

Supplementary Information to:

**A dominant homolytic O-Cl bond cleavage with
low-spin triplet-state Fe(IV)=O formed is revealed in
the mechanism of heme-dependent chlorite dismutase**

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1. Supplementary tables and figures

Table S1 Solvation effects of stationary points

Entry	Stationary points	Solvation effects (kcal/mol)
1	React _{II}	0.00
2	TS1 _{II,21}	-0.05
3	Int1 _{II,21}	0.04
4	Int1b _{II,21}	0.01
5	TS2 _{II,21}	-0.36
6	Int2 _{II,21}	0.01
7	Int2b _{II,21}	0.01
8	Prod _{II,21}	0.10
9	Prod _{IV,21}	0.06
10	TS _{II,hetero}	-0.52
11	Int1 _{II,01}	0.05
12	Int1 _{IV,21}	0.04
13	React _{IV}	-0.01
14	TS1 _{IV,41}	-0.12
16	Int1 _{IV,41}	0.00
16	React _{VI}	0.01
17	TS1 _{VI,41}	-0.10
18	Int1 _{VI,41}	0.01

Table S2 Dispersion effects of stationary points

Entry	Stationary points	Dispersion effects (kcal/mol)
1	React _{II}	0.0
2	TS1 _{II,21}	2.7
3	Int1 _{II,21}	0.5
4	Int1b _{II,21}	0.9
5	TS2 _{II,21}	0.5
6	Int2 _{II,21}	1.0
7	Int2b _{II,21}	3.6
8	Prod _{II,21}	5.8
9	Prod _{IV,21}	4.5
10	TS _{II,hetero}	2.7
11	Int1 _{II,01}	0.8
12	Int1 _{IV,21}	1.6
13	React _{IV}	3.8
14	TS1 _{IV,41}	3.2
15	Int1 _{IV,41}	2.6
16	React _{VI}	2.1
17	TS1 _{VI,41}	7.9
18	Int1 _{VI,41}	2.0

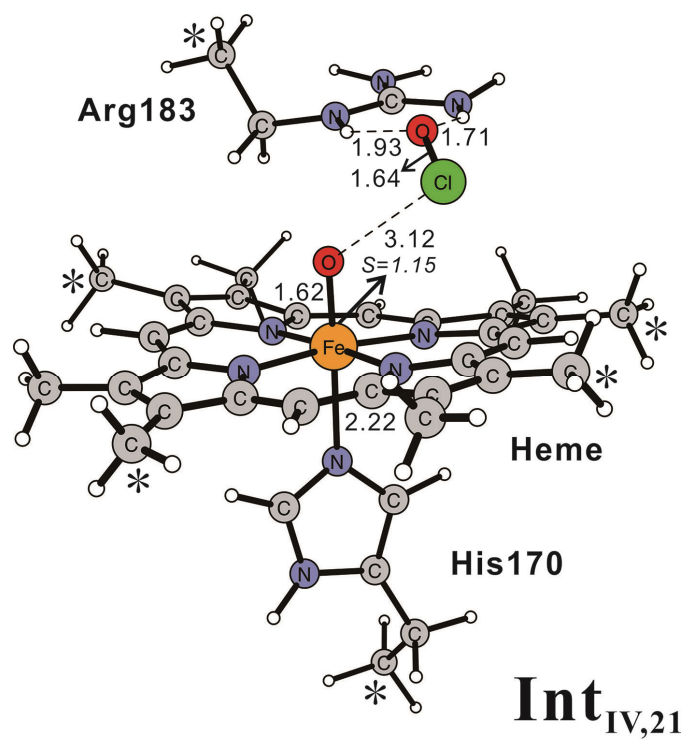


Fig. S1 Optimized structure of a quartet-state intermediate formed by ferromagnetical coupling between the low-spin triplet-state Fe(IV)=O diradicaloid and Cl-O[•] radical.

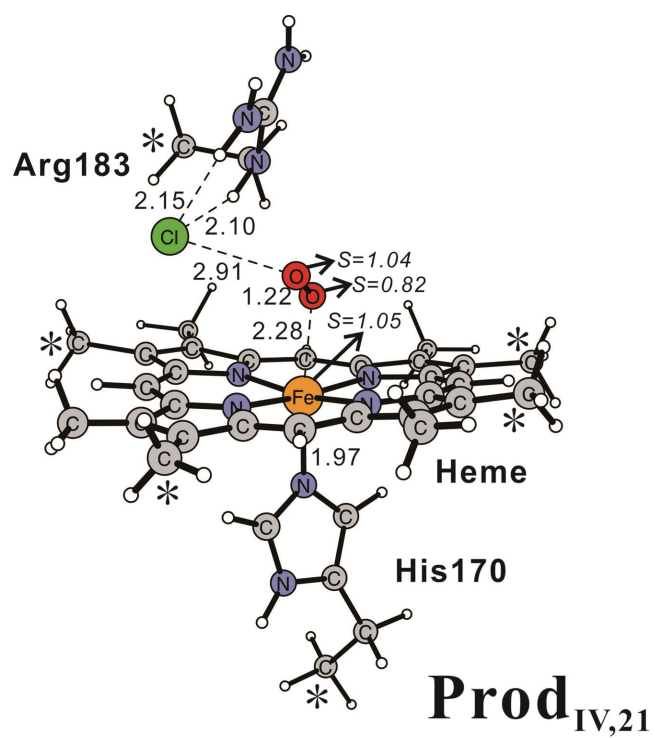


Fig. S2 Optimized structure of the quartet-state product formed by ferromagnetical coupling between low-spin Fe(III)(heme) cofactor and the triplet-state O₂.

2. The complete reference 38

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, Gaussian 03, Revision E.01, Gaussian, Inc., Wallingford CT, 2004.

3. Cartesian coordinates and absolute energies of all 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_{II}

Energy with the small basis set:	-2626.254279
Solution energy with the small basis set:	-2626.254306
Energy with larger basis sets:	-2626.936511
Zero-point energy:	0.779232
Dispersion effect:	-0.180650103

C	83.56100000	29.40899998	40.48999996
C	84.40751854	28.46158684	39.61534736
C	84.19983017	28.62718335	38.13877413
N	84.33770254	29.84645751	37.48894723
C	83.87862731	27.74169465	37.14163144
C	84.10281726	29.67080229	36.16976652
N	83.82240382	28.40048618	35.92632362
C	78.74700005	28.42299994	29.79600007
C	78.66103662	28.09248885	31.28455635
N	79.02766790	26.70559462	31.58147560
C	78.22773045	25.74486905	32.01812775
N	76.88132334	25.86403430	31.98037608
N	78.76692324	24.63612607	32.55928285
Fe	83.34866733	27.67997716	34.07515496
C	83.70213489	24.37699413	35.01590696
C	80.14559042	27.65309174	35.19184778
C	82.86539913	30.83990689	32.78028586
C	86.65034420	27.84650057	33.31356944
N	82.16538424	26.28334224	34.93127630
C	82.47096805	24.97808643	35.24891357
C	81.33476916	24.33102428	35.88765152
C	80.34777601	25.27951727	35.96683795
C	80.87706896	26.48581084	35.35738284
C	78.96877007	25.15163865	36.54147163
C	81.28899999	22.90700010	36.36999995
N	81.80574274	29.00619287	33.99215065
C	80.56053567	28.79637770	34.51758720
C	79.68326156	29.90950810	34.20546928
C	80.40985223	30.79234951	33.44382003
C	81.75561138	30.22350724	33.34895832

C	78.25437265	30.01839190	34.65043981
C	79.89800002	32.07999996	32.83400002
N	84.55639799	29.10663667	33.25151097
C	84.17216140	30.34135812	32.78459878
C	85.33399873	31.08225573	32.33360520
C	86.43866681	30.28757792	32.53231676
C	85.92281275	29.02028286	33.07693208
C	85.34618979	32.47117777	31.76467915
C	87.85999997	30.75899998	32.22300002
N	84.86427340	26.35036573	34.13622995
C	86.15811108	26.60778583	33.74664351
C	86.94983353	25.37892962	33.84065127
C	86.11192709	24.38049172	34.28755391
C	84.81991482	25.01882572	34.49053742
C	88.40105727	25.27888862	33.47587111
C	86.39099997	22.89700004	34.52599998
H	85.47105297	28.60146991	39.85418373
H	84.17666174	27.42145425	39.86670049
H	83.68663876	26.68352275	37.21247017
H	84.13620772	30.45963249	35.43606835
H	83.80032682	30.46186783	40.30234909
H	78.49887072	29.47631736	29.63413535
H	78.05823581	27.81340746	29.20165706
H	77.65726490	28.28361129	31.67709215
H	79.34095264	28.73231880	31.85381344
H	80.02253152	26.42239287	31.51595939
H	76.29674478	25.18585771	32.44135697
H	76.43715979	26.54272957	31.38464628
H	79.79489076	24.59202386	32.58041409
H	78.25642421	23.76729762	32.50651309
H	83.80810547	23.33289736	35.28702155
H	79.13441922	27.65443442	35.58195082
H	82.70954755	31.81603566	32.33509212
H	87.71206727	27.88661444	33.09300074
H	78.81028109	24.16917945	36.99246882
H	78.78444888	25.90126427	37.31942893
H	78.20006684	25.28763121	35.77084982
H	80.30938964	22.65859495	36.78444781
H	82.03317950	22.72281872	37.15376153
H	77.69218153	29.09819076	34.45277846
H	78.18156825	30.20935659	35.72834042
H	77.73645058	30.83662277	34.14416693
H	80.19837539	32.95861363	33.41838283
H	84.35337751	32.92523455	31.73204710

H	85.99067916	33.13691127	32.35191898
H	85.73955248	32.47395311	30.74100976
H	88.11833851	31.62514251	32.84254001
H	88.79334551	24.27864273	33.67439779
H	89.01158795	25.98963394	34.04545511
H	88.56417453	25.49150762	32.41269598
H	85.76489690	22.26993217	33.88161941
H	87.43480103	22.65518851	34.31431745
Cl	82.79439819	25.64016231	31.83101276
O	82.90166585	27.22154636	32.28737531
O	81.27376906	25.17097687	31.67588552
H	83.75207985	29.21746592	41.54953492
H	82.49213184	29.26878097	40.30347126
H	81.49523523	22.19681139	35.56000930
H	80.28202707	32.22143912	31.81854771
H	78.80706952	32.08030820	32.78141396
H	88.60671892	29.98239966	32.40797740
H	87.94591129	31.06493843	31.17471281
H	86.18679347	22.61462545	35.56487129
H	84.57573194	30.72571716	37.92408125
H	79.75959663	28.25334303	29.41823706

TS1_{II,21}

Energy with the small basis set:	-2626.244273
Solution energy with the small basis set:	-2626.244376
Energy with larger basis sets:	-2626.922041
Zero-point energy:	0.777279
Dispersion effect:	-0.176278391
Imaginary frequency:	-311 cm ⁻¹

C	4.81579500	4.35547800	-2.51176900
C	4.82711500	3.38995000	-1.31078100
C	3.74542900	2.35199400	-1.33631000
N	3.53578800	1.50714200	-2.41626200
C	2.80030400	1.97277000	-0.41580200
C	2.50780300	0.67484600	-2.12601900
N	2.04035000	0.93111100	-0.91640400
C	-5.74251700	-0.67116400	-1.18385800
C	-4.62416100	-0.13195200	-0.28411100
N	-4.28762000	-1.02059200	0.83119600
C	-4.90366200	-1.06211100	2.01058200
N	-6.04504100	-0.36990300	2.22538100
N	-4.37592800	-1.79441900	2.99809300

