

Electronic Supplementary Information to:

Asymmetric abstraction of two chemically-equivalent methylene hydrogens: significant enantioselectivity of endoperoxide presented by fumitremorgin B endoperoxidase

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Contents:

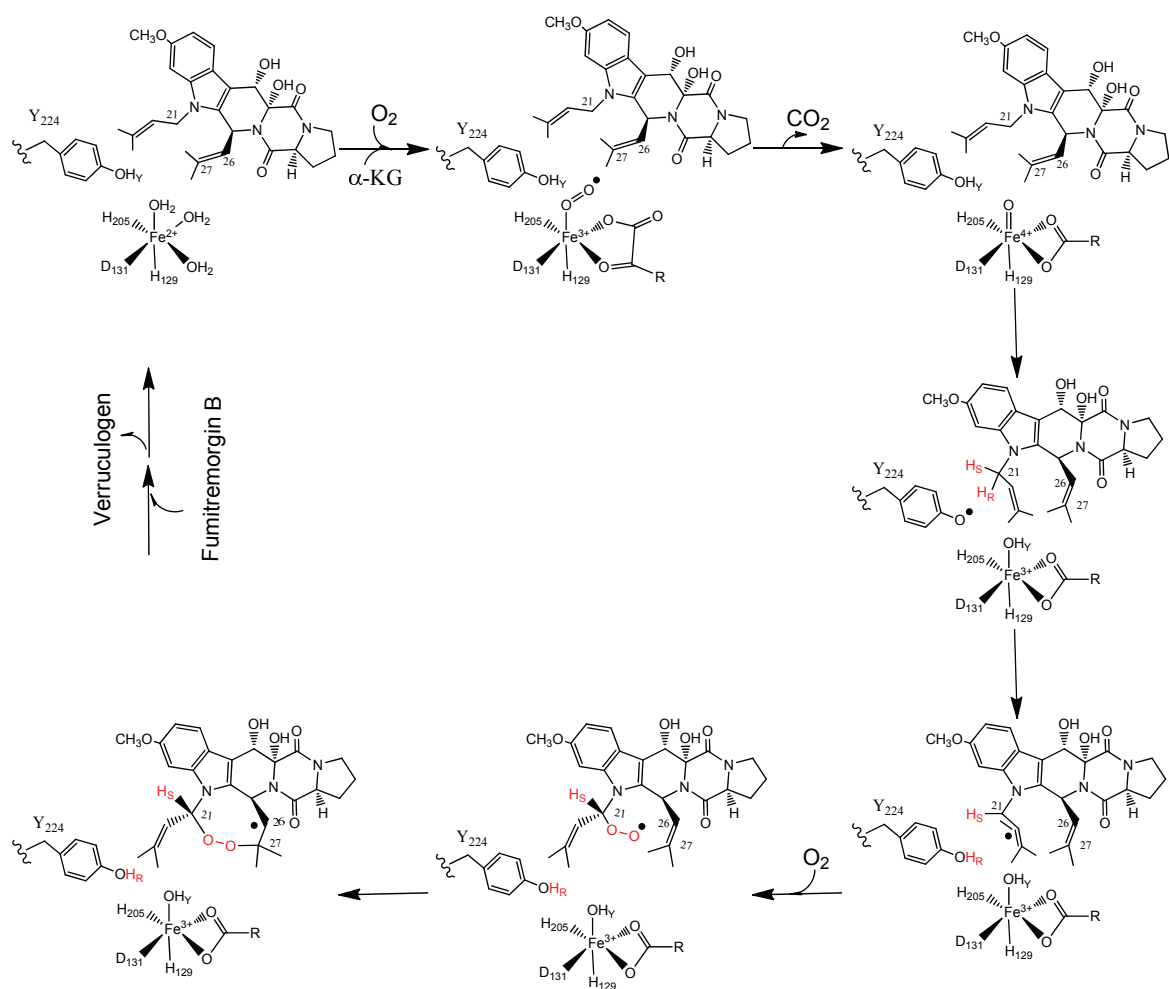
Table S1 Properties of $\text{Fe}^{\text{IV}}=\text{O}$ in various electronic states	S2
Table S2 Properties of $\text{Fe}^{\text{III}}-\text{OH}$ in various electronic states	S3
Scheme S1 A previously proposed mechanistic model of FtmOx1	S4
Fig. S1 Potential energy profile calculated by B3LYP-15%	S5
Fig. S2 Potential energy profile and optimized structures for α -ketoglutarate decarboxylation	S6
Fig. S3 Optimized structures of stationary points for the epoxidation	S7
Fig. S4 Potential energy profile for the epoxidation	S8
Cartesian coordinates and absolute energies of optimized structures	S9

Table S1 Properties of Fe^{IV}=O complex in the FtmOx1 active site in various electronic states. O_{Fe}: The oxygen binding to Fe.

entry	multiplicity	spin		energy (kcal mol ⁻¹)
		Fe	O _{Fe}	
1	1	0.31	-0.28	16.7
2	3	1.23	0.81	7.8
3	3	2.64	-0.70	19.1
4	5	3.04	0.61	0.0
5	7	4.03	1.22	15.6

Table S2 Properties of Fe^{III}–OH complex in the FtmOx1 active site in various electronic states.

entry	multiplicity	spin		energy (kcal mol ⁻¹)
		Fe	O _{Fe}	
1	1	0.93	-0.38	17.3
2	3	0.93	0.38	17.2
3	3	2.77	-0.38	10.4
4	5	2.77	0.38	10.4
5	5	4.05	-0.38	0.1
6	7	4.05	0.38	0.0



Scheme S1 A previously proposed mechanistic model of FtmOx1. α -KG: α -ketoglutarate. The atom numbers in the substrate is consistent with Fig. 1.A in the text.

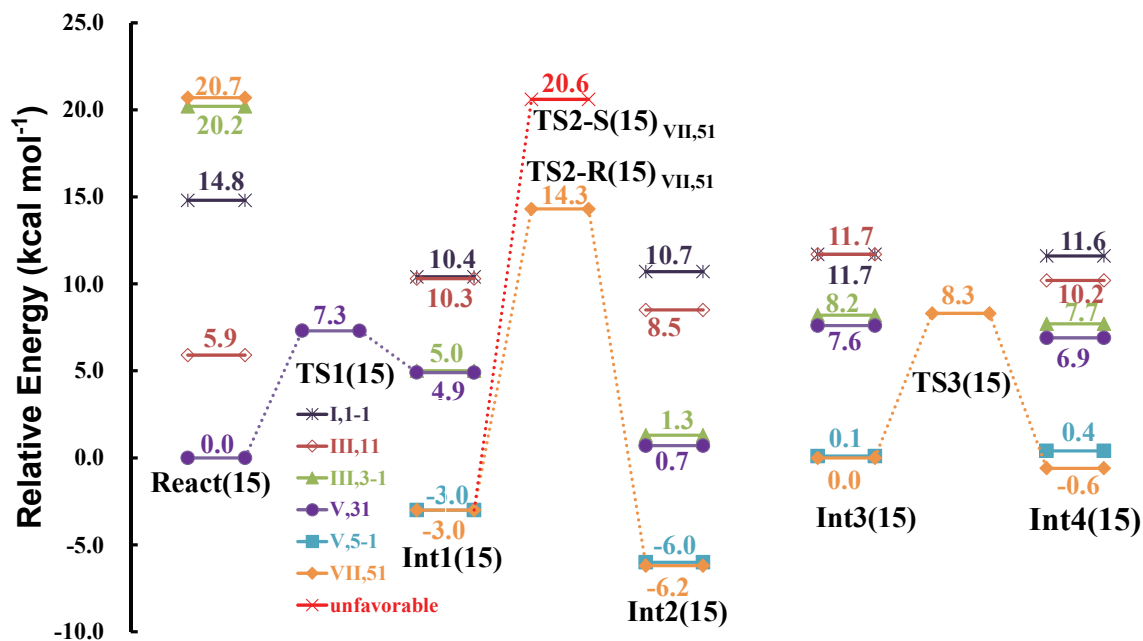


Fig. S1 Potential energy profile for hydrogen-atom transfer and epoxidation calculated by B3LYP-15%. Abbreviations signify the Fe^{IV}=O complex (**React(15)**), the TS for hydrogen-atom transfer from Tyr224 to Fe^{IV}=O (**TS1(15)**), the intermediate including Fe^{III}-OH and Tyr224 radical (**Int1(15)**), the TS for hydrogen-atom transfer from **C21** carbon (substrate chain A) to Tyr224 (**TS2(15)**), the intermediate of substrate-based radical (**C21** radical) (**Int2(15)**), the peroxy radical (**Int3(15)**), the TS for cyclization between peroxy radical and chain B (**TS3(15)**), and the intermediate of chain B radical (**Int4(15)**). In the legend, the Roman number before the comma indicates the multiplicity, the first Arabic number after the comma indicates the spin state of Fe, and the second Arabic number after the comma indicates the spin state of oxygen or carbon.

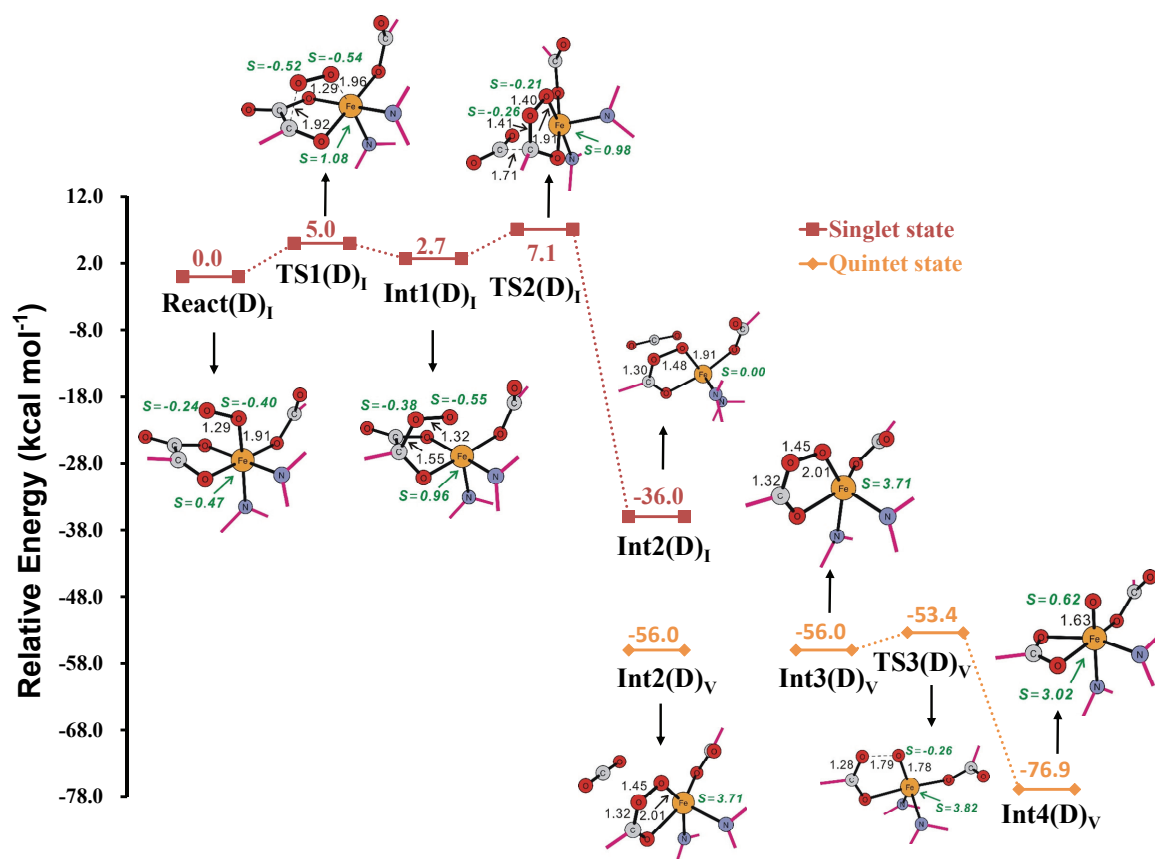


Fig. S2 Potential energy profile and optimized structures for α -ketoglutarate decarboxylation in FtmOx1.

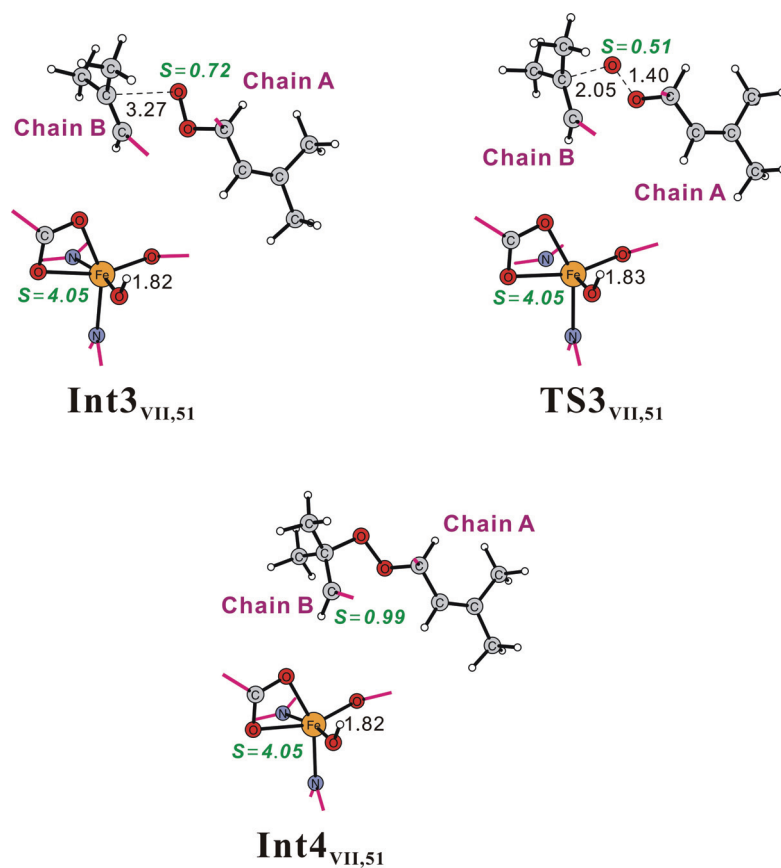


Fig. S3 Optimized structures of stationary points for the epoxidation. All distances are given in angstrom (Å). For clarity, some atoms that are not involved in reactions are omitted. The bonds connecting to the omitted atoms are indicated in magenta. The unpaired spin population is also shown with an indication of " S ".

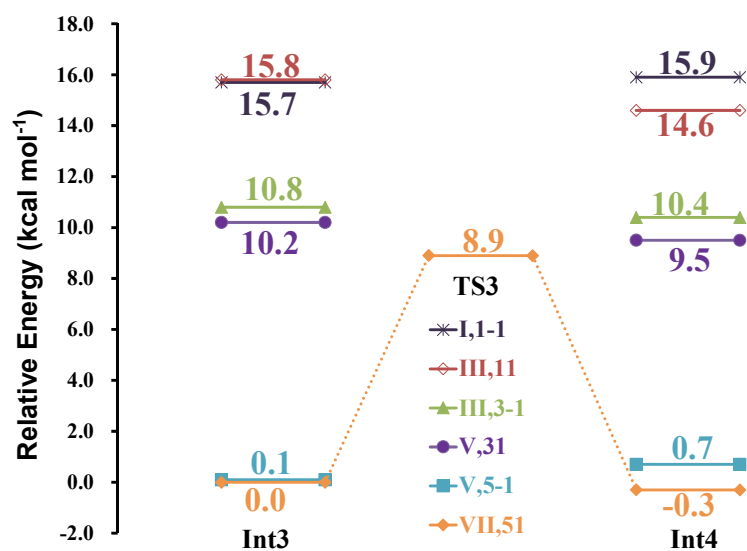


Fig. S4 Potential energy profile for the epoxidation. Abbreviations signify the peroxy radical (**Int3**), the TS for cyclization between peroxy radical and chain B (**TS3**), and the intermediate of chain B radical (**Int4**). The indications in the legend is the same as Figs. 3 and S1.

Cartesian coordinates and absolute energies of optimized structures

The abbreviations used here are consistent with those in the text. All energies here are the absolute energies in hartree. Frequencies are given in cm^{-1} .

