Supplementary Data

Mechanistic insights into $H_3B{\cdot}NMeH_2$ dehydrogenation by the Co-based complexes: A DFT perspective

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Complete Gaussian 09 reference

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Table S1. Selected donor-acceptor interactions involved in the bonding of the amidoborane fragment in **TS5-7** with the second order perturbation theory analysis (SOPT) of the Fock matrix in the natural bond orbital (NBO) basis. BD, LP, RY, denote bonding, lone pair, Rydberg orbitals, respectively. Asterisks denote antibonding NBO orbitals. Interaction energies, E_{SOPT}, are given in kcal/mol.

TS5-7	Donor	Contribution	Acceptor	Contribution	E_{SOPT}
N→H−H	LP N	s(16%)	BD* H−H	57% H s(99%)	19.03
		p(84%)		43% H s(99%)	
H−H→Co	BD H−H	57% H s(99%)	LP* Co	s (28%)	17.87
		43% H s(99%)		d (70%)	

Table S2. Selected donor-acceptor interactions involved in the bonding of the amidoborane fragment in **TS8-9**. Interaction energies, E_{SOPT}, are given in kcal/mol.

TS8-9	Donor	Contribution	Acceptor	Contribution	E_{SOPT}
H(B)→B	LP H	s(99%)	LP* B	s(3%) p(97%)	142.81
H→Co	LP H	s(99%)	LP* Co	s(80%) d(18%)	88.61
Co→H(B)	LP* Co	s(80%) d(18%)	RY* H	s(99%)	55.06

Table S3. Selected donor-acceptor interactions involved in the bonding of the amidoborane fragment in **TS11-12**. Interaction energies, E_{SOPT}, are given in kcal/mol.

TS11-12	Donor	Contribution	Acceptor	Contribution	E_{SOPT}
H(N)→Co	LP H	s(100%)	LP* Co	s(2%) p(97%)	77.16
N→Co	LP N	p(99%)	LP* Co	s(17%) p(71%) d(17%)	14.54

Table S4. Selected donor-acceptor interactions involved in the bonding of the amidoborane fragment in **TS12-13**. Interaction energies, E_{SOPT}, are given in kcal/mol.

TS12-13	Donor	Contribution	Acceptor	Contribution	E_{SOPT}
H(B)→B	LP H	s(100%)	LP* B	s(5%) p(95%)	788.74
Co−H→Co	BD* Co−H	43% Co s(21%) p(19%) d(60%) 57% H s(100%)	LP* Co	s(18%) p(69%) d(13%)	241.44
H→Co	LP H	s(100%)	LP* Co	s(18%) p(69%) d(13%)	107.85
Co→B	LP* Co	s(18%) p(69%) d(13%)	RY* B	p(86%) d(14%)	84.25

Table S5. Atom pair delta-g indices and percentage contributions of **TS5-7**.

TS5-7 Bond	Atomic pair delta-g indices	Percentage contributions
N5–H69	0.434473	35.82%
Co1–H70	0.178879	14.75%
Co1–H64	0.161790	13.34%
Co1–N62	0.083446	6.88%
Co1–H69	0.074999	6.18%
Co1–B59	0.043971	3.62%
N5–B59	0.042929	3.54%
N5–H58	0.035369	2.92%
Co1–H61	0.023748	1.96%
N5–H61	0.023369	1.93%
Co1–H58	0.023334	1.92%
Co1–C65	0.022362	1.84%
N5–N62	0.015214	1.25%
N5–H64	0.011072	0.91%
Co1–H68	0.009434	0.78%

Table S6. Atom pair delta-g indices and percentage contributions of **TS8-9**.

TS8-9 Bond	Atomic pair delta-g indices	Percentage contributions
Co1–H68	0.305374	45.62%
Co1–B59	0.096454	14.41%
N5–H68	0.045893	6.86%
Co1–N62	0.036378	5.44%
Co1–H60	0.030649	4.58%
Co1–H61	0.029410	4.39%
N5–B59	0.027533	4.11%
N5–N62	0.027153	4.06%
N5–C64	0.013015	1.94%
Co1–H63	0.009921	1.48%
Co1–C64	0.009580	1.43%
N5–H67	0.008606	1.29%
N5–H63	0.007988	1.19%
Co1–H65	0.005156	0.77%
N5–H65	0.004544	0.68%

Table S7. Atom pair delta-g indices and percentage contributions of **TS11-12**.

TS11-12 Bond	Atomic pair delta-g indices	Percentage contributions
N4–H65	0.435293	41.00%
Co1–H69	0.296436	27.92%
Co1–H65	0.065180	6.14%
Co1–H60	0.047561	4.48%
Co1–N59	0.038030	3.58%
N4–B57	0.026940	2.54%
Co1–B57	0.023890	2.25%
N4–H67	0.022488	2.12%
N4–H69	0.020103	1.89%
N4–H68	0.016374	1.54%
Co1–H67	0.015202	1.43%
Co1–H68	0.010999	1.04%
Co1–C61	0.010868	1.02%
N4–N59	0.008401	0.79%
N4–H60	0.007683	0.72%

Table S8. Atom pair delta-g indices and percentage contributions of **TS12-13**.

TS12-13 Bond	Atomic pair delta-g indices	Percentage contributions
N4–H65	0.435165	26.81%
Co1–H66	0.178879	22.71%
Co1–H68	0.290846	17.92%
Co1–B57	0.110943	6.84%
Co1–H65	0.083447	5.14%
N4–H68	0.059315	3.65%
N4–N59	0.043553	2.68%
Co1–N59	0.042493	2.62%
N4–B57	0.039904	2.46%
Co1–H69	0.034123	2.10%
Co1–H58	0.031345	1.93%
N4–H60	0.013654	0.84%
N4–C61	0.011307	0.70%
Co1–H60	0.010774	0.66%
Co1–C61	0.010154	0.63%

Cartesian coordinates of selected reactants, intermediates, and transition states.

NH_2MeBH_3

E_{gas} = -122.462390 a.u.

E_{solv} = -122.5941369 a.u.

Zero-point energy correction = 0.073061 a.u.

N	0.00878800	0.55042500	0.00000100
H	0.00866400	1.16253900	0.81520100
B	-1.40503400	-0.30751200	0.00000600
H	-1.36934700	-0.96930100	1.01447900
H	-2.27564300	0.53487700	-0.00004500
C	1.23377000	-0.28572400	-0.00000800
H	1.20753800	-0.92245100	0.88463500
H	1.20746700	-0.92250600	-0.88459900
H	2.14304900	0.32254000	-0.00003300
H	-1.36929600	-0.96933000	-1.01445300
H	0.00860200	1.16256500	-0.81517800

$NHMeBH_2$

E_{gas} = -121.305739 a.u.

E_{solv} = -121.3986866 a.u.

Zero-point energy correction = 0.051691 a.u.

N	0.14572700	-0.41747300	0.00015900
H	0.14122100	-1.42963200	-0.00012700
B	1.36375700	0.25184500	0.00011800
H	1.36931600	1.44847400	-0.00033000
H	2.37298600	-0.38926900	-0.00026400
C	-1.18539900	0.17114400	-0.00008200
H	-1.75854300	-0.12522800	0.88717700
H	-1.09261900	1.25874200	-0.00109200
H	-1.75884300	-0.12686600	-0.88658100

H_2

E_{gas} = -1.1798530 a.u.

E_{solv} = -1.1598602 a.u.

Zero-point energy correction = -0.001314 a.u.

H	2.11823590	-0.24302823	-0.02305752
H	1.51823590	-0.24302823	-0.02305752

$NMeH_3Cl$

E_{gas} = -556.641144 a.u.

E_{solv} = -556.76971360a.u.

Zero-point energy correction = 0.045731 a.u.

N	-1.15782500	0.67894700	0.00000200
H	-1.35489700	1.24974700	-0.81903900
C	-1.97055200	-0.55016800	0.00000000
H	-1.71528200	-1.14066000	-0.88261000
H	-1.71531000	-1.14064500	0.88262800
H	-3.05024900	-0.35952300	-0.00001900
H	0.35061900	0.30408300	-0.00003700
Cl	1.69224100	-0.09496300	0.00000100
H	-1.35489800	1.24974800	0.81904200

$NMeH_2$

E_{gas} = -95.822378 a.u.

E_{solv} = -95.9031196 a.u.

Zero-point energy correction = 0.041308 a.u.

N	0.75248200	0.00000200	-0.12584400
H	1.14307900	0.81126500	0.34765000
H	1.14316700	-0.81123100	0.34763900
C	-0.70546000	-0.00000200	0.01754700
H	-1.08664200	-0.00029800	1.05302300
H	-1.11711500	0.88053700	-0.48610300
H	-1.11709900	-0.88027200	-0.48658400

$H_2B(NMeH)_2Cl$

E_{gas} = -677.927989 a.u.

E_{solv} = -678.20717870 a.u.

Zero-point energy correction = 0.122530 a.u.

Cl	2.98054100	-0.27259800	0.11362900
B	-0.72213600	-0.91869000	0.23851800
N	-2.29971600	-0.77029000	-0.26412600
N	0.20006600	0.13934700	-0.41480000
H	1.30562100	-0.14778600	-0.12999100
H	-0.76393900	-0.78128400	1.43262900

H	-0.41260400	-2.01644900	-0.14513800
H	-2.71257800	-1.66681300	-0.00346100
C	-3.13041500	0.32562800	0.31033000
H	-2.34473800	-0.74172100	-1.28448000
H	-2.73990900	1.28532900	-0.02485500
H	-4.17455200	0.22898300	0.00322600
H	-3.05342300	0.27366500	1.39622600
C	0.11972100	1.57099800	-0.04051300
H	1.06789000	2.05178300	-0.29275500
H	-0.69956100	2.08749500	-0.55084300
H	-0.02432000	1.63857100	1.03878100
H	0.25530200	0.05269200	-1.43003400

INT1

E_{gas} = -2434.650860 a.u.

E_{solv} = -2436.3523132 a.u.

Zero-point energy correction = 0.4535090 a.u.

Co	0.00935400	-0.04735700	-0.30016200
C	-2.30536400	0.62529100	1.78312000
C	-1.34595200	-0.29504500	2.55322500
N	-0.05364600	-0.54466100	1.84062800
C	1.14765000	-0.08996800	2.58322600
C	2.43634800	-0.59568000	1.92166400
P	2.55845100	-0.09327400	0.11255400
C	3.70293000	1.40552100	0.16091700
C	3.19643500	2.46997900	1.14946300
C	3.85536900	2.01571300	-1.24308100
C	3.55470400	-1.52319200	-0.59828000
C	4.97354100	-1.68326400	-0.03335700
C	3.54554300	-1.52350800	-2.13602200
P	-2.52157200	0.04287600	0.01819500
C	-3.73275500	1.25067600	-0.78173200
C	-3.45519300	1.31689400	-2.29547600
C	-3.69629800	2.65931400	-0.16757500
C	-3.48105700	-1.56850900	0.19255100
C	-3.79608100	-2.15071100	-1.19627900
C	-4.73337900	-1.50754800	1.07857500
H	-1.87034400	1.62725100	1.71320200
H	-3.24581600	0.70860400	2.33920300
H	-1.82564400	-1.26109000	2.74299600
H	-1.12971900	0.14401600	3.53376500
H	0.03575800	-1.54808600	1.67618200
H	1.10607100	-0.44609500	3.62357200
H	1.12422700	1.00357800	2.60909600
H	2.44942800	-1.69225900	1.95336200
H	3.29922700	-0.25170700	2.50159400
H	4.68244300	1.04999400	0.50785400
H	3.17476500	2.10640600	2.18178500
H	3.86934400	3.33516700	1.12846200
H	2.19575100	2.81571000	0.87368800
H	4.29754800	1.31608900	-1.95693500
H	4.51016400	2.89370200	-1.19493500
H	2.88387600	2.33671100	-1.63031400
H	2.94619900	-2.38073900	-0.28504700
H	4.98915200	-1.72329000	1.06102000
H	5.41819300	-2.61527800	-0.40161400
H	5.63042600	-0.86600800	-0.34969300
H	2.52623000	-1.44767100	-2.52203000
H	3.97517400	-2.46203300	-2.50454400
H	4.14299700	-0.70679500	-2.55271700
H	-4.73559900	0.83258200	-0.62438800
H	-3.49412300	0.33221200	-2.77001000
H	-4.20310900	1.95301400	-2.78360400
H	-2.46527100	1.74324400	-2.48155700
H	-3.99209300	2.66387600	0.88591600
H	-4.39736000	3.30676700	-0.70715600
H	-2.69889100	3.09959200	-0.25477800
H	-2.75106100	-2.24393300	0.65736200
H	-2.89046900	-2.23574700	-1.80266900
H	-4.22579700	-3.15328900	-1.09055700
H	-4.52811200	-1.53847500	-1.73439700
H	-4.50945300	-1.19038800	2.10179000
H	-5.19810300	-2.49882700	1.13842900

H	-5.48662900	-0.82246100	0.67429300
Cl	0.04696700	-2.30255900	-0.98227100
Cl	-0.00215700	2.23356600	-0.83087700

INT2

E_{gas} = -2557.108537 a.u.

E_{solv} = -2558.9622866 a.u.

Zero-point energy correction = 0.5482950 a.u.

Co	0.01413200	-0.02563500	0.05433500
C	-2.31176200	-2.13197100	-0.74639600
C	-1.32065500	-2.14307400	-1.91847200
N	0.00048300	-1.54097800	-1.58866200
C	1.10660900	-2.50489200	-1.38901700
C	2.45341300	-1.77264200	-1.43214200
P	2.56255900	-0.36763900	-0.18123700
C	3.68716100	-0.99109200	1.20777800
C	3.53987800	-2.49138500	1.50860600
C	3.42663600	-0.16719400	2.48296200
C	3.62784700	0.86189900	-1.13606100
C	4.92269900	0.29207000	-1.73583800
C	3.92002300	2.12077300	-0.30445200
P	-2.52380800	-0.39810800	-0.08368000
C	-3.69054000	-0.53915600	1.40114500
C	-3.29294800	0.50945700	2.45500700
C	-3.74789900	-1.94176000	2.02655800
C	-3.56295200	0.44758200	-1.41448500
C	-3.83833100	1.90968800	-1.02519000
C	-4.85804700	-0.27395900	-1.81551600
H	-1.90814000	-2.72074300	0.08090600
H	-3.25438500	-2.59030800	-1.06394500
H	-1.73668500	-1.58178900	-2.76155800
H	-1.17783700	-3.17417200	-2.26829000
H	0.25337800	-0.90674900	-2.34537000
H	1.08600600	-3.27602000	-2.17464100
H	0.95389100	-2.99461000	-0.42356600
H	2.57449800	-1.32022100	-2.42465400
H	3.26786100	-2.49218000	-1.31446000
H	4.71644900	-0.80914400	0.87172200
H	3.82103300	-3.12380600	0.66073900
H	4.20226600	-2.75748300	2.34087600
H	2.51564900	-2.73221800	1.80520900
H	3.53586800	0.90804900	2.31934700
H	4.13726700	-0.46161800	3.26477700
H	2.41338800	-0.34799000	2.85118700
H	2.95459500	1.15571600	-1.95148400
H	4.74629900	-0.56801300	-2.38828400
H	5.42235200	1.06073900	-2.33763000
H	5.63019600	-0.01620700	-0.95818200
H	3.01063800	2.53637900	0.13615400
H	4.37639900	2.88846200	-0.94043600
H	4.62501600	1.91183400	0.50771600
H	-4.69206000	-0.29346300	1.02578400
H	-3.30142200	1.52552300	2.04699600
H	-3.99667700	0.48403100	3.29568400
H	-2.28788600	0.31220700	2.83701800
H	-4.11886000	-2.69534600	1.32523400
H	-4.43047600	-1.92783400	2.88460000
H	-2.76238800	-2.25184300	2.38403300
H	-2.88893500	0.47232000	-2.28011700
H	-2.90203400	2.45086300	-0.86187600
H	-4.37855000	2.42052500	-1.83046800
H	-4.45386800	1.98396300	-0.12131900
H	-4.67734900	-1.29283500	-2.17029700
H	-5.35505400	0.27041000	-2.62757400
H	-5.56860700	-0.33079000	-0.98373400
Cl	0.03198700	1.64277700	-1.82344000
Cl	-0.02974700	-1.62790600	1.84210100
H	-0.11139800	1.37058500	1.39361900
H	-0.15463600	3.15791100	-0.25218100
H	-1.41910900	3.47000300	0.73020800
B	0.21295800	2.50108700	1.77721600
H	-0.32510500	2.71573000	2.83726600
H	1.40882800	2.64959600	1.78172300

N	-0.40168700	3.52013200	0.68541800
C	0.03048100	4.92834800	0.84366000
H	1.11525700	4.96759500	0.74032000
H	-0.43504000	5.57134700	0.09165300
H	-0.23756300	5.27146600	1.84452600

TS2-3$_N$

E_{gas} = -2652.8960610 a.u.