Fe	0.38826300	-0.06977800	-0.02691400
C	1.01482100	1.18956800	3.09169900
C	-1.32304900	2.78646500	-0.82832700
C	-0.50760900	-1.42632300	-3.03380800
C	2.55078300	-2.65448900	0.53915600
N	-0.01138800	1.67577500	0.92592100
C	0.29617000	2.00432000	2.22307700
C	-0.20766800	3.33619600	2.54415400
C	-0.82639200	3.79306100	1.40979500
C	-0.71737300	2.73662000	0.41928100
C	-1.50730700	5.10819600	1.17469600
C	-0.05427300	4.05179800	3.86024900
N	-0.71650600	0.55836500	-1.64238000
C	-1.36766500	1.75347000	-1.75623100
C	-2.16233300	1.78500600	-2.97286000
C	-1.99802600	0.57140500	-3.59054300
C	-1.06164300	-0.18295300	-2.74671200
C	-2.98060900	2.96335500	-3.41162000
C	-2.64437500	0.12661300	-4.88425800
N	0.96963000	-1.71404900	-1.06492400
C	0.46172600	-2.09940200	-2.28195500
C	1.12464000	-3.30898800	-2.73119200
C	2.05311600	-3.65939600	-1.78012100
C	1.91325600	-2.65813000	-0.70693500
C	0.82275200	-4.01648300	-4.01934700
C	2.99274000	-4.86194900	-1.90953300
N	1.51700600	-0.64193800	1.52933800
C	2.33331500	-1.75171500	1.58874700
C	2.91468800	-1.85854900	2.92619900
C	2.44073200	-0.80096200	3.67228300
C	1.59422100	-0.03286900	2.76776500
C	3.84510300	-2.95509800	3.35199900
C	2.70341200	-0.44216900	5.13707200
H	5.80749600	2.89724800	-1.25288700
H	4.71941800	3.95633000	-0.38053200
H	2.61725600	2.37682100	0.56682200
H	2.13318500	-0.07786300	-2.80044100
H	4.97130200	3.82993900	-3.46063700
H	-5.92941200	0.02849400	-2.00375100
H	-6.68153900	-0.81304400	-0.63883300
H	-4.87923200	0.85771600	0.11525100
H	-3.70263000	0.00010900	-0.85472300
H	-3.46149400	-1.61871300	0.75294300
H	-6.36758600	-0.21697100	3.16731400

H	-6.43535400	0.21368300	1.50459500
H	-3.53859000	-2.36370600	2.74835300
H	-4.94616500	-2.05089000	3.78887300
H	1.17800700	1.56068400	4.09745800
H	-1.86426800	3.69266100	-1.07442000
H	-0.81956500	-1.90189700	-3.95746200
H	3.24820100	-3.46250900	0.73368400
H	-1.47399700	5.74157000	2.06354800
H	-1.03485500	5.66635800	0.35797100
H	-2.56248300	4.97738300	0.90672500
H	-0.53752400	5.03020600	3.83681400
H	1.00046200	4.21080700	4.11375900
H	-3.72153200	3.25008600	-2.65597700
H	-2.35121500	3.84299100	-3.59128400
H	-3.52054900	2.75843200	-4.33823400
H	-1.90692600	0.01253400	-5.68801700
H	0.91363500	-3.34929200	-4.88423700
H	1.50090400	-4.85693700	-4.18015800
H	-0.19814600	-4.41710200	-4.02713800
H	3.44591000	-4.88456100	-2.90414700
H	4.15942900	-2.82913500	4.39026100
H	4.75157000	-2.97554900	2.73571200
H	3.37438800	-3.94154400	3.26797100
H	1.76703900	-0.39212800	5.70257700
H	3.34362600	-1.18736900	5.61291500
Cl	-0.90992100	-2.39599200	1.85386100
O	-1.03277600	-0.76316300	0.51207200
O	-2.37825800	-3.04311400	1.69623400
H	5.61919800	5.09061800	-2.41446400
H	3.86528400	4.89290900	-2.57795700
H	-0.50024900	3.48222000	4.68407500
H	-3.14801700	-0.84024700	-4.77278800
H	-3.38684100	0.85206300	-5.22067600
H	3.80405200	-4.82639200	-1.17731000
H	2.45385900	-5.80399700	-1.76165300
H	3.19931200	0.53064900	5.22474400
H	4.05716100	1.51044600	-3.28029800
H	-5.46002900	-1.63566700	-1.61434800

Int1_{II,21}

Energy with the small basis set:	-2626.247408
Solution energy with the small basis set:	-2626.247379
Energy with larger basis sets:	-2626.924478
Zero-point energy:	0.775504
Dispersion effect:	-0.179863567

C	83.56100000	29.40899997	40.48999992
C	84.49102135	28.49612930	39.66757143
C	84.33708243	28.65947320	38.18663010
N	84.59158655	29.85281426	37.52829439
C	83.93119871	27.80261069	37.19470555
C	84.33918308	29.67991795	36.20710907
N	83.93600578	28.44464226	35.97128537
C	78.74700005	28.42299994	29.79600011
C	79.60299944	28.15029974	31.04362535
N	79.73719540	26.73226160	31.41098133
C	78.81859295	26.03880466	32.07573393
N	77.58408371	26.55663328	32.28518868
N	79.10931483	24.83250165	32.58022500
Fe	83.32276022	27.67533414	33.99419880
C	83.67475296	24.39201842	34.95360038
C	80.17312316	27.70804895	35.30544550
C	82.85473968	30.83409455	32.78237422
C	86.64669044	27.84727999	33.28190352
N	82.16880112	26.32332954	34.98196851
C	82.46299339	25.00123254	35.23962135
C	81.33823258	24.34749186	35.91585959
C	80.37893066	25.31207120	36.06147780
C	80.90713600	26.53028767	35.45050679
C	79.02612753	25.20461171	36.69754647
C	81.28899999	22.90700017	36.36999990
N	81.80733995	29.03472092	34.04996822
C	80.57280883	28.83617496	34.60242947
C	79.68833579	29.95570605	34.28457350
C	80.40188120	30.81416320	33.49186437
C	81.75165947	30.23115166	33.38471659
C	78.26654896	30.06217309	34.75274397
C	79.89800005	32.07999990	32.83400003
N	84.55162783	29.10247505	33.23418230
C	84.16152246	30.33388287	32.77886566
C	85.32768993	31.08994233	32.33360459
C	86.43226038	30.30093589	32.52318900

C	85.91497514	29.01800719	33.05388972
C	85.30812995	32.48208552	31.77709228
C	87.85999995	30.75899997	32.22300003
N	84.85843810	26.35830318	34.08732014
C	86.14710952	26.60578221	33.70505184
C	86.94214663	25.36664703	33.80117715
C	86.10090953	24.37342134	34.23585638
C	84.79714459	25.02695622	34.41882319
C	88.39899277	25.27851182	33.45961891
C	86.39099997	22.89700005	34.52599999
H	85.53488757	28.67988446	39.95730446
H	84.28981967	27.44771556	39.91024581
H	83.63688134	26.76876888	37.28127638
H	84.45692441	30.45689520	35.46874116
H	83.76005418	30.46955351	40.29949319
H	78.75554145	29.49572587	29.58054211
H	77.69893943	28.12164415	29.90881838
H	79.22099638	28.70468965	31.90795607
H	80.62264553	28.50425716	30.88076682
H	80.66602581	26.28864654	31.35192102
H	76.88366957	26.01674841	32.76691802
H	77.26780195	27.34689426	31.74845039
H	80.06079240	24.45465297	32.45794169
H	78.37053375	24.21798594	32.88214924
H	83.77130608	23.33937720	35.19570439
H	79.17184705	27.71627063	35.72147623
H	82.69769163	31.80576559	32.32777616
H	87.70795743	27.88904561	33.06110788
H	78.84479805	24.20248199	37.09303089
H	78.91436815	25.90996713	37.52920154
H	78.22544684	25.42656944	35.98069427
H	80.32339093	22.66716241	36.82023126
H	82.06388775	22.69335464	37.11572668
H	77.65946588	29.21777589	34.40202368
H	78.20426042	30.06507580	35.84758679
H	77.79108380	30.97937391	34.39795610
H	80.47615182	32.95922623	33.14265116
H	84.43322924	33.05024760	32.10354501
H	86.19657681	33.04235400	32.08516590
H	85.30121787	32.47286655	30.67997493
H	88.05897451	31.72068785	32.70699130
H	88.78433255	24.26801605	33.61414630
H	89.00012900	25.95740262	34.07669247
H	88.58318378	25.54554256	32.41193817

H	85.72395962	22.24433442	33.95267142
H	87.41958862	22.64344626	34.26138108
Cl	83.12375108	24.10857540	31.48360982
O	82.84708926	27.18204664	32.52231096
O	81.60106448	24.67528652	31.68535747
H	83.70310898	29.23683679	41.56099399
H	82.51120710	29.21773123	40.24832880
H	81.44860892	22.21638830	35.53343734
H	79.97177470	32.01680341	31.74198969
H	78.85363984	32.26554147	33.09015474
H	88.60573043	30.04477550	32.58172712
H	88.01282951	30.89004024	31.14616202
H	86.24982581	22.66918861	35.58858543
H	84.91595873	30.70798632	37.95527512
H	79.14520309	27.89614149	28.92418141

Int1b_{II,21}

Energy with the small basis set:	-2626.256947
Solution energy with the small basis set:	-2626.256955
Energy with larger basis sets:	-2626.933765
Zero-point energy:	0.777806
Dispersion effect:	-0.179202415

C	-3.85625000	3.23949199	4.71847699
C	-4.14812629	2.87554104	3.24870312
C	-3.23651643	1.83268999	2.67444865
N	-3.11465042	0.55750933	3.20561335
C	-2.38977175	1.83653569	1.59443911
C	-2.23031296	-0.14399983	2.45606486
N	-1.77166622	0.60523740	1.46868549
C	5.84501197	-0.92898699	-0.47938001
C	4.75458145	0.15116202	-0.53080663
N	3.65394437	-0.14666824	-1.45599115
C	3.73654826	-0.10133073	-2.78423884
N	4.84298003	0.37978003	-3.39534248
N	2.71568751	-0.53051821	-3.53051304
Fe	-0.31721575	-0.04147519	-0.01550478
C	-1.51608265	2.20914153	-2.30224074
C	1.67330584	2.40613121	1.32866377
C	1.05286463	-2.31077063	2.14474515
C	-2.68953528	-2.30832743	-0.94989637
N	-0.02570396	1.93791862	-0.38108669
C	-0.57857826	2.68515794	-1.39344008

C	-0.07364618	4.05289069	-1.34882755
C	0.79258509	4.10569951	-0.28665455
C	0.82933473	2.77405859	0.29083623
C	1.58402118	5.27362921	0.22415745
C	-0.45058299	5.17028498	-2.28765199
N	1.08700555	0.02988943	1.48293139
C	1.83158996	1.12210593	1.83496162
C	2.86825471	0.74394500	2.77883754
C	2.76039464	-0.61204354	2.97301946
C	1.61402854	-1.04027419	2.16710658
C	3.84000821	1.70690222	3.39725524
C	3.64410099	-1.46863300	3.85567100
N	-0.78900091	-1.93645003	0.53603259
C	-0.08893595	-2.69820860	1.44034024
C	-0.73178506	-3.98752269	1.59862493
C	-1.83534803	-4.01494151	0.77817476
C	-1.83420451	-2.71772100	0.07688914
C	-0.24485483	-5.07123843	2.51585347
C	-2.80047799	-5.20471398	0.69008800
N	-1.79724797	-0.04689795	-1.37460549
C	-2.63652647	-1.09823055	-1.65241626
C	-3.48346319	-0.75847710	-2.79700031
C	-3.13692462	0.50943641	-3.20791636
C	-2.08722559	0.94154465	-2.28975035
C	-4.51734803	-1.67661039	-3.37897540
C	-3.69932299	1.35088600	-4.35857500
H	-5.19154327	2.54284154	3.15709893
H	-4.06139554	3.76915921	2.62271871
H	-2.18649575	2.63850156	0.90358259
H	-1.95250686	-1.16656573	2.65319520
H	-3.97639150	2.37693843	5.38365653
H	6.61693578	-0.63669743	0.23910746
H	6.32872692	-1.08172850	-1.44916943
H	5.18324801	1.13458422	-0.77111738
H	4.29180681	0.25888770	0.45241673
H	2.70809313	-0.31464426	-1.08226709
H	5.00077371	0.20700683	-4.37492195
H	5.61120912	0.74592210	-2.85902181
H	1.90735102	-1.00983611	-3.10324823
H	2.69511610	-0.33450606	-4.51854465
H	-1.86203982	2.89922763	-3.06431234
H	2.30996828	3.18067037	1.74143246
H	1.51444302	-3.06590913	2.77246831
H	-3.44773456	-3.01823002	-1.26465610

