Ab Initio Calculations for Spin-Gaps of Non-Heme Iron Complexes

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Supporting Information Available

Computational Methodology

Here we describe the computational methodology used in this study.

The structures **1-10** were optimized using BP86-D3BJ/def2-TZVP, whereas structures **11** and **12** were taken from previous studies.[1,2] Using these optimized structures, we performed a series of single-point DFT calculations employing different functionals (BP86, B3LYP, TPSS, TPSSh, PBE0, M06, MN15, S12g, B97-D, OPBE and OLYP)[3–15] and the def2-TZVP basis set on all atoms.[16,17] The D3BJ dispersion correction[18,19] has been used in all DFT calculations.

The "reference" data were obtained with our recently proposed CASPT2/CC approach.[20,21] In this approach, dynamical correlation of valence electrons was described by CASPT2, whereas correlation of iron semi-core electrons (3s and 3p) was calculated with CCSD(T) with small basis set (cc-pwCVTZ-DK on Fe and minao on all other atoms). In the CASPT2 calculations, we used an extensive basis set, denoted as awC5Z/aTZ: aug-cc-pwCV5Z-DK for Fe, cc-pVTZ-DK for H, and aug-cc-pVTZ-DK for other ligand atoms.

In all CASSCF calculations, we used "standard" active spaces employed in a previous work.[1,21] The active spaces consist of one σ orbital describing the bonds between Fe and the equatorial coordinating ligand atoms, five Fe 3d, and three O 2p orbitals. To describe the 'double-shell' effect, three O 2p$'$ as well as three(four) Fe 3d$'$ were also included for the triplet(quintet) state. The resulting active spaces consist of 15 and 16 active orbitals for the triplet and quintet states, respectively. In **9**, we added one more sulfur 3p$_z$ orbital since it strongly mixes with σ_{z^2}. The active spaces and the natural orbital occupation numbers (NOONs) can be found in the Table S2.

Two different versions of local coupled cluster have been used: local coupled cluster with singles, doubles and non-iterative triples LUCCSD(T0),[22–25] as implemented in Molpro program package, and domain-based pair natural orbitals DLPNO-CCSD(T)[26–30] as imple-

mented in ORCA. In all local coupled cluster calculations, augmented triple zeta basis sets were used for Fe=O (aug-cc-pwCVTZ[31,32] for Fe and aug-cc-pVTZ-DK[33] for O) and augmented double zeta[33] for all other atoms, except for H where a double zeta basis set without augmented functions was used. Density fitting approximations were used throughout in LUCCSD(T0). In the case of Coulomb and exchange fitting, the aug-cc-pVTZ/JKFIT[34] auxiliary basis set was used for all atoms except Fe where the def2-QZVP/JKFIT basis set[35] was applied. For the correlation fitting, the aug-cc-pVTZ/MP2FIT[36] basis set was used for all atoms except for Fe in which case the aug-cc-pwCVTZ/MP2FIT[37] was applied. In the DLPNO-CCSD(T) calculations, the RIJCOSX approximation[38,39] was used. The RI-J auxiliary basis was automatically constructed from the orbitals basis set using the AutoAux keyword.[40] For the correlation fitting, the same basis set as in the case of the LUCCSD(T0) calculations was used.

All CASPT2 calculations have been performed using Molcas.[41] The ORCA program package[42] was used in the case of UKS-UCCSD(T) and DLPNO-CCSD(T) calculations. Molpro 2019[43] was used for LUCCSD(T0) and LUCCSD(T0)-*hotspot* calculations and CCSD(T) calculations for 3s3p correction. Most of the DFT (BP86, B3LYP, TPSS, TPSSh, PBE0, M06, MN15, S12g, B97-D) calculations have been carried out using TURBOMOLE V8.0 software,[44] while some of the DFT (OPBE, OLYP and MN15) calculations were performed using Gaussian 16.[45]

CASPT2/CC Results

Table S1: CASPT2 spin gap $\Delta E_{\mathrm{gas}}(E_{\mathrm{quintet}} - E_{\mathrm{triplet}})$ and the 3s3p, ZPE, thermal, and COSMO (acetonitrile) corrections to it. All values in kcal/mol.

	CASPT2	+3s3p(CC)[a]	+ZPE[b]	+thermal[b]	+COSMO[c]	ΔG°
1	7.8	2.5	–1.7	–1.3	1.0	8.3
2	5.7	2.5	–1.5	–1.2	1.8	7.3
3	4.0	2.6	–2.1	–1.4	2.2	5.4
4	9.8	2.2	–0.9	–1.3	–0.5	9.3
5_{ax}	8.4	2.1	–0.7	–1.5	2.3	10.6
5_{eq}	6.9	2.3	–1.0	–2.4	2.4	8.2
6_{ax}	1.8	2.1	–1.2	–1.1	2.8	4.5
6_{eq}	3.5	2.1	–1.3	–1.2	1.2	4.2
7	27.9	1.7	–2.0	–2.5	0.5	25.6
8	14.9	2.2	–0.8	–0.5	–2.4	13.4

[a]Calculated using UCCSD(T)/ROHF with small basis set. [b]Taken from the calculations at BP86-D3BJ/def2-TZVP level of theory. [c]Solvation correction obtained from BP86-D3BJ/def2-TZVP calculations with acetonitrile.

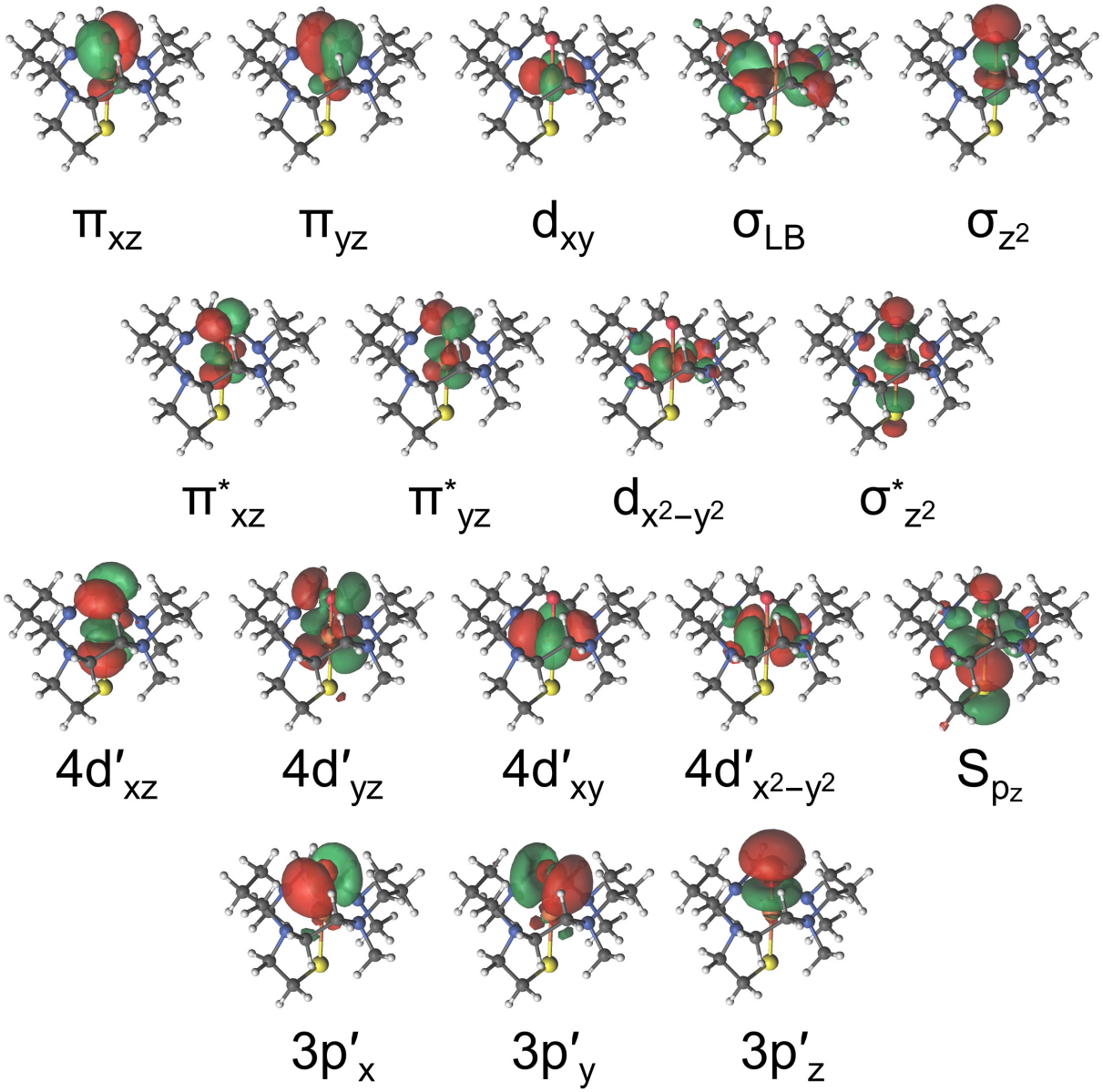

Figure S1: Active space used in CASPT2/CC calculations on the example of complex **9** in the quintet state.