React_{v,31}

Energy with the medium-sized basis set:	-3474.57085
Solution energy with the medium-sized basis set:	-3474.61754
Energy with larger basis sets:	-3475.65187
Zero-point energy:	1.22711

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Energy with larger basis sets:	-3475.63187
Zero-point energy:	1.21709
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O	-14.6918910000	0.4238840000	-42.9263960000
O	-11.2113330000	0.3025800000	-41.4042180000
C	-13.7341600000	-2.5271270000	-39.5112550000
C	-14.4194910000	-3.2903380000	-40.6593820000
C	-14.7911920000	-2.1899680000	-41.6702210000
H	-12.1465730000	9.7728870000	-32.0209760000
H	-11.2019820000	9.4361240000	-33.4749690000
H	-12.7329770000	7.7652210000	-33.9220650000
H	-11.5503090000	7.5132340000	-31.0977630000
H	-15.7054460000	-1.6709520000	-41.3639090000
H	-14.9459210000	-2.5593070000	-42.6853690000
H	-15.2844290000	-3.8643560000	-40.3164250000
H	-13.7132980000	-3.9947240000	-41.1136290000
H	-12.9445300000	-3.1009110000	-39.0168900000
H	-14.4455970000	-2.2137870000	-38.7365320000
H	-12.7880800000	-1.5519460000	-42.2501430000
H	-13.4183720000	9.2784360000	-35.4972940000
H	-14.5633530000	8.1906200000	-36.3122100000
H	-13.2627480000	8.9701250000	-37.2627160000
H	-14.1779010000	6.9514490000	-38.1367890000
H	-10.7454570000	3.5059190000	-36.9154440000
H	-11.0268520000	5.5628990000	-35.5439230000
H	-14.3032970000	6.5151280000	-40.6285730000
H	-14.9135110000	5.1607540000	-41.5548120000
H	-16.7066400000	4.7796740000	-39.7463710000
H	-16.3031500000	8.7889670000	-38.7640380000
H	-15.2223330000	8.2739430000	-40.0703710000
H	-16.8584950000	8.8318080000	-40.4290450000
H	-18.2147430000	7.2642200000	-37.9685540000
H	-18.5757970000	5.7863820000	-38.8818850000
H	-18.9126930000	7.3825590000	-39.5786680000
H	-11.0454730000	1.4946280000	-38.7860810000
H	-13.4632810000	2.9801130000	-42.2884540000
H	-15.7509130000	2.9575360000	-42.5020800000
H	-18.3891930000	2.9002600000	-40.2849420000
H	-17.9748660000	2.7028930000	-42.0012520000

H	-18.2585850000	1.2874310000	-40.9729610000
H	-15.0056240000	1.6837790000	-39.0064820000
H	-16.5739500000	2.3218100000	-38.4897870000
H	-16.4681050000	0.6942790000	-39.1429050000
H	-10.6229310000	3.2116430000	-40.9905520000
H	-10.5047070000	0.9855670000	-41.4154090000
H	-10.0895760000	8.4663530000	-31.4441900000
H	-10.5869520000	7.1721260000	-32.5458100000

Int1v₃₁

Energy with the medium-sized basis set:	-3474.56289
Solution energy with the medium-sized basis set:	-3474.61287
Energy with larger basis sets:	-3475.64281
Zero-point energy:	1.22350

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.3177250403	4.3779550323	-48.5185032837
C	-15.9652913583	4.2648390538	-47.8760188204
N	-15.1407924982	3.1665720363	-48.0745796500
C	-15.2719490377	5.0651395244	-46.9996232284
C	-14.0184808025	3.3154149492	-47.3291372240
N	-14.0744040293	4.4620130772	-46.6718889285
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.6008301815	8.4843477949	-43.5476072192
C	-13.4625944147	7.8571285440	-44.3675426352
O	-13.7799522845	6.7419928918	-44.9662760403
O	-12.3705479438	8.4310638166	-44.4014949009
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.2581502554	7.5843524753	-50.5074482574
C	-11.4389098938	7.1686504625	-49.0717885833
N	-10.8596631522	7.8941378817	-48.0333784620
C	-12.0133445684	6.0879931664	-48.4502969485
C	-11.0881155311	7.2594448710	-46.8602730835
N	-11.7822293013	6.1573730333	-47.0846272161
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.3659070615	8.8602643183	-37.7903473210
C	-10.4626315468	7.7362652086	-38.8003889247
C	-10.7133650566	7.9765195808	-40.1761616027
C	-10.3557820680	6.3937175912	-38.3626304860
C	-10.9319295733	6.9454806590	-41.0686251810
C	-10.5694797041	5.3424378139	-39.2187217890
C	-10.9261852386	5.5706833239	-40.6043672437

O	-11.2573878342	4.6081028278	-41.3618595542
Fe	-12.6033318169	5.2186555482	-45.4246219534
H	-18.0387239173	4.6681700093	-47.7454796422
H	-17.6338821343	3.3835167261	-48.8596677630
H	-15.5300797454	6.0141975254	-46.5561507842
H	-15.3658768470	2.3577096827	-48.6341994578
H	-13.2182967816	2.5977408626	-47.2421572943
H	-18.4632181987	5.4690919375	-50.0041603536
H	-14.2108242080	8.6266527457	-42.5344985798
H	-14.7686850736	9.4957237741	-43.9388021346
H	-15.6765452489	6.6246480722	-43.2902793836
H	-11.1723261733	8.6789821378	-50.5490247559
H	-10.2914774972	7.1995804179	-50.8634066649
H	-12.5712871729	5.2716973499	-48.8801516345
H	-10.3731989191	8.7729107090	-48.1299243470
H	-10.8474981434	7.6261439244	-45.8723747578
H	-12.0280824522	7.3075501182	-52.5156475090
H	-11.1860579350	8.7335361244	-37.0714168764
H	-10.5238982095	9.8233867625	-38.2893071667
H	-10.7603527262	9.0039069039	-40.5309195584
H	-10.1721394171	6.1912677400	-37.3120188101
H	-11.1593559473	7.1327535433	-42.1170255691
H	-10.5371281890	4.3138266873	-38.8767145854
H	-11.2421440588	5.2211585259	-43.6030078001
H	-8.1992517092	9.1082636972	-37.6858081652
C	-12.5763345804	2.8829642179	-44.3399606128
O	-11.9579603539	2.8098317930	-45.4258752492
C	-12.7479496209	1.7029999006	-43.4065330926
C	-11.9948307994	0.4456106769	-43.8305827645
H	-13.8251007371	1.5215958514	-43.3332640686
H	-12.4329096991	2.0347168069	-42.4121046144
H	-12.3155349266	0.1116342658	-44.8219009384
H	-10.9173140663	0.6285309004	-43.8797956611
H	-12.5491124578	6.0551459184	-51.3884872032
H	-13.2808681500	7.6502887300	-51.3469082600
H	-16.8361373000	5.1371404900	-50.5404367600
H	-17.1026046126	6.3790449918	-49.3429473979
H	-9.0234178500	9.5790658800	-36.2103454500
H	-8.8302973584	7.8919744521	-36.5791325445
H	-16.6115950000	8.0366627000	-42.8408657800
H	-16.3451355645	7.6571744958	-44.5314640771
H	-12.1793670234	-0.3636623744	-43.1161098521
O	-13.1195194357	3.9944088508	-43.9624958530
O	-11.1517410298	5.6387237191	-44.4792759979

C	-10.9580000000	7.9730000000	-31.8940000000
C	-12.2359452630	8.7554803935	-32.2261279690
O	-13.3661000068	7.9356890267	-32.4734919939
C	-13.7734092809	9.2126177047	-35.6077517765
O	-13.0159589697	8.0385574733	-35.3259947512
C	-13.1252216322	6.9708186400	-36.1956454099
C	-13.6605951909	7.0850849846	-37.4744266744
C	-13.7280367606	5.9111946709	-38.2314698791
C	-13.2594624888	4.6624239577	-37.7466407006
C	-12.7160968879	4.5905915424	-36.4545924531
C	-12.6495568961	5.7429860351	-35.6869927518
N	-14.2162889209	5.7276757043	-39.5161584076
C	-14.0876842307	4.3800581511	-39.8353850212
C	-13.4875017306	3.7162127232	-38.7984165541
C	-14.3849858626	6.8271076985	-40.4721754458
C	-15.5329163739	7.7333165261	-40.1356119403
C	-15.4790884644	9.0586736041	-39.9303341948
C	-14.2169813106	9.8892590770	-39.9594072493
C	-16.7381800780	9.8451613460	-39.6538594437
C	-13.0545269863	2.3133623857	-38.9683301274
C	-14.1301147132	1.4850967127	-39.7068845498
N	-14.8451403253	2.2654679742	-40.7546416451
C	-14.6622433972	3.7233809816	-41.0634170669
C	-15.9942591501	4.3426670935	-41.4711472365
C	-17.0686783683	4.5276261572	-40.6895443565
C	-18.3190808944	5.1557647511	-41.2593281666
C	-17.1706431314	4.1252809125	-39.2379361606
O	-11.8181622867	2.2180862302	-39.7125232664
C	-15.2155136179	0.9808363147	-38.7287554504
N	-16.2143899121	0.3422317727	-39.3791587660
C	-16.2934876341	0.2874210695	-40.8474679257
C	-15.7346764668	1.5504565414	-41.5147531914
O	-15.1881198618	1.1745027643	-37.5164333715
O	-16.1302324224	1.8860175132	-42.6262194580
O	-13.5142152608	0.3501395243	-40.2751525190
C	-17.4553441223	-0.0653813885	-38.7142326011
C	-18.2780945279	-0.6682821148	-39.8656844896
C	-17.8030227726	0.1181464762	-41.1009120544
H	-12.4973342792	9.4125764876	-31.3868050012
H	-12.0323294293	9.4104886092	-33.0898831274
H	-13.2940278983	7.6432460018	-33.3948633050
H	-10.9982600183	7.5154316144	-30.9018265146
H	-18.2739292923	1.1064943866	-41.1397875953
H	-18.0041132531	-0.3804217034	-42.0507609289

H	-19.3550255501	-0.5865461351	-39.6943228667
H	-18.0366121727	-1.7315949999	-39.9801580067
H	-17.2443242155	-0.7687994241	-37.9035552016
H	-17.9429613229	0.8133845830	-38.2706812398
H	-15.7269203273	-0.5731421027	-41.2236978109
H	-13.7088089609	9.8326703132	-34.7126945931
H	-14.8236399173	8.9678807165	-35.8084421224
H	-13.3606061379	9.7586191034	-36.4659937892
H	-14.0380320146	8.0190915914	-37.8637047401
H	-12.3631771832	3.6434813068	-36.0572732234
H	-12.2563727628	5.7251067217	-34.6748758488
H	-13.4394371061	7.3702689626	-40.5247172257
H	-14.5410610454	6.3779505104	-41.4538409310
H	-16.4969436195	7.2311835492	-40.0822245736
H	-14.1398248646	10.4961452680	-39.0464412156
H	-13.3040626971	9.2969789459	-40.0456636966
H	-14.2370335121	10.5933061566	-40.8013621839
H	-16.6751354765	10.3640631624	-38.6875496384
H	-17.6264876622	9.2070385819	-39.6415710541
H	-16.8876201017	10.6221564570	-40.4156874720
H	-12.8829136059	1.8132317718	-38.0136785223
H	-13.9753986970	3.8277328999	-41.9125394563
H	-16.0544402437	4.6100483293	-42.5206642158
H	-18.6189205342	6.0364174483	-40.6738153589
H	-18.1853794831	5.4679296102	-42.2989277693
H	-19.1634820884	4.4539533238	-41.2180598224
H	-16.2764913350	3.6407738282	-38.8484376646
H	-17.3778263284	5.0013010069	-38.6089683942
H	-18.0148318022	3.4355469104	-39.0984249770
H	-11.7351606844	2.9887148029	-40.3124218415
H	-12.5999276075	0.6437915590	-40.4572072634
H	-10.1292762400	8.6462920100	-31.9632444700
H	-10.8051016033	7.1792327452	-32.6346961680

Int1_{VII,51}

Energy with the medium-sized basis set:	-3474.56969
Solution energy with the medium-sized basis set:	-3474.61805
Energy with larger basis sets:	-3475.65794
Zero-point energy:	1.22056

C	-17.4200000000	5.3860000000	-49.6790000000
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C	-17.3249795435	4.3490428957	-48.5430555449
C	-15.9711621515	4.2305146414	-47.9064546255
N	-15.1164756948	3.1627897972	-48.1452706106
C	-15.2935245170	5.0194701418	-47.0082409909
C	-13.9947375089	3.3265088047	-47.3961353924
N	-14.0774580005	4.4469501594	-46.7018843126
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.6109685463	8.5023945563	-43.5449304470
C	-13.4696006375	7.9061703901	-44.3773037646
O	-13.7512230119	6.7509141762	-44.9290100217
O	-12.4036342258	8.5139356454	-44.4727088525
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.2462941364	7.6143970393	-50.5380140196
C	-11.4017982058	7.2063269720	-49.0989137022
N	-10.7962049316	7.9255916063	-48.0728774051
C	-11.9817309462	6.1343698317	-48.4666695344
C	-11.0183053967	7.2924166324	-46.8965406825
N	-11.7316821299	6.1997535527	-47.1061929256
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.3423970739	8.8856983336	-37.8294844475
C	-10.4159477111	7.7665475318	-38.8465725780
C	-10.6509081215	8.0090884499	-40.2246115929
C	-10.2932217845	6.4230963714	-38.4126709377
C	-10.8269508674	6.9782212200	-41.1266869377
C	-10.4583661171	5.3723446560	-39.2784971497
C	-10.7864792273	5.6005390662	-40.6706167848
O	-11.0613587804	4.6305427063	-41.4421345811
Fe	-12.5297261199	5.2852694123	-45.2877517877
H	-18.0457148017	4.6203016211	-47.7629620500
H	-17.6403875218	3.3634265589	-48.9096028681
H	-15.5829595584	5.9468338117	-46.5388446938
H	-15.3197811088	2.3690189632	-48.7341406551
H	-13.1722432355	2.6300416408	-47.3441629970
H	-18.4611871085	5.4881121072	-50.0052526873
H	-14.2183817950	8.6296873851	-42.5299971247
H	-14.7926490979	9.5182097709	-43.9168983713
H	-15.6650300533	6.6292529576	-43.2794221024
H	-11.1776509368	8.7096597632	-50.5929315133
H	-10.2805297464	7.2392660002	-50.9067321805
H	-12.5620375950	5.3278298399	-48.8857109989
H	-10.2968057945	8.7959511564	-48.1788854473
H	-10.7427250227	7.6560801895	-45.9173613944
H	-12.0464900483	7.2817818781	-52.5255574417
H	-11.1879452992	8.7645748986	-37.1391333085

H	-10.4725601869	9.8528323819	-38.3284939361
H	-10.7182151936	9.0371642563	-40.5740599104
H	-10.1305310708	6.2179275266	-37.3592642443
H	-11.0406659581	7.1605354640	-42.1786252948
H	-10.4049655831	4.3434853648	-38.9407582123
H	-10.9835830733	5.2229443078	-43.4460331666
H	-8.1761016033	9.0863967596	-37.6636267018
C	-12.6122965303	2.9357310523	-44.3165804548
O	-11.9330431397	3.0361668258	-45.3755012023
C	-12.6936434559	1.6507031728	-43.5239465308
C	-11.8395687471	0.5117427972	-44.0744607096
H	-13.7542693252	1.3823717939	-43.4734967000
H	-12.4074193549	1.8958590249	-42.4948799298
H	-12.1415660430	0.2513254878	-45.0936387433
H	-10.7832286177	0.7937769138	-44.1097037342
H	-12.5423829629	6.0573790297	-51.3579385175
H	-13.2808681500	7.6502887300	-51.3469082600
H	-16.8361373000	5.1371404900	-50.5404367600
H	-17.0873286124	6.3669075171	-49.3236466992
H	-9.0234178500	9.5790658800	-36.2103454500
H	-8.8640751637	7.8894305019	-36.5710325314
H	-16.6115950000	8.0366627000	-42.8408657800
H	-16.3448846207	7.6481075062	-44.5312045659
H	-11.9414921838	-0.3794350173	-43.4462358511
O	-13.2610925710	3.9555384270	-43.8782710478
O	-11.0540552877	5.7077524817	-44.2884129017
C	-10.9580000000	7.9730000000	-31.8940000000
C	-12.2426878146	8.7639619982	-32.1753247752
O	-13.3775807459	7.9498870949	-32.4189952365
C	-13.7796751044	9.2212078507	-35.5591645118
O	-13.0025469284	8.0645037259	-35.2637174236
C	-13.0689182729	6.9948056831	-36.1355386230
C	-13.6010730668	7.0902148062	-37.4175568431
C	-13.6243184178	5.9142891870	-38.1751411922
C	-13.1142055610	4.6831877755	-37.6876564339
C	-12.5766591041	4.6301236582	-36.3930859745
C	-12.5544584805	5.7843336676	-35.6245466942
N	-14.1002113001	5.7141376944	-39.4632401976
C	-13.9249944622	4.3702005255	-39.7786859131
C	-13.3024272268	3.7291607738	-38.7415593185
C	-14.2814656940	6.8050150202	-40.4286885651
C	-15.4523631949	7.6886411139	-40.1117834826
C	-15.4290257059	9.0151531554	-39.9078287665
C	-14.1836078828	9.8711439340	-39.9156957681