H	1.38360421	6.17760903	-0.35545262
H	1.34501942	5.49670796	1.27086526
H	2.66382562	5.08666594	0.17398983
H	0.08587462	6.08934316	-2.04281623
H	-1.52361350	5.39263559	-2.24353851
H	4.39883743	2.27072633	2.64058342
H	3.32683718	2.44317256	4.02765730
H	4.56905418	1.19417629	4.02872832
H	3.12380382	-1.78166710	4.76935268
H	-0.13555733	-4.71632284	3.54731882
H	-0.93309892	-5.91906363	2.53062233
H	0.73438104	-5.45365154	2.20218359
H	-3.04758106	-5.56758935	1.69150018
H	-5.03318662	-1.21151108	-4.22236219
H	-5.27963876	-1.94904982	-2.63902140
H	-4.06991450	-2.61007040	-3.74097631
H	-2.90974101	1.63570468	-5.06259777
H	-4.45816339	0.79440032	-4.91260583
Cl	1.50011663	-3.40506299	-1.76019953
O	0.87070667	-0.46403844	-1.06115568
O	0.66830949	-2.12980926	-2.42024263
H	-4.54636075	4.01518876	5.06272252
H	-2.83459122	3.61280638	4.83586353
H	-0.21736026	4.91892029	-3.32936997
H	3.96595010	-2.38092045	3.34092987
H	4.53993254	-0.92278039	4.15823753
H	-3.73688637	-4.93462252	0.19357177
H	-2.35465949	-6.03424508	0.13007151
H	-4.16253488	2.27160786	-3.98657816
H	-3.60369087	0.20315590	4.01448114
H	5.42285274	-1.88561713	-0.16007596

TS_{II,21}

Energy with the small basis set:	-2626.250959
Solution energy with the small basis set:	-2626.251564
Energy with larger basis sets:	-2626.928675
Zero-point energy:	0.777043
Dispersion effect:	-0.179881813
Imaginary frequency:	-344 cm ⁻¹

C	-3.85625000	3.23949200	4.71847700
C	-4.14114600	2.82608200	3.26119700
C	-3.18915000	1.81205700	2.70068100

N	-2.95454000	0.58264900	3.29838500
C	-2.40953200	1.79820100	1.57093700
C	-2.07066600	-0.10930000	2.54091800
N	-1.72047200	0.60173100	1.48272500
C	5.84501200	-0.92898700	-0.47938000
C	4.73994200	0.13013500	-0.59012700
N	3.66875700	-0.20550000	-1.53648400
C	3.75393000	-0.09792200	-2.86218500
N	4.87884600	0.37560700	-3.44339300
N	2.72095300	-0.44953500	-3.63122400
Fe	-0.33110600	-0.04791000	-0.01501600
C	-1.51797500	2.20529200	-2.30494000
C	1.68186400	2.39898200	1.31589800
C	1.06533500	-2.32048400	2.12289400
C	-2.71307800	-2.30179400	-0.93220500
N	-0.02078500	1.93248000	-0.39079200
C	-0.57518500	2.68100900	-1.40042500
C	-0.06669100	4.04857400	-1.35792600
C	0.80602000	4.09816900	-0.30187600
C	0.83865100	2.76723500	0.27738600
C	1.60268700	5.26258500	0.20623600
C	-0.45058300	5.17028500	-2.28765200
N	1.10361100	0.01996000	1.45954500
C	1.84009400	1.11453300	1.82119500
C	2.86781700	0.74008300	2.77694700
C	2.76462700	-0.61599600	2.96674100
C	1.62575400	-1.04772600	2.14990800
C	3.82533800	1.70861700	3.40749800
C	3.64410100	-1.46863300	3.85567100
N	-0.79410600	-1.93813100	0.53128900
C	-0.07901100	-2.70496200	1.41968400
C	-0.71657700	-3.99799300	1.57676800
C	-1.83303200	-4.01935200	0.77476200
C	-1.84392600	-2.71699400	0.08183700
C	-0.20647900	-5.08804300	2.47293100
C	-2.80047800	-5.20471400	0.69008800
N	-1.81529300	-0.04427600	-1.36124300
C	-2.66266700	-1.09012600	-1.63315000
C	-3.50713900	-0.75018600	-2.78028000
C	-3.15151000	0.51229300	-3.19819100
C	-2.09721900	0.94122300	-2.28242800
C	-4.54910100	-1.66279000	-3.35480400
C	-3.69932300	1.35088600	-4.35857500
H	-5.16826400	2.44244800	3.18954100

H	-4.10290100	3.70712800	2.61311300
H	-2.30164200	2.56306300	0.81933300
H	-1.71202700	-1.09584500	2.78454700
H	-3.92714000	2.38897000	5.40559500
H	6.58465600	-0.61166400	0.26134500
H	6.36638300	-1.09089200	-1.42808000
H	5.16014200	1.11180400	-0.84799700
H	4.25046400	0.25622900	0.37763600
H	2.72964300	-0.40707200	-1.16994500
H	5.00530200	0.31405500	-4.44020300
H	5.67964400	0.62853900	-2.89049100
H	1.86493200	-0.87038700	-3.22924400
H	2.75034800	-0.27986000	-4.62362900
H	-1.86344000	2.89325100	-3.06867400
H	2.31865500	3.17251900	1.72907800
H	1.52881100	-3.07633400	2.74737700
H	-3.47390200	-3.01010000	-1.24283600
H	1.43600800	6.15668300	-0.39804200
H	1.33685800	5.51265000	1.24004100
H	2.67937500	5.05571700	0.19202000
H	0.08831200	6.08752500	-2.04347700
H	-1.52268800	5.39253100	-2.23221300
H	4.39912500	2.26646900	2.65799800
H	3.29792200	2.44890000	4.02064000
H	4.54115500	1.20253700	4.05842300
H	3.11588700	-1.79090300	4.76129400
H	-0.07430200	-4.74215800	3.50446600
H	-0.88951700	-5.93929300	2.49623300
H	0.76602500	-5.46340900	2.13208000
H	-2.92076800	-5.66668700	1.67248900
H	-5.06734500	-1.19532500	-4.19486600
H	-5.30782500	-1.92898600	-2.60953000
H	-4.10989800	-2.59894600	-3.71867400
H	-2.90592700	1.60342700	-5.06994700
H	-4.47501800	0.80627300	-4.90009800
Cl	1.21386800	-3.21872400	-2.04582200
O	0.88331600	-0.46338200	-1.07264000
O	0.52895600	-1.73088000	-2.44544300
H	-4.58392200	3.98519200	5.04991200
H	-2.85504300	3.66860300	4.81850000
H	-0.22742800	4.92346700	-3.33230400
H	3.97943300	-2.37554300	3.34060700
H	4.53179900	-0.91800200	4.17180900
H	-3.79122800	-4.89527000	0.34510900

H	-2.43343400	-5.97059100	-0.00232300
H	-4.13662800	2.28834100	-3.99832100
H	-3.36834800	0.25316300	4.15781300
H	5.42703900	-1.88741900	-0.16076100

Int2_{II,21}

Energy with the small basis set:	-2626.280304
Solution energy with the small basis set:	-2626.280317
Energy with larger basis sets:	-2626.950567
Zero-point energy:	0.778377
Dispersion effect:	-0.179114872

C	83.56100000	29.40899994	40.48999982
C	84.47573467	28.52114851	39.62228692
C	84.25352723	28.67152918	38.14707738
N	84.29673325	29.90042582	37.50184942
C	83.98229799	27.76900440	37.15078334
C	84.05366228	29.71614609	36.18641421
N	83.86065612	28.42970551	35.94156366
C	78.74700012	28.42299993	29.79600018
C	78.97973349	27.62118142	31.08315951
N	80.17423244	26.76974961	31.04214344
C	80.28058576	25.63384520	30.35842628
N	79.21193701	25.09538608	29.73325206
N	81.45950787	25.00308701	30.30104963
Fe	83.36116333	27.70712687	34.12844825
C	83.69505346	24.38930649	34.99564834
C	80.14538654	27.67130284	35.24794303
C	82.86065706	30.84035913	32.81498340
C	86.65739954	27.85157425	33.31810787
N	82.17816733	26.31480172	34.99386207
C	82.47612004	24.99744460	35.27294131
C	81.34610712	24.34437776	35.91640878
C	80.36575858	25.29940719	36.02674674
C	80.89055160	26.51253131	35.42748691
C	78.99703158	25.17122096	36.62580507
C	81.28900002	22.90700050	36.36999976
N	81.79607813	29.01342771	34.02700028
C	80.54805345	28.80518934	34.55096184
C	79.66705178	29.91299777	34.22165377
C	80.39747980	30.79424643	33.45990587
C	81.74469188	30.22667854	33.37607847
C	78.23591784	30.01441409	34.66598995

C	79.89800017	32.07999963	32.83400012
N	84.55168903	29.09374586	33.26408933
C	84.16371367	30.33548970	32.81483759
C	85.31838267	31.08426512	32.36821244
C	86.43143311	30.29491603	32.54866844
C	85.92335703	29.01922343	33.08608313
C	85.27050648	32.47699217	31.81232557
C	87.85999977	30.75899988	32.22300010
N	84.86802074	26.36425337	34.13242296
C	86.16112604	26.61251104	33.74602538
C	86.94916048	25.37937240	33.83480681
C	86.10691729	24.38183992	34.27399207
C	84.81417352	25.02803942	34.47055122
C	88.40235612	25.28083592	33.47662637
C	86.39099993	22.89700011	34.52600000
H	85.52629070	28.73743754	39.86130095
H	84.31897349	27.46794149	39.87602197
H	83.86247897	26.69992543	37.21741892
H	84.01821143	30.50827548	35.45611070
H	83.72763396	30.47560335	40.30134025
H	77.85707827	29.05035640	29.90617144
H	78.59786039	27.77686225	28.92510149
H	78.10117920	27.01157637	31.33686818
H	79.13060493	28.29876705	31.92590132
H	81.00089958	27.04131867	31.59823680
H	79.31154712	24.29307670	29.13320779
H	78.30411879	25.52436961	29.79277578
H	82.30478259	25.46943859	30.64789828
H	81.55226457	24.12384106	29.81880967
H	83.79409993	23.33906686	35.24583964
H	79.13285188	27.66633257	35.63463286
H	82.71586038	31.81997161	32.37140519
H	87.71811882	27.89451980	33.09495192
H	78.81370982	24.16084076	36.99819092
H	78.86127622	25.85973807	37.46805765
H	78.21204517	25.39764943	35.89447842
H	80.30322376	22.65701736	36.76779160
H	82.02443484	22.70055514	37.15706489
H	77.63373747	29.16793161	34.31321959
H	78.15670660	30.02527817	35.75979573
H	77.76181308	30.92693907	34.29765972
H	80.49523813	32.94430689	33.14811118
H	84.71992323	33.16205079	32.46718065
H	86.27424838	32.88621696	31.67832198

H	84.77668967	32.49904134	30.83328654
H	88.06800699	31.71712683	32.70869435
H	88.78898035	24.27433323	33.65386028
H	89.01251570	25.97516346	34.06682749
H	88.57401459	25.51854238	32.41977169
H	85.77280972	22.26453224	33.87987215
H	87.43789431	22.66055138	34.32390179
Cl	83.91731881	27.87999075	30.16972508
O	82.63230698	27.03574910	32.42814062
O	83.49551075	26.57261687	31.51470724
H	83.75917750	29.23343343	41.55100134
H	82.50553139	29.19422603	40.29834570
H	81.49808409	22.21473878	35.54568158
H	79.94525624	32.04050456	31.73906301
H	78.86250439	32.27625393	33.11662782
H	88.60965647	30.04132511	32.56616474
H	87.99153375	30.89032798	31.14377698
H	86.17898486	22.62239046	35.56517137
H	84.47830749	30.79223564	37.93877405
H	79.60296711	29.07122754	29.58994821