Table S2: Occupation Numbers of Some Important Natural Orbitals

Complex	π_{xz}	π_{yz}	σ_{z^2}	d_{xy}	π^*_{xz}	π^*_{yz}	$\mathrm{d}_{x^2-y^2}$	$\sigma^*_{z^2}$
^{3}1	1.91	1.91	1.88	1.96	1.07	1.07	0.05	0.12
^{5}1	1.92	1.92	1.82	1.00	1.05	1.06	1.00	0.18
^{3}2	1.91	1.91	1.88	1.96	1.07	1.06	0.06	0.13
^{5}2	1.92	1.93	1.81	1.00	1.06	1.05	1.00	0.19
^{3}3	1.90	1.90	1.88	1.96	1.07	1.07	0.06	0.12
^{5}3	1.92	1.92	1.81	1.00	1.05	1.05	1.00	0.19
^{3}4	1.97	1.97	1.89	1.91	1.06	1.06	0.04	0.12
^{5}4	1.92	1.93	1.81	1.00	1.05	1.05	1.00	0.19
^{3}5$_{\mathrm{ax}}$	1.90	1.90	1.88	1.97	1.07	1.07	0.04	0.12
^{5}5$_{\mathrm{ax}}$	1.92	1.92	1.81	1.00	1.05	1.06	1.00	0.19
^{3}5$_{\mathrm{eq}}$	1.91	1.92	1.89	1.97	1.06	1.06	0.04	0.11
^{5}5$_{\mathrm{eq}}$	1.93	1.93	1.80	1.00	1.05	1.05	1.00	0.19
^{3}6$_{\mathrm{ax}}$	1.91	1.91	1.88	1.97	1.06	1.07	0.04	0.12
^{5}6$_{\mathrm{ax}}$	1.93	1.92	1.81	1.00	1.05	1.06	1.00	0.19
^{3}6$_{\mathrm{eq}}$	1.91	1.91	1.88	1.97	1.07	1.06	0.04	0.12
^{5}6$_{\mathrm{eq}}$	1.93	1.92	1.80	1.00	1.05	1.05	1.00	0.20
^{3}7	1.91	1.91	1.89	1.96	1.06	1.06	0.05	0.11
^{5}7	1.90	1.90	1.93	1.07	1.07	0.99	0.07	1.03
^{3}8	1.92	1.92	1.87	1.05	1.05	1.96	0.05	0.13
^{5}8	1.90	1.90	1.93	0.99	1.07	1.07	1.03	0.07
^{3}9	1.90	1.90	1.89	1.96	1.07	1.07	0.06	0.12
^{5}9	1.91	1.92	1.82	1.00	1.06	1.06	1.00	0.19
^{3}10	1.91	1.91	1.88	1.96	1.06	1.07	0.05	0.12
^{5}10	1.93	1.92	1.81	1.00	1.06	1.05	1.00	0.19

DFT Results

Table S3: ΔE_{gas} calculated with different DFT functionals compared to our best electronic CASPT2/CC results. All values in kcal/mol

	CASPT2/CC	BP86	B3LYP	TPSS	TPSSh	PBE0	M06	MN15	S12g	B97-D	OPBE	OLYP
1	10.2	10.6	1.3	14.4	9.6	0.3	−6.1	6.4	3.7	5.4	0.5	−0.3
2	8.1	9.2	0.2	13.1	8.5	−1.1	−8.2	5.9	2.1	3.7	−1.5	−2.2
3	6.6	6.5	−3.0	10.6	5.7	−4.1	−11.5	1.7	−1.2	0.1	−4.5	−5.3
4	11.9	22.2	9.4	22.9	16.9	6.7	−3.1	9.4	13.3	8.8	18.1	15.7
5_{ax}	10.5	12.4	2.2	16.2	11.4	1.8	−6.4	6.7	4.3	3.5	3.5	1.1
5_{eq}	9.1	12.0	1.0	15.7	10.6	0.9	−9.4	5.7	3.5	3.7	3.5	0.8
6_{ax}	4.0	9.3	1.5	12.0	7.9	−1.9	−11.7	1.8	−0.9	−3.3	3.9	3.2
6_{eq}	5.6	12.4	3.5	14.6	10.1	0.0	−9.9	3.5	2.7	−0.1	7.2	6.3
7	29.6	27.0	20.7	30.1	27.6	21.1	17.6	28.6	19.7	20.7	20.4	17.9
8	17.1	18.5	14.2	19.4	16.9	11.5	4.2	12.0	14.8	12.9	16.7	16.6
mean AE		3.3	6.2	5.6	2.0	7.8	15.7	3.1	5.4	5.7	6.0	6.8
max AE		10.2	9.7	10.9	5.0	10.7	18.5	5.1	9.8	8.8	11.1	11.9
min AE		0.2	2.1	0.5	0.1	5.3	12.0	1.0	1.4	3.2	0.1	0.4
SD		3.8	3.2	3.1	2.4	2.0	2.1	1.3	3.1	1.7	5.9	6.0
R^2		0.74	0.82	0.84	0.90	0.93	0.98	0.97	0.82	0.95	0.55	0.52

Table S4: ΔE_{gas} calculated with different DFT functionals compared to our best electronic CASPT2/CC results. All values in kcal/mol.

	$Linear fit$	R^2
BP86	$-2.53 + 0.99 * x$	0.74
B3LYP	$6.64 + 0.91 * x$	0.82
TPSS	$-8.26 + 1.16 * x$	0.84
TPSSh	$-2.48 + 1.10 * x$	0.90
PBE0	$7.99 + 0.93 * x$	0.93
M06	$14.87 + 0.81 * x$	0.98
MN15	$3.66 + 0.93 * x$	0.97
S12g	$5.46 + 0.94 * x$	0.82
B97-D	$5.59 + 1.02 * x$	0.95
OPBE	$6.99 + 0.63 * x$	0.55
OLYP	$7.85 + 0.64 * x$	0.52

Local Coupled-Cluster Results

Table S5: Local coupled-cluster energies (ΔE_{gas}) using different schemes in the case of LUCCSD(T0) (Pipek-Mezey localization (pipek), intrinsic bond orbitals (ibo) and ibos in combinations with *hotspot* approach) and different parameters in the case of DLPNO-CCSD(T). Statistical analyses of local coupled-cluster results compared to CASPT2/CC is also present (mean absolute error (AE), maximal AE, minimal AE, standard deviation (SD) and R^2). All values in kcal/mol.

	CASPT2/CC	LUCCSD(T)			DLPNO-CCSD(T)		
		pipek	ibo	ibo-*hotspot*	LoosePNO	NormalPNO	TightPNO
1	10.2	9.9	16.5	11.0	3.0	1.4	2.4
2	8.1	13.6	19.3	10.2	1.4	–0.3	
3	6.6	6.3	10.7	6.6	1.7	–3.2	–2.2
4	11.9	17.7	23.4	18.7	2.8	3.5	
5_{ax}	10.5	15.1	17.8	16.4	3.0	3.9	4.4
5_{eq}	9.1	13.6	12.8	13.2	0.3	1.6	2.5
6_{ax}	4.0	3.3	11.1	10.5	–6.3	–3.5	
6_{eq}	5.6	8.9	12.3	12.1	–4.7	–1.4	
7	29.6	47.4	40.0	38.4	19.4	25.7	
8	17.1	32.5	31.5	24.7	2.8	9.1	10.0
mean AE		5.8	8.3	4.9	8.9	7.6	-
max AE		17.8	14.5	8.9	14.3	9.8	-
min AE		0.3	3.7	0.0	4.9	3.8	-
SD		6.3	3.5	3.0	2.6	1.6	-
R^2		0.95	0.90	0.92	0.88	0.98	-

Table S6: Local coupled-cluster free energies ($\Delta G_{acetonitrile}$) using different schemes in the case of LUCCSD(T0) (Pipek-Mezey localization (pipek), intrinsic bond orbitals (ibo) and ibos in combinations with *hotspot* approach) and different parameters in the case of DLPNO-CCSD(T). Statistical analyses of local coupled-cluster results compared to CASPT2/CC is also present (mean absolute error (AE), maximal AE, minimal AE, standard deviation (SD) and R^2). All values in kcal/mol

	CASPT2/CC	LUCCSD(T)			DLPNO-CCSD(T)		
		pipek	nbo	nbo-*hotspot*	LoosePNO	NormalPNO	TightPNO
1	8.3	8.0	14.5	9.1	1.1	–0.5	0.5
2	7.3	12.7	18.4	9.3	0.5	–1.2	
3	5.4	5.1	9.4	5.3	0.4	–4.5	–3.4
4	9.2	15.0	20.7	16.0	0.1	0.8	
5_{ax}	10.6	15.2	17.9	16.5	3.1	4.0	4.5
5_{eq}	8.2	12.6	11.8	12.3	–0.7	0.6	1.5
6_{ax}	4.5	3.9	11.7	11.1	–5.8	–2.9	
6_{eq}	4.2	7.5	10.9	10.7	–6.1	–2.8	
7	25.6	43.4	36.0	34.4	15.4	21.7	
8	13.4	28.8	27.9	21.1	–0.9	5.5	6.3
mean AE		5.8	8.3	4.9	8.9	7.6	-
max AE		17.8	14.5	8.9	14.3	9.8	-
min AE		0.3	3.7	0.0	4.9	3.8	-
SD		6.3	3.5	3.0	2.6	1.6	-
R^2		0.93	0.87	0.90	0.83	0.98	-

[a]Corrections have been obtained from BP86-D3BJ calculations with def2-TZVP basis set. Solvent effects have been calculated using COSMO with acetonitrile as solvent.

