	C	0.52779000	-0.78621000	1.67910800
H	2.35585500	-1.29268500	1.53763100	H	1.42258300	-0.17043400	1.64279000
C	4.53076000	-0.18820800	-0.82456600	H	-0.27546200	-0.20370100	2.14260400
H	4.21019000	-0.34031100	-2.94764800	H	0.75601000	-1.67038600	2.28601900
H	4.53366700	-0.23296600	1.32996900	C	4.89626200	0.43299200	-0.25010200
H	5.50738800	0.27573400	-0.91045700	C	5.52060200	-0.81950300	-0.35319900
C	0.18167500	1.36900800	0.58616100	C	5.58782300	1.46126500	0.40426300
H	-0.87282900	1.34414400	0.87238200	C	6.79028800	-1.03518900	0.17559600
H	0.43984400	0.35798700	0.27666400	H	5.00469300	-1.64082800	-0.84414900
C	1.00777600	1.78756800	1.79754000	C	6.86054300	1.25259800	0.93471500
O	1.11415600	0.85256200	2.70920700	H	5.12542100	2.44003900	0.51008300
O	1.48966900	2.89568000	1.92117900	C	7.46315500	0.00277600	0.81987700
N	0.29998300	2.24556400	-0.62515700	H	7.25637700	-2.01199900	0.08641200
C	-0.41545400	1.53029900	-1.73308700	H	7.37738600	2.06340200	1.43952900
H	-1.44911700	1.34948300	-1.43448600	H	8.45283300	-0.16443700	1.23456400
H	-0.38081000	2.15472100	-2.62694500	Si	3.19801100	0.74998100	-0.97399100
H	0.08909800	0.57973200	-1.91039200	H	3.23204600	0.70274000	-2.45583500
C	1.73615600	2.43172600	-1.01572400	H	2.75335000	2.08087400	-0.50262200
H	2.23478700	3.01518400	-0.24547200	C	-3.27489400	1.02752500	0.79046100
H	2.19989000	1.44872500	-1.11019300	H	-3.28250300	1.22955900	1.86481700
H	1.76080700	2.95035900	-1.97506000	H	-2.97168700	-0.00890700	0.63493700
C	-0.35315800	3.57100400	-0.39079800	C	-2.23740800	1.96105800	0.10002100
H	-0.25381700	4.16949300	-1.29743300	O	-1.08034000	1.70219500	0.50187600
H	-1.40788800	3.39573300	-0.17282200	O	-2.63835600	2.80109600	-0.72115800

N	-4.71041300	1.13065800	0.31296100	H	-1.20497700	1.93194200	2.40747400
C	-5.51634500	0.11051600	1.04347800	C	-3.81273000	-0.53746600	-0.35894900
H	-5.45105700	0.30759000	2.11430200	C	-4.63220300	0.22962500	0.48409900
H	-6.55548000	0.17579100	0.71550900	C	-3.72126100	-1.91276400	-0.10760900
H	-5.10923500	-0.87808300	0.82398800	C	-5.33469600	-0.35639600	1.53385000
C	-4.78362600	0.84149200	-1.15625200	H	-4.70163200	1.30101200	0.32133600
H	-4.20201600	1.60319200	-1.67370800	C	-4.40391400	-2.50360700	0.95621500
H	-4.35436000	-0.14711100	-1.32448400	H	-3.10001900	-2.53139600	-0.75063400
H	-5.83242600	0.86020600	-1.45813300	C	-5.21586800	-1.72531900	1.77674200
C	-5.25577100	2.49560000	0.58855300	H	-5.97014000	0.25511900	2.16837300
H	-6.29076500	2.53481300	0.24417500	H	-4.30511100	-3.56989000	1.13905100
H	-5.21222000	2.67272200	1.66439100	H	-5.75492100	-2.18151600	2.60235100
H	-4.62760800	3.21063500	0.05735600	Si	-2.87067700	0.19018000	-1.82476700
C	-1.06755400	-1.73081600	0.08548100	H	-3.63358700	1.02004300	-2.78170400
C	-1.79410200	-2.33058700	1.13841900	H	-2.62774300	-1.07993300	-2.59837800
C	-1.66143400	-1.73504900	-1.19809700	C	2.45341400	-1.28347000	0.47048200
C	-3.03148400	-2.92256800	0.91090600	H	2.00611100	-1.88530100	1.26468500
H	-1.37968700	-2.34825700	2.13886100	H	2.50074600	-0.24383600	0.80418800
C	-2.89253300	-2.34441100	-1.40840100	C	1.55085300	-1.35056200	-0.78875500
H	-1.17770800	-1.22301300	-2.02089400	O	0.36833300	-1.06028900	-0.48243200
C	-3.59884200	-2.94141300	-0.36272900	O	2.04784000	-1.64067900	-1.88516000
H	-3.54901700	-3.38914000	1.74501800	N	3.88306500	-1.75955700	0.30885900
H	-3.31126500	-2.33993100	-2.41156100	C	4.56452400	-1.62366600	1.62820300
H	-4.55435400	-3.42497900	-0.54043300	H	4.04520500	-2.23850800	2.36417300
TS ₂₆₋₁₄				H	5.60019000	-1.95367700	1.53087300
C	-1.29899200	1.94845500	-0.78816600	H	4.53087800	-0.57620700	1.93121300
O	-1.13754800	0.55486000	-1.72988800	C	4.61305300	-0.92112300	-0.69769000
O	-2.58704500	1.95345400	-0.71887100	H	4.09760300	-1.02594200	-1.65110400
H	-0.53028400	-0.17265800	-1.35957700	H	4.57617800	0.11549500	-0.36178900
H	-0.80574200	2.65890300	-1.46169500	H	5.64455100	-1.27381700	-0.75293200
N	-0.55592000	1.79249800	0.40181700	C	3.90001200	-3.19193200	-0.12222400
C	-1.21197400	1.22720800	1.56909100	H	4.93693500	-3.52478900	-0.19159700
H	-2.24875400	1.02652200	1.30879100	H	3.36502000	-3.78422700	0.62164900
H	-0.72513100	0.29060000	1.86099000	H	3.39945200	-3.25301000	-1.08815400

C	0.81847200	1.99264000	0.41439100	H	3.57528200	-0.23776700	-2.91633600
C	1.50701000	2.12165300	1.63621500	H	2.62352200	1.99547000	-2.86878200
C	1.57466200	2.05776900	-0.77437700	C	-2.45917900	1.08440300	0.61115400
C	2.87797200	2.36059700	1.66356800	H	-2.20022700	1.46120600	1.60382700
H	0.96619000	2.05675600	2.57233900	H	-2.39223100	-0.00467100	0.62473900
C	2.94002500	2.31109500	-0.73177500	C	-1.43819800	1.63196500	-0.42661500
H	1.10525700	1.87554100	-1.73345700	O	-0.28684300	1.21984000	-0.16331300
C	3.60975900	2.46985600	0.48235900	O	-1.84424400	2.36301800	-1.34402300
H	3.37053000	2.48351500	2.62437700	N	-3.91782700	1.43018600	0.37835800
H	3.48747900	2.36620100	-1.66850400	C	-4.72691100	0.76363300	1.43831600
H	4.67383700	2.68562300	0.50644800	H	-4.40396100	1.12794700	2.41431500
XIV_A				H	-5.78180300	0.99724900	1.28348200
C	1.73650700	-2.52639900	-0.41451500	H	-4.56517900	-0.31323800	1.37405300
O	1.20416900	-0.00830000	-2.05111000	C	-4.36345400	0.92548600	-0.96108900
O	2.94688100	-2.47956700	-0.30467900	H	-3.76652000	1.43049600	-1.71936200
H	0.61055700	0.47315500	-1.43154200	H	-4.18474400	-0.14947000	-0.99166700
H	1.23997700	-3.08002900	-1.22610700	H	-5.42749300	1.14023600	-1.07450600
N	0.84987300	-1.94534900	0.45327200	C	-4.11902300	2.91133700	0.44940000
C	1.34451000	-1.15133900	1.57160600	H	-5.17744700	3.12670700	0.29336600
H	2.40400300	-0.96126800	1.39980500	H	-3.80879400	3.25536300	1.43732800
H	0.80788500	-0.19975100	1.59131600	H	-3.49901600	3.36308700	-0.32498900
H	1.23469200	-1.68101900	2.52441000	C	-0.53651500	-2.12309000	0.26829000
C	3.46216500	0.98723800	-0.46127100	C	-1.35720600	-2.42444900	1.36219500
C	4.55821400	0.23401100	-0.01982600	C	-1.10636700	-2.01998100	-1.00782100
C	2.91433200	1.93517800	0.41728800	C	-2.71618800	-2.66492900	1.17628600
C	5.09408500	0.41874500	1.25355500	H	-0.92446800	-2.49935300	2.35395400
H	4.98151000	-0.52915000	-0.66617800	C	-2.46138800	-2.28241400	-1.18666000
C	3.44287300	2.12123000	1.69265000	H	-0.48653600	-1.69917500	-1.83954800
H	2.04527000	2.51325500	0.11316100	C	-3.27454700	-2.61074200	-0.10076700
C	4.53565700	1.36286800	2.11243200	H	-3.33285300	-2.92631700	2.03191200
H	5.93850300	-0.18205200	1.57822900	H	-2.88535400	-2.21371800	-2.18435200
H	3.00263500	2.85636900	2.36062200	H	-4.32798300	-2.83083600	-0.24987300
H	4.95045200	1.50741400	3.10616300	XXVII			
Si	2.70643600	0.69068400	-2.15439200	C	-1.68998600	-0.47278600	-1.94616300