Int2b_{II,21}

Energy with the small basis set:	-2626.279397
Solution energy with the small basis set:	-2626.279414
Energy with larger basis sets:	-2626.951456
Zero-point energy:	0.775336
Dispersion effect:	-0.174979088

C	83.56100001	29.40899995	40.48999990
C	84.34326405	28.39628140	39.63295365
C	84.18604241	28.59327868	38.15565095
N	84.45664646	29.79390281	37.51661531
C	83.80000945	27.74575715	37.14973322
C	84.24038925	29.64584463	36.18983435
N	83.84124830	28.40990194	35.93759139
C	78.74700000	28.42299994	29.79600002
C	79.63520768	27.40122830	30.51178819
N	80.85718139	27.08517710	29.76888907
C	80.96668136	26.23033841	28.75657369
N	79.92165339	25.46916469	28.36921708
N	82.13824844	26.12120675	28.11821981
Fe	83.35600536	27.68273624	34.11950617
C	83.69754190	24.39860207	35.01996425

C	80.07418134	27.60570916	35.11380221
C	82.86981408	30.83553460	32.86030378
C	86.66475536	27.83993815	33.29550828
N	82.14257501	26.29472039	34.93775185
C	82.46402142	24.99315119	35.25884717
C	81.33021575	24.33129304	35.88787009
C	80.32354667	25.26152622	35.94578805
C	80.83570862	26.46837828	35.33240632
C	78.94155791	25.11324100	36.50896123
C	81.28900004	22.90700055	36.36999978
N	81.76872305	28.96775559	33.98064132
C	80.49616545	28.74536855	34.44298652
C	79.62765074	29.85570380	34.10968880
C	80.38795806	30.76910001	33.41971691
C	81.74101501	30.20565163	33.37188287
C	78.17372759	29.92494247	34.47665766
C	79.89800021	32.07999956	32.83400019
N	84.56410455	29.08065532	33.27569488
C	84.17160148	30.32837600	32.85525514
C	85.32334404	31.08840631	32.41231294
C	86.43697693	30.29520089	32.56246914
C	85.93404903	29.01188308	33.07956794
C	85.26585503	32.48752832	31.87515362
C	87.85999982	30.75899989	32.22300010
N	84.87185187	26.36659542	34.13703477
C	86.16708617	26.60730051	33.73333030
C	86.94687496	25.37533891	33.82439906
C	86.10559556	24.38392220	34.28274089
C	84.81624110	25.03426254	34.49087885
C	88.39521345	25.26576143	33.44804486
C	86.39099994	22.89700011	34.52600000
H	85.40870196	28.43800439	39.89879028
H	84.01324731	27.37924433	39.86764561
H	83.50477538	26.71150783	37.21204660
H	84.36707748	30.42945990	35.46106426
H	83.89702625	30.43766775	40.31673331
H	77.87150813	28.65481943	30.41046229
H	78.39417583	28.05192205	28.82829454
H	79.08891027	26.47467336	30.72989645
H	79.96658141	27.78558971	31.47920468
H	81.70869157	27.60774785	29.99433871
H	79.98659483	24.87136140	27.56180351
H	79.04611360	25.49552985	28.86374906
H	82.90940088	26.73389790	28.40096941

H	82.28587954	25.43425551	27.39712109
H	83.80397943	23.35401050	35.28962307
H	79.04703010	27.58519704	35.45832511
H	82.73234469	31.82735108	32.44259031
H	87.72365584	27.87783945	33.06267642
H	78.78778247	24.12214296	36.94153094
H	78.74969362	25.84830701	37.29906936
H	78.17343839	25.25699103	35.73967642
H	80.30467617	22.65199664	36.76787096
H	82.02334378	22.72500928	37.16425724
H	77.60281891	29.10208007	34.02992742
H	78.02961019	29.86155354	35.56180863
H	77.71517842	30.85830462	34.14319076
H	80.44862500	32.93696879	33.24029354
H	84.73530272	33.16683027	32.55256197
H	86.26721988	32.89479863	31.71874038
H	84.74540359	32.52155547	30.91014638
H	88.06763317	31.72439155	32.69353598
H	88.77885106	24.25912396	33.63038297
H	89.01657536	25.96215917	34.02378708
H	88.55457742	25.49178867	32.38682021
H	85.77331727	22.26968369	33.87456800
H	87.43820317	22.66283826	34.32415383
Cl	83.88321955	28.23813967	29.80470848
O	82.75076986	27.03714671	32.35909855
O	83.62195861	26.67996510	31.52492808
H	83.70508832	29.19702466	41.55317447
H	82.48936714	29.36464284	40.27433753
H	81.51095828	22.20061069	35.56095918
H	80.02310975	32.10755635	31.74486831
H	78.84047455	32.23242917	33.05347947
H	88.61412677	30.04916020	32.57284684
H	87.98631722	30.87433549	31.14130020
H	86.17686732	22.61539758	35.56283145
H	84.76210541	30.64685304	37.96186770
H	79.29657907	29.35228236	29.62251318

Prod_{II,21}

Energy with the small basis set:	-2626.299021
Solution energy with the small basis set:	-2626.298884
Energy with larger basis sets:	-2626.951456
Zero-point energy:	0.776381
Dispersion effect:	-0.17147725

C	83.56100001	29.40899993	40.48999981
C	84.48862423	28.51128841	39.65180236
C	84.25232889	28.65326774	38.18099455
N	84.23766001	29.89237269	37.55254885
C	83.98753462	27.75116201	37.18436698
C	83.97232804	29.72403050	36.24383505
N	83.81677583	28.43212083	35.99198921
C	78.74700019	28.42299984	29.79600017
C	79.63196763	27.23916036	29.39440687
N	80.86210607	27.69149592	28.74053862
C	81.06786615	27.79715139	27.42815716
N	80.39536670	27.02937659	26.53956906
N	81.97821578	28.67159684	26.99215242
Fe	83.40355335	27.74224669	34.22735853
C	83.71248858	24.39585702	35.02273900
C	80.12445977	27.62783066	35.14963500
C	82.88033539	30.85442143	32.86276085
C	86.67554931	27.87017688	33.36512976
N	82.18055066	26.30378983	34.94315505
C	82.48363267	24.99316869	35.26608553
C	81.35060984	24.33805994	35.89885433
C	80.35670806	25.28118487	35.96712444
C	80.87936896	26.48585454	35.35837628
C	78.97207566	25.14492981	36.52539757
C	81.28900003	22.90700071	36.36999968
N	81.80760555	28.98257428	33.98993440
C	80.54013543	28.76446140	34.47202011
C	79.66140934	29.86728802	34.14185218
C	80.40633398	30.78368410	33.44065941
C	81.75935341	30.22806852	33.38458508
C	78.20753734	29.92065372	34.51044225
C	79.89800025	32.07999953	32.83400021
N	84.57277854	29.11615680	33.34074509
C	84.18421063	30.35213928	32.87802138
C	85.32767268	31.09156220	32.39802193
C	86.44261812	30.30834388	32.58480791

C	85.94496416	29.04249950	33.14693652
C	85.24741525	32.43980542	31.74952243
C	87.85999965	30.75899981	32.22300015
N	84.88118517	26.38167216	34.17249843
C	86.18231431	26.62785474	33.79045015
C	86.96187316	25.39367744	33.86564636
C	86.11678590	24.39152266	34.29930213
C	84.83149459	25.03709117	34.50649085
C	88.41301574	25.29182391	33.49914893
C	86.39099988	22.89700019	34.52599995
H	85.53721354	28.74053327	39.88558287
H	84.33849396	27.46078681	39.91903747
H	83.90364756	26.67792362	37.23561220
H	83.89543269	30.52087382	35.52151337
H	83.72581249	30.47333440	40.28792848
H	77.87191785	28.06939920	30.35128189
H	78.39877033	28.96955211	28.91403258
H	79.08726824	26.54967199	28.74162061
H	79.92631031	26.66307140	30.27761960
H	81.43077152	28.37142550	29.28958570
H	80.47719670	27.19638077	25.55034893
H	79.86083093	26.23295578	26.84201796
H	82.35645318	29.34910670	27.67940840
H	82.32621951	28.64058429	26.04749006
H	83.81565598	23.34727011	35.28016368
H	79.09929632	27.61086406	35.50145812
H	82.73630379	31.82321175	32.40075392
H	87.73473676	27.91112413	33.13296799
H	78.82764842	24.17634998	37.00872129
H	78.76233112	25.91861175	37.27238266
H	78.21108990	25.23502994	35.74106971
H	80.34203931	22.69818503	36.87135903
H	82.09531953	22.67612834	37.07616366
H	77.64358998	29.09712149	34.05574570
H	78.06365784	29.84893268	35.59525784
H	77.74355618	30.85329188	34.18337458
H	80.35287391	32.95609743	33.31074096
H	84.78027435	33.18753222	32.40126956
H	86.23733372	32.81141094	31.47661788
H	84.64601837	32.37640524	30.83544686
H	88.05445862	31.75658373	32.62686327
H	88.79302371	24.27995267	33.65799541
H	89.03034658	25.97173840	34.09854095
H	88.58201952	25.54548386	32.44563476

H	85.74600689	22.28012090	33.89124369
H	87.42844202	22.65165533	34.28996353
Cl	82.45248793	30.14685148	29.68409290
O	83.02234115	27.02429817	32.09583741
O	83.63384889	27.39288090	31.10420190
H	83.74372481	29.25446533	41.55708659
H	82.50894041	29.18643589	40.28873389
H	81.38166257	22.20353918	35.53356453
H	80.13984569	32.12546793	31.76645876
H	78.81627744	32.16147103	32.94600867
H	88.62031570	30.08327665	32.62446174
H	87.99274878	30.80292568	31.13648175
H	86.20716752	22.61361931	35.56812108
H	84.39352265	30.78373042	38.00116753
H	79.30663247	29.11832450	30.42718779

Prod_{II,41}

Energy with the small basis set:	-2626.291223
Solution energy with the small basis set:	-2626.291151
Energy with larger basis sets:	-2626.961267
Zero-point energy:	0.776581
Dispersion effect:	-0.173553231

C	83.56100001	29.40899993	40.48999982
C	84.22466296	28.27319682	39.69113465
C	84.20605260	28.48352587	38.20871454
N	84.86924881	29.52284889	37.57215621
C	83.60016161	27.78673119	37.19819234
C	84.66775797	29.42971556	36.24031542
N	83.89719726	28.38061332	35.98305876
C	78.74700018	28.42299985	29.79600019
C	79.37899043	27.13584715	30.32990998
N	80.71728683	26.92323585	29.77172172
C	80.98296342	26.38225153	28.58055747
N	80.13357742	25.50925881	27.99425107
N	82.13999822	26.69089830	27.98937794
Fe	83.38848596	27.71632738	34.20234027
C	83.72198224	24.41297936	35.06596543
C	80.06025165	27.56984497	35.02817378
C	82.88982499	30.86205766	32.92928007
C	86.67462431	27.83996469	33.28527128
N	82.15671226	26.29565191	34.92811295