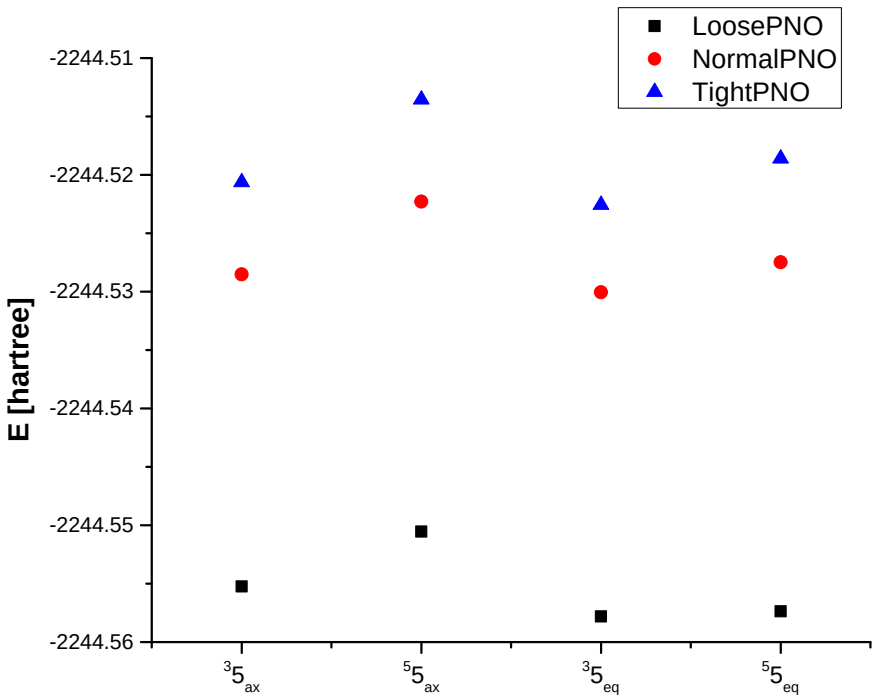

Figure S2: Absolute DLPNO-CCSD(T) energies using different parameters on the example of complex **5**.

Table S7: T_1 diagnostic obtained from different local coupled-cluster calculations.

	LUCCSD(T)			DLPNO-CCSD(T)
	ibo	ibo-*hotspot*	pipek	NormalPNO
^{5}1	0.04630	0.04005	0.04525	0.01610
^{3}1	0.05126	0.04187	0.05088	0.01402
^{5}2	0.04162	0.03601	0.03995	0.01533
^{3}2	0.04610	0.03833	0.04481	0.01344
^{5}3	0.05391	0.04552	0.05524	0.01672
^{3}3	0.05824	0.04669	0.06137	0.01498
^{5}4	0.04079	0.03432	0.03953	0.01502
^{3}4	0.04248	0.03478	0.04451	0.01294
^{5}5$_{ax}$	0.04415	0.03799	0.04271	0.01598
^{3}5$_{ax}$	0.04565	0.03848	0.04579	0.01362
^{5}5$_{eq}$	0.04340	0.03788	0.04324	0.01567
^{3}5$_{eq}$	0.04697	0.03907	0.04674	0.01351
^{5}6$_{ax}$	0.03856	0.03401	0.03838	0.01512
^{3}6$_{ax}$	0.04013	0.03434	0.04093	0.01288
^{5}6$_{eq}$	0.03845	0.03401	0.03833	0.01493
^{3}6$_{eq}$	0.04167	0.03495	0.04207	0.01279
^{5}7	0.04060	0.03599	0.04150	0.01492
^{3}7	0.04165	0.03545	0.04319	0.01313
^{5}8	0.04042	0.03514	0.04054	0.01524
^{3}8	0.04011	0.03442	0.04077	0.01325
^{5}9	0.04518	0.03813	0.04449	0.01577
^{3}9	0.04905	0.03928	0.04957	0.01409
^{5}10	0.04632	0.04027	0.04595	0.01587
^{3}10	0.05020	0.04177	0.05008	0.01373

It is important to notice also that the T_1 diagnostic (Table S7) obtained from DLPNO-CCSD(T) calculations is very small (around 0.015) and does not suggest any multireference character. On the contrary, in the case of LUCCSD(T0) the T_1 diagnostic is between 0.035 and 0.060 and it is above the recently proposed threshold of 0.03 for this scheme.[46] Therefore, one should be very cautious using T_1 diagnostic from local coupled-cluster calculations as an only diagnostic for the multireference character of the system.

We have employed Gaussian process regression (GPR), a less "parametric" tool to test how suitable is our linear fit. The statistical analyses were done with the scikit-learn library. We used the radial basis function (RBF) kernel. The parameters were optimized by

maximizing the log marginal likelihood. We used a noise up to 0.3 kcal/mol since smaller noise leads to unrealistic regressions. The results can be found in the Table S3. We found that indeed the relation between CASPT2/CC and DLPNO-CCSD(T)/LUCCSD(T)-*hotspot* can be well-described with a linear regression. Between CASPT2/CC and LUCCSD(T), the linear correlation is much less pronounced.

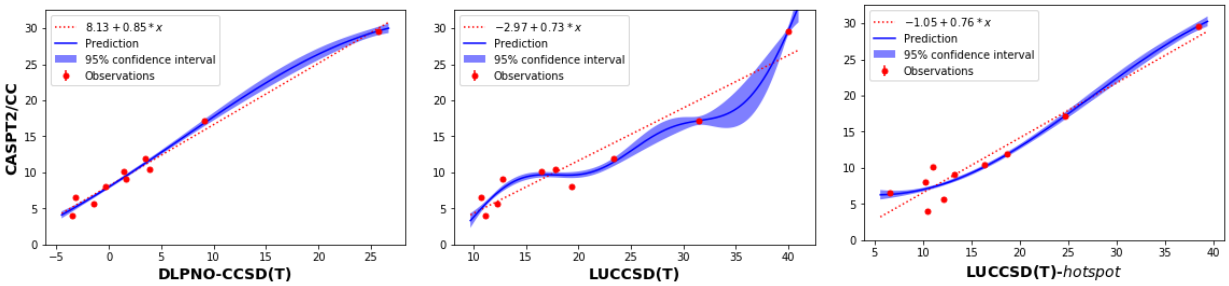

Figure S3: Gaussian process regression compared to linear regression for different methods.

Table S8: DLPNO-CCSD(T) and corrected DLPNO-CCSD(T) results of reaction mechanism of C-H activation by small non-heme iron complex compared to UCCSD(T) results. All values in kcal/mol

	UCCSD(T)	DLPNO-CCSD(T)	corrected DLPNO-CCSD(T)
^{3}SR	0.0	0.0	0.0
^{5}SR	0.6	–6.8	2.4
^{3}RC	–5.0	–4.9	–4.9
^{5}RC	–2.9	–9.8	–1.0
^{3}TS	24.6	27.0	27.0
^{5}TS	14.3	7.3	18.4
^{3}IM	13.6	14.1	14.1
^{5}IM	2.5	0.4	10.6
^{3}SP	20.6	20.7	20.7
^{5}SP	9.3	–4.2	7.7

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Cartesian Coordinates of the Molecules Studied in This Work

^{3}1 optimized with BP86-D3BJ/def2-TZVP

58

FE	-0.065670	-0.293302	0.000000
N	-1.455982	-0.324948	-1.575622
N	1.401864	-0.378285	-1.550228
N	1.401864	-0.378285	1.550228
N	-1.455982	-0.324948	1.575622
C	-0.726046	-1.102871	-2.628394
C	0.646125	-0.524795	-2.845974
C	2.220282	-1.617910	-1.305535
C	3.009792	-1.625381	0.000000
C	2.220282	-1.617910	1.305535
C	0.646125	-0.524795	2.845974
C	-0.726046	-1.102871	2.628394
C	-2.705806	-1.088972	1.260252
C	-3.426689	-0.646048	0.000000
C	-2.705806	-1.088972	-1.260252
C	-1.840852	1.011576	-2.101614
C	2.321479	0.775136	-1.750070
C	2.321479	0.775136	1.750070
C	-1.840852	1.011576	2.101614
O	-0.183587	-1.929501	0.000000
H	-2.495533	0.888619	-2.977251
H	-2.380035	1.573108	-1.333121
H	-0.957037	1.581634	-2.397315
H	2.961861	0.582573	-2.624257

H	1.743268	1.684727	-1.931506
H	2.966288	0.927474	-0.885015
H	-2.495533	0.888619	2.977251
H	-0.957037	1.581634	2.397315
H	-2.380035	1.573108	1.333121
H	2.961861	0.582573	2.624257
H	2.966288	0.927474	0.885015
H	1.743268	1.684727	1.931506
H	-2.418070	-2.142222	1.157228
H	-3.369517	-1.003225	2.135725
H	-4.410476	-1.137308	0.000000
H	-3.646532	0.431467	0.000000
H	-3.369517	-1.003225	-2.135725
H	-2.418070	-2.142222	-1.157228
H	-1.300186	-1.087770	-3.568517
H	-0.666462	-2.138039	-2.276198
H	1.223229	-1.154183	-3.539837
H	0.578180	0.468977	-3.304572
H	1.531939	-2.469541	-1.336445
H	2.927861	-1.711741	-2.145990
H	3.586771	-2.562528	0.000000
H	3.774767	-0.835505	0.000000
H	2.927861	-1.711741	2.145990
H	1.531939	-2.469541	1.336445
H	1.223229	-1.154183	3.539837
H	0.578180	0.468977	3.304572
H	-1.300186	-1.087770	3.568517

