Supporting Information

An Unprecedented Ring-contraction Mechanism in Cobalamin-dependent Radical S-adenosylmethionine Enzymes

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1. Computational methods

All calculations were performed using unrestricted density functional theory (UDFT) of the hybrid functional B3LYP[1-3] with Grimme's empirical D3-dispersion correction[4-7] included. Geometry optimizations were carried out using the Jaguar 8.7 package[8] with the LACVP** basis set, which implies a 6-31G(d,p) basis set[9,10] for the first- and second-row elements and an effective core potential[11] for the Fe and Co atoms. More accurate energies were evaluated on the basis of the optimized geometries by performing single-point calculations with larger basis sets, i.e., cc-pvtz(-f)+ for all the elements except for Co and [Fe_4S_4] cluster (SF4) which are calculated with LACVP** basis set. Using Gaussian 09 package,[12] frequency calculations were performed at the same level of theory as the optimizations to obtain zero-point energies (ZPE), which also further confirmed the nature of stationary points. The contributions of frozen atoms in vibrational analysis can be excluded in the Gaussian program to ensure that the fixation of atoms does not generate extra imaginary frequencies. Although the fixation of atoms may lead to inaccurate harmonic entropy effects, fortunately, in most enzymatic reactions especially without gas molecules participating, the entropy effects are not of such a magnitude that they will alter conclusions about the mechanism.[13,14] In the present work, the attempts to estimate entropy by excluding the contributions of frozen atoms to vibrational frequencies have been made. The energetics with this kind of entropy corrected (free energy profiles, given in Figures S4 and S5) are basically consistent with the ones without entropy (Figures 3 and 4) and do not change any conclusions about the mechanism. To explicate the effects of the ignored protein environment on the calculated energies, solvation effects were calculated at the same theory level as the optimizations by performing single-point calculations on the optimized structures using the self-consistent reaction field (SCRF) method with a Poisson-Boltzmann solver[15,16] as implemented in Jaguar 8.7. A standard dielectric constant (ε) of 4 was employed, which has been used in many previous studies modeling protein environment.[17-19]

Broken symmetry (BS)[20-24] method was used to correct the energies of the generation of 5'-dAdo$^{\bullet}$ involving the SF4 cluster (i.e., the step shown in Scheme 1.A.1). In the reduced $SF4^{1+}$ cluster, the four Fe atoms are supposed to consists of one high-spin ferric ion ($S(Fe^{III}) = 5/2$) and three high-spin ferrous ions ($S(Fe^{II}) = 2$). Only the highest spin state (HS) of S = 17/2 (HS_R in Table 1) with all the spins aligned parallelly is the pure spin state and can be approximated computationally. The

other spin states (BS states) are spin-contaminated and inaccurate by open-shell calculations. For example, a pure doublet-state reactant with a theoretical total spin ($< \boldsymbol{S^2} >_{\boldsymbol{p}}$) of 0.75 is calculated to have a total spin ($< \boldsymbol{S^2} >$) of 8.75 with the spin contamination. (shown in Table 1). The theoretical total spin of pure states ($< \boldsymbol{S^2} >_{\boldsymbol{p}}$) and the calculated total spin with the spin contamination ($< \boldsymbol{S^2} >$) of various spin states for the reactant (**React**), transition state (**TS1**) and intermediate (**Int1**) are given in Table 1. The corrected energy for the impure state can be estimated by the following formula, which is obtained from the broken symmetry (BS) theory proposed by L. Noodleman:

$$\Delta E_{HS-BS} = \frac{< S^2 >_p^{HS} - < S^2 >_p^{BS}}{< S^2 >^{HS} - < S^2 >^{BS}} \times \Delta E_{cal,HS-BS}$$

where $\Delta E_{cal,HS-BS}$ denotes the UDFT-calculated energy gap between the HS and BS states. Energies of all the possible antiferromagnetic couplings of HS states on the SF4 cluster are corrected with this theory and shown in Table S1.

Table S1. Calculated and corrected[a] energies (kcal/mol) for all spin states of stationary points in the S-C bond cleavage of SAM activated by $SF4^{1+}$ cluster (depicted in Scheme 1.A.1 in the paper).

complex	multiplicity	$< S^2 >_p$[b]	$< S^2 >$[c]	E_{cal}[d]	E_{cor}[e]
React[f]	II	0.75	8.75	0.0	-0.9
	VIII	15.75	20.75	3.9	3.5
	X	24.75	28.75	0.0	-0.6
	XVIII	80.75	80.75	7.9	7.9
TS1[g]	II	0.75	9.75	19.0	17.0
	VIII	15.75	21.75	22.7	21.5
	X	24.75	29.75	33.8	33.6
	XVIII	80.75	81.75	42.3	42.9
Int1[g]	II	0.75	9.73	10.7	9.3
	VIII	15.75	21.75	13.4	12.5
	X	24.75	29.75	16.6	16.0
	XVIII	80.75	81.75	24.1	24.1

[a]The Noodleman correction method is described above. [b]The theoretical total spin of a pure state. [c]The calculated total spin with the contamination. [d]The UDFT-calculated energy. [e]The energy corrected by the Noodleman correction method. [f]the doublet-state structure is shown in Figure 2A and the Cartesian coordinates of other spin-state structures are given below in the ESI. [g]the doublet-state structure is shown in Figure S1 and the Cartesian coordinates of other spin-state structures are given below in the ESI.

If not otherwise indicated, the energies reported in this paper have been corrected for ZPE, solvation, dispersion effects, and BS method for SF4-containing configurations, but not for entropy effects. Such a method of cluster modeling has been systematically benchmarked[17,25-29] and, despite still having some limitations,[17,30] successfully applied to a large number of metallo-enzymes especially Fe- and Cbl-containing enzymes in the past decades.[31-46]

The KIE_H (kinetic H-isotope effect) for the rate-limiting step via **TS2** was calculated by re-performing the frequency analysis using the structures of **TS2** and **Int1b** with the transferred hydrogen atom replaced by a deuterium atom. The new zero-point energies obtained were then used to update the corresponding barrier via **TS2** (ΔE_D). Using ΔE_D and the original barrier with hydrogen (ΔE_H), the KIE_H was predicted by the following formula (deduced from the Arrhenius equation):

$$KIE_H = \frac{k_H}{k_D} = \exp(-\frac{\Delta E_H - \Delta E_D}{RT})$$

2. Properties of three broken-symmetry states of the doublet-state React complex

Table S2. Spin densities and energies of three broken-symmetry states of the doublet-state **React** complex.

state	energy (kcal/mol)	spin density[a]			
		Fe1	Fe2	Fe3	Fe4
1	0.0	3.65	-3.60	3.67	-3.60
2	1.0	3.64	3.67	-3.60	-3.59
3	1.3	3.64	-3.60	-3.61	3.69

[a] The Fe coordinated by the SAM molecule is referred as Fe1, while the ones coordinated by Cys313, Cys318, and Cys321 as Fe2, Fe3, and Fe4, respectively.

3. Optimized structures of transition states and intermediates

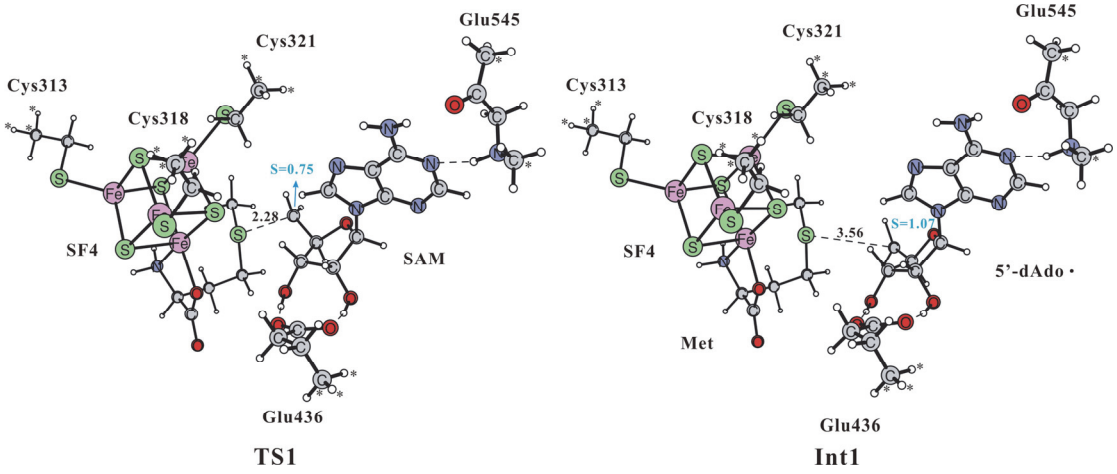

Figure S1. Optimized doublet-state structures of stationary points for the homolytic S-C cleavage of SAM in OxsB, including the transition state (**TS1**) and the resulting intermediate composed of a $SF4^{2+}$ cluster, a 5'-dAdo• radical, and a methionine (**Int1**). Some important distances are tagged in angstrom (Å). Asterisks indicate the atoms fixed to their X-ray crystal positions. The unpaired spin population is shown with an indication of "S".

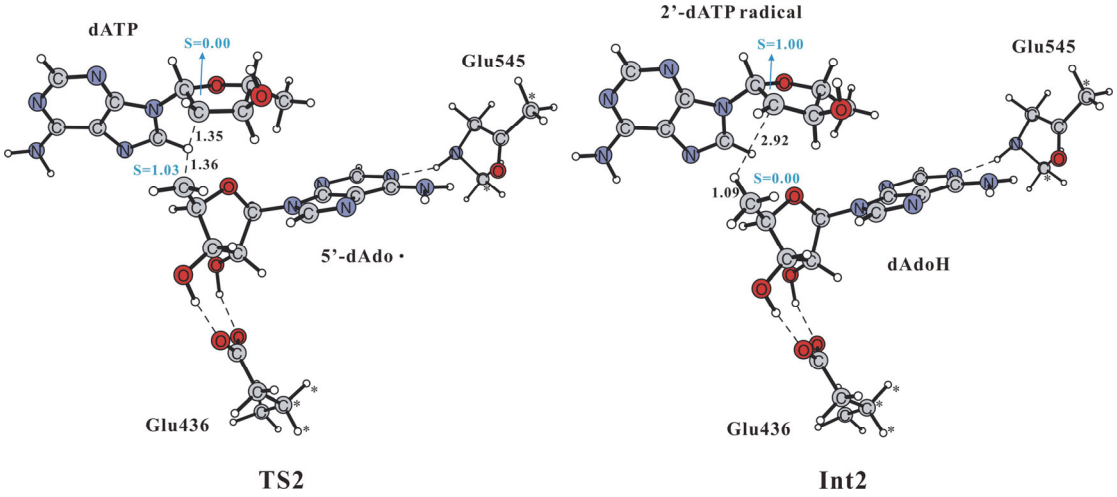

Figure S2. Optimized structures of stationary points for the H abstraction of dATP by 5'-dAdo• in OxsB, including the transition state (**TS2**) and the intermediate composed of a deoxyribose radical (2'-dATP radical) and a deoxyadenosine (dAdoH) (**Int2**).

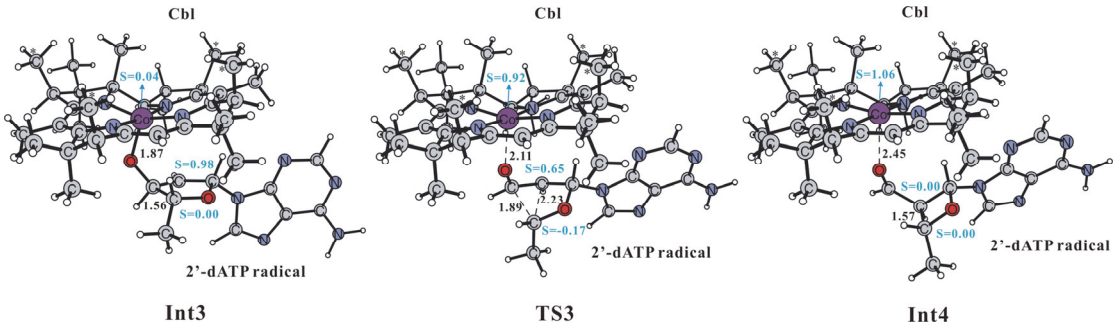

Figure S3. Optimized structures of stationary points for the Co^{III}Cbl-catalyzed ring contraction of 2'-dATP radical in OxsB, including the deprotonated 2'-dATP radical (**Int3**), the transition state (**TS3**), and the intermediate composed of an oxetane aldehyde and a Co^{II}Cbl (**Int4**).

4. The free energy profiles

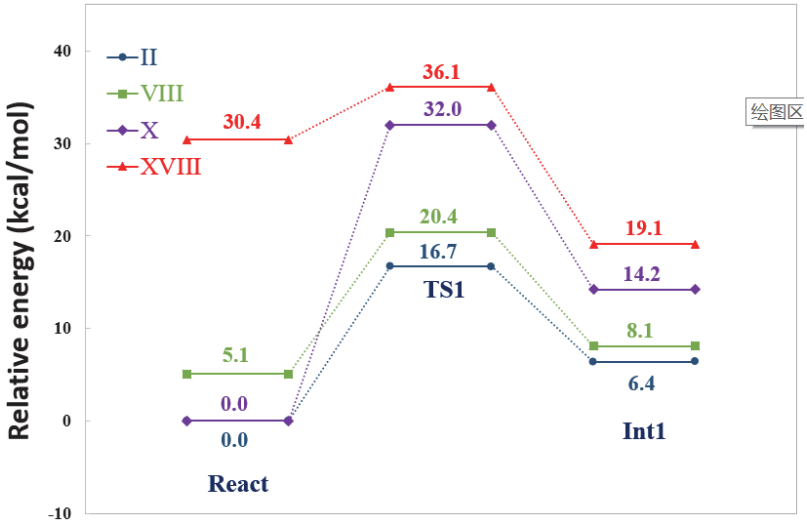

Figure S4. The free energy profile for the homolytic S-C cleavage of SAM in OxsB (shown in Scheme 1.A.1).

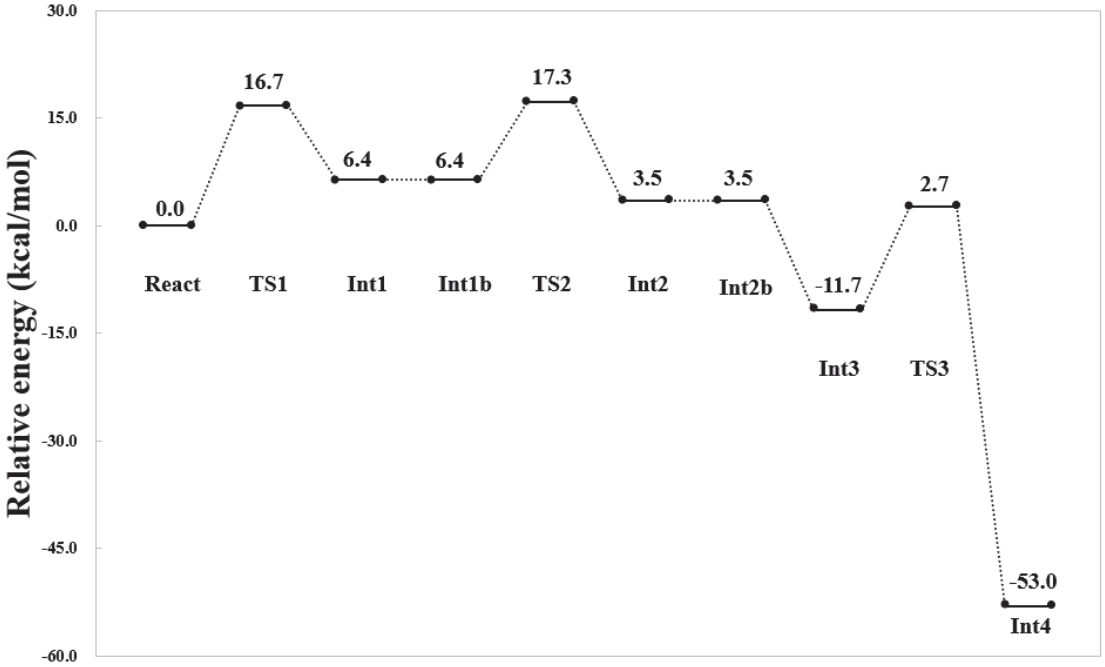

Figure S5. The free energy profile for the OxsB-catalyzed ring contraction of dATP.

5. Cartesian coordinates of optimized structures

The abbreviations used here are consistent with those in the text. All energies here are the absolute energies in hartree.

$React_{II}$

Energy with the medium-sized basis set: -5801.97733

Solution energy with the medium-sized basis set: -5802.33763

Energy with larger basis sets: -5802.86018

Zero-point energy: 0.74020

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6139585896	-35.5828134710	6.8104776669
C	-11.4646718532	-34.5940871230	7.2903341837
H	-11.2999003870	-34.5137879879	8.3697271761
H	-12.0526362952	-33.7226193041	6.9813161416
S	-12.4372838131	-36.1363241805	6.9543023561
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2221630162	-34.7239794043	7.3058790114
C	-19.7486163201	-34.7373826404	8.8885077442
H	-18.9049100889	-34.1317252380	9.2311295475
H	-20.4620058022	-34.7978301483	9.7182551845
S	-19.1515966567	-36.4528188599	8.5112192212
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1882672969	-30.1344164094	12.2093863745
C	-17.5898800801	-31.7616215412	10.9198848138
H	-18.0716150543	-32.5684510721	11.4796193675
H	-17.6385302186	-32.0430771368	9.8621037272
S	-15.7979221368	-31.7104239413	11.4114583779
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1258185604	-39.9374625918	15.8773942536
C	-23.0373923986	-39.4398523193	13.7928428893
H	-23.5159471843	-39.7659831322	12.8565295187
H	-23.4321013762	-38.4458770399	14.0325767393
C	-21.5233520695	-39.3327416771	13.5682604250
H	-21.0978893309	-40.3066448906	13.2957921614
H	-21.3104763728	-38.6707495308	12.7183323327
C	-20.7031607595	-38.7786651407	14.7556105502
O	-21.3395642591	-38.1020480393	15.6285874305
O	-19.4720233781	-39.0148853162	14.7299632274
N	-24.9094625552	-30.0606522919	18.5302372901
H	-24.5385015766	-30.6536565071	17.7829015138
C	-24.3991755365	-28.7374637374	18.2780915709

H	-24.6282963753	-28.0614431420	19.1174310104
C	-24.8603593197	-28.0757478371	16.9776822293
O	-25.3119619145	-28.7090969719	16.0391205565
Fe	-15.2176847436	-36.8989869589	11.4461299639
Fe	-16.9978519984	-36.0901754065	9.3202688453
Fe	-15.3630157346	-33.8783547518	10.5963332797
Fe	-14.1373293994	-36.0228526072	8.5683831865
S	-15.9108663122	-34.3378150448	8.2414348917
S	-13.4010980646	-35.2431660833	10.8368124440
S	-15.4832275983	-37.8970215756	9.2043861224
S	-17.1210949340	-35.3417754429	11.5381211135
N	-13.4144348363	-38.1933981843	12.0781706682
H	-12.5520790279	-37.6570631916	12.0803004761
H	-13.4488145871	-38.7473427024	11.2246240798
C	-13.7226354517	-38.9757073028	13.2730583031
H	-13.1953452858	-39.9394019785	13.2961145521
C	-15.2601364954	-39.2681656440	13.3083919277
O	-15.9784275473	-38.3641644813	12.7516536904
O	-15.6113415062	-40.2688165593	13.9383113948
C	-13.3578920028	-38.2387232708	14.5870782809
H	-13.2978297657	-39.0065973160	15.3663659989
H	-12.3581138107	-37.7857534366	14.5073153392
C	-14.3718491137	-37.2161192852	15.1403137094
H	-15.3729141030	-37.6543069391	15.2723532448
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H	-12.3317583731	-35.4406552534	13.6132759856
H	-12.9061096824	-34.6568099399	15.1551941094
C	-15.8278032119	-34.6568579135	14.7288359791
H	-15.2362355903	-33.8881406829	15.2329570759
H	-16.3159335443	-34.2267579889	13.8464384983
C	-16.8607026500	-35.2371707441	15.6979829574
H	-16.3719798015	-35.6500067163	16.5932832907
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C	-17.8358193554	-36.3052156284	15.1695494975
H	-17.8841478743	-36.2601144125	14.0717867392
O	-17.4074978758	-37.5601929252	15.6226342228
H	-18.1041538465	-38.2126273179	15.3310300925
C	-19.2227688765	-35.8708697720	15.7761102674
H	-19.9879188747	-35.9000842387	14.9892319090
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H	-19.3673320700	-30.5418266300	10.9979149600
H	-17.9102671400	-29.6574469000	10.5535050800
H	-19.6860130200	-34.0390303900	6.8556418600
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State 2 in Table S2

Energy with the medium-sized basis set:	-5801.97354
Solution energy with the medium-sized basis set:	-5802.86824
Energy with larger basis sets:	-5802.86824
Zero-point energy:	0.73987

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6125771583	-35.5800719287	6.8154172551

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H	-11.2222140314	-34.3559250728	8.3915988207
H	-12.0727282682	-33.7451524826	6.9712234917
S	-12.3859206600	-36.1523413734	7.2441742384
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2216201176	-34.7253171731	7.3080419062
C	-19.7458584189	-34.7390351342	8.8884851642
H	-18.8824924788	-34.1497957328	9.2136873551
H	-20.4526376435	-34.7654958636	9.7258190842
S	-19.1987584293	-36.4757091714	8.5297458323
C	-18.3150000000	-30.4390000000	11.1620000000
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H	-18.0575230443	-32.5670889785	11.4942141638
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S	-15.7948839928	-31.6733142033	11.4550237540
C	-23.3870000000	-40.4220000000	14.9300000000
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C	-13.2767301868	-38.1962644239	14.8352509839
H	-13.2587978004	-38.9986066644	15.5806814124
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H	-15.2610257475	-33.9311960702	15.4079478794
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H	-16.4034575322	-35.7350733931	16.7267105005
O	-17.6440466365	-34.1399917165	16.2345977799
C	-17.8603164728	-36.3371352853	15.2717548142
H	-17.9089525005	-36.2421490154	14.1768158712
O	-17.4288051742	-37.6093219493	15.6681638740
H	-18.1337758601	-38.2507843803	15.3664867374
C	-19.2448906382	-35.9238232238	15.8930919441
H	-20.0167665402	-35.9475292414	15.1128761274
O	-19.6283218998	-36.6975276776	16.9876294061
H	-20.2699325641	-37.3764598011	16.6072956505
C	-19.0147900464	-34.4733202482	16.3785963703
H	-19.3250128117	-34.4086782696	17.4254161913
N	-19.8019551183	-33.4641675765	15.6740391482
C	-19.7761563418	-33.1189394356	14.3317583602
H	-19.0744411327	-33.5781712926	13.6425648807
N	-20.6721207319	-32.2068062081	14.0114418821
C	-21.3252114464	-31.9448283106	15.2006753990
C	-22.4074591705	-31.1116024870	15.5334741299
N	-23.0117899805	-30.2980917692	14.6213331544
H	-23.9199019359	-29.9282960295	14.8689967358
H	-22.8132760182	-30.4913983777	13.6505848419
N	-22.8468675887	-31.1009301417	16.8095281196
C	-22.2176772229	-31.8783880718	17.7169494837
H	-22.6207968346	-31.8137263982	18.7274613435

N	-21.1955161174	-32.7038734421	17.5324402815
C	-20.7932766678	-32.7122122351	16.2481908047
C	-24.7296473400	-26.5691294600	16.9222566100
H	-23.7669727421	-26.2320605287	17.3239947653
H	-24.8450426656	-26.2269033160	15.8920006215
H	-25.5127561915	-26.1164056232	17.5442317518
C	-26.3586729200	-30.1235080600	18.6071865600
H	-26.8726939332	-29.7774878770	17.6946807713
H	-26.6565515385	-31.1629390914	18.7823946269
H	-26.7383744940	-29.5289489156	19.4519730077
H	-23.3095480774	-28.7629188690	18.2578097503
H	-24.4296321400	-40.6615236000	14.9511344400
H	-22.7325735700	-41.2640286700	14.8427431400
H	-9.4543576400	-33.8561806500	6.6796756600
H	-10.3106702900	-34.7224401900	5.4741079100
H	-19.3673320700	-30.5418266300	10.9979149600
H	-17.9102671400	-29.6574469000	10.5535050800
H	-19.6860130200	-34.0390303900	6.8556418600
H	-20.7882853400	-33.1267859900	7.8557695300

State 3 in Table S2

Energy with the medium-sized basis set: -5801.97290

Solution energy with the medium-sized basis set: -5802.33510

Energy with larger basis sets: -5802.86737

Zero-point energy: 0.73968

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6261711540	-35.5854853160	6.8218939745
C	-11.4504857679	-34.5432494629	7.3089369566
H	-11.2513507766	-34.3976517157	8.3761821057
H	-12.0296152919	-33.6786126073	6.9644349843
S	-12.4557688616	-36.0834991350	7.0994197916
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2244829209	-34.7192235324	7.3030254001
C	-19.7680691904	-34.7407748781	8.8989342582
H	-18.8848575269	-34.1749570102	9.2125380974
H	-20.4777358308	-34.7261363675	9.7343436931
S	-19.2836775408	-36.5027631866	8.5758750202
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1896510907	-30.1407820475	12.2109007479
C	-17.6183102403	-31.7827767694	10.9178550502