C	-16.7085316565	9.7759196326	-39.6539180505
C	-12.8349125543	2.3370508243	-38.9118526730
C	-13.9017320598	1.4775812296	-39.6244950043
N	-14.6378103404	2.2297904443	-40.6770110635
C	-14.4726307365	3.6881505889	-41.0039873167
C	-15.8015062932	4.2827343593	-41.4496799257
C	-16.8965217239	4.4567508140	-40.6951364763
C	-18.1449247197	5.0549308292	-41.2996307165
C	-17.0226483210	4.0611773545	-39.2434816058
O	-11.6107716631	2.2621528298	-39.6816299656
C	-14.9660776193	0.9701996148	-38.6258288501
N	-15.9602411300	0.3047695110	-39.2553339960
C	-16.0499184771	0.2239612382	-40.7219398845
C	-15.5238635290	1.4876241943	-41.4160061482
O	-14.9273698274	1.1838245397	-37.4171311001
O	-15.9410107093	1.7953300776	-42.5271490222
O	-13.2699968754	0.3456054180	-40.1824432781
C	-17.1869507425	-0.1159018840	-38.5729779341
C	-18.0050605989	-0.7579736836	-39.7064568811
C	-17.5568994685	0.0152574876	-40.9601286899
H	-12.4859605210	9.3972702865	-31.3127772962
H	-12.0587650328	9.4425895316	-33.0252589594
H	-13.3092017443	7.6600006635	-33.3415984128
H	-10.9764603884	7.4874715910	-30.9145329586
H	-18.0507776399	0.9914929802	-41.0149564333
H	-17.7534032678	-0.5062677022	-41.8985397747
H	-19.0822139822	-0.6966849170	-39.5280221978
H	-17.7409046795	-1.8177232620	-39.8029227554
H	-16.9547061606	-0.7987498252	-37.7505871777
H	-17.6900964616	0.7608125790	-38.1427821904
H	-15.4668478929	-0.6299470155	-41.0879312575
H	-13.7394495677	9.8450728266	-34.6652010274
H	-14.8223626481	8.9555156308	-35.7729436508
H	-13.3670749843	9.7735794703	-36.4137173810
H	-14.0106742582	8.0099441003	-37.8085845236
H	-12.1941704466	3.6955914824	-35.9933440990
H	-12.1678129828	5.7792041701	-34.6097850334
H	-13.3471721271	7.3683078578	-40.4747587248
H	-14.4184765195	6.3472209781	-41.4100251724
H	-16.4066946328	7.1671277457	-40.0733910474
H	-14.1351512476	10.4798469280	-39.0020196985
H	-13.2576180453	9.2971363081	-39.9845335933
H	-14.2026901815	10.5744823631	-40.7583819098
H	-16.6732219620	10.2957606703	-38.6866905172

H	-17.5836103088	9.1196995204	-39.6571639531
H	-16.8603449091	10.5498050774	-40.4184228632
H	-12.6288732426	1.8476530795	-37.9587824550
H	-13.7777359868	3.7889183647	-41.8453005643
H	-15.8348726295	4.5369509355	-42.5040152178
H	-18.4779304099	5.9338805360	-40.7295194409
H	-17.9914788794	5.3608828875	-42.3382849776
H	-18.9749900309	4.3354851131	-41.2736305532
H	-16.1215641958	3.6118000348	-38.8276262109
H	-17.2781183139	4.9327423176	-38.6260929813
H	-17.8444807781	3.3415116351	-39.1210360349
H	-11.5745896028	3.0030554417	-40.3197952007
H	-12.3626588964	0.6529641305	-40.3751890764
H	-10.1292762400	8.6462920100	-31.9632444700
H	-10.8222550575	7.2003812446	-32.6600532643

TS2-R_{VII,51}

Energy with the medium-sized basis set: -3474.53505

Solution energy with the medium-sized basis set: -3474.58586

Energy with larger basis sets: -3475.62600

Zero-point energy: 1.21459

Imaginary frequency: -1882.37

C	-17.4199890000	5.3859880000	-49.6790070000
C	-17.3463880000	4.4141510000	-48.4841620000
C	-15.9664470000	4.2312710000	-47.9267260000
N	-15.0799040000	3.2558390000	-48.3642180000
C	-15.2645890000	4.9291740000	-46.9762530000
C	-13.9156820000	3.3919270000	-47.6729430000
N	-13.9974250000	4.4040930000	-46.8295510000
C	-15.8870330000	7.6670240000	-43.5359660000
C	-15.2224530000	8.3664640000	-44.7238150000
C	-13.8552350000	7.7951430000	-45.1219930000
O	-13.7638410000	6.4974150000	-44.9676620000
O	-12.9798760000	8.5315250000	-45.5727970000
C	-12.3569880000	7.1289940000	-51.4869720000
C	-11.3181790000	7.8359580000	-50.6087540000
C	-11.2808990000	7.3149710000	-49.2040040000
N	-10.4627780000	7.8632860000	-48.2225250000
C	-11.9445630000	6.2988480000	-48.5679430000
C	-10.6606640000	7.1918460000	-47.0655350000
N	-11.5480380000	6.2306220000	-47.2458210000
C	-9.0339820000	8.8750110000	-37.0159870000
C	-7.9524350000	7.9594420000	-37.6276630000
C	-8.5361120000	7.0997540000	-38.7233890000

C	-8.4642810000	7.4897050000	-40.0703810000
C	-9.2811410000	5.9518490000	-38.4042510000
C	-9.1898010000	6.8253360000	-41.0532700000
C	-9.9986900000	5.2694120000	-39.3765130000
C	-10.0147700000	5.7334940000	-40.7090460000
O	-10.8313530000	5.1724500000	-41.6107350000
Fe	-12.3090660000	5.2769320000	-45.4622470000
H	-17.9903760000	4.7852590000	-47.6798030000
H	-17.7599640000	3.4396150000	-48.7746080000
H	-15.5789730000	5.7678540000	-46.3769250000
H	-15.2799120000	2.5359510000	-49.0424190000
H	-13.0538350000	2.7523280000	-47.7881400000
H	-18.4512030000	5.4880300000	-50.0318660000
H	-15.0924990000	9.4382520000	-44.5455630000
H	-15.8656150000	8.2824980000	-45.6125180000
H	-15.3074890000	7.7990830000	-42.6225810000
H	-11.5327730000	8.9137340000	-50.5908720000
H	-10.3244520000	7.7341140000	-51.0681520000
H	-12.6802600000	5.6194050000	-48.9655360000
H	-9.8586770000	8.6634550000	-48.3335560000
H	-10.1910050000	7.4126510000	-46.1198630000
H	-12.3515140000	7.5455890000	-52.4978770000
H	-7.1343300000	8.5725670000	-38.0232430000
H	-7.5239170000	7.3311200000	-36.8369860000
H	-7.8606150000	8.3529740000	-40.3423340000
H	-9.3220970000	5.6130200000	-37.3714350000
H	-9.1641700000	7.1492860000	-42.0885790000
H	-10.5981100000	4.4010270000	-39.1237710000
H	-10.7640130000	5.5341970000	-43.5896620000
H	-9.8409080000	8.2785570000	-36.5790910000
C	-11.9208270000	2.8573520000	-44.8683750000
O	-11.4748740000	3.2538930000	-45.9837320000
C	-11.6593070000	1.4550860000	-44.3636910000
C	-10.6809000000	0.6498700000	-45.2181600000
H	-12.6370860000	0.9643080000	-44.2947640000
H	-11.3031010000	1.5478010000	-43.3307610000
H	-11.0479650000	0.5418560000	-46.2427370000
H	-9.7055320000	1.1412890000	-45.2724160000
H	-12.1448610000	6.0578700000	-51.5628160000
H	-13.3641510000	7.2474280000	-51.0757920000
H	-16.8093020000	5.0338910000	-50.5171700000
H	-17.0552500000	6.3770140000	-49.3938540000
H	-8.6160900000	9.5113770000	-36.2277500000
H	-9.4695060000	9.5250610000	-37.7820120000

H	-16.8928900000	8.0665730000	-43.3616290000
H	-15.9686810000	6.5942350000	-43.7190750000
H	-10.5381820000	-0.3510820000	-44.7981580000
O	-12.6116530000	3.6639850000	-44.1486670000
O	-10.8680130000	5.8849970000	-44.4949330000
C	-10.9580080000	7.9729830000	-31.8940680000
C	-11.4520520000	9.0481080000	-32.8574080000
O	-12.7749670000	8.8086260000	-33.3169640000
C	-12.8858030000	8.6438330000	-36.4802530000
O	-12.7330850000	7.3695650000	-35.8479970000
C	-13.0323620000	6.2483730000	-36.5882750000
C	-13.0797620000	6.2684320000	-37.9822460000
C	-13.4546870000	5.0896910000	-38.6396430000
C	-13.7283810000	3.9024970000	-37.9222360000
C	-13.6327600000	3.8990750000	-36.5214420000
C	-13.2957250000	5.0719110000	-35.8595240000
N	-13.6446960000	4.8282290000	-40.0115770000
C	-14.0376930000	3.4897570000	-40.1366290000
C	-14.0836990000	2.9056560000	-38.9022420000
C	-13.2976260000	5.7129840000	-41.0835380000
C	-13.6162900000	7.1357430000	-40.7991680000
C	-13.0925030000	8.2692330000	-41.3152460000
C	-11.9929400000	8.3528300000	-42.3332160000
C	-13.6420080000	9.6046160000	-40.8734580000
C	-14.4589970000	1.4939770000	-38.6498550000
C	-14.4897070000	0.6377330000	-39.9577110000
N	-14.7679840000	1.3903790000	-41.1868330000
C	-14.4248670000	2.8353540000	-41.4315970000
C	-15.5601630000	3.5421860000	-42.1762460000
C	-16.8243860000	3.7421690000	-41.7728650000
C	-17.8182450000	4.4030210000	-42.6989030000
C	-17.4023040000	3.3257810000	-40.4436470000
O	-13.5319830000	0.8738990000	-37.7319370000
C	-15.6092000000	-0.4425020000	-39.7960360000
N	-15.7875540000	-1.1898500000	-40.9044650000
C	-15.1561590000	-0.8511330000	-42.1797370000
C	-14.9204890000	0.6495780000	-42.3419220000
O	-16.2462850000	-0.6031700000	-38.7588930000
O	-14.8610950000	1.1360180000	-43.4648380000
O	-13.2383230000	-0.0139570000	-40.1266370000
C	-16.8485750000	-2.1956290000	-41.0286990000
C	-16.7121570000	-2.6639410000	-42.4879910000
C	-16.1255950000	-1.4421130000	-43.2183430000
H	-11.4825620000	10.0189240000	-32.3501050000

H	-10.7486130000	9.1492200000	-33.7000740000
H	-12.7574610000	8.0318320000	-33.8978910000
H	-11.6417840000	7.8782870000	-31.0450620000
H	-16.9060020000	-0.7090560000	-43.4460530000
H	-15.6225130000	-1.6904200000	-44.1542720000
H	-17.6665230000	-2.9926960000	-42.9072810000
H	-16.0160020000	-3.5082290000	-42.5466160000
H	-16.7087220000	-2.9969940000	-40.2974400000
H	-17.8232670000	-1.7339550000	-40.8269210000
H	-14.1696930000	-1.3310770000	-42.2528380000
H	-12.8378370000	9.3734930000	-35.6722130000
H	-13.8564580000	8.7112450000	-36.9849560000
H	-12.0851190000	8.8310270000	-37.2036280000
H	-12.8246800000	7.1601830000	-38.5314000000
H	-13.8325660000	2.9898700000	-35.9635600000
H	-13.2443950000	5.1083010000	-34.7763430000
H	-12.0149250000	5.4880580000	-41.3453210000
H	-13.6813790000	5.3391120000	-42.0366170000
H	-14.4045880000	7.2633550000	-40.0580850000
H	-11.6682950000	7.3859320000	-42.7112830000
H	-12.3148310000	8.9440890000	-43.1975180000
H	-11.1269470000	8.8700880000	-41.9009540000
H	-12.8386560000	10.2447810000	-40.4855440000
H	-14.4107710000	9.5078220000	-40.1013250000
H	-14.0789310000	10.1429290000	-41.7244650000
H	-15.4349190000	1.3950880000	-38.1682260000
H	-13.5711910000	2.8522300000	-42.1201360000
H	-15.2768950000	3.8613840000	-43.1746320000
H	-18.2198650000	5.3247120000	-42.2575110000
H	-17.3733570000	4.6510650000	-43.6654290000
H	-18.6779340000	3.7429640000	-42.8776610000
H	-16.6688670000	2.8908500000	-39.7676520000
H	-17.8563420000	4.1878670000	-39.9377570000
H	-18.2079170000	2.5937540000	-40.5881290000
H	-12.7154890000	1.3922750000	-37.7746480000
H	-12.9613180000	-0.2387770000	-39.2196380000
H	-9.9595970000	8.2149280000	-31.5119880000
H	-10.8981690000	6.9981300000	-32.3921550000

TS2-S_{VII,51}

Energy with the medium-sized basis set:	-3474.51420
Solution energy with the medium-sized basis set:	-3474.56781
Energy with larger basis sets:	-3475.60869

Zero-point energy: 1.21504
Imaginary frequency: -1953.71

C	-17.4200170000	5.3859990000	-49.6790490000
C	-17.3872800000	4.9667790000	-48.1977440000
C	-16.0103930000	4.7210400000	-47.6621410000
N	-15.3152520000	3.5319260000	-47.8435740000
C	-15.1476720000	5.5180020000	-46.9523240000
C	-14.1000730000	3.6491800000	-47.2431740000
N	-13.9720250000	4.8430640000	-46.6977060000
C	-15.8868550000	7.6670150000	-43.5357560000
C	-14.7378460000	8.6553980000	-43.7782610000
C	-13.4155170000	7.9422640000	-44.0560860000
O	-13.4884010000	7.0649320000	-45.0169980000
O	-12.3998140000	8.2115160000	-43.4020020000
C	-12.3569980000	7.1289950000	-51.4870320000
C	-10.9780340000	7.3498770000	-50.8550990000
C	-10.9459960000	6.9682480000	-49.4071030000
N	-9.8647770000	7.2270530000	-48.5739960000
C	-11.8637450000	6.3503170000	-48.5979010000
C	-10.1613380000	6.7808570000	-47.3277710000
N	-11.3667420000	6.2411140000	-47.3150110000
C	-9.0340760000	8.8749920000	-37.0160990000
C	-8.7347740000	7.8150120000	-38.0940650000
C	-9.9896990000	7.1809820000	-38.6501310000
C	-10.6949540000	7.7849650000	-39.7058800000
C	-10.5050350000	5.9936750000	-38.1011000000
C	-11.8915930000	7.2583080000	-40.1739400000
C	-11.6899570000	5.4381580000	-38.5660960000
C	-12.4137270000	6.0744380000	-39.6023490000
O	-13.5646840000	5.5664040000	-40.0513130000
Fe	-12.2206270000	5.5949080000	-45.3920120000
H	-17.8473750000	5.7517800000	-47.5888370000
H	-18.0067630000	4.0716550000	-48.0536900000
H	-15.2833730000	6.5240770000	-46.5887040000
H	-15.6668770000	2.7039370000	-48.3006080000
H	-13.3539480000	2.8698060000	-47.2042170000
H	-18.4484610000	5.5609840000	-50.0105630000
H	-14.5938020000	9.3198380000	-42.9217880000
H	-14.9676440000	9.2830110000	-44.6495160000
H	-15.6817800000	7.0386220000	-42.6628320000
H	-10.6932660000	8.4058510000	-50.9624990000
H	-10.2237780000	6.7756780000	-51.4118550000
H	-12.8498850000	5.9924140000	-48.8436600000