E_{solv} = -2654.8507129 a.u.

Zero-point energy correction = 0.6009120 a.u.

Three lowest frequencies:

-146.0790 20.2825 24.4573

Co	0.23523000	-0.04226600	0.08227600
C	0.25687400	-2.94187900	-1.85408600
C	0.19791400	-1.76588900	-2.84161300
N	0.86114800	-0.56609500	-2.30531700
C	2.30341400	-0.51101000	-2.56431200
C	2.90823800	0.77077000	-1.98275400
P	2.52100400	0.95891100	-0.16119200
C	4.10885800	0.43883500	0.70583500
C	4.54183500	-0.96917200	0.26417100
C	3.94900200	0.49516300	2.23482700
C	2.39363800	2.83431400	-0.01413700
C	3.66070700	3.59467500	-0.43431300
C	1.88272700	3.30662500	1.35746800
P	-0.48092900	-2.42608700	-0.22010900
C	0.04477500	-3.78213900	0.96981400
C	-0.68669600	-3.66517900	2.31829900
C	1.56596800	-3.74122700	1.19054500
C	-2.32471500	-2.63164500	-0.54575500
C	-3.18679900	-1.83159200	0.44325300
C	-2.79216400	-4.08952600	-0.67552900
H	1.29636400	-3.24053100	-1.68377400
H	-0.26017800	-3.81206700	-2.27328100
H	-0.84349600	-1.49861600	-3.04022000
H	0.63778600	-2.07017600	-3.80504400
H	0.40640100	0.26318600	-2.68403300
H	2.52436700	-0.56314100	-3.64422100
H	2.76882000	-1.39053900	-2.10592900
H	2.46737800	1.63488000	-2.49365600
H	3.98606200	0.80463400	-2.17267300
H	4.88940700	1.14793000	0.40020500
H	4.76298500	-1.02719300	-0.80573300
H	5.45244100	-1.25877800	0.80027100
H	3.77298000	-1.71324700	0.49707400
H	3.77104500	1.50964700	2.59715000
H	4.86320600	0.12868000	2.71586200
H	3.11271200	-0.12458200	2.57325800
H	1.60038900	3.04221800	-0.74504900
H	4.01351800	3.30979800	-1.43023500
H	3.45830200	4.67170800	-0.45307100
H	4.47948800	3.43306900	0.27485300
H	1.03636200	2.71050900	1.70805100
H	1.57013200	4.35506100	1.28791200
H	2.66558900	3.25554500	2.12014900
H	-0.21763700	-4.73914700	0.50007400
H	-1.76452100	-3.81183900	2.21955500
H	-0.31183600	-4.43260300	3.00538200
H	-0.51771500	-2.68492200	2.77457100
H	2.13424600	-3.85573500	0.26220200
H	1.86545200	-4.55649600	1.85861400
H	1.86175900	-2.79900400	1.66354200
H	-2.43747500	-2.14654300	-1.52464400
H	-2.88551100	-0.78382200	0.47297500
H	-4.23419900	-1.84476000	0.12856700
H	-3.13177700	-2.23171200	1.45962900
H	-2.20974000	-4.66057400	-1.40626000
H	-3.83736000	-4.10897600	-1.00288500
H	-2.74226400	-4.61733600	0.28202800
Cl	-5.25129300	1.44959100	0.16396900
Cl	-0.19721000	0.21497100	2.40713800
H	-3.62757500	1.69214500	1.04450900
H	-2.03989300	1.38359100	1.78699900

B	-1.61817000	1.61571200	-2.14042800
H	-1.96798100	0.48757000	-2.35826100
H	-0.63254000	2.04772100	-2.69413500
N	-2.64041200	2.08280400	1.32269900
C	-2.81082400	3.30091600	2.14646700
H	-3.51755400	3.96065900	1.64178500
H	-3.22319100	3.01609100	3.11523800
H	-1.85268800	3.80334300	2.29039200
N	-2.59812100	2.55014500	-1.70933500
H	-3.52642800	2.21348200	-1.44390600
H	-2.21661400	2.28104000	0.40342100
C	-2.50143300	3.99628200	-1.80869800
H	-1.49038900	4.27593200	-2.11860700
H	-3.20464100	4.40333000	-2.54790000
H	-2.71570100	4.50184600	-0.85547400
H	-0.65144200	1.09352300	-0.71711700

TS2-3$_B$

E_{gas} = -2652.868205 a.u.

E_{solv} = -2654.8261349 a.u.

Zero-point energy correction = 0.605545 a.u.

Three lowest frequencies:

-438.6219 19.3518 26.3289

Co	0.15520600	-0.41355500	-0.32229100
C	2.77581800	-1.43584500	1.43131400
C	1.66646900	-1.02270200	2.40741500
N	0.31967400	-1.00626900	1.79008700
C	-0.44992600	-2.26114800	1.97441200
C	-1.94823500	-2.00729500	1.75605400
P	-2.31746700	-1.26743500	0.07019700
C	-3.08732600	-2.65406400	-0.96253800
C	-2.44501400	-4.03019900	-0.72483500
C	-3.01089600	-2.28406600	-2.45574500
C	-3.75938100	-0.13329800	0.51039800
C	-4.92828100	-0.81316700	1.24125400
C	-4.26629200	0.66374800	-0.70206800
P	2.80250000	-0.24852900	-0.00985900
C	4.16049200	-0.87879000	-1.17268400
C	3.82014600	-0.47368200	-2.61903000
C	4.39838200	-2.39443900	-1.08150800
C	3.56262000	1.31159300	0.74561800
C	3.75722100	2.37960300	-0.34503700
C	4.84519900	1.12458600	1.56932100
H	2.55439900	-2.42347600	1.01565000
H	3.73267200	-1.50556000	1.95997800
H	1.85267500	-0.01431200	2.79141300
H	1.67162700	-1.69298500	3.27925400
H	-0.20710100	-0.23322500	2.23024400
H	-0.30132800	-2.64545400	2.99526000
H	-0.07037600	-3.01192000	1.27366200
H	-2.28419700	-1.27055600	2.49370500
H	-2.51078500	-2.92887800	1.92996100
H	-4.14228500	-2.71182600	-0.66453000
H	-2.55999800	-4.37509500	0.30719700
H	-2.93224700	-4.77196400	-1.36913600
H	-1.38106400	-4.01341600	-0.97569600
H	-3.47524700	-1.31717500	-2.67163200
H	-3.53016700	-3.04210600	-3.05468800
H	-1.96783200	-2.24300300	-2.78210400
H	-3.27761400	0.56642700	1.20639600
H	-4.60362000	-1.35650900	2.13275400
H	-5.65188100	-0.05618300	1.56702100
H	-5.46524700	-1.51480200	0.59305800
H	-3.44799000	1.14572500	-1.24556500
H	-4.96333300	1.44330500	-0.36968500
H	-4.81168900	0.02734200	-1.40779800
H	5.08697400	-0.37048300	-0.87471500
H	3.67143100	0.60560800	-2.72302000
H	4.63545400	-0.76519500	-3.29263600
H	2.90400600	-0.97351700	-2.94558200
H	4.75219200	-2.70059700	-0.09235200
H	5.16445500	-2.68756500	-1.80963100
H	3.48442500	-2.94834300	-1.31357000

H	2.77442900	1.67219800	1.42025800
H	2.84780100	2.52122000	-0.93721100
H	4.03018200	3.34136800	0.10674000
H	4.56659100	2.10703200	-1.03107600
H	4.69746200	0.46084700	2.42613200
H	5.18741000	2.09019700	1.96225500
H	5.66180000	0.71464700	0.96470700
Cl	0.69101100	-2.34718500	-1.62701500
H	-1.18065600	4.36952100	-3.05929300
B	-0.63929300	2.91888900	-1.25909300
N	-1.31497000	4.66681000	-2.09550800
C	-2.71826000	5.06913500	-1.88418100
H	-2.83950400	5.45842500	-0.86898700
H	-3.06004100	5.84019300	-2.58422500
H	-3.35416300	4.18708900	-1.99299200
N	-0.82359100	3.32371400	0.24225400
H	-1.72291900	3.78773600	0.37618200
H	-0.90978000	2.48523200	0.88323100
C	0.24437600	4.16770100	0.84051500
H	0.03559900	4.30794800	1.90203400
H	1.19164500	3.64241400	0.72375500
H	0.29865300	5.13046500	0.32735600
H	0.08723800	1.19632300	-0.65028100
H	-0.68705500	5.45669800	-1.95480900
H	0.44183800	3.05672400	-1.73627200
H	-1.52397000	2.29393300	-1.75009600
Cl	-1.26212500	1.64840300	2.72417700

INT3$_N$

E_{gas} = -2652.911639 a.u.

E_{solv} = -2654.8588514 a.u.

Zero-point energy correction = 0.603945 a.u.

Co	0.02213300	0.49814100	-0.01628700
C	2.35614900	-0.00172500	-2.16390400
C	1.14633000	0.62927600	-2.85793300
N	-0.08861900	0.14404000	-2.22311600
C	-1.30424500	0.78997800	-2.74877800
C	-2.52364700	0.24952500	-1.99872500
P	-2.30359900	0.40598300	-0.14505000
C	-3.39899300	1.82454100	0.45978300
C	-3.53611000	2.98302700	-0.54145000
C	-2.89211400	2.33932000	1.81967000
C	-3.23593000	-1.13390500	0.42995000
C	-4.65633100	-1.27703400	-0.14339900
C	-3.25226200	-1.28561400	1.95807300
P	2.31989600	0.32941100	-0.32074700
C	3.51820300	1.75421300	0.00976300
C	3.22033200	2.39966500	1.37588800
C	3.53635600	2.82224000	-1.09633500
C	3.25334000	-1.18129300	0.32393800
C	3.46364200	-1.15042100	1.84506800
C	4.57814900	-1.47944400	-0.39859300
H	3.29159400	0.32992500	-2.62400800
H	2.30149700	-1.09018300	-2.28608000
H	-0.17287500	-0.86773900	-2.39163200
H	-1.42408600	0.59726300	-3.82622500
H	-1.19933400	1.86830000	-2.60077800
H	-2.60847500	-0.82283400	-2.20924600
H	-3.44234300	0.72993100	-2.34626200
H	-4.39364400	1.38396500	0.60431300
H	-3.99006800	2.66761700	-1.48546200
H	-4.18684100	3.75360700	-0.11108800
H	-2.56447600	3.43578700	-0.75062900
H	-2.82071000	1.54175700	2.56598200
H	-3.58331600	3.09566200	2.21031900
H	-1.90599800	2.79678700	1.70619000
H	-2.62771500	-1.93980500	-0.00110700
H	-4.67366100	-1.23754100	-1.23504500
H	-5.07929800	-2.24312000	0.15626700
H	-5.32892400	-0.50128500	0.23700600
H	-2.25644900	-1.19670500	2.39935100
H	-3.66243400	-2.26417400	2.23700100
H	-3.89446300	-0.53050700	2.42343600

H	4.51365600	1.29285200	0.05055800
H	3.23499400	1.67365500	2.19416800
H	3.97819900	3.16070800	1.59682300
H	2.23973700	2.88149500	1.35913100
H	3.83045100	2.41485100	-2.06818100
H	4.26824000	3.59577400	-0.83504600
H	2.55843400	3.29906400	-1.19342000
H	2.55258500	-1.99435000	0.09565800
H	2.53630000	-0.95781300	2.38997300
H	3.85901500	-2.11428700	2.18727300
H	4.19458800	-0.38677600	2.12987000
H	4.45464600	-1.58820700	-1.47901400
H	5.00316200	-2.41650200	-0.01964800
H	5.32284300	-0.69670100	-0.22046300
Cl	-0.68553200	-3.13632300	-2.71266800
N	0.14804000	-0.70593400	3.64362800
N	-0.28790100	-3.43667300	0.16477300
H	-0.52000400	-3.40075700	-0.91901400
C	0.21132000	0.49693500	4.46539400
H	-0.66233500	1.13755100	4.29973900
H	0.24100100	0.21324300	5.51945200
H	1.10614900	1.08745700	4.23708900
C	0.81904100	-4.38822700	0.42774200
H	1.64459000	-4.14159900	-0.24003800
H	1.13895100	-4.32010400	1.46841600
H	0.47830000	-5.39981000	0.20324400
H	-0.05077800	-2.44554100	0.40572000
Cl	0.03677200	2.84339800	-0.27136500
H	0.05129000	-0.89745000	0.62722700
H	1.16772700	1.71819200	-2.75601200
H	1.16874700	0.38665600	-3.93187600
H	-1.12581100	-3.68098100	0.69208100
H	0.11421200	-0.51885100	2.64240600
B	0.12981600	-2.02035700	4.08562000
H	0.07149900	-2.90014900	3.26897600
H	0.16941400	-2.26388900	5.25588600

$INT3_B$

$E_{solv} = E_{solv(H2B(NMeH)2Cl)} + E_{solv(INT4)}$ = -2654.25605740 a.u.

INT4

E_{gas} = -1974.976162 a.u.

E_{solv} = -1976.6370187 a.u.

Zero-point energy correction = 0.465610 a.u.

Co	0.01482400	-0.04339900	-0.24751700
Cl	-0.01440500	2.28662000	0.27784600
C	-2.35043600	0.18403000	1.77584900
C	-1.37339900	-0.72380000	2.54661800
N	-0.03914700	-0.82227300	1.90417400
C	1.08467300	-0.14277600	2.57308400
C	2.39285700	-0.51041700	1.85496100
P	2.26328200	-0.24019100	-0.00817000
C	3.47229700	1.13532600	-0.47508000
C	3.62640200	2.22181500	0.60168800
C	3.02368600	1.76219300	-1.80887700
C	3.06469800	-1.81515700	-0.66564100
C	4.49301900	-2.08934200	-0.17050800
C	2.97844900	-1.89255400	-2.19718000
P	-2.23356700	-0.13953100	-0.06094500
C	-3.39924900	1.07428900	-0.91594400
C	-2.79405700	1.48418900	-2.27113000
C	-3.73690400	2.31662700	-0.07596300
C	-3.05005200	-1.81922900	-0.29689600
C	-3.04176100	-2.21598100	-1.78201700
C	-4.44988300	-1.96939600	0.31728300
H	-2.05091600	1.22829200	1.89336900
H	-3.36209300	0.06881400	2.18062600
H	-1.79137300	-1.73484600	2.61261900
H	-1.27397400	-0.36123300	3.57871000
H	0.19644200	-1.80404400	1.79427800
H	1.15837900	-0.42432000	3.63696700
H	0.90476600	0.93380400	2.51032900
H	2.60065700	-1.57670000	2.01233100
H	3.22851400	0.03980800	2.29393900
H	4.44803500	0.65483900	-0.62151400

H	4.07724500	1.83870800	1.52240500
H	4.28733800	3.01118600	0.22453300
H	2.66041300	2.67379100	0.84098400
H	2.92239800	1.02012900	-2.60642900
H	3.76121700	2.50454800	-2.13677400
H	2.05961200	2.26213100	-1.68304400
H	2.39811200	-2.58894800	-0.26102400
H	4.57467000	-2.05980400	0.92047200
H	4.81847000	-3.08410600	-0.49739800
H	5.20895900	-1.36848200	-0.57896000
H	1.95805200	-1.70496000	-2.54280300
H	3.28097700	-2.88798300	-2.54278800
H	3.64649000	-1.16699400	-2.67368100
H	-4.32920800	0.52163700	-1.10081600
H	-2.57804500	0.61937600	-2.90604200
H	-3.49288000	2.13274200	-2.81310900
H	-1.86071000	2.03316000	-2.11610100
H	-4.24744800	2.06167500	0.85771300
H	-4.40526000	2.97061900	-0.64867700
H	-2.83206100	2.88144500	0.16355300
H	-2.36402900	-2.49935300	0.22518700
H	-2.03572100	-2.13886900	-2.20348200
H	-3.38561300	-3.25019200	-1.89981000
H	-3.71406100	-1.58165700	-2.37077400
H	-4.45803500	-1.77215900	1.39348300
H	-4.81764000	-2.99157900	0.16849500
H	-5.17514200	-1.29542000	-0.15173200
H	0.01435200	-1.41299300	-0.86942000

INT5

E_{gas} = -2097.4228460 a.u.