C	82.48288684	24.99930832	35.28079047
C	81.33980856	24.33003413	35.88350012
C	80.31841603	25.24587315	35.89324994
C	80.83247870	26.44916402	35.28136290
C	78.91547971	25.08276096	36.39714536
C	81.28900001	22.90700060	36.36999972
N	81.78636101	28.94927300	33.95816431
C	80.49532345	28.71125152	34.37465646
C	79.62750626	29.81829902	34.04006859
C	80.39825336	30.76239630	33.40679265
C	81.75834572	30.21336238	33.39248869
C	78.15831076	29.85144876	34.34482709
C	79.89800019	32.07999962	32.83400016
N	84.57138389	29.08568619	33.31158998
C	84.18640329	30.34840610	32.92365560
C	85.33449239	31.10756399	32.47975448
C	86.44488891	30.30257947	32.59470189
C	85.94403326	29.01481960	33.09291037
C	85.27304491	32.50650416	31.94379688
C	87.85999972	30.75899986	32.22300012
N	84.88751120	26.37995383	34.16045448
C	86.17982549	26.60837438	33.73162410
C	86.95009441	25.37287788	33.80629875
C	86.11216532	24.38779199	34.28998137
C	84.83492250	25.04600375	34.52499229
C	88.38682160	25.25099393	33.39135498
C	86.39099990	22.89700015	34.52599996
H	85.26060205	28.13718992	40.02995286
H	83.71221029	27.32788243	39.89601638
H	82.98984728	26.90232009	37.25808510
H	85.07438616	30.11074400	35.51207527
H	84.07267723	30.36604921	40.33902978
H	77.78393419	28.61064739	30.28256442
H	78.57629135	28.35943658	28.71637836
H	78.74129850	26.26560714	30.13697656
H	79.50192565	27.18786449	31.41570828
H	81.41001895	27.65706804	30.03036952
H	80.29042489	25.18846906	27.05320673
H	79.31063625	25.18426410	28.47224454
H	82.64880386	27.51920248	28.35285932
H	82.43039217	26.24174158	27.13589265
H	83.83242961	23.37110559	35.34423143
H	79.02265773	27.53769728	35.33716303
H	82.75765151	31.85843905	32.52367819

H	87.72910267	27.87451636	33.03301848
H	78.77076841	24.11212514	36.87622997
H	78.66147550	25.85272450	37.13425512
H	78.18385033	25.15753756	35.58388932
H	80.32127241	22.67777161	36.82007743
H	82.06024527	22.70555994	37.12301304
H	77.62066270	29.05009274	33.82403476
H	77.96577642	29.72540390	35.41681452
H	77.70390519	30.79713962	34.04323733
H	80.42807664	32.93656443	33.26674499
H	84.73359695	33.18286623	32.61658734
H	86.27263428	32.91965405	31.79171123
H	84.75663166	32.52694213	30.97644526
H	88.07934784	31.72781155	32.68091560
H	88.76180718	24.23710833	33.54878301
H	89.03165932	25.93054475	33.96148800
H	88.52202002	25.49098213	32.32998437
H	85.73240293	22.27390017	33.91141376
H	87.42322667	22.64950993	34.27075984
Cl	82.82303920	29.18225429	29.71059351
O	82.99602595	26.74328499	32.17711115
O	83.73561752	26.86694107	31.21255221
H	83.59008451	29.18804380	41.56069709
H	82.51547956	29.53772804	40.19520384
H	81.44815145	22.19599740	35.54999070
H	80.04868385	32.12027022	31.74914742
H	78.83423073	32.20938835	33.03472675
H	88.62123706	30.05039003	32.56072767
H	87.96191502	30.86704052	31.13790828
H	86.22855668	22.62375456	35.57439974
H	85.41772424	30.24111057	38.02332809
H	79.40911505	29.27198591	29.98563973

TS_{II,hetero}

Energy with the small basis set:	-2626.201775
Solution energy with the small basis set:	-2626.202627
Energy with larger basis sets:	-2626.881462
Zero-point energy:	0.777410
Dispersion effect:	-0.176435028
Imaginary frequency:	-316 cm ⁻¹

C	4.81579500	4.35547800	-2.51176900
C	4.82180100	3.40182300	-1.30147400

C	3.74942100	2.35405000	-1.32814000
N	3.56708200	1.48572100	-2.39436600
C	2.79014800	1.98568400	-0.41803200
C	2.54060900	0.65063900	-2.10608600
N	2.04789000	0.92786200	-0.91121500
C	-5.74251700	-0.67116400	-1.18385800
C	-4.58052200	-0.14724100	-0.33138600
N	-4.28046100	-0.98405300	0.83314600
C	-4.86963800	-0.90685600	2.02400000
N	-5.97017900	-0.14387700	2.20973000
N	-4.35585700	-1.59206600	3.05222700
Fe	0.39153500	-0.06972300	-0.02721800
C	1.01734500	1.19009400	3.09157800
C	-1.31264400	2.78973200	-0.83251200
C	-0.50921600	-1.42707500	-3.03375700
C	2.54855200	-2.65616600	0.54001900
N	-0.00518200	1.67694500	0.92425800
C	0.29945800	2.00480100	2.22244200
C	-0.20454000	3.33658600	2.54317900
C	-0.82061800	3.79398500	1.40754200
C	-0.70953000	2.73819000	0.41644400
C	-1.50474800	5.10762400	1.17289900
C	-0.05427300	4.05179800	3.86024900
N	-0.71310300	0.55943900	-1.64420900
C	-1.35929300	1.75668800	-1.76038900
C	-2.15317200	1.78946600	-2.97770800
C	-1.99482600	0.57356700	-3.59255400
C	-1.06058500	-0.18237500	-2.74757600
C	-2.96613000	2.97048200	-3.41868600
C	-2.64437500	0.12661300	-4.88425800
N	0.96826200	-1.71460900	-1.06504400
C	0.45928000	-2.10077600	-2.28152700
C	1.12169200	-3.31089300	-2.73022700
C	2.05126900	-3.66059000	-1.77970400
C	1.91189700	-2.65899700	-0.70680400
C	0.81936200	-4.01893500	-4.01808000
C	2.99274000	-4.86194900	-1.90953300
N	1.51513400	-0.64388400	1.53096600
C	2.33088800	-1.75433100	1.59034500
C	2.91350900	-1.86055200	2.92736100
C	2.44167500	-0.80126300	3.67255100
C	1.59530100	-0.03315600	2.76837900
C	3.84042700	-2.95970300	3.35394000
C	2.70341200	-0.44216900	5.13707200

H	5.80557600	2.91811100	-1.22757500
H	4.69844000	3.97591600	-0.37796400
H	2.58605100	2.40783700	0.55267800
H	2.18595400	-0.12072300	-2.77017100
H	4.99309200	3.82287300	-3.45280400
H	-5.89061800	-0.01829200	-2.04898800
H	-6.68364000	-0.71168100	-0.62540100
H	-4.76920500	0.87895700	0.00782100
H	-3.66137200	-0.10635300	-0.91936600
H	-3.48349000	-1.62487400	0.78813500
H	-6.25975600	0.09760600	3.14378900
H	-6.34997800	0.40126300	1.45403600
H	-3.54202400	-2.20417900	2.83226700
H	-4.92053100	-1.76875500	3.86828700
H	1.18075100	1.56110700	4.09722300
H	-1.84994000	3.69821200	-1.07934700
H	-0.82173800	-1.90335400	-3.95681300
H	3.24578900	-3.46468900	0.73366900
H	-1.42365900	5.76301900	2.04254300
H	-1.07026400	5.64169800	0.32017100
H	-2.57289500	4.97754700	0.96086500
H	-0.54927200	5.02440900	3.84005600
H	0.99945800	4.22247500	4.11026300
H	-3.70193300	3.26498200	-2.66107300
H	-2.33208700	3.84537700	-3.60485200
H	-3.51116200	2.76447400	-4.34204600
H	-1.90892400	0.01012200	-5.68945700
H	0.94170300	-3.36096700	-4.88635300
H	1.47620400	-4.87907000	-4.16219200
H	-0.21208200	-4.39075900	-4.03835700
H	3.44630100	-4.88322500	-2.90393500
H	4.17734900	-2.81944400	4.38330700
H	4.73369700	-3.00197800	2.71988800
H	3.35680100	-3.94202500	3.29735000
H	1.77155200	-0.43781800	5.71241400
H	3.38071400	-1.16195500	5.60061000
Cl	-0.92412700	-2.34187800	1.90422700
O	-1.03345000	-0.75711400	0.51001900
O	-2.40613400	-2.96799500	1.79394200
H	5.60720400	5.10289300	-2.40946200
H	3.85892100	4.87861700	-2.59764900
H	-0.49103900	3.47610300	4.68462100
H	-3.14871200	-0.83945900	-4.76930700
H	-3.38701600	0.85206000	-5.22040000

H	3.80343300	-4.82462000	-1.17673400
H	2.45541700	-5.80494100	-1.76188900
H	3.15692800	0.55068500	5.22737100
H	4.10578100	1.47442100	-3.24764700
H	-5.52991400	-1.67973800	-1.54861300

Int1_{II,01}

Energy with the small basis set:	-2626.233099
Solution energy with the small basis set:	-2626.233049
Energy with larger basis sets:	-2626.910297
Zero-point energy:	0.775469
Dispersion effect:	-0.179381661

C	83.56100000	29.40899998	40.48999993
C	84.50950823	28.51784128	39.66532281
C	84.34131729	28.67573823	38.18562756
N	84.55023139	29.87820309	37.52786132
C	83.95579882	27.80769441	37.19541608
C	84.29279415	29.69950062	36.20863444
N	83.92914746	28.45194838	35.97341057
C	78.74700006	28.42299995	29.79600009
C	79.64624574	28.13413160	31.00698814
N	79.84843850	26.70787473	31.29410696
C	78.98808478	25.94282383	31.95816837
N	77.74933661	26.40589059	32.26299074
N	79.35360668	24.72424084	32.37196178
Fe	83.32385295	27.66953960	34.00639981
C	83.68239945	24.39432990	34.98132771
C	80.15840635	27.69266921	35.28655438
C	82.85719860	30.83407477	32.80623161
C	86.64761126	27.84575550	33.28246319
N	82.17215582	26.32238108	35.00004606
C	82.47061691	25.00627965	35.26811920
C	81.33909742	24.34812823	35.92790910
C	80.36959211	25.30445735	36.05409008
C	80.89869462	26.52321415	35.44718382
C	79.00789030	25.18855758	36.66938504
C	81.28899999	22.90700015	36.36999992
N	81.80030330	29.02559932	34.04966645
C	80.56150435	28.82296210	34.58645591
C	79.67602144	29.94115047	34.26283991
C	80.39637772	30.80770238	33.48578034
C	81.74937246	30.22709094	33.39091732

C	78.24841038	30.03868685	34.71456984
C	79.89800004	32.07999990	32.83400003
N	84.55361689	29.09878319	33.24368595
C	84.16417517	30.33187824	32.79879273
C	85.32763697	31.09218955	32.35260052
C	86.43322812	30.30266725	32.53193029
C	85.91769071	29.01619880	33.05895507
C	85.29588393	32.48531858	31.79895236
C	87.85999994	30.75899997	32.22300003
N	84.86128597	26.35983186	34.10111439
C	86.14632595	26.60496296	33.71087359
C	86.94072179	25.36495583	33.80091895
C	86.10095517	24.37266828	34.24048496
C	84.79974473	25.02658352	34.43430191
C	88.39473918	25.27498318	33.44873112
C	86.39099997	22.89700005	34.52599999
H	85.55006422	28.72886322	39.94834425
H	84.33643146	27.46516790	39.91113813
H	83.69597710	26.76465401	37.28218383
H	84.37793143	30.48176370	35.47142498
H	83.73055024	30.47367532	40.29397055
H	78.68921783	29.50378952	29.63489911
H	77.72104736	28.05601516	29.91825287
H	79.26172583	28.62654426	31.90668858
H	80.64431412	28.54259366	30.83849275
H	80.78374569	26.29918211	31.15964173
H	77.08067053	25.78752671	32.69384130
H	77.37414087	27.19136493	31.75700493
H	80.30693495	24.39565477	32.13091846
H	78.65833206	24.06219927	32.67708830
H	83.77982570	23.34255454	35.22653570
H	79.15104994	27.69480439	35.68742781
H	82.70446931	31.80967381	32.35785520
H	87.70823247	27.88468024	33.05820065
H	78.82377120	24.18286708	37.05434977
H	78.88320879	25.88690095	37.50515127
H	78.21632458	25.41456031	35.94389390
H	80.32233064	22.66241660	36.81547250
H	82.06164216	22.68606837	37.11605354
H	77.65444314	29.18326047	34.36852097
H	78.17429308	30.05492002	35.80862782
H	77.76707028	30.94598323	34.34275839
H	80.46417871	32.95801660	33.16726903
H	84.48101088	33.08105093	32.21999944