H	-9.0062710000	7.6848360000	-48.8413820000
H	-9.5296980000	6.8658110000	-46.4558340000
H	-12.3489890000	7.4250320000	-52.5395970000
H	-8.1671420000	8.2820160000	-38.9080440000
H	-8.0882390000	7.0392870000	-37.6665220000
H	-10.2953690000	8.6850670000	-40.1676700000
H	-9.9586940000	5.4993710000	-37.3005370000
H	-12.4115190000	7.7150090000	-41.0104480000
H	-12.0670760000	4.5045580000	-38.1579360000
H	-11.0776010000	7.0267160000	-43.9804580000
H	-9.5738130000	8.4331860000	-36.1720300000
C	-12.2107520000	3.3114770000	-44.4004360000
O	-11.6252340000	3.4905020000	-45.5215350000
C	-12.0826810000	2.0029120000	-43.6497010000
C	-11.8165770000	0.7939100000	-44.5492760000
H	-12.9748980000	1.8726630000	-43.0298350000
H	-11.2461210000	2.1417370000	-42.9507650000
H	-12.6649520000	0.5998870000	-45.2151290000
H	-10.9348060000	0.9597150000	-45.1730890000
H	-12.6486620000	6.0753700000	-51.4375110000
H	-13.1228450000	7.7175000000	-50.9731570000
H	-16.9867950000	4.6135390000	-50.3236130000
H	-16.8491930000	6.3064240000	-49.8333100000
H	-8.1086040000	9.3191400000	-36.6337910000
H	-9.6550460000	9.6801540000	-37.4220800000
H	-16.8299460000	8.1985970000	-43.3634080000
H	-16.0171720000	7.0026390000	-44.3921290000
H	-11.6530730000	-0.1082920000	-43.9503480000
O	-12.8790810000	4.2647580000	-43.8934530000
O	-10.7530660000	6.2911240000	-44.5499120000
C	-10.9580540000	7.9729990000	-31.8940650000
C	-11.8130370000	9.2291460000	-32.0517850000
O	-13.0660670000	9.1319690000	-31.3922780000
C	-15.2209170000	8.9548060000	-33.8337930000
O	-14.7898500000	7.7424830000	-33.2242230000
C	-14.7303500000	6.6001820000	-33.9867800000
C	-15.0560490000	6.5600770000	-35.3417110000
C	-14.9226500000	5.3265730000	-35.9928380000
C	-14.5030220000	4.1533780000	-35.3211470000
C	-14.2049460000	4.2251580000	-33.9489050000
C	-14.3150150000	5.4420150000	-33.2939300000
N	-15.1716510000	5.0101580000	-37.3262300000
C	-14.9032300000	3.6470800000	-37.4995570000
C	-14.4896790000	3.1067880000	-36.3124640000

C	-15.3952260000	6.0135140000	-38.3369610000
C	-16.7256120000	6.1079410000	-38.9350580000
C	-17.2462550000	7.1922840000	-39.5636510000
C	-16.5284700000	8.5060620000	-39.7252490000
C	-18.6303420000	7.1403620000	-40.1554920000
C	-14.0230180000	1.7021500000	-36.1623880000
C	-13.5987360000	1.0952910000	-37.5388410000
N	-14.3829190000	1.5613150000	-38.6831390000
C	-15.0200290000	2.9145370000	-38.8038900000
C	-16.4395000000	2.7981400000	-39.3654540000
C	-17.5191890000	2.2069200000	-38.8300140000
C	-18.8173280000	2.1672560000	-39.6029430000
C	-17.5694300000	1.5134070000	-37.4924900000
O	-12.8797860000	1.6336110000	-35.2882220000
C	-13.7534470000	-0.4561730000	-37.4587140000
N	-13.4948690000	-1.0759480000	-38.6303530000
C	-13.3367700000	-0.3378280000	-39.8859460000
C	-14.1355000000	0.9631900000	-39.9045330000
O	-14.0665510000	-1.0486940000	-36.4306410000
O	-14.5173160000	1.4394440000	-40.9658860000
O	-12.2352940000	1.4204410000	-37.7901620000
C	-13.6816900000	-2.5183390000	-38.8253030000
C	-13.3885100000	-2.7056650000	-40.3237920000
C	-13.7811320000	-1.3556130000	-40.9505500000
H	-11.3020060000	10.0887830000	-31.6035800000
H	-11.9405120000	9.4582980000	-33.1233030000
H	-13.5713740000	8.4281580000	-31.8294730000
H	-10.8035110000	7.7468460000	-30.8344850000
H	-14.8648580000	-1.2882170000	-41.0896910000
H	-13.3121380000	-1.1681370000	-41.9178860000
H	-13.9375830000	-3.5491090000	-40.7502160000
H	-12.3197210000	-2.8947720000	-40.4749170000
H	-13.0111270000	-3.0859790000	-38.1737350000
H	-14.7095760000	-2.7987530000	-38.5625480000
H	-12.2837020000	-0.0584010000	-40.0311380000
H	-15.1134670000	9.7201880000	-33.0651950000
H	-16.2666970000	8.8852010000	-34.1566470000
H	-14.5915680000	9.2155570000	-34.6936570000
H	-15.4098010000	7.4366040000	-35.8679140000
H	-13.8951560000	3.3375710000	-33.4064120000
H	-14.0963280000	5.5286250000	-32.2347180000
H	-14.9771560000	6.9605480000	-37.9916790000
H	-14.4934100000	5.7638400000	-39.2970610000
H	-17.3227600000	5.2010670000	-38.8965060000

H	-17.1357870000	9.3292490000	-39.3259000000
H	-15.5511010000	8.5334140000	-39.2403410000
H	-16.3688800000	8.7247210000	-40.7883900000
H	-19.2772890000	7.9112100000	-39.7149800000
H	-19.1050310000	6.1674600000	-40.0037320000
H	-18.6012940000	7.3412410000	-41.2350570000
H	-14.7658360000	1.0370970000	-35.7141540000
H	-14.4418640000	3.4639230000	-39.5549990000
H	-16.5366900000	3.2260070000	-40.3587390000
H	-19.6275240000	2.6484330000	-39.0386670000
H	-18.7324190000	2.6611470000	-40.5745950000
H	-19.1358670000	1.1306830000	-39.7768490000
H	-16.6810660000	1.6834490000	-36.8879560000
H	-18.4382950000	1.8551290000	-36.9159410000
H	-17.6911960000	0.4301870000	-37.6250880000
H	-12.5086040000	2.5266370000	-35.2523090000
H	-11.7957370000	1.2955350000	-36.9302410000
H	-9.9786290000	8.1006680000	-32.3694390000
H	-11.4458780000	7.1084730000	-32.3594700000

Int2_{VII,51}

Energy with the medium-sized basis set:	-3474.58477
Solution energy with the medium-sized basis set:	-3474.62742
Energy with larger basis sets:	-3475.67134
Zero-point energy:	1.22415

C	-17.4199890000	5.3859880000	-49.6790070000
C	-17.2540670089	5.8393699319	-48.2098658067
C	-15.9774050093	5.4125366366	-47.5461156575
N	-15.6858858957	4.0924950102	-47.2169560810
C	-14.8833644546	6.1187890632	-47.1110055584
C	-14.4662983627	4.0516411516	-46.6165064818
N	-13.9533128186	5.2649331870	-46.5421817274
C	-15.8870330000	7.6670240000	-43.5359660000
C	-15.0043071299	8.7647590819	-44.1218048676
C	-13.6784893900	8.2933629430	-44.7284686008
O	-13.3543675857	7.0510305263	-44.4701440687
O	-13.0049505342	9.0781553358	-45.3997998512
C	-12.3569880000	7.1289940000	-51.4869720000
C	-11.5792939779	8.2017848067	-50.7201477327
C	-11.4864326691	7.8664334691	-49.2669752687
N	-10.7954326818	8.6429891620	-48.3434112995

C	-11.9859762690	6.8210932830	-48.5372546087
C	-10.8948955618	8.0641444133	-47.1272209189
N	-11.6097493437	6.9562985926	-47.2157571350
C	-9.0339820000	8.8750110000	-37.0159870000
C	-9.3891818578	7.3812709106	-37.0843061514
C	-9.4421850581	6.7936108977	-38.4863989346
C	-8.6404539370	7.2658266666	-39.5350456222
C	-10.3244126909	5.7427944647	-38.7724704707
C	-8.7357673984	6.7363545114	-40.8211194023
C	-10.4372325386	5.2038916249	-40.0535823316
C	-9.6522132054	5.7180221151	-41.0901780014
O	-9.7371921023	5.2556929082	-42.3775385584
Fe	-12.0366807484	5.9514581626	-45.3785034527
H	-17.2970971579	6.9326713889	-48.1602740224
H	-18.1089995122	5.4769746946	-47.6215571530
H	-14.6952523364	7.1804396617	-47.1664504392
H	-16.2956609019	3.2992776977	-47.3456711436
H	-14.0137137773	3.1563290371	-46.2245350655
H	-18.3713548503	5.7426762136	-50.0852874630
H	-14.7464914683	9.5036762439	-43.3552043208
H	-15.5230586493	9.3218214617	-44.9114808033
H	-15.3820569089	7.1457915323	-42.7251077795
H	-12.0663545349	9.1790029673	-50.8497014328
H	-10.5707344029	8.3042346904	-51.1455925392
H	-12.5852911520	5.9869258332	-48.8604610398
H	-10.3226196039	9.5130598301	-48.5359201106
H	-10.4726598666	8.4412140807	-46.2117564969
H	-12.4243012852	7.3800578222	-52.5494189738
H	-8.6668054401	6.8202249586	-36.4739521899
H	-10.3630905431	7.2266526028	-36.6063972246
H	-7.9370357937	8.0750268896	-39.3588948811
H	-10.9609198819	5.3528061743	-37.9838862273
H	-8.1294718737	7.1216496230	-41.6354751973
H	-11.1511086031	4.4086873522	-40.2547294958
H	-9.9943288205	6.2399526619	-44.0072397264
H	-9.6688240530	9.4644557091	-37.6855325561
C	-11.6644067049	3.5583095615	-44.4915515656
O	-11.6254395415	3.8104597856	-45.7272434861
C	-11.2973597518	2.1957518531	-43.9540941201
C	-9.7650098650	2.0487537661	-43.8972861995
H	-11.7316461177	1.4412070310	-44.6172735687
H	-11.7272660038	2.0759017250	-42.9554256291
H	-9.3311694826	2.1519766827	-44.8963519785
H	-9.3256368503	2.8174797063	-43.2537162373

H	-11.8674871226	6.1540083477	-51.3985887478
H	-13.3752988315	7.0318486096	-51.0963909029
H	-17.4048381356	4.2936501648	-49.7648760694
H	-16.6086975354	5.7798123239	-50.2994642160
H	-9.1651917958	9.2570962927	-35.9979556062
H	-7.9944315200	9.0621368446	-37.3045455562
H	-16.8254381097	8.0830402621	-43.1509195106
H	-16.1336901384	6.9293268453	-44.3053864938
H	-9.4917649806	1.0672124777	-43.4982640697
O	-11.9580362202	4.5077969197	-43.6726077947
O	-10.3722204922	6.5199628401	-44.8595412532
C	-10.9580080000	7.9729830000	-31.8940680000
C	-11.0462085882	8.9794599446	-33.0404658996
O	-12.3869823545	9.1942825758	-33.4626159675
C	-12.6825299532	9.2405520188	-36.5707279482
O	-12.7862095147	7.9369766762	-35.9923085838
C	-13.1559737283	6.8968431261	-36.8132729480
C	-13.2574991939	7.0291821088	-38.1938184079
C	-13.6313544836	5.8962547246	-38.9243100209
C	-13.8700029256	4.6465706758	-38.3036807636
C	-13.7526517099	4.5436684048	-36.9058689073
C	-13.4036987014	5.6662009881	-36.1686651083
N	-13.7517214064	5.7321112062	-40.3121769766
C	-14.0767501855	4.3910546436	-40.5474531107
C	-14.1427549668	3.7096777250	-39.3656050304
C	-13.2641665365	6.6272477194	-41.2791744198
C	-13.3283105192	8.0184534399	-41.1065827016
C	-12.5156198370	8.9641231927	-41.7002384215
C	-11.3084657178	8.6303740706	-42.5267831698
C	-12.7822856376	10.4314568728	-41.5028653983
C	-14.4339685700	2.2591969187	-39.2660086499
C	-14.2470863189	1.5248359173	-40.6407441629
N	-14.4980226710	2.3465825184	-41.8264903789
C	-14.4094932814	3.8401778953	-41.8959563040
C	-15.6799124803	4.4082168450	-42.5146255332
C	-16.9295975157	4.3085151008	-42.0391402257
C	-18.0901438404	4.8762506501	-42.8209151405
C	-17.2950365432	3.6259245196	-40.7374260444
O	-13.5520215555	1.6251412251	-38.3143227567
C	-15.2399568776	0.3186112023	-40.6941526826
N	-15.2039305259	-0.3414958494	-41.8720315909
C	-14.5075555366	0.1988915018	-43.0412707634
C	-14.4932352781	1.7238118447	-43.0479813403
O	-15.9792912117	0.0058130771	-39.7659265076

O	-14.4646021325	2.3326289917	-44.1162253506
O	-12.9110349574	1.0459786984	-40.7454627510
C	-16.1420911772	-1.4200952951	-42.2019110602
C	-15.7796463934	-1.7522334202	-43.6595037590
C	-15.2784170334	-0.4103337871	-44.2251368687
H	-10.6681580917	9.9546147071	-32.7099553660
H	-10.4105580353	8.6556763110	-33.8812962586
H	-12.6443366227	8.4515711627	-34.0301777520
H	-11.5848602636	8.2989971378	-31.0584863836
H	-16.1175105822	0.2448091627	-44.4826446144
H	-14.6515094328	-0.5121434554	-45.1131541458
H	-16.6281550435	-2.1597277581	-44.2156419736
H	-14.9746893565	-2.4959140652	-43.6846212094
H	-16.0181689502	-2.2595601249	-41.5120112175
H	-17.1737027099	-1.0583593239	-42.0994265455
H	-13.4574690576	-0.1250737738	-43.0402809381
H	-12.4581708795	9.9058156381	-35.7376077718
H	-13.6279231313	9.5333433028	-37.0446648112
H	-11.8776924960	9.2820054999	-37.3124080524
H	-13.0048895635	7.9508528328	-38.6910471264
H	-13.9290736690	3.5917311720	-36.4141317465
H	-13.3124291308	5.6228904887	-35.0879270855
H	-10.6161933982	4.8601600498	-42.5727868682
H	-12.7931260120	6.1738248642	-42.1404558355
H	-14.0981117324	8.3859893604	-40.4282047961
H	-11.1721426351	7.5625454104	-42.6756167292
H	-11.3693805556	9.0934504539	-43.5177973048
H	-10.4043301990	9.0165153711	-42.0344265812
H	-11.9084906544	10.9371087724	-41.0663840176
H	-13.6454243065	10.6191624577	-40.8551469676
H	-12.9686076700	10.9237576952	-42.4685181004
H	-15.4441380348	2.0496214823	-38.9081018554
H	-13.5957579528	4.0668350911	-42.5867882575
H	-15.5116910773	4.8964025789	-43.4675228872
H	-18.6139791606	5.6455334192	-42.2373266147
H	-17.7746834164	5.3240423560	-43.7667617059
H	-18.8300526448	4.0931438263	-43.0384895999
H	-16.7576337159	4.0623051552	-39.8906254834
H	-18.3663161425	3.7120047458	-40.5330270535
H	-17.0510959895	2.5579316095	-40.7541254194
H	-12.8020221776	2.2262721373	-38.1981923510
H	-12.6846799455	0.7629226296	-39.8407343949
H	-9.9264331817	7.8659028085	-31.5382700654
H	-11.3090185325	6.9857206961	-32.2171811447