H	-18.1520638629	-32.5844201252	11.4378728975
H	-17.6258881255	-32.0385959549	9.8533693885
S	-15.8490649989	-31.8179660011	11.4896289042
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1243517324	-39.9432890877	15.8797414048
C	-23.0379633998	-39.4315933796	13.7998277583
H	-23.5304965282	-39.7413651089	12.8652266898
H	-23.4219796922	-38.4368640325	14.0544836130
C	-21.5262540656	-39.3358918374	13.5539913411
H	-21.1178194736	-40.3108223105	13.2588470519
H	-21.3192652337	-38.6654617222	12.7094608266
C	-20.6730268341	-38.8136320689	14.7329010860
O	-21.2861656193	-38.2012446030	15.6675643257
O	-19.4385674709	-39.0142912411	14.6400684791
N	-24.9106957691	-30.0117794849	18.6412241391
H	-24.4563680610	-30.6340663246	17.9641941055
C	-24.4204597137	-28.6858993747	18.3696819246
H	-24.7116733244	-27.9849046949	19.1692452668
C	-24.8237862688	-28.0755602478	17.0245433184
O	-25.2088638076	-28.7495794443	16.0842395505
Fe	-15.0910405723	-36.9724423604	11.5765827393
Fe	-17.1309423283	-36.3341484455	9.4391346913
Fe	-15.5045908577	-34.0303064610	10.6983213680
Fe	-14.0497119880	-35.8525953099	8.8049553481
S	-15.9417062696	-34.3245238931	8.4647934098
S	-13.4215966414	-35.0184698252	11.0269779243
S	-15.2580229597	-37.8943377089	9.4298308942
S	-17.0498336187	-35.4471510220	11.7529180920
N	-13.1915342615	-38.0039196025	12.3308448777
H	-12.3511863960	-37.4345793379	12.3806875230
H	-13.1637868408	-38.5081261591	11.4438245214
C	-13.4421985852	-38.9024862679	13.4604117196
H	-12.8130075099	-39.8022673345	13.4301877314
C	-14.9437133090	-39.3592200101	13.4487833075
O	-15.7493801232	-38.5161686783	12.9320547432
O	-15.1761963308	-40.4236572718	14.0344374626
C	-13.1925802691	-38.2216109907	14.8246035528
H	-13.1499686721	-39.0269730703	15.5659700120
H	-12.2133049187	-37.7186027780	14.8362600182
C	-14.2904210251	-37.2726753362	15.3442429161
H	-15.2711516535	-37.7658177018	15.4117203755
H	-14.0207939848	-36.8535233142	16.3196307878
S	-14.5932837259	-35.8882628764	14.1828237222
C	-13.0750925114	-34.9038370560	14.3348609565

H	-13.2579046609	-33.9890179312	13.7686416856
H	-12.2821407904	-35.4480007596	13.8247183765
H	-12.8463780308	-34.7175949077	15.3890314205
C	-15.7707796249	-34.7421699434	15.0044955410
H	-15.1802340790	-33.9989481326	15.5473005425
H	-16.2636599368	-34.2732578037	14.1452148624
C	-16.7932339551	-35.3835287725	15.9471209985
H	-16.2948731472	-35.8809689266	16.7912216582
O	-17.5275877063	-34.2495219512	16.4326738956
C	-17.7913397731	-36.3841146572	15.3392093221
H	-17.8436810179	-36.2475452617	14.2493255449
O	-17.3804296010	-37.6768000914	15.6843224691
H	-18.0778456904	-38.2929094741	15.3209118225
C	-19.1694774282	-35.9730182642	15.9814329940
H	-19.9361752508	-35.9264259432	15.1967563233
O	-19.5752712168	-36.8004538047	17.0256397805
H	-20.2148932160	-37.4590373476	16.6038446890
C	-18.9048762583	-34.5612411516	16.5572481615
H	-19.2173517911	-34.5573899265	17.6056666374
N	-19.6572219239	-33.4830960232	15.9158954366
C	-19.4987982378	-32.9582306939	14.6440039722
H	-18.7322443662	-33.3258635248	13.9713338839
N	-20.3627740740	-32.0039407524	14.3614148551
C	-21.1347345416	-31.9037065147	15.5018568574
C	-22.2452734945	-31.1088989894	15.8313448065
N	-22.7395473851	-30.1629894011	14.9793111672
H	-23.6896162909	-29.8567692383	15.1445797411
H	-22.4291494804	-30.2405273009	14.0211072413
N	-22.8194871694	-31.2690369238	17.0411763845
C	-22.2874971492	-32.1726682088	17.8921850972
H	-22.7931200418	-32.2437259381	18.8547081136
N	-21.2474044432	-32.9756309403	17.7052063851
C	-20.7103318590	-32.8129570692	16.4824783301
C	-24.7296473400	-26.5691294600	16.9222566100
H	-23.7933473824	-26.2024025799	17.3586534551
H	-24.8043570462	-26.2563874027	15.8791118378
H	-25.5494231375	-26.1166458197	17.4951387120
C	-26.3586729200	-30.1235080600	18.6071865600
H	-26.8263111738	-29.8365044190	17.6511756470
H	-26.6419097989	-31.1601892557	18.8183604924
H	-26.7998115928	-29.4978159074	19.3978489578
H	-23.3202654156	-28.7124659285	18.3632294858
H	-24.4296321400	-40.6615236000	14.9511344400
H	-22.7325735700	-41.2640286700	14.8427431400

H	-9.4543576400	-33.8561806500	6.6796756600
H	-10.3106702900	-34.7224401900	5.4741079100
H	-19.3673320700	-30.5418266300	10.9979149600
H	-17.9102671400	-29.6574469000	10.5535050800
H	-19.6860130200	-34.0390303900	6.8556418600
H	-20.7882853400	-33.1267859900	7.8557695300

React$_{VIII}$

Energy with the medium-sized basis set: -5801.97023

Solution energy with the medium-sized basis set: -5802.33056

Energy with larger basis sets: -5802.85362

Zero-point energy: 0.73979

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6020047652	-35.5779568597	6.8046234844
C	-11.4580827962	-34.6189124985	7.3014876805
H	-11.2846256009	-34.4841711223	8.3741562954
H	-12.0917689083	-33.7916278183	6.9634229320
S	-12.3536155211	-36.2246334195	7.0487344565
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2217257215	-34.7248579121	7.3068948486
C	-19.7394982156	-34.7413622068	8.8826669138
H	-18.8951338576	-34.1359492380	9.2249153591
H	-20.4473668826	-34.8112764357	9.7163819197
S	-19.1345103808	-36.4498346338	8.4872927128
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1888001644	-30.1316979391	12.2087660307
C	-17.5875717792	-31.7627422132	10.9258478227
H	-18.0702798948	-32.5687025951	11.4864191337
H	-17.6313316852	-32.0468071167	9.8685920993
S	-15.7978741193	-31.7045752826	11.4254564222
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1265985805	-39.9405828668	15.8793123153
C	-23.0307503704	-39.4365554819	13.7979903149
H	-23.5037584879	-39.7593791957	12.8577413629
H	-23.4264210893	-38.4430248253	14.0382082852
C	-21.5149989537	-39.3294391994	13.5818948988
H	-21.0883758611	-40.3043556514	13.3143074389
H	-21.2977755258	-38.6711241003	12.7302623294
C	-20.6973824853	-38.7708122101	14.7698130791
O	-21.3386441037	-38.1116521819	15.6522293515

O	-19.4623289413	-38.9853472665	14.7336825918
N	-24.9104086308	-30.0666171111	18.5131561803
H	-24.5541198111	-30.6521610385	17.7537123806
C	-24.4004945841	-28.7425951334	18.2643190196
H	-24.6223790135	-28.0717699875	19.1096617918
C	-24.8742569194	-28.0741603582	16.9725935522
O	-25.3471844268	-28.6994557062	16.0392885515
Fe	-15.1957178963	-37.0301871423	11.6047727941
Fe	-16.9831979607	-36.1154310759	9.3190451621
Fe	-15.3247513744	-33.8735508373	10.6222074228
Fe	-14.0825489857	-36.0240470741	8.6181784260
S	-15.8513395406	-34.3586142971	8.2630916114
S	-13.3857325123	-35.2750833992	10.9168017103
S	-15.4857865308	-37.8952786247	9.2790183579
S	-17.0901442822	-35.3874423865	11.5354237398
N	-13.3282611915	-38.2156447660	12.2163520570
H	-12.5147718967	-37.6074346188	12.1968722586
H	-13.3068590129	-38.8139650527	11.3939720830
C	-13.6007153889	-38.9487746165	13.4511931885
H	-13.0226051023	-39.8801040417	13.5258391312
C	-15.1188664049	-39.3241934697	13.4981975792
O	-15.8851843331	-38.4892314325	12.8949580383
O	-15.4215550435	-40.3115469946	14.1711442177
C	-13.2834593631	-38.1316109228	14.7307491661
H	-13.2000288383	-38.8599660323	15.5449750035
H	-12.3019611738	-37.6434268683	14.6382980920
C	-14.3423942142	-37.1256533780	15.2301833320
H	-15.3336630068	-37.5879026235	15.3509572773
H	-14.0337101285	-36.6713335035	16.1778321002
S	-14.6287984058	-35.7907707095	14.0095639761
C	-13.1252373804	-34.7834403950	14.1497201646
H	-13.3087117374	-33.9012093288	13.5336023832
H	-12.3169526007	-35.3414675574	13.6798208466
H	-12.9322148274	-34.5424572322	15.2005187716
C	-15.8497830017	-34.6123766478	14.7147473463
H	-15.2848549689	-33.8150611746	15.2042319235
H	-16.3302399806	-34.2218175836	13.8094145270
C	-16.8879535014	-35.1851208907	15.6822863153
H	-16.4079186966	-35.5692924562	16.5952416964
O	-17.6726699997	-34.0266776531	15.9979456723
C	-17.8414708394	-36.2770277534	15.1641878379
H	-17.8851804656	-36.2448836998	14.0657037242
O	-17.3963842947	-37.5203858568	15.6333996389
H	-18.0842637790	-38.1827370021	15.3472335618

C	-19.2380408028	-35.8576177357	15.7571357424
H	-19.9999106637	-35.9179042092	14.9690929446
O	-19.6249287090	-36.5929979916	16.8757679803
H	-20.2649503224	-37.2893526627	16.5249874493
C	-19.0291909986	-34.3885115778	16.1947033740
H	-19.3087593213	-34.3039144581	17.2488466931
N	-19.8623606572	-33.4195199638	15.4900766606
C	-19.9267428071	-33.1534258012	14.1315799249
H	-19.2622139463	-33.6453895818	13.4283106497
N	-20.8516654042	-32.2684082462	13.8174654596
C	-21.4300712534	-31.9416825099	15.0291745120
C	-22.4972207289	-31.0978453428	15.3837523157
N	-23.1692969845	-30.3415964310	14.4702421685
H	-24.0563734679	-29.9527804822	14.7602611845
H	-23.0348339695	-30.5838071939	13.4999824293
N	-22.8535508710	-31.0162186341	16.6824183690
C	-22.1606089340	-31.7371582889	17.5893419620
H	-22.5021173625	-31.6216283451	18.6175855115
N	-21.1432364132	-32.5644343468	17.3867788913
C	-20.8236185256	-32.6431011294	16.0823792043
C	-24.7296473400	-26.5691294600	16.9222566100
H	-23.7454087031	-26.2566788539	17.2901107800
H	-24.8791081001	-26.2075762688	15.9030464843
H	-25.4784376206	-26.1123861066	17.5823107966
C	-26.3586729200	-30.1235080600	18.6071865600
H	-26.8980299000	-29.7475268728	17.7219442579
H	-26.6670150927	-31.1620301467	18.7686110624
H	-26.6981160582	-29.5438280432	19.4784754020
H	-23.3055838439	-28.7972117355	18.1799468132
H	-24.4296321400	-40.6615236000	14.9511344400
H	-22.7325735700	-41.2640286700	14.8427431400
H	-9.4543576400	-33.8561806500	6.6796756600
H	-10.3106702900	-34.7224401900	5.4741079100
H	-19.3673320700	-30.5418266300	10.9979149600
H	-17.9102671400	-29.6574469000	10.5535050800
H	-19.6860130200	-34.0390303900	6.8556418600
H	-20.7882853400	-33.1267859900	7.8557695300

React$_X$

Energy with the medium-sized basis set:	-5801.97582
Solution energy with the medium-sized basis set:	-5802.33776
Energy with larger basis sets:	-5802.85861

Zero-point energy: 0.74021

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6173819849	-35.5839237814	6.8132382152
C	-11.4607001586	-34.5801227150	7.2958302848
H	-11.2854495717	-34.4848477862	8.3726980418
H	-12.0436245188	-33.7074051323	6.9798594780
S	-12.4507010885	-36.1178453157	6.9926259615
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2202936463	-34.7292370508	7.3116073136
C	-19.7383702534	-34.7271842282	8.8900710678
H	-18.8998188552	-34.1110013637	9.2265622942
H	-20.4486826435	-34.7898506997	9.7222301930
S	-19.1219773481	-36.4379195921	8.5214666555
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1872217848	-30.1339978055	12.2091537935
C	-17.5844055162	-31.7587281846	10.9186928482
H	-18.0526176677	-32.5666076368	11.4881328241
H	-17.6424514904	-32.0441520701	9.8625458594
S	-15.7870238819	-31.6879884114	11.3871319515
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1258188318	-39.9398725054	15.8785338551
C	-23.0330938462	-39.4379261931	13.7960806187
H	-23.5127431987	-39.7583259532	12.8583942813
H	-23.4233395550	-38.4428505785	14.0387716564
C	-21.5183780321	-39.3380485847	13.5716988451
H	-21.0994062045	-40.3129983278	13.2925602205
H	-21.3014906658	-38.6725999522	12.7255597432
C	-20.6924766580	-38.7972117534	14.7614226672
O	-21.3254790903	-38.1401885272	15.6514409029
O	-19.4597166057	-39.0236825864	14.7205218029
N	-24.9100818910	-30.0659948718	18.5171899469
H	-24.5484837184	-30.6555463702	17.7626044402
C	-24.3971069766	-28.7432113378	18.2675771452
H	-24.6205592855	-28.0697687328	19.1104941958
C	-24.8628692449	-28.0758904013	16.9715774899
O	-25.3203381690	-28.7047298001	16.0330034168
Fe	-15.2277681118	-36.9522895588	11.5022951372
Fe	-16.9749015049	-36.0729604387	9.3595131038
Fe	-15.3371695386	-33.8763771194	10.5688197881
Fe	-14.1293169452	-35.9182512974	8.6081834136
S	-15.9006191284	-34.3062970213	8.2270389923
S	-13.3966373816	-35.1918027451	10.8654811473
S	-15.4474957972	-37.8582410036	9.2351194609
S	-17.1172956560	-35.3426715376	11.5795903662

N	-13.3549873845	-38.1329833745	12.1250847416
H	-12.5187247542	-37.5567807646	12.1274884237
H	-13.3548054457	-38.6933639618	11.2747771057
C	-13.6287998112	-38.9231438770	13.3248988945
H	-13.0539460276	-39.8588739067	13.3535648837
C	-15.1488453010	-39.2934918198	13.3593439049
O	-15.9122959194	-38.4348023891	12.7890666776
O	-15.4519266806	-40.3025230143	13.9995505207
C	-13.3053598431	-38.1649643882	14.6372348264
H	-13.2297345364	-38.9267324066	15.4210197476
H	-12.3197185903	-37.6808209964	14.5666815657
C	-14.3583450945	-37.1719894263	15.1714855455
H	-15.3492228997	-37.6365887175	15.2876366101
H	-14.0429419277	-36.7420290087	16.1283337824
S	-14.6542692583	-35.8062282618	13.9882405859
C	-13.1434038903	-34.8111440326	14.1324949348
H	-13.3293430301	-33.9106400436	13.5437515617
H	-12.3421200213	-35.3608104399	13.6407735667
H	-12.9337039610	-34.5981068093	15.1858583958
C	-15.8546892827	-34.6390219096	14.7445086399
H	-15.2761394088	-33.8601855077	15.2482869178
H	-16.3461122721	-34.2225295002	13.8570881325
C	-16.8805049412	-35.2338081054	15.7124652314
H	-16.3877947008	-35.6445537515	16.6065249357
O	-17.6552000290	-34.0819293295	16.0751118901
C	-17.8433148365	-36.3089370014	15.1776046281
H	-17.8948819513	-36.2532751784	14.0805484338
O	-17.3992013746	-37.5636366009	15.6174363400
H	-18.0925420209	-38.2189616664	15.3254249037
C	-19.2327781777	-35.8954243701	15.7893437799
H	-20.0027727162	-35.9424497877	15.0084698414
O	-19.6092316642	-36.6484725367	16.9002343707
H	-20.2511210778	-37.3388882964	16.5409491073
C	-19.0177839040	-34.4338427662	16.2469647693
H	-19.3111690030	-34.3587567975	17.2978957451
N	-19.8337848319	-33.4486119149	15.5426934719
C	-19.8544303033	-33.1398203751	14.1915206803
H	-19.1691418219	-33.6111437115	13.4934565351
N	-20.7701572640	-32.2455502748	13.8758870671
C	-21.3863064786	-31.9559241557	15.0783077468
C	-22.4634389745	-31.1214810218	15.4248363875
N	-23.1033395692	-30.3341566125	14.5140848589
H	-24.0008863115	-29.9559216223	14.7854018729
H	-22.9367386310	-30.5465699803	13.5416734285

N	-22.8626082175	-31.0809182983	16.7131499518
C	-22.1992504425	-31.8307362098	17.6190489059
H	-22.5723278107	-31.7450450729	18.6392479443
N	-21.1760674143	-32.6524778942	17.4232355175
C	-20.8140813339	-32.6906704477	16.1279201806
C	-24.7296473400	-26.5691294600	16.9222566100
H	-23.7524075319	-26.2487181751	17.3017301894
H	-24.8699674195	-26.2095699356	15.9010691255
H	-25.4899682029	-26.1182713201	17.5731199542
C	-26.3586729200	-30.1235080600	18.6071865600
H	-26.8957000751	-29.7506796537	17.7189812181
H	-26.6668366405	-31.1618415959	18.7705482347
H	-26.7016104409	-29.5412569051	19.4755688105
H	-23.3017093805	-28.8007049594	18.1887213241
H	-24.4296321400	-40.6615236000	14.9511344400
H	-22.7325735700	-41.2640286700	14.8427431400
H	-9.4543576400	-33.8561806500	6.6796756600
H	-10.3106702900	-34.7224401900	5.4741079100
H	-19.3673320700	-30.5418266300	10.9979149600
H	-17.9102671400	-29.6574469000	10.5535050800
H	-19.6860130200	-34.0390303900	6.8556418600
H	-20.7882853400	-33.1267859900	7.8557695300

$\mathbf{React_{XVIII}}$

Energy with the medium-sized basis set: -5801.96203

Solution energy with the medium-sized basis set: -5802.32477

Energy with larger basis sets: -5802.84469

Zero-point energy: 0.73970

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6145434398	-35.5818010749	6.8137344751
C	-11.4516558021	-34.5761422580	7.3108321309
H	-11.2576854048	-34.4275715577	8.3784406576
H	-12.0595810019	-33.7317858777	6.9671550809
S	-12.4001592993	-36.1499763548	7.0911827604
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2271802718	-34.7131751869	7.2980057658
C	-19.7837300956	-34.7474387085	8.9017391930
H	-18.8862734835	-34.2026491363	9.2109747927
H	-20.4914455850	-34.7066069214	9.7378935421
S	-19.3477960555	-36.5233797156	8.5952083716
C	-18.3150000000	-30.4390000000	11.1620000000

H	-18.1707884037	-30.1581247048	12.2128013512
C	-17.6353725155	-31.7819297969	10.8733462450
H	-18.1284277694	-32.5802722360	11.4357702819
H	-17.7313046789	-32.0380399364	9.8128019953
S	-15.8273244786	-31.8205569209	11.2994806814
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1284484576	-39.9460231982	15.8825722982
C	-23.0250202080	-39.4303269651	13.8060177523
H	-23.4955800878	-39.7431073445	12.8614525671
H	-23.4172152272	-38.4369425803	14.0525196514
C	-21.5077979003	-39.3303613008	13.5967369493
H	-21.0888821234	-40.3020288200	13.3065794603
H	-21.2817130524	-38.6527929807	12.7627495124
C	-20.6915027570	-38.8109064033	14.8017567940
O	-21.3271186095	-38.1588965077	15.6933413017
O	-19.4594785842	-39.0474923901	14.7722213178
N	-24.9085512041	-30.0551657005	18.5442428458
H	-24.5258880428	-30.6543492445	17.8081246145
C	-24.3998030098	-28.7318526719	18.2888424755
H	-24.6380307915	-28.0522844194	19.1227998359
C	-24.8515508500	-28.0770598139	16.9813441953
O	-25.2902817480	-28.7160774107	16.0406967765
Fe	-15.2505378928	-37.0235722315	11.6407667153
Fe	-17.1501085757	-36.3588055810	9.4026899039
Fe	-15.5855097535	-34.0593703423	10.5224632803
Fe	-14.1352769142	-35.9989336497	8.6945950851
S	-15.9982666124	-34.3966988683	8.2805253421
S	-13.5381694750	-35.1334830728	10.9795028750
S	-15.3689097524	-37.9696321543	9.3335774635
S	-17.1739233493	-35.3827611787	11.6750075974
N	-13.3349876620	-38.1498279439	12.2195049208
H	-12.4916595975	-37.5843326017	12.2319090872
H	-13.3500370867	-38.6801217536	11.3486980136
C	-13.5930539781	-38.9816354237	13.3953007838
H	-12.9916356603	-39.9009336074	13.4038815841
C	-15.1013092445	-39.3984481078	13.4164622355
O	-15.8928995648	-38.5509624256	12.8667135788
O	-15.3739410974	-40.4303915699	14.0326288316
C	-13.3038637622	-38.2490144406	14.7288687900
H	-13.2499085087	-39.0264998842	15.4988624191
H	-12.3164757845	-37.7645332377	14.6933077128
C	-14.3698782208	-37.2638666047	15.2523894228
H	-15.3629368909	-37.7280687400	15.3488419916
H	-14.0723507043	-36.8404044818	16.2176069478

S	-14.6462205909	-35.8877631199	14.0747451498
C	-13.1181808284	-34.9206896788	14.2352991324
H	-13.2775781972	-34.0185509225	13.6425731655
H	-12.3216344654	-35.4881727411	13.7570029587
H	-12.9158229691	-34.7142403943	15.2913971774
C	-15.8390975338	-34.7087700945	14.8253858802
H	-15.2557859968	-33.9284076385	15.3212404652
H	-16.3337960306	-34.3043261170	13.9333736552
C	-16.8661242994	-35.2938784134	15.7987371617
H	-16.3746137329	-35.7077787177	16.6920198256
O	-17.6318548894	-34.1362599976	16.1619699152
C	-17.8373187509	-36.3612687559	15.2633971364
H	-17.8865878333	-36.3046593747	14.1666190665
O	-17.4069504495	-37.6207732922	15.7032802838
H	-18.1091398385	-38.2666306796	15.4062662247
C	-19.2255584627	-35.9349446141	15.8685500361
H	-19.9904376076	-35.9727820023	15.0822879131
O	-19.6178326612	-36.6875831756	16.9741722609
H	-20.2604686469	-37.3722572826	16.6044963012
C	-18.9989817808	-34.4762812270	16.3294349254
H	-19.2936315910	-34.3991629463	17.3798268377
N	-19.8057608795	-33.4850313863	15.6232695035
C	-19.8376282336	-33.1961509639	14.2674404408
H	-19.1643265123	-33.6847484606	13.5686843729
N	-20.7485674850	-32.2983030795	13.9488438126
C	-21.3512120212	-31.9866531006	15.1526042746
C	-22.4214537936	-31.1415298180	15.4954436814
N	-23.0663308128	-30.3672826529	14.5773577187
H	-23.9615581241	-29.9836603774	14.8493058065
H	-22.9103840877	-30.5996352974	13.6076866132
N	-22.8088192642	-31.0780546230	16.7866435111
C	-22.1423995320	-31.8195516104	17.6969744966
H	-22.5066750742	-31.7180237542	18.7189031327
N	-21.1261258675	-32.6511252104	17.5046400111
C	-20.7747440854	-32.7105930063	16.2071347022
C	-24.7296473400	-26.5691294600	16.9222566100
H	-23.7605867676	-26.2380498339	17.3133593091
H	-24.8579551737	-26.2188835395	15.8963117973
H	-25.5028264622	-26.1194277630	17.5585098422
C	-26.3586729200	-30.1235080600	18.6071865600
H	-26.8811050003	-29.7681968963	17.7033298426
H	-26.6613641704	-31.1618112111	18.7801897576
H	-26.7225254448	-29.5311771122	19.4599981370
H	-23.3031963449	-28.7846625815	18.2249141800

H	-24.4296321400	-40.6615236000	14.9511344400
H	-22.7325735700	-41.2640286700	14.8427431400
H	-9.4543576400	-33.8561806500	6.6796756600
H	-10.3106702900	-34.7224401900	5.4741079100
H	-19.3673320700	-30.5418266300	10.9979149600
H	-17.9102671400	-29.6574469000	10.5535050800
H	-19.6860130200	-34.0390303900	6.8556418600
H	-20.7882853400	-33.1267859900	7.8557695300

$TS1_{II}$

Energy with the medium-sized basis set: -5801.94197

Solution energy with the medium-sized basis set: -5802.30247

Energy with larger basis sets: -5802.82595

Zero-point energy: 0.73643

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6404920000	-35.5903300000	6.8286740000
C	-11.4747620000	-34.5311660000	7.2665350000
H	-11.3309160000	-34.4947550000	8.3509680000
H	-11.9878010000	-33.6088130000	6.9717790000
S	-12.5489220000	-35.9830140000	6.8590390000
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2268920000	-34.7082630000	7.2892730000
C	-19.7937650000	-34.7615090000	8.8958440000
H	-18.9416190000	-34.1856400000	9.2645410000
H	-20.5282950000	-34.8072300000	9.7072240000
S	-19.2512950000	-36.4974090000	8.5202600000
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1780980000	-30.1459080000	12.2101960000
C	-17.6130470000	-31.7741040000	10.9000330000
H	-18.0818420000	-32.5689830000	11.4875690000
H	-17.7110870000	-32.0568110000	9.8461310000
S	-15.8007330000	-31.7473940000	11.3174870000
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1173390000	-39.9482050000	15.8790380000
C	-23.0512760000	-39.4265020000	13.8018840000
H	-23.5823410000	-39.7143450000	12.8813680000
H	-23.4124820000	-38.4287760000	14.0790720000
C	-21.5510680000	-39.3524450000	13.4945040000
H	-21.1773520000	-40.3349410000	13.1767840000
H	-21.3672800000	-38.6867120000	12.6422290000
C	-20.6218910000	-38.8612590000	14.6291810000