H	86.23042861	33.01435004	32.00733520
H	85.16708412	32.47940602	30.70914900
H	88.05498386	31.73196449	32.68472997
H	88.77952029	24.26358991	33.59854353
H	89.00131200	25.95190727	34.06265920
H	88.57164080	25.54359650	32.40020312
H	85.72677734	22.24549954	33.94782087
H	87.42065701	22.64487072	34.26417569
Cl	83.30684799	24.26298874	31.43406724
O	82.84626621	27.15635244	32.54015599
O	81.72798043	24.63386715	31.19714998
H	83.71445236	29.24554404	41.56080669
H	82.51512999	29.18877341	40.25608614
H	81.45112007	22.22281307	35.52838014
H	79.99528782	32.03184768	31.74318960
H	78.84739158	32.25506463	33.07095256
H	88.60688810	30.05565052	32.60043449
H	88.01481999	30.86415410	31.14367153
H	86.24637830	22.66474482	35.58718586
H	84.84911628	30.74301971	37.95411468
H	79.15098390	27.96322886	28.88958097

Int1_{IV,21}

Energy with the small basis set:	-2626.247078
Solution energy with the small basis set:	-2626.247044
Energy with larger basis sets:	-2626.924673
Zero-point energy:	0.775159
Dispersion effect:	-0.178091669

C	83.56100000	29.40899998	40.48999995
C	84.40437337	28.39368561	39.69507799
C	84.32443349	28.57450957	38.21036091
N	84.80133637	29.69869828	37.55451494
C	83.80219558	27.79315481	37.21123130
C	84.55885646	29.55987849	36.22663167
N	83.95216262	28.41156982	35.98469597
C	78.74700005	28.42299994	29.79600009
C	79.57894484	28.07862154	31.04184273
N	79.86113102	26.64818352	31.21780594
C	79.00535644	25.76814898	31.72922993
N	77.71959142	26.11719161	31.96750492
N	79.41799720	24.53435282	32.04921724
Fe	83.31789155	27.67000741	33.99614182

C	83.67572772	24.38996565	34.96608452
C	80.14282881	27.67828012	35.24731399
C	82.85930025	30.84598361	32.81590018
C	86.64119776	27.83988212	33.26653420
N	82.16145058	26.31484807	34.97421844
C	82.46396712	24.99986496	35.25007928
C	81.33340642	24.34272957	35.91178902
C	80.35772339	25.29452865	36.02411632
C	80.88516422	26.51101703	35.41258178
C	78.99233385	25.17725791	36.63141707
C	81.28899999	22.90700013	36.36999993
N	81.80127213	29.02970389	34.05279240
C	80.55414600	28.81558659	34.56586929
C	79.66775428	29.92956013	34.23581246
C	80.39458109	30.80325260	33.47423902
C	81.75176095	30.23263533	33.39663090
C	78.23508065	30.02375675	34.67084618
C	79.89800003	32.07999994	32.83400002
N	84.55118565	29.10461248	33.24378753
C	84.16546249	30.34432726	32.80749040
C	85.33265878	31.09985659	32.36208790
C	86.43415945	30.30135070	32.53348560
C	85.91369214	29.01544250	33.05177388
C	85.33024607	32.49880879	31.81953800
C	87.85999996	30.75899997	32.22300003
N	84.85405456	26.35359737	34.08215087
C	86.14058068	26.59957481	33.69144644
C	86.93606209	25.36098456	33.78502961
C	86.09752180	24.37003563	34.22933529
C	84.79412008	25.02374566	34.41841921
C	88.39085734	25.27138774	33.43535377
C	86.39099996	22.89700005	34.52599999
H	85.45180262	28.45035615	40.02200775
H	84.07045546	27.37658175	39.92473696
H	83.32954296	26.82805395	37.29607094
H	84.83637445	30.29560127	35.48905781
H	83.89156988	30.43840261	40.31192917
H	78.61426409	29.50741926	29.73659772
H	77.74973584	27.96833899	29.80132601
H	79.09874925	28.45939809	31.94956251
H	80.55470080	28.56458197	30.98903112
H	80.82803758	26.31289042	31.10798750
H	77.07771246	25.45546180	32.37175880
H	77.33906537	26.96999416	31.59409233

H	80.40088303	24.28623435	31.82808995
H	78.74008971	23.79860140	32.17197869
H	83.77579932	23.33956523	35.21608522
H	79.13040166	27.67481297	35.63521643
H	82.70252138	31.82215162	32.37134242
H	87.70119890	27.87844711	33.03913122
H	78.81634718	24.17849037	37.03737644
H	78.85305772	25.89269754	37.45023477
H	78.20427945	25.37632828	35.89452072
H	80.33366559	22.67185194	36.84392935
H	82.08077256	22.69030276	37.09688968
H	77.66430158	29.12905462	34.39304852
H	78.15344964	30.12597131	35.75996856
H	77.73332252	30.88629768	34.22626456
H	80.32597582	32.96976899	33.31208500
H	84.38529969	33.01809127	31.99507106
H	86.12335025	33.10083699	32.27734927
H	85.51233235	32.50560065	30.73736124
H	88.08385652	31.68909901	32.75625975
H	88.77604274	24.26056464	33.58805876
H	88.99625089	25.94991871	34.04868965
H	88.56923024	25.53770512	32.38651278
H	85.72860224	22.23908297	33.95301875
H	87.42142720	22.64566724	34.26648164
Cl	83.43071096	24.32767082	31.41455681
O	82.82983648	27.17748049	32.52733551
O	81.87413697	24.69543869	31.05653971
H	83.64281741	29.21878910	41.56435468
H	82.50535540	29.34461494	40.20977176
H	81.42478123	22.21290380	35.53167623
H	80.16699660	32.12486480	31.77293283
H	78.81196779	32.15698469	32.90880408
H	88.60675884	30.01689280	32.51670743
H	87.98286109	30.95293739	31.15175277
H	86.24647459	22.67344496	35.58906060
H	85.26095029	30.48702276	37.98626018
H	79.25162067	28.08931338	28.88481133

React_{IV}

Energy with the small basis set:	-2626.246978
Solution energy with the small basis set:	-2626.247025
Energy with larger basis sets:	-2626.93359
Zero-point energy:	0.776997
Dispersion effect:	-0.174537618

C	83.56100000	29.40899998	40.48999996
C	84.33025896	28.29692659	39.75510321
C	84.32678305	28.46981102	38.26935942
N	84.99437195	29.49947001	37.62417572
C	83.69515466	27.78696538	37.26183920
C	84.75106246	29.40210982	36.29252475
N	83.96467197	28.37219717	36.04075943
C	78.74700004	28.42299994	29.79600007
C	79.15304251	27.82392731	31.14329450
N	79.54133899	26.41631614	31.06026250
C	78.78430645	25.36806375	31.34566533
N	77.44151793	25.47730486	31.46382029
N	79.37559694	24.18058594	31.56769301
Fe	83.32197762	27.63856050	33.94176553
C	83.68824646	24.35984591	34.93319698
C	80.10418956	27.60565193	35.08491031
C	82.86537453	30.83774888	32.78332353
C	86.64539295	27.81278271	33.20230905
N	82.14121353	26.25715724	34.84617920
C	82.45952919	24.95803338	35.18129686
C	81.33652530	24.31926557	35.85323423
C	80.34203231	25.26265771	35.92115630
C	80.85104318	26.45462242	35.27611235
C	78.97319971	25.14120652	36.52116061
C	81.28899999	22.90700009	36.36999995
N	81.77710703	28.95632921	33.89856133
C	80.52215024	28.74430927	34.40900293
C	79.65722038	29.86508645	34.11430843
C	80.40095306	30.76854746	33.39370626
C	81.74465879	30.20021658	33.30090952
C	78.22462379	29.97843441	34.54513154
C	79.89800002	32.07999997	32.83400001
N	84.55221258	29.07992495	33.19161124
C	84.17127798	30.33946191	32.78890359
C	85.33517068	31.09469308	32.37755281
C	86.43891691	30.28232055	32.52650583

C	85.92197782	28.99554188	33.00614343
C	85.35574840	32.50974664	31.87924469
C	87.85999997	30.75899998	32.22300002
N	84.84262867	26.31722373	33.99161561
C	86.14600563	26.57323545	33.61922278
C	86.93705355	25.35298752	33.74931791
C	86.09725799	24.36333523	34.21794171
C	84.79935313	24.99604124	34.38686737
C	88.39505573	25.25106622	33.41160745
C	86.39099997	22.89700004	34.52599999
H	85.36274738	28.24990678	40.12721010
H	83.88142087	27.32430421	39.98149687
H	83.06665360	26.91347594	37.33725888
H	85.15953138	30.07819280	35.55822072
H	84.00386455	30.39458795	40.30845589
H	78.49992004	29.48210997	29.91788328
H	77.87388604	27.91981135	29.36487856
H	78.34861464	27.92320654	31.88009747
H	80.01903053	28.35282846	31.54731986
H	80.52801638	26.17451521	30.86544941
H	76.89395240	24.70244330	31.80113684
H	76.95454585	26.27287270	31.08557604
H	80.40692326	24.17702607	31.47976549
H	78.86646321	23.33060877	31.37742061
H	83.80484547	23.32251425	35.22471422
H	79.09236492	27.60521046	35.47174976
H	82.71871542	31.83297902	32.38007832
H	87.70757134	27.85357078	32.98548221
H	78.82125890	24.16401071	36.98467244
H	78.80457027	25.89964347	37.29408892
H	78.18892514	25.27052882	35.76553161
H	80.34524704	22.70305712	36.87966851
H	82.09829424	22.70863662	37.08266357
H	77.67791481	29.03897268	34.40794268
H	78.14374919	30.24343153	35.60684511
H	77.69663751	30.75134089	33.98114134
H	80.12009088	32.92070046	33.50303297
H	84.37181294	32.98256891	31.90285254
H	86.03108494	33.13150069	32.47933639
H	85.71795957	32.55733654	30.84520483
H	88.12271420	31.60891571	32.86260096
H	88.77537108	24.24274295	33.59064183
H	88.99841243	25.94050751	34.01431983
H	88.58339354	25.49200277	32.35858859

H	85.73966947	22.23452125	33.94561696
H	87.42548146	22.64480959	34.28333452
Cl	83.15277284	25.67179839	31.32886731
O	82.74785928	27.11447544	31.98452729
O	81.84285975	24.94813692	30.73425383
H	83.57124019	29.23759367	41.57079165
H	82.51893496	29.44583909	40.15872478
H	81.39162619	22.17603470	35.55847618
H	80.35566625	32.30612126	31.86581977
H	78.81518087	32.05245831	32.69234394
H	88.60552725	29.97606641	32.38377154
H	87.94065854	31.09151473	31.18242822
H	86.23242618	22.67517418	35.58730235
H	85.57204265	30.19967188	38.06621626
H	79.56517213	28.34571016	29.07415414

TS1_{IV,41}

Energy with the small basis set:	-2626.212532
Solution energy with the small basis set:	-2626.212753
Energy with larger basis sets:	-2626.89373
Zero-point energy:	0.775994
Dispersion effect:	-0.175620931
Imaginary frequency:	-407 cm ⁻¹

C	4.38916900	0.41708100	5.35565600
C	4.45823800	-0.35061400	4.02143400
C	3.50773500	0.13948200	2.97024500
N	3.45352500	1.46247600	2.55602100
C	2.56739400	-0.50025900	2.20232100
C	2.51680500	1.57974000	1.58636400
N	1.96169900	0.40337600	1.34781100
C	-5.61812400	1.66523700	-0.71102600
C	-4.55362400	0.60858900	-0.39442200
N	-4.17484600	-0.20725200	-1.55156700
C	-4.79714600	-1.30630100	-1.97097700
N	-5.98608700	-1.67654000	-1.44650400
N	-4.22848100	-2.05907200	-2.92062400
Fe	0.39494900	0.06737800	-0.03581500
C	0.88049000	-3.33377300	-0.00602200
C	-1.63295000	-0.22587600	2.73463800
C	-0.28183800	3.42382300	-0.16659600
C	2.78172700	0.42629100	-2.47124500