H	-0.666462	-2.138039	2.276198
N	0.040934	1.734807	0.000000
C	0.106436	2.893488	0.000000
C	0.185180	4.335456	0.000000
H	-0.310840	4.739875	0.894392
H	-0.310840	4.739875	-0.894392
H	1.237057	4.655963	0.000000

[5]1 optimized with BP86-D3BJ/def2-TZVP

58

FE	-0.101122	-0.278426	0.000000
N	-1.497736	-0.313896	-1.682244
N	1.449021	-0.384783	-1.620089
N	1.449021	-0.384783	1.620089
N	-1.497736	-0.313896	1.682244
C	-0.728534	-1.128012	-2.670439
C	0.667649	-0.570432	-2.888720
C	2.257716	-1.614207	-1.317436
C	3.035758	-1.586344	0.000000
C	2.257716	-1.614207	1.317436
C	0.667649	-0.570432	2.888720
C	-0.728534	-1.128012	2.670439
C	-2.738333	-1.055713	1.286743
C	-3.402572	-0.569225	0.000000
C	-2.738333	-1.055713	-1.286743
C	-1.867055	1.001103	-2.256460

C	2.350461	0.775461	-1.822146
C	2.350461	0.775461	1.822146
C	-1.867055	1.001103	2.256460
O	-0.215649	-1.911678	0.000000
H	-2.493996	0.859104	-3.150718
H	-2.430474	1.584494	-1.521287
H	-0.972722	1.564663	-2.538313
H	3.028870	0.586326	-2.669292
H	1.759041	1.670280	-2.039251
H	2.957075	0.960243	-0.933663
H	-2.493996	0.859104	3.150718
H	-0.972722	1.564663	2.538313
H	-2.430474	1.584494	1.521287
H	3.028870	0.586326	2.669292
H	2.957075	0.960243	0.933663
H	1.759041	1.670280	2.039251
H	-2.460488	-2.110703	1.173290
H	-3.449186	-0.985165	2.127096
H	-4.423862	-0.977326	0.000000
H	-3.538818	0.522722	0.000000
H	-3.449186	-0.985165	-2.127096
H	-2.460488	-2.110703	-1.173290
H	-1.262497	-1.150109	-3.634653
H	-0.683978	-2.150888	-2.281191
H	1.221795	-1.235531	-3.569614
H	0.610095	0.406029	-3.384549
H	1.567677	-2.466135	-1.326955

H	2.977208	-1.747697	-2.143458
H	3.646538	-2.502119	0.000000
H	3.773565	-0.771314	0.000000
H	2.977208	-1.747697	2.143458
H	1.567677	-2.466135	1.326955
H	1.221795	-1.235531	3.569614
H	0.610095	0.406029	3.384549
H	-1.262497	-1.150109	3.634653
H	-0.683978	-2.150888	2.281191
N	-0.000487	1.734562	0.000000
C	0.063940	2.892498	0.000000
C	0.144331	4.333214	0.000000
H	-0.351089	4.737170	0.894934
H	-0.351089	4.737170	-0.894934
H	1.197343	4.650233	0.000000

^{3}2 optimized with BP86-D3BJ/def2-TZVP

60

FE	0.956643	-0.114309	0.049166
N	0.686440	-1.435119	-1.570120
N	1.542283	1.317495	-1.372298
N	1.019108	1.238186	1.677509
N	0.782719	-1.626846	1.498536
C	0.999076	-0.622776	-2.793815
C	2.017422	0.447915	-2.496634
C	2.729541	2.090070	-0.880674

C	2.544229	2.830499	0.435424
C	2.337291	1.944079	1.660541
C	0.893611	0.391365	2.909788
C	1.441682	-0.992196	2.684469
C	1.612398	-2.824782	1.142748
C	1.351515	-3.457899	-0.216114
C	1.651179	-2.568420	-1.420063
C	-0.673872	-2.011601	-1.776326
C	0.507268	2.257856	-1.872422
C	-0.062562	2.258296	1.764885
C	-0.597820	-2.039757	1.850106
O	2.570503	-0.435528	0.149760
H	-1.367680	-1.229574	-2.085585
H	-1.051130	-2.467626	-0.862227
H	-0.613899	-2.782866	-2.561176
H	0.958271	2.939243	-2.610591
H	-0.316580	1.714264	-2.341517
H	0.093535	2.847392	-1.051619
H	-1.213202	-1.166704	2.076102
H	-1.061503	-2.561604	1.010380
H	-0.571649	-2.716032	2.718758
H	-0.102419	2.877185	0.869682
H	0.125561	2.900872	2.639766
H	-1.029810	1.768703	1.868800
H	1.461021	-3.576830	1.935942
H	2.656356	-2.494726	1.177909
H	0.341094	-3.883129	-0.280346

H	2.028975	-4.322398	-0.282578
H	2.659995	-2.148189	-1.338612
H	1.590647	-3.174131	-2.339824
H	1.356821	-1.284653	-3.598583
H	0.056882	-0.175930	-3.131105
H	2.968686	0.004078	-2.183051
H	2.199166	1.063638	-3.392623
H	3.002466	2.807804	-1.671878
H	3.546821	1.369379	-0.770118
H	1.760158	3.596586	0.361854
H	3.475131	3.391748	0.606266
H	2.389967	2.566311	2.570047
H	3.124429	1.182421	1.709033
H	1.409227	0.879474	3.751677
H	-0.171240	0.346045	3.165935
H	2.515112	-0.952096	2.472250
H	1.285632	-1.618352	3.578060
O	-1.022999	0.202896	0.025146
C	-3.597237	-0.110873	0.211142
F	-3.507246	-0.000304	1.556595
F	-3.487316	-1.419213	-0.112764
F	-4.784537	0.341428	-0.190596
S	-2.229003	0.884381	-0.599637
O	-2.337227	0.621406	-2.028930
O	-2.412783	2.246011	-0.138492

[5]2 optimized with BP86-D3BJ/def2-TZVP

60

FE	0.928703	-0.101041	0.061989
N	0.695877	-1.623512	-1.548602
N	1.558446	1.250455	-1.522706
N	0.954874	1.426976	1.692680
N	0.779750	-1.549694	1.689159
C	1.074043	-0.863490	-2.778458
C	2.069021	0.260464	-2.520935
C	2.706087	2.067000	-1.012220
C	2.437522	2.897027	0.243189
C	2.260814	2.137562	1.563880
C	0.879991	0.615879	2.943939
C	1.435774	-0.791079	2.795836
C	1.626108	-2.744907	1.377579
C	1.347261	-3.467670	0.060297
C	1.667658	-2.709649	-1.233070
C	-0.647139	-2.219304	-1.761827
C	0.536517	2.130642	-2.134599
C	-0.149635	2.414810	1.729927
C	-0.595524	-1.947407	2.056642
O	2.543628	-0.390043	0.210605
H	-1.337204	-1.457871	-2.129132
H	-1.047380	-2.617467	-0.827251
H	-0.574905	-3.040291	-2.495252
H	1.001795	2.752853	-2.916349
H	-0.267869	1.537465	-2.577603

H	0.090570	2.782009	-1.377433
H	-1.210890	-1.063654	2.242959
H	-1.056943	-2.500895	1.234274
H	-0.578250	-2.585238	2.955432
H	-0.205638	2.979305	0.798349
H	0.005240	3.113817	2.569122
H	-1.103152	1.899231	1.854046
H	1.512032	-3.459903	2.211587
H	2.664943	-2.395591	1.372690
H	0.326363	-3.872102	0.033986
H	1.999091	-4.354126	0.069584
H	2.668438	-2.266205	-1.167318
H	1.658801	-3.425129	-2.075371
H	1.494251	-1.551756	-3.531513
H	0.145926	-0.454600	-3.194877
H	3.010029	-0.139065	-2.128017
H	2.284801	0.773922	-3.473296
H	3.019302	2.741110	-1.828047
H	3.527138	1.370225	-0.811748
H	1.610449	3.601575	0.082250
H	3.326013	3.533278	0.373653
H	2.338841	2.856219	2.399621
H	3.059797	1.394402	1.673210
H	1.414317	1.131354	3.759630
H	-0.176614	0.572419	3.234361
H	2.506749	-0.756868	2.569422
H	1.303308	-1.333182	3.747662

O	-1.021082	0.158473	0.008919
C	-3.592041	-0.062776	0.182489
F	-3.507633	0.170526	1.511240
F	-3.507617	-1.394931	-0.021710
F	-4.764009	0.380545	-0.270668
S	-2.195606	0.821630	-0.705767
O	-2.283718	0.428052	-2.103657
O	-2.334985	2.224854	-0.375151