O	-21.1648600000	-38.4294220000	15.6970710000
O	-19.3973750000	-38.9163550000	14.3684540000
N	-24.9080690000	-30.0366770000	18.5920420000
H	-24.4823790000	-30.6573140000	17.8983670000
C	-24.4006110000	-28.7151260000	18.3274450000
H	-24.6656680000	-28.0225240000	19.1421920000
C	-24.8134040000	-28.0813900000	16.9952490000
O	-25.1913870000	-28.7428420000	16.0436220000
Fe	-15.1311670000	-36.9803710000	11.3617820000
Fe	-17.0872840000	-36.1552320000	9.2425930000
Fe	-15.5175640000	-33.9259650000	10.4668750000
Fe	-14.2633270000	-35.8922110000	8.4525110000
S	-16.1243250000	-34.3042120000	8.1667480000
S	-13.5014530000	-35.1131600000	10.6952620000
S	-15.4761920000	-37.8325090000	9.0275020000
S	-17.1032690000	-35.4442880000	11.4579410000
N	-13.2070620000	-38.1421890000	11.6682530000
H	-12.4110400000	-37.5126640000	11.6976860000
H	-13.1986700000	-38.6328570000	10.7771300000
C	-13.3684700000	-39.0429100000	12.8092620000
H	-12.7337500000	-39.9361140000	12.7300970000
C	-14.8542280000	-39.5171900000	12.8712190000
O	-15.6983420000	-38.6646520000	12.4156610000
O	-15.0692440000	-40.6024830000	13.4178000000
C	-13.0267990000	-38.3587020000	14.1554670000
H	-12.8121190000	-39.1640610000	14.8683240000
H	-12.1024290000	-37.7720670000	14.0519210000
C	-14.1227620000	-37.5112870000	14.8254630000
H	-15.0572370000	-38.0658830000	14.9532350000
H	-13.7855310000	-37.1714750000	15.8119490000
S	-14.6586750000	-36.0344830000	13.8910940000
C	-13.1735590000	-34.9882330000	13.9710310000
H	-13.4455050000	-34.0454850000	13.4940010000
H	-12.3782230000	-35.4373720000	13.3791710000
H	-12.8753570000	-34.8396450000	15.0140760000
C	-15.7287990000	-34.7204160000	15.4098990000
H	-14.9046420000	-34.3402840000	16.0133590000
H	-16.0831830000	-34.0088780000	14.6643310000
C	-16.8188540000	-35.4328010000	16.1501660000
H	-16.4182180000	-36.0614410000	16.9562890000
O	-17.6571090000	-34.3935020000	16.7393550000
C	-17.7550920000	-36.3131940000	15.3064470000
H	-17.8328440000	-35.8884100000	14.2901310000
O	-17.2584580000	-37.6166900000	15.2829270000

H	-17.9894070000	-38.1993110000	14.9370120000
C	-19.1321210000	-36.1558420000	16.0239900000
H	-19.9508110000	-36.1857570000	15.2951780000
O	-19.3429200000	-37.0971360000	17.0356640000
H	-19.9942100000	-37.7472090000	16.6324010000
C	-19.0217720000	-34.7564820000	16.6654840000
H	-19.4691670000	-34.7837500000	17.6621550000
N	-19.7605480000	-33.7087330000	15.9438270000
C	-19.6691520000	-33.3381610000	14.6130940000
H	-18.9673510000	-33.8157070000	13.9387680000
N	-20.5082810000	-32.3789890000	14.2736030000
C	-21.1898080000	-32.1041160000	15.4423690000
C	-22.2437080000	-31.2243220000	15.7458850000
N	-22.7737130000	-30.3701020000	14.8221100000
H	-23.6851820000	-29.9837870000	15.0295290000
H	-22.5466510000	-30.5663660000	13.8582230000
N	-22.7314280000	-31.2066560000	17.0040260000
C	-22.1774040000	-32.0312110000	17.9194240000
H	-22.6144200000	-31.9607940000	18.9148180000
N	-21.1928060000	-32.9069610000	17.7594180000
C	-20.7354290000	-32.9165100000	16.4935210000
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.7800380000	-26.2106350000	17.3357950000
H	-24.8386930000	-26.2346940000	15.8891290000
H	-25.5302990000	-26.1331280000	17.5330680000
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.8539510000	-29.7931140000	17.6788350000
H	-26.6533080000	-31.1618740000	18.7912420000
H	-26.7587680000	-29.5189650000	19.4346690000
H	-23.3021410000	-28.7655420000	18.2987600000
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

TS1$_{VIII}$

Energy with the medium-sized basis set: -5801.94811

Solution energy with the medium-sized basis set: -5802.29653

Energy with larger basis sets: -5802.83247

Zero-point energy: 0.73678

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6332060000	-35.5885410000	6.8228010000
C	-11.4829050000	-34.5610280000	7.2539500000
H	-11.3568830000	-34.5492420000	8.3411300000
H	-12.0078750000	-33.6415430000	6.9721770000
S	-12.5273120000	-36.0229890000	6.7918710000
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2236620000	-34.7189270000	7.3018750000
C	-19.7655590000	-34.7433300000	8.8938120000
H	-18.9143490000	-34.1516790000	9.2404040000
H	-20.4849200000	-34.7921950000	9.7185620000
S	-19.1982460000	-36.4719500000	8.5273360000
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1823090000	-30.1398290000	12.2092700000
C	-17.6017120000	-31.7692280000	10.9134740000
H	-18.0760900000	-32.5646510000	11.4960810000
H	-17.6799250000	-32.0533290000	9.8581990000
S	-15.7975550000	-31.7161580000	11.3688370000
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1199520000	-39.9521970000	15.8817080000
C	-23.0506360000	-39.4192850000	13.8096060000
H	-23.5681860000	-39.7079370000	12.8817710000
H	-23.4255840000	-38.4267620000	14.0875150000
C	-21.5478870000	-39.3291240000	13.5207220000
H	-21.1629700000	-40.3037000000	13.1925490000
H	-21.3582090000	-38.6487260000	12.6814500000
C	-20.6372700000	-38.8516140000	14.6750900000
O	-21.1951780000	-38.4364850000	15.7413280000
O	-19.4087010000	-38.9023450000	14.4306310000
N	-24.9116520000	-30.0032220000	18.6608300000
H	-24.4387230000	-30.6318060000	18.0047840000
C	-24.4205810000	-28.6776900000	18.3876240000
H	-24.7319060000	-27.9723390000	19.1749060000
C	-24.7911720000	-28.0799560000	17.0266860000
O	-25.1217670000	-28.7679380000	16.0761420000
Fe	-15.1809680000	-36.9776260000	11.4945010000
Fe	-17.0328540000	-36.1360510000	9.2508690000
Fe	-15.4274580000	-33.8606040000	10.4908360000
Fe	-14.1894070000	-35.9448500000	8.4299780000
S	-16.0376340000	-34.3176480000	8.1835400000
S	-13.4596360000	-35.2362600000	10.6979090000

S	-15.4924270000	-37.8555850000	9.1099620000
S	-17.0423300000	-35.4911900000	11.5038600000
N	-13.2541910000	-38.1135270000	11.7850880000
H	-12.4696400000	-37.4686950000	11.8048520000
H	-13.2541780000	-38.5869340000	10.8837170000
C	-13.3837310000	-39.0297830000	12.9136390000
H	-12.7313520000	-39.9083840000	12.8192580000
C	-14.8591380000	-39.5279420000	12.9727720000
O	-15.7100170000	-38.6893690000	12.4970410000
O	-15.0702590000	-40.6096560000	13.5242940000
C	-13.0440390000	-38.3331820000	14.2517250000
H	-12.7590600000	-39.1224340000	14.9579450000
H	-12.1599070000	-37.6927370000	14.1219860000
C	-14.1652600000	-37.5568140000	14.9576120000
H	-15.0519880000	-38.1749380000	15.1241790000
H	-13.8081980000	-37.2002520000	15.9297170000
S	-14.8704020000	-36.1004090000	14.0958860000
C	-13.4450270000	-34.9728230000	13.9970570000
H	-13.8298440000	-34.0467900000	13.5645200000
H	-12.7132680000	-35.3698960000	13.2960070000
H	-13.0247690000	-34.8032690000	14.9928180000
C	-15.5938890000	-34.9967140000	15.9358960000
H	-14.7132790000	-34.9757850000	16.5793600000
H	-15.7750900000	-34.0452930000	15.4363250000
C	-16.8401540000	-35.5947310000	16.5190160000
H	-16.6056970000	-36.2847580000	17.3414050000
O	-17.6541980000	-34.4995150000	17.0245380000
C	-17.7561930000	-36.3686640000	15.5560700000
H	-17.7671560000	-35.8538060000	14.5776190000
O	-17.2993530000	-37.6794320000	15.4471210000
H	-18.0433790000	-38.2238110000	15.0606670000
C	-19.1533340000	-36.2036320000	16.2208060000
H	-19.9462610000	-36.1906380000	15.4633670000
O	-19.4206250000	-37.1706410000	17.1946030000
H	-20.0600580000	-37.7999920000	16.7414620000
C	-19.0273290000	-34.8256140000	16.9094020000
H	-19.5058810000	-34.8708370000	17.8913980000
N	-19.7137030000	-33.7413130000	16.1947710000
C	-19.5659010000	-33.3448590000	14.8764920000
H	-18.8432980000	-33.8168810000	14.2218410000
N	-20.3799300000	-32.3699650000	14.5237070000
C	-21.1040070000	-32.1113430000	15.6698450000
C	-22.1633870000	-31.2293660000	15.9444150000
N	-22.6492650000	-30.3591390000	15.0117410000

H	-23.5716120000	-29.9792540000	15.1798220000
H	-22.3790140000	-30.5443070000	14.0565920000
N	-22.7004530000	-31.2291670000	17.1823390000
C	-22.1908350000	-32.0747970000	18.1042370000
H	-22.6653950000	-32.0162390000	19.0830820000
N	-21.2095640000	-32.9584960000	17.9680870000
C	-20.7011020000	-32.9490290000	16.7218460000
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.8021560000	-26.1850820000	17.3622880000
H	-24.8054470000	-26.2598660000	15.8783980000
H	-25.5594760000	-26.1331450000	17.4928060000
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.8145910000	-29.8324240000	17.6463460000
H	-26.6388780000	-31.1627950000	18.8079830000
H	-26.8131460000	-29.5048790000	19.3954350000
H	-23.3208970000	-28.7049020000	18.4053940000
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

$TS1_X$

Energy with the medium-sized basis set: -5801.93492

Solution energy with the medium-sized basis set: -5802.27275

Energy with larger basis sets: -5802.82463

Zero-point energy: 0.73611

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6348880000	-35.5883510000	6.8264750000
C	-11.4681130000	-34.5374800000	7.2791420000
H	-11.3082060000	-34.4617590000	8.3595310000
H	-12.0075430000	-33.6373290000	6.9634940000
S	-12.5241050000	-36.0257580000	6.9514080000
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2201760000	-34.7270060000	7.3089360000
C	-19.7459840000	-34.7317230000	8.8905600000
H	-18.9145310000	-34.1140200000	9.2410600000
H	-20.4621560000	-34.8076360000	9.7158030000

S	-19.1225180000	-36.4366380000	8.5063780000
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1825640000	-30.1393190000	12.2092030000
C	-17.5926800000	-31.7637100000	10.9111530000
H	-18.0532050000	-32.5648970000	11.4966520000
H	-17.6705480000	-32.0514060000	9.8571890000
S	-15.7887790000	-31.6875300000	11.3507040000
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1184740000	-39.9490380000	15.8796830000
C	-23.0493110000	-39.4262450000	13.8030220000
H	-23.5797610000	-39.7112370000	12.8813910000
H	-23.4071390000	-38.4277380000	14.0813310000
C	-21.5481530000	-39.3583240000	13.5001320000
H	-21.1794310000	-40.3381610000	13.1693560000
H	-21.3564110000	-38.6803260000	12.6592090000
C	-20.6236870000	-38.8901370000	14.6470790000
O	-21.1710410000	-38.4378190000	15.7034430000
O	-19.3962960000	-38.9814380000	14.4069510000
N	-24.9081190000	-30.0342530000	18.5988940000
H	-24.4760090000	-30.6597970000	17.9130580000
C	-24.4002970000	-28.7134010000	18.3319650000
H	-24.6676300000	-28.0184730000	19.1441010000
C	-24.8092950000	-28.0819030000	16.9970840000
O	-25.1818360000	-28.7455350000	16.0448530000
Fe	-15.1430900000	-37.0794770000	11.4311240000
Fe	-16.9794030000	-36.0478270000	9.2938190000
Fe	-15.3257290000	-33.8663060000	10.5776640000
Fe	-14.1782270000	-35.7650990000	8.5677480000
S	-15.9377730000	-34.2277400000	8.2008030000
S	-13.3559710000	-35.1527670000	10.7190900000
S	-15.3842490000	-37.7469240000	9.0492060000
S	-17.0101920000	-35.4515400000	11.5358210000
N	-13.2052520000	-38.1926240000	11.6897380000
H	-12.4035430000	-37.5763230000	11.7790090000
H	-13.1819380000	-38.6018040000	10.7574410000
C	-13.3659510000	-39.1964950000	12.7435030000
H	-12.7131120000	-40.0666480000	12.5918870000
C	-14.8417720000	-39.7016450000	12.7444460000
O	-15.6961270000	-38.8380020000	12.3277250000
O	-15.0460460000	-40.8229610000	13.2157690000
C	-13.0545080000	-38.6281690000	14.1480600000
H	-12.8700890000	-39.4909280000	14.7992850000
H	-12.1217740000	-38.0468590000	14.1158280000
C	-14.1611420000	-37.8182660000	14.8473510000

H	-15.0942040000	-38.3800020000	14.9353780000
H	-13.8383780000	-37.5289350000	15.8544820000
S	-14.6902350000	-36.2987670000	13.9801490000
C	-13.1654600000	-35.3122270000	14.0210380000
H	-13.4359340000	-34.3166080000	13.6662900000
H	-12.4434480000	-35.7185550000	13.3141810000
H	-12.7692610000	-35.2760760000	15.0408430000
C	-15.6666670000	-34.8723390000	15.5191430000
H	-14.8038180000	-34.5916670000	16.1218640000
H	-15.9417280000	-34.1371060000	14.7635180000
C	-16.8219650000	-35.5076800000	16.2229910000
H	-16.4914860000	-36.1386880000	17.0593200000
O	-17.6433820000	-34.4206810000	16.7391150000
C	-17.7567300000	-36.3602960000	15.3505250000
H	-17.8094540000	-35.9169000000	14.3406080000
O	-17.2819140000	-37.6717050000	15.3144230000
H	-18.0271640000	-38.2451840000	14.9769670000
C	-19.1366960000	-36.1817370000	16.0525920000
H	-19.9499580000	-36.2055720000	15.3174300000
O	-19.3670270000	-37.1148400000	17.0685670000
H	-20.0140620000	-37.7647000000	16.6587330000
C	-19.0128220000	-34.7785960000	16.6867690000
H	-19.4491200000	-34.8028890000	17.6888710000
N	-19.7502700000	-33.7293110000	15.9717360000
C	-19.6516060000	-33.3495920000	14.6435020000
H	-18.9405840000	-33.8174320000	13.9717790000
N	-20.4947360000	-32.3938130000	14.3052960000
C	-21.1856800000	-32.1306440000	15.4711480000
C	-22.2444980000	-31.2560880000	15.7733600000
N	-22.7701430000	-30.3977360000	14.8518170000
H	-23.6812450000	-30.0088680000	15.0556310000
H	-22.5321090000	-30.5820920000	13.8883160000
N	-22.7406470000	-31.2482040000	17.0285180000
C	-22.1890170000	-32.0761170000	17.9421970000
H	-22.6319410000	-32.0130420000	18.9354770000
N	-21.1995440000	-32.9468100000	17.7832880000
C	-20.7340260000	-32.9467350000	16.5202900000
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.7820620000	-26.2075680000	17.3377820000
H	-24.8368090000	-26.2366050000	15.8883380000
H	-25.5330500000	-26.1344990000	17.5304080000
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.8498530000	-29.7991460000	17.6744970000
H	-26.6523420000	-31.1613910000	18.7954570000

H	-26.7641390000	-29.5150290000	19.4292140000
H	-23.3016230000	-28.7633650000	18.3073420000
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

TS1$_{XVIII}$

Energy with the medium-sized basis set: -5801.92293

Solution energy with the medium-sized basis set: -5802.27199

Energy with larger basis sets: -5802.80873

Zero-point energy: 0.73675

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6227530000	-35.5848620000	6.8170990000
C	-11.4798410000	-34.5863660000	7.2616110000
H	-11.3405000000	-34.5322250000	8.3460740000
H	-12.0445040000	-33.6987000000	6.9568660000
S	-12.4699960000	-36.1084310000	6.8594170000
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2203040000	-34.7274220000	7.3104820000
C	-19.7384990000	-34.7367150000	8.8842970000
H	-18.8980970000	-34.1250710000	9.2260160000
H	-20.4471030000	-34.8094230000	9.7163410000
S	-19.1346040000	-36.4481160000	8.4962850000
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1943770000	-30.1246650000	12.2069130000
C	-17.5836580000	-31.7633680000	10.9468810000
H	-18.0704900000	-32.5610490000	11.5158160000
H	-17.6098480000	-32.0555610000	9.8915570000
S	-15.8013770000	-31.6760530000	11.4789820000
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1218390000	-39.9584750000	15.8852210000
C	-23.0384740000	-39.4146300000	13.8180940000
H	-23.5515140000	-39.6925780000	12.8846290000
H	-23.4074080000	-38.4208960000	14.0998020000
C	-21.5322470000	-39.3361390000	13.5406120000
H	-21.1569540000	-40.3093410000	13.1973740000

H	-21.3284940000	-38.6432700000	12.7150350000
C	-20.6239340000	-38.8915980000	14.7100070000
O	-21.1846640000	-38.4965270000	15.7822900000
O	-19.3938490000	-38.9462300000	14.4724730000
N	-24.9148510000	-29.9869830000	18.6934550000
H	-24.4195000000	-30.6226050000	18.0597700000
C	-24.4304600000	-28.6607490000	18.4138650000
H	-24.7619020000	-27.9486660000	19.1870480000
C	-24.7814030000	-28.0791740000	17.0405400000
O	-25.0912060000	-28.7782040000	16.0910450000
Fe	-15.1379990000	-37.0716840000	11.5421330000
Fe	-16.9521750000	-36.0665070000	9.1898190000
Fe	-15.3466100000	-33.8235730000	10.6505340000
Fe	-14.1018330000	-35.8506110000	8.5437580000
S	-15.9187910000	-34.2036390000	8.2382210000
S	-13.3685300000	-35.1913200000	10.7406240000
S	-15.4090580000	-37.8418670000	9.1506470000
S	-16.9624150000	-35.5280940000	11.5486040000
N	-13.1719750000	-38.0695780000	11.8506770000
H	-12.4220160000	-37.3841700000	11.8690920000
H	-13.1321160000	-38.5549950000	10.9553020000
C	-13.2598290000	-38.9792170000	12.9924940000
H	-12.5612420000	-39.8216010000	12.9060480000
C	-14.7056830000	-39.5532800000	13.0518920000
O	-15.5987910000	-38.7630770000	12.5621570000
O	-14.8679240000	-40.6367200000	13.6124050000
C	-12.9615960000	-38.2506820000	14.3237880000
H	-12.6307810000	-39.0161990000	15.0360140000
H	-12.1153370000	-37.5629420000	14.1865510000
C	-14.1239830000	-37.5314190000	15.0252760000
H	-14.9753680000	-38.1965300000	15.1954060000
H	-13.7842990000	-37.1586310000	15.9972470000
S	-14.9134620000	-36.1159440000	14.1646080000
C	-13.5470770000	-34.9205790000	14.0333390000
H	-13.9767560000	-34.0328210000	13.5631410000
H	-12.7828670000	-35.3006070000	13.3585020000
H	-13.1474270000	-34.6872040000	15.0241330000
C	-15.6364730000	-35.0186930000	16.0472750000
H	-14.7443270000	-35.0023250000	16.6742360000
H	-15.8306070000	-34.0676620000	15.5526100000
C	-16.8676040000	-35.6452750000	16.6269360000
H	-16.6193440000	-36.3488160000	17.4333990000
O	-17.6961560000	-34.5740790000	17.1599660000
C	-17.7726580000	-36.4120720000	15.6479210000

H	-17.7871140000	-35.8796120000	14.6793030000
O	-17.2975800000	-37.7144470000	15.5132080000
H	-18.0363050000	-38.2614210000	15.1202240000
C	-19.1722610000	-36.2740930000	16.3114300000
H	-19.9646160000	-36.2631260000	15.5536020000
O	-19.4274270000	-37.2567730000	17.2728360000
H	-20.0603770000	-37.8840820000	16.8082020000
C	-19.0657150000	-34.9026720000	17.0141330000
H	-19.5618860000	-34.9557910000	17.9867380000
N	-19.7430870000	-33.8158150000	16.2937050000
C	-19.5837450000	-33.4185430000	14.9767060000
H	-18.8605930000	-33.8943140000	14.3255530000
N	-20.3885880000	-32.4378760000	14.6198240000
C	-21.1180200000	-32.1755150000	15.7613400000
C	-22.1722750000	-31.2852930000	16.0286850000
N	-22.6442050000	-30.4121350000	15.0928550000
H	-23.5623220000	-30.0192220000	15.2539350000
H	-22.3646610000	-30.5952830000	14.1400770000
N	-22.7172060000	-31.2818150000	17.2632750000
C	-22.2206700000	-32.1322060000	18.1878070000
H	-22.7009410000	-32.0701980000	19.1636790000
N	-21.2455940000	-33.0236770000	18.0578230000
C	-20.7283460000	-33.0168690000	16.8150220000
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.8126930000	-26.1735770000	17.3740560000
H	-24.7901560000	-26.2707270000	15.8742650000
H	-25.5722290000	-26.1339190000	17.4743920000
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.7943950000	-29.8541120000	17.6308730000
H	-26.6327050000	-31.1622070000	18.8192950000
H	-26.8389020000	-29.4964500000	19.3733740000
H	-23.3309650000	-28.6766990000	18.4531400000
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

$\mathbf{Int1_{II}}$

Energy with the medium-sized basis set: -5801.98077

Solution energy with the medium-sized basis set: -5802.31376

Energy with larger basis sets: -5802.86502

Zero-point energy: 0.73483

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6305492812	-35.5864653007	6.8248610571
C	-11.4550068425	-34.5338290408	7.3023091145
H	-11.2666488732	-34.4173449453	8.3744044121
H	-12.0165434430	-33.6534357048	6.9701034322
S	-12.4840574396	-36.0503797374	7.0431655740
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2238831542	-34.7173782897	7.2990171274
C	-19.7608108868	-34.7517188320	8.8873058424
H	-18.9182841584	-34.1561544852	9.2481511911
H	-20.4805183021	-34.8270038901	9.7093813249
S	-19.1691683799	-36.4678773450	8.4908749901
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1647811417	-30.1618891280	12.2122635612
C	-17.6359106469	-31.7808876113	10.8644805291
H	-18.0891178976	-32.5748997733	11.4642850445
H	-17.7708946012	-32.0521844842	9.8119672801
S	-15.8126330747	-31.7791034372	11.2161033788
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1401723576	-39.9763733556	15.8998701847
C	-23.0121782960	-39.3813257543	13.8607048985
H	-23.4237965918	-39.6700987004	12.8814557158
H	-23.4576948575	-38.4147580961	14.1260402619
C	-21.4910320951	-39.2162301395	13.7319576557
H	-21.0277249635	-40.1523777802	13.3954822635
H	-21.2482849197	-38.4784134120	12.9563524650
C	-20.7382786998	-38.7716464041	15.0082436106
O	-21.4333799998	-38.3203559221	15.9758159804
O	-19.4895326294	-38.8780455752	14.9609564959
N	-24.9372220007	-29.9124895993	18.8196118800
H	-24.3667736884	-30.5292394374	18.2335029353
C	-24.4948150225	-28.5723836217	18.5341841533
H	-24.9356572391	-27.8507830473	19.2409545035
C	-24.7401796108	-28.0700056263	17.1091427944
O	-24.9389001885	-28.8227950096	16.1710249861
Fe	-15.1660028979	-36.9647471901	11.6413117108
Fe	-17.0338140319	-36.1467237836	9.2773977008
Fe	-15.4956293682	-33.9862430037	10.5301658789
Fe	-14.1696528844	-35.8900656510	8.6668814511
S	-16.0051288715	-34.2936600838	8.2471736693