O	-1.73729600	0.22183700	-2.93967000	C	0.32753100	3.67814100	0.08430600
O	-0.51906600	-0.81579300	-1.37668800	H	2.15305600	3.21869100	1.12623000
C	-0.28200200	-0.87814100	2.33916200	H	-1.61753800	3.80825300	-0.84312600
H	0.12058100	-0.51786400	3.29729200	H	0.69729100	4.60418400	-0.34518200
H	-0.87494800	-1.77373500	2.53612600	TS ₂₇₋₂₈			
H	0.56903500	-1.16390000	1.70100400	C	-1.00102600	-1.52122400	-0.25133100
H	-2.00819600	-0.27277100	1.29679500	O	-1.17851900	-1.14907800	-1.44502300
H	-2.54620300	-0.87079800	-1.37760900	O	0.32978200	-1.48588000	0.12202000
Si	0.90320100	-0.07228600	-1.93410300	C	-1.46569900	-0.74762800	2.28456200
H	0.85449700	1.39871400	-1.82744100	H	-1.79947000	-0.00027300	3.01095900
H	1.17452300	-0.49961200	-3.32920800	H	-2.03819700	-1.66349000	2.44694600
N	-1.13822100	0.09769700	1.71836300	H	-0.40268200	-0.96133700	2.42201700
C	2.23047000	-0.74896100	-0.79633700	H	-2.80475400	-0.40401300	0.75148400
C	2.26336900	-2.10339300	-0.43572100	H	-1.54348300	-2.37510500	0.17732600
C	3.21461300	0.09734000	-0.27039500	Si	1.09348500	-0.78901900	-1.25131700
C	3.24379000	-2.59507700	0.42311800	H	0.78042000	0.59425600	-1.67415500
H	1.49655400	-2.77853900	-0.80675000	H	1.24176500	-1.74351600	-2.37714800
C	4.20195400	-0.38853600	0.58471800	N	-1.73103500	-0.29900300	0.91904000
H	3.18904900	1.15886600	-0.50377000	C	2.84173100	-0.59752800	-0.52067200
C	4.21651400	-1.73705700	0.93439600	C	3.61011400	-1.70374900	-0.12572200
H	3.24285000	-3.64519100	0.70092900	C	3.40916900	0.67236000	-0.34904100
H	4.94900700	0.28844400	0.98962500	C	4.88419800	-1.55212700	0.41723500
H	4.97694700	-2.11649500	1.61127800	H	3.20030900	-2.70524600	-0.23938600
C	-4.42530700	-1.44778000	0.99234500	C	4.68443300	0.83766800	0.19392700
H	-4.51939100	-1.24828700	2.09406700	H	2.83624800	1.55179300	-0.63738100
O	-5.34966100	-2.07207000	0.45414900	C	5.42614500	-0.27678300	0.57894500
O	-3.36327000	-0.99331600	0.46388700	H	5.45538900	-2.42729900	0.71650500
C	-0.63548100	1.25106500	1.19117000	H	5.09826200	1.83513200	0.31868000
C	0.67593500	1.70173400	1.45070700	H	6.41844000	-0.15377200	1.00479800
C	-1.45021200	2.04809200	0.35034500	C	-4.91509600	-0.88609000	-0.28091200
C	1.13615800	2.89965600	0.90644500	H	-4.27508300	-0.88087800	-1.20030400
H	1.34047200	1.10786900	2.06907800	O	-6.12296700	-1.10116000	-0.42422700
C	-0.97162000	3.22985700	-0.18795900	O	-4.28281200	-0.66485200	0.80712200
H	-2.45485900	1.70010300	0.12531100	C	-1.25845100	0.98524000	0.55478000

C	-0.13243300	1.56440400	1.14626600	H	5.46995200	0.63504000	-0.03753200
C	-1.88280100	1.62877000	-0.51914800	C	-4.32890800	-0.07716600	-0.93858400
C	0.36048000	2.77614300	0.66732200	H	-3.48422500	-0.72184900	-1.24113800
H	0.37716800	1.06399300	1.96167800	O	-5.39787300	-0.07624700	-1.51146400
C	-1.38172800	2.83468800	-0.99238700	O	-4.06809000	0.69145200	0.10757100
H	-2.74543800	1.16193800	-0.98070400	C	-0.61509700	1.09659300	0.52794300
C	-0.25648600	3.41415900	-0.40520300	C	0.46731700	1.58130100	1.26381300
H	1.24180400	3.21177500	1.12965700	C	-0.71168200	1.42854000	-0.82742600
H	-1.86825200	3.31997600	-1.83318200	C	1.43774700	2.37404000	0.65582700
H	0.13684200	4.35329000	-0.78348400	H	0.58436400	1.30534500	2.30521000
XXVIII				C	0.26256800	2.21279400	-1.43338100
C	-1.36910800	-1.22891500	0.78350200	H	-1.53946700	1.03856200	-1.40664300
O	-1.29990600	-1.41835600	-0.58897200	C	1.34434900	2.68906000	-0.69519600
O	-0.17961400	-1.69308600	1.23623900	H	2.29161200	2.71092700	1.23589400
C	-1.80925800	0.38974000	2.53391800	H	0.17985400	2.44019400	-2.49213000
H	-1.96131100	1.44553200	2.77272500	H	2.11752300	3.28276100	-1.17351600
H	-2.70963400	-0.16239300	2.82122300	TS ₂₈₋₂₉			
H	-0.96566300	-0.00592700	3.11411200	C	-0.38873100	0.35853300	-0.98425700
H	-3.11730300	0.53759700	0.43643500	O	0.19723600	1.59168500	-0.66699000
H	-2.24703600	-1.73683200	1.22609300	O	0.66770300	-0.36137300	-1.45203400
Si	0.33676800	-2.08795100	-0.56651500	H	-1.21584400	1.72686400	0.92332600
H	0.36407000	-2.12969400	-2.09365500	H	-1.19882500	0.47549600	-1.71824900
H	0.50311500	-3.55053300	-0.27853200	Si	1.79726300	1.15089300	-1.26272800
N	-1.61618100	0.23634500	1.09233800	N	-1.01921600	-0.20355400	0.24518400
C	2.00671000	-1.16422200	-0.37542900	C	-0.05146200	-0.73435900	1.19149900
C	2.62533000	-0.99506400	0.87370700	H	0.74888900	-0.00229100	1.31387100
C	2.67950700	-0.65784300	-1.49378500	H	-0.53602900	-0.87837900	2.16203800
C	3.86243700	-0.36744200	0.99807100	H	0.40784500	-1.67437700	0.85870700
H	2.10414200	-1.34784400	1.75905100	C	3.16829300	0.13115000	-0.37656400
C	3.91073200	-0.00848700	-1.38145900	C	4.22428300	0.78043100	0.27768100
H	2.21995100	-0.76763600	-2.47390000	C	3.18921000	-1.27352300	-0.38279200
C	4.50951800	0.13379500	-0.13254800	C	5.25810500	0.07302200	0.89455800
H	4.32017600	-0.25561700	1.97861200	H	4.22969900	1.86837100	0.30721200
H	4.39927900	0.38879500	-2.26829300	C	4.21706900	-1.99221700	0.22614800

H	2.36858200	-1.79418200	-0.86832300	C	-3.15639200	0.13406600	0.29043300
C	5.25775200	-1.32018500	0.86874900	C	-4.27444300	0.64950400	-0.37998100
H	6.06105100	0.60765900	1.39725900	C	-3.17795500	-1.23287300	0.61229400
H	4.20641100	-3.07977700	0.20301000	C	-5.37017100	-0.14957500	-0.71036000
H	6.05857200	-1.87801600	1.34855200	H	-4.27965100	1.70294400	-0.65344400
H	-2.85266800	3.82015100	1.91873700	C	-4.26464000	-2.04292100	0.28448800
C	-2.54184600	3.08874100	1.15541200	H	-2.31375700	-1.65470200	1.11713300
O	-1.53715000	2.36649600	1.60680900	C	-5.36729700	-1.50297600	-0.37805600
O	-3.08336000	2.99865400	0.07653700	H	-6.22217500	0.28165100	-1.23091000
C	-2.22642700	-0.90075900	0.09399100	H	-4.25119500	-3.09941400	0.54276600
C	-2.42885700	-2.18614200	0.62220500	H	-6.21405200	-2.13382600	-0.63811700
C	-3.30587600	-0.28053800	-0.56558600	H	2.88954400	4.44929700	-1.03767300
C	-3.65761500	-2.82980400	0.48197000	C	2.37320100	3.60722800	-0.54463700
H	-1.62043700	-2.69510000	1.13434000	O	1.21828700	3.37452500	-1.11055600
C	-4.51895900	-0.93811500	-0.71431300	O	2.86828500	3.01651900	0.39669500
H	-3.19766300	0.74223300	-0.91156200	C	2.28215200	-1.12780000	-0.19278900
C	-4.70992900	-2.21982800	-0.19309200	C	2.54122900	-2.47756000	-0.49934700
H	-3.78381400	-3.82469200	0.90178400	C	3.35857600	-0.34817000	0.28697700
H	-5.33513600	-0.43015700	-1.22111300	C	3.81041600	-3.02424900	-0.31911600
H	-5.66517700	-2.72483300	-0.30266700	H	1.74268200	-3.11371100	-0.86357100
H	2.35946500	2.51035800	-0.83715200	C	4.61166000	-0.91277400	0.47647800
H	2.07240900	1.24091900	-2.73610500	H	3.21742800	0.71150600	0.47348600
XXIX				C	4.85781100	-2.25547500	0.17799700
C	0.48235700	0.37685000	0.57713600	H	3.97115500	-4.07229400	-0.56026500
O	-0.11686700	1.49286600	-0.05908900	H	5.41632900	-0.28085600	0.84346000
O	-0.59274600	-0.11427500	1.27135300	H	5.84429800	-2.68616200	0.32174500
H	0.70075300	2.60468700	-0.66213300	H	-2.23495800	2.49739200	-0.00188500
H	1.30432100	0.70334300	1.22348800	H	-1.85846400	1.82314100	2.16106800
Si	-1.69623000	1.28885200	0.76777300	TS ₂₉₋₃₀			
N	1.03067300	-0.56149300	-0.39812600	C	0.21308900	-0.36966000	1.62935500
C	0.04068300	-1.29262000	-1.15958800	O	0.00193900	1.06634200	0.70420100
H	-0.78744200	-0.62058100	-1.38890700	O	-0.91006500	-0.60698200	2.16524600
H	0.47899000	-1.62788200	-2.10521800	H	0.83447500	1.69693800	-0.37133000
H	-0.37007700	-2.15902300	-0.62175300	H	1.03719300	0.00476500	2.25201100

Si	-1.56640000	1.55989300	0.89574200	XXX			
N	0.72010100	-1.32587200	0.67795400	C	-0.77008600	-0.89066100	2.59634500
C	-0.23205400	-2.23122200	0.07632500	O	0.60406200	2.01469100	1.39420900
H	-1.19884600	-2.03228300	0.53750600	O	-1.71511600	-0.60765500	3.31825200
H	-0.30528600	-2.07323300	-1.00782400	H	1.37131500	2.11876300	0.73802100
H	0.03045100	-3.28078500	0.26564600	H	0.27381200	-0.73494400	2.90096300
C	-2.90467200	0.51496000	0.05190200	Si	-0.84434300	2.52574400	0.82670800
C	-3.28470300	0.81230200	-1.26427900	N	-0.89667100	-1.43579800	1.35143900
C	-3.56345700	-0.54431700	0.69501300	C	-2.23213400	-1.69926400	0.84272900
C	-4.27603200	0.08261900	-1.92219200	H	-2.91714800	-0.98532500	1.29971900
H	-2.79342500	1.62943600	-1.78866900	H	-2.23496900	-1.56339000	-0.24024300
C	-4.56431400	-1.26913600	0.05110700	H	-2.56957300	-2.71336900	1.09236300
H	-3.25455200	-0.81247300	1.70121000	C	-1.46836100	1.46435300	-0.60596900
C	-4.92157200	-0.96016800	-1.26199900	C	-0.56320200	0.81011600	-1.45505200
H	-4.54127800	0.32648200	-2.94788200	C	-2.83872700	1.30500800	-0.85426100
H	-5.05903800	-2.08686900	0.56954100	C	-1.01613400	0.00707700	-2.50102100
H	-5.69621000	-1.53161900	-1.76740900	H	0.50552800	0.93166100	-1.29251100
H	2.77586700	3.24435000	-1.87429800	C	-3.29793400	0.51939800	-1.91066100
C	2.34148600	2.83876400	-0.94308500	H	-3.56434100	1.78805600	-0.20164900
O	1.28762400	2.11247900	-1.20533300	C	-2.38341000	-0.13766900	-2.73353500
O	2.83133100	3.07665100	0.14473600	H	-0.29710400	-0.50933600	-3.13053200
C	2.01903900	-1.27206700	0.20603600	H	-4.36537000	0.40589300	-2.08207000
C	2.52765600	-2.29943400	-0.61757600	H	-2.73536600	-0.76434400	-3.54901100
C	2.88748900	-0.20171000	0.51415100	H	4.03840400	2.48009100	-1.48443500
C	3.84060300	-2.26942500	-1.07819500	C	3.50984100	2.00679200	-0.61965900
H	1.89223300	-3.13022300	-0.90102400	O	2.29509900	2.35302500	-0.50441800
C	4.19503100	-0.18967800	0.04876400	O	4.16321000	1.22141200	0.08648200
H	2.53449000	0.65697900	1.07051000	C	0.23667300	-1.83701800	0.59486100
C	4.69509200	-1.22140700	-0.74655900	C	0.17302900	-3.00028000	-0.17905600
H	4.19263800	-3.08073600	-1.71112400	C	1.40473400	-1.07045000	0.59368500
H	4.81743100	0.66649600	0.29403000	C	1.27326600	-3.39258700	-0.93715000
H	5.71621600	-1.19648400	-1.11552900	H	-0.73397800	-3.59622500	-0.19336500
H	-1.62878900	2.84600500	0.12364200	C	2.50741800	-1.47845000	-0.15133500
H	-1.98738700	1.88541500	2.28153200	H	1.44036700	-0.12144900	1.11866100