^{3}3 optimized with BP86-D3BJ/def2-TZVP

55

FE	-0.016424	0.007887	0.000000
N	-1.361876	0.366601	1.576369
N	1.445109	-0.232267	1.534704
N	1.445109	-0.232267	-1.534704
N	-1.361876	0.366601	-1.576369
C	-0.462256	0.940069	2.622352
C	0.729166	0.042846	2.824795
C	2.498721	0.807672	1.308606
C	3.275426	0.667469	0.000000
C	2.498721	0.807672	-1.308606
C	0.729166	0.042846	-2.824795
C	-0.462256	0.940069	-2.622352
C	-2.386647	1.405921	-1.261502
C	-3.191618	1.140758	0.000000
C	-2.386647	1.405921	1.261502

C	-2.052894	-0.837162	2.104658
C	2.082370	-1.564646	1.707547
C	2.082370	-1.564646	-1.707547
C	-2.052894	-0.837162	-2.104658
O	0.239570	1.660861	0.000000
H	-2.621908	-0.566714	3.008303
H	-2.745800	-1.235139	1.358822
H	-1.333309	-1.620920	2.347912
H	2.645846	-1.577576	2.653740
H	1.308076	-2.336462	1.711605
H	2.776292	-1.778069	0.895640
H	-2.621908	-0.566714	-3.008303
H	-1.333309	-1.620920	-2.347912
H	-2.745800	-1.235139	-1.358822
H	2.645846	-1.577576	-2.653740
H	2.776292	-1.778069	-0.895640
H	1.308076	-2.336462	-1.711605
H	-1.849706	2.355449	-1.148461
H	-3.054585	1.488778	-2.135513
H	-4.040134	1.840569	0.000000
H	-3.642306	0.138018	0.000000
H	-3.054585	1.488778	2.135513
H	-1.849706	2.355449	1.148461
H	-1.016405	1.058686	3.568831
H	-0.151055	1.927745	2.266894
H	1.430027	0.487282	3.549404
H	0.414893	-0.923552	3.236055

H	1.997646	1.781314	1.338923
H	3.212963	0.747023	2.148903
H	4.020336	1.478373	0.000000
H	3.870921	-0.255687	0.000000
H	3.212963	0.747023	-2.148903
H	1.997646	1.781314	-1.338923
H	1.430027	0.487282	-3.549404
H	0.414893	-0.923552	-3.236055
H	-1.016405	1.058686	-3.568831
H	-0.151055	1.927745	-2.266894
N	-0.285005	-1.925712	0.000000
N	-1.195649	-2.718257	0.000000
N	-2.044452	-3.508038	0.000000

^{5}3 optimized with BP86-D3BJ/def2-TZVP

55

FE	-0.060541	-0.014579	0.000000
N	-1.405815	0.360817	1.689043
N	1.497237	-0.237413	1.604721
N	1.497237	-0.237413	-1.604721
N	-1.405815	0.360817	-1.689043
C	-0.455898	0.966741	2.662650
C	0.764962	0.085631	2.867930
C	2.537264	0.795152	1.319030
C	3.297267	0.619506	0.000000
C	2.537264	0.795152	-1.319030

C	0.764962	0.085631	-2.867930
C	-0.455898	0.966741	-2.662650
C	-2.427398	1.372503	-1.287832
C	-3.185340	1.044325	0.000000
C	-2.427398	1.372503	1.287832
C	-2.075333	-0.820925	2.275532
C	2.111646	-1.572059	1.783608
C	2.111646	-1.572059	-1.783608
C	-2.075333	-0.820925	-2.275532
O	0.197558	1.636074	0.000000
H	-2.601445	-0.534928	3.201488
H	-2.805240	-1.231779	1.571550
H	-1.346799	-1.604378	2.499804
H	2.728967	-1.588362	2.697294
H	1.322769	-2.327831	1.848290
H	2.748795	-1.822977	0.934267
H	-2.601445	-0.534928	-3.201488
H	-1.346799	-1.604378	-2.499804
H	-2.805240	-1.231779	-1.571550
H	2.728967	-1.588362	-2.697294
H	2.748795	-1.822977	-0.934267
H	1.322769	-2.327831	-1.848290
H	-1.900748	2.326078	-1.160065
H	-3.138929	1.485481	-2.124197
H	-4.094865	1.662140	0.000000
H	-3.547832	0.005165	0.000000
H	-3.138929	1.485481	2.124197

H	-1.900748	2.326078	1.160065
H	-0.958058	1.118324	3.634117
H	-0.164341	1.943497	2.262803
H	1.451155	0.573150	3.580566
H	0.465272	-0.867146	3.321153
H	2.031777	1.768065	1.322971
H	3.270789	0.779436	2.146649
H	4.074935	1.399230	0.000000
H	3.857449	-0.325664	0.000000
H	3.270789	0.779436	-2.146649
H	2.031777	1.768065	-1.322971
H	1.451155	0.573150	-3.580566
H	0.465272	-0.867146	-3.321153
H	-0.958058	1.118324	-3.634117
H	-0.164341	1.943497	-2.262803
N	-0.331484	-1.931108	0.000000
N	-1.304525	-2.650630	0.000000
N	-2.203882	-3.378607	0.000000

^{3}4 optimized with BP86-D3BJ/def2-TZVP

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FE	-0.098510	-0.816688	0.000000
N	1.341529	-0.759045	-1.342966
N	-1.438582	-0.378827	-1.367326
N	1.341529	-0.759045	1.342966
N	-1.438582	-0.378827	1.367326

N	0.219950	1.236859	0.000000
O	-0.346937	-2.442170	0.000000
C	-3.315330	-0.882086	-2.756084
C	-2.334244	-1.264437	-1.848676
C	-1.480167	0.916368	-1.764736
C	-2.450294	1.361232	-2.657793
C	-3.380193	0.451375	-3.162670
C	-2.334244	-1.264437	1.848676
C	-1.480167	0.916368	1.764736
C	-2.450294	1.361232	2.657793
C	-3.380193	0.451375	3.162670
C	-3.315330	-0.882086	2.756084
C	1.590071	-1.654116	-2.313511
C	2.642832	-1.464182	-3.207237
C	3.439674	-0.324521	-3.091852
C	3.174905	0.600002	-2.074459
C	2.117346	0.346903	-1.211964
C	3.174905	0.600002	2.074459
C	3.439674	-0.324521	3.091852
C	2.642832	-1.464182	3.207237
C	1.590071	-1.654116	2.313511
C	2.117346	0.346903	1.211964
C	-0.376789	1.803786	1.243966
C	-0.376789	1.803786	-1.243966
C	1.728306	1.173885	0.000000
H	-4.019539	-1.624282	-3.128731
H	-2.232170	-2.284630	-1.480646

H	-2.471322	2.408733	-2.958271
H	-4.146175	0.781053	-3.864197
H	-2.232170	-2.284630	1.480646
H	-2.471322	2.408733	2.958271
H	-4.146175	0.781053	3.864197
H	-4.019539	-1.624282	3.128731
H	0.937207	-2.525395	-2.341935
H	2.830651	-2.208406	-3.979629
H	4.263601	-0.154474	-3.784460
H	3.780489	1.497932	-1.955723
H	3.780489	1.497932	1.955723
H	4.263601	-0.154474	3.784460
H	2.830651	-2.208406	3.979629
H	0.937207	-2.525395	2.341935
H	0.410858	1.872279	2.009060
H	-0.738297	2.826683	1.070160
H	0.410858	1.872279	-2.009060
H	-0.738297	2.826683	-1.070160
H	2.205068	2.164221	0.000000

[5]4 optimized with BP86-D3BJ/def2-TZVP

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FE	-0.234423	-0.969774	0.000000
N	1.368908	-0.971129	-1.405082
N	-1.564569	-0.298800	-1.452059
N	1.368908	-0.971129	1.405082

N	-1.564569	-0.298800	1.452059
N	0.307998	1.062800	0.000000
O	-0.659173	-2.546737	0.000000
C	-3.563293	-0.456282	-2.750696
C	-2.590785	-1.025101	-1.936005
C	-1.460658	1.017174	-1.749426
C	-2.410567	1.652527	-2.543686
C	-3.474685	0.904144	-3.052996
C	-2.590785	-1.025101	1.936005
C	-1.460658	1.017174	1.749426
C	-2.410567	1.652527	2.543686
C	-3.474685	0.904144	3.052996
C	-3.563293	-0.456282	2.750696
C	1.617718	-1.848702	-2.389693
C	2.711113	-1.688915	-3.241084
C	3.552847	-0.590738	-3.060972
C	3.288897	0.319603	-2.029911
C	2.184756	0.091947	-1.218697
C	3.288897	0.319603	2.029911
C	3.552847	-0.590738	3.060972
C	2.711113	-1.688915	3.241084
C	1.617718	-1.848702	2.389693
C	2.184756	0.091947	1.218697
C	-0.220285	1.708870	1.242636
C	-0.220285	1.708870	-1.242636
C	1.810914	0.919748	0.000000
H	-4.377560	-1.070028	-3.132958

H	-2.606762	-2.075635	-1.645034
H	-2.317191	2.715156	-2.767814
H	-4.228437	1.381207	-3.679371
H	-2.606762	-2.075635	1.645034
H	-2.317191	2.715156	2.767814
H	-4.228437	1.381207	3.679371
H	-4.377560	-1.070028	3.132958
H	0.926110	-2.686670	-2.475959
H	2.894991	-2.418129	-4.028658
H	4.411605	-0.440923	-3.715202
H	3.931144	1.184279	-1.864780
H	3.931144	1.184279	1.864780
H	4.411605	-0.440923	3.715202
H	2.894991	-2.418129	4.028658
H	0.926110	-2.686670	2.475959
H	0.556134	1.637202	2.019124
H	-0.402587	2.779107	1.071843
H	0.556134	1.637202	-2.019124
H	-0.402587	2.779107	-1.071843
H	2.320995	1.893635	0.000000