S	-13.5071494292	-35.0646917159	10.8996884196
S	-15.4221473154	-37.7953783346	9.1649752964
S	-17.1169543613	-35.3814833390	11.4828357668
N	-13.2677676604	-38.0971738144	11.9400981920
H	-12.4824679406	-37.4794854994	12.1230897992
H	-13.1509431630	-38.4948760465	11.0105947456
C	-13.5102046188	-39.1187288343	12.9670113055
H	-12.8560508447	-39.9916348379	12.8373614033
C	-14.9854389269	-39.6120010528	12.8615690791
O	-15.8147713132	-38.7294568696	12.4247467555
O	-15.2267583762	-40.7512802147	13.2652588617
C	-13.2751152726	-38.5642795933	14.3913817259
H	-13.1030119637	-39.4308359071	15.0423436507
H	-12.3447963518	-37.9756164529	14.4016393357
C	-14.4128162574	-37.7645346934	15.0469484076
H	-15.3291520942	-38.3554290992	15.1311873567
H	-14.1198892162	-37.4942019856	16.0672470361
S	-14.9758593849	-36.2317865568	14.2162152090
C	-13.5092902074	-35.1650225619	14.3741498325
H	-13.7545939362	-34.2393698209	13.8500382576
H	-12.6403985393	-35.6000384192	13.8755852601
H	-13.2929125919	-34.9627576814	15.4295104554
C	-15.6965990488	-35.6143333171	17.6459012235
H	-14.9613154501	-36.3891019926	17.8305598675
H	-15.4022816651	-34.7382818547	17.0777964335
C	-17.1293806009	-35.9317572893	17.7852779096
H	-17.3067830471	-36.6260884737	18.6233896066
O	-17.8662236956	-34.7024160294	17.9868875733
C	-17.8280731331	-36.5733656983	16.5550578401
H	-17.5425014018	-35.9803061469	15.6687153991
O	-17.4904782591	-37.9149631207	16.4251915181
H	-18.2320081018	-38.3525635256	15.9186761345
C	-19.3182645168	-36.2858658129	16.8939929792
H	-19.9172617818	-36.1952901901	15.9795709576
O	-19.8755179442	-37.2361342271	17.7537170764
H	-20.4714119551	-37.7899647838	17.1584113419
C	-19.2224635925	-34.9325909858	17.6432803032
H	-19.8541638141	-34.9791771116	18.5356572187
N	-19.7217366808	-33.7930322824	16.8725001566
C	-19.4776021293	-33.4739241191	15.5472664820
H	-18.7646718528	-34.0348088151	14.9556962993
N	-20.1947406827	-32.4611878342	15.1070927539
C	-20.9515539200	-32.0907046782	16.2001688480
C	-21.9737312110	-31.1414495261	16.3657983464

N	-22.3702010961	-30.3142375225	15.3545917726
H	-23.2952079181	-29.9123767241	15.4403306357
H	-22.0618682266	-30.5848093699	14.4311416336
N	-22.5699381094	-31.0403792944	17.5716025283
C	-22.1643825515	-31.8641294428	18.5620836148
H	-22.6862784233	-31.7251404859	19.5084662972
N	-21.2397939469	-32.8154914218	18.5248435152
C	-20.6672341121	-32.9009867964	17.3099343947
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.8761917732	-26.1155695577	17.4398428848
H	-24.6977825927	-26.3204396363	15.8598437579
H	-25.6374416592	-26.1423895540	17.3679008299
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.7156074586	-29.9009065049	17.5881939065
H	-26.6003265544	-31.1696466934	18.8227846180
H	-26.9372589461	-29.5037508277	19.3087454543
H	-23.4045400741	-28.5275430616	18.6754913157
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

$\mathbf{Int1_{VIII}}$

Energy with the medium-sized basis set:	-5801.97550
Solution energy with the medium-sized basis set:	-5802.30976
Energy with larger basis sets:	-5802.85955
Zero-point energy:	0.73492

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6330593102	-35.5873044965	6.8261775011
C	-11.4556002930	-34.5281307369	7.3003049116
H	-11.2688371190	-34.4232730106	8.3739012112
H	-12.0069338617	-33.6389489272	6.9744339888
S	-12.5012387419	-36.0306937490	7.0242596793
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2235920189	-34.7180519173	7.2995902181
C	-19.7639287375	-34.7478296778	8.8916509726
H	-18.9224110916	-34.1509198396	9.2527661070

H	-20.4874786049	-34.8187097556	9.7110200824
S	-19.1694548262	-36.4642302625	8.5064599728
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1688466509	-30.1581039948	12.2119570841
C	-17.6363648385	-31.7844731535	10.8764692992
H	-18.1104590465	-32.5764037795	11.4633430318
H	-17.7467398623	-32.0524755941	9.8202047979
S	-15.8222277682	-31.7930860833	11.2753533647
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1385520013	-39.9734905166	15.8978649613
C	-23.0175222116	-39.3847535614	13.8555688077
H	-23.4324551713	-39.6786976884	12.8792078115
H	-23.4649308665	-38.4181296588	14.1179854290
C	-21.4979527460	-39.2160601093	13.7187281336
H	-21.0335935508	-40.1554036215	13.3920327681
H	-21.2595881085	-38.4882406195	12.9325762120
C	-20.7395249553	-38.7550066082	14.9854556319
O	-21.4301511153	-38.3339324701	15.9689306220
O	-19.4886426323	-38.8198339860	14.9133708189
N	-24.9346714058	-29.9192012680	18.8045170581
H	-24.3761776486	-30.5290332763	18.2006012729
C	-24.4918187716	-28.5781525425	18.5241579878
H	-24.9257965720	-27.8599133873	19.2383432853
C	-24.7480494290	-28.0699522468	17.1035224133
O	-24.9606257499	-28.8185743017	16.1650281339
Fe	-15.2088097539	-37.1173963188	11.6920808825
Fe	-17.0395915464	-36.1547745855	9.3179290743
Fe	-15.4979040530	-34.0014246026	10.5962712951
Fe	-14.1540877082	-35.8900849371	8.6807233047
S	-16.0123137147	-34.2941592898	8.3095231979
S	-13.5255786073	-35.0862745266	10.9529430458
S	-15.4470142202	-37.8089502405	9.2081096652
S	-17.1087741817	-35.4429236144	11.5368007376
N	-13.2537026440	-38.0979261051	12.0308900425
H	-12.5171607708	-37.4313728774	12.2435150763
H	-13.0848936737	-38.4589961408	11.0938736739
C	-13.4414727464	-39.1652184321	13.0221530898
H	-12.7176567907	-39.9802316240	12.8857228765
C	-14.8704813858	-39.7749483051	12.8675197437
O	-15.7529340007	-38.9767863896	12.3820818503
O	-15.0270166546	-40.9246836292	13.2894310121
C	-13.2822825453	-38.6356477511	14.4644960361
H	-13.0964460641	-39.5101526440	15.1005081421
H	-12.3805889374	-38.0066427256	14.5234058112

C	-14.4791691944	-37.9037527144	15.0919301440
H	-15.3671681787	-38.5393999733	15.1310242779
H	-14.2377920705	-37.6383782663	16.1265490921
S	-15.0945904440	-36.3888022611	14.2656819175
C	-13.6729924812	-35.2618756308	14.4258254345
H	-13.9481799765	-34.3562673086	13.8815959186
H	-12.7791003197	-35.6666944594	13.9470102408
H	-13.4814038896	-35.0344185651	15.4802715562
C	-15.7268162061	-35.5359926015	17.5743442817
H	-14.9638781716	-36.2920911764	17.7174386939
H	-15.4737931131	-34.6329524910	17.0291548007
C	-17.1468995937	-35.8924139605	17.7518013863
H	-17.2831277706	-36.5974312025	18.5887057940
O	-17.9034862871	-34.6816486247	17.9880574971
C	-17.8618427797	-36.5420772522	16.5363220193
H	-17.5946763268	-35.9518412081	15.6429688173
O	-17.5148836515	-37.8809397275	16.4075029746
H	-18.2486778064	-38.3177166566	15.8878050556
C	-19.3495981514	-36.2665205952	16.8906903623
H	-19.9568917231	-36.1802641163	15.9811879434
O	-19.8945888703	-37.2204250344	17.7548258947
H	-20.4773482214	-37.7861832697	17.1592948284
C	-19.2564518957	-34.9125944938	17.6352955339
H	-19.8946263653	-34.9506209186	18.5231951369
N	-19.7474401179	-33.7762106542	16.8529287359
C	-19.4913486084	-33.4598209559	15.5293898495
H	-18.7784436058	-34.0258179971	14.9427278707
N	-20.1965284797	-32.4406548385	15.0842041981
C	-20.9604813608	-32.0658069821	16.1707726976
C	-21.9778438409	-31.1107237766	16.3299298907
N	-22.3653950185	-30.2810013932	15.3166377187
H	-23.2909541271	-29.8793667063	15.3975037296
H	-22.0549366246	-30.5543839370	14.3946543672
N	-22.5788959073	-31.0053092560	17.5325484041
C	-22.1864336130	-31.8319913226	18.5257993710
H	-22.7137865255	-31.6892040463	19.4685131511
N	-21.2696744656	-32.7906626153	18.4936727120
C	-20.6894810453	-32.8780502696	17.2827330576
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.8646213988	-26.1239777365	17.4278000026
H	-24.7127180495	-26.3159908265	15.8605295128
H	-25.6268344484	-26.1373631269	17.3841938072
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.7283942034	-29.8847059325	17.5964446865

H	-26.6002048430	-31.1722871677	18.8098083754
H	-26.9271122491	-29.5136104661	19.3255163113
H	-23.4003550070	-28.5366819644	18.6562472468
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

$\mathbf{Int1_X}$

Energy with the medium-sized basis set: -5801.97336

Solution energy with the medium-sized basis set: -5802.30592

Energy with larger basis sets: -5802.85637

Zero-point energy: 0.73503

C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6269079958	-35.5853891876	6.8226517369
C	-11.4459557681	-34.5329352063	7.3203277989
H	-11.2335795769	-34.3850478368	8.3844365592
H	-12.0219924743	-33.6655465104	6.9781629021
S	-12.4707715154	-36.0640069180	7.1296533466
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2235737817	-34.7189453231	7.3016607187
C	-19.7471549053	-34.7559508392	8.8801426562
H	-18.8923882730	-34.1695710334	9.2275804860
H	-20.4547562413	-34.8281271814	9.7125245376
S	-19.1744915513	-36.4775053579	8.4728656956
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1758557256	-30.1497703836	12.2109466082
C	-17.6159305524	-31.7752226963	10.8917444457
H	-18.0955242376	-32.5772760405	11.4591958870
H	-17.6820361529	-32.0424614392	9.8319302456
S	-15.8155336166	-31.7580270613	11.3592724111
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1473597094	-39.9831823464	15.9053561318
C	-23.0107346148	-39.3682580058	13.8755149243
H	-23.3929606052	-39.6571232518	12.8846394795
H	-23.4803711341	-38.4127812640	14.1389448745
C	-21.4902594566	-39.1738477332	13.7894001296

H	-21.0000370259	-40.0925274710	13.4447887233
H	-21.2421764331	-38.4111188594	13.0396991457
C	-20.7877964730	-38.7471545636	15.0990730934
O	-21.5121667493	-38.2461799661	16.0191730399
O	-19.5446471204	-38.9159503077	15.1246726536
N	-24.9482529986	-29.8862910726	18.8638729773
H	-24.3511858656	-30.4980679634	18.3008588580
C	-24.5197703581	-28.5418702818	18.5760468148
H	-24.9988764946	-27.8193637190	19.2562735098
C	-24.7229686185	-28.0661099872	17.1355627138
O	-24.8759512476	-28.8384980617	16.2046985204
Fe	-15.3586237984	-37.1477846403	11.8243395263
Fe	-17.0456617696	-36.2388066093	9.3277641330
Fe	-15.4537320007	-33.9641546343	10.7154555699
Fe	-14.1151032310	-35.8882552162	8.7773965925
S	-15.9508465726	-34.2984421623	8.4021379178
S	-13.5483873499	-35.1300325605	11.0518429730
S	-15.4215133909	-37.8392254940	9.2979978181
S	-17.1641265778	-35.4147075092	11.5630144959
N	-13.4156147306	-38.1691854243	12.1358993484
H	-12.6572871053	-37.5189266498	12.3193140448
H	-13.2722893713	-38.5689613383	11.2105898399
C	-13.6213292910	-39.1935275581	13.1696920463
H	-12.9283712771	-40.0371716789	13.0496805856
C	-15.0707933590	-39.7559709211	13.0580480724
O	-15.9367101361	-38.9209300945	12.5921873707
O	-15.2667707449	-40.8958795333	13.4813179117
C	-13.4183411284	-38.6204564544	14.5915103255
H	-13.2286810271	-39.4766921797	15.2512414764
H	-12.5050531575	-38.0062773294	14.6052587437
C	-14.5840793741	-37.8471289518	15.2290732895
H	-15.4825388227	-38.4642047098	15.3160860313
H	-14.3064817201	-37.5558843273	16.2474229499
S	-15.1895883734	-36.3413338822	14.3758247516
C	-13.7508120280	-35.2335242756	14.5133119171
H	-14.0199045975	-34.3225125168	13.9751857009
H	-12.8701991372	-35.6520348209	14.0214561520
H	-13.5402316858	-35.0093837198	15.5653298587
C	-15.7768832911	-35.7618628140	17.9307107495
H	-15.0736982303	-36.5628790956	18.1271757973
H	-15.4406191807	-34.8949360314	17.3712829834
C	-17.2227354702	-36.0274216953	18.0428985107
H	-17.4406850816	-36.7219581455	18.8711114634
O	-17.9207677286	-34.7760927242	18.2389319050

C	-17.9112236118	-36.6339661775	16.7902246186
H	-17.5805518561	-36.0426924176	15.9192344385
O	-17.6122397288	-37.9836204553	16.6586212977
H	-18.3505156813	-38.3989687503	16.1249748588
C	-19.3991652437	-36.2931311298	17.0838840535
H	-19.9609247445	-36.1633568650	16.1502333150
O	-20.0282391049	-37.2330727821	17.9044201548
H	-20.6060030568	-37.7622500874	17.2706491297
C	-19.2750731203	-34.9541245596	17.8557405432
H	-19.9324271258	-34.9888784974	18.7300788976
N	-19.7096173230	-33.7879402377	17.0865141422
C	-19.4044021474	-33.4586897596	15.7763536093
H	-18.6883615673	-34.0349165687	15.2037039866
N	-20.0697567018	-32.4163441385	15.3250214462
C	-20.8578530455	-32.0379522437	16.3928717271
C	-21.8613936153	-31.0649026841	16.5292569925
N	-22.1980058988	-30.2187841729	15.5103467497
H	-23.1281372257	-29.8213728738	15.5530522409
H	-21.8572698093	-30.4942387936	14.5992952899
N	-22.5008422252	-30.9602590782	17.7122063010
C	-22.1577698836	-31.8072008226	18.7067760020
H	-22.7129054904	-31.6655866247	19.6336174753
N	-21.2604443040	-32.7853145363	18.6929576500
C	-20.6422287393	-32.8715914028	17.5009782212
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.9047272542	-26.0914576568	17.4638526325
H	-24.6612619856	-26.3385480231	15.8574711279
H	-25.6612153859	-26.1507692821	17.3247681914
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.6860259220	-29.9139867570	17.5757189042
H	-26.5889430029	-31.1722631271	18.8222285874
H	-26.9698122287	-29.5093806877	19.2855682867
H	-23.4361218822	-28.4757969805	18.7547334804
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

Int1$_{XVIII}$

Energy with the medium-sized basis set:			-5801.96142
Solution energy with the medium-sized basis set:			-5802.29444
Energy with larger basis sets:			-5802.84379
Zero-point energy:			0.73499
C	-10.1420000000	-34.6620000000	6.5290000000
H	-9.6194268943	-35.5817410729	6.8206168072
C	-11.4407780502	-34.5449298027	7.3291004906
H	-11.2229157598	-34.3377338788	8.3819437690
H	-12.0567995127	-33.7204039029	6.9533165965
S	-12.3991600402	-36.1262716490	7.2249522970
C	-20.3890000000	-34.1000000000	7.6600000000
H	-21.2233952571	-34.7222230655	7.3077131440
C	-19.7568909345	-34.7317817775	8.8982211353
H	-18.8878396835	-34.1507462352	9.2192070532
H	-20.4636826616	-34.7517831801	9.7341701016
S	-19.2276121029	-36.4813578704	8.5636481683
C	-18.3150000000	-30.4390000000	11.1620000000
H	-18.1718348451	-30.1522710107	12.2110122295
C	-17.6059470819	-31.7656090233	10.8804083645
H	-18.0508412274	-32.5700116295	11.4715286397
H	-17.7025132276	-32.0437744148	9.8258336482
S	-15.7912327594	-31.7026442243	11.2833617834
C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1499791313	-39.9863203301	15.9074094731
C	-23.0042666004	-39.3645681898	13.8818743896
H	-23.3721324378	-39.6533795354	12.8855815581
H	-23.4817705431	-38.4119291375	14.1412671246
C	-21.4832529221	-39.1621310814	13.8165650009
H	-20.9832992482	-40.0783425222	13.4793100808
H	-21.2287082240	-38.3983333452	13.0701510537
C	-20.8022426630	-38.7319803355	15.1367765322
O	-21.5461553977	-38.2409271687	16.0474436875
O	-19.5582728129	-38.8874741470	15.1813967113
N	-24.9556435891	-29.8706140833	18.8888830269
H	-24.3428613239	-30.4793773772	18.3393654883
C	-24.5359431806	-28.5239693414	18.5990885153
H	-25.0383818125	-27.8010390861	19.2617707719
C	-24.7117472237	-28.0637148730	17.1498847278
O	-24.8348944690	-28.8463044884	16.2232621714
Fe	-15.3964122372	-37.0520806006	11.9717945739
Fe	-17.1214323018	-36.2607930632	9.4817790173
Fe	-15.4275886524	-33.9284145746	10.7027520330

Fe	-14.0479631376	-35.9383939868	8.8977961597
S	-15.9869709271	-34.3819335495	8.4338519634
S	-13.4969070861	-35.0548102498	11.1380022129
S	-15.4268655076	-37.8459475989	9.4908127251
S	-17.1610573018	-35.3138986584	11.6499511018
N	-13.4603662203	-38.0663094881	12.3438810289
H	-12.7106933702	-37.4013589002	12.5110735062
H	-13.3018648932	-38.5028258308	11.4381712323
C	-13.6796055984	-39.0493778707	13.4151177389
H	-12.9972161376	-39.9052058665	13.3267560166
C	-15.1361462187	-39.5947157190	13.3222237251
O	-15.9946621843	-38.7455795407	12.8625125679
O	-15.3472389801	-40.7285816857	13.7505944866
C	-13.4718537788	-38.4280899991	14.8150760336
H	-13.3225298332	-39.2643014075	15.5100002488
H	-12.5360581661	-37.8485928078	14.8158151533
C	-14.6152157232	-37.5875306470	15.4067798593
H	-15.5346135604	-38.1706250316	15.5172718247
H	-14.3333075131	-37.2583120059	16.4122912038
S	-15.1572136730	-36.0987158617	14.4819232923
C	-13.6776022119	-35.0418342525	14.5968128321
H	-13.9085096161	-34.1341573918	14.0363290067
H	-12.8130084531	-35.5056849730	14.1181311344
H	-13.4611139630	-34.8024951675	15.6443792699
C	-15.8587010690	-35.8674393842	18.2374401602
H	-15.1848329852	-36.6662874885	18.5257263963
H	-15.4665490055	-35.0271536207	17.6731260644
C	-17.3137822879	-36.1021688511	18.2557802259
H	-17.5982619485	-36.8004113094	19.0597004069
O	-17.9966374265	-34.8371010289	18.4228221160
C	-17.9388992325	-36.6738980130	16.9538282619
H	-17.5566903717	-36.0646061701	16.1161955501
O	-17.6516683945	-38.0241712919	16.8025692501
H	-18.3750794928	-38.4170990995	16.2333910203
C	-19.4353040646	-36.3223672557	17.1822238101
H	-19.9545600203	-36.1818161172	16.2258878622
O	-20.1026993770	-37.2643164765	17.9686674986
H	-20.6714216082	-37.7766199543	17.3107294958
C	-19.3340513554	-34.9930946603	17.9734097662
H	-20.0306217918	-35.0329519487	18.8165043304
N	-19.7225878626	-33.8130890298	17.2022612324
C	-19.3825823701	-33.4806451533	15.9011488396
H	-18.6625877416	-34.0641051898	15.3408230765
N	-20.0213354972	-32.4252699585	15.4420011425

C	-20.8287594464	-32.0418351063	16.4936088210
C	-21.8258120079	-31.0594581775	16.6108593429
N	-22.1321254681	-30.2075676526	15.5870770261
H	-23.0614699254	-29.8065924157	15.6089377825
H	-21.7735724870	-30.4845932199	14.6832561623
N	-22.4909643347	-30.9528441881	17.7794626064
C	-22.1804754741	-31.8083952435	18.7773535897
H	-22.7542207542	-31.6642752296	19.6924302586
N	-21.2956893756	-32.7979628859	18.7785161804
C	-20.6508313424	-32.8850378841	17.6008744325
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.9257576334	-26.0763777784	17.4816635361
H	-24.6350341064	-26.3474898468	15.8575807262
H	-25.6769203873	-26.1584928900	17.2949884854
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.6682559148	-29.9241247634	17.5682123247
H	-26.5827347547	-31.1730662041	18.8248071984
H	-26.9886299011	-29.5109465302	19.2695907567
H	-23.4573990058	-28.4431735762	18.8016018663
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
H	-9.4543580000	-33.8561810000	6.6796760000
H	-10.3106700000	-34.7224400000	5.4741080000
H	-19.3673320000	-30.5418270000	10.9979150000
H	-17.9102670000	-29.6574470000	10.5535050000
H	-19.6860130000	-34.0390300000	6.8556420000
H	-20.7882850000	-33.1267860000	7.8557700000

Int1b

Energy with the medium-sized basis set:	-2295.91052
Solution energy with the medium-sized basis set:	-2295.99904
Energy with larger basis sets:	-2296.69168
Zero-point energy:	0.68468

C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1172222804	-39.9468873248	15.8758975930
C	-23.0813329364	-39.4349619504	13.7845648784
H	-23.6417629714	-39.7320412822	12.8851156242
H	-23.4419314883	-38.4352886826	14.0579270744
C	-21.5960552441	-39.3530051095	13.4105378335
H	-21.2311072516	-40.3483157948	13.1167095927
H	-21.4540546946	-38.7209879347	12.5252268516

C	-20.6232263492	-38.8308965122	14.4904610680
O	-21.0688336088	-38.6785903471	15.6642337007
O	-19.4489218083	-38.6119667344	14.0817452476
N	-24.9616733323	-29.8606104389	18.9190730285
H	-24.3331583966	-30.5354267154	18.4710467740
C	-24.5334838445	-28.5227837402	18.6102780579
H	-25.0495453273	-27.7913329276	19.2532759519
C	-24.6916885919	-28.0614421509	17.1564101898
O	-24.7917170461	-28.8451733309	16.2253283595
C	-15.5670215492	-35.6309837770	16.7797722685
H	-14.7228579768	-36.3088296771	16.8033494899
H	-15.4811294640	-34.7096817095	16.2105269500
C	-16.9053122029	-36.1079104117	17.1762801243
H	-16.8474125617	-36.9375515899	17.8910253275
O	-17.6543695991	-35.0065043991	17.7724704744
C	-17.8092012185	-36.5751398565	16.0087652606
H	-17.7200046970	-35.8229114597	15.1965497063
O	-17.4570312205	-37.8455560703	15.5951423473
H	-18.2197363191	-38.2032670900	15.0448603303
C	-19.2225007038	-36.4322713701	16.6510659801
H	-19.9872858977	-36.2582133635	15.8825569803
O	-19.5486262946	-37.5273087698	17.4476904530
H	-20.0746235197	-38.1245625297	16.8371215809
C	-19.0507531164	-35.1924316956	17.5562558986
H	-19.5783038038	-35.3488191917	18.5002194205
N	-19.6020848979	-33.9655391129	16.9817608546
C	-19.2792113980	-33.3788102836	15.7714960046
H	-18.4406126271	-33.7355794183	15.1918589670
N	-20.0624256300	-32.3777467520	15.4379328470
C	-20.9549215106	-32.2952989730	16.4907458937
C	-22.0686651373	-31.4663304939	16.7226973008
N	-22.4520936308	-30.5132584759	15.8384237195
H	-23.3780275725	-30.1110415497	15.9367884761
H	-22.0381705116	-30.5572725447	14.9198450753
N	-22.7558253006	-31.6223758533	17.8730741719
C	-22.3528245128	-32.5736722682	18.7396935103
H	-22.9376546822	-32.6358725845	19.6555534015
N	-21.3490476562	-33.4393532836	18.6191331777
C	-20.6847298586	-33.2646882814	17.4644152358
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.9454282000	-26.0618597651	17.4960773833
H	-24.6210369931	-26.3504038540	15.8587376218
H	-25.6891562679	-26.1719671216	17.2763231504
C	-26.3586730000	-30.1235080000	18.6071870000

H	-26.6309969505	-29.9889482424	17.5477112490
H	-26.5979304563	-31.1547936168	18.8853189753
H	-27.0033685728	-29.4650116010	19.2067038283
H	-23.4618095304	-28.4203593532	18.8421629568
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
C	-18.2080938490	-31.7400996923	19.3663217464
H	-18.8005027790	-31.3425467296	18.5366889695
H	-18.3971397117	-32.8137965776	19.4352126405
C	-16.7387285931	-31.4776063468	19.1046924664
H	-16.5530818999	-30.3865290842	19.0591127066
O	-15.9474343830	-32.0394827535	20.1669774563
C	-16.1793376675	-32.1163675049	17.8232900779
H	-16.6153457426	-33.1098461380	17.7044993425
O	-16.4986909342	-31.4192443407	16.6336233845
H	-16.1674410999	-30.5141880327	16.7172836227
C	-14.6828782191	-32.2137757598	18.1541672059
H	-14.1628596129	-33.0060130123	17.6130367823
H	-14.1934021985	-31.2580033811	17.9260363351
C	-14.6770765350	-32.4492426432	19.6779717483
H	-13.8728655018	-31.8972130297	20.1764008539
N	-14.4644759472	-33.8456468973	20.0490729887
C	-15.3637131142	-34.8983955919	19.9767875807
H	-16.3839478554	-34.7438818087	19.6554575841
N	-14.8378363561	-36.0562699049	20.3099731597
C	-13.5214825202	-35.7570695705	20.6066170163
C	-12.4262560655	-36.5529319250	20.9904229449
N	-12.5516490663	-37.8957714611	21.1851629072
H	-11.6990438882	-38.4325325194	21.2232144989
H	-13.3797004917	-38.3394398780	20.8164503708
N	-11.2290672694	-35.9702179956	21.1885679219
C	-11.1389600179	-34.6399484568	21.0125591078
H	-10.1516264320	-34.2161427018	21.1896597755
N	-12.0866935682	-33.7724461264	20.6432450249
C	-13.2627896973	-34.3898359100	20.4511452975
H	-18.5368291604	-31.2653482134	20.2952568198