Int3_{VII,51}

Energy with the medium-sized basis set: -3624.91768
Solution energy with the medium-sized basis set: -3624.96348
Energy with larger basis sets: -3626.06291
Zero-point energy: 1.23244

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.5043453215	4.9343321830	-48.2085346671
C	-16.1798215416	4.5221324884	-47.6505777756
N	-15.4744731417	3.4231560339	-48.1258721934
C	-15.3680961792	5.0636461521	-46.6860941076
C	-14.2990230967	3.3383472593	-47.4497953597
N	-14.2110886020	4.3203565010	-46.5718005895
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4711297324	7.7777942472	-42.9569466695
C	-13.3761164981	7.2193333775	-43.8683121499
O	-13.5976736747	6.0320169559	-44.3369057065
O	-12.3651625083	7.9110450266	-44.0890842736
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.7796231423	7.9864758266	-50.3475065588
C	-11.6959803183	7.3012760807	-49.0097829042
N	-10.7698334364	7.7040759315	-48.0531727599
C	-12.3990719912	6.2933334537	-48.3961287970
C	-10.9288115863	6.9524071726	-46.9390568851
N	-11.9114208913	6.0861143716	-47.1155576372
C	-9.0340000000	8.8750000000	-37.0160000000
C	-8.2213607281	9.3275785975	-38.2428121419
C	-8.7317806114	8.7607890986	-39.5535290139
C	-9.8077312804	9.3430975524	-40.2378195922
C	-8.1461600039	7.6203693495	-40.1219182817
C	-10.2688489615	8.8294533596	-41.4525412048
C	-8.5858320206	7.0966549197	-41.3342416259
C	-9.6389768665	7.7126939005	-42.0180349584
O	-9.9829659581	7.2221203594	-43.2385449233
Fe	-12.3874062940	4.8047649199	-45.3674727317
H	-17.8896706765	5.7502929368	-47.5892039048
H	-18.2263203474	4.1109491459	-48.1160225885
H	-15.5233041921	5.9295070215	-46.0617384129
H	-15.7910787823	2.7787773515	-48.8348641939
H	-13.5418873080	2.5851579901	-47.6041360584
H	-18.4028308587	5.6915115518	-50.0517709580

H	-14.4098333085	7.2136384109	-42.0167295400
H	-14.2164174273	8.8168656547	-42.7319898034
H	-16.1221001102	6.6250542857	-43.7734859367
H	-12.3780762476	8.9037209854	-50.2483384061
H	-10.7712694522	8.3191393917	-50.6298481445
H	-13.2180620579	5.7052434150	-48.7795552802
H	-10.0827765994	8.4342934438	-48.1687961456
H	-10.3437030617	7.0346475857	-46.0365210869
H	-12.3882795032	7.7037352664	-52.4169490583
H	-8.2236971858	10.4247681336	-38.2901928823
H	-7.1739462460	9.0300066389	-38.1083536905
H	-10.2857145803	10.2298172583	-39.8238801132
H	-7.3189694052	7.1364811074	-39.6063270224
H	-11.0949836075	9.2946281050	-41.9841711767
H	-8.1304896935	6.2140133726	-41.7705189352
H	-10.4055316724	5.5443872638	-43.9257468382
H	-9.0986021378	7.7840720510	-36.9635634488
C	-12.1172540742	2.3227893782	-45.0146395406
O	-11.7917035421	2.8225536472	-46.1377092669
C	-11.6895151463	0.9254316131	-44.6301316710
C	-11.4177297086	0.0008759140	-45.8165264969
H	-12.4241229026	0.4929425170	-43.9472846184
H	-10.7729755611	1.0505740454	-44.0366058601
H	-12.3274042307	-0.1599104278	-46.4068215684
H	-10.6617592728	0.4302558856	-46.4793687198
H	-11.7487501922	6.2342081314	-51.6512855922
H	-13.3779346227	6.8045358952	-51.2577170868
H	-17.0557753090	4.5792447967	-50.3255769439
H	-16.7332690547	6.2319582328	-49.7839897726
H	-8.5825013501	9.2393903364	-36.0858498877
H	-10.0571726390	9.2578161989	-37.0623429812
H	-16.6331655265	8.0359222635	-42.8247038941
H	-15.9820134423	8.2540747941	-44.4569661126
H	-11.0705140495	-0.9733256112	-45.4600721744
O	-12.7646694147	3.0368527151	-44.1755165950
O	-10.7331366060	5.0920915359	-44.7260847337
C	-10.9580000000	7.9730000000	-31.8940000000
C	-10.9069884324	8.1744518651	-33.4059808180
O	-11.8135908451	7.2585739668	-34.0017583745
C	-12.3825552919	7.9981759917	-37.8589601796
O	-11.8109014408	7.0880793632	-36.9236503212
C	-11.6507109101	5.7787413326	-37.3169344768
C	-11.9255644008	5.3335933892	-38.6072168443
C	-11.7622502982	3.9648332389	-38.8411783547

C	-11.3099446105	3.0605806516	-37.8537144372
C	-11.0115163991	3.5547591117	-36.5716332452
C	-11.1923525704	4.9027477199	-36.3062122740
N	-12.0280045279	3.2396752786	-39.9979171014
C	-11.7350544462	1.9011450628	-39.7532246996
C	-11.3054704782	1.7518820211	-38.4673825558
C	-12.5219377927	3.7833792679	-41.2265508357
C	-13.8903702889	4.3936620716	-41.2510248035
C	-14.9013944476	4.3009782061	-40.3705055220
C	-14.8909811779	3.5840202556	-39.0394762010
C	-16.2165192238	4.9758062227	-40.6903316518
C	-10.9102117619	0.4521398699	-37.8723154678
C	-10.7943610808	-0.6994254635	-38.9442253508
N	-11.5348569543	-0.4861902640	-40.1993827089
C	-12.0056999536	0.8120526109	-40.7380521866
C	-13.4821481186	0.7635235209	-41.1320582996
C	-14.5131423395	0.3365444195	-40.3899124932
C	-15.9140799215	0.3794672582	-40.9518867504
C	-14.4100054597	-0.2256004681	-38.9930694778
O	-9.6377988340	0.5678413744	-37.1979780964
C	-11.3521074496	-2.0245385765	-38.3244652681
N	-11.3393953275	-3.0502954691	-39.2024347736
C	-11.0438655792	-2.8625799935	-40.6263327643
C	-11.5149271728	-1.5017532393	-41.1299773101
O	-11.7553463309	-2.1252859405	-37.1686528104
O	-11.8588900414	-1.3482448741	-42.2965390832
O	-9.4315962707	-0.8853683578	-39.2873253874
C	-11.9065423033	-4.3675227765	-38.8973534144
C	-11.6987233876	-5.1408297541	-40.2113515814
C	-11.7632866791	-4.0465794318	-41.2932814898
H	-11.1748977567	9.2178678900	-33.6480230664
H	-9.8771827454	8.0175166413	-33.7705376010
H	-11.8090182737	7.3802993915	-34.9650883055
H	-11.9739568673	8.1452896672	-31.5250299772
H	-12.7995888433	-3.7655822792	-41.5083246090
H	-11.2952434240	-4.3301517565	-42.2376526376
H	-12.4448240875	-5.9272008805	-40.3534340427
H	-10.7095192911	-5.6136524960	-40.2132945181
H	-11.3995104783	-4.8121785085	-38.0361884455
H	-12.9684250066	-4.2639778865	-38.6377139952
H	-9.9595035561	-2.9084668014	-40.7943041947
H	-12.4844853001	8.9477412839	-37.3306030092
H	-13.3732267118	7.6564429777	-38.1868153506
H	-11.7326431129	8.1368906865	-38.7306877660

H	-12.2518049901	5.9923726446	-39.3996815622
H	-10.6588860237	2.8819843567	-35.7963517789
H	-11.0181410669	5.3129670611	-35.3166048360
H	-10.8590389162	7.5671385290	-43.5463528942
H	-12.4371896541	3.0469780169	-42.0257832601
H	-14.0618441754	4.9036125140	-42.1971165217
H	-15.8932989826	3.2024893662	-38.8130329625
H	-14.1975557618	2.7464574207	-39.0063360113
H	-14.6185448632	4.2762366687	-38.2330320690
H	-17.0236903030	4.2334215816	-40.7513505617
H	-16.1876360635	5.5268678149	-41.6334145164
H	-16.4970199019	5.6741773495	-39.8898743241
H	-11.6043149000	0.1111348734	-37.1007125667
H	-11.4367190634	1.0049010683	-41.6558790221
H	-13.6868371171	1.1464516667	-42.1284827370
H	-16.5564189249	1.0224483212	-40.3345895352
H	-15.9358806076	0.7588686460	-41.9774513020
H	-16.3712655843	-0.6195602250	-40.9443920670
H	-13.4902567539	0.0524697177	-38.4836910518
H	-15.2485718243	0.1233330258	-38.3782454858
H	-14.4624418380	-1.3225943446	-39.0075833702
H	-9.2017410309	1.3463057461	-37.5744947116
H	-8.9465813590	-0.6489994016	-38.4745959309
H	-10.2767559493	8.6637995295	-31.3856203140
H	-10.6725399405	6.9474287793	-31.6395203335
O	-11.6041819439	4.8828073114	-41.6656780558
O	-10.3991983843	4.4050021711	-41.9063029528

TS3_{VII,51}

Energy with the medium-sized basis set:	-3624.89547
Solution energy with the medium-sized basis set:	-3624.94312
Energy with larger basis sets:	-3626.04460
Zero-point energy:	1.23007
Imaginary frequency:	-333.66

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.3621730000	4.5050220000	-48.4175080000
C	-15.9669190000	4.2174540000	-47.9589920000
N	-15.1613630000	3.2454350000	-48.5381300000
C	-15.1697730000	4.8042120000	-47.0087520000
C	-13.9472850000	3.2739800000	-47.9282660000
N	-13.9237420000	4.2115770000	-46.9987570000

C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.5244830000	8.0620050000	-44.1275400000
C	-13.5191860000	6.9222900000	-43.9834750000
O	-13.4485700000	6.1212550000	-44.9918740000
O	-12.8901050000	6.8194120000	-42.9150540000
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.0448810000	7.4282370000	-50.7529160000
C	-10.9924700000	6.8247100000	-49.3820460000
N	-9.8558380000	6.8596210000	-48.5837170000
C	-11.9252920000	6.1663260000	-48.6227510000
C	-10.1304040000	6.2420480000	-47.4084600000
N	-11.3779170000	5.8087460000	-47.4060800000
C	-9.0340000000	8.8750000000	-37.0160000000
C	-8.1017260000	8.4455350000	-38.1635720000
C	-8.8122830000	7.6215790000	-39.2164900000
C	-9.7273370000	8.2191150000	-40.0930760000
C	-8.6216000000	6.2374120000	-39.3274370000
C	-10.4547800000	7.4745510000	-41.0186500000
C	-9.3409080000	5.4703300000	-40.2478000000
C	-10.2836850000	6.0835250000	-41.0830380000
O	-11.0060700000	5.2952770000	-41.9296790000
Fe	-12.1454860000	4.7651840000	-45.6369110000
H	-17.8932860000	5.0010350000	-47.5988850000
H	-17.8972530000	3.5636860000	-48.5998200000
H	-15.3939810000	5.6001410000	-46.3165430000
H	-15.4392400000	2.6013610000	-49.2635420000
H	-13.1247770000	2.6158170000	-48.1626550000
H	-18.4562470000	5.5730950000	-49.9771290000
H	-14.1290900000	8.9317550000	-43.5941300000
H	-14.6226350000	8.3202740000	-45.1863100000
H	-15.7743970000	7.3260990000	-42.5035680000
H	-10.9071340000	8.5166460000	-50.6838070000
H	-10.2003560000	7.0550920000	-51.3489530000
H	-12.9480230000	5.9280830000	-48.8644530000
H	-8.9687230000	7.2712240000	-48.8326790000
H	-9.4455030000	6.1183370000	-46.5828300000
H	-12.3511840000	7.5829450000	-52.4815760000
H	-7.6658590000	9.3420970000	-38.6241220000
H	-7.2629300000	7.8709140000	-37.7531550000
H	-9.8806500000	9.2957200000	-40.0503730000
H	-7.8978980000	5.7459590000	-38.6800030000
H	-11.1590860000	7.9538690000	-41.6896100000
H	-9.1814530000	4.3997530000	-40.3370360000
H	-10.5065600000	5.0396610000	-43.8313340000

H	-9.4635570000	8.0019110000	-36.5142630000
C	-12.0076540000	2.2782060000	-45.3960370000
O	-11.4799360000	2.7972670000	-46.4283120000
C	-11.9577400000	0.7863500000	-45.1653310000
C	-13.3410770000	0.1830920000	-44.8886440000
H	-11.3242170000	0.6139570000	-44.2894530000
H	-11.4833170000	0.3276010000	-46.0376210000
H	-13.7984610000	0.6723210000	-44.0270020000
H	-14.0113930000	0.2988500000	-45.7479910000
H	-12.5039440000	6.0511160000	-51.6063280000
H	-13.2155270000	7.5303300000	-50.9396600000
H	-16.9096680000	4.9093560000	-50.5232100000
H	-16.9359700000	6.3505010000	-49.4996450000
H	-8.4949320000	9.4676580000	-36.2686620000
H	-9.8651820000	9.4807670000	-37.3920020000
H	-16.5794190000	8.5150490000	-43.5497600000
H	-16.3432000000	6.8500590000	-44.1057450000
H	-13.2545340000	-0.8854220000	-44.6693760000
O	-12.5928640000	3.0439830000	-44.5544270000
O	-10.5972890000	5.2268210000	-44.7833000000
C	-10.9580000000	7.9730000000	-31.8940000000
C	-12.2628700000	7.8291970000	-32.6607790000
O	-13.1123510000	6.9507090000	-31.9351280000
C	-16.2022820000	6.5476540000	-34.4157560000
O	-14.9553010000	6.0169120000	-33.9961570000
C	-14.2117500000	5.2810860000	-34.8980270000
C	-14.5889090000	5.0897660000	-36.2241990000
C	-13.7265240000	4.3264810000	-37.0325210000
C	-12.5280960000	3.7852920000	-36.5239630000
C	-12.1769600000	3.9970570000	-35.1807560000
C	-13.0184580000	4.7377330000	-34.3710300000
N	-13.8369200000	3.9795960000	-38.3805730000
C	-12.7031050000	3.2234880000	-38.7232120000
C	-11.9040670000	3.0963570000	-37.6126320000
C	-14.8977080000	4.6239360000	-39.1881540000
C	-14.4285340000	5.9514180000	-39.7207720000
C	-15.0334680000	7.1372540000	-39.5454330000
C	-16.3559690000	7.3478180000	-38.8489400000
C	-14.3958560000	8.4036950000	-40.0646420000
C	-10.5601060000	2.4811080000	-37.5780440000
C	-10.2632920000	1.5445830000	-38.7925420000
N	-11.3263920000	1.5080500000	-39.8265660000
C	-12.3732280000	2.5801610000	-40.0569220000
C	-13.5438970000	1.9649180000	-40.7971770000