C	2.44587800	-2.63963700	-0.92033700	O	3.83270000	0.86407900	0.79452700
H	1.20955700	-4.29508500	-1.53950300	C	0.67509800	1.04526900	-0.23199700
H	3.38511000	-0.83607500	-0.14446500	C	0.53336500	1.46201500	1.09597600
H	3.30100100	-2.94531700	-1.51627200	C	-0.24109700	1.49396200	-1.18349700
H	-0.81266700	3.94701900	0.36644100	C	-0.51669400	2.29602400	1.46102600
H	-1.86022500	2.43140300	1.91020800	H	1.23460600	1.09649600	1.83631600
XXVIII₂				C	-1.28689900	2.33682900	-0.81466300
C	1.42513200	-1.30523800	-0.15324400	H	-0.17039500	1.15011900	-2.20866500
O	1.06652400	-1.36770900	1.18245200	C	-1.43384600	2.73747300	0.50851500
O	0.34595300	-1.80713800	-0.80388600	H	-0.62718300	2.58957200	2.50100700
C	2.16815900	0.15052900	-1.95053900	H	-2.01281500	2.64428700	-1.56135200
H	2.35349800	1.18126400	-2.26556600	H	-2.26668900	3.37089100	0.79939500
H	3.10540300	-0.40769400	-2.02208800	TS _{28-29_2}			
H	1.42168100	-0.31268500	-2.60615400	C	1.45044400	-0.83360100	-0.99344700
H	2.98329900	0.52960300	0.23808200	O	1.26692400	-1.60931700	0.15697600
H	2.37089000	-1.83473100	-0.35854300	O	0.29169100	-1.03541100	-1.68037600
N	1.74408800	0.13850500	-0.54686600	C	2.54048500	1.24685100	-1.63534700
C	-2.11534700	-1.12620500	0.27547300	H	2.80536500	2.25186800	-1.29332700
C	-2.44800000	-1.03022600	-1.08538300	H	3.46779600	0.68416000	-1.76759100
C	-3.00952100	-0.55750500	1.19050900	H	2.03125100	1.32730400	-2.60993400
C	-3.62076800	-0.41044900	-1.51038100	H	2.74176000	-0.42160200	1.01982100
H	-1.75019100	-1.43178600	-1.81458300	H	2.35059200	-1.15736500	-1.54333900
C	-4.18046300	0.08230400	0.77804700	N	1.74275700	0.58081200	-0.61931400
H	-2.77503500	-0.61052100	2.25176300	C	-2.01641400	-1.33075700	-0.16309100
C	-4.49243500	0.15331400	-0.57730600	C	-2.43784400	-0.31267900	-1.03270100
H	-3.85115400	-0.35290500	-2.57214300	C	-2.88658300	-1.68243000	0.87763700
H	-4.84731500	0.52581900	1.51420200	C	-3.66770100	0.32208500	-0.87063400
H	-5.40342500	0.64812400	-0.90625100	H	-1.76101500	-0.00182900	-1.82270400
Si	-0.53591600	-2.03594000	0.87891700	C	-4.12224800	-1.05628700	1.04942700
H	-0.67893700	-3.51774100	0.68663100	H	-2.57806700	-2.45505000	1.57944300
H	-0.88258700	-1.95147800	2.36709000	C	-4.51694100	-0.04775800	0.17232000
C	4.95040300	0.31046200	0.41222300	H	-3.95858300	1.11907300	-1.55106500
H	5.79667100	0.64208400	1.04028000	H	-4.77295100	-1.34879400	1.87090600
O	5.11124600	-0.47128700	-0.50868600	H	-5.47370500	0.45216000	0.30542700

Si	-0.32198300	-2.21835700	-0.34480700	C	-3.93014100	-1.93058800	0.69762500
H	-0.40430700	-3.38045000	-1.29447900	H	-2.15476300	-3.10048700	1.01492200
H	-0.44615000	-3.00220400	0.96762500	C	-4.48661400	-0.82600400	0.05489600
C	4.63594600	-0.33838100	1.24988200	H	-4.11151200	0.81824200	-1.28602400
H	5.36966000	-0.26219100	2.06867700	H	-4.53802100	-2.53488700	1.36749400
O	4.96027800	-0.39601100	0.08446100	H	-5.52833800	-0.56220700	0.22235500
O	3.41434300	-0.35586000	1.74019600	Si	0.06722800	-1.98797100	-0.60313400
C	0.64698500	1.31907300	-0.10444400	H	0.24868000	-2.98936300	-1.70939600
C	0.07520300	0.94510600	1.12211500	H	0.09533400	-2.97099800	0.57223900
C	0.10919200	2.43073000	-0.76751300	C	4.64389900	-0.91539100	1.05753100
C	-1.01280700	1.63429100	1.64066900	H	5.48098300	-0.98551300	1.77446400
H	0.47584900	0.08752100	1.64824500	O	4.79158700	-0.44891800	-0.05522500
C	-0.96838000	3.13246200	-0.23006600	O	3.54570900	-1.39415900	1.58477000
H	0.51514400	2.74056300	-1.72396600	C	0.41760100	1.69372600	0.11452600
C	-1.54418100	2.73571800	0.97238000	C	-0.16234100	1.06961700	1.23310100
H	-1.45754500	1.29554100	2.57167100	C	-0.21510800	2.83431300	-0.40207600
H	-1.37146200	3.98403600	-0.77259400	C	-1.34390600	1.54903800	1.78110400
H	-2.40198300	3.26483700	1.37650300	H	0.32230400	0.19595800	1.65060500
XXIX_{2A}				C	-1.38948800	3.32273400	0.16858800
C	1.57896600	-0.19924400	-0.93865400	H	0.19402900	3.33403500	-1.27307200
O	1.49762700	-1.15443700	0.09906100	C	-1.96920600	2.68108900	1.25792800
O	0.47489600	-0.53264700	-1.67866200	H	-1.78474400	1.02571400	2.62469700
C	2.36230700	2.06327400	-1.30728500	H	-1.86059000	4.20414100	-0.25975300
H	2.49843100	3.03385500	-0.82027400	H	-2.89482600	3.05001900	1.68980900
H	3.35041700	1.62400400	-1.46642600	XXIX_{2B}			
H	1.89009600	2.22790000	-2.29139100	C	1.43137500	0.32873000	1.06923700
H	2.73225100	-1.31693600	0.96029700	O	1.52291100	0.83819400	-0.26301000
H	2.52711300	-0.32471600	-1.47982600	O	0.28982600	0.93364000	1.49017100
N	1.60810200	1.18250400	-0.43661100	C	2.73433200	-1.67592400	0.78768000
C	-1.77128100	-1.49891700	-0.36538400	H	3.03949400	-1.53224800	-0.26210200
C	-2.35636700	-0.39450800	-1.00375900	H	3.47230900	-1.16300700	1.40846800
C	-2.58789100	-2.25096800	0.49002400	H	2.76058500	-2.74586800	1.01741300
C	-3.69240300	-0.05706400	-0.79572600	H	2.81947600	0.98042300	-0.99373600
H	-1.73145400	0.21995400	-1.64476200	H	2.33050400	0.62181100	1.63201300

N	1.41807300	-1.14061600	1.08525600	C	1.86986900	1.86541900	0.90039200
C	-1.80556300	1.54328600	-0.14052900	H	1.83713300	1.06549200	1.65521800
C	-2.57098300	1.45792200	1.03425000	H	2.88548900	1.88783000	0.49465900
C	-2.47654500	1.35577200	-1.35376300	H	1.66212200	2.82485900	1.38632600
C	-3.93955000	1.20204400	0.99890600	H	3.01212000	-0.84561700	0.46012400
H	-2.07174900	1.57278900	1.99292100	H	2.41526800	0.94571700	-1.47809100
C	-3.84434800	1.07676400	-1.40361900	N	0.94646700	1.65849600	-0.19509300
H	-1.91016600	1.41625400	-2.28083800	C	-1.01701200	-1.84969600	-0.29755000
C	-4.58176100	1.00265500	-0.22495100	C	-1.98743900	-1.10407900	-0.98191600
H	-4.50606600	1.14545900	1.92579700	C	-1.43100000	-2.58830300	0.82059000
H	-4.33233100	0.91535400	-2.36198000	C	-3.31589200	-1.09541400	-0.56398700
H	-5.64756700	0.78912100	-0.25694200	H	-1.67169400	-0.49746100	-1.82470400
Si	0.08137600	1.89061500	-0.09938500	C	-2.75923500	-2.58137300	1.24795400
H	0.34560600	3.23860500	0.50180300	H	-0.70071100	-3.17580400	1.37328000
H	0.18255500	2.23400100	-1.58447500	C	-3.70617900	-1.83280500	0.55288900
C	4.77471400	1.06116600	-0.84394100	H	-4.04267600	-0.48871100	-1.09697700
H	5.66448000	1.18118400	-1.48725200	H	-3.05204200	-3.15446100	2.12452700
O	3.68069200	1.07014900	-1.55973200	H	-4.74095000	-1.81395700	0.88641400
O	4.87013900	0.93673400	0.36214400	Si	0.79803000	-1.90650000	-0.82022100
C	0.32472400	-1.79324200	0.47575100	H	0.94975100	-2.32214800	-2.23563000
C	0.48768100	-2.71725800	-0.56763300	H	1.32341000	-3.06198200	-0.01342400
C	-0.97941700	-1.55398600	0.94416800	C	4.89747700	-0.33388600	0.79766400
C	-0.61363600	-3.36267200	-1.13089200	H	5.75260700	-0.64327600	1.42621600
H	1.47420600	-2.92277100	-0.96677600	O	3.84850000	-1.06967800	1.04753600
C	-2.07219700	-2.17290700	0.35487200	O	4.99150700	0.58289400	0.00287600
H	-1.11277500	-0.84589800	1.74997400	C	-0.42497900	1.81792300	0.05548800
C	-1.90185900	-3.08959800	-0.68436200	C	-0.97074500	1.68253800	1.33860600
H	-0.45503600	-4.07136300	-1.94013000	C	-1.28423700	2.18978400	-0.99480400
H	-3.06906400	-1.92936800	0.71209400	C	-2.32806700	1.91043000	1.56638400
H	-2.76057300	-3.57504200	-1.13929100	H	-0.33700900	1.37255600	2.16252700
TS _{29-30_2}				C	-2.63302700	2.41150400	-0.76081600
C	1.38728600	0.67670800	-1.17905700	H	-0.86464200	2.28161800	-1.98879000
O	1.76440500	-0.65787300	-0.28023200	C	-3.16986000	2.27612700	0.52245000
O	0.55126800	0.28411700	-2.05854300	H	-2.72829900	1.78063200	2.56863300