TS2

Energy with the medium-sized basis set:	-2295.88584
Solution energy with the medium-sized basis set:	-2295.97449
Energy with larger basis sets:	-2296.66609

Zero-point energy: 0.68125

C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1146990000	-39.9461840000	15.8745280000
C	-23.0783600000	-39.4425540000	13.7785450000
H	-23.6673620000	-39.7219220000	12.8919210000
H	-23.4015920000	-38.4324700000	14.0596030000
C	-21.6005050000	-39.4066200000	13.3705330000
H	-21.2751440000	-40.4114770000	13.0631720000
H	-21.4577720000	-38.7734020000	12.4862730000
C	-20.5904890000	-38.9222150000	14.4326550000
O	-21.0097530000	-38.7662540000	15.6155290000
O	-19.4192770000	-38.7307240000	14.0025650000
N	-24.9364720000	-29.9113040000	18.8323810000
H	-24.3549070000	-30.5734270000	18.3110440000
C	-24.4920930000	-28.5748380000	18.5406440000
H	-24.9547260000	-27.8522740000	19.2316510000
C	-24.7121300000	-28.0688150000	17.1104630000
O	-24.8719600000	-28.8237560000	16.1642890000
C	-15.5741960000	-35.4460660000	16.3534980000
H	-14.7576100000	-36.1673120000	16.3752340000
H	-15.6309630000	-34.9120780000	15.4010200000
C	-16.8920330000	-35.9787610000	16.8329100000
H	-16.7623890000	-36.7323940000	17.6181780000
O	-17.6729050000	-34.8680090000	17.3569670000
C	-17.7922590000	-36.5899510000	15.7460720000
H	-17.7647460000	-35.9061930000	14.8695900000
O	-17.3909110000	-37.8731750000	15.4235810000
H	-18.1518970000	-38.2926180000	14.9185910000
C	-19.1972160000	-36.4628490000	16.4101670000
H	-19.9838600000	-36.3780160000	15.6496610000
O	-19.4605890000	-37.5106750000	17.2888910000
H	-19.9953950000	-38.1555450000	16.7376040000
C	-19.0637280000	-35.1534510000	17.2171740000
H	-19.5421610000	-35.2702500000	18.1925230000
N	-19.7082300000	-34.0049350000	16.5853320000
C	-19.5086810000	-33.5222910000	15.3057990000
H	-18.7564080000	-33.9580770000	14.6637710000
N	-20.3005560000	-32.5237520000	14.9817970000
C	-21.0719730000	-32.3375010000	16.1143080000
C	-22.1375670000	-31.4620170000	16.4018090000
N	-22.5919640000	-30.5556030000	15.5029430000
H	-23.4841170000	-30.1074950000	15.6794120000
H	-22.2725670000	-30.6536220000	14.5519150000
N	-22.7067830000	-31.5261060000	17.6234270000

C	-22.2342540000	-32.4248320000	18.5105660000
H	-22.7283360000	-32.4131410000	19.4802010000
N	-21.2596710000	-33.3171600000	18.3510630000
C	-20.7176570000	-33.2399690000	17.1243720000
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.9070670000	-26.0958840000	17.4705950000
H	-24.6697980000	-26.3195470000	15.8617180000
H	-25.6614710000	-26.1644540000	17.3367340000
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.6987910000	-29.9340610000	17.5758510000
H	-26.6093710000	-31.1592360000	18.8570620000
H	-26.9405210000	-29.4757610000	19.2780280000
H	-23.4071820000	-28.5081300000	18.7165480000
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
C	-17.9656120000	-31.5861890000	18.7520200000
H	-18.3150390000	-30.9017790000	17.9727200000
H	-18.4381030000	-32.5580100000	18.6021170000
C	-16.4589220000	-31.7374650000	18.6673730000
H	-15.9649200000	-30.7695350000	18.8748050000
O	-16.0382430000	-32.6950310000	19.6455000000
C	-15.9243270000	-32.2370770000	17.2975430000
H	-16.7255620000	-32.7351450000	16.7456510000
O	-15.4952270000	-31.1714610000	16.4555970000
H	-14.7549010000	-30.7340790000	16.8985760000
C	-14.8393360000	-33.2350770000	17.6888330000
H	-15.1893680000	-34.4261390000	17.1583330000
H	-13.8650710000	-33.0655590000	17.2278750000
C	-14.8354210000	-33.3030690000	19.2124960000
H	-13.9508680000	-32.7958810000	19.6295850000
N	-14.8072220000	-34.6461270000	19.7756190000
C	-15.8750940000	-35.5146360000	19.9295970000
H	-16.8678120000	-35.2120330000	19.6305350000
N	-15.5304040000	-36.6797730000	20.4307510000
C	-14.1626300000	-36.5781510000	20.6089490000
C	-13.1912410000	-37.4836700000	21.0742800000
N	-13.5244990000	-38.7324340000	21.5094320000
H	-12.7714140000	-39.3981070000	21.5908490000
H	-14.4363320000	-39.0791730000	21.2504850000
N	-11.9012000000	-37.0999560000	21.1122890000
C	-11.6006230000	-35.8538770000	20.7049710000
H	-10.5452840000	-35.5911760000	20.7591660000
N	-12.4145150000	-34.9020850000	20.2369380000
C	-13.6886940000	-35.3223750000	20.2085030000

H	-18.2701600000	-31.1969280000	19.7275510000

Int2

Energy with the medium-sized basis set: -2295.91558

Solution energy with the medium-sized basis set: -2296.00399

Energy with larger basis sets: -2296.69666

Zero-point energy: 0.68496

C	-23.3870000000	-40.4220000000	14.9300000000
H	-23.1099895547	-39.9333241129	15.8660270991
C	-23.1026513890	-39.4584284490	13.7566389388
H	-23.7122680684	-39.7536493495	12.8891257220
H	-23.4236568503	-38.4448446856	14.0282686310
C	-21.6362864988	-39.4229363620	13.3108910959
H	-21.3102807294	-40.4349209450	13.0272816100
H	-21.5199199198	-38.8161860815	12.4046572263
C	-20.6094057517	-38.8990406367	14.3367345356
O	-20.9910742648	-38.7678790581	15.5347892061
O	-19.4630852199	-38.6595694234	13.8640735551
N	-24.9431634113	-29.8969088537	18.8590029742
H	-24.3508202735	-30.5660797058	18.3566626727
C	-24.5038314803	-28.5598081890	18.5615877184
H	-24.9806472756	-27.8339338018	19.2399197788
C	-24.7117605184	-28.0665250656	17.1247728414
O	-24.8660657022	-28.8289248380	16.1835671212
C	-15.5660142882	-35.5474546655	16.2990556001
H	-15.0836227078	-36.3843381448	15.7849496740
H	-15.6848716268	-34.7210788578	15.5891034109
C	-16.9181094442	-36.0169490055	16.7911225207
H	-16.8092874420	-36.8005593328	17.5512380384
O	-17.6481793853	-34.8969417483	17.3691143376
C	-17.8466115615	-36.5513792030	15.7031360256
H	-17.8172392167	-35.8366042464	14.8515968373
O	-17.4667178156	-37.8289593700	15.3267280391
H	-18.2232177179	-38.2183901235	14.7889285934
C	-19.2338032955	-36.4189904468	16.3960258908
H	-20.0413040986	-36.2938408507	15.6630982637
O	-19.4954789502	-37.4858569721	17.2562456156
H	-19.9923820225	-38.1376094867	16.6815431510
C	-19.0510459828	-35.1381867329	17.2426345302
H	-19.5197951426	-35.2712333408	18.2206441899
N	-19.6753396732	-33.9564537158	16.6492995943

C	-19.4542458578	-33.4310349731	15.3892471552
H	-18.6630776966	-33.8170533749	14.7628521894
N	-20.2740257038	-32.4560597094	15.0656569007
C	-21.0900784827	-32.3330291194	16.1748948702
C	-22.1908926736	-31.4990704014	16.4514319263
N	-22.6463592624	-30.5895573690	15.5594964730
H	-23.5410928141	-30.1439282356	15.7285163974
H	-22.2868010445	-30.6433980546	14.6194815428
N	-22.7906559610	-31.6090380475	17.6552668269
C	-22.3161648059	-32.5168503987	18.5318059148
H	-22.8349458630	-32.5430297716	19.4883659753
N	-21.3118708040	-33.3767235214	18.3791579303
C	-20.7351470419	-33.2494784350	17.1720988689
C	-24.7296470000	-26.5691290000	16.9222570000
H	-23.9164303831	-26.0877258507	17.4775781648
H	-24.6552765331	-26.3299389257	15.8601748018
H	-25.6687193341	-26.1630828958	17.3185854200
C	-26.3586730000	-30.1235080000	18.6071870000
H	-26.6776068883	-29.9540947693	17.5657560292
H	-26.6063578679	-31.1572416827	18.8684947328
H	-26.9604235001	-29.4693885605	19.2541352609
H	-23.4220556643	-28.4809019796	18.7518280099
H	-24.4296320000	-40.6615240000	14.9511340000
H	-22.7325740000	-41.2640290000	14.8427430000
C	-18.3339551401	-31.6408088609	19.0483478896
H	-18.8783941100	-31.1458389956	18.2381835504
H	-18.5760478093	-32.7050879643	19.0244275522
C	-16.8447846339	-31.4373983903	18.8591868915
H	-16.5930232418	-30.3640077996	18.9300727573
O	-16.1370728137	-32.1514439357	19.8913765475
C	-16.2742779960	-31.9573714250	17.5136276339
H	-16.8782198879	-32.7991009758	17.1497511959
O	-16.3038504737	-30.9871442885	16.4706772456
H	-15.6729977852	-30.2939952576	16.7110749944
C	-14.9193928091	-32.4145230045	17.9276078341
H	-14.9206645459	-35.2182339435	17.1181984864
H	-14.1416446048	-32.7687200069	17.2634694048
C	-14.8654725307	-32.5656885052	19.4149163849
H	-14.0489441613	-31.9884064060	19.8765006227
N	-14.6393099021	-33.9458425648	19.8509206141
C	-15.5318536308	-35.0044766866	19.7691642724
H	-16.5323948860	-34.8563360560	19.3868123778
N	-15.0159143219	-36.1481524697	20.1566192531
C	-13.7137555348	-35.8338417768	20.5005909535

C	-12.6320852615	-36.6159862091	20.9458023065
N	-12.7619620906	-37.9525376498	21.1716468756
H	-11.9113720306	-38.4867012529	21.2575628312
H	-13.5774193511	-38.4082379647	20.7900495553
N	-11.4439660987	-36.0242669896	21.1698897388
C	-11.3505204779	-34.6992317330	20.9606153334
H	-10.3707282253	-34.2681865155	21.1595397221
N	-12.2862978623	-33.8445496828	20.5349686781
C	-13.4530966712	-34.4704302606	20.3182532304
H	-18.6714876471	-31.2292109816	20.0038295774

$\mathbf{Int2b_{II,BS}}$

Energy with the medium-sized basis set: -2502.74794

Solution energy with the medium-sized basis set: -2502.90010

Energy with larger basis sets: -2503.42384

Zero-point energy: 1.01574

Co	-11.8422907414	-31.6042060842	20.2935138591
N	-12.1034107365	-30.9094899778	18.5637684391
N	-13.4955138873	-30.7755473103	20.8756086892
N	-11.2123276964	-32.0674060908	22.0539926559
N	-10.3038095586	-32.3949246664	19.5162212652
C	-10.9431814214	-31.0544597833	17.6429298392
C	-9.9008432174	-29.9685390612	17.9809043052
H	-9.5649324254	-30.0713281933	19.0163175203
H	-10.3162090512	-28.9703795654	17.8688997778
H	-9.0266779499	-30.0338787328	17.3309236604
C	-11.6091487569	-30.8848700563	16.2318991180
C	-10.6725594300	-30.3242118826	15.1558924964
H	-11.2130541513	-30.1989992499	14.2126115038
H	-9.8422177481	-31.0130541152	14.9671917089
H	-10.2480860580	-29.3551242931	15.4232227831
C	-12.2127095252	-32.2119247167	15.7208911048
H	-12.7675944552	-32.0341488686	14.7949614708
H	-11.4478878000	-32.9588818697	15.5009622060
C	-12.8202423493	-29.9483932509	16.5800919672
H	-13.6443608472	-30.1723934360	15.8975255473
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5523071975	-27.9140069367	16.7530207044
H	-11.8935096115	-28.0813899704	17.3121159651
C	-13.1375983115	-30.3532151815	18.0044768415
C	-14.3960215448	-30.1082271915	18.6861411433

C	-15.5685399912	-29.6597677740	17.8337467533
H	-15.7375885060	-28.5800991828	17.8950091057
H	-16.4935598144	-30.1543614737	18.1298603258
H	-15.4123579962	-29.9024111201	16.7827853022
C	-14.5187880797	-30.2769191886	20.0422036917
C	-15.7861259041	-30.0825557922	20.8933671185
C	-16.6850062126	-28.8763394036	20.5758457499
H	-17.3507999511	-28.6980598197	21.4256517783
H	-17.3250420384	-29.0501816433	19.7120031905
H	-16.1109543777	-27.9634790381	20.4006266090
C	-16.6079798306	-31.3959967957	20.8052777335
H	-17.4768819767	-31.3348295078	21.4678152326
H	-16.0067978260	-32.2631433045	21.0998980490
C	-15.1610835023	-29.9785465755	22.3151145033
H	-15.8117806223	-30.4268873054	23.0733340522
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6773934059	-27.9365277530	22.9082637946
H	-14.1584098393	-28.0542677244	21.9982174579
C	-13.8870295908	-30.7541929265	22.1428099481
C	-13.1893470448	-31.3247550858	23.2406000428
H	-13.6747444820	-31.2316283143	24.2051781433
C	-11.9574623889	-31.9237219990	23.2102159546
C	-11.2036635549	-32.4618558022	24.4120658884
C	-11.5497908625	-33.9564607998	24.6306127653
H	-10.9965764937	-34.3244004760	25.5002673522
H	-11.2970160651	-34.5679591974	23.7655113039
H	-12.6185232846	-34.0775242839	24.8330812592
C	-11.5007548185	-31.6945943853	25.7096377317
H	-10.8203681656	-32.0184036084	26.5023248123
H	-12.5152140105	-31.9149874160	26.0551083775
H	-11.4090653921	-30.6118208976	25.5969075501
C	-9.7387438365	-32.3381849467	23.8806230949
H	-9.1290590128	-33.1736859048	24.2340376410
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.6986765663	-30.1472770153	23.9908725891
H	-8.9420013769	-30.9618459868	25.3742082431
C	-9.9409599481	-32.4086889771	22.3658162002
C	-8.9249500306	-32.7674437856	21.4328994472
C	-7.6244029259	-33.2609122912	21.9858406164
H	-6.8053140061	-33.1680996350	21.2785124689
H	-7.7502862392	-34.3301944472	22.2291202966
H	-7.3374577218	-32.7477007186	22.9043596897
C	-9.1549963497	-32.7898610341	19.9941826443
C	-8.2392153602	-33.3479086441	18.8707470587

C	-8.1676882700	-34.8833084612	19.0308295712
H	-7.5155237253	-35.3119403342	18.2659680726
H	-9.1486386563	-35.3544271042	18.9331179185
H	-7.7606046296	-35.1619694269	20.0053735016
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1159820661	-33.1842824366	19.4833008658
H	-6.4232228737	-33.0141840052	17.7671478523
C	-8.9967320499	-32.8846396736	17.5675255682
H	-8.4701736948	-31.9958508968	17.2121496040
C	-8.9965610199	-33.8938859862	16.4171954786
H	-9.6055426520	-34.7765905822	16.6373343791
H	-9.3831994933	-33.4385876395	15.5017441610
C	-10.3862305343	-32.4525678445	18.0446102304
H	-11.1441846039	-33.2033265443	17.8078490681
H	-14.2277543870	-28.5643885382	23.6942631339
H	-8.0970369834	-30.8737404361	23.8271363239
H	-6.8141720083	-31.6778637931	18.8599194960
H	-12.2546736854	-28.0936441780	15.5785736303
H	-7.9813133713	-34.2345656112	16.1948990994
H	-16.9723931268	-31.5687412624	19.7890830349
C	-14.3392070157	-36.3171486537	21.5441813222
H	-15.3790651104	-36.1689745763	21.2353270953
H	-13.9385772165	-37.1797952485	21.0025212252
C	-13.5146897841	-35.0634499588	21.2804061495
H	-13.9557874168	-34.1931198944	21.7769929523
O	-12.1787744719	-35.2026944748	21.8133066100
C	-13.3153931767	-34.7563932791	19.7859758222
H	-14.1141468033	-35.1772776587	19.1660770659
O	-13.3185146629	-33.3074484120	19.6145554249
H	-13.4981461617	-33.0945848638	18.6887658655
C	-11.9747174160	-35.3377322771	19.5100417423
H	-11.5583184243	-35.5482190839	18.5329912499
C	-11.2483146016	-35.5329694740	20.7984990944
H	-10.3924427941	-34.8571892064	20.9196682129
N	-10.6848304738	-36.8672736078	20.9514106424
C	-11.1559954247	-38.0810836647	20.4658246081
H	-12.0261401593	-38.1305536518	19.8251403307
N	-10.4394859264	-39.1104715767	20.8467687822
C	-9.4513462420	-38.5649693882	21.6363358670
C	-8.3683753410	-39.1405754003	22.3498967519
N	-8.1211221123	-40.4562669818	22.3443355799
H	-7.3360856271	-40.8142859410	22.8699797826
H	-8.7180966240	-41.0894755922	21.8326799325
N	-7.5555284387	-38.3214594435	23.0561854382

C	-7.8037861685	-37.0150360788	23.0523585341
H	-7.1194514999	-36.4045939626	23.6378795581
N	-8.7944162765	-36.3425215494	22.4216439199
C	-9.5782194373	-37.1725118377	21.7269647067
H	-14.3231491834	-36.5523558744	22.6108500263
H	-12.9184683111	-32.6511458534	16.4380924489

Int2b$_{II}$

Energy with the medium-sized basis set: -2502.74804

Solution energy with the medium-sized basis set: -2502.90009

Energy with larger basis sets: -2503.44282

Zero-point energy: 1.01565

Co	-11.8560484062	-31.6206404566	20.2826497719
N	-12.1055958974	-30.9085323651	18.5558224148
N	-13.4983349606	-30.7711966777	20.8672529271
N	-11.2087663024	-32.0558264070	22.0503978425
N	-10.3002900162	-32.3901446217	19.5084730224
C	-10.9426310162	-31.0498237636	17.6358564401
C	-9.9046574662	-29.9606240237	17.9774707650
H	-9.5741422323	-30.0618927599	19.0146075963
H	-10.3207326178	-28.9632911609	17.8616969131
H	-9.0271952388	-30.0258020056	17.3317776136
C	-11.6075578673	-30.8819930362	16.2245385758
C	-10.6707593852	-30.3202064157	15.1493603975
H	-11.2107273446	-30.1944798381	14.2058560087
H	-9.8400232651	-31.0084746751	14.9606577958
H	-10.2465289615	-29.3513669743	15.4178201411
C	-12.2087812915	-32.2101434131	15.7133640145
H	-12.7603756294	-32.0335737000	14.7858361327
H	-11.4431953814	-32.9571639113	15.4968072183
C	-12.8201780295	-29.9477123323	16.5717788212
H	-13.6421355940	-30.1695542230	15.8859630103
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5555486734	-27.9166222612	16.7408014529
H	-11.9054484368	-28.0832782437	17.3239559763
C	-13.1394106192	-30.3559828522	17.9946326312
C	-14.3996588368	-30.1128104623	18.6770392261
C	-15.5725233088	-29.6694587212	17.8232701577
H	-15.7382318504	-28.5885899095	17.8760224654
H	-16.4986780462	-30.1580221864	18.1257978915

H	-15.4186007033	-29.9210068348	16.7739018121
C	-14.5217674147	-30.2752052279	20.0348911946
C	-15.7886517248	-30.0751503909	20.8861944145
C	-16.6803304274	-28.8639153058	20.5676511242
H	-17.3480507114	-28.6832872114	21.4153958912
H	-17.3183529054	-29.0330835660	19.7013663735
H	-16.1008473923	-27.9538093988	20.3957419559
C	-16.6175476932	-31.3841428109	20.7976395476
H	-17.4860516072	-31.3188854453	21.4603821896
H	-16.0208982905	-32.2543222974	21.0924767375
C	-15.1638058633	-29.9752143150	22.3089049169
H	-15.8161136859	-30.4252667654	23.0646871995
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6755299309	-27.9339169921	22.9090829710
H	-14.1551361608	-28.0528913957	22.0017520305
C	-13.8904148360	-30.7523821394	22.1350292036
C	-13.1920021387	-31.3242472536	23.2290469540
H	-13.6789477606	-31.2368051908	24.1935561119
C	-11.9534453255	-31.9173046891	23.2010779050
C	-11.2053506095	-32.4576151617	24.4060014097
C	-11.5583323908	-33.9513662572	24.6184154058
H	-11.0155861676	-34.3226829146	25.4932335457
H	-11.2975744690	-34.5616535407	23.7546065912
H	-12.6294833900	-34.0702367415	24.8096654880
C	-11.5049519610	-31.6915994954	25.7037045714
H	-10.8268086151	-32.0167757548	26.4977517103
H	-12.5204386571	-31.9112939977	26.0467570801
H	-11.4116932466	-30.6087111514	25.5926077226
C	-9.7388434329	-32.3378181583	23.8795048091
H	-9.1328215325	-33.1738723560	24.2376343109
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.6957812303	-30.1466757095	23.9865994366
H	-8.9461516978	-30.9602699590	25.3746835114
C	-9.9373517380	-32.4117963700	22.3626668210
C	-8.9294076773	-32.7773613254	21.4309971909
C	-7.6293602336	-33.2781928017	21.9796761219
H	-6.8079680201	-33.1711591241	21.2768544308
H	-7.7534949655	-34.3514647994	22.2034970709
H	-7.3471164497	-32.7800010692	22.9077313403
C	-9.1578313271	-32.7940811520	19.9871641741
C	-8.2394764400	-33.3476747741	18.8629808079
C	-8.1692155729	-34.8845533909	19.0123988510
H	-7.5090447051	-35.3070518069	18.2505732443
H	-9.1490785670	-35.3554586662	18.9005921759

H	-7.7719844277	-35.1713017265	19.9886942930
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1175450169	-33.1915238166	19.4806146363
H	-6.4215772485	-33.0055612043	17.7656821282
C	-8.9921910535	-32.8746896850	17.5603537085
H	-8.4643169122	-31.9832073194	17.2140688316
C	-8.9874066412	-33.8750742237	16.4023687838
H	-9.5978344723	-34.7590839281	16.6128327695
H	-9.3693291431	-33.4127696797	15.4885053571
C	-10.3825655179	-32.4456511661	18.0366546863
H	-11.1383851432	-33.1987836898	17.7993668206
H	-14.2295677006	-28.5699692928	23.6952235441
H	-8.0949145603	-30.8767417104	23.8306353666
H	-6.8132436288	-31.6788191968	18.8696429907
H	-12.2412939147	-28.0891117994	15.5850276947
H	-7.9713127095	-34.2146343157	16.1824317041
H	-16.9836572692	-31.5554849323	19.7817532147
C	-14.3314328942	-36.2947985881	21.5461598381
H	-15.3745555255	-36.1424369686	21.2508166864
H	-13.9394183778	-37.1560759366	20.9961807035
C	-13.5059263779	-35.0425661001	21.2782125629
H	-13.9352148702	-34.1737018041	21.7875729656
O	-12.1625437801	-35.1911258222	21.7878738227
C	-13.3278636299	-34.7282336610	19.7827973494
H	-14.1420540913	-35.1334485613	19.1729224959
O	-13.3178052145	-33.2771744788	19.6182768741
H	-13.5070685030	-33.0597193404	18.6951706017
C	-11.9982039456	-35.3220182639	19.4809769474
H	-11.6021779778	-35.5384357404	18.4967603009
C	-11.2543631687	-35.5324149201	20.7561573773
H	-10.3878860815	-34.8686610481	20.8670979985
N	-10.7068620142	-36.8735731696	20.8932092568
C	-11.1845713053	-38.0827476371	20.4004762791
H	-12.0558643044	-38.1247156995	19.7607960309
N	-10.4715476774	-39.1171213690	20.7733107538
C	-9.4795700650	-38.5814821066	21.5658051168
C	-8.3986039938	-39.1658275665	22.2758747827
N	-8.1540117068	-40.4821287051	22.2618552782
H	-7.3705758142	-40.8446421354	22.7867847279
H	-8.7508069546	-41.1112368784	21.7451689328
N	-7.5840334050	-38.3542729607	22.9887127841
C	-7.8264447437	-37.0466253171	22.9920867791
H	-7.1396926545	-36.4428099220	23.5817248092
N	-8.8133811225	-36.3666313390	22.3645063932

C	-9.6006886906	-37.1898893848	21.6654619915
H	-14.3027353608	-36.5347575678	22.6115022992
H	-12.9160694782	-32.6490228132	16.4283342995