$^{3}5_{\mathrm{ax}}$ optimized with BP86-D3BJ/def2-TZVP

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C	-3.879369	1.538382	0.096381
C	-4.600537	0.397335	-0.257037
C	-3.907928	-0.740947	-0.673350

C	-2.518514	-0.708022	-0.724428
N	-1.823545	0.401780	-0.358954
C	-2.490710	1.504238	0.032820
C	-1.668527	-1.829705	-1.242085
N	-0.336526	-1.773354	-0.565126
C	-0.406867	-2.346769	0.830856
C	-0.551944	-1.256084	1.879215
N	0.384198	-0.136296	1.579394
C	0.046874	1.031611	2.431663
FE	0.140521	0.163126	-0.545699
C	0.746574	-2.417577	-1.375442
C	2.090647	-1.952383	-0.841845
N	2.096006	-0.451510	-0.631857
C	2.852952	0.199859	-1.736972
C	2.702150	-0.084465	0.682494
C	1.812123	-0.543262	1.822061
O	0.041176	0.233903	-2.194448
H	-1.886694	2.371993	0.287634
H	-4.381525	2.450253	0.415704
H	-5.689425	0.393584	-0.213195
H	-4.439874	-1.646200	-0.965116
H	-2.139460	-2.813726	-1.104483
H	-1.496487	-1.670263	-2.316610
H	0.663439	-3.514699	-1.338660
H	0.605759	-2.085529	-2.410196
H	-1.245544	-3.052752	0.895457
H	0.505626	-2.928456	0.998115

H	2.330362	-2.438636	0.111193
H	2.889539	-2.228407	-1.542419
H	-1.567719	-0.845089	1.883126
H	-0.361758	-1.671123	2.883121
H	1.855533	-1.632712	1.938082
H	2.167841	-0.120349	2.771426
H	2.811978	1.007077	0.688333
H	3.709978	-0.520618	0.776961
H	3.895775	-0.149439	-1.726722
H	2.378331	-0.047362	-2.691144
H	2.830863	1.285097	-1.604174
H	0.102053	0.757990	3.496353
H	0.751903	1.845344	2.236068
H	-0.969290	1.372366	2.207950
H	0.604025	4.952588	-1.613466
H	0.704819	5.149738	0.163607
H	2.172419	4.745990	-0.777431
N	0.576103	2.044131	-0.422106
C	0.804651	3.175775	-0.537785
C	1.088026	4.583576	-0.697262

$^{5}5_{\mathrm{ax}}$ optimized with BP86-D3BJ/def2-TZVP

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C	-4.004053	1.463990	0.094412
C	-4.682683	0.303090	-0.280944
C	-3.949733	-0.811551	-0.690069

C	-2.559270	-0.739703	-0.717087
N	-1.913417	0.384112	-0.332717
C	-2.614477	1.466827	0.055172
C	-1.688135	-1.856478	-1.234025
N	-0.372496	-1.846587	-0.560306
C	-0.430396	-2.382866	0.830796
C	-0.545990	-1.274354	1.872945
N	0.409264	-0.157896	1.598558
C	0.088269	0.986990	2.490529
FE	0.169407	0.324418	-0.516613
C	0.714990	-2.432284	-1.382273
C	2.075896	-2.004925	-0.841692
N	2.159545	-0.520897	-0.630872
C	2.925444	0.118992	-1.731339
C	2.741425	-0.158742	0.693761
C	1.832074	-0.601287	1.825752
O	0.072948	0.457559	-2.150441
H	-2.036371	2.348376	0.331862
H	-4.538992	2.356787	0.414369
H	-5.771693	0.266341	-0.256936
H	-4.449948	-1.730718	-0.995034
H	-2.189057	-2.830996	-1.122873
H	-1.516608	-1.685044	-2.307626
H	0.655384	-3.532660	-1.407967
H	0.580225	-2.056434	-2.404031
H	-1.283438	-3.069229	0.937384
H	0.468720	-2.984714	1.003969

H	2.295451	-2.507651	0.107676
H	2.859360	-2.317226	-1.545412
H	-1.553760	-0.844870	1.875001
H	-0.365026	-1.688012	2.879103
H	1.845368	-1.692146	1.932027
H	2.199718	-0.195037	2.777802
H	2.864959	0.932798	0.700678
H	3.744230	-0.603069	0.811543
H	3.964868	-0.242730	-1.725812
H	2.449714	-0.118566	-2.688025
H	2.918957	1.205898	-1.598649
H	0.129995	0.674494	3.545095
H	0.807567	1.794973	2.325232
H	-0.920652	1.353391	2.270782
H	0.640806	5.140372	-1.751609
H	0.795783	5.526399	-0.005924
H	2.236116	5.031806	-0.946489
N	0.688268	2.379970	-0.238186
C	0.896226	3.493244	-0.495416
C	1.155217	4.875843	-0.816079

$^{3}5_{\mathrm{eq}}$ optimized with BP86-D3BJ/def2-TZVP

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C	3.892755	-0.661178	-1.360054
C	4.434741	-0.720455	-0.075330
C	3.606903	-0.481498	1.024113

C	2.261572	-0.199404	0.812337
N	1.739682	-0.183119	-0.442216
C	2.537029	-0.389490	-1.510163
C	1.298318	0.178901	1.908440
N	-0.082744	-0.203785	1.507990
C	-0.329306	-1.665910	1.745527
C	-0.084604	-2.463626	0.475587
N	-0.713200	-1.768147	-0.688302
C	-0.240821	-2.395260	-1.954532
FE	-0.189782	0.209680	-0.541194
C	-1.152001	0.653491	2.096249
C	-2.433919	0.473810	1.290717
N	-2.171565	0.565563	-0.196757
C	-2.642404	1.876526	-0.724504
C	-2.854478	-0.529498	-0.954986
C	-2.221587	-1.860496	-0.616334
O	-0.298114	0.404962	-2.175182
H	2.052574	-0.317908	-2.483447
H	4.507621	-0.825102	-2.243778
H	5.491295	-0.944340	0.071020
H	4.001849	-0.507251	2.039738
H	1.580778	-0.272551	2.871162
H	1.321185	1.270708	2.039388
H	-1.329625	0.414039	3.157093
H	-0.804194	1.691784	2.039963
H	0.315697	-2.032768	2.556244
H	-1.361406	-1.787849	2.092079

H	-2.894408	-0.497677	1.503008
H	-3.169805	1.235399	1.580761
H	0.986491	-2.555106	0.263374
H	-0.489944	-3.483277	0.571823
H	-2.501880	-2.188126	0.390902
H	-2.572869	-2.636410	-1.309157
H	-2.727341	-0.295475	-2.018586
H	-3.932470	-0.540351	-0.727286
H	-3.740340	1.921469	-0.673174
H	-2.223984	2.687355	-0.121444
H	-2.312177	1.981060	-1.762836
H	-0.536500	-3.454298	-1.969917
H	-0.679479	-1.865945	-2.805678
H	0.849329	-2.326975	-2.013831
H	0.917520	4.911538	-1.493420
H	0.590546	5.177496	0.245934
H	2.202561	4.605978	-0.286315
N	0.305509	2.077238	-0.290485
C	0.675104	3.173524	-0.367180
C	1.121890	4.542754	-0.477360

$^{5}5_{\mathrm{eq}}$ optimized with BP86-D3BJ/def2-TZVP

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C	4.003829	-0.637247	-1.270910
C	4.491774	-0.759062	0.032315
C	3.630790	-0.547255	1.113587

C	2.302480	-0.222326	0.864632
N	1.836640	-0.125489	-0.409368
C	2.663944	-0.318959	-1.457879
C	1.300052	0.118614	1.936749
N	-0.071657	-0.261616	1.490413
C	-0.325419	-1.734037	1.690433
C	-0.118255	-2.542681	0.416098
N	-0.795367	-1.898703	-0.736372
C	-0.350729	-2.487487	-2.020725
FE	-0.152085	0.247324	-0.558380
C	-1.143618	0.578010	2.112798
C	-2.444208	0.412245	1.334778
N	-2.218952	0.541356	-0.151807
C	-2.694079	1.862330	-0.647484
C	-2.887795	-0.549278	-0.927328
C	-2.284298	-1.913661	-0.619764
O	-0.233554	0.517906	-2.173895
H	2.214093	-0.203533	-2.444137
H	4.649542	-0.788460	-2.134651
H	5.536260	-1.016954	0.208287
H	3.989491	-0.631055	2.139284
H	1.554004	-0.355074	2.896373
H	1.311407	1.208052	2.089502
H	-1.291937	0.314282	3.172286
H	-0.802015	1.618835	2.065367
H	0.329735	-2.117694	2.484865
H	-1.351701	-1.849499	2.055970