H	-3.27651200	2.69583000	-1.59009100	C	-3.28975100	-0.59453300	-1.65775700
H	-4.22825400	2.44548600	0.69970900	H	-1.24304300	-0.31873400	-2.19120100
XXX₂				C	-3.71033200	-1.75066200	0.39488500
C	0.59772400	-1.88386700	1.00895800	H	-1.98094100	-2.40647600	1.49035400
O	2.66823100	1.52386000	-0.67633700	C	-4.19972300	-1.09328100	-0.73177000
O	0.04214200	-2.12346100	2.07294300	H	-3.64016600	-0.06542100	-2.53947100
C	0.84411900	-1.23129800	-1.30582600	H	-4.40082400	-2.14915600	1.13355400
H	0.81406400	-0.16411500	-1.54467200	H	-5.26803500	-0.96932700	-0.88264900
H	1.87528600	-1.47625000	-1.03857700	XXII_B			
H	0.54073500	-1.81758700	-2.17961700	H	2.77998800	0.57915400	2.25663300
H	3.47131900	0.90543800	-0.75707400	C	0.03255800	0.23443200	-0.22225400
H	1.69200100	-1.91298900	0.89378100	C	0.03821300	0.02519800	1.16339500
N	-0.02663100	-1.54523100	-0.17110800	C	-0.57996600	1.39574000	-0.72052900
C	0.11517800	1.90902800	0.54361400	C	-0.54021600	0.95774300	2.02555100
C	-0.81229000	1.39628100	1.45983800	H	0.50361000	-0.86684600	1.57376800
C	-0.37978000	2.60774000	-0.56805900	C	-1.17145500	2.31820300	0.13592500
C	-2.18282200	1.58432100	1.28461300	H	-0.60642900	1.58426600	-1.79247500
H	-0.46631700	0.80553800	2.30538900	C	-1.14986000	2.10094600	1.51367100
C	-1.74742500	2.80486600	-0.74607600	H	-0.54112300	0.77748300	3.09646400
H	0.31929700	2.98735900	-1.30976600	H	-1.68210200	3.18762500	-0.26325300
C	-2.65245800	2.29541700	0.18421800	H	-1.65501200	2.79711600	2.17273400
H	-2.88332300	1.14782100	1.99035800	C	2.47121700	-2.64653400	0.03500700
H	-2.10979800	3.34256000	-1.61864500	O	2.64862000	-3.53743000	0.81973700
H	-3.72058100	2.42658800	0.03591700	Si	0.87757400	-0.96023000	-1.37067600
Si	1.97019300	1.68339200	0.79322900	H	2.11819900	-0.43251300	-1.97980100
H	2.16088400	0.51626400	1.69613900	O	1.25891800	-2.33841500	-0.45193500
H	2.47710000	2.88955900	1.52143700	H	3.28257900	-2.01366900	-0.36188500
C	4.71927800	-1.18868500	-0.43876700	H	-0.05114800	-1.43372900	-2.42574900
H	5.71127000	-1.70270300	-0.44730000	N	3.38334200	0.04134000	1.65272300
O	4.74638100	0.01525900	-0.82108500	C	4.36460600	-0.77288500	2.34457300
O	3.73996400	-1.86327000	-0.06245000	C	3.68969800	0.68445100	0.45998100
C	-1.42221400	-1.40139000	-0.32856600	C	2.90876000	1.77514400	0.03767600
C	-1.92117400	-0.74513400	-1.46424000	C	3.13534400	2.37104500	-1.19358300
C	-2.34482200	-1.91019400	0.60327300	C	4.14841200	1.90816700	-2.03634600

C	4.72579300	0.23871700	-0.37564100	C	0.77899800	1.18515200	-2.11470800
C	4.94202800	0.84750800	-1.61176400	H	0.33503900	-0.85705300	-2.60746900
H	5.32266600	-0.25264300	2.48662800	C	0.76269800	1.74129600	0.23079000
H	3.96173600	-1.04410000	3.32145400	H	0.27819600	0.14707400	1.57647400
H	4.54954200	-1.70816900	1.80726400	C	0.94841100	2.12280000	-1.09654700
H	2.10673300	2.13779400	0.67559300	H	0.93648500	1.47447000	-3.14966700
H	2.51128400	3.20604900	-1.49811200	H	0.92761500	2.46205800	1.02466100
H	4.32189300	2.37700500	-2.99896900	H	1.27268300	3.13174000	-1.32548600
H	5.36831600	-0.57886800	-0.06481200	C	-3.33677600	-1.75520800	0.93815500
H	5.74588400	0.48359000	-2.24477500	O	-4.08425900	-2.59852500	1.33677800
N	-3.95279700	-1.20010200	-0.37245500	Si	-0.31628800	-2.30073000	-0.07053000
C	-3.39536500	-0.73442700	-1.68192500	H	0.07628700	-2.51904400	1.36080600
H	-3.94786100	0.16079500	-1.96851700	O	-1.90578000	-2.45781500	-0.33343400
H	-3.50591700	-1.53861600	-2.41184900	H	-2.60181300	-1.18670400	1.51645700
H	-2.34152700	-0.50244600	-1.53185900	H	0.50835700	-3.22188000	-0.91548400
C	-5.39857900	-1.54204100	-0.53983600	N	-3.72960100	-0.92264300	-0.33055800
H	-5.91164000	-0.62950700	-0.84609800	C	-4.92836800	-1.48143900	-0.99554700
H	-5.78384900	-1.89466900	0.41828900	C	-3.76786700	0.50467400	-0.05053600
H	-5.48825600	-2.32835700	-1.29165400	C	-2.79613700	1.33062400	-0.60185400
C	-3.19648300	-2.40483700	0.07172200	C	-2.81375900	2.69017500	-0.29785500
H	-3.60558600	-2.75362900	1.02075300	C	-3.79016500	3.20675800	0.54883400
H	-2.14650900	-2.13754400	0.20135000	C	-4.74427800	1.00416900	0.80824900
H	-3.29089100	-3.18718700	-0.68380400	C	-4.75347500	2.36340300	1.10234400
C	-3.79778800	-0.11557400	0.68271600	H	-5.11693500	-0.90534700	-1.90130900
H	-2.72531700	0.04015400	0.80513100	H	-4.72094300	-2.52439000	-1.23092200
H	-4.19804500	-0.52903000	1.61157700	H	-5.78229000	-1.42918100	-0.32131600
C	-4.48338600	1.26728900	0.40091800	H	-2.02129000	0.92363400	-1.24521100
O	-5.09789600	1.39899800	-0.68083200	H	-2.05017800	3.33612500	-0.71713600
O	-4.29117600	2.05251500	1.33903400	H	-3.79755400	4.26573100	0.78473700
TS ₂₂₋₁₄				H	-5.48044200	0.33988900	1.25074100
H	-2.87397600	-1.21300600	-0.86861600	H	-5.50820000	2.76120900	1.77238000
C	0.25874400	-0.54383000	-0.47090200	N	4.31749100	-0.99952600	0.13873900
C	0.44563100	-0.13345800	-1.80126600	C	3.57199400	-1.21443000	1.42024400
C	0.41450500	0.42625700	0.53289300	H	3.89832100	-0.44436800	2.11890000

H	3.79370200	-2.21918600	1.78477000	H	2.33314700	-0.82843300	-2.15161100
H	2.50660800	-1.11671000	1.21267800	H	-0.02361500	-3.02043500	2.28042800
C	5.78591600	-1.12406400	0.38844200	N	3.80891600	-0.74726500	-0.71084100
H	6.06065900	-0.33840300	1.09349800	C	5.10305800	-1.23494700	-0.23082500
H	6.30812900	-0.98834200	-0.56001700	C	3.40516400	0.57797000	-0.34462500
H	5.98964000	-2.11838900	0.79023100	C	3.12672200	0.86884600	0.99180100
C	3.88456600	-2.03072200	-0.84599100	C	2.73510300	2.15230700	1.35168300
H	4.42515100	-1.87961200	-1.78125000	C	2.60401300	3.14589600	0.38294600
H	2.81276400	-1.92431000	-1.01904500	C	3.29329600	1.57432400	-1.31386600
H	4.09974700	-3.02292100	-0.44476000	C	2.87941200	2.85401900	-0.94876800
C	4.00414100	0.37497700	-0.43290900	H	5.17815600	-1.07562700	0.84595900
H	2.93829200	0.37416000	-0.66051200	H	5.17922000	-2.29953300	-0.45221800
H	4.56035900	0.45400800	-1.37030800	H	5.92271200	-0.70664900	-0.72946000
C	4.33396300	1.62015700	0.46275200	H	3.18743800	0.08501500	1.74055300
O	4.85178900	1.40786400	1.58187600	H	2.50452600	2.36861700	2.38939600
O	4.01149300	2.67102700	-0.10837000	H	2.27917100	4.14179900	0.66571600
XIV_c				H	3.53663800	1.35393900	-2.34892100
H	2.77712400	-2.04535500	0.66386200	H	2.78181400	3.62272900	-1.70835800
C	-0.01403300	-0.55668800	1.06228000	N	-4.14129200	-1.05486300	-0.16756700
C	-0.37663400	0.13584800	2.22726300	C	-3.09495200	-1.57827500	-1.10341900
C	-0.08351900	0.13416600	-0.16001300	H	-3.11457100	-0.95057900	-1.99448300
C	-0.79744900	1.46499700	2.17115600	H	-3.32262900	-2.62186900	-1.32880900
H	-0.33254300	-0.36630800	3.19161800	H	-2.12869300	-1.49990100	-0.60557500
C	-0.50722500	1.45673600	-0.22310500	C	-5.48516400	-1.15319800	-0.81593000
H	0.17567100	-0.37691400	-1.08568400	H	-5.45700000	-0.53272800	-1.71270300
C	-0.86980200	2.12365600	0.94605700	H	-6.23353300	-0.77933400	-0.11530400
H	-1.08862700	1.98028400	3.08165600	H	-5.68394700	-2.19981800	-1.05391000
H	-0.59777300	1.96004000	-1.17935700	C	-4.12244400	-1.87069100	1.07802400
H	-1.25296800	3.13576200	0.88509300	H	-4.88893200	-1.50061000	1.76013400
C	3.25309400	-1.33928000	-1.82023000	H	-3.14047000	-1.77583100	1.54426500
O	3.68403900	-2.33838300	-2.36121000	H	-4.31895000	-2.91536700	0.82889200
Si	0.59042300	-2.32379200	1.12589400	C	-3.85203900	0.39249000	0.20141800
H	0.18739300	-2.97326800	-0.15317000	H	-2.88667000	0.39238800	0.71113500
O	2.23386200	-2.44787700	1.35396600	H	-4.62455000	0.69029300	0.91428500