Int2b$_{IV}$

Energy with the medium-sized basis set: -2502.74775

Solution energy with the medium-sized basis set: -2502.89882

Energy with larger basis sets: -2503.44201

Zero-point energy: 1.01584

Co	-11.8257801203	-31.5852779297	20.3102247993
N	-12.0944132248	-30.8899780806	18.5813294834
N	-13.4775702845	-30.7675922387	20.9008636450
N	-11.1911018250	-32.0685943471	22.0604345894
N	-10.2894733783	-32.3672983963	19.5289723643
C	-10.9449427165	-31.0505936380	17.6494016647
C	-9.8941632064	-29.9650218402	17.9627680503
H	-9.5516811286	-30.0529814246	18.9973817497
H	-10.3056300692	-28.9668252740	17.8375800634
H	-9.0248687400	-30.0444899479	17.3077313604
C	-11.6252176042	-30.8933454025	16.2443300489
C	-10.6981006226	-30.3494973684	15.1513266056
H	-11.2494826426	-30.2300514996	14.2136156061
H	-9.8747210625	-31.0457000357	14.9592864348
H	-10.2640018470	-29.3807177539	15.4036666705
C	-12.2393728295	-32.2230845543	15.7531005491
H	-12.7981162323	-32.0538752686	14.8280214340
H	-11.4802306587	-32.9776674190	15.5391761610
C	-12.8276790127	-29.9468385802	16.5958426224
H	-13.6593723572	-30.1735260766	15.9233985616
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5498795128	-27.9097484784	16.7516775498
H	-11.8903724883	-28.0771107702	17.3070795528
C	-13.1328514155	-30.3356132508	18.0274172458
C	-14.3866880730	-30.0896535196	18.7173287629
C	-15.5644444487	-29.6325363011	17.8763859361
H	-15.7651955882	-28.5629999088	17.9910196228
H	-16.4772306017	-30.1683767294	18.1391424802
H	-15.3938756557	-29.8152786702	16.8160505615
C	-14.5062567356	-30.2738488844	20.0719645830
C	-15.7769692322	-30.1146844701	20.9261078883
C	-16.7183852126	-28.9387296042	20.6193048529

H	-17.3825924959	-28.7871531060	21.4756195454
H	-17.3593880408	-29.1323237445	19.7603286657
H	-16.1788882967	-28.0054566282	20.4431703192
C	-16.5592810114	-31.4519362847	20.8358761409
H	-17.4270132228	-31.4194921103	21.5018930851
H	-15.9323111252	-32.3030031313	21.1224239930
C	-15.1465384608	-29.9911652685	22.3436406787
H	-15.7887799607	-30.4358047693	23.1109436830
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6841719688	-27.9481169168	22.9134063216
H	-14.1788350780	-28.0581811661	21.9793507749
C	-13.8661537160	-30.7576437162	22.1695948471
C	-13.1666905201	-31.3429327567	23.2591298705
H	-13.6505233382	-31.2628576746	24.2256966548
C	-11.9362157106	-31.9477270898	23.2178439894
C	-11.1765852452	-32.5030991493	24.4090639842
C	-11.4940595211	-34.0092234146	24.5942475925
H	-10.9596972050	-34.3744253589	25.4769857974
H	-11.1899365643	-34.6015389548	23.7325143740
H	-12.5651413178	-34.1617408312	24.7568596777
C	-11.4834877659	-31.7680346213	25.7222909885
H	-10.7939679989	-32.0946640895	26.5059200334
H	-12.4927264610	-32.0135162649	26.0665185083
H	-11.4111842335	-30.6816791730	25.6306927152
C	-9.7140560257	-32.3464276938	23.8805995216
H	-9.0898683800	-33.1745064328	24.2248899081
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.7168873446	-30.1584391689	23.9969505319
H	-8.9374651056	-30.9594736206	25.3738681711
C	-9.9142342022	-32.4007602165	22.3681895437
C	-8.8928693127	-32.7234163799	21.4349361472
C	-7.5624697977	-33.1551902813	21.9722463924
H	-6.7484920265	-32.9518273124	21.2816541175
H	-7.5969042932	-34.2403433186	22.1533562437
H	-7.3210921907	-32.6789274746	22.9221224918
C	-9.1380150168	-32.7602459418	20.0006004722
C	-8.2401109585	-33.3386378708	18.8789733419
C	-8.1899382664	-34.8731397763	19.0605748297
H	-7.5546221908	-35.3243962757	18.2943259212
H	-9.1815332916	-35.3285575516	18.9838331288
H	-7.7746411110	-35.1418367834	20.0345438701
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1133172042	-33.1960418659	19.4735282456
H	-6.4313091207	-33.0091633576	17.7625450347

C	-9.0041900742	-32.8868673305	17.5762794999
H	-8.4785389975	-32.0022801490	17.2092619717
C	-9.0142598115	-33.9066865268	16.4356381742
H	-9.6226701294	-34.7862513148	16.6690047047
H	-9.4071776645	-33.4592602833	15.5189151355
C	-10.3884155358	-32.4469808768	18.0618146780
H	-11.1511410445	-33.2024792444	17.8469726607
H	-14.2117366138	-28.5400849488	23.6848995597
H	-8.1021508181	-30.8516575327	23.8232210271
H	-6.8064267141	-31.6786181770	18.8663513481
H	-12.2567969461	-28.1040145993	15.5744161320
H	-8.0009120714	-34.2504003046	16.2090188108
H	-16.9218213769	-31.6290138277	19.8196421113
C	-14.4705759102	-36.2262963922	21.5405698139
H	-15.5189318062	-36.1195570651	21.2440043752
H	-14.0508413250	-37.0896871977	21.0147932214
C	-13.6900082158	-34.9543562835	21.2340947425
H	-14.1559331403	-34.0839686329	21.7064305890
O	-12.3445211673	-35.0226320810	21.7582496396
C	-13.4924671032	-34.6937694078	19.7342933747
H	-14.3272085589	-35.0576957520	19.1270390662
O	-13.3666949555	-33.2529284486	19.5548563977
H	-13.4767532196	-33.0371750371	18.6193518686
C	-12.1909235641	-35.3665502768	19.4681203298
H	-11.7905053573	-35.6387314340	18.4994268966
C	-11.4315050482	-35.4338772031	20.7542027274
H	-10.5877560862	-34.7385395057	20.7915068868
N	-10.8498207024	-36.7422290526	21.0244318741
C	-11.2520256584	-37.9957005016	20.5874202446
H	-12.0690783186	-38.1119901358	19.8883103602
N	-10.5373931279	-38.9785400000	21.0844426723
C	-9.6258426555	-38.3560809550	21.9050415747
C	-8.5779635168	-38.8499960299	22.7252168678
N	-8.2912142096	-40.1537293615	22.8201727081
H	-7.5414843104	-40.4525887969	23.4282526281
H	-8.8320321639	-40.8377329274	22.3109991728
N	-7.8447613311	-37.9624711019	23.4374780419
C	-8.1323231374	-36.6685815346	23.3355009849
H	-7.5182436282	-36.0018744157	23.9375619366
N	-9.0830085641	-36.0669296598	22.5811094246
C	-9.7953569240	-36.9642556695	21.8952534220
H	-14.4316616766	-36.4324265278	22.6127498954
H	-12.9447218129	-32.6501241846	16.4776264565

Int2b$_{VI}$

Energy with the medium-sized basis set:	-2502.72938
Solution energy with the medium-sized basis set:	-2502.88208
Energy with larger basis sets:	-2503.42546
Zero-point energy:	1.01406

Co	-12.2483439246	-32.2434350896	20.2010819718
N	-12.2420707115	-31.1101885459	18.5096849356
N	-13.7071868995	-30.9358572258	20.8114303438
N	-11.2270589381	-31.9958583650	21.9929657389
N	-10.4141508420	-32.6929095938	19.4213316079
C	-11.0275786998	-31.1706984168	17.6698587966
C	-10.0612389553	-30.0879859444	18.2003048855
H	-9.8403983141	-30.2625893939	19.2556155599
H	-10.5080597588	-29.0994719400	18.1247696588
H	-9.1212746136	-30.0671725930	17.6466051881
C	-11.5858986423	-30.8721477307	16.2315281349
C	-10.5652383183	-30.2347466762	15.2819372154
H	-11.0272958655	-30.0228806766	14.3127294229
H	-9.7279951394	-30.9170260538	15.1011588468
H	-10.1561855434	-29.2978298793	15.6636174634
C	-12.1487490195	-32.1463890267	15.5656095351
H	-12.6314187198	-31.8890990380	14.6182793360
H	-11.3710635860	-32.8804332042	15.3440752854
C	-12.8192364932	-29.9501872528	16.5703975178
H	-13.6186353785	-30.1633995997	15.8531313814
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5481291346	-27.9118695083	16.7622640452
H	-11.8829914255	-28.0865025373	17.3046380958
C	-13.2047832746	-30.4381701286	17.9623704966
C	-14.4816350319	-30.1489213357	18.6313363075
C	-15.5950001354	-29.5978360729	17.7635761176
H	-15.6690380993	-28.5064928403	17.8181260010
H	-16.5624299115	-30.0066650062	18.0543702817
H	-15.4468318524	-29.8579861748	16.7149377867
C	-14.6628835602	-30.3275952591	19.9825199057
C	-15.8915132064	-29.9802372106	20.8485475248
C	-16.6447804564	-28.6819633610	20.5195123704
H	-17.3023535617	-28.4261994351	21.3555591640
H	-17.2832964921	-28.7876892369	19.6431339683
H	-15.9682847667	-27.8405052928	20.3520812223
C	-16.8682424662	-31.1831715944	20.7839776797

H	-17.7248321414	-31.0037076890	21.4413485486
H	-16.3826794281	-32.1119936693	21.1047853042
C	-15.2431515908	-29.9378067825	22.2749273344
H	-15.9164175796	-30.3642063366	23.0274814731
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6382827789	-27.8839788983	22.9137045924
H	-14.1179398724	-28.0739535089	22.0204774236
C	-14.0179681087	-30.7922808971	22.0880749189
C	-13.2509355818	-31.3177386300	23.1724275347
H	-13.7074962239	-31.2202224155	24.1516926616
C	-11.9834429717	-31.8634102716	23.1369704882
C	-11.2375302376	-32.4293786418	24.3329699207
C	-11.6171252371	-33.9298446167	24.4588973681
H	-11.0496946547	-34.3802208939	25.2793256534
H	-11.3981916561	-34.4776802352	23.5418526990
H	-12.6834302397	-34.0351515154	24.6840275037
C	-11.5362918734	-31.7202027493	25.6594132359
H	-10.8715592277	-32.0926499792	26.4440390682
H	-12.5593683385	-31.9318477667	25.9849363094
H	-11.4183960775	-30.6363714011	25.5937021577
C	-9.7633478235	-32.3033979088	23.8206033745
H	-9.1766786183	-33.1642620514	24.1526795204
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.6702252702	-30.1201968347	24.0121471062
H	-8.9581154220	-31.0045572460	25.3767754050
C	-9.9655316206	-32.3520789231	22.3004627918
C	-8.9705536849	-32.7321375969	21.3508173908
C	-7.5665009303	-32.9497364028	21.8354559324
H	-6.9124152542	-32.1441094329	21.4818886862
H	-7.1579936983	-33.8858148047	21.4510570002
H	-7.4957277793	-32.9730765738	22.9202071725
C	-9.2213993687	-32.8761403977	19.9152601666
C	-8.2392866828	-33.3476128607	18.8064055978
C	-8.1799407541	-34.8914832420	18.9304046374
H	-7.4872641616	-35.3008969572	18.1908426712
H	-9.1602040709	-35.3492993018	18.7635512932
H	-7.8412777907	-35.2039845948	19.9204352084
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1504840682	-33.1926893876	19.5093529385
H	-6.3819286797	-32.9993312752	17.7810306551
C	-8.9831813191	-32.8793868088	17.5004953185
H	-8.5191971939	-31.9343708246	17.2075298563
C	-8.8637540663	-33.8257441890	16.3028684469
H	-9.4120258224	-34.7607013764	16.4542496592

H	-9.2516565071	-33.3522779145	15.3968169987
C	-10.4253353265	-32.5952839606	17.9543596760
H	-11.1284881308	-33.3498415345	17.5843270998
H	-14.2418716814	-28.6240036865	23.6992362285
H	-8.0867563775	-30.8864823993	23.8463635272
H	-6.8204358678	-31.6785176875	18.8702573099
H	-12.2608807513	-28.0933577218	15.5769719496
H	-7.8180885067	-34.0785825383	16.1041511763
H	-17.2474128171	-31.3350586502	19.7697923470
C	-14.6723030129	-35.5844057816	21.9978387553
H	-15.7621103673	-35.5234102143	21.9164299491
H	-14.3673104437	-36.5987755414	21.7368201689
C	-14.0338186536	-34.5312056348	21.1099794733
H	-14.4336133543	-33.5436864151	21.3539007955
O	-12.5859548674	-34.4181587401	21.2878756048
C	-14.1060870294	-34.7802610714	19.6007228192
H	-15.0735675385	-35.1279756018	19.2317720000
O	-13.8007518628	-33.4594247972	19.0280386220
H	-13.6870064709	-33.5207163720	18.0689840412
C	-12.9517747138	-35.6968170948	19.3825622284
H	-12.8044370263	-36.3731228976	18.5502897612
C	-11.9389313603	-35.4253305478	20.4538180910
H	-11.0333161544	-34.9361098523	20.0865076427
N	-11.5071808159	-36.5871805781	21.1864923145
C	-12.0723029094	-37.8657391205	21.2551487814
H	-12.9658584461	-38.1152351565	20.6991327496
N	-11.3957529758	-38.6870539405	22.0070081508
C	-10.3287334905	-37.9389014168	22.4737103939
C	-9.2397461877	-38.2604958180	23.3211132130
N	-9.0727011324	-39.4769097345	23.8577696047
H	-8.2705476366	-39.6528458916	24.4444524085
H	-9.7255179871	-40.2196030358	23.6593252316
N	-8.3378371424	-37.2901167483	23.5921345794
C	-8.5023777376	-36.0885737549	23.0415287975
H	-7.7406079984	-35.3558104600	23.2967189824
N	-9.4764897488	-35.6594768883	22.2147271550
C	-10.3649304224	-36.6363404481	21.9761833612
H	-14.3916040364	-35.4013816643	23.0377681542
H	-12.9088198167	-32.6351164435	16.1891959055

Int2b$_{III}$

Energy with the medium-sized basis set: -2503.07031

Solution energy with the medium-sized basis set: -2503.12493

Energy with larger basis sets: -2503.77258

Zero-point energy: 1.01661

Co	-11.8056262524	-31.5712941190	20.3277273683
N	-12.0834291918	-30.8909319955	18.5953222856
N	-13.4516619711	-30.7549513052	20.9160795708
N	-11.1753435425	-32.0529748230	22.0665937635
N	-10.2784386566	-32.3664797035	19.5404178989
C	-10.9422204211	-31.0508803983	17.6607427752
C	-9.8859952727	-29.9675145164	17.9681148542
H	-9.5284350892	-30.0789459341	18.9943963206
H	-10.3022569641	-28.9675353630	17.8709834728
H	-9.0275849229	-30.0353134813	17.2968627237
C	-11.6258273968	-30.8899970686	16.2568210912
C	-10.7008635730	-30.3461625032	15.1617953217
H	-11.2514701343	-30.2312227529	14.2222906281
H	-9.8732098343	-31.0390975276	14.9747409620
H	-10.2711991227	-29.3748722860	15.4132416730
C	-12.2400099701	-32.2186961167	15.7618185712
H	-12.7997638508	-32.0462878288	14.8371941684
H	-11.4806606683	-32.9732499646	15.5483023822
C	-12.8270161112	-29.9453297075	16.6086788428
H	-13.6602896210	-30.1771191105	15.9387123710
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5441470477	-27.9100993866	16.7805194968
H	-11.8698606230	-28.0797475770	17.2882637423
C	-13.1280315688	-30.3336583817	18.0448462197
C	-14.3653003306	-30.0868295789	18.7355425007
C	-15.5531989597	-29.6294876861	17.9077730495
H	-15.7881494530	-28.5713185517	18.0570627750
H	-16.4520718780	-30.2012703794	18.1452046950
H	-15.3743499327	-29.7694084075	16.8418273492
C	-14.4720249730	-30.2781003381	20.0992144115
C	-15.7543647627	-30.1384736890	20.9461531086
C	-16.7202721513	-28.9831556913	20.6364345005
H	-17.3843446026	-28.8390109137	21.4949664472
H	-17.3589419300	-29.1916685369	19.7786818449
H	-16.1986315679	-28.0406089834	20.4545377822
C	-16.5098808670	-31.4894455191	20.8512521905
H	-17.3817613184	-31.4777461340	21.5138488995
H	-15.8642506366	-32.3259283451	21.1373939742
C	-15.1327248857	-29.9986936596	22.3648606004
H	-15.7824568952	-30.4347475689	23.1312783543

C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6838884242	-27.9424031670	22.8963988816
H	-14.1705042555	-28.0710636748	21.9775168023
C	-13.8512313438	-30.7761629937	22.2037189459
C	-13.1728730624	-31.3763210734	23.2595244335
H	-13.6488300516	-31.3253387807	24.2314792274
C	-11.9064111297	-31.9558655462	23.1952212384
C	-11.1543029965	-32.5133592619	24.3962718705
C	-11.4836026269	-34.0146648899	24.5732458244
H	-10.9444823883	-34.3988361004	25.4457576391
H	-11.2000071609	-34.5991761802	23.6990122926
H	-12.5552696800	-34.1600128970	24.7447577225
C	-11.4677693962	-31.7835853119	25.7108098407
H	-10.7783924277	-32.1091723545	26.4960298314
H	-12.4782392608	-32.0308936659	26.0506356639
H	-11.3996473963	-30.6966960289	25.6215916243
C	-9.6903367119	-32.3564745046	23.8811232004
H	-9.0635198784	-33.1728734051	24.2491975766
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.7224067026	-30.1706104545	23.9744698200
H	-8.9499333263	-30.9397573116	25.3753062517
C	-9.8703003344	-32.4317689187	22.3619041968
C	-8.8838090381	-32.7697208598	21.4510008713
C	-7.5374798079	-33.2142499700	21.9879345084
H	-6.7272746076	-33.0091086087	21.2918351961
H	-7.5548676921	-34.2896152693	22.1925950862
H	-7.2841640334	-32.7032197179	22.9180912893
C	-9.1364578569	-32.7821121149	20.0193591470
C	-8.2377517360	-33.3464943914	18.8845806620
C	-8.1651291464	-34.8807415827	19.0452450667
H	-7.5111913919	-35.3157730023	18.2842092955
H	-9.1473458481	-35.3500823810	18.9474323755
H	-7.7685275725	-35.1541618197	20.0253339129
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1127776174	-33.1880606111	19.4776416578
H	-6.4308681738	-33.0082094798	17.7617628103
C	-9.0007880319	-32.8839080323	17.5860816799
H	-8.4729121854	-31.9986389550	17.2226068495
C	-9.0142514413	-33.8958787375	16.4386420394
H	-9.6243870053	-34.7752657057	16.6692230870
H	-9.4100293763	-33.4433860097	15.5248826466
C	-10.3826130533	-32.4444142616	18.0759300278
H	-11.1414954283	-33.1987988812	17.8478786739
H	-14.2156782159	-28.5297781338	23.6869063962

H	-8.0993798180	-30.8500697438	23.8286226806
H	-6.8152720462	-31.6783300882	18.8672393795
H	-12.2813980653	-28.1025090847	15.5657181477
H	-8.0023854217	-34.2434901164	16.2090981342
H	-16.8631023151	-31.6717968492	19.8318896769
C	-14.4242745851	-36.2265040588	21.5603470887
H	-15.4603551469	-36.0127697829	21.2768724867
H	-14.0835027468	-37.1048748441	21.0022057915
C	-13.5272633875	-35.0254246345	21.2870983788
H	-13.8995053942	-34.1317493465	21.7998798107
O	-12.2003288172	-35.2693961203	21.7895539884
C	-13.3556938562	-34.7150611140	19.7885714230
H	-14.1805752244	-35.1184909938	19.1889720700
O	-13.3391434096	-33.2710362948	19.6327114641
H	-13.4264310350	-33.0460512497	18.6967066391
C	-12.0393067216	-35.3313904733	19.4773445923
H	-11.6357431367	-35.5084616485	18.4883402651
C	-11.2840249844	-35.5571432460	20.7445884480
H	-10.4294069859	-34.8824829604	20.8704885664
N	-10.7277555754	-36.8984253776	20.8510659348
C	-11.2335609425	-38.0974661154	20.3623877176
H	-12.1134347093	-38.1142139249	19.7329874671
N	-10.5381007154	-39.1456125195	20.7210216546
C	-9.5215239316	-38.6258211396	21.5061346381
C	-8.4441980629	-39.2267255231	22.1967636541
N	-8.2236214753	-40.5559948864	22.1731791872
H	-7.4592476999	-40.9360536907	22.7087916603
H	-8.8544534728	-41.1668232117	21.6798299058
N	-7.6081511105	-38.4356750114	22.8997254830
C	-7.8313162742	-37.1159620678	22.9050859049
H	-7.1244100704	-36.5264949563	23.4864351843
N	-8.8032233568	-36.4222622854	22.2927905689
C	-9.6195569936	-37.2360141026	21.6086820928
H	-14.3965470756	-36.4726907579	22.6244945402
H	-12.9427128549	-32.6448059429	16.4881915072

Int2b$_V$

Energy with the medium-sized basis set:	-2503.03886
Solution energy with the medium-sized basis set:	-2503.09276
Energy with larger basis sets:	-2503.74306
Zero-point energy:	1.01330

Co	-12.0695972510	-31.9894256666	20.2616237021
N	-12.2257164333	-31.0698707280	18.4808994724
N	-13.6230365347	-30.8523173772	20.8440247556
N	-11.2381381397	-32.1192059060	22.0509305167
N	-10.3691894513	-32.5964392569	19.4304630559
C	-11.0253303694	-31.1401844341	17.6260503969
C	-10.0371214571	-30.0470036355	18.0968165592
H	-9.7354297655	-30.2394916947	19.1284812955
H	-10.4949272270	-29.0612386343	18.0721376264
H	-9.1394651650	-30.0115989057	17.4763918653
C	-11.6253530704	-30.8769446356	16.1971261747
C	-10.6398495561	-30.2656689487	15.1949620462
H	-11.1349022065	-30.0823126307	14.2354303778
H	-9.8053618486	-30.9501965520	15.0081079143
H	-10.2214587353	-29.3174023444	15.5371104695
C	-12.2054723455	-32.1714902300	15.5864470933
H	-12.7242684131	-31.9439833324	14.6499268793
H	-11.4286409291	-32.9057064774	15.3604047035
C	-12.8457584250	-29.9435543718	16.5471575989
H	-13.6536215019	-30.1388359597	15.8339119584
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5423292241	-27.9056386529	16.7777057785
H	-11.8810380853	-28.1111180895	17.3119666631
C	-13.2126037748	-30.4133011152	17.9518598232
C	-14.4561409095	-30.1234516026	18.6559979315
C	-15.6054431071	-29.5911544394	17.8177841814
H	-15.7513361449	-28.5124190085	17.9346699155
H	-16.5477888395	-30.0777978219	18.0753477399
H	-15.4428762717	-29.7794551755	16.7557272502
C	-14.5976097209	-30.2993546060	20.0213432752
C	-15.8496879050	-30.0305933810	20.8868503879
C	-16.6902482754	-28.7830998074	20.5739783862
H	-17.3525065755	-28.5743018030	21.4203850270
H	-17.3298009119	-28.9238759045	19.7028269617
H	-16.0714725406	-27.8985226761	20.4043697344
C	-16.7407556292	-31.2961060224	20.8035458874
H	-17.6054399992	-31.1916030747	21.4673973648
H	-16.1835761906	-32.1911583617	21.1001587971
C	-15.2110747921	-29.9608755599	22.3126056190
H	-15.8837190749	-30.3835312427	23.0672203461
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6490601166	-27.8942953302	22.9017751434
H	-14.1307576958	-28.0835580176	22.0027192386
C	-13.9609411721	-30.7939744240	22.1389908738

C	-13.2357197773	-31.3484174763	23.2095479371
H	-13.6900509733	-31.2375156858	24.1874514650
C	-11.9663600805	-31.9361041377	23.1727251956
C	-11.2048092510	-32.4586425281	24.3840257459
C	-11.5520131848	-33.9578321876	24.5711675158
H	-11.0000347956	-34.3514825816	25.4313535309
H	-11.2927832613	-34.5446222428	23.6892417697
H	-12.6218471340	-34.0871543873	24.7649532687
C	-11.5075902874	-31.7097894954	25.6878896708
H	-10.8307361154	-32.0397983942	26.4820640773
H	-12.5256712697	-31.9304189516	26.0237113187
H	-11.4152016848	-30.6259574996	25.5843471518
C	-9.7334298011	-32.3314973898	23.8590730449
H	-9.1329951928	-33.1661082836	24.2325824778
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.6826574209	-30.1428059607	23.9700005509
H	-8.9669185160	-30.9558338154	25.3776156646
C	-9.9232060914	-32.4458569801	22.3311390652
C	-8.9505622880	-32.7819685928	21.3887522489
C	-7.5457044453	-33.0776420989	21.8744373065
H	-6.8272014574	-32.3340283428	21.5147945833
H	-7.2095898213	-34.0627101682	21.5433893335
H	-7.4869675567	-33.0803653376	22.9619270746
C	-9.1955864938	-32.8526306203	19.9453783948
C	-8.2360694934	-33.3435703239	18.8180294662
C	-8.1861204751	-34.8858282574	18.9229307696
H	-7.5174204204	-35.3011323618	18.1638060871
H	-9.1757869417	-35.3298388139	18.7782361526
H	-7.8269048715	-35.2064915578	19.9027048487
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1542589060	-33.1829998820	19.5190331953
H	-6.3787205490	-33.0064781706	17.7832759295
C	-8.9701253304	-32.8531327652	17.5137457652
H	-8.4885433310	-31.9138222076	17.2295505507
C	-8.8653906825	-33.7901588975	16.3081579289
H	-9.4206029003	-34.7216357963	16.4589760009
H	-9.2600476274	-33.3085902088	15.4084700596
C	-10.4042489074	-32.5482379644	17.9653564530
H	-11.1023009300	-33.3211246386	17.6236720374
H	-14.2313865452	-28.5932478352	23.6947862422
H	-8.0861657360	-30.8907084988	23.8453594102
H	-6.8235984709	-31.6779939203	18.8659158673
H	-12.2575380141	-28.0730918900	15.5841223092
H	-7.8234428841	-34.0526598399	16.0993252371