E_{solv} = -2099.2465706 a.u.

Zero-point energy correction = 0.558491 a.u.

Co	0.04489000	-0.11987500	-0.09298400
Cl	0.19800200	-2.69165600	-0.17180900
C	2.45105100	-0.95337000	1.68629400
C	1.46469100	-0.25794000	2.63310500
N	0.10578100	-0.09800600	2.03327600
C	-0.93735000	-1.01822800	2.54912000
C	-2.30709000	-0.58708900	2.00450400
P	-2.21793100	-0.28383400	0.15050800
C	-3.00396200	-1.79785100	-0.63243300
C	-2.69525800	-1.88322100	-2.13664900
C	-4.49434400	-2.02328500	-0.34058900
C	-3.31776000	1.22774100	-0.09509500
C	-4.66657600	1.25757400	0.64519800
C	-3.50504400	1.54866200	-1.58796000
P	2.31591100	-0.18524200	-0.00910700
C	3.37172700	-1.21021000	-1.19550900
C	2.67172800	-1.34010600	-2.55924200
C	3.77401400	-2.58920000	-0.64899700
C	3.27905900	1.43449500	0.11977300
C	3.39065000	2.10107400	-1.26454600
C	4.66193800	1.33385400	0.78266700
H	2.15593400	-1.99548700	1.54596200
H	3.46294700	-0.92515200	2.10318000
H	1.82837500	0.74497700	2.88133000
H	1.39396000	-0.81363500	3.57693500
H	-0.95490100	-1.00829800	3.64968200
H	-0.68207500	-2.02250200	2.20322000
H	-2.60592700	0.35601100	2.47787000
H	-3.06783600	-1.33029400	2.26241500
H	-2.41903600	-2.59141500	-0.15443200
H	-1.62360300	-1.77731500	-2.31347800
H	-3.00865700	-2.86331700	-2.51431300
H	-3.23028200	-1.12165000	-2.71320200
H	-4.74163100	-1.93520200	0.72231100
H	-4.77385700	-3.03522600	-0.65650900
H	-5.13061500	-1.32639800	-0.89531600
H	-2.69308400	2.01715000	0.34344800
H	-4.56822200	1.03572300	1.71146000
H	-5.10166400	2.26105200	0.56373500
H	-5.38661300	0.55473200	0.22021200
H	-2.56045500	1.50957200	-2.13908500
H	-3.93315800	2.55137000	-1.70614400
H	-4.19688000	0.84639000	-2.06281300

H	4.28924700	-0.62286700	-1.33119000
H	2.43097500	-0.36497700	-2.99276600
H	3.32835900	-1.87018600	-3.25996400
H	1.74042400	-1.90126900	-2.45271400
H	4.34756300	-2.51755000	0.28055000
H	4.40690300	-3.09546200	-1.38751000
H	2.89074400	-3.20746600	-0.47231400
H	2.64112400	2.06497200	0.75243900
H	2.43514300	2.11264400	-1.79997500
H	3.75080900	3.13229200	-1.16495300
H	4.10535600	1.57442000	-1.90557400
H	4.60309300	0.98038700	1.81590000
H	5.14154400	2.31979900	0.80305800
H	5.32870600	0.65962700	0.23357800
H	0.65673500	2.75379300	1.65685500
B	-0.11785100	3.52168500	1.11463700
H	0.16212500	4.67799700	1.33748400
H	-1.27738100	3.26543600	1.36639200
N	0.07822200	3.30595600	-0.49281600
H	1.05953500	3.47271600	-0.71158700
H	-0.08624700	2.32093700	-0.75542700
C	-0.75721800	4.19606300	-1.33652700
H	-0.52186500	5.23104600	-1.08480100
H	-0.57928500	4.01663400	-2.40035100
H	-1.80548500	4.01077500	-1.10305900
H	-0.19089700	0.86007900	2.22747400
H	-0.04801000	0.32819700	-1.54279600

TS5-7

E_{gas} = -2097.388207 a.u.

E_{solv} = -2099.2065932 a.u.

Zero-point energy correction = 0.553402 a.u.

Three lowest frequencies:

-426.7848 35.4520 42.1335

Co	0.05823600	-0.16258200	-0.27231100
Cl	0.11592200	-2.49401900	-0.45107900
C	2.41209500	-0.77946600	1.76292400
C	1.41370900	0.10575100	2.52296400
N	0.08866200	0.22914400	1.85075100
C	-0.99844800	-0.54594700	2.49841100
C	-2.37200800	-0.09543100	1.98537000
P	-2.48652300	-0.15725500	0.11602200
C	-3.32115500	-1.80613200	-0.23666600
C	-3.27273100	-2.14505000	-1.73722900
C	-4.72791000	-2.02989600	0.33865200
C	-3.62662800	1.29174700	-0.26588900
C	-4.91929100	1.41217600	0.55796300
C	-3.91734700	1.40884100	-1.77157800
P	2.59032500	-0.17414700	0.00751200
C	3.76559700	-1.37159800	-0.86438500
C	3.37202100	-1.48769600	-2.34845600
C	3.84622900	-2.76121000	-0.21297100
C	3.58924700	1.41786200	0.16545400
C	3.93404600	1.96692500	-1.23074400
C	4.84263400	1.33189100	1.04828600
H	2.02705800	-1.80052400	1.69285300
H	3.36056700	-0.81461200	2.30941800
H	1.81224400	1.11952800	2.62528400
H	1.27384800	-0.28756200	3.53783500
H	-0.95917500	-0.40501600	3.58829200
H	-0.82910000	-1.60747300	2.29148200
H	-2.53480900	0.94704000	2.27966300
H	-3.15429000	-0.69417500	2.46256600
H	-2.62678000	-2.49494800	0.26067300
H	-2.25592400	-2.06321300	-2.12738800
H	-3.60690700	-3.17737900	-1.89148900
H	-3.93167100	-1.49695100	-2.32360800
H	-4.81038700	-1.75618600	1.39509300
H	-4.98965400	-3.09148900	0.25657000
H	-5.48578900	-1.46797800	-0.21522100
H	-2.97559900	2.12929400	0.01841400
H	-4.74290700	1.31977700	1.63319300
H	-5.36753800	2.39837300	0.38748100
H	-5.66181200	0.66301900	0.27130400
H	-3.00939000	1.32476700	-2.37588100
H	-4.37406000	2.38148500	-1.98778400

H	-4.62018400	0.63962400	-2.10716100
H	4.75964100	-0.90992600	-0.80335200
H	3.33887700	-0.51345300	-2.84590400
H	4.10107700	-2.10925900	-2.88171200
H	2.38697100	-1.95261800	-2.44714700
H	4.21895200	-2.71717100	0.81466700
H	4.53797700	-3.38924000	-0.78654600
H	2.86949400	-3.25260000	-0.20976600
H	2.88341400	2.11550100	0.63430200
H	3.05402700	2.02752000	-1.87948900
H	4.35917300	2.97308600	-1.14565300
H	4.67679200	1.34180700	-1.73830500
H	4.60517500	1.06070200	2.08062800
H	5.34680300	2.30498300	1.07662200
H	5.56558600	0.60273800	0.66591000
H	0.82166200	2.81130100	1.49539300
B	-0.08303500	3.26976800	0.79960000
H	-0.07184500	4.48737100	0.88638200
H	-1.17384400	2.84544500	1.18094500
N	0.16308700	2.82320000	-0.69939800
H	1.14489600	2.98329900	-0.92097800
H	0.03821300	1.36993700	-1.46098300
C	-0.63555700	3.58158700	-1.67130300
H	-0.41222700	4.65598000	-1.63028300
H	-0.47260100	3.22863800	-2.69931200
H	-1.69664100	3.46249000	-1.43598700
H	-0.15681500	1.22949100	1.85132400
H	-0.01664700	0.65627800	-1.91689500

INT6

E_{gas} = -1973.810996 a.u.

E_{solv} = -1975.4399985 a.u.

Zero-point energy correction = 0.44316500 a.u.

Co	0.00001900	0.09241900	-0.06587900
Cl	-0.00010300	1.75019900	1.51197400
C	2.44612200	-1.04550400	-1.68599300
C	1.20016800	-1.93430800	-1.79321000
N	0.00005500	-1.19201800	-1.42235200
C	-1.20010500	-1.93410600	-1.79343700
C	-2.44595000	-1.04510500	-1.68649000
P	-2.25018400	-0.08803300	-0.11574700
C	-3.29132300	1.46140700	-0.24301500
C	-4.78317800	1.24217500	-0.53773000
C	-2.64887200	2.41803000	-1.26326300
C	-2.91389900	-1.16277900	1.28089900
C	-4.16236900	-2.00522500	0.97679600
C	-3.07810000	-0.33220900	2.56589400
P	2.25016900	-0.08804200	-0.11549600
C	3.29137800	1.46131900	-0.24351100
C	2.64836200	2.41800400	-1.26332900
C	4.78296600	1.24171800	-0.53937800
C	2.91400200	-1.16222400	1.28154600
C	3.07854800	-0.33110900	2.56614500
C	4.16235600	-2.00490900	0.97766700
H	2.43910500	-0.31416300	-2.50104600
H	3.37369600	-1.62160800	-1.75366600
H	1.34310400	-2.83993800	-1.16945500
H	1.11132000	-2.30411000	-2.82944000
H	-1.34331700	-2.83969600	-1.16968300
H	-1.11110400	-2.30397000	-2.82963600
H	-3.37359700	-1.62104700	-1.75456000
H	-2.43851400	-0.31365200	-2.50143100
H	-3.18186500	1.92133500	0.74634500
H	-5.28935900	0.68922200	0.25760200
H	-5.28827900	2.21049900	-0.63509600
H	-4.93482500	0.69968800	-1.47739400
H	-1.60110700	2.60692700	-1.01770600
H	-3.18163800	3.37571800	-1.25813800
H	-2.70101400	2.01999900	-2.28302700
H	-2.07709700	-1.85548400	1.44256100
H	-4.01582500	-2.67063500	0.12132600
H	-4.39722000	-2.63483800	1.84334800
H	-5.04138300	-1.38624200	0.77630400
H	-2.18620200	0.26440800	2.77775300
H	-3.25953300	-0.99794300	3.41733300
H	-3.93459400	0.34744600	2.49556600

H	3.18283300	1.92132900	0.74591000
H	1.60091200	2.60739500	-1.01681500
H	3.18158000	3.37544400	-1.25896700
H	2.69929900	2.01971000	-2.28305600
H	5.28958700	0.68845300	0.25545700
H	5.28827600	2.20991500	-0.63694300
H	4.93373800	0.69938100	-1.47927400
H	2.07713000	-1.85474200	1.44364600
H	2.18682100	0.26579300	2.77791100
H	3.25999000	-0.99650000	3.41785400
H	3.93520200	0.34829300	2.49535100
H	4.01576200	-2.67057400	0.12240500
H	4.39717900	-2.63424900	1.84441900
H	5.04140500	-1.38603800	0.77696400

INT7

E_{gas} = -2096.264602 a.u.

E_{solv} = -2098.0539877 a.u.

Zero-point energy correction = 0.5377220 a.u.

Co	-0.11969300	-0.18821600	-0.30352400
Cl	-0.08367600	2.10610200	-0.77492600
C	-2.38547000	0.64494400	1.84375500
C	-1.40869400	-0.31910000	2.52977700
N	-0.08166500	-0.38140100	1.85862600
C	0.94273900	0.52701600	2.43080900
C	2.34909300	0.06762900	2.03322500
P	2.60924800	-0.01040700	0.17307100
C	3.37649800	1.67447400	-0.19324600
C	3.40594000	1.95501200	-1.70677300
C	4.73017100	1.99878100	0.45702900
C	3.93470100	-1.35967000	0.03653600
C	5.02270900	-1.41175100	1.12277000
C	4.57725700	-1.39048600	-1.36160900
P	-2.72598900	0.06935400	0.09850300
C	-3.85010400	1.38685700	-0.66527000
C	-3.60805900	1.44427900	-2.18510700
C	-3.69347500	2.78300500	-0.04202000
C	-3.86990700	-1.41415600	0.35033800
C	-4.36801700	-1.94267700	-1.00671400
C	-5.04253900	-1.20800700	1.32088100
H	-1.93414500	1.63819000	1.76632700
H	-3.29406100	0.73837500	2.44725100
H	-1.81678700	-1.33388700	2.52445600
H	-1.27513000	-0.03119300	3.58181400
H	0.86276300	0.53709000	3.52820200
H	0.73968900	1.53998400	2.06970900
H	2.50719900	-0.94359900	2.42684200
H	3.09109900	0.71145300	2.51650100
H	2.61636900	2.34374000	0.22997000
H	2.41919400	1.80878800	-2.15108700
H	3.70028600	2.99628900	-1.88240800
H	4.12889900	1.31930900	-2.22714300
H	4.75466100	1.78612000	1.53050100
H	4.95148600	3.06558900	0.33198300
H	5.54786000	1.44412100	-0.01382200
H	3.31730100	-2.26278700	0.13633100
H	4.61148100	-1.45097500	2.13479600
H	5.62715700	-2.31691000	0.98697200
H	5.70013900	-0.55577600	1.06821800
H	3.83849200	-1.32951600	-2.16557100
H	5.13528800	-2.32441700	-1.49351000
H	5.28571800	-0.56688100	-1.49535700
H	-4.87928600	1.04924100	-0.48753600
H	-3.74468200	0.46980700	-2.66435900
H	-4.31175400	2.14418300	-2.65127700
H	-2.59108200	1.78764100	-2.39570900
H	-3.96614300	2.79864900	1.01756400
H	-4.35484400	3.48724600	-0.56042100
H	-2.66774800	3.14727300	-0.14621900
H	-3.19919500	-2.17757500	0.76343600
H	-3.54384500	-2.13174700	-1.70184000
H	-4.90282300	-2.88844600	-0.86626000
H	-5.06199400	-1.24356000	-1.48621000
H	-4.71125100	-0.95270300	2.33180600
H	-5.63082700	-2.13027400	1.39698500
H	-5.72268500	-0.41852100	0.98221900

H	-0.95806900	-2.71215800	0.54820100
B	-0.07785200	-2.95262100	-0.27581800
H	-0.23922100	-4.06875900	-0.73834700
H	1.02958900	-2.85706600	0.24479700
N	-0.18142600	-1.85423800	-1.43470200
H	-1.11822100	-1.90274900	-1.82971000
C	0.77656700	-2.05641900	-2.53132700
H	0.62823200	-3.03470900	-3.00715100
H	0.68994400	-1.27162300	-3.29198900
H	1.78827100	-2.03482300	-2.12474500
H	0.25243300	-1.34433100	1.92436200

INT8 (1a)

E_{gas} = -2096.260382 a.u.

E_{solv} = -2098.0535789 a.u.

Zero-point energy correction = 0.5362610 a.u.