C	-3.80806100	1.43609200	-0.96918600	H	-4.34199100	0.25914900	-1.23759500
O	-3.94674700	1.00389700	-2.13486600	H	-4.91261700	-2.10201300	-1.65057700
O	-3.62341200	2.57987300	-0.53202100	H	-4.68158000	-3.79820300	0.16551200
XXII₂				H	-3.28762400	-0.71906000	2.82015700
H	-3.37496200	1.85254700	0.19002800	H	-3.86176100	-3.06826500	2.39792900
C	0.35081900	0.26005700	-0.95679300	C	3.53899400	1.32965400	0.78575000
C	-0.57330300	-0.49567800	-0.22495100	O	3.72830000	2.30444000	1.49602900
C	0.92941300	-0.33164700	-2.08887700	O	2.72945000	1.16522700	-0.18623600
C	-0.88814700	-1.80684000	-0.58143100	C	4.43773000	0.11132800	1.13761500
H	-1.07144400	-0.05518800	0.63357500	H	5.47331900	0.35843300	0.89056900
C	0.61679700	-1.63830300	-2.45920800	H	4.37036100	-0.04707200	2.21570500
H	1.63541200	0.23805600	-2.69002200	C	4.31302200	-1.13565500	-1.00530800
C	-0.28575800	-2.38308900	-1.69745000	H	3.61916200	-0.38590200	-1.37889300
H	-1.62408300	-2.35782000	-0.00302300	H	5.34499200	-0.84734400	-1.21154500
H	1.06362200	-2.07235500	-3.34999400	H	4.09921200	-2.11457700	-1.43609200
H	-0.53814400	-3.39872800	-1.98836200	C	5.09147500	-2.23207700	1.02241300
C	-1.60185800	2.81808200	-1.46106500	H	4.94451900	-2.32261500	2.09909400
O	-2.81694500	2.89614600	-1.45572800	H	4.90191900	-3.19309200	0.54229500
Si	0.80612400	1.99654500	-0.37050200	H	6.11217300	-1.90901000	0.81459400
H	1.39067400	2.88096000	-1.40202700	C	2.73551900	-1.66323800	0.79607200
O	-0.87740000	2.64815700	-0.38774200	H	2.57317000	-2.64721300	0.35465500
H	-1.03537100	2.89646000	-2.40848500	H	2.62416000	-1.71027400	1.88014100
H	0.92959300	2.24815400	1.07347300	H	2.03745000	-0.94677300	0.36967800
N	-3.47928300	1.27657700	1.02018500	N	4.13534200	-1.22212800	0.48037100
C	-2.79895400	1.74787600	2.19840900	TS _{22-14_2}			
C	-3.77920600	-0.04649700	0.82109200	H	-2.78211600	-1.70299600	-0.70277000
C	-4.24433400	-0.47406300	-0.44188100	C	0.39824200	0.18507300	-0.19545400
C	-4.55971000	-1.80313800	-0.66740400	C	0.54358500	1.13049100	-1.22105000
C	-4.42758300	-2.75887200	0.34664100	C	0.26874700	0.66907500	1.11545700
C	-3.64170800	-1.01103700	1.83702600	C	0.53854900	2.49954000	-0.95317700
C	-3.96877400	-2.34528400	1.59338400	H	0.68511300	0.78648400	-2.24220400
H	-3.42452300	1.64010400	3.09352700	C	0.26138200	2.03582600	1.39563400
H	-1.84723900	1.22271500	2.38285500	H	0.16884000	-0.03630600	1.94013700
H	-2.57040200	2.80491100	2.06118900	C	0.39068300	2.95667800	0.35667500

H	0.65448200	3.21149300	-1.76581200	H	4.18160100	-1.54194000	1.88240900
H	0.14551000	2.38242800	2.41921700	H	3.07769300	-0.20456400	2.33621900
H	0.37729500	4.02270500	0.56535500	C	5.52948100	0.73291700	1.91608600
C	-2.57685300	-1.54135600	1.18629300	H	6.21456900	1.45204700	1.46527000
O	-2.73913000	-2.37361400	2.03104000	H	4.99760000	1.19909000	2.74788700
Si	0.21258100	-1.66787700	-0.57327300	H	6.08963900	-0.13232200	2.27291800
H	1.12960400	-2.40042200	0.34919500	C	3.77758500	1.47588500	0.39802100
O	-1.35009200	-2.07669100	-0.30095800	H	3.24774100	1.92935500	1.23707800
H	-2.10232000	-0.56136600	1.29250500	H	4.48650600	2.18393900	-0.03450400
H	0.58115800	-1.89293000	-1.98887100	H	3.07864600	1.11947800	-0.35781600
N	-3.58717400	-1.46975300	-0.03069200	N	4.54439100	0.28841900	0.89349700
C	-4.55563400	-2.57784000	0.01421800	XIV_{2B}			
C	-4.09443300	-0.12519300	-0.23035200	H	-2.11355700	1.98810400	-1.05296200
C	-3.19594500	0.83560200	-0.69338900	C	0.14794200	0.30116600	0.34224300
C	-3.62145100	2.14995000	-0.85113000	C	0.31997100	0.51525300	1.71664800
C	-4.93718300	2.50157900	-0.55693200	C	-0.05293800	-1.01497200	-0.09387800
C	-5.40804100	0.21581500	0.07715300	C	0.28676000	-0.54338200	2.62249300
C	-5.82584500	1.53396100	-0.09545400	H	0.49795000	1.52340300	2.08119700
H	-5.12349500	-2.54766500	0.94470700	C	-0.07604000	-2.08480100	0.80187000
H	-5.21675100	-2.50595400	-0.84988800	H	-0.21231600	-1.21625000	-1.15160900
H	-3.99070600	-3.50823400	-0.01675600	C	0.09014700	-1.84801600	2.16572100
H	-2.17031600	0.56204500	-0.92072900	H	0.41771400	-0.35372000	3.68408500
H	-2.91574300	2.89363100	-1.20586500	H	-0.25551800	-3.09169200	0.43621100
H	-5.26965700	3.52621900	-0.68693500	H	0.05875300	-2.67392000	2.87063500
H	-6.10710100	-0.52699700	0.44387800	C	-3.16813700	-2.47857900	-0.31529200
H	-6.85211300	1.80040900	0.13487200	O	-2.78395200	-3.48944600	-0.88114800
C	4.43129800	-0.88220400	-1.47661100	Si	0.15348500	1.73897100	-0.87748500
O	5.16354700	-1.33666400	-2.36054400	H	1.03407100	1.47640100	-2.03190800
O	3.18769400	-0.77032100	-1.39212500	O	-1.36020000	1.79541700	-1.61964600
C	5.28903800	-0.36483900	-0.26059600	H	-3.47327300	-2.47715100	0.74300600
H	5.84170000	-1.20725800	0.16203600	H	0.39126100	3.00505000	-0.15740100
H	6.00444500	0.37459900	-0.62764200	N	-3.27645500	-1.25287000	-0.90258100
C	3.60144900	-0.69451600	1.51370900	C	-2.98389000	-1.11334100	-2.32529200
H	2.90745900	-1.01569300	0.73838300	C	-3.64597100	-0.11083700	-0.14933600

C	-3.14048900	0.08778900	1.13899100	O	0.00000000	0.00000000	-1.16935600
C	-3.48510300	1.23089100	1.85415500	C	0.00000000	0.00000000	0.00000000
C	-4.31157100	2.19874400	1.28848700	CH ₃ COO ⁻ (the black line in section 4.6.5.1)			
C	-4.48149100	0.85689600	-0.71641500	C	0.20920900	0.00114600	0.00000300
C	-4.80400600	2.00741600	-0.00174000	O	0.80506900	-1.11092700	-0.00000800
H	-3.90124200	-1.13492400	-2.92351800	C	-1.35403400	-0.04912000	0.00000800
H	-2.45105900	-0.17384100	-2.48987300	H	-1.74105200	0.47868600	-0.88303000
H	-2.36403700	-1.95965900	-2.62295000	H	-1.72857300	-1.07996300	-0.00012900
H	-2.43770300	-0.62096700	1.56335100	H	-1.74102400	0.47842700	0.88321400
H	-3.07086300	1.37735000	2.84657200	O	0.70488000	1.16226500	-0.00000700
H	-4.56021000	3.09902600	1.84053000	PhSiH ₃ (the black line in section 4.6.5.1)			
H	-4.87087300	0.71593800	-1.71885400	Si	-2.35175900	0.00021100	0.00491300
H	-5.44604200	2.75481900	-0.45685900	H	-2.84882000	1.33412600	-0.42503700
C	4.01368300	1.77948200	-0.19732800	H	-2.87924000	-1.04577400	-0.91221300
O	4.67401300	2.80939400	-0.34016700	H	-2.88539500	-0.28118500	1.36647900
O	2.78982800	1.59302900	0.00950500	C	-0.46977400	-0.00061000	-0.01152700
C	4.92655300	0.50259300	-0.28338200	C	0.25748800	-1.20630700	-0.00834900
H	5.47226700	0.52915200	-1.22918200	C	0.25583100	1.20502800	-0.00839400
H	5.64857400	0.53329500	0.53603600	C	1.65449100	-1.20879900	0.00275500
C	3.26613300	-0.99366000	-1.33438000	H	-0.26894300	-2.15918400	-0.01868800
H	2.53404600	-0.19521600	-1.22922700	C	1.65404400	1.20860200	0.00255900
H	3.80596500	-0.89808400	-2.27776300	H	-0.27289300	2.15611400	-0.01874100
H	2.78985200	-1.97265400	-1.26326300	C	2.35602700	0.00068700	0.00911300
C	5.28023100	-1.91992100	-0.33623700	H	2.19480000	-2.15243300	0.00365600
H	6.00298500	-1.81349300	0.47361300	H	2.19322000	2.15288600	0.00317200
H	4.79628600	-2.89638400	-0.27523800	H	3.44324800	0.00089500	0.01564400
H	5.78738300	-1.81569900	-1.29612700	(IM1a+Si-1a) ₂			
C	3.53505200	-1.01149100	1.09801900	C	-3.29550700	-2.38961100	-1.19444500
H	3.03958000	-1.98339800	1.11629500	O	-4.17539200	-2.90451800	-1.89446400
H	4.27486100	-0.94396200	1.89727300	C	-2.88165200	-3.08015700	0.11094500
H	2.80886300	-0.20368000	1.17391000	H	-3.52394300	-3.94738500	0.28486700
N	4.24630600	-0.85541400	-0.21193900	H	-1.83603300	-3.40501200	0.05629400
CO ₂ (the black line in section 4.6.5.1)				H	-2.95667500	-2.38902300	0.95896700
O	0.00000000	0.00000000	1.16935600	O	-2.69199300	-1.27728300	-1.50582900
				Si	3.04779100	-0.02660100	-1.63136600