H	-2.900908	-0.563587	1.534976
H	-3.170846	1.167174	1.664448
H	0.948058	-2.614977	0.167971
H	-0.485543	-3.572175	0.568628
H	-2.559248	-2.246580	0.388418
H	-2.704927	-2.655797	-1.313161
H	-2.755341	-0.300299	-1.987824
H	-3.968108	-0.557727	-0.709659
H	-3.788399	1.925526	-0.550535
H	-2.232098	2.659159	-0.057126
H	-2.407017	1.975477	-1.698270
H	-0.635456	-3.549958	-2.076181
H	-0.806438	-1.936465	-2.849747
H	0.738631	-2.405277	-2.103843
H	0.916755	5.015486	-1.762171
H	0.673185	5.567494	-0.075768
H	2.254194	4.896164	-0.577939
N	0.350419	2.429054	-0.056081
C	0.718763	3.491655	-0.347350
C	1.165950	4.816771	-0.709824

^{3}6$_{ax}$ optimized with BP86-D3BJ/def2-TZVP

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C	-0.947039	4.471563	-0.262279
C	-1.869161	3.505389	-0.671675
C	-1.471153	2.175032	-0.723130

N	-0.216283	1.799842	-0.363380
C	0.677743	2.725882	0.025313
C	0.343273	4.076012	0.085288
C	-2.331285	1.055098	-1.238726
N	-1.932930	-0.214100	-0.562354
C	-2.232073	-1.435186	-1.372483
C	-1.404153	-2.594964	-0.833732
N	0.032797	-2.183988	-0.625862
C	0.567316	-2.639391	0.688277
C	-0.143147	-1.928828	1.826402
N	-0.171573	-0.447860	1.592212
FE	0.066682	-0.142947	-0.547114
O	1.973105	-0.117547	-0.174376
C	-2.507934	-0.308619	0.823879
C	-1.505916	0.130882	1.882020
C	0.858896	0.211605	2.429592
O	0.112997	-0.037925	-2.192114
C	0.879093	-2.726081	-1.724643
H	1.675198	2.364535	0.259148
H	1.096382	4.799198	0.393250
H	-1.234903	5.521807	-0.221882
H	-2.883341	3.780939	-0.959115
H	-3.404741	1.258563	-1.108271
H	-2.119505	0.926854	-2.310313
H	-3.307529	-1.674275	-1.348005
H	-1.936803	-1.204818	-2.402076
H	-3.421500	0.298140	0.887505

H	-2.809415	-1.349092	0.989604
H	-1.809738	-2.957171	0.118746
H	-1.447923	-3.440130	-1.533840
H	-1.395204	1.221557	1.883223
H	-1.864052	-0.165029	2.882897
H	-1.173771	-2.290920	1.934134
H	0.362078	-2.149425	2.777802
H	1.635288	-2.389407	0.685563
H	0.466936	-3.732974	0.790012
H	0.847989	-3.826435	-1.700046
H	0.497462	-2.353696	-2.680151
H	1.906766	-2.369875	-1.608477
H	0.638089	0.055742	3.497878
H	1.841705	-0.199674	2.185491
H	0.871387	1.285703	2.219196
S	3.071796	0.290712	-1.181347
O	2.852672	1.609537	-1.741556
C	4.451057	0.489778	0.080722
F	5.578132	0.839513	-0.542738
F	4.122175	1.455090	0.975162
F	4.650100	-0.660335	0.755096
O	3.463962	-0.808278	-2.038731

$^{5}6_{ax}$ optimized with BP86-D3BJ/def2-TZVP

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C	-1.208067	4.561032	-0.363184

C	-2.083460	3.525453	-0.695996
C	-1.605726	2.218148	-0.711948
N	-0.328352	1.940351	-0.381310
C	0.529777	2.931549	-0.081748
C	0.120794	4.261944	-0.062876
C	-2.425870	1.043291	-1.190121
N	-1.999745	-0.207208	-0.532916
C	-2.246991	-1.419446	-1.349404
C	-1.414452	-2.591667	-0.830115
N	0.021391	-2.221044	-0.660673
C	0.588139	-2.649828	0.645104
C	-0.079073	-1.914476	1.795634
N	-0.111468	-0.428660	1.564991
FE	0.215281	-0.073379	-0.563365
O	2.102143	-0.007470	-0.127728
C	-2.498664	-0.317525	0.863388
C	-1.452955	0.135303	1.877275
C	0.904752	0.236831	2.419743
O	0.251077	0.062474	-2.198454
C	0.844848	-2.741598	-1.781545
H	1.562156	2.638251	0.108997
H	0.839749	5.043078	0.178535
H	-1.559324	5.592644	-0.350483
H	-3.122433	3.728616	-0.955637
H	-3.502966	1.229420	-1.048012
H	-2.236977	0.929415	-2.268571
H	-3.315185	-1.695598	-1.356829

H	-1.942047	-1.175090	-2.374465
H	-3.414931	0.279099	0.992234
H	-2.783422	-1.360601	1.046550
H	-1.807277	-2.949696	0.129631
H	-1.499502	-3.433065	-1.532409
H	-1.352971	1.226598	1.866101
H	-1.766358	-0.155509	2.894402
H	-1.107949	-2.268598	1.938015
H	0.454661	-2.132476	2.731611
H	1.659894	-2.416474	0.612355
H	0.482103	-3.740354	0.781171
H	0.849577	-3.843282	-1.763274
H	0.427191	-2.381379	-2.726928
H	1.867588	-2.358168	-1.699834
H	0.654138	0.097414	3.483592
H	1.891144	-0.183972	2.210228
H	0.929515	1.307982	2.192351
S	3.292742	0.333461	-1.060141
O	3.279560	1.736659	-1.417577
C	4.656084	0.115955	0.215681
F	5.846574	0.302807	-0.356198
F	4.494469	1.007182	1.216281
F	4.600530	-1.128471	0.738478
O	3.500289	-0.689924	-2.060614

$^{3}6_{\mathrm{eq}}$ optimized with BP86-D3BJ/def2-TZVP

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C	-0.788752	2.378079	-1.525792
C	-1.335636	3.647169	-1.386638
C	-1.659288	4.109595	-0.111338
C	-1.439450	3.279629	0.988438
C	-0.897886	2.014904	0.786124
N	-0.555546	1.593234	-0.456371
C	-0.747733	0.990680	1.880690
N	0.303897	0.005054	1.517241
C	0.055101	-1.363990	2.049703
C	0.877202	-2.371416	1.251801
N	0.737771	-2.149682	-0.233505
C	2.054601	-2.183636	-0.931649
C	2.889987	-0.984633	-0.524108
N	2.078008	0.284549	-0.598560
FE	0.095674	-0.243914	-0.559603
O	-1.711446	-0.829393	-0.136025
S	-2.905958	-0.730679	-1.113341
O	-2.991562	-1.886641	-1.977018
C	1.675115	0.505859	1.828051
C	2.307786	1.143439	0.598739
C	2.433600	1.036430	-1.829349
O	0.042277	-0.405435	-2.196239
C	-0.169542	-3.168786	-0.830529
C	-4.240583	-0.933157	0.195507
F	-4.112630	0.035497	1.138343
F	-5.446236	-0.832669	-0.366485

F	-4.126406	-2.129692	0.805405
H	-0.551771	1.935895	-2.491823
H	-1.518484	4.251055	-2.273541
H	-2.091615	5.100283	0.026182
H	-1.701108	3.599672	1.996604
H	-0.538170	1.463321	2.852963
H	-1.699393	0.447881	1.960688
H	0.299874	-1.434699	3.122482
H	-1.013329	-1.564521	1.919293
H	1.642371	1.231573	2.653854
H	2.278664	-0.338845	2.180277
H	1.939601	-2.305780	1.516084
H	0.554963	-3.391638	1.499727
H	1.852731	2.118470	0.387972
H	3.386890	1.304988	0.756028
H	3.263850	-1.097176	0.500858
H	3.771209	-0.896495	-1.173120
H	1.832171	-2.153648	-2.004918
H	2.591080	-3.121780	-0.710965
H	0.303668	-4.160876	-0.768385
H	-1.119250	-3.169065	-0.290957
H	-0.368642	-2.900099	-1.872503
H	3.500180	1.307571	-1.806462
H	2.211793	0.414912	-2.702102
H	1.829233	1.946820	-1.884674
O	-3.078881	0.601786	-1.657055

^{5}6$_{eq}$ optimized with BP86-D3BJ/def2-TZVP

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C	-0.835470	2.550031	-1.490461
C	-1.410943	3.799967	-1.294538
C	-1.726034	4.196716	0.005329
C	-1.476906	3.327102	1.068946
C	-0.911960	2.084285	0.801921
N	-0.576635	1.727714	-0.458754
C	-0.752174	1.007866	1.845818
N	0.294631	0.028225	1.445767
C	0.052939	-1.332421	2.014753
C	0.903624	-2.367788	1.281471
N	0.793734	-2.217266	-0.205142
C	2.109895	-2.239982	-0.890074
C	2.958327	-1.032838	-0.503696
N	2.201889	0.245608	-0.642470
FE	0.031251	-0.246091	-0.638878
O	-1.805908	-0.820994	-0.172346
S	-3.016942	-0.773161	-1.132920
O	-3.072451	-1.944660	-1.976570
C	1.672714	0.531487	1.755838
C	2.358544	1.131337	0.534408
C	2.575142	0.948770	-1.888611
O	-0.006137	-0.380005	-2.270364
C	-0.111883	-3.241154	-0.787802
C	-4.353322	-0.974516	0.172783