N	-0.19544200	-1.50151100	1.21319800
C	0.07621700	-2.82462700	1.02192200
C	-0.59083000	-3.60877900	2.05364600
C	-1.27346200	-2.72340200	2.84783300
C	-1.03290700	-1.40305400	2.28857800
C	-2.11997900	-3.00102200	4.05344800
C	-0.51195600	-5.09092600	2.18497400
N	-0.75212900	1.38275700	1.09896700
C	-1.54502900	1.04248100	2.15735800
C	-2.33010600	2.19564500	2.56894600
C	-2.00122800	3.22340400	1.72040700
C	-0.98381400	2.70027800	0.80531500
C	-3.29454400	2.19572700	3.71758700
C	-2.56682500	4.61206000	1.72489100
N	1.17989700	1.67748200	-1.11556400
C	0.73857200	2.96795900	-1.01848700
C	1.52924500	3.81095100	-1.90254400
C	2.45115500	3.00284600	-2.52857600
C	2.18860300	1.63272000	-2.04444600
C	1.32708500	5.28909600	-2.05888900
C	3.50851500	3.48320400	-3.50270300
N	1.57684800	-1.23920600	-1.09188600
C	2.47973900	-0.89302900	-2.07188100
C	3.04630700	-2.12244300	-2.63704200
C	2.47453900	-3.19259100	-1.97629300
C	1.57900000	-2.61331900	-0.98013300
C	4.05391100	-2.14923000	-3.74750600
C	2.67222100	-4.69286700	-2.18920100
H	5.48556000	-0.31125500	3.63389400
H	4.24119600	-1.40946500	4.19285900
H	2.28667000	-1.54073900	2.20676200
H	2.26727900	2.50557900	1.09469100
H	4.65421400	1.47332900	5.23414500
H	-5.83206700	2.25538600	0.18482300
H	-6.55752500	1.21992500	-1.05522300
H	-4.88042300	-0.05533300	0.41537300
H	-3.63448200	1.08248500	-0.04404400
H	-3.30799400	0.01749400	-2.04311200
H	-6.33008400	-2.61188900	-1.59303100
H	-6.41750700	-1.13471100	-0.71652000
H	-3.34659400	-1.69253700	-3.33087000
H	-4.78820400	-2.71965900	-3.43691100
H	0.99943400	-4.41197600	-0.03412300
H	-2.29015400	-0.31769600	3.59308700

H	-0.53326600	4.47636600	-0.25066100
H	3.54279400	0.51953900	-3.24016400
H	-2.12803200	-4.06423200	4.30347400
H	-1.75518000	-2.46070600	4.93473900
H	-3.16154900	-2.69444100	3.89760100
H	-1.10122400	-5.45323400	3.03025900
H	0.51934800	-5.43188300	2.33748900
H	-4.06592900	1.42495200	3.60220000
H	-2.78496100	1.99642000	4.66780900
H	-3.80382800	3.15635400	3.81914500
H	-1.80718200	5.36155500	1.97957500
H	1.35439000	5.80770100	-1.09366100
H	2.09231200	5.73846800	-2.69453500
H	0.35554200	5.51195900	-2.51658100
H	3.68680600	4.55361900	-3.38674900
H	4.35665000	-3.17058700	-3.98857100
H	4.96019300	-1.59309100	-3.48082200
H	3.65726000	-1.69829100	-4.66479800
H	1.72949000	-5.17600600	-2.46750700
H	3.39542300	-4.88624400	-2.98394000
Cl	-0.69837900	-0.89592400	-2.89967900
O	-0.97519100	-0.07600000	-1.02042500
O	-2.09543100	-0.52585300	-3.59638500
H	5.09148400	-0.01132200	6.07577500
H	3.38479000	0.37053400	5.78659300
H	-0.88419100	-5.59951100	1.28718500
H	-2.96794700	4.88967700	0.74306100
H	-3.37571200	4.71151100	2.45137200
H	4.46243300	2.96876100	-3.34573900
H	3.21345600	3.30622900	-4.54426700
H	3.03906300	-5.17811800	-1.27822600
H	4.01560400	2.21932600	2.91629900
H	-5.26730700	2.34487600	-1.49236300

Int1_{IV,41}

Energy with the small basis set:	-2626.224388
Solution energy with the small basis set:	-2626.224408
Energy with larger basis sets:	-2626.906635
Zero-point energy:	0.773791
Dispersion effect:	-0.176564462

C	83.56100000	29.40899998	40.48999995
C	84.47967796	28.44084519	39.72114692

C	84.39948202	28.60734310	38.23586934
N	84.86235942	29.73379041	37.57420014
C	83.86626206	27.82353237	37.24521699
C	84.60299262	29.59553085	36.25044163
N	83.99679846	28.44453516	36.01828571
C	78.74700001	28.42299994	29.79600008
C	79.52749654	28.09906707	31.07946466
N	79.71433598	26.66581054	31.32868660
C	78.80102531	25.86392916	31.86221031
N	77.54382584	26.30846570	32.10064104
N	79.13304893	24.61334156	32.21967248
Fe	83.30922305	27.70193938	34.04096833
C	83.69110136	24.42585401	35.05731901
C	80.11179388	27.69184157	35.29911952
C	82.86263752	30.90114035	32.92716798
C	86.64064610	27.85292388	33.25648135
N	82.14564492	26.33216463	35.10286181
C	82.46510532	25.02191577	35.34874244
C	81.31794839	24.34655969	35.96138988
C	80.32210405	25.27981198	36.05815705
C	80.85421024	26.51769329	35.48726095
C	78.93716834	25.12338877	36.60770176
C	81.28900000	22.90700019	36.36999990
N	81.77138985	29.10593479	34.17731384
C	80.51411735	28.85466408	34.64144562
C	79.62268644	29.95549767	34.26710492
C	80.37008469	30.83423805	33.52911009
C	81.73937743	30.29081154	33.50260380
C	78.17034190	30.03098476	34.63431999
C	79.89800007	32.07999987	32.83400003
N	84.57495978	29.16778780	33.28088530
C	84.17778517	30.40996732	32.87557739
C	85.34639316	31.15900306	32.41345394
C	86.43864607	30.33828216	32.54702428
C	85.92260130	29.04966924	33.06135143
C	85.34822387	32.56724001	31.89697957
C	87.85999996	30.75899997	32.22300003
N	84.89874200	26.35668066	34.14628633
C	86.16432261	26.60310487	33.70376069
C	86.94939912	25.34985801	33.77190036
C	86.11358071	24.37030638	34.24957574
C	84.82162384	25.03646055	34.48720778
C	88.38685310	25.23811769	33.36407756
C	86.39099996	22.89700006	34.52600000

H	85.51743711	28.56982337	40.05748588
H	84.20967169	27.40682988	39.95871170
H	83.39671707	26.85771058	37.33496914
H	84.86802023	30.33190852	35.50949766
H	83.82083845	30.45502107	40.29308027
H	78.68015112	29.50807904	29.67158590
H	77.72491695	28.02708539	29.80118596
H	79.05073679	28.55372026	31.95482334
H	80.53280943	28.52156041	31.02783806
H	80.64638870	26.23862247	31.19256570
H	76.85817925	25.69411478	32.50853275
H	77.21100267	27.15587433	31.67232191
H	80.09749827	24.30398319	31.99570593
H	78.40885226	23.91938717	32.32251072
H	83.78570092	23.37296388	35.29940300
H	79.08414951	27.66673564	35.64530168
H	82.70015791	31.87983694	32.48778879
H	87.69236371	27.88571100	32.98993336
H	78.78173838	24.12896724	37.03275218
H	78.73307879	25.85412305	37.39876728
H	78.17770210	25.27147170	35.82964040
H	80.33590070	22.63790811	36.83133997
H	82.08036834	22.67420382	37.09275411
H	77.62505385	29.13104168	34.32299792
H	78.03596954	30.12260056	35.71914513
H	77.67985642	30.89132290	34.17285722
H	80.35536133	32.98371458	33.25587727
H	84.44038425	33.11241065	32.16736544
H	86.19948014	33.13243487	32.29242890
H	85.43201703	32.59149577	30.80292526
H	88.10549609	31.70081950	32.72579667
H	88.76686342	24.22413802	33.50891158
H	89.02438818	25.91520695	33.94578674
H	88.52421751	25.49451562	32.30652532
H	85.71258713	22.25374219	33.95453152
H	87.41427598	22.63092366	34.25236229
Cl	83.15544154	24.33573067	31.50625984
O	82.78692251	27.20854557	32.58655097
O	81.57555277	24.65756059	31.17428565
H	83.64487686	29.24581663	41.56873954
H	82.51542522	29.26530947	40.20166749
H	81.43817301	22.24279886	35.50956927
H	80.15513464	32.06107466	31.76866305
H	78.81488691	32.19509909	32.91363902

H	88.59369318	30.01295111	32.53936372
H	87.99138643	30.91860733	31.14656667
H	86.25561725	22.66216282	35.58801667
H	85.32625380	30.52289316	38.00012205
H	79.25237376	28.00915194	28.91872300

React_{VI}

Energy with the small basis set:	-2626.23897
Solution energy with the small basis set:	-2626.238987
Energy with larger basis sets:	-2626.9315
Zero-point energy:	0.776136
Dispersion effect:	-0.177378573

C	83.56100000	29.40899997	40.48999995
C	84.42427471	28.37615771	39.74348705
C	84.37613070	28.54371957	38.25792179
N	84.93097115	29.63097017	37.59982628
C	83.78829020	27.80453316	37.26419433
C	84.67040673	29.51253409	36.27440934
N	83.97672194	28.41354748	36.03941569
C	78.74700008	28.42299993	29.79600008
C	79.31990821	28.02030830	31.15363783
N	79.51921473	26.57694551	31.29124421
C	78.71810557	25.72773116	31.91686312
N	77.43633580	26.04969146	32.20363563
N	79.20694044	24.53788247	32.30311849
Fe	83.32072575	27.66819268	33.98263614
C	83.69749308	24.38659165	35.00246348
C	80.08308059	27.62656148	35.15109935
C	82.85792366	30.86941855	32.84719124
C	86.65209249	27.83066503	33.22463951
N	82.11898738	26.26766883	34.94106051
C	82.45283333	24.97233967	35.25164275
C	81.31876838	24.32036450	35.88830299
C	80.31119907	25.25163408	35.95674251
C	80.82332235	26.46217346	35.34634818
C	78.93388094	25.09834045	36.52800574
C	81.28899999	22.90700009	36.36999996
N	81.74295781	29.01264725	33.98732559
C	80.48995684	28.78597198	34.48896028
C	79.62445497	29.90591272	34.17928169
C	80.37764646	30.80127831	33.45474370
C	81.72524542	30.24364777	33.37705986

C	78.18405081	30.00952642	34.58788404
C	79.89800001	32.07999999	32.83400001
N	84.56819789	29.12411380	33.20167408
C	84.17593622	30.38158777	32.81339823
C	85.34054390	31.13041624	32.38682847
C	86.44185820	30.30804481	32.52873423
C	85.93207868	29.02404134	33.01630407
C	85.36438332	32.54699645	31.89470903
C	87.85999995	30.75899997	32.22300002
N	84.88563963	26.31798906	34.05737228
C	86.17746445	26.57979406	33.66321111
C	86.96454180	25.35243901	33.78160051
C	86.12026339	24.36672285	34.25741635
C	84.82739585	25.00412406	34.45155431
C	88.41557602	25.23558625	33.42130206
C	86.39099997	22.89700005	34.52599998
H	85.46288613	28.43427875	40.09616203
H	84.07925483	27.36434014	39.97944654
H	83.24448958	26.87713205	37.34899103
H	84.99851458	30.22208069	35.53182585
H	83.89918953	30.43318288	40.29752476
H	78.64932206	29.51152128	29.73955492
H	77.75731641	27.98630649	29.61882361
H	78.68349220	28.36718819	31.97308726
H	80.30179607	28.47529281	31.30856118
H	80.43747304	26.17453381	31.04502056
H	76.87430052	25.44652204	32.78167028
H	76.98222923	26.81708488	31.73636916
H	80.20954663	24.38051282	32.11411619
H	78.58994610	23.74805182	32.41250703
H	83.80806911	23.34671850	35.28986582
H	79.06491966	27.61686393	35.52428394
H	82.70671677	31.86714563	32.44824631
H	87.71197859	27.87354931	32.99377117
H	78.76144617	24.08754072	36.90484350
H	78.76346917	25.79115295	37.36023615
H	78.16263209	25.30620041	35.77613316
H	80.30109203	22.62766869	36.74343219
H	82.00343485	22.74263867	37.18578544
H	77.61187098	29.11837059	34.30101803
H	78.08264625	30.11330305	35.67518169
H	77.69446770	30.87442628	34.13427117
H	80.32869996	32.96089785	33.32591226
H	84.36372411	32.94332644	31.70772643