C	-14.5255890000	1.1359430000	-40.2790870000
C	-15.4653000000	0.4557030000	-41.2481610000
C	-14.4364760000	0.4769600000	-38.9245200000
O	-9.5313550000	3.4982800000	-37.5019290000
C	-10.0901380000	0.0816360000	-38.2737340000
N	-9.9070850000	-0.7991870000	-39.2784540000
C	-10.0265250000	-0.4131870000	-40.6845390000
C	-11.0673180000	0.6865230000	-40.8982190000
O	-10.0962180000	-0.2298120000	-37.0867630000
O	-11.6352480000	0.7758610000	-41.9830100000
O	-9.0389510000	1.9247940000	-39.3898090000
C	-9.7903850000	-2.2467020000	-39.0774350000
C	-9.6479480000	-2.7848780000	-40.5126380000
C	-10.3763690000	-1.7406160000	-41.3791980000
H	-12.7328350000	8.8196220000	-32.7871900000
H	-12.0578790000	7.4369870000	-33.6690000000
H	-13.8661500000	6.7329260000	-32.5059490000
H	-11.1475480000	8.3557170000	-30.8862400000
H	-11.4597990000	-1.8950630000	-41.3508330000
H	-10.0674860000	-1.7500380000	-42.4257730000
H	-10.0632590000	-3.7901690000	-40.6205730000
H	-8.5892570000	-2.8318510000	-40.7912600000
H	-8.9347090000	-2.4798210000	-38.4369160000
H	-10.6889140000	-2.6276700000	-38.5760520000
H	-9.0694500000	-0.0217700000	-41.0557410000
H	-16.6326670000	7.0397940000	-33.5421300000
H	-16.8799320000	5.7542920000	-34.7546450000
H	-16.0786890000	7.2832010000	-35.2214580000
H	-15.4984650000	5.5257890000	-36.6100480000
H	-11.2528760000	3.5896750000	-34.7820550000
H	-12.7794000000	4.9369620000	-33.3320250000
H	-11.7425300000	5.8240610000	-42.3533170000
H	-15.7403570000	4.7229390000	-38.5017540000
H	-13.4939860000	5.9127670000	-40.2749010000
H	-17.0837320000	7.7687010000	-39.5543950000
H	-16.7944150000	6.4356750000	-38.4398040000
H	-16.2538840000	8.0794400000	-38.0369830000
H	-15.1141700000	8.9923840000	-40.6492510000
H	-13.5326690000	8.1900740000	-40.6972440000
H	-14.0758100000	9.0407900000	-39.2289920000
H	-10.4196890000	1.8704020000	-36.6841420000
H	-11.9343550000	3.3318670000	-40.7270140000
H	-13.6751410000	2.3209230000	-41.8115860000
H	-16.4575960000	0.3365260000	-40.8031110000

H	-15.5692610000	1.0274870000	-42.1727810000
H	-15.0867710000	-0.5438900000	-41.5005820000
H	-13.8041900000	1.0196710000	-38.2227490000
H	-15.4363610000	0.3846010000	-38.4892900000
H	-14.0324960000	-0.5388420000	-39.0305700000
H	-9.8702130000	4.2981340000	-37.9365210000
H	-8.7053520000	2.6413020000	-38.8083740000
H	-10.2798660000	8.6634930000	-32.4061060000
H	-10.4614100000	7.0024510000	-31.7999940000
O	-15.3276550000	3.8702930000	-40.3016300000
O	-15.8488270000	2.6449410000	-39.8575250000

Int4_{vII,51}

Energy with the medium-sized basis set:	-3624.92300
Solution energy with the medium-sized basis set:	-3624.96843
Energy with larger basis sets:	-3626.06493
Zero-point energy:	1.23355

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.3787883544	4.5461325616	-48.3893302930
C	-15.9837238653	4.2876475827	-47.9182204319
N	-15.1647059802	3.3079067235	-48.4658499797
C	-15.1957251653	4.9203573843	-46.9912820886
C	-13.9504471648	3.3721559583	-47.8572649500
N	-13.9438633560	4.3425353740	-46.9628275399
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.6027389130	8.2206250287	-44.1816918839
C	-13.4720913888	7.2025699066	-44.0721967790
O	-13.4919389446	6.2766828135	-44.9705865031
O	-12.6604277624	7.2953863828	-43.1306999503
C	-12.3570000000	7.1290000000	-51.4870000000
C	-10.9711898530	7.2293331881	-50.8380117470
C	-10.9618545012	6.7072338710	-49.4343482828
N	-9.8208565849	6.6952614807	-48.6412128105
C	-11.9405097176	6.1662920055	-48.6410386479
C	-10.1351993442	6.1669266768	-47.4334010409
N	-11.4138920194	5.8369414751	-47.4069415864
C	-9.0340000000	8.8750000000	-37.0160000000
C	-8.0383208965	8.2829667219	-38.0316456031
C	-8.7454945479	7.5635436303	-39.1607362694
C	-9.4832125130	8.2868669511	-40.1071724071
C	-8.7462095330	6.1665293981	-39.2665329272

C	-10.2125517433	7.6519961660	-41.1075961702
C	-9.4798764936	5.5061407838	-40.2564439742
C	-10.2288844427	6.2514724709	-41.1759244183
O	-10.9792668823	5.5841411055	-42.0948239841
Fe	-12.2096579486	4.9073489330	-45.6025726039
H	-17.9170989306	5.0676733791	-47.5910473513
H	-17.9060331216	3.5951297138	-48.5446204447
H	-15.4273043743	5.7408628559	-46.3317320837
H	-15.4373245106	2.6351195304	-49.1668306863
H	-13.1185367366	2.7137971299	-48.0543563211
H	-18.4512871214	5.5600694398	-50.0029471042
H	-14.2931220962	9.1403630559	-43.6782301636
H	-14.7770068410	8.4393647581	-45.2409914790
H	-15.7208357994	7.4275040171	-42.4822012196
H	-10.6371217385	8.2767106497	-50.8440768630
H	-10.2397477209	6.6740616903	-51.4425884474
H	-12.9812735462	5.9950686741	-48.8633115942
H	-8.9064885993	7.0229533568	-48.9150504472
H	-9.4645219241	6.0293925016	-46.5985669753
H	-12.3351939249	7.5176185773	-52.5089744044
H	-7.4140844158	9.0910479253	-38.4368168119
H	-7.3581920627	7.5922507877	-37.5187590565
H	-9.4926710167	9.3741914409	-40.0566659560
H	-8.1645639332	5.5789873069	-38.5583855624
H	-10.7826004179	8.2211539241	-41.8341099921
H	-9.4884792924	4.4211929003	-40.3218499824
H	-10.5046933453	5.1147899959	-43.8471198941
H	-9.6526294520	8.0859948982	-36.5740747077
C	-12.1641858397	2.4519333921	-45.1777188004
O	-11.5836817287	2.8607245515	-46.2308592824
C	-12.1181022384	0.9949984704	-44.7862445868
C	-13.4384409653	0.5070448124	-44.1855578764
H	-11.3297494092	0.9104259832	-44.0296086092
H	-11.8184865389	0.4167783725	-45.6658534481
H	-13.6508571252	1.0795122067	-43.2812929058
H	-14.2733586600	0.6420329254	-44.8823184416
H	-12.6963099747	6.0886803216	-51.5249604585
H	-13.0948121547	7.7045420250	-50.9193689393
H	-16.8898034327	4.8840333426	-50.4962226080
H	-16.9408693582	6.3569327593	-49.5190306514
H	-8.5136510289	9.3960044494	-36.2040062536
H	-9.7079712851	9.5896715525	-37.5005940542
H	-16.6994262622	8.3983922092	-43.6020246341
H	-16.2092991749	6.7499387497	-44.0406391565

H	-13.3795421656	-0.5550403151	-43.9267934482
O	-12.7894580168	3.2953981844	-44.4436124892
O	-10.6215611103	5.3008602882	-44.7973282081
C	-10.9580000000	7.9730000000	-31.8940000000
C	-12.0759919178	8.6168321514	-32.7041290815
O	-13.3164784919	8.2803272503	-32.0928382097
C	-16.0843838354	8.7283602083	-34.9458713100
O	-15.1456555542	7.8653376313	-34.3232596343
C	-14.5181271637	6.9102685517	-35.0989096361
C	-14.7236449202	6.7814763572	-36.4701826563
C	-13.9876190051	5.7842659205	-37.1325463464
C	-13.0589257676	4.9689024735	-36.4535273970
C	-12.8824861714	5.1212977249	-35.0694864472
C	-13.6193100419	6.0781507548	-34.3934646417
N	-13.9679781449	5.4360389492	-38.4804830644
C	-13.0224727775	4.4208468755	-38.6623804789
C	-12.4651101892	4.1205368693	-37.4433575125
C	-14.8932530391	6.0803548519	-39.4216057400
C	-14.2368967642	7.2228372243	-40.1421948953
C	-14.5647758962	8.5210646044	-40.0496160348
C	-15.7109163340	9.0791611360	-39.2408787970
C	-13.7446736296	9.5591676370	-40.7769506043
C	-11.2738376719	3.2697894228	-37.2616029702
C	-11.0919645881	2.2263642520	-38.3902183728
N	-11.7269751376	2.6048536770	-39.6823181363
C	-12.6112468896	3.7994092521	-39.9751904699
C	-13.7248481012	3.3840941838	-40.8982663112
C	-15.0671272745	2.8926114236	-40.4569913856
C	-15.9077014349	2.4672423116	-41.6649243396
C	-15.0024660310	1.7888361728	-39.3898813680
O	-10.0786068696	4.0869429346	-37.1798537644
C	-11.7071787271	0.8613835474	-38.0024032457
N	-11.5661702066	-0.0404867029	-38.9996063537
C	-11.0424473631	0.3283548984	-40.3238200063
C	-11.4283103084	1.7606790430	-40.7263559934
O	-12.2739336673	0.6365917663	-36.9373123781
O	-11.5122361819	2.0617013848	-41.9109014633
O	-9.7090881122	2.0211163145	-38.5839647221
C	-12.1893670255	-1.3664356251	-38.9679943763
C	-11.7842410104	-1.9647844260	-40.3262725497
C	-11.6749241402	-0.7326006087	-41.2420575455
H	-11.9372674900	9.7119157937	-32.7348760933
H	-12.0338759871	8.2538298232	-33.7426163770
H	-14.0145355509	8.3521388211	-32.7621385794

H	-11.0089387923	8.3004241445	-30.8503606474
H	-12.6682126371	-0.3956900990	-41.5539409063
H	-11.0838590330	-0.9003573993	-42.1444558152
H	-12.5051142922	-2.7034223420	-40.6879060727
H	-10.8097624529	-2.4601385838	-40.2413426181
H	-11.8323190694	-1.9388967257	-38.1068909021
H	-13.2785536124	-1.2637545969	-38.8682354553
H	-9.9485353650	0.2581339376	-40.3324466464
H	-16.4692858935	9.3790677582	-34.1584734907
H	-16.9155624162	8.1632757062	-35.3881272931
H	-15.6150780154	9.3423608647	-35.7271225227
H	-15.3930655907	7.4411126130	-37.0015641450
H	-12.1716058129	4.4974542410	-34.5356686055
H	-13.5089800940	6.2328586714	-33.3260615370
H	-11.6084920001	6.2104813655	-42.5609787352
H	-15.7428800524	6.3953677797	-38.8095615251
H	-13.4027021365	6.9284006643	-40.7739437549
H	-16.3266551011	9.7378441936	-39.8657643514
H	-16.3706448581	8.3164817116	-38.8224148326
H	-15.3327364929	9.6963450796	-38.4145607834
H	-14.3924818819	10.2179769032	-41.3706072690
H	-13.0165473295	9.0969183155	-41.4457085896
H	-13.2152473744	10.2021547562	-40.0602884818
H	-11.3114082781	2.7096699007	-36.3250306314
H	-12.0079801797	4.5139010631	-40.5416742425
H	-13.5256510296	3.4811531520	-41.9587327485
H	-16.9138915942	2.1859319017	-41.3394375299
H	-15.9848822228	3.2949246818	-42.3760172359
H	-15.4510120503	1.6159662057	-42.1786214460
H	-14.3824482723	2.0826436332	-38.5407324606
H	-16.0085205659	1.5600991743	-39.0227222171
H	-14.5824471749	0.8785826094	-39.8296675059
H	-10.2201452087	4.8605223952	-37.7493422388
H	-9.2954604751	2.8119773944	-38.1804168955
H	-9.9762092218	8.2445535994	-32.2976214188
H	-11.0550455097	6.8825885435	-31.9141617631
O	-15.3609955954	5.2127545198	-40.4336950455
O	-15.7977522815	3.9804510333	-39.7794496617

React(D)₁

Energy with the medium-sized basis set:	-1918.72266
Solution energy with the medium-sized basis set:	-1918.76227
Energy with larger basis sets:	-1919.33339
Zero-point energy:	0.58980

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.6033436517	4.7681163609	-48.2821699613
C	-16.2836298264	4.3823529008	-47.7036514303
N	-15.6286245442	3.2043826467	-48.0395921259
C	-15.3882348937	5.0812278065	-46.9398650547
C	-14.3958038462	3.2184763950	-47.4788086392
N	-14.2295268589	4.3485628814	-46.8163124470
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.5123277898	7.3774545548	-42.9175693968
C	-13.4226573732	7.0036397455	-43.9223621279
O	-13.7516023049	6.0751421510	-44.7608833754
O	-12.3127914545	7.5673076999	-43.8708864406
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.7501059856	8.0329898855	-50.4073508842
C	-11.8893097293	7.4897316476	-49.0160849706
N	-11.4951308216	8.2231539878	-47.9034767489
C	-12.3546032680	6.3058197634	-48.5018504005
C	-11.7221340755	7.4947931206	-46.7851402645
N	-12.2475345979	6.3293638389	-47.1224317508
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.5139067679	8.4745317910	-37.1579226588
C	-10.7676567933	7.7471879598	-38.4592785106
C	-11.0632052250	8.4498738600	-39.6328978901
C	-10.6183939165	6.3564685269	-38.5534212162
C	-11.1921655432	7.8041700042	-40.8611855383
C	-10.7419570084	5.6910352910	-39.7694021704
C	-11.0183012394	6.4135096089	-40.9377715381
O	-11.1004180325	5.7211328725	-42.1002733364
Fe	-12.6213169744	4.8857150949	-45.7700802786
H	-18.0828769102	5.4883645039	-47.6116940869
H	-18.2699788025	3.8975794673	-48.3329582403
H	-15.4785289217	6.0384104287	-46.4537591832
H	-16.0178744242	2.4467499408	-48.5809770204
H	-13.6684320912	2.4279009676	-47.5588926166
H	-18.3822107074	5.6755323359	-50.1141802347

H	-14.5884663329	6.5283911578	-42.2262866637
H	-14.1470877166	8.2324517419	-42.3429489303
H	-16.2438959483	6.7964096075	-44.0946998987
H	-12.2225304143	9.0245545828	-50.4539803830
H	-10.6853602765	8.1961724423	-50.6263838658
H	-12.7516189461	5.4457271493	-49.0153612288
H	-11.1010290619	9.1520152906	-47.9185487231
H	-11.5396933780	7.7989470228	-45.7611769771
H	-12.2292867778	7.5744154446	-52.4772121949
H	-10.8021529590	7.8404475029	-36.3095145608
H	-11.1405452133	9.3742084663	-37.1014456970
H	-11.1906504738	9.5305541023	-39.5883478356
H	-10.3941534503	5.7835823212	-37.6552263936
H	-11.4328402298	8.3558102747	-41.7643494957
H	-10.6241382182	4.6140681939	-39.8416785862
H	-11.2898154486	6.3272267100	-42.8401772162
H	-8.7307505326	9.5265916979	-37.8426997749
C	-12.0348363852	2.5327982741	-44.6511173938
O	-12.8835752750	3.5112488712	-44.5068527235
O	-11.9398644760	1.5092138260	-43.9930129164
C	-11.1365869712	2.7469700506	-45.8776232395
O	-11.5720038301	3.5419640234	-46.7579519267
C	-10.0053867968	1.8089091858	-46.1443780379
C	-9.0087613257	2.3321821157	-47.1778481788
H	-10.4600669715	0.8585716506	-46.4626741476
H	-9.5408699030	1.5915656253	-45.1777007970
H	-9.5011653197	2.5302342683	-48.1341856030
H	-8.5633230704	3.2687642590	-46.8298943669
H	-11.8741986719	6.1462772144	-51.4917208213
H	-13.4279864114	6.9784760296	-51.3149909313
H	-16.9399436324	4.6781121667	-50.3638724368
H	-16.7860793638	6.2761960490	-49.6218045646
H	-8.8462205823	9.4054473191	-36.0745381687
H	-8.3912119026	7.9884647319	-37.0435363531
H	-16.6208550724	7.9016915560	-42.7586402028
H	-15.8403472494	8.5200403387	-44.2230981196
H	-8.2070692040	1.6066106585	-47.3428409638
O	-10.1388127628	4.3675364581	-44.7477377720
O	-10.9408809967	5.3520449653	-44.9812819988