Co	-0.01597300	0.40910200	0.64422100
Cl	0.04116400	-0.69276200	2.70436600
C	-2.18801300	-0.11378100	-1.94809500
C	-1.38196300	1.17735200	-2.18292900
N	-0.03218200	1.12427400	-1.59782700
C	0.96482200	0.52520700	-2.49546700
C	2.35125200	0.47884700	-1.83619700
P	2.25971400	-0.32435500	-0.15481700
C	2.67346900	-2.14302100	-0.40144700
C	4.10480800	-2.48167400	-0.84552200
C	1.65352400	-2.78412500	-1.35821200
C	3.64244000	0.47261500	0.83960800
C	4.97324900	0.73786900	0.11694300
C	3.83745800	-0.27148900	2.17274700
P	-2.25887500	-0.45996500	-0.11908000
C	-2.97786900	-2.19048000	0.10854700
C	-1.88460900	-3.20198500	0.49009400
C	-3.82381400	-2.70654900	-1.06717700
C	-3.59048400	0.70444900	0.52461100
C	-3.59641200	0.68689500	2.06347300
C	-5.00032000	0.50062900	-0.04827800
H	-1.68474800	-0.96275800	-2.42534600
H	-3.17759900	-0.03003400	-2.40946700
H	-1.90207300	2.02356500	-1.72360800
H	-1.33706200	1.38689800	-3.26361800
H	0.25395700	2.10240100	-1.33446700
H	1.03283300	1.09179000	-3.43966500
H	0.64219400	-0.48730000	-2.76303400
H	2.70186100	1.50409500	-1.67324200
H	3.07549900	-0.00621800	-2.49916300
H	2.50579300	-2.56420000	0.59778600
H	4.84953200	-2.19880800	-0.09940900
H	4.19485500	-3.56319000	-1.00378400
H	4.36632700	-1.99338700	-1.79129900
H	0.62582800	-2.52496400	-1.09210200
H	1.74426000	-3.87549000	-1.32712100
H	1.83086100	-2.47332600	-2.39409900
H	3.19402700	1.44562100	1.07782800
H	4.83955200	1.28676900	-0.82012300
H	5.61645900	1.34800200	0.76198600
H	5.51846500	-0.18178200	-0.10798400
H	2.88778700	-0.40219000	2.69946400
H	4.51135600	0.30262900	2.81836400
H	4.29051600	-1.25825300	2.02505800
H	-3.63390400	-2.07119200	0.98032600
H	-1.27060200	-2.83788700	1.31803000
H	-2.34359300	-4.15365500	0.78315600
H	-1.22655400	-3.41074200	-0.36091600
H	-4.64479300	-2.03497100	-1.33011000
H	-4.26023300	-3.67819200	-0.80750500
H	-3.21206200	-2.85858800	-1.96302700
H	-3.22536700	1.69104200	0.21187500
H	-2.60017600	0.87036500	2.47311700
H	-4.27612200	1.45912200	2.44069700
H	-3.94595100	-0.27541600	2.45454000
H	-5.02274000	0.53358600	-1.14227700
H	-5.66461100	1.29305400	0.31584100
H	-5.43085900	-0.45345900	0.27277000

B	0.15938500	2.81108300	1.00084400
H	-0.06906100	3.46258400	1.99964100
H	-0.88601300	2.11981600	0.80380100
N	0.48376800	3.58467100	-0.29108800
H	1.44527700	3.91587700	-0.25073700
C	-0.38086200	4.73949900	-0.54187400
H	-0.37523700	5.48111100	0.27406300
H	-0.10474200	5.25352800	-1.47201600
H	-1.41824400	4.40045500	-0.65071500
H	1.08588900	2.02011900	1.25001000

TS8-9

E_{gas} = -2096.250864 a.u.

E_{solv} = -2098.0375908 a.u.

Zero-point energy correction = 0.5371830 a.u.

Three lowest frequencies:

-149.8052 36.4210 44.9105

Co	0.02052600	-0.31097200	0.22580600
Cl	0.06411400	-2.46002600	-0.78087100
C	-2.29864500	-0.21318500	-1.85373900
C	-1.37794100	0.93309700	-2.31106300
N	-0.05091200	0.90352200	-1.65311600
C	1.08620000	0.47291400	-2.48141700
C	2.39562800	0.65698900	-1.69770900
P	2.32580100	-0.15196500	0.00002700
C	3.29231600	-1.75165100	-0.21211500
C	3.14498700	-2.66764100	1.01514400
C	4.76074200	-1.64068100	-0.64951600
C	3.27573200	1.06272500	1.07498400
C	4.66590300	1.51308900	0.59615200
C	3.30381900	0.61505500	2.54495400
P	-2.26764100	-0.37547700	0.00554800
C	-3.13707100	-2.01125600	0.32387800
C	-4.63922900	-2.06625900	0.01247300
C	-2.82057900	-2.54874200	1.73005100
C	-3.30760900	1.05801100	0.64175500
C	-3.55820300	0.93521400	2.15364500
C	-4.60157000	1.39029200	-0.11995700
H	-1.90807100	-1.16747000	-2.21822700
H	-3.30637000	-0.07345100	-2.26011100
H	-1.84951000	1.89432200	-2.07779300
H	-1.26472500	0.89921200	-3.40352200
H	0.14529800	1.81771200	-1.24210900
H	1.14500100	1.04540300	-3.42266100
H	0.93883700	-0.58142000	-2.73405700
H	2.56862500	1.72816400	-1.53602000
H	3.23944200	0.28528700	-2.28723900
H	2.71822900	-2.22095300	-1.01918800
H	2.09419100	-2.79741200	1.28222800
H	3.55524300	-3.65733200	0.78360000
H	3.69052500	-2.28278300	1.88288500
H	4.91508600	-0.94050900	-1.47647700
H	5.11189000	-2.62340500	-0.98593400
H	5.40901400	-1.33360600	0.17623300
H	2.60776800	1.93024200	1.02823000
H	4.67535900	1.81256300	-0.45652000
H	4.98965700	2.37972500	1.18533800
H	5.41925800	0.73316000	0.72872300
H	2.30807000	0.32822000	2.89396700
H	3.65638400	1.43778000	3.17735500
H	3.98267600	-0.22963000	2.69839200
H	-2.60762500	-2.65890300	-0.38351700
H	-4.87297900	-1.69055500	-0.98849200
H	-4.98468000	-3.10581800	0.06152600
H	-5.22901700	-1.49616900	0.73711300
H	-1.74106500	-2.58427500	1.89764800
H	-3.20965500	-3.56881500	1.83062400
H	-3.27629200	-1.94391900	2.52020000
H	-2.61774700	1.89874800	0.50927900
H	-2.63240600	0.73310700	2.69939200
H	-3.97376500	1.87294600	2.53954200
H	-4.27603500	0.14055700	2.38060000
H	-4.42716600	1.56121000	-1.18651300

H	-5.03605400	2.31098400	0.28838800
H	-5.35564700	0.60515000	-0.02596900
B	0.01143200	2.67098400	1.46572300
H	0.91129500	2.48987600	2.23453200
H	-1.11510500	2.67534400	1.87276500
N	0.28412600	3.46714800	0.29457600
H	1.24069000	3.75460900	0.13230600
C	-0.67888600	4.30080600	-0.40982700
H	-1.69010300	4.00281400	-0.12166000
H	-0.57060800	5.36720000	-0.16355400
H	-0.59902200	4.21130500	-1.50351800
H	-0.01866100	0.98683400	1.08162600

INT9

E_{gas} = -2096.268755 a.u.

E_{solv} = -2098.04156760 a.u.

Zero-point energy correction = 0.52775800 a.u.

Co	0.06354800	-0.63461400	-0.18353400
Cl	0.14659800	-2.34583700	1.48277200
C	2.35257800	0.34440300	1.68825100
C	1.32750000	1.48162200	1.84749000
N	0.00805400	1.16181400	1.25167400
C	-1.08517200	0.83498900	2.18303300
C	-2.39636400	0.67713700	1.39472500
P	-2.19367900	-0.48791500	-0.07506500
C	-3.15196300	-2.02313600	0.43132800
C	-2.86539200	-3.19346600	-0.52456400
C	-4.65548400	-1.87182800	0.70391800
C	-3.05649800	0.44901000	-1.46253300
C	-4.49073400	0.94387600	-1.21615200
C	-2.94524700	-0.30286600	-2.79841300
P	2.29671100	-0.35869300	-0.04155900
C	3.38922200	-1.88049200	0.07561900
C	4.88788200	-1.65135500	0.31819400
C	3.13963300	-2.83511000	-1.10455800
C	3.06353600	0.97009700	-1.13422400
C	3.21472400	0.47913900	-2.58333700
C	4.34608300	1.65154900	-0.63174600
H	2.07432000	-0.49756500	2.32921700
H	3.34669800	0.69398400	1.98917600
H	1.70723100	2.38224800	1.35155200
H	1.21955300	1.73315800	2.91220000
H	-0.28225200	1.94350000	0.66958500
H	-1.21390100	1.61380200	2.95471000
H	-0.82883300	-0.10403500	2.68101700
H	-2.70480700	1.65535500	1.00482500
H	-3.19437400	0.33910100	2.06312000
H	-2.64179200	-2.26071700	1.37333700
H	-1.78953000	-3.34505900	-0.63881400
H	-3.29313900	-4.11647800	-0.11635800
H	-3.30953300	-3.03510400	-1.51303200
H	-4.89336000	-1.00751300	1.33227800
H	-5.02398500	-2.76417400	1.22388100
H	-5.22858600	-1.78065500	-0.22364900
H	-2.39848300	1.32613600	-1.53637800
H	-4.60616300	1.45226800	-0.25348800
H	-4.77341100	1.65715400	-1.99999900
H	-5.21445900	0.12576200	-1.24798400
H	-1.91670300	-0.62410000	-2.98383100
H	-3.25308600	0.35063300	-3.62303700
H	-3.59502500	-1.18393300	-2.82093100
H	2.95611700	-2.35967500	0.96238400
H	5.07942200	-0.96568000	1.14936700
H	5.37199300	-2.60496200	0.56100600
H	5.38725400	-1.25427600	-0.57151800
H	2.07348400	-3.05285500	-1.20857800
H	3.66242400	-3.78297400	-0.93112200
H	3.50471300	-2.42627700	-2.05226900
H	2.26139700	1.72021700	-1.13777200
H	2.29070100	0.01845500	-2.94414900
H	3.45257800	1.32249000	-3.24187900
H	4.02702400	-0.24895800	-2.67992200
H	4.23892200	2.04972800	0.38185500

H	4.59465000	2.49468600	-1.28773000
H	5.20271200	0.97280500	-0.63489900
B	-0.35451100	4.17065200	-1.30693700
H	-0.98132100	3.70702200	-2.21129800
H	0.81506500	4.40816000	-1.39313600
N	-1.00925200	4.44331900	-0.10659100
H	-2.00625300	4.27657800	-0.04447600
C	-0.44898900	5.07261400	1.08356000
H	0.61776300	5.24369600	0.92631700
H	-0.92529700	6.03901500	1.28803000
H	-0.57209800	4.44146800	1.97207500
H	0.03798000	0.19418600	-1.43646500

INT10

E_{gas} = -1974.368122 a.u.

E_{solv} = -1976.0212299 a.u.

Zero-point energy correction = 0.4572360 a.u.

Co	-0.00189500	-0.02051500	-0.33038400
Cl	-0.05162800	-2.30724500	-0.55022900
C	2.34567700	1.80522800	0.67326700
C	1.36231100	2.67417000	-0.11683600
N	0.01802300	2.02708100	-0.24041800
C	-0.98002100	2.50763000	0.75707800
C	-2.37245300	1.98182900	0.38202000
P	-2.20790400	0.16901000	-0.08830300
C	-2.92086300	-0.81367300	1.34710400
C	-4.42554000	-0.68676000	1.62244800
C	-2.10685200	-0.51154800	2.61684600
C	-3.36173800	-0.03468500	-1.57141000
C	-4.72528400	0.67618000	-1.54617700
C	-3.49721900	-1.52464500	-1.93231800
P	2.19070900	0.07125100	-0.00687900
C	3.02068800	-1.04618400	1.25533800
C	2.08287400	-1.24857500	2.45735200
C	4.42834600	-0.63083500	1.70963100
C	3.26459500	0.04881300	-1.56866000
C	3.46834100	-1.40452200	-2.03293200
C	4.58097200	0.84123100	-1.57582500
H	2.05860800	1.76719900	1.72980200
H	3.35280700	2.23120200	0.62059700
H	1.74423400	2.81503700	-1.13355500
H	1.26174700	3.67332200	0.32897700
H	-0.34456600	2.27914800	-1.16104900
H	-0.97948200	3.60793400	0.79873700
H	-0.67425800	2.13275300	1.73678500
H	-2.74647600	2.53409900	-0.48892400
H	-3.08199500	2.16108500	1.19579000
H	-2.69241500	-1.84499100	1.05079200
H	-5.03306200	-1.06480700	0.79759400
H	-4.68885700	-1.26870100	2.51420600
H	-4.72259600	0.35092400	1.81593400
H	-1.03481100	-0.61401500	2.43100700
H	-2.38863400	-1.20563700	3.41694900
H	-2.30071900	0.50358200	2.98578200
H	-2.76173100	0.43438900	-2.36424800
H	-4.64116100	1.74527800	-1.32635900
H	-5.20184600	0.58468300	-2.53007800
H	-5.40825000	0.23930400	-0.81403200
H	-2.52255700	-2.01985700	-1.95969800
H	-3.97336200	-1.62887000	-2.91434900
H	-4.12511000	-2.05569300	-1.20830300
H	3.08268000	-2.00821900	0.73280100
H	1.11560900	-1.63355100	2.12863600
H	2.52578900	-1.96664300	3.15788500
H	1.92080700	-0.31459900	3.00952300
H	5.14986900	-0.62249200	0.88944900
H	4.79888500	-1.33602800	2.46334200
H	4.42969900	0.36380800	2.16985300
H	2.59207100	0.52194100	-2.29670600
H	2.52619300	-1.96103300	-2.02910500
H	3.87670800	-1.41891500	-3.05021200
H	4.18028300	-1.93300900	-1.38896900
H	4.44484500	1.89056700	-1.29366700

H	5.00848800	0.83166300	-2.58608500
H	5.33015800	0.41080400	-0.90574400

INT11

E_{gas} = -2096.834072 a.u.

E_{solv} = -2098.640081 a.u.

Zero-point energy correction = 0.55113300 a.u.

Co	0.04373200	-0.00843900	-0.04759900
Cl	-0.05584600	0.47821400	-2.30460400
C	2.38767700	-0.97789000	1.79216500
C	1.41914200	-0.14642700	2.63615300
N	0.07109800	-0.06339400	2.00047900
C	-0.89477300	-1.05375000	2.54776900
C	-2.29648400	-0.77596300	1.99476600
P	-2.15806800	-0.43100200	0.15970800
C	-2.66620700	-2.02055700	-0.71386400
C	-4.11540900	-2.49359500	-0.53236000
C	-1.67951100	-3.14212800	-0.34533500
C	-3.50720200	0.85144900	-0.16659900
C	-4.84502300	0.69928300	0.57737300
C	-3.71501400	1.04139600	-1.67954800
P	2.26315600	-0.32738200	0.04587000
C	3.15774000	-1.58296200	-1.04593400
C	2.15718200	-2.50743400	-1.75803900
C	4.24143300	-2.40625800	-0.32786500
C	3.39821100	1.18783600	0.05088100
C	3.33175900	1.90002200	-1.31263200
C	4.85666000	0.97839100	0.48420100
H	2.07390600	-2.02748700	1.77546400
H	3.39612100	-0.94411100	2.21734300
H	1.78960000	0.87875000	2.72669500
H	1.33459600	-0.54932400	3.65457400
H	-0.11260400	2.22058500	-0.23384200
H	-0.90272000	-1.00890700	3.64713600
H	-0.55170500	-2.05116900	2.25892100
H	-2.69635900	0.12666000	2.47018000
H	-2.97904200	-1.59695800	2.23718400
H	-2.50033400	-1.77084300	-1.76934500
H	-4.83814700	-1.80711900	-0.97802500
H	-4.25040900	-3.46796800	-1.01756800
H	-4.37493900	-2.62094500	0.52488300
H	-0.64478300	-2.80933900	-0.46199900
H	-1.84059400	-4.01259500	-0.99170100
H	-1.82256300	-3.47604500	0.68976200
H	-3.02772300	1.75916500	0.22308200
H	-4.71659900	0.59914500	1.65912300
H	-5.45476100	1.59499700	0.40727500
H	-5.42464800	-0.15783200	0.22701800
H	-2.76430000	1.16693000	-2.20497900
H	-4.33878400	1.92447500	-1.86275900
H	-4.23266100	0.18317200	-2.12203700
H	3.64258400	-0.96594000	-1.81319500
H	1.39677000	-1.93392600	-2.29202500
H	2.68658300	-3.15017300	-2.47218700
H	1.64997700	-3.16446600	-1.04179000
H	4.98717500	-1.78820800	0.17719500
H	4.76806300	-3.03679900	-1.05392400
H	3.80013500	-3.07597800	0.41814400
H	2.91356500	1.83904900	0.79193000
H	2.30368700	2.01716000	-1.66671600
H	3.80767900	2.88618300	-1.24802200
H	3.86994400	1.33485600	-2.08198500
H	4.94433200	0.47844300	1.45375900
H	5.36176500	1.94803400	0.57133400
H	5.41317700	0.39127200	-0.25330200
B	-0.33215600	3.40132500	1.60976400
H	-0.34302400	4.58714300	1.85252600
H	-1.40464300	2.86991100	1.84366300
N	-0.07142600	3.22947500	0.01705500
H	0.88509400	3.51061000	-0.19520300
C	-0.99278400	3.98116700	-0.86953200
H	-0.86006500	5.04946100	-0.69055100
H	-0.80373200	3.73662000	-1.91720400

H	-2.01690800	3.71018300	-0.61146400
H	0.59643500	2.83731500	2.16690800
H	-0.28815900	0.87532300	2.20433800

INT11'

E_{gas} = -2096.783493 a.u.