H	-17.1121793396	-31.4528127349	19.7867038751
C	-14.4662691429	-36.3790704627	21.4963667972
H	-15.5125824872	-36.2674266453	21.1933121173
H	-14.0541459735	-37.2656285046	21.0043515892
C	-13.6651673126	-35.1308771121	21.1463910374
H	-14.1216442776	-34.2390564041	21.5894347850
O	-12.3276726278	-35.2108812263	21.6750196972
C	-13.4868962870	-34.9185236290	19.6324794902
H	-14.2950748134	-35.3670692262	19.0450982291
O	-13.5040493292	-33.4749859173	19.3906689924
H	-13.4821444968	-33.2989020835	18.4388742350
C	-12.1444782297	-35.5060099647	19.3804969011
H	-11.7177681121	-35.7312082071	18.4111195985
C	-11.3926888673	-35.5867979936	20.6694242603
H	-10.5612571662	-34.8773587312	20.7304351979
N	-10.7911611638	-36.8876473948	20.9136295369
C	-11.2339634126	-38.1560790900	20.5546604924
H	-12.1187367664	-38.2864702535	19.9459605137
N	-10.4720642428	-39.1214570623	21.0000044575
C	-9.4722389730	-38.4698990296	21.7046779432
C	-8.3439183313	-38.9345090851	22.4193069171
N	-8.0464838750	-40.2445219718	22.5254237171
H	-7.2460038980	-40.5236053169	23.0703712735
H	-8.6523968505	-40.9378045315	22.1170933191
N	-7.5371101225	-38.0285686305	23.0091562969
C	-7.8379895665	-36.7294656897	22.8878671365
H	-7.1512981962	-36.0436458502	23.3808249942
N	-8.8664136247	-36.1591888846	22.2420840221
C	-9.6485386417	-37.0852006137	21.6706873916
H	-14.4303336173	-36.5458332173	22.5754783453
H	-12.9357179876	-32.6475819367	16.2523361560

$\mathbf{Int3_{II}}$

Energy with the medium-sized basis set: -2502.42115

Solution energy with the medium-sized basis set: -2502.47587

Energy with larger basis sets: -2503.12793

Zero-point energy: 1.00542

Co	-11.8959852554	-31.7585143354	20.3040955540
N	-12.0649279122	-30.8930691047	18.6380571934
N	-13.4648425847	-30.8244598708	20.9263845184
N	-11.2023163933	-32.1040034778	22.0688936698

N	-10.3096518166	-32.4547628092	19.5498303307
C	-10.9243223127	-31.0726833335	17.7009034931
C	-9.8607000398	-30.0042907027	18.0245596847
H	-9.5063663658	-30.1294134645	19.0507690623
H	-10.2740297556	-29.0009824027	17.9385314121
H	-9.0021520579	-30.0687586798	17.3534956123
C	-11.6051895903	-30.8953891703	16.2965457868
C	-10.6726018066	-30.3492412616	15.2104755221
H	-11.2168723654	-30.2363125786	14.2671863968
H	-9.8440022147	-31.0425446881	15.0290647284
H	-10.2454739774	-29.3768933997	15.4640784621
C	-12.2328059644	-32.2188427250	15.8042433718
H	-12.8108240419	-32.0334218170	14.8933050661
H	-11.4764172868	-32.9669204836	15.5593064310
C	-12.8056437803	-29.9494022334	16.6472547703
H	-13.6410369855	-30.2003982472	15.9881218447
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5384638472	-27.9119207328	16.8097899422
H	-11.8370727520	-28.0586793551	17.2444407765
C	-13.1069251337	-30.3497631738	18.0808436092
C	-14.3651787814	-30.1389036161	18.7520508136
C	-15.5484728152	-29.7031948584	17.9089038567
H	-15.7673867385	-28.6353763969	18.0104714196
H	-16.4516317864	-30.2529335107	18.1765201713
H	-15.3744119220	-29.8964008347	16.8508859321
C	-14.4866677317	-30.3390298607	20.1062626925
C	-15.7585755908	-30.1700399612	20.9591055849
C	-16.7164485852	-29.0143061026	20.6298129854
H	-17.3773179836	-28.8495455516	21.4869087273
H	-17.3590935723	-29.2352426834	19.7783399001
H	-16.1885805262	-28.0790788965	20.4284347903
C	-16.5212672100	-31.5186079209	20.9040492515
H	-17.3868036542	-31.4844825907	21.5738603202
H	-15.8776966455	-32.3509320086	21.2059935616
C	-15.1255765128	-30.0023129430	22.3705408986
H	-15.7658419672	-30.4369949739	23.1457289968
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6887180291	-27.9495611627	22.8936055309
H	-14.1742203314	-28.0688360095	21.9758414307
C	-13.8470788089	-30.7838816132	22.2133380217
C	-13.1576925076	-31.3442595113	23.2862998577
H	-13.6211325917	-31.2548716913	24.2611661197
C	-11.9121626233	-31.9471712073	23.2175866900
C	-11.1600463381	-32.4943521114	24.4187266601

C	-11.5201623614	-33.9886130716	24.6046841414
H	-10.9539047182	-34.3906129318	25.4514391970
H	-11.2987075249	-34.5856277667	23.7191628361
H	-12.5865521966	-34.1047495701	24.8252443459
C	-11.4574626611	-31.7516516609	25.7295630674
H	-10.7698845840	-32.0839127519	26.5132531090
H	-12.4696053412	-31.9821848944	26.0758810059
H	-11.3729141539	-30.6665131999	25.6346363075
C	-9.7003234798	-32.3588854850	23.8910939588
H	-9.0764095099	-33.1735515858	24.2681208116
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.7197630946	-30.1684115554	23.9752583673
H	-8.9431429124	-30.9399335266	25.3739518014
C	-9.8920503416	-32.4727356941	22.3716001305
C	-8.9119697709	-32.8361969927	21.4648985330
C	-7.5748962689	-33.2974799662	22.0096309485
H	-6.7751150910	-33.1869106155	21.2817799859
H	-7.6351429638	-34.3556568096	22.2913027077
H	-7.2791722449	-32.7243839836	22.8896123552
C	-9.1594125361	-32.8463865926	20.0319017042
C	-8.2339769013	-33.3744026612	18.8917551178
C	-8.1145624212	-34.9066336703	19.0568707435
H	-7.4655403687	-35.3222091158	18.2808382140
H	-9.0815658391	-35.4078316463	18.9867506662
H	-7.6850397784	-35.1673287768	20.0262254648
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1056103981	-33.1619620966	19.4852732601
H	-6.4317474101	-33.0213161006	17.7651738800
C	-9.0151544153	-32.9311379466	17.5940360555
H	-8.4914778074	-32.0528674525	17.2081346273
C	-9.0407318100	-33.9635800774	16.4644512161
H	-9.6419324073	-34.8417513923	16.7195501420
H	-9.4555075644	-33.5279251419	15.5512679435
C	-10.3992818904	-32.4874608755	18.0836894971
H	-11.1788353887	-33.2094480774	17.8397639425
H	-14.2166429038	-28.5227856538	23.6873229360
H	-8.1013323721	-30.8577076387	23.8222901478
H	-6.8353517276	-31.6766046284	18.8467877794
H	-12.3279595546	-28.1272915653	15.5446064681
H	-8.0303877707	-34.3078419712	16.2235333307
H	-16.8810528206	-31.7257270472	19.8924655823
C	-14.5475500688	-35.4706744566	21.7688863041
H	-15.4041002887	-34.8475366785	21.4886371911
H	-14.5954855245	-36.4066457085	21.2027744601

C	-13.2458663754	-34.7415698934	21.4800827002
H	-13.2178532112	-33.7923487750	22.0230861053
O	-12.1543976993	-35.5683012795	21.9354317400
C	-12.9979939896	-34.4398314675	19.9738576768
H	-13.8283212612	-34.8567642601	19.3753799533
O	-13.0139934085	-33.0799602675	19.6044367742
C	-11.7466935178	-35.1946370789	19.6903358221
H	-11.3158330538	-35.3426335932	18.7095131023
C	-11.1171584528	-35.6508645112	20.9576761475
H	-10.2697434806	-35.0183796179	21.2617893254
N	-10.5828136441	-36.9959295787	20.9283947245
C	-11.2230463152	-38.1510314147	20.4978238013
H	-12.1808024690	-38.0977564222	19.9975037804
N	-10.5583627488	-39.2469797623	20.7582048594
C	-9.4204669828	-38.8054726098	21.4152961659
C	-8.3122625928	-39.4859741050	21.9675607088
N	-8.1876529251	-40.8270455055	21.9087788406
H	-7.4050828698	-41.2667323812	22.3668003158
H	-8.9266417297	-41.3862770217	21.5140725376
N	-7.3454288403	-38.7633464908	22.5700320377
C	-7.4787555010	-37.4327540944	22.6155756783
H	-6.6691583258	-36.9000025816	23.1113077834
N	-8.4713330681	-36.6677951973	22.1352768901
C	-9.4168954058	-37.4144536481	21.5456390370
H	-14.6252731268	-35.7119855055	22.8326853941
H	-12.9085679551	-32.6490708963	16.5512741837

$\mathbf{Int3_{II,BS}}$

Energy with the medium-sized basis set:	-2502.41445
Solution energy with the medium-sized basis set:	-2502.46807
Energy with larger basis sets:	-2503.10115
Zero-point energy:	1.00420

Co	-11.9648822112	-31.8772890166	20.2817692434
N	-12.0750810202	-30.9374807824	18.6212611614
N	-13.5089770072	-30.8539900192	20.8866576365
N	-11.1819618803	-32.0381365117	22.0483830159
N	-10.3527712683	-32.5650843642	19.5234208288
C	-10.9238714498	-31.1072279316	17.7017479785
C	-9.8653658671	-30.0494169214	18.0709862051
H	-9.5384820149	-30.1921715976	19.1041284846
H	-10.2798304420	-29.0452960798	17.9934446061

H	-8.9894921919	-30.0988681486	17.4215155740
C	-11.5783585122	-30.8905778321	16.2877127122
C	-10.6219647828	-30.3155786262	15.2375608041
H	-11.1455299931	-30.1739508641	14.2865366028
H	-9.7907988395	-31.0052678361	15.0539615931
H	-10.1994135916	-29.3518692077	15.5287492475
C	-12.1947380804	-32.1984463697	15.7409383750
H	-12.7431356792	-31.9866518869	14.8173503510
H	-11.4351009508	-32.9450254227	15.5008735335
C	-12.7875704225	-29.9529522106	16.6369752879
H	-13.6172893615	-30.2079519848	15.9718752363
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5431134534	-27.9221700977	16.8095545792
H	-11.8411710045	-28.0566621752	17.2488376914
C	-13.1041765201	-30.3572670825	18.0651453450
C	-14.3619915416	-30.1124739254	18.7179167341
C	-15.5244135485	-29.6291737774	17.8710539384
H	-15.7277269872	-28.5613485591	17.9991783972
H	-16.4392201521	-30.1715835922	18.1131535720
H	-15.3423564161	-29.7963672246	16.8099834275
C	-14.5024168852	-30.3253639714	20.0700855638
C	-15.7717685636	-30.1276824992	20.9208248580
C	-16.6987714283	-28.9460698072	20.5981086947
H	-17.3688738715	-28.7830219860	21.4483439117
H	-17.3328703140	-29.1380636946	19.7334125846
H	-16.1482885492	-28.0187430044	20.4223136576
C	-16.5651694854	-31.4585441841	20.8445726041
H	-17.4228926161	-31.4186996327	21.5241702079
H	-15.9357828396	-32.3116407533	21.1170000039
C	-15.1406529242	-29.9917381042	22.3380512192
H	-15.7904467526	-30.4313303842	23.1028504987
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6832447144	-27.9418864186	22.8955763783
H	-14.1601403535	-28.0614095561	21.9917389798
C	-13.8756988205	-30.7968901237	22.1759042764
C	-13.1817640565	-31.3542631547	23.2464268465
H	-13.6455764239	-31.2732621307	24.2215775269
C	-11.9180895309	-31.9224054884	23.1803139598
C	-11.1729642201	-32.4798544384	24.3827072044
C	-11.5427532595	-33.9728187853	24.5539491812
H	-10.9803716309	-34.3867351626	25.3977113728
H	-11.3231160295	-34.5585252696	23.6608042249
H	-12.6101300686	-34.0817219231	24.7733561465
C	-11.4782640838	-31.7435317746	25.6953193462

H	-10.7975957183	-32.0821702285	26.4823276110
H	-12.4935651963	-31.9727145340	26.0325172457
H	-11.3894886354	-30.6586489076	25.6050443468
C	-9.7062804898	-32.3472098155	23.8698020202
H	-9.0913286399	-33.1716396801	24.2401226996
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.7106143207	-30.1595759395	23.9805167473
H	-8.9512119728	-30.9539550922	25.3756091616
C	-9.8857629658	-32.4369138612	22.3488980919
C	-8.9168088410	-32.8286770620	21.4425362041
C	-7.5831924868	-33.2991940886	21.9906562790
H	-6.7813520946	-33.2013399462	21.2634273093
H	-7.6509659033	-34.3549665320	22.2795715244
H	-7.2821091492	-32.7214360703	22.8658489978
C	-9.1781682910	-32.8731865943	20.0129442221
C	-8.2320594195	-33.3824432545	18.8785747219
C	-8.0982258177	-34.9141408866	19.0415948584
H	-7.4197535680	-35.3152183106	18.2833901160
H	-9.0552819405	-35.4276525557	18.9361330179
H	-7.6945840595	-35.1752881273	20.0216773883
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1104552220	-33.1595352069	19.4906384202
H	-6.4222798803	-33.0185706620	17.7682099702
C	-9.0119791951	-32.9565284691	17.5762000764
H	-8.5044692038	-32.0684778601	17.1915150415
C	-9.0112713153	-33.9896626003	16.4463678474
H	-9.5969542874	-34.8794627820	16.6971743413
H	-9.4289836382	-33.5611552950	15.5310000143
C	-10.4116194845	-32.5399795555	18.0542124732
H	-11.1793699194	-33.2546976168	17.7546052750
H	-14.2263689726	-28.5501122776	23.6931151642
H	-8.0963235676	-30.8590027871	23.8322468205
H	-6.8412461661	-31.6767680956	18.8473859387
H	-12.3256480177	-28.1192311424	15.5474826414
H	-7.9932395626	-34.3146262467	16.2112554997
H	-16.9417023621	-31.6324352489	19.8325805118
C	-14.2256161796	-36.4756329755	21.4752491872
H	-15.2544324281	-36.1945054757	21.2254714334
H	-13.9014466285	-37.2505830663	20.7727574303
C	-13.3089043520	-35.2602806931	21.4138016204
H	-13.6820123689	-34.4580139908	22.0590769129
O	-11.9916267999	-35.6031931953	21.8988091995
C	-13.1008063373	-34.6921476388	19.9806376439
H	-13.9009380429	-35.0475706870	19.3114607586

O	-13.1717427156	-33.2863909019	19.9877972197
C	-11.7868561352	-35.2995123987	19.6105076636
H	-11.3856234895	-35.3817583211	18.6092937604
C	-11.0515117165	-35.7119079234	20.8388178859
H	-10.2054101416	-35.0560621995	21.0795728529
N	-10.4691804531	-37.0460771911	20.7751950724
C	-11.0419859546	-38.2119692211	20.2829011881
H	-11.9647061869	-38.1810493055	19.7195271103
N	-10.3542663753	-39.2916914267	20.5532731638
C	-9.2697411204	-38.8287556207	21.2811026122
C	-8.1690990035	-39.4849320155	21.8767602989
N	-7.9971780615	-40.8199411263	21.7985573352
H	-7.2274328881	-41.2436506951	22.2920833355
H	-8.6989401401	-41.3947175416	21.3606103020
N	-7.2586835607	-38.7446492442	22.5417819654
C	-7.4372519749	-37.4197703141	22.6040576924
H	-6.6699808909	-36.8712574107	23.1476478751
N	-8.4301737309	-36.6778254528	22.0904275870
C	-9.3212231979	-37.4417504131	21.4405898139
H	-14.2141155976	-36.9047483450	22.4806892102
H	-12.9001359502	-32.6449543207	16.4506583764

$\mathbf{Int3_{III}}$

Energy with the medium-sized basis set:	-2502.60589
Solution energy with the medium-sized basis set:	-2502.62796
Energy with larger basis sets:	-2503.31827
Zero-point energy:	1.00327

Co	-11.8558096054	-31.6179979293	20.2907732891
N	-12.0787125404	-30.8086239926	18.6005212719
N	-13.4940111219	-30.8086632947	20.9059682682
N	-11.1925659901	-32.0816884617	22.0472842954
N	-10.2749448291	-32.2957966741	19.5283764905
C	-10.9643088576	-31.0111669460	17.6454398167
C	-9.8873783280	-29.9309783940	17.8877425355
H	-9.4907091733	-30.0354301130	18.9005024825
H	-10.2930970522	-28.9264034229	17.7945488015
H	-9.0583411455	-30.0182467403	17.1815791335
C	-11.6878567851	-30.9066691326	16.2587734288
C	-10.8016773005	-30.4225010860	15.1070785374
H	-11.3859670675	-30.3529440950	14.1823863528
H	-9.9829627939	-31.1277184828	14.9257373815

H	-10.3585405211	-29.4413480668	15.2939136325
C	-12.3367271303	-32.2577490881	15.8779141862
H	-12.9954850466	-32.1209580995	15.0127225324
H	-11.5853034593	-33.0007959533	15.5999795327
C	-12.8633658757	-29.9376375922	16.6078931182
H	-13.7051382513	-30.1547548331	15.9440457898
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5340324785	-27.8897139024	16.7807299136
H	-11.8673953621	-28.0985599798	17.2932275008
C	-13.1430349955	-30.3099914146	18.0520370749
C	-14.3897566019	-30.0840625923	18.7432003643
C	-15.5781164230	-29.6336451623	17.9124229962
H	-15.8043461532	-28.5673813436	18.0278959864
H	-16.4821281201	-30.1901782323	18.1681579284
H	-15.4058969199	-29.8086179081	16.8502783166
C	-14.5046088824	-30.2995560625	20.0963572231
C	-15.7789367670	-30.1364259151	20.9532225694
C	-16.7244269152	-28.9641302115	20.6439898232
H	-17.3857362712	-28.8034886443	21.5027125983
H	-17.3662300222	-29.1630552642	19.7858011281
H	-16.1846253516	-28.0325504036	20.4560329132
C	-16.5639779567	-31.4691129123	20.8761301000
H	-17.4354492137	-31.4318707829	21.5399447936
H	-15.9363916935	-32.3149756681	21.1706292934
C	-15.1430009052	-29.9988998029	22.3670664493
H	-15.7929820333	-30.4274133063	23.1388664785
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6780588483	-27.9333131318	22.9003898785
H	-14.1705433742	-28.0794214100	21.9722819673
C	-13.8717659263	-30.7997888737	22.1945540332
C	-13.1831261982	-31.3945656116	23.2498872571
H	-13.6504479528	-31.3349257774	24.2257647720
C	-11.9196124341	-31.9802747916	23.1761113978
C	-11.1563061659	-32.5171043042	24.3820222099
C	-11.4597330963	-34.0199289149	24.5814088619
H	-10.9189366271	-34.3813467138	25.4641241788
H	-11.1551190980	-34.6068644514	23.7177814232
H	-12.5303904721	-34.1848800769	24.7364912062
C	-11.4765868099	-31.7780427633	25.6899570913
H	-10.7853284998	-32.0881695754	26.4807301136
H	-12.4860942727	-32.0309397927	26.0295837769
H	-11.4200155640	-30.6911353101	25.5884272292
C	-9.6952492434	-32.3443261013	23.8664588698
H	-9.0707450211	-33.1687305970	24.2214199750

C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.7105873293	-30.1631588199	23.9687510831
H	-8.9596809739	-30.9393274593	25.3775883611
C	-9.8719235427	-32.4052293458	22.3457769360
C	-8.8719747153	-32.6770595724	21.4330095310
C	-7.4701603806	-32.9788828286	21.9152427534
H	-6.7442717481	-32.2534222048	21.5307049152
H	-7.1458315398	-33.9759967058	21.6061171225
H	-7.4043174936	-32.9568900930	23.0017395344
C	-9.1348970024	-32.7000484208	20.0023197621
C	-8.2549364374	-33.3007475792	18.8752429150
C	-8.2547546433	-34.8351986749	19.0574859143
H	-7.6446907319	-35.3187719823	18.2879386840
H	-9.2680979577	-35.2409034029	18.9951656481
H	-7.8541286464	-35.1179395391	20.0334475092
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1525933640	-33.1582358300	19.5313817666
H	-6.4044298198	-33.0725062503	17.7894402879
C	-9.0150994308	-32.8384695897	17.5765173366
H	-8.4783658775	-31.9595247681	17.2081413031
C	-9.0391184961	-33.8576026930	16.4353618937
H	-9.6497671388	-34.7317513043	16.6806525636
H	-9.4515119556	-33.4098240196	15.5263534937
C	-10.3977823370	-32.4009714801	18.0730527382
H	-11.1724158023	-33.1497305833	17.9028598093
H	-14.2076923889	-28.5353321796	23.6824646380
H	-8.0934316536	-30.8603415938	23.8369039613
H	-6.7952329199	-31.6737082317	18.8052806186
H	-12.2711485551	-28.1011069078	15.5682518360
H	-8.0290498711	-34.2069298674	16.1939858061
H	-16.9165208275	-31.6579277345	19.8580606455
C	-14.8118193538	-35.6374101695	21.4895438658
H	-15.7903728683	-35.2979274262	21.1297687048
H	-14.5759079243	-36.5873672012	20.9957180538
C	-13.7359326281	-34.6025179311	21.1859042883
H	-14.0044724542	-33.6194286798	21.5853690297
O	-12.5072577317	-34.9963091517	21.8477378198
C	-13.3989462084	-34.4566023611	19.6776470835
H	-14.2570761422	-34.8196145466	19.0768333278
O	-13.0139798908	-33.1906443612	19.2877471864
C	-12.1929789356	-35.3510376068	19.5740493169
H	-11.6487831423	-35.5003633875	18.6468692092
C	-11.5029023202	-35.3201735576	20.8959226175
H	-10.6947344551	-34.5855325491	20.9757126221

N	-10.8741665049	-36.5992554213	21.2572690511
C	-11.3566595156	-37.8678757266	21.0019380786
H	-12.2410411038	-37.9984970075	20.3936187243
N	-10.6462191836	-38.8316200597	21.5432460042
C	-9.6380614135	-38.1582587550	22.2118755966
C	-8.5616073293	-38.6020050265	23.0058245329
N	-8.3189060894	-39.9235071626	23.2102838379
H	-7.6614188561	-40.1711911741	23.9330827110
H	-9.0369249045	-40.5831582829	22.9542856235
N	-7.7379128629	-37.6935074628	23.5612967514
C	-7.9804290116	-36.3945557905	23.3195206761
H	-7.2856704260	-35.6972732178	23.7857030124
N	-8.9543086026	-35.8408418462	22.5900315036
C	-9.7633982440	-36.7716555567	22.0566555311
H	-14.8795992464	-35.8207133196	22.5665629401
H	-12.9228425879	-32.6645519450	16.7098108223

Int3$_{VI}$

Energy with the medium-sized basis set: -2502.40080

Solution energy with the medium-sized basis set: -2502.45359

Energy with larger basis sets: -2503.08785

Zero-point energy: 1.00229

Co	-12.1916578461	-32.1907895457	20.2299248559
N	-12.1692729122	-31.0236498451	18.5838223951
N	-13.6037153965	-30.8467819723	20.8595355396
N	-11.2457449819	-32.0746870261	22.0234134019
N	-10.3677747831	-32.6174666615	19.4868300806
C	-10.9850971490	-31.1374858370	17.7028436602
C	-9.9759571351	-30.0609684610	18.1549636259
H	-9.6983835277	-30.2277774830	19.1979787864
H	-10.4133936242	-29.0666844513	18.0889568258
H	-9.0688789805	-30.0669514002	17.5475677160
C	-11.5899335525	-30.8851115977	16.2740851457
C	-10.5998959237	-30.2847775033	15.2700438384
H	-11.0904480208	-30.1180288768	14.3053299828
H	-9.7633758667	-30.9706168288	15.0973293466
H	-10.1859079007	-29.3298176153	15.5998500812
C	-12.1831565409	-32.1815290302	15.6782748494
H	-12.7097695173	-31.9516939594	14.7462874187
H	-11.4110611469	-32.9162519741	15.4396730967
C	-12.8087628895	-29.9514198598	16.6113947257

H	-13.6235465502	-30.1876248938	15.9195944034
C	-12.6042351200	-28.4244251600	16.5600578000
H	-13.5419552977	-27.9147098437	16.7971223906
H	-11.8517892697	-28.0729309250	17.2674004238
C	-13.1612515734	-30.3901644100	18.0260194384
C	-14.4235016337	-30.1112552700	18.6853744629
C	-15.5657886506	-29.5976899367	17.8292436349
H	-15.7144013016	-28.5176918185	17.9315824503
H	-16.5076147127	-30.0837264913	18.0894181792
H	-15.3952397338	-29.8010811596	16.7719169882
C	-14.5834123793	-30.2964835943	20.0432921554
C	-15.8441359509	-30.0420181674	20.8951456593
C	-16.6965254653	-28.8045349275	20.5748982607
H	-17.3646630964	-28.6025522859	21.4182247923
H	-17.3308723262	-28.9548634744	19.7017225018
H	-16.0879313173	-27.9126380910	20.4065790207
C	-16.7158416540	-31.3210981418	20.8074570139
H	-17.5808526616	-31.2297560264	21.4726789107
H	-16.1450777836	-32.2096193625	21.0968775181
C	-15.2109360249	-29.9609522852	22.3189504303
H	-15.8791896097	-30.3854091271	23.0761728364
C	-14.7834948900	-28.5435965800	22.7519140700
H	-15.6494234588	-27.8940879800	22.8986186040
H	-14.1307600802	-28.0855647503	22.0015368672
C	-13.9611179537	-30.7874530489	22.1475665554
C	-13.2393475847	-31.3350355509	23.2138156873
H	-13.6910589553	-31.2372200502	24.1938582498
C	-11.9713224789	-31.9093165076	23.1572963123
C	-11.2221422182	-32.4287008968	24.3766369161
C	-11.5995648309	-33.9153354017	24.5900542382
H	-11.0422502875	-34.3094958852	25.4464492323
H	-11.3751716978	-34.5239983365	23.7132086681
H	-12.6682942436	-34.0137134193	24.8088435658
C	-11.5204057472	-31.6524456351	25.6674636095
H	-10.8458544469	-31.9758978008	26.4659229083
H	-12.5388434730	-31.8596636369	26.0099517294
H	-11.4187080043	-30.5716991567	25.5461385623
C	-9.7521066826	-32.3265098147	23.8566856778
H	-9.1597453557	-33.1663791545	24.2307791855
C	-9.0787890500	-30.9973449100	24.2922969900
H	-9.6768171674	-30.1358584176	23.9788143549
H	-8.9610283306	-30.9662609886	25.3769351737
C	-9.9433556823	-32.4435292022	22.3312633801
C	-8.9669226700	-32.8475072794	21.4261976757