H	4.10631800	-0.45844500	-2.57677600	C	2.80300100	2.57474500	1.83250300
C	3.51350900	-0.59418300	0.09084900	H	3.42778000	3.36153700	2.26172100
C	2.53669000	-0.77478800	1.09016100	H	1.95631100	2.37351800	2.49874100
C	4.85717700	-0.86495000	0.41459000	H	3.37838100	1.64468600	1.75899800
C	2.89706900	-1.20573300	2.37009600	O	1.58297900	2.15098400	-0.22781600
H	1.49119100	-0.57478000	0.86589900	Si	-2.69431900	-1.87575500	-0.49271300
C	5.21942900	-1.29450500	1.69394000	H	-3.60271400	-3.05906300	-0.56091400
H	5.63176600	-0.74099900	-0.34047700	C	-3.80395300	-0.36365600	-0.36916200
C	4.23680600	-1.46468100	2.67421600	C	-3.27993900	0.94401200	-0.35515800
H	2.12872100	-1.34130400	3.12752000	C	-5.20153600	-0.51349900	-0.30820400
H	6.26301700	-1.49754500	1.92480200	C	-4.12176400	2.05641700	-0.28248700
H	4.51454200	-1.80126400	3.67088500	H	-2.20474400	1.09763600	-0.40071900
O	3.08930000	1.67377900	-1.77262500	C	-6.04959900	0.59675900	-0.23665600
C	2.09293100	2.56603600	-1.56493000	H	-5.63615600	-1.51175000	-0.31155200
H	1.13603800	2.11305700	-1.25628800	C	-5.50898800	1.88521500	-0.22381100
O	2.26335600	3.75297800	-1.70527700	H	-3.69300100	3.05577600	-0.27168400
H	1.71580300	-0.51829200	-2.03740900	H	-7.12751500	0.45556000	-0.18727200
Si	-1.28037000	-0.16524500	-0.70321400	H	-6.16411700	2.75211100	-0.16636600
H	-0.63081600	-1.42360700	-0.20056700	O	-1.70115800	-1.98750400	0.83864000
H	-1.04968900	0.25802500	-2.11819100	C	-0.34943400	-2.42452200	0.85432400
H	-0.09310400	0.72037600	-0.15016100	H	-0.09022700	-2.93910100	-0.08925600
C	-2.57056800	0.76213100	0.38987300	O	0.15037400	-2.74105000	1.93095200
C	-3.95882500	0.74366800	0.14580500	H	-1.87986900	-1.84592700	-1.73905200
C	-2.12877800	1.53558500	1.48105500	Si	0.99673800	0.40433200	0.08751800
C	-4.85569500	1.45618400	0.94988800	H	0.63260600	0.67273900	1.51170100
H	-4.33686700	0.16275700	-0.68960400	H	0.00589500	0.61980900	-1.00854000
C	-3.01840300	2.23476700	2.30435300	H	0.32377100	-1.10452800	0.32817400
H	-1.06129200	1.59620400	1.68303700	C	2.67654100	-0.41539700	-0.32190400
C	-4.39036600	2.20064200	2.03816000	C	3.57189300	0.15341400	-1.24893200
H	-5.92099500	1.42599800	0.72619800	C	3.05222100	-1.63223400	0.28200500
H	-2.63938000	2.81433700	3.14506800	C	4.78425600	-0.46789400	-1.56923900
H	-5.08758100	2.75066600	2.66827400	H	3.31819400	1.10014200	-1.71896400
TS _{2a} (the black line in section 4.6.5.1)				C	4.27385000	-2.24570700	-0.01712600
C	2.30605000	3.01203400	0.45633300	H	2.38196300	-2.10640700	0.99584200
O	2.57861100	4.13093900	0.02388900	C	5.14223600	-1.66907600	-0.94957000

H	5.45214100	-0.00853400	-2.29627400	C	2.07371500	1.43858000	0.29903200
H	4.54291900	-3.17883300	0.47512300	C	4.37334400	2.78747400	-0.55967900
H	6.08905300	-2.15006800	-1.18979200	H	5.42233100	0.95560600	-0.15888000
IM3a				C	1.99190900	2.77167600	-0.11595900
C	2.41928600	-2.56239200	-1.30520900	H	1.16933200	0.92975900	0.62899500
O	2.61939000	-3.56712400	-1.95418800	C	3.13830800	3.44618300	-0.54474500
C	1.19688800	-1.68906200	-1.44682500	H	5.26843500	3.31055200	-0.89052000
H	0.49209500	-2.16690700	-2.12974100	H	1.02525600	3.26861800	-0.10381000
H	0.69604700	-1.48585800	-0.49016300	H	3.07249400	4.48375500	-0.86648800
H	1.48808300	-0.71465700	-1.85835700	TS _{2a_2}			
O	3.36381400	-2.15685300	-0.41000300	C	-2.99032900	-2.41316400	0.74517100
Si	-1.96790600	0.62460900	1.12445500	O	-3.33837800	-3.56162300	0.94416200
H	-1.24454400	1.52464400	0.10002500	C	-2.65780600	-1.43829200	1.84959200
C	-3.55436700	0.42347000	0.04071500	H	-2.76113100	-1.93944600	2.81432000
C	-4.61163200	-0.43652600	0.40007700	H	-1.63526200	-1.06893000	1.70240400
C	-3.71933700	1.17438800	-1.13813600	H	-3.32853400	-0.57225400	1.81024600
C	-5.77489800	-0.53492100	-0.37195800	O	-2.89904800	-1.95547600	-0.51960800
H	-4.49919000	-1.03612200	1.29936500	Si	1.70256000	-0.11200900	-0.03530300
C	-4.87908100	1.08846300	-1.91788400	H	1.40230500	0.74810500	1.16582500
H	-2.91552400	1.83944500	-1.45126700	C	3.63533900	0.17675800	0.01396200
C	-5.91474800	0.22991300	-1.53550000	C	4.58448600	-0.77880000	-0.39965200
H	-6.57420500	-1.21001500	-0.06723100	C	4.14212100	1.42169800	0.43247000
H	-4.97236500	1.68445200	-2.82535800	C	5.95817200	-0.50590900	-0.40326400
H	-6.81801000	0.15375000	-2.13944300	H	4.23363300	-1.75847900	-0.71538900
O	-2.38861600	-0.77904900	2.27997900	C	5.51109900	1.71335100	0.42987900
C	-1.12821600	-1.32972300	2.12059000	H	3.44532000	2.18805700	0.77642900
H	-0.54043200	-1.33764200	3.06082600	C	6.42932900	0.74508200	0.00945000
O	-0.53860800	-0.43748000	1.17588200	H	6.66329400	-1.27136500	-0.72677700
H	-2.18450000	1.69660700	2.16536500	H	5.86268100	2.69041400	0.76079900
Si	3.42669600	-1.02025000	0.85087600	H	7.49679800	0.96100100	0.00827700
H	2.37511600	-1.34143200	1.83883100	O	1.82587600	-1.83683200	-0.12892300
H	4.78041600	-1.26280500	1.40996000	C	0.42866100	-2.11353700	-0.12771300
H	-1.15515300	-2.35907600	1.70951500	H	0.13667000	-2.56805000	-1.09498300
C	3.30810900	0.75872300	0.28574600	O	-0.12997700	-0.85761200	0.06790300
C	4.45462000	1.45548100	-0.14686700	H	1.40074000	0.65869000	-1.28954200

Si	-2.49133800	-0.56819300	-1.41368300	H	7.70103200	0.31417300	0.09354500
H	-1.27415200	-0.78630500	-2.21196000	O	1.50912700	-1.38863300	-0.05350700
H	-3.63466600	-0.57046000	-2.38075000	C	0.13721600	-1.80430700	-0.22884500
H	0.18657000	-2.82366500	0.68549800	H	0.06661700	-2.25034400	-1.23507200
C	-2.70445500	1.10829900	-0.56705900	O	-0.71381400	-0.73518200	-0.07301100
C	-3.90822400	1.80230600	-0.80732900	H	1.46709400	0.96639700	-1.27286600
C	-1.74217200	1.73245000	0.25008300	Si	-2.16896200	-0.56581200	-1.21755400
C	-4.14802700	3.06498100	-0.25523500	H	-1.21397500	-0.70806900	-2.37751600
H	-4.67077300	1.35113600	-1.43936900	H	-3.42393200	-0.52513900	-2.10387100
C	-1.97469000	2.99697100	0.79786700	H	-0.03579800	-2.58619200	0.52620300
H	-0.81191700	1.21886900	0.46029800	C	-2.56920500	1.16993800	-0.45329400
C	-3.17720500	3.66659900	0.54981800	C	-3.66609300	1.88466400	-0.97186500
H	-5.08763200	3.57634600	-0.45608300	C	-1.84409400	1.79392100	0.58272700
H	-1.21124800	3.45799200	1.42081100	C	-4.02033300	3.15427700	-0.49998100
H	-3.35538700	4.65076600	0.97924100	H	-4.25611800	1.42765100	-1.76413000
IM2a_2				C	-2.19317300	3.05738600	1.07097700
C	-3.10889400	-2.63953700	0.57670500	H	-0.99376300	1.27379900	1.00905400
O	-3.33568200	-3.83692400	0.72217900	C	-3.28341300	3.74660700	0.52897800
C	-3.22820300	-1.66135200	1.73620800	H	-4.87355100	3.67650200	-0.93116600
H	-3.48979500	-2.20122600	2.64937900	H	-1.61108900	3.50607200	1.87496900
H	-2.28325500	-1.12379900	1.86581200	H	-3.55531700	4.73133500	0.90630000
H	-3.99739800	-0.91007900	1.52047800	CO ₂ (the red line in section 4.6.5.1)			
O	-2.78036200	-2.13001500	-0.59647700	O	0.00000000	0.00000000	1.16935600
Si	1.88623000	0.22991200	-0.05065700	O	0.00000000	0.00000000	-1.16935600
H	1.42024600	0.99105200	1.14176300	C	0.00000000	0.00000000	0.00000000
C	3.78172200	0.23797800	0.01441300	CH ₃ COO ⁻ (the red line in section 4.6.5.1)			
C	4.53705400	-0.93045500	-0.19274300	C	0.20919000	0.00118200	0.00005000
C	4.48502900	1.43266400	0.25615100	O	0.80548300	-1.11072500	-0.00002900
C	5.93579100	-0.90634400	-0.16513200	C	-1.35418500	-0.04946400	0.00001800
H	4.01681300	-1.86804700	-0.37143700	H	-1.74122800	0.47822900	-0.88304200
C	5.88250700	1.46718900	0.28330500	H	-1.72766300	-1.08059700	-0.00012800
H	3.93475000	2.35760900	0.42905100	H	-1.74123700	0.47796800	0.88323000
C	6.61316300	0.29338700	0.07175800	O	0.70452900	1.16248600	-0.00002900
H	6.49673000	-1.82494800	-0.32722200	PhSiH ₃ (the red line in section 4.6.5.1)			
H	6.40034900	2.40578500	0.47204900	Si	-2.35175900	0.00021100	0.00491300