E_{solv} = -2098.6106319 a.u.

Zero-point energy correction = 0.55303300 a.u.

Co	-0.01446300	-0.02151600	0.07630500
Cl	-0.30709100	-2.21753800	1.49887700
C	-2.29113600	-1.57870300	-1.31710200
C	-1.19076600	-1.38133600	-2.35558300
N	0.10859700	-1.05653300	-1.69358700
C	0.97652100	-2.26112500	-1.51968000
C	2.27975700	-1.92750300	-0.76123400
P	2.24148400	-0.17479600	-0.10727000
C	3.43471400	-0.19195100	1.34887000
C	4.83424400	-0.75397000	1.04872900
C	2.80759300	-0.90419400	2.55880000
C	3.11022500	0.85950400	-1.46378400
C	4.13283200	0.15733100	-2.37260000
C	3.69597800	2.15753300	-0.88213700
P	-2.31409300	-0.06627200	-0.22469200
C	-3.55870300	-0.44291500	1.15825300
C	-3.06237600	0.14583200	2.48911400
C	-3.89332700	-1.93434300	1.31994400
C	-3.29345600	1.18610800	-1.28548800
C	-3.67440300	2.43919000	-0.47926300
C	-4.54073500	0.62725300	-1.99007800
H	-2.02806600	-2.40733800	-0.65476300
H	-3.24602800	-1.80276600	-1.80149000
H	-1.44050500	-0.54813700	-3.02240100
H	-1.07516000	-2.27414000	-2.98519500
H	1.19290300	-2.69714400	-2.50557500
H	0.39591300	-2.96943600	-0.92866200
H	3.16612900	-2.14017500	-1.36368100
H	2.31809800	-2.55180400	0.13482100
H	3.53243100	0.86916000	1.60945100
H	5.36950100	-0.18490400	0.28410500
H	5.44255700	-0.72755600	1.96066800
H	4.78736800	-1.79880000	0.72355400
H	1.81719100	-0.51472500	2.79393200
H	3.46031700	-0.77161900	3.43033800
H	2.68988400	-1.97698700	2.38440800
H	2.26034300	1.15255800	-2.09616700
H	3.69289100	-0.68122200	-2.92024600
H	4.51374900	0.86582600	-3.11881500
H	4.99351800	-0.22422700	-1.81683500
H	2.98832900	2.67009800	-0.22290400
H	3.96514100	2.84924400	-1.68883300
H	4.60299700	1.96534400	-0.30090300
H	-4.48151500	0.07712300	0.86938400
H	-2.86254800	1.21967600	2.42230600
H	-3.81981900	-0.00719200	3.26764800
H	-2.13834600	-0.35036200	2.79590300
H	-4.33767700	-2.36248700	0.41574900
H	-4.62379900	-2.05063800	2.12994100
H	-2.99720900	-2.50345000	1.58071800
H	-2.57093400	1.49253800	-2.05380200
H	-2.82488800	2.88004200	0.05303900
H	-4.08180400	3.21137500	-1.14184300
H	-4.43844500	2.21892000	0.27285400
H	-4.29521500	-0.15273800	-2.71559800
H	-5.05960100	1.42533900	-2.53550100
H	-5.25562800	0.20601600	-1.27479200
B	0.24616700	1.98415700	1.85732100
H	1.41221900	2.03996300	2.15701500
H	-0.50270400	2.35466100	2.72915800
N	0.03191100	2.94751300	0.57771000
H	0.44804900	2.42441600	-0.21175500
C	0.55422800	4.32715900	0.72902000
H	1.62571700	4.27451300	0.92344600
H	0.36767400	4.92391100	-0.16792900

H	0.06937500	4.79042500	1.59015800
H	-0.10721000	0.82401600	1.56216500
H	0.59631800	-0.41110200	-2.31227000
H	-0.96283000	2.96802400	0.35732700

TS11-12

E_{gas} = -2096.785962 a.u.

E_{solv} = -2098.5760743 a.u.

Zero-point energy correction = 0.535221 a.u.

Three lowest frequencies:

-153.6012 29.4739 32.2128

Co	0.02023900	-0.22202500	-0.34933300
C	2.35239700	-0.70492900	1.83839200
C	1.37666200	0.29351400	2.47599400
N	0.05296700	0.33440500	1.79908600
C	-1.00619400	-0.46876800	2.45774500
C	-2.39585600	-0.08697100	1.92065800
P	-2.50542400	-0.19030000	0.04839700
C	-3.42236900	-1.79841500	-0.27762800
C	-3.35511800	-2.18163100	-1.76603600
C	-4.85069700	-1.92247400	0.27351400
C	-3.52915900	1.32619900	-0.39406700
C	-4.87447600	1.51402300	0.32588300
C	-3.68262400	1.47340800	-1.91750800
P	2.50583800	-0.35680800	0.01221300
C	3.68990600	-1.65335100	-0.68699300
C	3.31508100	-1.95203200	-2.15049100
C	3.74019500	-2.95189500	0.13354000
C	3.46066100	1.26315000	-0.07317100
C	3.74931300	1.62790200	-1.53953500
C	4.73463500	1.33363100	0.78166300
H	1.95426200	-1.72066200	1.91628000
H	3.30988600	-0.67561000	2.36988500
H	1.78907400	1.30599000	2.42802200
H	1.24577100	0.05545500	3.54076300
H	-0.98846200	-0.30366400	3.54572800
H	-0.79562800	-1.52600900	2.27041000
H	-2.61620200	0.94820900	2.20412000
H	-3.15320300	-0.71794300	2.39670600
H	-2.77323300	-2.50387000	0.25641700
H	-2.32290100	-2.18261400	-2.12374900
H	-3.75680200	-3.19197500	-1.90309800
H	-3.94870700	-1.50596400	-2.39058200
H	-4.93873200	-1.60011200	1.31570000
H	-5.16810600	-2.97093100	0.22811400
H	-5.56430600	-1.34296000	-0.31943700
H	-2.85805200	2.12526200	-0.04954800
H	-4.79157800	1.39438200	1.41008900
H	-5.25012400	2.52689700	0.13826900
H	-5.63129100	0.81273100	-0.03436600
H	-2.72656800	1.35479100	-2.43703700
H	-4.07897900	2.46641900	-2.15821900
H	-4.38216600	0.73679100	-2.32534200
H	4.68748200	-1.19503600	-0.66569900
H	3.29975700	-1.04902400	-2.76801600
H	4.04347500	-2.64463600	-2.58885500
H	2.32513900	-2.41422900	-2.20108600
H	4.10387600	-2.78681500	1.15214000
H	4.42541900	-3.65852300	-0.34949600
H	2.75373100	-3.42104100	0.18521100
H	2.73956200	1.99663000	0.30969100
H	2.84096500	1.58465100	-2.14784400
H	4.15499700	2.64421000	-1.60163300
H	4.49160900	0.95574400	-1.98389700
H	4.53239700	1.18127000	1.84591500
H	5.20245700	2.31991400	0.67745500
H	5.47641700	0.58946400	0.47079500
B	-0.24336400	3.65743700	0.94373000
H	-0.42322500	4.84696600	1.16678400
N	-0.05030800	3.47336800	-0.55075500
H	-0.48250600	2.70098300	-1.05662400
C	0.82208400	4.29501100	-1.35266500
H	1.61600600	4.71892000	-0.73150400
H	1.26336300	3.72310000	-2.17401100
H	0.25873900	5.13592300	-1.78782300
H	-0.24586800	1.31398600	1.78185500

Cl	0.02168200	-2.62483600	-0.27092200
H	-1.17052600	2.96665500	1.33323400
H	0.80786300	3.37411900	1.53131500
H	0.27521400	1.07581800	-1.30126100

TS11-12$_B$

E_{gas} = -2096.773461 a.u.

E_{solv} = -2098.5881996 a.u.

Zero-point energy correction = 0.55351800 a.u.

Three lowest frequencies:

-95.3865 26.8419 37.9343

Co	-0.00818900	-0.10497300	-0.02589700
Cl	0.02769700	-1.65428800	-1.98497100
C	2.16137900	-1.84268200	1.19498500
C	1.25133800	-1.50271500	2.37480000
N	-0.00055300	-0.79883800	1.93137700
C	-1.22414200	-1.57084100	2.27275700
C	-2.46987700	-0.75446400	1.93367800
P	-2.29123900	-0.11505000	0.18351500
C	-3.28087100	-1.33230200	-0.87447700
C	-4.81197100	-1.21551200	-0.84430000
C	-2.86400600	-2.77937200	-0.55434500
C	-3.25996300	1.51559300	0.25108300
C	-4.58596500	1.55187200	1.03228000
C	-3.41463300	2.12875100	-1.15214400
P	2.27976100	-0.32749400	0.11801600
C	3.48032500	-0.77016200	-1.27277000
C	3.15819600	0.03131500	-2.54618400
C	3.53803000	-2.27581200	-1.58134100
C	3.31625200	0.85233900	1.19411100
C	3.74361200	2.09657800	0.39746000
C	4.52970800	0.22357100	1.89751200
H	1.69251100	-2.60706900	0.56897900
H	3.12093500	-2.22952300	1.55341300
H	1.77815600	-0.85599800	3.08556500
H	0.97560700	-2.41051500	2.92313600
H	-1.21744900	-1.84064000	3.34003500
H	-1.19688100	-2.49573300	1.69219800
H	-2.53706800	0.10855100	2.60822400
H	-3.37409700	-1.35225700	2.08672400
H	-2.91481600	-1.11590100	-1.88478900
H	-5.17818500	-0.25738700	-1.21878700
H	-5.24289600	-1.99702600	-1.48141300
H	-5.21512600	-1.36563100	0.16407800
H	-1.78256500	-2.90241200	-0.63565600
H	-3.32721500	-3.45359800	-1.28363300
H	-3.21315900	-3.09172100	0.43806500
H	-2.55231700	2.13831200	0.81972700
H	-4.49218300	1.13898500	2.04118800
H	-4.91664700	2.59272500	1.13715000
H	-5.38287200	1.00925600	0.52173700
H	-2.46818700	2.16262100	-1.69846300
H	-3.80644400	3.15080700	-1.07780600
H	-4.12415400	1.55845900	-1.75890300
H	4.46872800	-0.46333800	-0.90453300
H	3.14872800	1.10996200	-2.37185900
H	3.91455800	-0.18282400	-3.31133900
H	2.17598200	-0.25599100	-2.92888100
H	3.87460600	-2.86727100	-0.72387900
H	4.25392100	-2.44452400	-2.39482500
H	2.55997400	-2.63944700	-1.90574100
H	2.60509100	1.18194300	1.96489700
H	2.91202300	2.54014500	-0.15642800
H	4.16014800	2.85484400	1.07155100
H	4.52215000	1.85108600	-0.33205900
H	4.24904100	-0.57882400	2.58617700
H	5.06319500	0.98315200	2.48214900
H	5.24430700	-0.19019600	1.17778600
B	0.27110300	2.52458900	-1.63515700
H	-0.46492900	3.07058900	-2.42670300
H	1.44145900	2.69812100	-1.87672100
N	-0.00983200	3.20846200	-0.17663000
H	-1.01612800	3.19447400	-0.01906400
C	0.50977500	4.58291300	0.00714100
H	0.08478400	5.21879600	-0.77150500
H	0.25456300	4.98310900	0.99309500

H	1.59281900	4.56493700	-0.11530000
H	-0.00767300	1.33500800	-1.48462500
H	-0.05678900	0.08532500	2.43443400
H	0.37097700	2.53722000	0.50443600

TS11-12$_N$

E_{gas} = -2096.773453 a.u.

E_{solv} = -2098.58461420 a.u.

Zero-point energy correction = 0.54889200 a.u.

Three lowest frequencies:

-847.1970 35.6207 40.3107

Co	0.02069100	0.03126000	-0.09277900
Cl	0.26120000	-2.52792800	-0.64586700
C	2.27938500	-1.01517000	1.76084100
C	1.17136600	-0.43798400	2.64072000
N	-0.12881000	-0.37415100	1.90361100
C	-1.00168300	-1.56119200	2.16490200
C	-2.26764700	-1.56512900	1.27847700
P	-2.23441800	-0.16415800	0.04355300
C	-3.35106100	-0.71445900	-1.36273900
C	-4.67252400	-1.34521200	-0.89257300
C	-2.61841900	-1.62545800	-2.35899600
C	-3.15220800	1.28871600	0.88084700
C	-4.02290100	0.93548300	2.09761400
C	-3.94972100	2.13792200	-0.12493800
P	2.30597300	-0.04605000	0.16999800
C	3.49589300	-0.93464200	-1.00168800
C	2.96051000	-0.87842000	-2.44284600
C	3.83180900	-2.37736200	-0.59219700
C	3.26819500	1.53430400	0.60374000
C	3.68928400	2.30224700	-0.66545700
C	4.48547200	1.32662300	1.51904200
H	2.03030900	-2.03946500	1.47280400
H	3.23217900	-1.02326700	2.29793400
H	1.42397600	0.58326300	2.94654800
H	1.04909700	-1.02896200	3.55826700
H	-1.26564700	-1.58098400	3.23148200
H	-0.40251800	-2.43923900	1.92601400
H	-3.18093700	-1.57968400	1.87737900
H	-2.24267700	-2.46839500	0.66433200
H	-3.57771100	0.22250800	-1.88319400
H	-5.24248900	-0.69294700	-0.22443400
H	-5.30542200	-1.56179500	-1.76088500
H	-4.49992000	-2.29365600	-0.37380400
H	-1.71283100	-1.15151200	-2.73966400
H	-3.28607500	-1.83861700	-3.20285400
H	-2.31536100	-2.57229000	-1.90683700
H	-2.32142000	1.91191500	1.23704900
H	-3.45516600	0.44127800	2.89232800
H	-4.44776200	1.85188000	2.52457300
H	-4.85990000	0.28200100	1.83189800
H	-3.36365200	2.38830100	-1.01291200
H	-4.26166000	3.07606200	0.34851800
H	-4.85732100	1.62266400	-0.45492200
H	4.42367700	-0.35125300	-0.94985600
H	2.74588500	0.14347700	-2.76835400
H	3.70404300	-1.30390700	-3.12756100
H	2.03728600	-1.45774100	-2.51883900
H	4.30282400	-2.43152100	0.39484200
H	4.54145400	-2.79509900	-1.31626000
H	2.93377900	-2.99926700	-0.59375400
H	2.53341900	2.14907900	1.14113900
H	2.88718800	2.39428100	-1.40378900
H	4.02424900	3.31131900	-0.39930800
H	4.52644900	1.80793200	-1.16812800
H	4.21014200	0.93351100	2.50186600
H	5.00123500	2.28062700	1.68258700
H	5.21163300	0.63765000	1.07319800
B	-0.14895100	1.69895000	-2.05943000
H	-1.31509800	1.73655200	-2.37964400
H	0.60826300	1.84774800	-2.99648500
N	0.11270600	2.69393200	-0.86835100
H	-0.06245700	1.60995300	0.06777400
C	-0.61461300	3.96608300	-0.88522700
H	-1.68810600	3.77431200	-0.83337100
H	-0.33399500	4.59294800	-0.03079800

H	-0.42796700	4.53598600	-1.80799900
H	0.11095100	0.47655800	-1.69190100
H	-0.61786700	0.44772900	2.25264500
H	1.10419200	2.88261400	-0.76292400

INT12

E_{gas} = -2096.820884 a.u.