C	-7.6407505200	-33.3177776589	21.9896548921
H	-6.8363550995	-33.2493964189	21.2617941980
H	-7.7256929628	-34.3673694376	22.2977057659
H	-7.3336354812	-32.7294303816	22.8555633242
C	-9.1948221966	-32.9005828034	19.9839196973
C	-8.2291448503	-33.3778256166	18.8515371350
C	-8.1208140685	-34.9150327541	18.9806658956
H	-7.4469311380	-35.3152120692	18.2180422356
H	-9.0904946429	-35.4044670100	18.8580458670
H	-7.7295618790	-35.2034320149	19.9590849171
C	-6.8178668600	-32.7676303200	18.7575435900
H	-6.1184108668	-33.1714245926	19.4928500831
H	-6.4065534547	-32.9996712795	17.7698855069
C	-8.9922417906	-32.9135272968	17.5510626908
H	-8.4997907644	-31.9959472902	17.2186201218
C	-8.9386029136	-33.8970032934	16.3792269899
H	-9.5103390772	-34.8088381825	16.5787165971
H	-9.3441663666	-33.4404943864	15.4718659712
C	-10.4116862482	-32.5611983498	18.0234649439
H	-11.1439920029	-33.3041164451	17.6943312597
H	-14.2323553490	-28.5877467790	23.6957613665
H	-8.0880525446	-30.8926662231	23.8417112362
H	-6.8411228221	-31.6785213721	18.8673270901
H	-12.3036185088	-28.1087247261	15.5572740048
H	-7.9079994335	-34.1903963706	16.1563204174
H	-17.0856658912	-31.4783721040	19.7904438792
C	-14.1698665900	-36.6631427744	21.7132066181
H	-15.2292593605	-36.4867145215	21.4984886930
H	-13.8215897949	-37.4835007617	21.0779690363
C	-13.3582259284	-35.3957636885	21.4756003641
H	-13.7570287805	-34.5641096712	22.0662013093
O	-11.9883691051	-35.5751839858	21.8975766226
C	-13.2756003733	-34.9693522137	19.9893352860
H	-14.1170844727	-35.3737772355	19.4091442941
O	-13.3050007947	-33.5626232501	19.8400333237
C	-11.9555374139	-35.5387365589	19.5789593053
H	-11.5851144884	-35.5909447654	18.5633308028
C	-11.1280692209	-35.8118043313	20.7907256047
H	-10.2720217148	-35.1369944499	20.9017842416
N	-10.5512958256	-37.1499297857	20.8123056059
C	-11.0968300300	-38.3410923427	20.3480310718
H	-12.0194339038	-38.3464715297	19.7836040891
N	-10.3801440542	-39.3960360716	20.6385660948
C	-9.3028219859	-38.8890780298	21.3468378691

C	-8.1788204946	-39.5037486726	21.9433663912
N	-7.9742549349	-40.8351915684	21.8920824494
H	-7.1839409606	-41.2286818731	22.3779937113
H	-8.6619761776	-41.4364683990	21.4675388723
N	-7.2800273653	-38.7250595732	22.5794934575
C	-7.4911182529	-37.4037801339	22.6126529514
H	-6.7314841496	-36.8239543178	23.1339622704
N	-8.5082047338	-36.6985067874	22.0941176749
C	-9.3862995900	-37.5000706278	21.4732692610
H	-14.0719369565	-36.9789599338	22.7549897440
H	-12.9008990591	-32.6513226200	16.3599220763

$TS3_{II}$

Energy with the medium-sized basis set: -2502.39514

Solution energy with the medium-sized basis set: -2502.44867

Energy with larger basis sets: -2503.10083

Zero-point energy: 1.00239

Co	-0.0829120000	1.0375770000	1.9873680000
N	-0.3443530000	1.7362820000	0.2648660000
N	-1.6759340000	1.9471480000	2.5829330000
N	0.6148220000	0.6667780000	3.7360440000
N	1.4612240000	0.2549980000	1.2061020000
C	0.8224070000	1.6203650000	-0.6423560000
C	1.8511720000	2.7120880000	-0.2701830000
H	2.2063180000	2.5585320000	0.7511040000
H	1.4100600000	3.7045870000	-0.3162580000
H	2.7137450000	2.7020400000	-0.9386250000
C	0.1722120000	1.8197880000	-2.0558990000
C	1.1218630000	2.3841720000	-3.1176240000
H	0.5942590000	2.5135940000	-4.0680630000
H	1.9540280000	1.6951870000	-3.2965710000
H	1.5433850000	3.3515700000	-2.8398660000
C	-0.4385980000	0.5043320000	-2.5868190000
H	-0.9912970000	0.7018410000	-3.5104320000
H	0.3267090000	-0.2388780000	-2.8196220000
C	-1.0300530000	2.7624750000	-1.7035460000
H	-1.8543430000	2.5463210000	-2.3896070000
C	-0.7985770000	4.2836700000	-1.7345320000
H	-1.7350230000	4.8018960000	-1.5078600000
H	-0.0606280000	4.6189620000	-1.0063170000
C	-1.3611990000	2.3355790000	-0.2832060000

C	-2.5991830000	2.5992440000	0.4037510000
C	-3.7803170000	3.0603800000	-0.4305690000
H	-3.9934900000	4.1272640000	-0.3100360000
H	-4.6897500000	2.5137180000	-0.1756590000
H	-3.6059640000	2.8863100000	-1.4921740000
C	-2.6995410000	2.4257260000	1.7677150000
C	-3.9691320000	2.5994450000	2.6257400000
C	-4.9050940000	3.7775260000	2.3148650000
H	-5.5692820000	3.9374890000	3.1702950000
H	-5.5440040000	3.5857460000	1.4537610000
H	-4.3589190000	4.7068270000	2.1363160000
C	-4.7510160000	1.2634760000	2.5408540000
H	-5.6062130000	1.2846090000	3.2243870000
H	-4.1083040000	0.4177040000	2.8046560000
C	-3.3389870000	2.7233320000	4.0416220000
H	-3.9865730000	2.2779070000	4.8041710000
C	-2.9778370000	4.1644980000	4.4573240000
H	-3.8720450000	4.7737090000	4.6075000000
H	-2.3548850000	4.6450190000	3.6961490000
C	-2.0625920000	1.9446350000	3.8687260000
C	-1.3752130000	1.3605230000	4.9315520000
H	-1.8480650000	1.4233110000	5.9040620000
C	-0.1152710000	0.7814320000	4.8679100000
C	0.6305670000	0.2090390000	6.0602090000
C	0.2710230000	-1.2928260000	6.1834520000
H	0.8132510000	-1.7294760000	7.0282160000
H	0.5472880000	-1.8523690000	5.2902340000
H	-0.8014490000	-1.4187780000	6.3585890000
C	0.3186550000	0.9023340000	7.3924430000
H	1.0008140000	0.5476860000	8.1708990000
H	-0.6957450000	0.6579930000	7.7217170000
H	0.3996960000	1.9898910000	7.3317630000
C	2.0980440000	0.3701970000	5.5542770000
H	2.7112090000	-0.4632500000	5.9051330000
C	2.7268690000	1.7107500000	5.9977070000
H	2.1047640000	2.5556160000	5.6854180000
H	2.8422230000	1.7470360000	7.0829680000
C	1.9219920000	0.3107210000	4.0337070000
C	2.9069350000	-0.0125590000	3.1116010000
C	4.3140910000	-0.2944670000	3.5924490000
H	5.0121370000	0.4795790000	3.2567070000
H	4.6861640000	-1.2558760000	3.2322800000
H	4.3692330000	-0.3310760000	4.6784720000
C	2.6313040000	-0.0771680000	1.6892490000

C	3.5559370000	-0.6200010000	0.5622450000
C	3.6087790000	-2.1572470000	0.7065820000
H	4.2382870000	-2.5968250000	-0.0715350000
H	2.6140450000	-2.6018970000	0.6288270000
H	4.0251180000	-2.4490580000	1.6727440000
C	4.9877910000	-0.0595350000	0.4629540000
H	5.6570300000	-0.4573990000	1.2278920000
H	5.4038780000	-0.3397230000	-0.5099740000
C	2.8040170000	-0.1531480000	-0.7368970000
H	3.3092770000	0.7581090000	-1.0659010000
C	2.8436750000	-1.1349680000	-1.9091000000
H	2.2610330000	-2.0394230000	-1.7087720000
H	2.4417520000	-0.6727670000	-2.8146540000
C	1.3950300000	0.2238290000	-0.2655160000
H	0.6606770000	-0.5344440000	-0.5459280000
H	-2.4162380000	4.1551540000	5.3958540000
H	3.7156580000	1.8423090000	5.5495900000
H	4.9968790000	1.0328340000	0.5329900000
H	-0.4770140000	4.6113090000	-2.7267380000
H	3.8702220000	-1.4388860000	-2.1347010000
H	-5.1299040000	1.0939410000	1.5291900000
C	-2.3657670000	-4.2406850000	1.6919440000
H	-3.1086160000	-4.0198540000	0.9201400000
H	-1.5602070000	-4.8331490000	1.2567590000
C	-1.8748640000	-2.9705060000	2.3370930000
H	-2.6751960000	-2.3661330000	2.7638510000
O	-0.8211960000	-3.0816080000	3.2482380000
C	-1.2314320000	-1.6799730000	1.1198550000
H	-1.8210050000	-1.7799880000	0.1918510000
O	-1.3984060000	-0.6030400000	1.8298010000
C	-0.0362820000	-2.4981870000	1.1604640000
H	0.1852290000	-3.1769950000	0.3438790000
C	0.4212250000	-2.8173150000	2.5624040000
H	0.9001640000	-1.9672080000	3.0528920000
N	1.3483560000	-3.9144780000	2.6587050000
C	1.3706110000	-5.1222510000	1.9647570000
H	0.6443820000	-5.3479300000	1.1970160000
N	2.3382770000	-5.9200950000	2.3316500000
C	2.9953440000	-5.2236480000	3.3334110000
C	4.1194970000	-5.5331610000	4.1333910000
N	4.7999590000	-6.6891190000	4.0073210000
H	5.5546160000	-6.8840130000	4.6462670000
H	4.4708490000	-7.4044600000	3.3792570000
N	4.5266730000	-4.6287260000	5.0471870000

C	3.8494080000	-3.4793430000	5.1546720000
H	4.2204420000	-2.7888560000	5.9093290000
N	2.7799640000	-3.0646670000	4.4594030000
C	2.3984080000	-3.9832710000	3.5637190000
H	-2.8539360000	-4.8450420000	2.4666410000
H	-1.1377600000	0.0623450000	-1.8690980000

$TS3_{epoxide}$

Energy with the medium-sized basis set: -2502.41848

Solution energy with the medium-sized basis set: -2502.47166

Energy with larger basis sets: -2503.10259

Zero-point energy: 1.00489

Co	-11.9396360000	-31.7315600000	20.2638700000
N	-12.1045850000	-30.8425880000	18.6087540000
N	-13.5418050000	-30.8652850000	20.8808990000
N	-11.2362570000	-32.0861280000	22.0339330000
N	-10.3111510000	-32.3415770000	19.5230660000
C	-10.9612100000	-31.0088940000	17.6686750000
C	-9.9109780000	-29.9201940000	17.9762480000
H	-9.5209610000	-30.0583170000	18.9872300000
H	-10.3385870000	-28.9222610000	17.9245320000
H	-9.0748510000	-29.9573200000	17.2764840000
C	-11.6534230000	-30.8783450000	16.2677640000
C	-10.7397700000	-30.3488710000	15.1582910000
H	-11.2976380000	-30.2561440000	14.2209770000
H	-9.9113750000	-31.0413020000	14.9778550000
H	-10.3125430000	-29.3714290000	15.3881090000
C	-12.2702290000	-32.2209450000	15.8155230000
H	-12.8742210000	-32.0601820000	14.9171310000
H	-11.5055390000	-32.9576760000	15.5627070000
C	-12.8512190000	-29.9375200000	16.6131310000
H	-13.6831330000	-30.1607110000	15.9401450000
C	-12.6042350000	-28.4244250000	16.5600580000
H	-13.5319920000	-27.8890460000	16.7858300000
H	-11.8568760000	-28.0866940000	17.2765670000
C	-13.1610320000	-30.3399680000	18.0444230000
C	-14.4269080000	-30.1474540000	18.7096020000
C	-15.6041090000	-29.7154590000	17.8564750000
H	-15.7683600000	-28.6327580000	17.8776690000
H	-16.5280160000	-30.1963010000	18.1764660000
H	-15.4571850000	-29.9991410000	16.8142580000

C	-14.5508960000	-30.3470920000	20.0643380000
C	-15.8070700000	-30.1152500000	20.9269830000
C	-16.6901530000	-28.9030200000	20.5918470000
H	-17.3460430000	-28.6953190000	21.4429220000
H	-17.3377290000	-29.0845310000	19.7352880000
H	-16.1020730000	-28.0042910000	20.3917780000
C	-16.6539350000	-31.4123670000	20.8807850000
H	-17.5219800000	-31.3135370000	21.5402890000
H	-16.0713370000	-32.2793170000	21.2076820000
C	-15.1627450000	-29.9856800000	22.3402090000
H	-15.8151400000	-30.4139860000	23.1086220000
C	-14.7834950000	-28.5435970000	22.7519140000
H	-15.6727220000	-27.9270300000	22.8973270000
H	-14.1531350000	-28.0715480000	21.9916320000
C	-13.9057480000	-30.8012240000	22.1754870000
C	-13.2129520000	-31.3679840000	23.2414180000
H	-13.6710800000	-31.2757610000	24.2180220000
C	-11.9561850000	-31.9602540000	23.1743870000
C	-11.1939000000	-32.4678770000	24.3881500000
C	-11.5004310000	-33.9660340000	24.6345090000
H	-10.9846190000	-34.2802210000	25.5476730000
H	-11.1607740000	-34.5874930000	23.8084900000
H	-12.5725790000	-34.1346150000	24.7667860000
C	-11.5106070000	-31.6904030000	25.6748190000
H	-10.8173710000	-31.9812710000	26.4689680000
H	-12.5168560000	-31.9354480000	26.0277040000
H	-11.4514750000	-30.6073190000	25.5445970000
C	-9.7339300000	-32.3265340000	23.8634750000
H	-9.1283930000	-33.1621640000	24.2229980000
C	-9.0787890000	-30.9973450000	24.2922970000
H	-9.6807520000	-30.1403660000	23.9734010000
H	-8.9617880000	-30.9542570000	25.3768530000
C	-9.9141400000	-32.4161710000	22.3436800000
C	-8.9161050000	-32.7172690000	21.4374470000
C	-7.5183310000	-33.0266420000	21.9227260000
H	-6.8050010000	-32.2627100000	21.5961680000
H	-7.1740440000	-33.9913990000	21.5454360000
H	-7.4669060000	-33.0798200000	23.0083270000
C	-9.1670280000	-32.7305370000	20.0069310000
C	-8.2629610000	-33.2913430000	18.8719200000
C	-8.2870970000	-34.8303940000	19.0222950000
H	-7.6688240000	-35.3012290000	18.2535910000
H	-9.3053440000	-35.2198240000	18.9261420000
H	-7.9143540000	-35.1439710000	19.9988180000

C	-6.8178670000	-32.7676300000	18.7575440000
H	-6.1526840000	-33.1746630000	19.5221670000
H	-6.4164520000	-33.0678030000	17.7848080000
C	-9.0036360000	-32.7976040000	17.5774990000
H	-8.4778370000	-31.8958980000	17.2553920000
C	-8.9841590000	-33.7745180000	16.4006140000
H	-9.5943310000	-34.6620590000	16.5916290000
H	-9.3643810000	-33.2965880000	15.4941500000
C	-10.3994380000	-32.3999820000	18.0599660000
H	-11.1501450000	-33.1578400000	17.8343770000
H	-14.2255830000	-28.5582630000	23.6923630000
H	-8.0873560000	-30.8901740000	23.8436360000
H	-6.7828480000	-31.6752960000	18.8173680000
H	-12.2891140000	-28.1141080000	15.5605360000
H	-7.9646310000	-34.1060410000	16.1821480000
H	-17.0170970000	-31.6135570000	19.8694680000
C	-14.9180850000	-35.3449300000	21.7212990000
H	-15.8764250000	-34.9281550000	21.3930850000
H	-14.7834440000	-36.3201590000	21.2419420000
C	-13.7688050000	-34.4074030000	21.3719780000
H	-13.9474370000	-33.4117490000	21.7813170000
O	-12.5446900000	-34.8956510000	21.9566450000
C	-13.4949720000	-34.3230070000	19.8628700000
H	-14.4138820000	-34.4764240000	19.2822730000
O	-12.8643450000	-33.1453090000	19.3878580000
C	-12.4447290000	-35.3581530000	19.6834580000
H	-12.0587260000	-35.6925670000	18.7285890000
C	-11.6553690000	-35.3833410000	20.9501490000
H	-10.7836950000	-34.7165790000	20.9112010000
N	-11.1237770000	-36.6777270000	21.3158860000
C	-11.7366130000	-37.9204330000	21.2274070000
H	-12.6875940000	-38.0328390000	20.7243370000
N	-11.0500790000	-38.8842010000	21.7866930000
C	-9.9278120000	-38.2497140000	22.2953470000
C	-8.8080570000	-38.7203570000	23.0181960000
N	-8.6514940000	-40.0198000000	23.3382660000
H	-7.8453340000	-40.3018780000	23.8725240000
H	-9.3546510000	-40.6931300000	23.0808090000
N	-7.8651890000	-37.8330990000	23.3984040000
C	-8.0307010000	-36.5462120000	23.0704260000
H	-7.2406040000	-35.8753220000	23.4028700000
N	-9.0337150000	-35.9721280000	22.3888970000
C	-9.9540500000	-36.8798060000	22.0269980000
H	-14.9555230000	-35.5003330000	22.8024120000

H	-12.9150590000	-32.6510440000	16.5887850000

Int4

Energy with the medium-sized basis set:	-2502.48821
Solution energy with the medium-sized basis set:	-2502.54277
Energy with larger basis sets:	-2503.19032
Zero-point energy:	1.00597

Co	-0.4714991449	1.3745394083	-0.1462851240
N	-0.7613736438	2.0436431986	-1.8754172817
N	-2.1382655848	2.1498747035	0.4359660988
N	0.1649850300	0.8957610506	1.5922298826
N	1.0558615428	0.5904737529	-0.9346316112
C	0.3805768631	1.8918722883	-2.8127466616
C	1.4312622896	2.9840209264	-2.5124030005
H	1.8059606036	2.8688801481	-1.4924791433
H	1.0080492037	3.9820405533	-2.5954597785
H	2.2800108896	2.9281653385	-3.1968790025
C	-0.3096049596	2.0407864747	-4.2123512614
C	0.6064344000	2.5698753878	-5.3212116805
H	0.0466445448	2.6760541866	-6.2564695876
H	1.4301651841	1.8727504275	-5.5095492248
H	1.0422942679	3.5425185464	-5.0852818562
C	-0.9376255720	0.7074528044	-4.6785757139
H	-1.5211662254	0.8720457055	-5.5902519490
H	-0.1802457194	-0.0450905107	-4.9093615076
C	-1.5016481839	2.9931873973	-3.8573518387
H	-2.3336680861	2.7779470870	-4.5338702822
C	-1.2597200000	4.5125190000	-3.8866120000
H	-2.2019062260	5.0358465137	-3.6947880667
H	-0.5492240932	4.8465997363	-3.1311267597
C	-1.8074835718	2.5926929213	-2.4251927759
C	-3.0475299041	2.8387764482	-1.7373817897
C	-4.2298459199	3.3057615596	-2.5668970395
H	-4.4465596668	4.3698570348	-2.4310447487
H	-5.1366982674	2.7514717992	-2.3194892368
H	-4.0561077748	3.1477637885	-3.6311549019
C	-3.1567961952	2.6439117187	-0.3772968258
C	-4.4286681096	2.8190297025	0.4794169569
C	-5.3617405449	4.0004210361	0.1673438365
H	-6.0235251670	4.1638421321	1.0241357550
H	-6.0040507556	3.8081432903	-0.6914594629

H	-4.8136075895	4.9277996088	-0.0150928033
C	-5.2259277339	1.4919674701	0.3984007374
H	-6.1020444502	1.5415656854	1.0539748032
H	-4.6106271899	0.6407483341	0.7080957226
C	-3.7979857254	2.9462374877	1.8960999491
H	-4.4471715779	2.5058094127	2.6607264990
C	-3.4389800000	4.3933470000	2.3052440000
H	-4.3354084082	4.9994493708	2.4538457547
H	-2.8189641467	4.8722470259	1.5402387780
C	-2.5227140122	2.1598140238	1.7275580859
C	-1.8301859109	1.5855206988	2.7878975042
H	-2.2975727625	1.6513039222	3.7630397849
C	-0.5683424019	1.0034147203	2.7208866023
C	0.1748678940	0.4354941129	3.9179093615
C	-0.1906581345	-1.0617018315	4.0619560708
H	0.3472184489	-1.4872396997	4.9160640718
H	0.0828036080	-1.6372081234	3.1794288519
H	-1.2641758563	-1.1815408590	4.2383990686
C	-0.1370688965	1.1482348935	5.2415970567
H	0.5451994153	0.8031066491	6.0247690236
H	-1.1516794331	0.9076078150	5.5735740222
H	-0.0558879281	2.2354843538	5.1687818093
C	1.6433027933	0.5926156588	3.4130407046
H	2.2581186631	-0.2368553299	3.7698114228
C	2.2657260000	1.9395990000	3.8456270000
H	1.6384490149	2.7788183590	3.5275309249
H	2.3826015447	1.9867208212	4.9305823851
C	1.4760172677	0.5342955366	1.8920489342
C	2.4671363159	0.2319070180	0.9740656207
C	3.8764493510	-0.0439524213	1.4530651631
H	4.5683297971	0.7376410276	1.1205795476
H	4.2563672648	-0.9997701728	1.0852510350
H	3.9340823423	-0.0857095369	2.5389746551
C	2.2010925805	0.1923060970	-0.4519983775
C	3.0964243831	-0.3832820900	-1.5816910742
C	3.1149780481	-1.9194905964	-1.4254555041
H	3.7159033554	-2.3834351329	-2.2125891810
H	2.1066866174	-2.3421161914	-1.4753515098
H	3.5429505909	-2.2145433327	-0.4652435872
C	4.5266480000	0.1693140000	-1.6891260000
H	5.1979279639	-0.2219855586	-0.9218947191
H	4.9430750053	-0.1178205726	-2.6603976014
C	2.3477991061	0.0898979380	-2.8820027391
H	2.8731292517	0.9846524015	-3.2251046903

C	2.3528341756	-0.9039696196	-4.0452812793
H	1.7527573158	-1.7942860957	-3.8307865433
H	1.9523994175	-0.4417051169	-4.9520570999
C	0.9566814617	0.5063994291	-2.3987352868
H	0.2103574785	-0.2565106865	-2.6355691062
H	-2.8751580348	4.3884151494	3.2425695733
H	3.2530991294	2.0728288980	3.3943910379
H	4.5361702059	1.2622752017	-1.6272310430
H	-0.9014915827	4.8394889311	-4.8670771154
H	3.3703595916	-1.2336313299	-4.2775628469
H	-5.5763201389	1.3032936360	-0.6205950968
C	-2.8262947074	-4.6858426775	0.7299675198
H	-3.6089738269	-4.7748233491	-0.0311710068
H	-2.0766639576	-5.4661254942	0.5668049971
C	-2.1907123977	-3.3144345952	0.6849695922
H	-2.9289521048	-2.5154074778	0.8247245590
O	-1.1086754352	-3.1730021114	1.6368400950
C	-1.5575239095	-1.7751899971	-1.2837195478
H	-1.7567284262	-1.8926748363	-2.3686345923
O	-1.6531325189	-0.6797625431	-0.7614774611
C	-1.2198809099	-3.0175541839	-0.5120657374
H	-1.0798247970	-3.8644146545	-1.1845113983
C	-0.1597428950	-2.8572961221	0.6086216199
H	0.2320619771	-1.8427172200	0.7277785581
N	0.9578716878	-3.7704094219	0.5885948393
C	1.1129463823	-4.9820687574	-0.0850683705
H	0.4069458094	-5.3116412154	-0.8333746076
N	2.1860426820	-5.6432017772	0.2589433753
C	2.7718399740	-4.8588891605	1.2381029003
C	3.9308897729	-5.0298478577	2.0293198449
N	4.7464603661	-6.0952010676	1.8946551847
H	5.5031334790	-6.2122573881	2.5505895987
H	4.4844952114	-6.8556388606	1.2876264560
N	4.2293717775	-4.0862041874	2.9447177152
C	3.4133613320	-3.0310806538	3.0596891148
H	3.6971471985	-2.3063948287	3.8205994400
N	2.2989890469	-2.7471074896	2.3709717416
C	2.0278455505	-3.7001830228	1.4719822579
H	-3.2783691450	-4.8494864059	1.7130040654
H	-1.6140699131	0.2933229136	-3.9224017038

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