H	85.85160424	33.21578064	32.61589716
H	85.92869312	32.62717897	30.95897679
H	88.14146765	31.60736105	32.85716811
H	88.79975964	24.23404485	33.62861983
H	89.02948542	25.94623790	33.98753156
H	88.58482336	25.43969196	32.35708506
H	85.77871296	22.26177584	33.87641150
H	87.43831650	22.64490867	34.34493871
Cl	83.03351231	25.56928995	31.54342001
O	82.73379712	27.08571521	32.09521418
O	81.66396717	24.84938502	31.12025249
H	83.60833308	29.24402033	41.57076409
H	82.51463552	29.33970424	40.17820917
H	81.55067027	22.20035595	35.57290417
H	80.17558211	32.13875508	31.77570540
H	78.81221271	32.17083305	32.89907630
H	88.59322197	29.96494144	32.38587390
H	87.94933255	31.08692079	31.18105613
H	86.15960696	22.63096762	35.56345296
H	85.45011458	30.38229608	38.03038494
H	79.40243657	28.09872553	28.98238486

TS1_{VI,41}

Energy with the small basis set:	-2626.214773
Solution energy with the small basis set:	-2626.21496
Energy with larger basis sets:	-2626.896512
Zero-point energy:	0.773349
Dispersion effect:	-0.168020122

C	6.30054500	-2.25092600	2.77688000
C	5.99790800	-1.38589600	1.54050700
C	4.61323300	-0.81677600	1.52139700
N	4.12501500	0.02034800	2.51218400
C	3.56892700	-0.94574400	0.63942600
C	2.84531400	0.35434300	2.19771300
N	2.47706400	-0.21527900	1.06641200
C	-5.23426700	-2.20676000	0.44137500
C	-4.39092200	-1.59960900	-0.68546700
N	-4.72450500	-0.20517200	-0.97427800
C	-5.62525200	0.22344400	-1.85219300
N	-6.54228600	-0.61192300	-2.39471900
N	-5.61227100	1.51551600	-2.20341300
Fe	0.34184400	0.05636100	-0.05221200

C	1.96013200	-0.41034500	-3.03666700
C	0.02620500	-3.36017300	0.28423000
C	-1.05764400	0.47902600	3.03276200
C	1.28576300	3.39486300	-0.07161500
N	0.91858500	-1.60210200	-1.16807100
C	1.54023900	-1.58370600	-2.37174500
C	1.71456100	-2.95296600	-2.85862200
C	1.17680700	-3.78342200	-1.91279500
C	0.67371500	-2.92402300	-0.85671800
C	1.09524200	-5.27963800	-1.90516200
C	2.37250400	-3.34004300	-4.13663700
N	-0.38404700	-1.22671900	1.40743900
C	-0.49765700	-2.56852100	1.32501300
C	-1.26311900	-3.08682800	2.44921200
C	-1.61526400	-2.00354400	3.20671400
C	-1.03416000	-0.82555800	2.56057700
C	-1.57084900	-4.53626300	2.67069400
C	-2.43530100	-2.01110500	4.44829400
N	0.18498900	1.69725100	1.29040700
C	-0.45412000	1.64716300	2.47545300
C	-0.41115100	2.95449900	3.12385400
C	0.28069900	3.79998000	2.28675000
C	0.63920600	2.98746600	1.10050600
C	-1.01978700	3.25133500	4.46201600
C	0.61391000	5.25049900	2.58195600
N	1.44585500	1.28901300	-1.34920300
C	1.62819800	2.62522900	-1.22917700
C	2.23025700	3.14846100	-2.46494800
C	2.39506000	2.07619600	-3.31535500
C	1.91134500	0.90784800	-2.58251700
C	2.56873400	4.58927300	-2.70359300
C	2.93228000	2.02316400	-4.73120200
H	6.73533500	-0.57404000	1.47402500
H	6.12362000	-1.98313100	0.63191400
H	3.53879100	-1.51673800	-0.27561000
H	2.23537400	1.00241200	2.80721100
H	6.22532300	-1.67399200	3.70523700
H	-4.92503000	-3.23999300	0.62626900
H	-6.30269500	-2.21131000	0.20062600
H	-4.48495700	-2.18831900	-1.60686300
H	-3.32929500	-1.60006600	-0.42547800
H	-4.13486300	0.55352100	-0.58974900
H	-7.00735400	-0.34839900	-3.24885200
H	-6.54011900	-1.59016400	-2.15776000

H	-4.87832300	2.08998500	-1.73423800
H	-6.43367300	1.93930300	-2.60521500
H	2.40000600	-0.55910700	-4.01809200
H	-0.11215100	-4.43174400	0.38177100
H	-1.57946800	0.63113200	3.97288600
H	1.55496200	4.44644100	-0.12231700
H	1.53598800	-5.71200800	-2.80557600
H	1.62276400	-5.70741600	-1.04461900
H	0.05612300	-5.62534900	-1.85239700
H	2.38065700	-4.42304900	-4.27388200
H	3.41398200	-2.99793700	-4.17757400
H	-2.10705700	-4.97169300	1.81904500
H	-0.65471300	-5.12355400	2.80658100
H	-2.18763600	-4.68868700	3.55867300
H	-1.86292100	-1.67054000	5.32046800
H	-0.55578100	2.65814200	5.25934800
H	-0.90753200	4.30230400	4.73443500
H	-2.09226800	3.02443400	4.47233300
H	-0.01541600	5.64042800	3.38317700
H	2.99920200	4.73868000	-3.69629200
H	3.29768000	4.95953900	-1.97265400
H	1.68228800	5.23026700	-2.63018700
H	2.17488500	1.64328700	-5.42551500
H	3.23540300	3.01276700	-5.07989500
Cl	-2.13709600	2.03837400	-1.40753800
O	-1.26048800	0.22858600	-0.82685500
O	-3.56305200	2.28089600	-0.62890300
H	7.31641200	-2.65286500	2.72493400
H	5.60308300	-3.09061900	2.84898400
H	1.86186900	-2.90553000	-5.00501700
H	-3.30497400	-1.34835400	4.36407900
H	-2.80749000	-3.01135400	4.67751200
H	1.66019300	5.36553200	2.88973000
H	0.46332700	5.88631100	1.70300100
H	3.80650800	1.36626200	-4.80248400
H	4.63118700	0.33105200	3.32810100
H	-5.10470700	-1.64020800	1.36747500

Int1_{VI,41}

Energy with the small basis set:	-2626.223782
Solution energy with the small basis set:	-2626.223798
Energy with larger basis sets:	-2626.905801
Zero-point energy:	0.772347
Dispersion effect:	-0.177531321

C	83.56100000	29.40899997	40.48999995
C	84.44527521	28.40867202	39.72213042
C	84.37948443	28.58062151	38.23660391
N	84.87903941	29.69326405	37.57797144
C	83.82907852	27.81327334	37.24250884
C	84.62342100	29.56212446	36.25259554
N	83.98506935	28.42989487	36.01621477
C	78.74700005	28.42299994	29.79600007
C	79.58517105	28.10932672	31.04228454
N	79.68507187	26.67904211	31.35326765
C	78.77709073	25.98494091	32.02661242
N	77.56355996	26.51610422	32.30633238
N	79.07116597	24.75474832	32.47600971
Fe	83.30200387	27.69317131	34.02670889
C	83.69267307	24.42887543	35.06303499
C	80.10628308	27.68682731	35.29358708
C	82.85932206	30.89220325	32.91602614
C	86.64157456	27.85152614	33.25733961
N	82.13757154	26.32715598	35.09235703
C	82.45902396	25.02310888	35.34530050
C	81.31390945	24.34585393	35.95897407
C	80.31518667	25.27702285	36.05383358
C	80.84345253	26.51440784	35.47993895
C	78.92957803	25.11791162	36.60156114
C	81.28900000	22.90700012	36.36999994
N	81.76728976	29.09495291	34.16423791
C	80.51484945	28.85005087	34.63181742
C	79.62505135	29.95276576	34.26106936
C	80.37128570	30.83011455	33.51971160
C	81.73838856	30.28561073	33.48879248
C	78.17521151	30.03101942	34.63498032
C	79.89800004	32.07999994	32.83400002
N	84.57386418	29.16302576	33.27871422
C	84.17864629	30.39905917	32.86742508
C	85.34507040	31.14544393	32.39658673
C	86.43947117	30.32866915	32.53721590

C	85.92657488	29.04370383	33.05906720
C	85.35217372	32.55478955	31.88456950
C	87.85999994	30.75899997	32.22300003
N	84.89829039	26.35537555	34.14639734
C	86.16160237	26.59860866	33.70535349
C	86.94735320	25.34809841	33.77359396
C	86.11299046	24.36956050	34.25585514
C	84.82031600	25.03395767	34.49449382
C	88.38439824	25.23621773	33.36331280
C	86.39099997	22.89700005	34.52599999
H	85.48551969	28.49541239	40.06427728
H	84.13383614	27.38519533	39.95476659
H	83.33088770	26.86183820	37.32993141
H	84.91395258	30.29008166	35.51283766
H	83.86441656	30.44481875	40.30169410
H	78.74633504	29.50233744	29.61577234
H	77.70220428	28.10408099	29.88971464
H	79.19535610	28.63500198	31.92037210
H	80.61173328	28.45638133	30.90859390
H	80.56901769	26.17558161	31.16979045
H	76.90026789	26.00412891	32.86450608
H	77.23545172	27.33349417	31.81980924
H	80.00878675	24.38385521	32.24835185
H	78.32532014	24.10629102	32.67522944
H	83.78765111	23.37744230	35.31243526
H	79.07928848	27.66909593	35.64333459
H	82.69957845	31.87113832	32.47629480
H	87.69451660	27.88275878	32.99554825
H	78.76684752	24.11507175	37.00356898
H	78.72717617	25.83220332	37.40856818
H	78.17212103	25.28874076	35.82592660
H	80.31707928	22.62142516	36.77942218
H	82.04335552	22.69041683	37.13635487
H	77.62563969	29.14073844	34.30520737
H	78.04500393	30.09928571	35.72193717
H	77.68854727	30.90411422	34.19416722
H	80.32896703	32.98131719	33.28692378
H	84.35081405	32.91512438	31.63699873
H	85.77593915	33.25006387	32.62075919
H	85.96391875	32.63902705	30.98015707
H	88.16212999	31.59468096	32.86447133
H	88.76716326	24.22459398	33.51724724
H	89.02183006	25.91978327	33.93746599
H	88.51949175	25.48263439	32.30308163

H	85.73402362	22.25541474	33.92787608
H	87.42378237	22.63924730	34.28166554
Cl	83.05598973	24.32252299	31.48597369
O	82.80043691	27.19573257	32.56473675
O	81.44825059	24.57432563	31.25795846
H	83.63043719	29.23640943	41.56831855
H	82.51258117	29.30952186	40.19364771
H	81.49729016	22.24336920	35.52178604
H	80.18229861	32.08808837	31.77522262
H	78.81149638	32.17716326	32.88765840
H	88.58132613	29.95104788	32.36999434
H	87.94614046	31.09705501	31.18408314
H	86.22417154	22.65028972	35.58078538
H	85.36232244	30.46912857	38.00659613
H	79.16017352	27.92942775	28.91167033