E_{solv} = -2098.62560270 a.u.

Zero-point energy correction = 0.54935200 a.u.

Co	0.08218700	-0.16521000	-0.20360800
C	2.45010700	0.04724000	1.79103000
C	1.40257400	1.06803600	2.26300800
N	0.07156400	0.90069500	1.61215400
C	-1.00983700	0.39356100	2.48499500
C	-2.35010100	0.44042200	1.73276300
P	-2.18078300	-0.28965900	0.00752500
C	-2.93241300	-2.00692600	0.12595800
C	-2.60618100	-2.85515900	-1.11490600
C	-4.42415700	-2.08432100	0.48536800
C	-3.25075500	0.82733500	-1.05552200
C	-4.67974500	1.11551800	-0.56545900
C	-3.23216300	0.39481000	-2.53055200
P	2.34609900	-0.13012400	-0.06570800
C	3.42051100	-1.60002800	-0.57345900
C	2.76533400	-2.37525500	-1.72936000
C	3.80699800	-2.53924400	0.58012200
C	3.29755400	1.33722400	-0.75620400
C	3.36345700	1.25061900	-2.29082700
C	4.69156800	1.55648600	-0.14707400
H	2.21149500	-0.93926400	2.19197300
H	3.44485300	0.33451700	2.14763500
H	1.74924700	2.08216600	2.03136400
H	1.29790000	1.01393000	3.35413200
H	-1.08444300	0.99408500	3.40512800
H	-0.76296500	-0.63416300	2.76232100
H	-2.66457400	1.48370800	1.61272500
H	-3.12750000	-0.06265000	2.31644700
H	-2.35092100	-2.42614000	0.95356400
H	-1.53830200	-2.82156000	-1.33734100
H	-2.88390200	-3.89835800	-0.92519100
H	-3.16310200	-2.52189800	-1.99627100
H	-4.70007700	-1.43830200	1.32486400
H	-4.67063900	-3.11360000	0.77145400
H	-5.06249100	-1.82556200	-0.36426400
H	-2.68337300	1.76182400	-1.00124400
H	-4.71726100	1.39685300	0.49155200
H	-5.09539400	1.95174000	-1.14036800
H	-5.34590200	0.26192400	-0.70826600
H	-2.21272800	0.20997000	-2.87917900
H	-3.66449800	1.18740600	-3.15185100
H	-3.82496700	-0.51041200	-2.69541800
H	4.34380200	-1.14264600	-0.95024800
H	2.55024000	-1.72975400	-2.58550000
H	3.44034000	-3.17157800	-2.06578400
H	1.82473700	-2.82314200	-1.40205800
H	4.35037400	-2.01960400	1.37559500
H	4.46467700	-3.32727600	0.19449800
H	2.92335500	-3.01404300	1.01169400
H	2.66971300	2.19986900	-0.50855800
H	2.37133700	1.11231700	-2.72718600
H	3.78463500	2.17645000	-2.69837500
H	4.00590200	0.42695300	-2.62088200
H	4.65455000	1.74056100	0.93069300
H	5.16385300	2.43030900	-0.61135200
H	5.35616000	0.70265800	-0.31840900
B	-0.08295300	2.67119400	-1.20524800
H	-1.06521700	2.64835800	-1.89764200
N	-0.19921500	3.41653900	0.06305800
H	0.64845900	3.89284600	0.34834400
C	-1.37890700	4.20794300	0.40158300
H	-2.28406000	3.63602000	0.17908900
H	-1.40019500	4.46074000	1.46968200
H	-1.44795700	5.14998400	-0.16367600
H	-0.18959900	1.82994500	1.24260400
H	0.06642800	-0.76725700	-1.52919400
Cl	0.25094500	-2.27777000	0.87905000

H	0.97546100	2.74730100	-1.76474700
H	-0.01705000	1.18811500	-0.95505300

INT12'

E_{gas} = -2096.790847 a.u.

E_{solv} = -2098.6074344 a.u.

Zero-point energy correction = 0.55514700 a.u.

Co	0.05409800	0.07481200	-0.00544700
Cl	0.17065400	-2.40673000	-0.54703700
C	2.43359300	-1.19714500	1.56097800
C	1.47561600	-0.63959300	2.62065200
N	0.11852400	-0.34538300	2.07546800
C	-0.93439900	-1.32964200	2.41603900
C	-2.29361900	-0.77868800	1.96551800
P	-2.21326800	-0.19658300	0.17813700
C	-2.99602900	-1.60486300	-0.79833200
C	-2.71630900	-1.47879400	-2.30563800
C	-4.47501400	-1.90977000	-0.51883100
C	-3.41878900	1.26670900	0.15303800
C	-4.69831300	1.15558000	1.00099100
C	-3.77084400	1.69875900	-1.28284700
P	2.32631800	-0.11567400	0.03823800
C	3.30557800	-0.96818600	-1.34483000
C	2.57620200	-0.83681700	-2.69201200
C	3.68084600	-2.43051800	-1.05670900
C	3.47160000	1.33051400	0.46189600
C	3.55512700	2.31583300	-0.71490800
C	4.87823300	0.94331700	0.94616400
H	2.10187800	-2.18741300	1.24438900
H	3.44315800	-1.28081100	1.97609500
H	1.87409200	0.29914700	3.02067500
H	1.39792800	-1.33737600	3.46545500
H	-0.95269400	-1.52165900	3.50066400
H	-0.69798100	-2.25944700	1.89411500
H	-2.54897700	0.09161600	2.58191600
H	-3.07934400	-1.52423100	2.12262400
H	-2.39081300	-2.44744100	-0.44861300
H	-1.65238500	-1.31154400	-2.48196900
H	-3.00226800	-2.41074600	-2.80722100
H	-3.29032500	-0.66940700	-2.76874200
H	-4.70191900	-1.99011700	0.54920600
H	-4.73749100	-2.86997000	-0.97902100
H	-5.14252600	-1.15672000	-0.95001900
H	-2.80519500	2.05576800	0.60397600
H	-4.48896600	0.90456700	2.04396400
H	-5.22077000	2.12057000	1.00075300
H	-5.39267200	0.40914000	0.60917600
H	-2.90171400	1.71532000	-1.95050200
H	-4.21878600	2.69993600	-1.27863800
H	-4.49951000	1.02141000	-1.73763500
H	4.23991600	-0.39709700	-1.41077300
H	2.38150200	0.20910200	-2.94925400
H	3.19260500	-1.27206700	-3.48867300
H	1.61765700	-1.35840700	-2.65653100
H	4.27166900	-2.53431800	-0.14084600
H	4.28836800	-2.81631400	-1.88460000
H	2.78584400	-3.05027000	-0.96984700
H	2.95504600	1.84526000	1.27909700
H	2.56207400	2.65168600	-1.02387500
H	4.13464400	3.20188200	-0.42993600
H	4.04757300	1.87065000	-1.58631300
H	4.85496600	0.33495200	1.85440300
H	5.45402600	1.84813100	1.17704500
H	5.44130900	0.38896500	0.18751000
B	-0.01139600	2.07833700	0.52108600
H	1.03418000	2.52802400	0.94276200
H	-0.91064200	2.31557100	1.31869300
N	-0.34485600	2.97171600	-0.80375200
H	0.34119100	2.68047800	-1.50016700
C	-0.35949800	4.44622300	-0.63625700
H	0.61791200	4.75866000	-0.26694900
H	-0.58468100	4.95838100	-1.57724000
H	-1.11036100	4.70008200	0.11343300

H	-0.17165100	0.55507100	2.45069900
H	-1.23428500	2.64193700	-1.17585800
H	-0.00166100	0.49389400	-1.42930200

TS12-13

E_{gas} = -2096.82018 a.u.

E_{solv} = -2098.6257203 a.u.

Zero-point energy correction = 0.550027 a.u.

Three lowest frequencies:

-64.1047 35.4437 43.0432

Co	0.08521600	-0.17015000	-0.19992900
C	2.45242400	0.07515800	1.78632600
C	1.39678300	1.09189900	2.24949100
N	0.06289700	0.90236300	1.60901900
C	-1.00399300	0.37691700	2.49018100
C	-2.35032300	0.39568700	1.74750200
P	-2.17228000	-0.30527900	0.00875200
C	-2.91594000	-2.02847800	0.08952300
C	-2.57131200	-2.84951500	-1.16441700
C	-4.40997200	-2.12230300	0.43411300
C	-3.24771000	0.82850200	-1.03134700
C	-4.68339500	1.08960500	-0.54557200
C	-3.21423800	0.43500500	-2.51705500
P	2.34295200	-0.12485200	-0.06905100
C	3.41943200	-1.59841800	-0.56476000
C	2.75064000	-2.39804900	-1.69588000
C	3.82492900	-2.51390300	0.60106700
C	3.28623300	1.33794100	-0.77873900
C	3.32264500	1.24760400	-2.31411500
C	4.69117600	1.55794800	-0.19593300
H	2.22499700	-0.90888700	2.20012400
H	3.44457400	0.37749700	2.13790300
H	1.73201800	2.10536400	2.00016700
H	1.29860400	1.05383900	3.34201800
H	-1.08239400	0.97741200	3.41004400
H	-0.73479400	-0.64532900	2.76511400
H	-2.69837100	1.43018700	1.64530500
H	-3.10761400	-0.13937500	2.32928800
H	-2.33851500	-2.45908700	0.91399700
H	-1.50043900	-2.80836200	-1.37073900
H	-2.84960500	-3.89704200	-1.00109500
H	-3.11592100	-2.49846800	-2.04682500
H	-4.69666500	-1.48903900	1.27950800
H	-4.65178400	-3.15702600	0.70407000
H	-5.04280600	-1.85606800	-0.41741500
H	-2.69022700	1.76692000	-0.94718900
H	-4.73428700	1.33023700	0.52091800
H	-5.09992700	1.94338800	-1.09347700
H	-5.34126500	0.23710000	-0.72748600
H	-2.19036800	0.27029900	-2.86270600
H	-3.65200000	1.23780600	-3.12136700
H	-3.79521100	-0.47271700	-2.70864000
H	4.33540300	-1.14503100	-0.96374100
H	2.52159500	-1.77041300	-2.56165900
H	3.42297100	-3.19944200	-2.02595400
H	1.81592400	-2.84096400	-1.34568200
H	4.37497800	-1.97621700	1.37971100
H	4.48152900	-3.30619200	0.22245100
H	2.94849600	-2.98437400	1.05191500
H	2.66548600	2.20271100	-0.52034400
H	2.32178800	1.11073600	-2.73069200
H	3.73973700	2.17033400	-2.73285000
H	3.95523200	0.42018300	-2.65380900
H	4.67469000	1.72903700	0.88448000
H	5.14965700	2.43971400	-0.65918100
H	5.35659000	0.70998200	-0.39068400
B	-0.09611100	2.73332700	-1.20899100
H	-1.07741600	2.67244600	-1.89653900
N	-0.21988400	3.46695200	0.04853500
H	0.62709800	3.91159200	0.38133900
C	-1.40917900	4.21261700	0.44612500
H	-2.30196700	3.69731800	0.08320600
H	-1.49260500	4.29945300	1.53798100
H	-1.43422300	5.23161200	0.03182600
H	-0.21788000	1.82267000	1.24248100
H	0.07697100	-0.77679000	-1.52345900

Cl	0.25951500	-2.28234100	0.90955800
H	-0.01511700	1.17022200	-0.94866600
H	0.97065000	2.77743900	-1.75057600

TS12'-10

E_{gas} = -2096.777950 a.u.

E_{solv} = -2098.5725259 a.u.

Zero-point energy correction = 0.5400500 a.u.

Three lowest frequencies:

-1453.2433 31.4416 38.2815

Co	0.02583200	-0.23884000	-0.26542600
C	2.34114800	-0.62870300	1.81614900
C	1.40291900	0.36252500	2.52349100
N	0.05724400	0.42419100	1.90466300
C	-0.98371100	-0.38428400	2.56752000
C	-2.35329900	-0.10396500	1.92735300
P	-2.28833800	-0.22210800	0.05137700
C	-3.22106100	-1.80226300	-0.35895200
C	-3.08075400	-2.15407500	-1.84938600
C	-4.67588400	-1.93056700	0.11642800
C	-3.28035700	1.30099000	-0.46015100
C	-4.71637900	1.44084800	0.07103700
C	-3.22454000	1.53026600	-1.97988000
P	2.32218400	-0.31351300	-0.02407000
C	3.43738400	-1.61603700	-0.82271900
C	2.87223400	-2.00137500	-2.20173200
C	3.67104900	-2.86516200	0.04160100
C	3.31170300	1.28130800	-0.22207100
C	3.47088700	1.62660800	-1.71256600
C	4.66528000	1.32071500	0.50377300
H	1.96740600	-1.64864700	1.93682400
H	3.34289800	-0.57708600	2.25681700
H	1.82424500	1.37286600	2.47634300
H	1.33011200	0.10318000	3.59000100
H	-1.03631300	-0.16282700	3.64627700
H	-0.71971400	-1.43768600	2.44310100
H	-2.66779800	0.91554100	2.18131700
H	-3.10182900	-0.78407600	2.34571500
H	-2.60665200	-2.52626300	0.18904000
H	-2.03145100	-2.14698700	-2.15419700
H	-3.47410400	-3.16113900	-2.02929700
H	-3.64191700	-1.46501700	-2.49020800
H	-4.81864100	-1.61437700	1.15443000
H	-4.98507300	-2.98059700	0.05166700
H	-5.36417600	-1.35400100	-0.50820900
H	-2.68392000	2.08721900	0.02332700
H	-4.78954400	1.24039800	1.14387800
H	-5.07357000	2.46440900	-0.09602900
H	-5.40600100	0.76887800	-0.44505100
H	-2.20326600	1.44303400	-2.36287700
H	-3.60898600	2.52719100	-2.23020100
H	-3.84591100	0.80558100	-2.51522600
H	4.40633000	-1.12186100	-0.97086000
H	2.74220100	-1.13033200	-2.85203000
H	3.55526100	-2.69607300	-2.70549500
H	1.90066400	-2.48973700	-2.08757300
H	4.15522900	-2.62639100	0.99347700
H	4.32809200	-3.55915700	-0.49634500
H	2.72826300	-3.37816400	0.24688400
H	2.65947200	2.03914400	0.23117900
H	2.51023000	1.60618700	-2.23548700
H	3.90441100	2.62706900	-1.82887700
H	4.14461300	0.92436000	-2.21546600
H	4.56128700	1.19037000	1.58459000
H	5.15401100	2.28826600	0.33696000
H	5.34821800	0.54688900	0.13660200
B	-0.31928400	3.71263300	1.13112900
H	0.73346900	3.85122900	1.67760100
N	-0.27948900	3.40013300	-0.35785500
H	-0.09867300	2.27237300	-0.61505200
C	0.72279300	4.13874100	-1.17074800
H	1.69819500	4.03390200	-0.69569300
H	0.76629000	3.71892600	-2.18083400
H	0.46491000	5.19874100	-1.21103000
H	-0.23776400	1.40762100	1.91305500
Cl	0.02922400	-2.64277200	0.12058600

H	-1.38952400	3.68543200	1.65960900
H	0.05423300	1.17295000	-1.03804800
H	-1.20149900	3.55190200	-0.76588500

INT13

E_{gas} = -2096.841035 a.u.