H	-2.84882000	1.33412600	-0.42503700	O	-3.16152600	-2.22007900	0.93229300
H	-2.87924000	-1.04577400	-0.91221300	C	-2.21138400	-2.16096600	1.89435400
H	-2.88539500	-0.28118500	1.36647900	H	-1.31004700	-1.58926000	1.61192300
C	-0.46977400	-0.00061000	-0.01152700	O	-2.35636700	-2.70017400	2.96457900
C	0.25748800	-1.20630700	-0.00834900	H	-1.80465100	-1.73252500	-1.22884400
C	0.25583100	1.20502800	-0.00839400	Si	1.34566700	0.65922500	0.41196200
C	1.65449100	-1.20879900	0.00275500	H	1.44216300	0.91891400	1.88446500
H	-0.26894300	-2.15918400	-0.01868800	H	0.55030500	1.58511600	-0.45334900
C	1.65404400	1.20860200	0.00255900	H	0.14222800	-0.34829000	0.59594100
H	-0.27289300	2.15611400	-0.01874100	C	2.45039500	-0.69269100	-0.40405700
C	2.35602700	0.00068700	0.00911300	C	3.50845400	-0.40114500	-1.28821700
H	2.19480000	-2.15243300	0.00365600	C	2.19171300	-2.05338100	-0.14975400
H	2.19322000	2.15288600	0.00317200	C	4.26333700	-1.41508200	-1.88912600
H	3.44324800	0.00089500	0.01564400	H	3.74161300	0.63761200	-1.50171600
(IM1a+Si-1a) ₃				C	2.95633100	-3.07467600	-0.72441200
C	3.82147500	2.40606800	0.76110900	H	1.37049200	-2.31748000	0.51361500
O	4.55485300	3.32372600	0.37264500	C	3.99509800	-2.75772100	-1.60506800
C	4.17482700	1.66258300	2.05462200	H	5.06805500	-1.15386800	-2.57473400
H	5.12799200	2.03156400	2.44234000	H	2.73609700	-4.11553500	-0.49122000
H	3.39139100	1.81179200	2.80681300	H	4.58789500	-3.54733200	-2.06414200
H	4.24238700	0.58280200	1.87596500	TS _{2a} (the red line in section 4.6.5.1)			
O	2.74884600	2.02762300	0.12580400	C	2.30410800	3.01231000	0.45583400
Si	-3.14340600	-1.53681900	-0.63235200	O	2.57595300	4.13145100	0.02355700
H	-4.17779400	-2.33274600	-1.33678400	C	2.80095600	2.57530000	1.83212900
C	-3.63622700	0.26537800	-0.63045500	H	3.42521400	3.36242800	2.26149100
C	-2.66302700	1.27985700	-0.54087500	H	1.95420200	2.37365800	2.49816000
C	-4.98995700	0.64331900	-0.72818000	H	3.37683200	1.64553900	1.75878000
C	-3.03388700	2.62766200	-0.54460200	O	1.58192800	2.15074700	-0.22862500
H	-1.60893700	1.02457800	-0.46242200	Si	-2.69426600	-1.87620200	-0.49290400
C	-5.36260700	1.98956000	-0.72968200	H	-3.60285600	-3.05937600	-0.56081600
H	-5.76259900	-0.12008800	-0.80478200	C	-3.80366100	-0.36396100	-0.36888900
C	-4.38231000	2.98345000	-0.63739500	C	-3.27954400	0.94367500	-0.35559400
H	-2.26527600	3.39310600	-0.47524900	C	-5.20121100	-0.51367800	-0.30682600
H	-6.41292500	2.26319500	-0.80430700	C	-4.12122900	2.05616200	-0.28254600
H	-4.66986200	4.03269200	-0.64019200	H	-2.20437500	1.09722000	-0.40199500

C	-6.04913600	0.59666000	-0.23489100	H	-1.34406000	-2.12960500	1.59912300
H	-5.63591400	-1.51189500	-0.30961400	C	-2.85111500	-0.35834900	0.54388300
C	-5.50841900	1.88508000	-0.22276700	C	-3.52763600	0.35321600	-0.46757900
H	-3.69237700	3.05548800	-0.27229900	C	-2.74159000	0.27268000	1.79782700
H	-7.12702400	0.45555200	-0.18465100	C	-4.06706200	1.62508600	-0.23904400
H	-6.16343900	2.75203800	-0.16502400	H	-3.62015800	-0.11458000	-1.44423300
O	-1.70062300	-1.98823700	0.83806600	C	-3.28575900	1.53914600	2.04370500
C	-0.34889800	-2.42529300	0.85325900	H	-2.21258300	-0.24424800	2.59777400
H	-0.08995700	-2.93956000	-0.09056400	C	-3.95070000	2.22358300	1.02069300
O	0.15115000	-2.74225100	1.92965800	H	-4.58163300	2.15037200	-1.04324200
H	-1.88027400	-1.84641000	-1.73954400	H	-3.18544100	1.99541600	3.02823800
Si	0.99646900	0.40383900	0.08673300	H	-4.36949600	3.21254500	1.20167100
H	0.63149400	0.67241300	1.51067000	O	-2.58979300	-2.19744900	-1.53564600
H	0.00603500	0.61849200	-1.00984700	C	-1.32434700	-2.65970000	-1.85787900
H	0.32421000	-1.10529500	0.32752400	H	-1.33472600	-3.68966700	-2.26964300
C	2.67686000	-0.41511100	-0.32185200	O	-0.67591700	-2.64155300	-0.59064100
C	3.57238200	0.15411500	-1.24846400	H	-3.17251300	-3.16116000	0.69589200
C	3.05282200	-1.63177000	0.28224000	Si	1.80260100	0.50061700	-1.57249200
C	4.78519000	-0.46661900	-1.56819100	H	0.38690700	0.08350200	-1.58664000
H	3.31844500	1.10070900	-1.71863900	H	2.42455000	0.31032000	-2.90594600
C	4.27488300	-2.24466700	-0.01631400	H	-0.79300900	-1.99910100	-2.57415200
H	2.38244000	-2.10627100	0.99574100	C	2.75552100	-0.37240300	-0.21829400
C	5.14344300	-1.66762700	-0.94834200	C	4.02114000	0.08947600	0.19652700
H	5.45320200	-0.00694900	-2.29491500	C	2.22304300	-1.52646700	0.38977600
H	4.54415200	-3.17766900	0.47606000	C	4.73819700	-0.57937900	1.19072200
H	6.09060100	-2.14817400	-1.18811100	H	4.44811100	0.98435300	-0.25363700
IM3a_2				C	2.94637200	-2.19603200	1.38413500
C	1.35828200	3.05843200	-0.49728800	H	1.24303700	-1.90647900	0.09659200
O	1.69726000	4.22314100	-0.50288700	C	4.19936500	-1.72670900	1.78527000
C	0.31203500	2.48909200	0.43478300	H	5.71179700	-0.20687500	1.50299600
H	-0.04689900	3.27476000	1.10073300	H	2.51637900	-3.08029100	1.84827000
H	-0.53775400	2.07976300	-0.12324300	H	4.75503200	-2.24814100	2.56238600
H	0.72648400	1.66806400	1.03142900	TS _{2a_3}			
O	1.92811800	2.19144100	-1.37417300	C	1.56124900	3.07419300	-0.58512700
Si	-2.14016100	-2.14158900	0.28099100	O	2.05960300	4.16934600	-0.74538500

C	0.56371300	2.76209500	0.51072400	H	5.74383500	-0.20110000	1.22371500
H	0.42745400	3.64667200	1.13481800	H	2.71762800	-3.20290600	1.86167900
H	-0.40396700	2.46524000	0.09085400	H	4.98442200	-2.29000100	2.34767900
H	0.91013700	1.92782700	1.13196100	IM2a_3			
O	1.88468300	2.05867700	-1.42107500	C	3.92384400	2.54957400	-0.17056900
Si	-2.15554300	-2.10573300	0.30988700	O	4.77876200	3.23305200	-0.73897500
H	-1.30048600	-2.07679100	1.59073200	C	3.87574600	2.51489300	1.35867000
C	-2.84867000	-0.31630800	0.56961300	H	4.71813200	3.08260000	1.76144800
C	-3.57861000	0.37076300	-0.42125300	H	2.93631400	2.94791200	1.72124800
C	-2.66529600	0.34825700	1.79732800	H	3.91430000	1.48339000	1.72727900
C	-4.09773900	1.65192200	-0.19872000	O	3.03672900	1.83998800	-0.82205700
H	-3.72736300	-0.12299800	-1.37802200	Si	-2.50171400	0.22903200	0.39885100
C	-3.18788100	1.62494000	2.03752400	H	-2.09266700	1.63367400	0.13449800
H	-2.09490500	-0.14977000	2.58060000	C	-4.38665700	0.16333800	0.17245400
C	-3.90646100	2.28495600	1.03480000	C	-5.01058100	-0.80871000	-0.63052100
H	-4.65467500	2.15779000	-0.98696800	C	-5.21565500	1.09669100	0.82244600
H	-3.02987100	2.10758100	3.00171400	C	-6.40190700	-0.85063700	-0.77451400
H	-4.30978700	3.28114100	1.21149000	H	-4.39241800	-1.53579500	-1.15080900
O	-2.69500000	-2.21081800	-1.48034500	C	-6.60679600	1.06223700	0.68652600
C	-1.42923700	-2.62297600	-1.86239300	H	-4.77037400	1.87065200	1.44789500
H	-1.41810600	-3.65168700	-2.27649600	C	-7.20499400	0.08459100	-0.11533200
O	-0.72295600	-2.58042900	-0.62614700	H	-6.85887600	-1.61236100	-1.40373000
H	-3.16515900	-3.11915900	0.79117200	H	-7.22247700	1.79782500	1.20095200
Si	1.50369000	0.38973300	-1.40923700	H	-8.28716400	0.05438800	-0.22664000
H	0.07682800	0.20097400	-1.09517100	O	-1.96697100	-0.91334500	-0.69570400
H	1.80239700	-0.00089600	-2.80771900	C	-0.54216900	-1.11060300	-0.78704400
H	-0.95748700	-1.94111100	-2.60047300	H	-0.35888900	-2.17441400	-0.55904900
C	2.62856300	-0.46162900	-0.17436900	O	0.09078200	-0.27617700	0.09981900
C	3.91230700	0.04440000	0.10997400	H	-2.22684700	-0.09529600	1.82557700
C	2.20947300	-1.64380200	0.46802000	Si	1.62171200	0.67097100	-0.31348500
C	4.75695600	-0.60790000	1.01203700	H	1.29913700	1.53232500	0.85541300
H	4.25433400	0.95929400	-0.37053000	H	1.14836900	0.86581000	-1.71420100
C	3.05875300	-2.29520700	1.36926700	H	-0.25503200	-0.90823000	-1.83360200
H	1.22104500	-2.05433300	0.26210700	C	2.81501100	-0.80936600	-0.01668300
C	4.32938300	-1.78136800	1.64280200	C	4.06761300	-0.90495200	-0.65491100

C	2.45871400	-1.86191900	0.84946800
C	4.91847000	-1.99602100	-0.44507600
H	4.38151500	-0.10660900	-1.32177800
C	3.31113100	-2.94710400	1.08194800
H	1.49227600	-1.82451500	1.34614800
C	4.54585900	-3.02103400	0.42995900
H	5.87642400	-2.04098900	-0.96091400
H	3.00865200	-3.73736800	1.76777900
H	5.20946600	-3.86706000	0.60177100

8.4. Supporting information for chapter 5.4.2

Table S8.4.1. Energy of species involved in figure 5.4.2.1 to figure 5.4.2.3

	ω B97XD/6-31+G(d,p)		SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)		SMD(CH ₃ CN) M06-2X/6-311++G(d,p)	
	ϵ (hartree)	G (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)
A	-326.8235558	-326.707709	-326.896965	-326.781118	-326.862070	-326.746224
B	-402.2270179	-402.092700	-402.359810	-402.225492	-402.309348	-402.175030
CO ₂	-188.5269446	-188.535860	-188.581469	-188.590384	-188.575118	-188.584034
PhSiH ₃	-522.8548462	-522.770631	-522.924458	-522.840243	-522.878682	-522.794467
I	-1113.6323641	-1113.388560	-1113.879403	-1113.635599	-1113.777955	-1113.534151
TS ₁₋₂	-1113.5911617	-1113.337940	-1113.869532	-1113.616310	-1113.774801	-1113.521579
II	-1113.6567417	-1113.402029	-1113.908890	-1113.654177	-1113.815629	-1113.560916
III	-1636.5401604	-1636.176426	-1636.845900	-1636.482166	-1636.705442	-1636.341707
TS ₃₋₄	-1636.4779843	-1636.113110	-1636.801064	-1636.436190	-1636.666868	-1636.301993
IV	-1636.5172515	-1636.146056	-1636.828617	-1636.457421	-1636.697381	-1636.326186
TS ₄₋₅	-1636.5169993	-1636.144686	-1636.827284	-1636.454970	-1636.696696	-1636.324382
V_A	-1636.5621860	-1636.192670	-1636.865087	-1636.495571	-1636.732688	-1636.363172
V'_B	-1234.3072065	-1234.097465	-1234.495756	-1234.286014	-1234.413004	-1234.203263
TS' ₅₋₆	-1234.2601704	-1234.050178	-1234.451049	-1234.241057	-1234.367872	-1234.157880
VI'	-1234.2976613	-1234.096264	-1234.489369	-1234.287972	-1234.403097	-1234.201700
VII'	-441.3022128	-441.164519	-441.407768	-441.270074	-441.361745	-441.224051
TS' ₇₋₈	-441.2547303	-441.114199	-441.364656	-441.224125	-441.319430	-441.178898
VIII'	-441.3189717	-441.172805	-441.420857	-441.274690	-441.378513	-441.232346

Note: $G_{\text{sol}} = \epsilon_{\text{sol}} + G - \epsilon$. This formula applies to every table in the supporting information.