TS1(D)_I

Energy with the medium-sized basis set:	-1918.71349
Solution energy with the medium-sized basis set:	-1918.75319
Energy with larger basis sets:	-1919.32492
Zero-point energy:	0.58937

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.6070270000	4.8727430000	-48.2406410000
C	-16.3001530000	4.4883390000	-47.6289560000
N	-15.6879730000	3.2626970000	-47.8561360000
C	-15.3796140000	5.2163700000	-46.9235410000
C	-14.4555780000	3.2819580000	-47.2967410000
N	-14.2444770000	4.4593570000	-46.7358270000
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4564740000	7.6772740000	-42.9897990000
C	-13.3575530000	7.1506750000	-43.9169180000
O	-13.7055160000	6.2118570000	-44.7312950000
O	-12.2099180000	7.6298020000	-43.8225290000
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.7877910000	8.0987020000	-50.4465010000
C	-11.9093830000	7.5952390000	-49.0400530000
N	-11.5236370000	8.3522930000	-47.9413310000
C	-12.3625230000	6.4171150000	-48.5046990000
C	-11.7441560000	7.6387360000	-46.8121520000
N	-12.2597690000	6.4615100000	-47.1271670000
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.3101010000	8.0180500000	-37.0382290000
C	-10.5224600000	7.4032610000	-38.4012310000
C	-11.0566350000	8.1642890000	-39.4477670000
C	-10.0849920000	6.1050080000	-38.6948730000
C	-11.1313310000	7.6696900000	-40.7469100000
C	-10.1559250000	5.5885490000	-39.9853180000
C	-10.6662720000	6.3753290000	-41.0268180000
O	-10.6779990000	5.8455450000	-42.2721450000
Fe	-12.6013940000	5.0053990000	-45.7668660000
H	-18.0651890000	5.6520870000	-47.6238150000
H	-18.3003850000	4.0223810000	-48.2278890000
H	-15.4460270000	6.2144160000	-46.5229040000
H	-16.1019900000	2.4724150000	-48.3279290000
H	-13.7597780000	2.4596350000	-47.3109160000
H	-18.3793380000	5.6715750000	-50.1223860000

H	-14.3992980000	7.0550600000	-42.0864050000
H	-14.1570680000	8.6841850000	-42.6855910000
H	-16.1834280000	6.6567890000	-43.8303300000
H	-12.3007690000	9.0669210000	-50.5315900000
H	-10.7309160000	8.2967860000	-50.6736680000
H	-12.7438780000	5.5438730000	-49.0081720000
H	-11.1336830000	9.2826160000	-47.9697970000
H	-11.5479120000	7.9675080000	-45.7986680000
H	-12.2465060000	7.5405040000	-52.4936800000
H	-10.2380290000	7.2325320000	-36.2760300000
H	-11.1703380000	8.6421310000	-36.7628250000
H	-11.4089580000	9.1746090000	-39.2459080000
H	-9.6708960000	5.4895130000	-37.8985310000
H	-11.5377230000	8.2709290000	-41.5539050000
H	-9.8149220000	4.5832760000	-40.2121200000
H	-11.0747250000	6.4757780000	-42.9054250000
H	-9.0951290000	9.6797000000	-37.7558520000
C	-11.8743870000	2.6938200000	-44.6388870000
O	-12.7717020000	3.6319180000	-44.4862570000
O	-11.7361840000	1.6748150000	-43.9844510000
C	-10.9919110000	2.9996910000	-45.8617480000
O	-11.5860560000	3.6996090000	-46.7659040000
C	-9.8844510000	2.0520260000	-46.2235200000
C	-8.9639920000	2.5543450000	-47.3363340000
H	-10.3717030000	1.1095070000	-46.5100200000
H	-9.3381390000	1.8253610000	-45.3031090000
H	-9.5279210000	2.7645760000	-48.2492180000
H	-8.4580710000	3.4755630000	-47.0339580000
H	-11.8347890000	6.1677340000	-51.4575980000
H	-13.4212880000	6.9429480000	-51.3122240000
H	-16.9700030000	4.6198250000	-50.3190720000
H	-16.7629470000	6.2603900000	-49.6921380000
H	-8.8678800000	9.3302290000	-36.0320950000
H	-8.1564690000	8.2685000000	-37.2628740000
H	-16.5896830000	8.0250170000	-42.7770850000
H	-15.9837400000	8.3184840000	-44.4123360000
H	-8.2003960000	1.8060240000	-47.5675290000
O	-10.0423450000	4.4097470000	-44.9691120000
O	-10.8282330000	5.4340480000	-45.0564910000

Int1(D)₁

Energy with the medium-sized basis set:	-1918.72378
Solution energy with the medium-sized basis set:	-1918.76030
Energy with larger basis sets:	-1919.33316
Zero-point energy:	0.59074

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.5154245847	4.7126177531	-48.2982444369
C	-16.1636925052	4.4334002279	-47.7271759839
N	-15.4240923907	3.3048582598	-48.0549726079
C	-15.3336588082	5.1852387549	-46.9377667512
C	-14.2068459463	3.3936004569	-47.4652396831
N	-14.1326872404	4.5278352495	-46.7941363863
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4840784001	7.5329608753	-42.9330596624
C	-13.3958215156	7.1918845656	-43.9431091407
O	-13.7341165262	6.3202536475	-44.8399315424
O	-12.2709114511	7.7200128833	-43.8638987914
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.4938296746	7.9214657792	-50.4967357331
C	-11.7132802651	7.5058141340	-49.0736742140
N	-11.4129180028	8.3307066765	-47.9972662286
C	-12.1798231567	6.3481053300	-48.5056742189
C	-11.6933105076	7.6771380068	-46.8440625249
N	-12.1628069047	6.4753868699	-47.1327353724
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.5383970506	8.5631388152	-37.1156801351
C	-10.8595756244	7.8265883530	-38.3964766483
C	-11.0552902192	8.5265189538	-39.5927888088
C	-10.8654298767	6.4265060740	-38.4518148749
C	-11.2325910600	7.8664442541	-40.8062619850
C	-11.0400652708	5.7456992145	-39.6538874591
C	-11.2108313883	6.4641265597	-40.8432155929
O	-11.3492181352	5.7590149539	-41.9957616330
Fe	-12.5801609010	5.1031485285	-45.7595726327
H	-18.0598940117	5.3605561986	-47.6039707540
H	-18.0934677016	3.7822418667	-48.3698136069
H	-15.4983405593	6.1306125486	-46.4489318691
H	-15.7514785876	2.5247089872	-48.6046934710
H	-13.4168708872	2.6633255410	-47.5247152650
H	-18.4149322665	5.5811280548	-50.0921273535

H	-14.4664906246	6.7165655749	-42.1988174430
H	-14.1784571909	8.4410063724	-42.4069492608
H	-16.1745555273	6.7401333967	-44.0395200918
H	-11.7103792989	8.9935835910	-50.5967361138
H	-10.4331665136	7.8012716192	-50.7575901897
H	-12.5153214978	5.4370739435	-48.9720204935
H	-11.0482027682	9.2695612984	-48.0580318121
H	-11.5777748274	8.0552289340	-45.8353901815
H	-12.1635369985	7.4536880882	-52.5132558271
H	-10.8471577945	7.9662201528	-36.2481705269
H	-11.1070488697	9.5010551884	-37.0677455693
H	-11.0619350797	9.6153410573	-39.5773644177
H	-10.7208441005	5.8570361069	-37.5354978304
H	-11.3947721349	8.4161896130	-41.7279478502
H	-11.0395609039	4.6608393345	-39.6971953470
H	-11.4141884543	6.3735466225	-42.7479428314
H	-8.7108104960	9.4799919309	-37.8696444791
C	-11.8931166304	2.8460764884	-44.5075785322
O	-12.8538401640	3.7250615049	-44.4691872857
O	-11.7815249825	1.8078058925	-43.8840329693
C	-10.8370866736	3.2910222382	-45.5859592100
O	-11.4970535016	3.8510835374	-46.6187320980
C	-9.7641586909	2.2794064387	-45.9224638270
C	-8.7628375950	2.7863967956	-46.9619531948
H	-10.2905860993	1.3874617082	-46.2788115165
H	-9.2786017583	1.9904682127	-44.9851674256
H	-9.2790781098	3.0826129040	-47.8796749408
H	-8.2186401959	3.6585412865	-46.5864535020
H	-12.1382381318	6.0578474296	-51.4294263788
H	-13.4214137634	7.2682042552	-51.2748101229
H	-16.8763466705	4.7542509622	-50.3897875429
H	-16.8857674962	6.3378801610	-49.6031032293
H	-8.7931626529	9.4222245104	-36.0965746024
H	-8.4478285780	7.9498776865	-37.0279075132
H	-16.6259534342	7.8820076570	-42.7576802413
H	-15.9251007500	8.4806858245	-44.2694727180
H	-8.0326548092	2.0097259943	-47.2085114096
O	-10.1026363242	4.4352101616	-44.8435140625
O	-10.8742739886	5.5113135503	-44.8262592299

TS2(D)_I

Energy with the medium-sized basis set:	-1918.71575
Solution energy with the medium-sized basis set:	-1918.74990
Energy with larger basis sets:	-1919.32619
Zero-point energy:	0.58851

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.4653550000	4.7835250000	-48.2631940000
C	-16.1018050000	4.5228130000	-47.7082410000
N	-15.3559040000	3.3928810000	-48.0183030000
C	-15.2721340000	5.2892920000	-46.9323940000
C	-14.1382020000	3.5010340000	-47.4330640000
N	-14.0637560000	4.6458750000	-46.7781950000
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4496140000	7.8889960000	-43.0596740000
C	-13.3481750000	7.4676810000	-44.0321490000
O	-13.6634520000	6.4843730000	-44.8273990000
O	-12.2523030000	8.0412540000	-44.0116470000
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.6204850000	8.0644120000	-50.5208390000
C	-11.7227720000	7.6333030000	-49.0887880000
N	-11.3016710000	8.4308010000	-48.0317790000
C	-12.1923110000	6.4918610000	-48.4936110000
C	-11.5192750000	7.7767480000	-46.8666050000
N	-12.0653350000	6.5992850000	-47.1219450000
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.5303270000	8.8257880000	-37.3699410000
C	-10.8114120000	7.9793930000	-38.5922000000
C	-10.7544980000	8.5259890000	-39.8801710000
C	-11.0850940000	6.6087710000	-38.4809230000
C	-10.9509500000	7.7472120000	-41.0200650000
C	-11.2825330000	5.8120660000	-39.6051270000
C	-11.2106990000	6.3758660000	-40.8865140000
O	-11.4150630000	5.5487000000	-41.9443160000
Fe	-12.4930010000	5.2667510000	-45.7133390000
H	-17.9840030000	5.4702680000	-47.5869440000
H	-18.0537600000	3.8570270000	-48.2679960000
H	-15.4495960000	6.2391850000	-46.4551740000
H	-15.6765150000	2.6008510000	-48.5551520000
H	-13.3489340000	2.7688030000	-47.4904700000
H	-18.4305140000	5.5731880000	-50.0556780000

H	-14.2666370000	7.3116260000	-42.1436200000
H	-14.2675850000	8.9365040000	-42.8025920000
H	-16.0583030000	6.6137910000	-43.7718500000
H	-12.0240970000	9.0814650000	-50.6213050000
H	-10.5628800000	8.1299680000	-50.8128510000
H	-12.6051350000	5.6085250000	-48.9512140000
H	-10.9026730000	9.3544590000	-48.1078310000
H	-11.3356120000	8.1528140000	-45.8673190000
H	-12.2602080000	7.4883230000	-52.5149240000
H	-11.0903820000	8.4345280000	-36.5112450000
H	-10.8937700000	9.8480710000	-37.5353410000
H	-10.5576060000	9.5900720000	-39.9988740000
H	-11.1441660000	6.1548550000	-37.4934610000
H	-10.9428690000	8.1949350000	-42.0088510000
H	-11.4936790000	4.7509860000	-39.5150990000
H	-11.2468740000	5.9936090000	-42.7943990000
H	-8.4510990000	9.2888120000	-37.8455480000
C	-11.8991690000	2.9837060000	-44.3432530000
O	-12.8026220000	3.8746030000	-44.3567170000
O	-11.7552380000	1.9218640000	-43.7827700000
C	-10.6945180000	3.4934010000	-45.4493830000
O	-11.4192960000	3.9301460000	-46.4885300000
C	-9.6497340000	2.4225320000	-45.7190180000
C	-8.6051440000	2.8561570000	-46.7526450000
H	-10.1907080000	1.5333000000	-46.0557060000
H	-9.1848650000	2.1629110000	-44.7636170000
H	-9.0809810000	3.1146380000	-47.7027500000
H	-8.0476010000	3.7298660000	-46.4032200000
H	-11.9447240000	6.1159130000	-51.4469130000
H	-13.4225790000	7.0724470000	-51.2445410000
H	-16.9192430000	4.7131780000	-50.3833210000
H	-16.8742940000	6.3340460000	-49.6771270000
H	-8.8519340000	9.4943480000	-36.1299220000
H	-8.6486000000	7.8702120000	-36.8134290000
H	-16.6005610000	7.9672340000	-42.7617720000
H	-16.1052260000	8.2562680000	-44.4343920000
H	-7.8909430000	2.0473000000	-46.9348500000
O	-10.1004790000	4.5375180000	-44.7086690000
O	-10.8978380000	5.6894630000	-44.7448290000

Int2(D)_I

Energy with the medium-sized basis set:	-1918.79058
Solution energy with the medium-sized basis set:	-1918.82008
Energy with larger basis sets:	-1919.39938
Zero-point energy:	0.58823

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.3783083725	4.9220656077	-48.2092534664
C	-15.9932111046	4.6809001438	-47.6959774358
N	-15.1911971336	3.6377903946	-48.1424776379
C	-15.2187699384	5.3557132800	-46.7871984022
C	-13.9927488838	3.7111320784	-47.5032080671
N	-13.9851036527	4.7447134772	-46.6799073885
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4854231771	8.1105728753	-43.1036236188
C	-13.3670558772	7.6761679455	-44.0557551710
O	-13.6297388066	6.5849078665	-44.7086874459
O	-12.3244094883	8.3403105393	-44.1301171982
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.6336870827	8.1351834467	-50.5818304454
C	-11.6364942096	7.7020675626	-49.1486198082
N	-11.1786489832	8.4956820685	-48.1041331232
C	-12.0563125204	6.5453970456	-48.5448347365
C	-11.3306519175	7.8191377679	-46.9357445119
N	-11.8605520574	6.6342108418	-47.1818981360
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.4656763160	8.6426926589	-37.5384225408
C	-10.5243650898	7.7549712827	-38.7671611140
C	-10.8482641357	8.2598612398	-40.0323712510
C	-10.2384369132	6.3845556058	-38.6723665995
C	-10.8862559098	7.4472294455	-41.1681058996
C	-10.2649273793	5.5563974978	-39.7898420642
C	-10.5854038473	6.0831527331	-41.0492856273
O	-10.5857113506	5.2304844813	-42.1049404352
Fe	-12.4100928220	5.4406894771	-45.6514874798
H	-17.8412370157	5.6802142076	-47.5695295129
H	-17.9838665435	4.0124036159	-48.0931333768
H	-15.4362744901	6.2251922718	-46.1888753356
H	-15.4626395750	2.9247727344	-48.8021231605
H	-13.1685217109	3.0300285290	-47.6470452521
H	-18.4512710141	5.5534669197	-50.0050201201