E_{solv} = -2098.6354269 a.u.

Zero-point energy correction = 0.54592300 a.u.

Co	0.03530100	-0.34367300	-0.15354100
C	2.43489700	-0.65053300	1.78030400
C	1.42495400	0.21374000	2.55044400
N	0.07971700	0.26228300	1.89991300
C	-1.01296800	-0.44504200	2.61091400
C	-2.35007800	-0.11986700	1.92617400
P	-2.19285100	-0.30209300	0.05836600
C	-3.13373900	-1.87473200	-0.34564700
C	-2.86328500	-2.33731600	-1.78680700
C	-4.63265500	-1.89611700	-0.01302600
C	-3.07045200	1.22866700	-0.59553700
C	-4.48970100	1.51218800	-0.07654400
C	-3.00785500	1.30082800	-2.12996600
P	2.26290300	-0.32138500	-0.04878200
C	3.35750500	-1.55655100	-0.96211800
C	2.68096200	-1.98079600	-2.27732500
C	3.74522900	-2.78658000	-0.12552400
C	3.10592100	1.33805900	-0.32490500
C	3.03488100	1.72762500	-1.81105200
C	4.53879500	1.45329600	0.21735000
H	2.18323200	-1.70607100	1.90274000
H	3.44547400	-0.48663900	2.16983300
H	1.79304700	1.24340200	2.61685200
H	1.32781400	-0.15292400	3.57980100
H	0.01176500	1.05167600	-0.61689300
H	-1.05128400	-0.14380900	3.66897100
H	-0.80138900	-1.51481400	2.55190500
H	-2.62936800	0.91883600	2.14114000
H	-3.14468900	-0.75368700	2.33136000
H	-2.61395900	-2.58177900	0.31202300
H	-1.79066000	-2.36694800	-1.98737900
H	-3.26808300	-3.34607100	-1.92851100
H	-3.34378400	-1.68445000	-2.52317900
H	-4.85605800	-1.51729500	0.98942000
H	-4.99887500	-2.92838300	-0.06018000
H	-5.21722000	-1.31428600	-0.73177000
H	-2.40919400	2.01541600	-0.20754700
H	-4.56437100	1.44055800	1.01279500
H	-4.78437100	2.53060900	-0.35699400
H	-5.22657300	0.83091500	-0.50854400
H	-1.99660900	1.10584400	-2.49664000
H	-3.31412000	2.29730900	-2.46978100
H	-3.68622200	0.57763500	-2.59380700
H	4.27648400	-1.00697700	-1.20296400
H	2.44989500	-1.12419000	-2.91684400
H	3.34535500	-2.65216700	-2.83469600
H	1.74393700	-2.50156900	-2.06624600
H	4.30146000	-2.51829700	0.77805100
H	4.38845200	-3.44106000	-0.72553700
H	2.85784200	-3.35468500	0.16466900
H	2.46940500	2.04025900	0.22840000
H	2.01203300	1.65544800	-2.19098300
H	3.38621100	2.75691300	-1.94943300
H	3.67231200	1.08289600	-2.42632900
H	4.59569500	1.26523200	1.29367200
H	4.92389800	2.46469600	0.04172700
H	5.22208900	0.75736500	-0.28117900
B	-0.15307500	4.15549200	1.34174700
H	-0.19498300	3.27932500	2.16352700
H	-0.20598700	5.30467000	1.66909700
N	-0.04219400	3.81259400	0.00310900
H	0.00176800	2.82825600	-0.26266400
C	0.02235900	4.72736600	-1.12924500
H	0.95965700	4.60724300	-1.68519300
H	-0.80532700	4.55594400	-1.82757900
H	-0.03692000	5.75614400	-0.76776300
H	-0.18325400	1.24409800	1.84834700
Cl	0.09181100	-2.68820600	0.39184500

H	-0.01513900	-0.61073800	-1.58002500

TS13-10

E_{gas} = -1975.516732 a.u.

E_{solv} = -1977.2009908 a.u.

Zero-point energy correction = 0.4738720 a.u.

Three lowest frequencies:

-71.4530 25.5584 43.1304

Co	-0.07396000	-0.03803700	-0.35392300
C	2.40595700	1.95653500	-0.65455800
C	1.23816600	2.71955400	-0.03315400
N	-0.04631600	2.10763200	-0.44752800
C	-1.20608500	2.74287600	0.21781900
C	-2.50732400	2.07818400	-0.22907300
P	-2.31842000	0.20862800	-0.12885000
C	-3.26516800	-0.19132700	1.45348300
C	-2.49724500	0.34300600	2.67458200
C	-3.56080700	-1.69080600	1.62267900
C	-3.43722900	-0.32785800	-1.55399800
C	-4.91751700	0.05557300	-1.40337400
C	-3.26798800	-1.81237600	-1.91880300
P	2.17853600	0.14195800	-0.24806700
C	2.98676800	-0.08210000	1.45155400
C	4.09585600	0.91943200	1.81112500
C	3.44736400	-1.52854400	1.70342400
C	3.22946000	-0.67817700	-1.57912300
C	3.01247700	-2.20048200	-1.64373300
C	4.72177100	-0.31173300	-1.59297400
H	3.36023300	2.37789300	-0.32764700
H	2.37060100	2.04923300	-1.74760700
H	-2.71969300	2.34214400	-1.27293100
H	-3.34639500	2.44750800	0.37021000
H	-4.21861200	0.34986200	1.37391900
H	-2.37113600	1.43058400	2.64524200
H	-3.05289600	0.10770700	3.59016300
H	-1.51129700	-0.12623100	2.73571800
H	-4.23865900	-2.06939800	0.85304400
H	-4.04608600	-1.85622000	2.59228200
H	-2.63575200	-2.27202600	1.59632500
H	-3.01593300	0.25534900	-2.38593500
H	-5.05403700	1.12193600	-1.19534000
H	-5.46165800	-0.17132000	-2.32802400
H	-5.39873500	-0.50794600	-0.59787500
H	-2.21402500	-2.08483900	-2.01137900
H	-3.76265000	-2.01771700	-2.87564400
H	-3.71503200	-2.47129500	-1.17022900
H	2.12957000	0.08921700	2.11312000
H	3.74934200	1.95755900	1.80589200
H	4.45862700	0.70879000	2.82422800
H	4.95548100	0.84720600	1.13695100
H	2.64961600	-2.23928100	1.48040100
H	3.71173900	-1.64061500	2.76162100
H	4.33806000	-1.78070100	1.11860900
H	2.76872000	-0.25192800	-2.48259800
H	1.95253500	-2.45840900	-1.57731600
H	3.40826800	-2.59008800	-2.58915200
H	3.52916300	-2.71777700	-0.83180100
H	4.88657700	0.77047400	-1.60527600
H	5.20055400	-0.72721300	-2.48807800
H	5.24604700	-0.72317600	-0.72535900
H	-0.11773700	-0.36098900	-2.03188300
Cl	-0.01721800	-1.92735400	1.09985200
H	-0.11093500	-1.10098200	-1.67272700
H	-1.06159100	2.61340900	1.29379300
H	-1.23044400	3.82575400	0.01247600
H	1.28424400	2.65993600	1.05972000
H	1.26942300	3.78667800	-0.30581900
H	-0.14414700	2.25615100	-1.45145100

TS1a-1b

E_{gas} = -2217.542721 a.u.

E_{solv} = -2219.4569728 a.u.

Zero-point energy correction = 0.606102 a.u.

Three lowest frequencies:

-129.6203 12.6000 24.9084

Co	-0.28222200	-0.10657700	0.70740000

Cl	-1.04255400	-1.40761800	2.49553300
C	-2.16010600	1.02531000	-1.94334600
C	-0.75574800	1.65346900	-1.95467000
N	0.27664500	0.75660700	-1.39673700
C	0.77154300	-0.23535600	-2.37042800
C	1.89927500	-1.08987000	-1.77464700
P	1.39293000	-1.78532200	-0.11972300
C	0.85022400	-3.56013500	-0.40997500
C	1.92702600	-4.55135000	-0.87551700
C	-0.35350600	-3.57529500	-1.36618000
C	2.95798700	-1.79147100	0.91945700
C	4.26336800	-2.23371700	0.23884200
C	2.70531900	-2.53446000	2.24308100
P	-2.58426500	0.48263300	-0.21116800
C	-4.13431600	-0.58750100	-0.32959700
C	-3.78658900	-2.08082000	-0.22386100
C	-5.02580300	-0.31592400	-1.55290200
C	-3.14734500	2.05928200	0.65125800
C	-3.31057700	1.79344700	2.15848700
C	-4.38415000	2.75532200	0.06529100
H	-2.18397600	0.13698200	-2.58472700
H	-2.88486100	1.73276800	-2.35945200
H	-0.75266400	2.56175700	-1.34627200
H	-0.49593300	1.95729100	-2.98040300
H	1.05795300	1.34266200	-1.08837600
H	1.13569400	0.26501000	-3.28145700
H	-0.06903600	-0.87202600	-2.66621300
H	2.77123300	-0.45138900	-1.60247400
H	2.20061100	-1.86624700	-2.48575300
H	0.48920800	-3.86492200	0.58018300
H	2.70380600	-4.70223300	-0.12352500
H	1.46821200	-5.52770800	-1.07263900
H	2.41026900	-4.22659000	-1.80393200
H	-1.13281500	-2.88433600	-1.03797400
H	-0.78972600	-4.57964400	-1.40395800
H	-0.05883100	-3.31087400	-2.38860800
H	3.05480200	-0.72453500	1.15608200
H	4.45589600	-1.68925700	-0.69016700
H	5.10414500	-2.03136400	0.91288600
H	4.27811900	-3.30275700	0.01396300
H	1.79249400	-2.18426100	2.73368300
H	3.54752000	-2.37016000	2.92445300
H	2.61738200	-3.61573200	2.08835700
H	-4.69157000	-0.31339900	0.57525900
H	-3.14840100	-2.28486900	0.63997100
H	-4.70449700	-2.67294000	-0.12999700
H	-3.27086800	-2.42799800	-1.12649200
H	-5.32228200	0.73166800	-1.64120100
H	-5.94051300	-0.91614200	-1.48268900
H	-4.52347900	-0.60361400	-2.48281300
H	-2.28375900	2.72501600	0.52967400
H	-2.41565200	1.33728200	2.58812400
H	-3.50616700	2.73606800	2.68175000
H	-4.15625800	1.12603500	2.36014100
H	-4.28683000	2.96866700	-1.00414100
H	-4.54200600	3.71299700	0.57499400
H	-5.29057200	2.15937400	0.21319800
B	0.91671200	1.81055800	1.58568900
H	0.72261000	2.15621200	2.73448700
H	-0.22204800	1.77121400	1.04610700
N	1.82526400	2.74662500	0.75407600
H	2.72517400	2.76845400	1.22978500
C	1.33067000	4.12609000	0.71956900
H	1.14912600	4.55063100	1.71991800
H	2.03389500	4.77949400	0.18936600
H	0.37611100	4.15902600	0.18015400
H	1.37916700	0.65619900	1.59845800
B	3.28566200	2.51475300	-1.14187700
H	2.41878200	2.63265200	-1.96426000
H	3.63340300	1.43271400	-0.75427100
N	4.18892500	3.58882300	-0.99185500
H	3.97352700	4.47774000	-1.42180000
C	5.38576400	3.61093900	-0.16960700
H	5.58417000	2.60066500	0.19774700
H	6.26636500	3.93993100	-0.73790600
H	5.29060200	4.27320100	0.70329500

1b

E_{gas} = -2217.557021 a.u.

E_{solv} = -2219.4777476 a.u.

Zero-point energy correction = 0.610157 a.u.

Co	0.20976500	-0.05774300	-0.58668500
Cl	0.76303100	-1.24524700	-2.52417700
C	2.38189700	0.53587700	2.04082700
C	1.03828800	1.24581400	2.27258800
N	-0.10177400	0.52173100	1.67819200
C	-0.58986500	-0.59508500	2.50931400
C	-1.87555200	-1.19529400	1.92204600
P	-1.63056300	-1.60239200	0.11843600
C	-1.29225700	-3.44543200	0.00571600
C	-2.42699400	-4.38805700	0.43253400
C	0.00688300	-3.77333400	0.75949800
C	-3.26777800	-1.22824900	-0.71806600
C	-4.55249500	-1.65401400	0.01026600
C	-3.23120300	-1.71621800	-2.17693500
P	2.61863500	0.22618900	0.21961400
C	4.05943900	-0.98001700	0.06186100
C	3.55226700	-2.41802400	-0.13151600
C	5.09556000	-0.91261400	1.19678200
C	3.24646000	1.86129400	-0.47108900
C	3.29702800	1.78596800	-2.00788000
C	4.56429900	2.39549100	0.10807500
H	-0.86252400	1.19813100	1.55323700
H	-0.78038900	-0.25703200	3.54059600
H	0.19427200	-1.35815800	2.56278900
H	-2.67432300	-0.44863900	1.97655400
H	-2.19417800	-2.06128800	2.51138000
H	-1.09291000	-3.58495700	-1.06387300
H	-3.30114600	-4.30487600	-0.21607700
H	-2.08016800	-5.42711000	0.38257700
H	-2.74963200	-4.20352000	1.46348700
H	0.82576100	-3.12600400	0.43914700
H	0.30213300	-4.80973300	0.56187800
H	-0.11890700	-3.67333800	1.84422200
H	-3.24715200	-0.13163000	-0.73001700
H	-4.59078800	-1.28451800	1.03911600
H	-5.41742100	-1.23296100	-0.51555700
H	-4.68281200	-2.73857500	0.03432700
H	-2.32338300	-1.38735600	-2.69129400
H	-4.09660900	-1.32062400	-2.72016600
H	-3.27980100	-2.80914200	-2.23852400
H	4.54335200	-0.67013000	-0.87310000
H	2.83908900	-2.48260600	-0.95720600
H	4.39520000	-3.08631400	-0.34283400
H	3.06680900	-2.78968600	0.77870800
H	5.50078300	0.09014100	1.34816800
H	5.93468800	-1.57979200	0.96772000
H	4.66724100	-1.24999100	2.14672300
H	2.44271000	2.55939500	-0.20402600
H	2.34716600	1.44930400	-2.42950400
H	3.52778100	2.77482700	-2.41949000
H	4.07918500	1.09904900	-2.35051400
H	4.55519800	2.46007700	1.20081100
H	4.75047800	3.40525500	-0.27597900
H	5.41566100	1.77575000	-0.19078900
B	-0.75437000	2.00049100	-1.45400300
H	-0.34184600	2.31000000	-2.54500100
H	0.22577400	1.88482800	-0.68438100
N	-1.71500700	3.09263600	-0.85198600
H	-2.55560400	3.07535600	-1.43201300
C	-1.15534700	4.46086100	-0.99646700
H	-0.94094100	4.68460300	-2.04535500
H	-1.86682400	5.18006700	-0.58469000
H	-0.22326500	4.51446800	-0.42768100
H	-1.34928400	0.92463500	-1.52644500
B	-2.27570400	2.86557400	0.67064500
H	-1.31014800	3.06800700	1.40125800
H	-2.63093200	1.68545000	0.70377700
N	-3.39211000	3.84018800	0.95185800

H	-3.26731300	4.35196600	1.81604900
C	-4.76919500	3.39511000	0.82370700
H	-5.06477000	2.58649900	1.52070300
H	-5.47373500	4.22547100	0.96845900
H	-4.94913200	3.00816700	-0.18817800
H	0.88472200	1.39707700	3.35248000
H	1.05345200	2.23932600	1.81555400
H	3.19332300	1.12292300	2.48303100
H	2.38890400	-0.43816400	2.54347700

2a

E_{gas} = -2562.933958 a.u.

E_{solv} = -2565.1605574 a.u.

Zero-point energy correction = 0.787713 a.u.