Table S8.4.2. Energy of species involved in figure 5.4.2.4 to figure 5.4.2.6

	ω B97XD/6-31+G(d,p)		SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)		SMD(CH ₃ CN) M06-2X/6-311++G(d,p)	
	ϵ (hartree)	G (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)
IM2	-1113.6644969	-1113.409141	-1113.908140	-1113.652784	-1113.814737	-1113.559381
TS _{IM}	-1113.6287974	-1113.372760	-1113.877867	-1113.621829	-1113.787207	-1113.531170
IM3	-1113.6379844	-1113.383188	-1113.886260	-1113.631463	-1113.795521	-1113.540724
IX	-1365.6895193	-1365.282652	-1366.024703	-1365.617835	-1365.895586	-1365.488719
TS ₉₋₁₅	-1365.6703099	-1365.266659	-1366.004111	-1365.600460	-1365.873020	-1365.469369
XV	-1365.6723316	-1365.270347	-1366.005123	-1365.603138	-1365.874570	-1365.472585
XVIII	-1152.6902455	-1152.426442	-1152.938229	-1152.674426	-1152.848715	-1152.584911
TS ₁₈₋₁₉	-1152.6884667	-1152.425078	-1152.935803	-1152.672415	-1152.846891	-1152.583502
XIX	-1152.8083181	-1152.541905	-1153.026237	-1152.759824	-1152.942033	-1152.675620
XX	-1365.6925048	-1365.291590	-1366.020123	-1365.619208	-1365.886818	-1365.485904
TS ₂₀₋₂₁	-1365.6569084	-1365.256600	-1366.002387	-1365.602079	-1365.869270	-1365.468962
XXI	-1365.7517715	-1365.340076	-1366.081631	-1365.669936	-1365.959568	-1365.547872
XVI	-1478.9755683	-1478.565385	-1479.347054	-1478.936870	-1479.213510	-1478.803327
TS ₁₆₋₁₇	-1478.9739402	-1478.562571	-1479.345019	-1478.933650	-1479.212214	-1478.800845
XVII	-1478.9914118	-1478.576294	-1479.352093	-1478.936975	-1479.220556	-1478.805439
XXIII	-881.4667811	-881.178433	-881.665340	-881.376992	-881.584674	-881.296325
TS ₂₃₋₂₄	-881.4285371	-881.142039	-881.639229	-881.352730	-881.554706	-881.268208
XXIV	-881.4750235	-881.182014	-881.673717	-881.380707	-881.592649	-881.299639

Table S8.4.3. Energy of species involved in figure 5.4.2.7

	ω B97XD/6-31+G(d,p)		SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)		SMD(CH ₃ CN) M06-2X/6-311++G(d,p)	
	ϵ (hartree)	G (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)
A	-326.8235558	-326.707709	-326.896965	-326.781118	-326.862070	-326.746224
B	-402.2270179	-402.092700	-402.359810	-402.225492	-402.309348	-402.175030
CO ₂	-188.5269446	-188.535860	-188.581469	-188.590384	-188.575118	-188.584034
PhSiH ₃	-522.8548462	-522.770631	-522.924458	-522.840243	-522.878682	-522.794467
X'	-515.3575242	-515.237874	-515.483915	-515.364265	-515.443870	-515.324219
TS' ₁₀₋₁₁	-515.2926030	-515.170916	-515.420342	-515.298655	-515.381879	-515.260192
XI'	-515.3499623	-515.225731	-515.478139	-515.353908	-515.440371	-515.316140
XII_A	-1440.4704901	-1440.081971	-1440.784570	-1440.396051	-1440.650972	-1440.262453
TS ₁₂₋₁₃	-1440.4111774	-1440.017674	-1440.745528	-1440.352025	-1440.621535	-1440.228032
XIII	-1440.4887949	-1440.091839	-1440.799482	-1440.402526	-1440.675649	-1440.278693
XII'	-1038.2257247	-1037.992168	-1038.416990	-1038.183434	-1038.334196	-1038.100640
TS' ₁₂₋₁₄	-1038.1337090	-1037.901113	-1038.327660	-1038.095064	-1038.248869	-1038.016273
XIV'_A	-1038.2555947	-1038.021377	-1038.449485	-1038.215267	-1038.369171	-1038.134953

Table S8.4.4. Energy of species involved in figure 5.4.2.8 and figure 5.4.2.9

	ω B97XD/6-31+G(d,p)		SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)		SMD(CH ₃ CN) M06-2X/6-311++G(d,p)	
	ϵ (hartree)	G (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)
A	-326.8235558	-326.707709	-326.896965	-326.781118	-326.862070	-326.746224
B	-402.2270179	-402.092700	-402.359810	-402.225492	-402.309348	-402.175030
CO ₂	-188.5269446	-188.535860	-188.581469	-188.590384	-188.575118	-188.584034
PhSiH ₃	-522.8548462	-522.770631	-522.924458	-522.840243	-522.878682	-522.794467
I	-1113.6323641	-1113.388560	-1113.879403	-1113.635599	-1113.777955	-1113.534151
TS ₁₋₂	-1113.5911617	-1113.337940	-1113.869532	-1113.616310	-1113.774801	-1113.521579
II	-1113.6567417	-1113.402029	-1113.908890	-1113.654177	-1113.815629	-1113.560916
XXII_A	-1440.5064474	-1440.115714	-1440.812208	-1440.421475	-1440.681336	-1440.290603
TS ₂₂₋₂₅	-1440.4912954	-1440.096621	-1440.790822	-1440.396147	-1440.662880	-1440.268206
XXV_A	-1440.4916616	-1440.096553	-1440.788977	-1440.393869	-1440.661456	-1440.266348
XXV_B	-1440.4932520	-1440.094404	-1440.791646	-1440.392798	-1440.663387	-1440.264539
TS ₂₅₋₂₆	-1440.4715629	-1440.073927	-1440.779771	-1440.382136	-1440.654906	-1440.257271
XXVI_A	-1440.4942507	-1440.091962	-1440.792648	-1440.390360	-1440.667315	-1440.265026
XXVI_B	-1440.4968084	-1440.103523	-1440.802054	-1440.408769	-1440.676522	-1440.283237
TS ₂₆₋₁₄	-1440.4692567	-1440.074470	-1440.778620	-1440.383834	-1440.652285	-1440.257499
XIV_A	-1440.5139925	-1440.121500	-1440.825396	-1440.432904	-1440.694101	-1440.301609

Table S8.4.5. Energy of species involved in figure 5.4.2.10 and figure 5.4.2.11

	ω B97XD/6-31+G(d,p)		SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)		SMD(CH ₃ CN) M06-2X/6-311++G(d,p)	
	ϵ (hartree)	G (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)
A	-326.8235558	-326.707709	-326.896965	-326.781118	-326.862070	-326.746224
B	-402.2270179	-402.092700	-402.359810	-402.225492	-402.309348	-402.175030
CO ₂	-188.5269446	-188.535860	-188.581469	-188.590384	-188.575118	-188.584034
PhSiH ₃	-522.8548462	-522.770631	-522.924458	-522.840243	-522.878682	-522.794467
I	-1113.6323641	-1113.388560	-1113.879403	-1113.635599	-1113.777955	-1113.534151
TS ₁₋₂	-1113.5911617	-1113.337940	-1113.869532	-1113.616310	-1113.774801	-1113.521579
II	-1113.6567417	-1113.402029	-1113.908890	-1113.654177	-1113.815629	-1113.560916
XXVII	-1227.4430594	-1227.196436	-1227.745861	-1227.499238	-1227.655349	-1227.408725
TS ₂₇₋₂₈	-1227.4189550	-1227.166018	-1227.723109	-1227.470172	-1227.636778	-1227.383841
XXVIII	-1227.4350060	-1227.176898	-1227.729490	-1227.471381	-1227.647301	-1227.389193
TS ₂₈₋₂₉	-1227.4270777	-1227.171120	-1227.722708	-1227.466750	-1227.641337	-1227.385379
XXIX	-1227.4361550	-1227.180493	-1227.728811	-1227.473149	-1227.646811	-1227.391149
TS ₂₉₋₃₀	-1227.4231041	-1227.171206	-1227.719731	-1227.467833	-1227.636376	-1227.384478
XXX	-1227.4623201	-1227.214877	-1227.763562	-1227.516118	-1227.673583	-1227.42614

Table S8.4.6. Energy of species involved in figure 5.4.2.12

	ω B97XD/6-31+G(d,p)		SMD(CH ₃ CN) ω B97XD/6-311++G(d,p)		SMD(CH ₃ CN) M06-2X/6-311++G(d,p)	
	ϵ (hartree)	G (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)	ϵ_{sol} (hartree)	G_{sol} (hartree)
A	-326.8235558	-326.707709	-326.896965	-326.781118	-326.862070	-326.746224
B	-402.2270179	-402.092700	-402.359810	-402.225492	-402.309348	-402.175030
CO ₂	-188.5269446	-188.535860	-188.581469	-188.590384	-188.575118	-188.584034
PhSiH ₃	-522.8548462	-522.770631	-522.924458	-522.840243	-522.878682	-522.794467
I	-1113.6323641	-1113.388560	-1113.879403	-1113.635599	-1113.777955	-1113.534151
TS ₁₋₂	-1113.5911617	-1113.337940	-1113.869532	-1113.616310	-1113.774801	-1113.521579
II	-1113.6567417	-1113.402029	-1113.908890	-1113.654177	-1113.815629	-1113.560916
XXII'	-1038.2443916	-1038.011263	-1038.437070	-1038.203942	-1038.356811	-1038.123682
TS' ₂₂₋₁₄	-1038.1886695	-1037.953688	-1038.388659	-1038.153678	-1038.306507	-1038.071525
XIV'B	-1038.2545625	-1038.021332	-1038.448282	-1038.215052	-1038.367713	-1038.134483