H	-14.2363999922	7.6776682769	-42.1246956765
H	-14.4199290395	9.1968026768	-42.9855106158
H	-15.9259331849	6.5800620300	-43.6400597231
H	-12.1149409158	9.1194913130	-50.6697830192
H	-10.6007306922	8.2707709227	-50.9333930270
H	-12.4946650606	5.6659423547	-48.9881924894
H	-10.8142179413	9.4326012103	-48.1880259486
H	-11.1391080281	8.1909894687	-45.9368233223
H	-12.3519355060	7.4685195867	-52.5264107939
H	-11.0665882781	8.1968750065	-36.7335115833
H	-10.9292458012	9.6107922725	-37.7650928869
H	-11.0846331079	9.3170979392	-40.1395518388
H	-9.9903668672	5.9575525145	-37.7019932594
H	-11.1569349848	7.8599345470	-42.1374164586
H	-10.0380103420	4.4968543370	-39.7129807074
H	-10.7399295281	5.6920073322	-42.9676731748
H	-8.4164489659	9.3579429688	-37.7809328203
C	-11.8881102606	3.0532624909	-43.0807424759
O	-12.9267749815	3.5725398816	-42.9487919220
O	-10.8824151410	2.4789529763	-43.2507704724
C	-10.1154709796	4.0173982163	-45.7416133890
O	-11.2783999850	3.8677568318	-46.1765913303
C	-9.0179977415	3.0135921937	-45.9845946403
C	-9.1457454439	2.3268739901	-47.3468243560
H	-9.1036498781	2.2826964559	-45.1707731570
H	-8.0526486250	3.5122973014	-45.8625817197
H	-10.1186474542	1.8375837784	-47.4399747392
H	-9.0507926401	3.0489733595	-48.1640860419
H	-11.8699253198	6.1492310072	-51.4490758012
H	-13.3977616648	7.0014696234	-51.1724808713
H	-16.9753813871	4.6391342972	-50.3470296415
H	-16.8616706952	6.3189443924	-49.8046251513
H	-9.0342210395	9.5101137179	-36.1225845389
H	-8.5544255146	7.9248280320	-36.7574029241
H	-16.6439378309	7.9778846205	-42.8072125112
H	-16.1552679550	8.1069094348	-44.5043200915
H	-8.3642409451	1.5712947671	-47.4658448426
O	-9.7489809572	5.0293234020	-45.0080921325
O	-10.8664342528	5.9368158498	-44.6444409148

Int2(D)_v

Energy with the medium-sized basis set:	-1918.81715
Solution energy with the medium-sized basis set:	-1918.84714
Energy with larger basis sets:	-1919.42938
Zero-point energy:	0.58666

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.2859787024	4.4773566856	-48.4382783039
C	-15.8827989503	4.3038193354	-47.9389591534
N	-14.9665240852	3.4279267665	-48.5096660478
C	-15.1973403630	4.8938567566	-46.9065048072
C	-13.7983113747	3.5140632353	-47.8134975780
N	-13.9089463144	4.3993556809	-46.8411799278
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4285756145	7.9120340915	-43.1430699904
C	-13.4538253883	7.1174435095	-43.9952276204
O	-13.9085405039	6.0510893745	-44.5557337438
O	-12.2648176140	7.4842550216	-44.1351622558
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.7319060790	8.2039000728	-50.5896652150
C	-11.7130223703	7.7866864155	-49.1524361907
N	-11.2835852642	8.6129677030	-48.1213159956
C	-12.0830782121	6.6222765964	-48.5310603479
C	-11.4094867568	7.9431843303	-46.9467600841
N	-11.8901376549	6.7334944215	-47.1684289424
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.3984259338	8.6902808993	-37.7096842202
C	-10.3842747927	7.6830455499	-38.8452561550
C	-10.6489191378	8.0529573399	-40.1697460931
C	-10.1170001185	6.3273024749	-38.5984738241
C	-10.6460506302	7.1261926824	-41.2158503838
C	-10.0984569870	5.3887122007	-39.6249970446
C	-10.3563967313	5.7808409053	-40.9473042107
O	-10.3088521782	4.8220429905	-41.9050644193
Fe	-12.2936652061	5.3668495812	-45.5617279144
H	-17.8782022146	4.8962950346	-47.6179726567
H	-17.7236215876	3.4933470639	-48.6558143518
H	-15.5262393043	5.6287911935	-46.1891934034
H	-15.1508915624	2.7997619285	-49.2774021736
H	-12.9108736714	2.9374322366	-48.0252518308
H	-18.4674063897	5.4713475459	-49.9849187162

H	-14.2505273230	7.6142767541	-42.1008602214
H	-14.1533953923	8.9698323783	-43.2098196427
H	-16.1296206579	6.6055142170	-43.4494287653
H	-12.2934286278	9.1430875133	-50.6944116256
H	-10.7097240598	8.4215108236	-50.9308407570
H	-12.4848255586	5.7193180275	-48.9608193169
H	-10.9436070460	9.5576102003	-48.2225883701
H	-11.1890521236	8.3370719785	-45.9655579587
H	-12.3709640760	7.4551313525	-52.5305701276
H	-11.1358684877	8.3810377726	-36.9551323806
H	-10.7432609300	9.6598486988	-38.0901828163
H	-10.8737227408	9.0940763010	-40.3961669083
H	-9.9205093424	5.9983737458	-37.5794408674
H	-10.8892045997	7.4317267054	-42.2302507377
H	-9.8844313832	4.3421877424	-39.4281786334
H	-10.4113251124	5.1868380671	-42.8192986438
H	-8.2805983139	9.2266309200	-37.7290228011
C	-11.9239256872	2.8597548421	-43.0269184846
O	-12.8877793965	3.4884690329	-42.8263634496
O	-10.9999575141	2.1776308971	-43.2551127049
C	-10.0792863404	3.4330102875	-45.8475498337
O	-11.1843946525	3.5689281210	-46.3840530804
C	-9.1317217943	2.2913347853	-46.1255455290
C	-9.2520842901	1.7644210599	-47.5564667491
H	-9.3891971609	1.5108131703	-45.3980592339
H	-8.1136595018	2.6140417928	-45.8885261701
H	-10.2779971272	1.4487188390	-47.7639142535
H	-8.9829053028	2.5353200868	-48.2856768057
H	-11.7884076454	6.1952609155	-51.4311487694
H	-13.3864913222	6.9171802231	-51.1810014906
H	-16.8509007666	4.9884941053	-50.5269643748
H	-17.0395142543	6.3891311893	-49.4633052591
H	-9.1008132006	9.6026636120	-36.1992107578
H	-8.6745631775	7.9291635466	-36.5971686492
H	-16.5708047725	8.2378422197	-42.8980247711
H	-16.0668130450	7.9649598089	-44.5752792635
H	-8.5891179365	0.9074421174	-47.7053150144
O	-9.6132999949	4.2541696440	-44.9301888151
O	-10.5779529842	5.2558467164	-44.5301495205

Int3(D)_v

Energy with the medium-sized basis set:	-1730.22446
Solution energy with the medium-sized basis set:	-1730.25724
Energy with larger basis sets:	-1730.76346
Zero-point energy:	0.57404

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.3286458910	4.5204429617	-48.4054148859
C	-15.9328804724	4.3129714318	-47.9017992666
N	-15.0431904879	3.4036260765	-48.4610964042
C	-15.2273850718	4.9029391830	-46.8829379167
C	-13.8699018289	3.4716729116	-47.7704800575
N	-13.9529812137	4.3763056259	-46.8144948143
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4286620094	7.7887680035	-43.0803677233
C	-13.4970250557	6.9547715254	-43.9399986523
O	-13.9516329653	5.8394361811	-44.3900656260
O	-12.3319712510	7.3405815133	-44.2088339082
C	-12.3570000000	7.1290000000	-51.4870000000
C	-11.6284745674	8.1104885132	-50.5613025324
C	-11.6335977919	7.6594461069	-49.1330268449
N	-11.1445629812	8.4428552042	-48.0948605364
C	-12.0727315901	6.5126716037	-48.5224886208
C	-11.3063212029	7.7684220674	-46.9284180118
N	-11.8634328740	6.5930828825	-47.1584354270
C	-9.0340000000	8.8750000000	-37.0160000000
C	-10.3320139169	8.9655497817	-37.8459032318
C	-10.5074040049	7.8684338052	-38.8831513526
C	-10.5825854431	8.1493134499	-40.2536108268
C	-10.6426075194	6.5250189129	-38.4982761048
C	-10.7865964252	7.1501456819	-41.2097036852
C	-10.8372861862	5.5130335492	-39.4328990741
C	-10.9118241982	5.8126287363	-40.8034386311
O	-11.1218284094	4.7853679291	-41.6588503895
Fe	-12.3206580392	5.2741601797	-45.5010765261
H	-17.9034981874	4.9936260996	-47.6024421879
H	-17.8053311565	3.5474088687	-48.5874924918
H	-15.5384134235	5.6526465863	-46.1727475192
H	-15.2486666517	2.7658955928	-49.2154517048
H	-13.0009861318	2.8638740448	-47.9718872421
H	-18.4614731295	5.5056430152	-49.9938158322

H	-14.3168571323	7.4300985125	-42.0485531801
H	-14.0758247564	8.8242698201	-43.0932557898
H	-16.2018380410	6.6213147716	-43.5143123189
H	-12.1000901176	9.1008624895	-50.6332779546
H	-10.5930714286	8.2425959009	-50.9068479264
H	-12.5353861150	5.6437144820	-48.9614195349
H	-10.7499248262	9.3671369480	-48.1865559864
H	-11.0580308205	8.1425540088	-45.9467832337
H	-12.3452716774	7.4893936710	-52.5192398259
H	-11.1869694489	8.9493430273	-37.1544758787
H	-10.3690652291	9.9413767607	-38.3465003034
H	-10.4956063254	9.1817323077	-40.5891172286
H	-10.6008126037	6.2655578999	-37.4416345625
H	-10.8838877503	7.3974022618	-42.2632892997
H	-10.9400586271	4.4762511397	-39.1259814175
H	-10.9879201694	5.0423412536	-42.6039350541
H	-8.1531708513	8.9389800350	-37.6639556161
C	-10.3420174157	3.1109034921	-45.5004528700
O	-11.3070754230	3.4079210793	-46.2147019979
C	-9.5476997956	1.8338621328	-45.6495820844
C	-9.3054812675	1.4790251847	-47.1207586919
H	-10.1318040399	1.0430039395	-45.1608100620
H	-8.6118661297	1.9306989926	-45.0924052516
H	-10.2551103532	1.4042834854	-47.6573232559
H	-8.6976095620	2.2437342035	-47.6151279601
H	-11.8783843393	6.1445469924	-51.4661487204
H	-13.4000803465	7.0041580361	-51.1789659079
H	-16.8660050564	4.9326837656	-50.5088918492
H	-16.9966140645	6.3790679000	-49.4992932520
H	-8.9799805542	9.6852589356	-36.2802235546
H	-8.9771641428	7.9237511366	-36.4761387603
H	-16.5540654918	8.2498602064	-42.8916861836
H	-16.0074506907	8.0328116374	-44.5625089653
H	-8.7823711029	0.5220230404	-47.2028408480
O	-9.9097155393	3.8641224605	-44.5125045025
O	-10.7066833512	5.0543602988	-44.3218589873

TS3(D)_v

Energy with the medium-sized basis set: -1730.21183
Solution energy with the medium-sized basis set: -1730.24445
Energy with larger basis sets: -1730.75812
Zero-point energy: 0.57269

C	-17.4199580000	5.3859830000	-49.6789380000
C	-17.4900480000	4.8168380000	-48.2470760000
C	-16.1509430000	4.5721770000	-47.6208760000
N	-15.3698440000	3.4541920000	-47.8925310000
C	-15.3917900000	5.3223050000	-46.7603450000
C	-14.2034190000	3.5646150000	-47.2087840000
N	-14.1868480000	4.6900910000	-46.5159790000
C	-15.8870140000	7.6670350000	-43.5359910000
C	-14.5283840000	8.3338680000	-43.3029730000
C	-13.5872670000	8.2444140000	-44.4985270000
O	-13.6728520000	7.1266840000	-45.1794710000
O	-12.8190200000	9.1658650000	-44.7831430000
C	-12.3569970000	7.1290110000	-51.4870280000
C	-10.9798310000	7.0970100000	-50.7938810000
C	-11.1027690000	7.1297040000	-49.3038610000
N	-11.3553990000	8.2956460000	-48.5897920000
C	-11.1859430000	6.1303830000	-48.3710020000
C	-11.5907020000	7.9803180000	-47.2942160000
N	-11.4977350000	6.6674370000	-47.1362400000
C	-9.0340320000	8.8749700000	-37.0160440000
C	-9.6368760000	9.4803040000	-38.2967910000
C	-10.3886350000	8.4840280000	-39.1579380000
C	-9.8667560000	8.0189170000	-40.3711910000
C	-11.6443700000	7.9938730000	-38.7667540000
C	-10.5596050000	7.1100020000	-41.1730180000
C	-12.3498490000	7.0854630000	-39.5496040000
C	-11.8157730000	6.6374230000	-40.7679410000
O	-12.5572640000	5.7698400000	-41.5024440000
Fe	-12.4747300000	5.6376520000	-45.5492650000
H	-18.0346740000	5.5166750000	-47.6053900000
H	-18.0758610000	3.8880610000	-48.2473480000
H	-15.6049690000	6.2744400000	-46.3013690000
H	-15.6333950000	2.6771560000	-48.4799890000
H	-13.4002950000	2.8448140000	-47.2383180000
H	-18.4258080000	5.5534070000	-50.0761720000

H	-14.0188970000	7.8287650000	-42.4723710000
H	-14.6311980000	9.3878050000	-43.0300370000
H	-15.7611880000	6.6055720000	-43.7604120000
H	-10.3644470000	7.9350870000	-51.1459410000
H	-10.4450360000	6.1850680000	-51.0787260000
H	-11.0607330000	5.0658040000	-48.4964320000
H	-11.3621350000	9.2319570000	-48.9663650000
H	-11.8736600000	8.6758580000	-46.5041520000
H	-12.2480970000	7.1003260000	-52.5761510000
H	-10.3097920000	10.3012960000	-38.0142930000
H	-8.8350380000	9.9359890000	-38.8902200000
H	-8.8976710000	8.3824390000	-40.7076300000
H	-12.0851770000	8.3385890000	-37.8330740000
H	-10.1446970000	6.7742910000	-42.1192510000
H	-13.3241550000	6.7170260000	-39.2428280000
H	-12.1084680000	5.5453990000	-42.3519620000
H	-8.3178480000	8.0825290000	-37.2577300000
C	-10.6847140000	3.3690350000	-45.2631690000
O	-11.4326550000	3.8048710000	-46.1779180000
C	-9.8642300000	2.1009790000	-45.4840170000
C	-9.3130860000	1.9843800000	-46.9074870000
H	-10.5340610000	1.2584750000	-45.2659540000
H	-9.0668820000	2.0690700000	-44.7374050000
H	-10.1220260000	2.0265610000	-47.6408490000
H	-8.6152000000	2.7979290000	-47.1284600000
H	-12.9618880000	6.2714710000	-51.1783980000
H	-12.9111870000	8.0371640000	-51.2283680000
H	-16.9005620000	4.7011310000	-50.3578840000
H	-16.8828720000	6.3387610000	-49.6902230000
H	-8.5135930000	9.6369970000	-36.4248230000
H	-9.8125380000	8.4326210000	-36.3854840000
H	-16.5195540000	7.7550580000	-42.6463060000
H	-16.4248480000	8.1323240000	-44.3707980000
H	-8.7785520000	1.0381120000	-47.0332060000
O	-10.5503390000	3.8868330000	-44.1025820000
O	-11.6361130000	5.3038660000	-44.0183830000

Int4(D)_v

Energy with the medium-sized basis set: -1730.24725
Solution energy with the medium-sized basis set: -1730.28168
Energy with larger basis sets: -1730.79664
Zero-point energy: 0.57555

C	-17.4200000000	5.3860000000	-49.6790000000
C	-17.3520443564	4.8636120491	-48.2300580605
C	-15.9614314351	4.6020973413	-47.7407633174
N	-15.1595497719	3.5761680272	-48.2273678416
C	-15.1878035434	5.2306974758	-46.7997572523
C	-13.9668578831	3.6113365353	-47.5803408084
N	-13.9602480097	4.6062183670	-46.7102184767
C	-15.8870000000	7.6670000000	-43.5360000000
C	-14.4711518605	7.7966948177	-42.9608506424
C	-13.3851490031	7.4988077180	-43.9843268882
O	-13.6248764797	6.4032945105	-44.6820142956
O	-12.4064693152	8.2266742625	-44.1246794408
C	-12.3570000000	7.1290000000	-51.4870000000
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