Co	0.13470600	-1.02776300	-0.26801000
C	-2.24051300	-0.52045100	2.17841700
C	-1.25435900	-1.65012600	2.52553600
N	0.10713900	-1.38663400	2.03657900
C	0.86744600	-0.44351200	2.86501300
C	2.28302200	-0.24273800	2.30502000
P	2.22905000	0.16476400	0.47868100
P	-2.14129800	-0.11265800	0.35682000
H	-1.97878400	0.39250200	2.72611000
H	-3.25088700	-0.79452000	2.49510800
H	-1.58454100	-2.58167000	2.05645000
H	-1.26163200	-1.81909400	3.61487800
H	0.61531000	-2.30423000	1.95847600
H	0.93284300	-0.79462100	3.90897200
H	0.33873800	0.51685100	2.89175100
H	2.84217200	-1.17981900	2.40421200
H	2.82060400	0.51642600	2.88339500
Cl	0.06909500	-0.35414100	-2.50366200
C	-3.62135400	-0.90932700	-0.49236700
C	-3.21592100	-2.22473400	-1.21110100
C	-4.87759100	-1.15318700	0.36575400
C	-4.44795400	-3.07484900	-1.61378100
H	-2.60960200	-1.97385600	-2.08684300
C	-6.09485400	-1.47246700	-0.54072100
H	-4.68504100	-2.00049400	1.03649500
C	-5.68758800	-2.20151800	-1.84268500
H	-4.21300300	-3.65911300	-2.50962700
H	-6.80605400	-2.08545700	0.02593900
H	-6.52481500	-2.80283600	-2.21395900
C	-2.48136600	1.73076000	0.30547500
C	-2.27383900	2.29564000	-1.12792600
C	-3.82680600	2.20983100	0.88403500
C	-2.96555800	3.66610700	-1.32304100
H	-1.20052700	2.37360500	-1.32551200
C	-3.82943500	3.74975700	1.06078100
H	-4.63311100	1.91412000	0.20243800
C	-2.98761700	4.47181900	-0.01870000
H	-2.45774400	4.22281100	-2.11804600
H	-4.86570100	4.10660700	1.02822000
H	-3.37883500	5.48076000	-0.18924600
H	-6.62137000	-0.54308000	-0.78982500
H	-5.11230300	-0.29929800	1.00781200
H	-3.88211700	-0.17112400	-1.26245600
H	-2.56586200	-2.82314300	-0.56440200
H	-4.67272500	-3.80493600	-0.82496000
H	-5.46814500	-1.46848600	-2.62965000
H	-1.68815000	2.13567700	0.95049400
H	-4.04394200	1.73166900	1.84524100
H	-2.64810700	1.59319700	-1.88037600
H	-3.44828500	4.00677800	2.05649400
H	-1.95631300	4.60244200	0.33571200
H	-3.99783400	3.51955700	-1.66700800
C	2.51447200	2.01593200	0.38449700
C	2.57603100	2.49577000	-1.09679800
C	1.44637900	2.81212000	1.15888700
C	2.13025900	3.96711900	-1.26111700
H	3.60537000	2.38890400	-1.45611700
C	1.81171000	4.31484300	1.22913900
H	0.48149900	2.68445800	0.65444900
C	2.53497500	4.80970300	-0.04653300
H	2.55922400	4.37694100	-2.18192900
H	0.89227000	4.89169200	1.38711800

H	2.31964000	5.87051400	-0.21514500
C	3.78688200	-0.66152600	-0.15838800
C	3.89116700	-0.69593100	-1.69667500
C	5.11951800	-0.18214300	0.47265900
C	4.91952200	-1.76853400	-2.13165600
H	2.91687600	-0.89624100	-2.15096600
C	6.34492300	-0.61448000	-0.37388800
H	5.13274600	0.90899900	0.57704700
C	6.07767200	-1.93000000	-1.11625600
H	4.40973300	-2.72958400	-2.26259400
H	6.57745800	0.16593400	-1.10958500
H	3.60698500	-1.69766300	0.15951400
H	5.20605400	-0.58910600	1.48752100
H	7.22726000	-0.69893700	0.27068500
H	6.98450600	-2.27483100	-1.62531200
H	5.82961400	-2.70855700	-0.38253200
H	5.32070300	-1.49495700	-3.11449300
H	4.20829700	0.28878900	-2.05843600
H	3.48096800	2.21241600	0.86831400
H	1.95265700	1.85646500	-1.73177200
H	1.04091100	4.01485300	-1.38724700
H	3.62226300	4.73715100	0.08839700
H	2.44306500	4.49963600	2.10653700
H	1.31840800	2.42650600	2.17601900
H	1.53782200	-2.50024400	-0.63124100
N	1.20764300	-3.85196000	1.17380500
H	2.21664400	-3.98317800	1.18098500
B	0.76335500	-3.37900400	-0.22350700
H	0.64285400	-4.22648900	-1.08534500
C	0.58631000	-5.09887800	1.62406000
H	0.94308900	-5.38773700	2.62158000
H	-0.49941200	-4.96068000	1.69273700
H	0.75403900	-5.94792900	0.94076900
H	-0.38718200	-2.85074900	-0.12023600

TS2a-2b

E_{gas} = -2684.213987 a.u.

E_{solv} = -2686.564678 a.u.

Zero-point energy correction = 0.860058 a.u.

Three lowest frequencies:

-133.4234 17.5366 23.0269

Co	0.12856600	-0.56169100	-0.53325900
C	-2.04079400	-1.25381500	2.05678500
C	-0.71023500	-2.01610900	2.17315000
N	0.43703800	-1.22912700	1.68239100
C	0.87517700	-0.17694300	2.61699300
C	2.08052100	0.59299300	2.06182700
P	1.77228700	1.14777000	0.30184800
P	-2.25349000	-0.56462200	0.33050500
H	-2.05638100	-0.40437200	2.74913600
H	-2.86607500	-1.90802200	2.35107800
H	-0.75291800	-2.92400600	1.56581100
H	-0.55422300	-2.33125000	3.21673100
H	1.13212000	-0.60749100	3.59755700
H	0.03554900	0.50819600	2.77711100
H	2.94917100	-0.07211300	2.04456200
H	2.32680400	1.43324400	2.71984500
Cl	-0.37001400	0.36017700	-2.61762500
C	-3.48614800	-1.66196000	-0.57743300
C	-2.76806300	-2.64584200	-1.53995900
C	-4.50797000	-2.43041000	0.28259000
C	-3.71095600	-3.77349900	-2.03235400
H	-2.36087600	-2.07913600	-2.38276700
C	-5.65279600	-2.98155200	-0.60701000
H	-3.99297400	-3.26330400	0.77863500
C	-5.17702800	-3.32387300	-2.03834300
H	-3.40047400	-4.10075800	-3.03013800
H	-6.07374900	-3.87373000	-0.12802400
H	-5.82019300	-4.09711600	-2.47281700
C	-3.16210400	1.05045600	0.61822100
C	-3.29504400	1.85707800	-0.70412900
C	-4.52216200	0.96926700	1.33798000
C	-4.39893500	2.93867700	-0.62172800
H	-2.32794300	2.31017900	-0.94152100
C	-4.99178400	2.37853000	1.78062800
H	-5.26021900	0.53024000	0.65633900
C	-4.53789500	3.48886600	0.80269600

H	-4.17710300	3.74289000	-1.33152300
H	-6.08512800	2.37593800	1.86297900
H	-5.24304400	4.32674000	0.83049400
H	-6.46598000	-2.24716800	-0.65618600
H	-4.92879700	-1.81002100	1.07915100
H	-4.04288100	-0.93899700	-1.18828900
H	-1.90313200	-3.09635800	-1.04303100
H	-3.61539400	-4.65218500	-1.38074900
H	-5.27891000	-2.44466000	-2.68751100
H	-2.47471100	1.59432900	1.28200000
H	-4.47637300	0.30881700	2.21057800
H	-3.50733500	1.19003300	-1.54655900
H	-4.60954200	2.59533600	2.78542100
H	-3.56959600	3.89686500	1.12229500
H	-5.36257600	2.51546600	-0.93420600
C	1.43973500	2.98785800	0.42960700
C	1.25953400	3.62904400	-0.97807800
C	0.21794600	3.29779200	1.31583500
C	0.37028000	4.89396700	-0.94082800
H	2.24759000	3.89315700	-1.37061100
C	0.09140000	4.81837900	1.57750800
H	-0.68180700	2.92888800	0.81016100
C	0.55600500	5.66712100	0.36958600
H	0.60078700	5.52733500	-1.80429300
H	-0.95427400	5.04735600	1.81704100
H	0.01219500	6.61782700	0.34497300
C	3.45835700	0.93923400	-0.48741200
C	3.45059500	1.08905800	-2.02227900
C	4.60880000	1.76679700	0.14131700
C	4.73408500	0.46163400	-2.61954100
H	2.56168600	0.62357700	-2.45684600
C	5.84120200	1.84115400	-0.79716700
H	4.27911200	2.78729700	0.36883300
C	5.95376800	0.58743300	-1.67386400
H	4.55209800	-0.59526000	-2.84477700
H	5.75669100	2.72131800	-1.44738700
H	3.64466500	-0.12306600	-0.27913400
H	4.89671600	1.31448400	1.09781100
H	6.74969400	1.98717800	-0.20184800
H	6.88369300	0.60547500	-2.25310400
H	6.01881900	-0.29534800	-1.02408400
H	4.95270800	0.94839800	-3.57724400
H	3.40359500	2.15295900	-2.28132200
H	2.31804500	3.43097700	0.91870500
H	0.82616200	2.90312200	-1.67479300
H	-0.68489700	4.61059400	-1.04641300
H	1.61724800	5.92591100	0.48114900
H	0.67506900	5.08956700	2.46540800
H	0.27377500	2.77122100	2.27498900
H	1.86221800	-1.47468300	-1.12197200
N	2.11700800	-3.46851500	-0.00842800
H	3.05663300	-3.57994800	-0.38430000
B	1.34570500	-2.60165100	-1.03537900
H	1.25979700	-3.07588800	-2.15033600
C	1.55267500	-4.81553100	0.12490700
H	2.16525200	-5.43022200	0.79528900
H	0.54788200	-4.74978300	0.55909300
H	1.45381400	-5.34297500	-0.83703900
H	0.15839400	-2.46228900	-0.63429800
B	3.37925700	-3.07417800	1.97172800
H	2.43425400	-3.05453000	2.71231900
H	3.82436000	-2.06029000	1.50573600
N	4.23863300	-4.19315800	2.04604700
H	3.93548500	-5.01472100	2.55049200
C	5.50588700	-4.36315900	1.35808900
H	6.30756200	-4.66517900	2.04576500
H	5.45945700	-5.11486000	0.55628500
H	5.79613800	-3.41100100	0.90592900
H	1.21136900	-1.87989200	1.51835400

2b

E_{gas} = -2684.218865 a.u.

E_{solv} = -2686.576841 a.u.

Zero-point energy correction = 0.865203 a.u.

Co	0.05256200	0.09500000	0.01899000
C	-2.39932600	-0.90587100	1.76498000

C	-1.25068000	-0.48601800	2.68448100
N	0.05604700	-0.55261100	1.97391200
C	1.15689100	-0.03452800	2.83063000
C	2.50015600	-0.10685100	2.10090200
P	2.31699100	0.50430900	0.34417700
P	-2.25290900	0.07409600	0.19219400
H	-3.35970100	-0.78206900	2.27416800
H	-2.28534100	-1.96432600	1.51360900
H	2.81095600	-1.15480300	2.03247200
H	3.26992300	0.43627600	2.65961700
Cl	0.01434800	1.12749100	-2.01190700
C	-3.41972300	-0.64956600	-1.08389300
C	-2.66257600	-1.44350300	-2.18520300
C	-4.56970800	-1.49753700	-0.50105200
C	-3.59394300	-2.42670200	-2.93278200
H	-2.21776300	-0.72788800	-2.88235300
C	-5.64089700	-1.77266700	-1.58622600
H	-4.15798900	-2.44627600	-0.13638300
C	-5.03170100	-1.89830800	-3.00315100
H	-3.19689600	-2.61057700	-3.93672400
H	-6.17567800	-2.69317200	-1.32365100
H	-5.65850500	-2.54717500	-3.62472800
C	-2.97766600	1.74825900	0.63729700
C	-2.76972400	2.78631200	-0.50259800
C	-4.45207700	1.74600900	1.08972700
C	-3.74149700	3.98526700	-0.38703900
H	-1.73247900	3.13121000	-0.48069100
C	-4.83006400	3.10728500	1.72638100
H	-5.09004800	1.55378700	0.21886600
C	-4.07882100	4.29357500	1.07613900
H	-3.30189800	4.85936000	-0.87951700
H	-5.91276400	3.25089300	1.63080500
H	-4.67702300	5.20776400	1.15536500
H	-6.38843500	-0.97001700	-1.57599800
H	-5.03915400	-1.01406000	0.36110700
H	-3.86753700	0.23929000	-1.54743700
H	-1.82065400	-1.99208600	-1.75658900
H	-3.59734800	-3.40048800	-2.42536500
H	-5.02650400	-0.91746900	-3.49665600
H	-2.37122100	2.06509300	1.49793200
H	-4.65889900	0.94330500	1.80488700
H	-2.89153600	2.31555200	-1.48365700
H	-4.61804800	3.08211500	2.80206400
H	-3.14689200	4.49231900	1.62191100
H	-4.67176700	3.76810800	-0.92807600
C	2.78350000	2.32084000	0.41153800
C	3.07768500	2.90860500	-0.99977200
C	1.70516600	3.16894300	1.11658300
C	2.85247100	4.43826200	-1.06122900
H	4.11587000	2.68083600	-1.26558500
C	2.21046000	4.60890000	1.38050600
H	0.81490500	3.18778900	0.47700000
C	3.17458700	5.10771900	0.27892300
H	3.46076200	4.86368800	-1.86686200
H	1.34351100	5.27686800	1.44978500
H	3.12089700	6.19877800	0.19584400
C	3.67624200	-0.40375700	-0.55673100
C	3.56851400	-0.36030400	-2.09428500
C	5.11475800	-0.06572600	-0.08136600
C	4.44236100	-1.48082800	-2.70907800
H	2.52891000	-0.47400000	-2.41055500
C	6.17469900	-0.51910500	-1.11712200
H	5.23386300	1.00875600	0.09793800
C	5.71514000	-1.77084200	-1.87527900
H	3.84675300	-2.39539700	-2.79751900
H	6.35305400	0.28851200	-1.83865400
H	3.44691900	-1.43668800	-0.27026300
H	5.30041900	-0.56210200	0.87899100
H	7.13095900	-0.69412800	-0.61106000
H	6.51706700	-2.14305000	-2.52250600
H	5.51481300	-2.57107800	-1.15079100
H	4.72243200	-1.18930400	-3.72828200
H	3.90263400	0.61643600	-2.45986100
H	3.69834200	2.37102700	1.01855900
H	2.43813300	2.42942600	-1.74540500
H	1.80795800	4.64537900	-1.32584600

H	4.21146000	4.87385000	0.55489300
H	2.71040100	4.65246200	2.35570400
H	1.39726800	2.72152000	2.06687400
H	1.88277700	-2.61743100	-0.58582700
N	0.32205600	-4.07668900	0.18040200
H	1.07214200	-4.74711000	0.00656600
B	0.69971300	-2.82183500	-0.72803300
H	0.40426500	-3.03490200	-1.88543200
C	-0.92538200	-4.76352500	-0.22881900
H	-1.09501600	-5.62645600	0.42064600
H	-1.76134100	-4.06694200	-0.12047700
H	-0.87036900	-5.07722000	-1.27536300
H	0.03406400	-1.82385500	-0.34977100
B	0.35654700	-3.87665200	1.79519700
H	-0.71061800	-3.34831100	2.09257000
H	1.30496700	-3.11207500	2.01389200
N	0.48707500	-5.22223000	2.47226900
C	1.81453300	-5.69510300	2.82833200
H	1.78147800	-6.71520300	3.23534600
H	2.45249200	-5.73761600	1.93530400
H	2.35379500	-5.06317100	3.56118100
H	-0.14174000	-5.32908500	3.25873200
H	1.20036700	-0.61767600	3.76065200
H	0.90963900	0.99646200	3.10130600
H	-1.21870400	-1.13407700	3.56982600
H	-1.38879800	0.54402400	3.03298500
H	0.25433400	-1.55431400	1.82792200