F	-4.227728	0.000098	1.108752
F	-5.560344	-0.884340	-0.388350
F	-4.229300	-2.166869	0.787459
H	-0.590424	2.160395	-2.477945
H	-1.617234	4.441458	-2.149408
H	-2.176510	5.171645	0.190952
H	-1.735688	3.601770	2.091225
H	-0.539649	1.432552	2.839392
H	-1.707040	0.465961	1.902434
H	0.267740	-1.355513	3.096156
H	-1.010464	-1.549689	1.866006
H	1.625919	1.280038	2.560150
H	2.258121	-0.307745	2.148404
H	1.958761	-2.281770	1.568499
H	0.582633	-3.376057	1.579477
H	1.906472	2.096478	0.274771
H	3.424045	1.316566	0.758671
H	3.311661	-1.124786	0.531312
H	3.858037	-1.004871	-1.134614
H	1.897119	-2.227040	-1.966628
H	2.658323	-3.169866	-0.659990
H	0.339108	-4.241803	-0.693001
H	-1.073371	-3.213069	-0.267949
H	-0.291705	-3.005135	-1.842021
H	3.641304	1.228582	-1.873431
H	2.367277	0.298555	-2.744303
H	1.966748	1.853826	-1.991030

O	-3.199737	0.552397	-1.689399

^{3}7 optimized with BP86-D3BJ/def2-TZVP

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FE	-0.017436	0.296258	0.000000
O	-0.132769	1.956165	0.000000
C	1.460839	0.302805	-1.305480
C	-1.450172	0.155801	1.435096
C	-1.450172	0.155801	-1.435096
C	1.460839	0.302805	1.305480
N	0.026479	-1.762231	0.000000
N	-1.576606	0.656646	-2.698995
N	-2.669561	-0.417735	-1.202103
N	-2.669561	-0.417735	1.202103
N	-1.576606	0.656646	2.698995
N	1.597984	1.079071	2.406218
N	2.666647	-0.327019	1.185701
N	2.666647	-0.327019	-1.185701
N	1.597984	1.079071	-2.406218
C	-2.838816	0.395041	-3.226547
H	-3.129875	0.722535	-4.217180
C	-3.532721	-0.283918	-2.281400
H	-4.545888	-0.666941	-2.278332
C	-3.015418	-1.149400	0.000000
H	-4.097088	-1.316873	0.000000
H	-2.509607	-2.122651	0.000000

C	-3.532721	-0.283918	2.281400
H	-4.545888	-0.666941	2.278332
C	-2.838816	0.395041	3.226547
H	-3.129875	0.722535	4.217180
C	-0.586185	1.323765	3.564264
H	-0.210032	0.582459	4.285545
H	-1.139243	2.085218	4.129462
C	0.570160	2.011797	2.866770
H	0.228061	2.593223	2.000226
H	1.044795	2.691414	3.584412
C	2.859051	0.935187	2.977273
H	3.160259	1.473770	3.867588
C	3.541226	0.050389	2.202411
H	4.548498	-0.339100	2.285946
C	3.028235	-1.091333	0.000000
H	2.515021	-2.058005	0.000000
H	4.109562	-1.257866	0.000000
C	3.541226	0.050389	-2.202411
H	4.548498	-0.339100	-2.285946
C	2.859051	0.935187	-2.977273
H	3.160259	1.473770	-3.867588
C	0.570160	2.011797	-2.866770
H	1.044795	2.691414	-3.584412
H	0.228061	2.593223	-2.000226
C	-0.586185	1.323765	-3.564264
H	-1.139243	2.085218	-4.129462
H	-0.210032	0.582459	-4.285545

C	0.020575	-2.922617	0.000000
C	0.020564	-4.370873	0.000000
H	0.532918	-4.749085	-0.895810
H	-1.010799	-4.751222	0.000000
H	0.532918	-4.749085	0.895810

^{5}7 optimized with BP86-D3BJ/def2-TZVP

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FE	-0.057235	0.961656	0.000000
O	-0.126200	2.691132	0.000000
C	1.377591	0.635695	-1.299454
C	-1.376001	0.529259	1.449525
C	-1.376001	0.529259	-1.449525
C	1.377591	0.635695	1.299454
N	0.084626	-3.096906	0.000000
N	-1.551251	0.956667	-2.730132
N	-2.459943	-0.263678	-1.206215
N	-2.459943	-0.263678	1.206215
N	-1.551251	0.956667	2.730132
N	1.533710	1.285522	2.477072
N	2.461608	-0.173815	1.188460
N	2.461608	-0.173815	-1.188460
N	1.533710	1.285522	-2.477072
C	-2.725798	0.439719	-3.267018
H	-3.050129	0.668349	-4.275184
C	-3.303533	-0.327492	-2.304124

H	-4.225522	-0.896309	-2.308009
C	-2.593451	-1.067523	0.000000
H	-3.581242	-1.538182	0.000000
H	-1.805885	-1.837762	0.000000
C	-3.303533	-0.327492	2.304124
H	-4.225522	-0.896309	2.308009
C	-2.725798	0.439719	3.267018
H	-3.050129	0.668349	4.275184
C	-0.660729	1.777931	3.576411
H	-0.399506	1.164209	4.450964
H	-1.245572	2.638109	3.931346
C	0.594463	2.323554	2.914822
H	0.346451	2.924176	2.026508
H	1.108367	2.960551	3.644545
C	2.699111	0.877384	3.111855
H	3.017408	1.278299	4.066771
C	3.293152	-0.041993	2.294173
H	4.219362	-0.592881	2.404445
C	2.675630	-0.996113	0.000000
H	1.951760	-1.825137	0.000000
H	3.701145	-1.376731	0.000000
C	3.293152	-0.041993	-2.294173
H	4.219362	-0.592881	-2.404445
C	2.699111	0.877384	-3.111855
H	3.017408	1.278299	-4.066771
C	0.594463	2.323554	-2.914822
H	1.108367	2.960551	-3.644545

H	0.346451	2.924176	-2.026508
C	-0.660729	1.777931	-3.576411
H	-1.245572	2.638109	-3.931346
H	-0.399506	1.164209	-4.450964
C	0.086543	-4.260521	0.000000
C	0.089759	-5.711648	0.000000
H	0.604542	-6.088610	-0.894169
H	-0.941013	-6.091560	0.000000
H	0.604542	-6.088610	0.894169

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FE	0.010878	-0.165700	0.000000
O	0.351006	-1.765834	0.000000
C	1.346836	0.387887	1.307511
C	-1.400635	-0.181825	-1.421589
C	-1.400635	-0.181825	1.421589
C	1.346836	0.387887	-1.307511
N	-1.434424	-0.623600	2.714111
N	-2.675926	0.265692	1.203487
N	-2.675926	0.265692	-1.203487
N	-1.434424	-0.623600	-2.714111
N	1.663206	-0.228737	-2.471249
N	2.260066	1.392409	-1.188221
N	2.260066	1.392409	1.188221
N	1.663206	-0.228737	2.471249

C	-2.696474	-0.454478	3.270728
H	-2.928170	-0.761502	4.283841
C	-3.481802	0.115159	2.320075
H	-4.521652	0.418383	2.344911
C	-3.099082	0.961072	0.000000
H	-4.192280	1.018285	0.000000
H	-2.696840	1.984280	0.000000
C	-3.481802	0.115159	-2.320075
H	-4.521652	0.418383	-2.344911
C	-2.696474	-0.454478	-3.270728
H	-2.928170	-0.761502	-4.283841
C	-0.364669	-1.179766	-3.569861
H	-0.248239	-0.490460	-4.418879
H	-0.733231	-2.136831	-3.964537
C	0.979667	-1.444267	-2.920107
H	0.882710	-2.109395	-2.052662
H	1.617832	-1.931798	-3.666653
C	2.754015	0.379322	-3.080258
H	3.173746	0.028105	-4.015458
C	3.131945	1.410446	-2.272072
H	3.925021	2.140912	-2.378776
C	2.332957	2.236028	0.000000
H	1.509539	2.963620	0.000000
H	3.284175	2.776939	0.000000
C	3.131945	1.410446	2.272072
H	3.925021	2.140912	2.378776
C	2.754015	0.379322	3.080258

H	3.173746	0.028105	4.015458
C	0.979667	-1.444267	2.920107
H	1.617832	-1.931798	3.666653
H	0.882710	-2.109395	2.052662
C	-0.364669	-1.179766	3.569861
H	-0.733231	-2.136831	3.964537
H	-0.248239	-0.490460	4.418879

[5]8 optimized with BP86-D3BJ/def2-TZVP

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FE	0.017055	-0.245714	0.000000
O	0.354929	-1.940004	0.000000
C	1.352049	0.382786	1.300799
C	-1.376712	-0.166322	-1.449643
C	-1.376712	-0.166322	1.449643
C	1.352049	0.382786	-1.300799
N	-1.437310	-0.642802	2.723612
N	-2.637774	0.299817	1.205783
N	-2.637774	0.299817	-1.205783
N	-1.437310	-0.642802	-2.723612
N	1.660555	-0.232816	-2.466642
N	2.245133	1.401645	-1.188091
N	2.245133	1.401645	1.188091
N	1.660555	-0.232816	2.466642
C	-2.712187	-0.477089	3.254836
H	-2.966834	-0.798183	4.258026

C	-3.473904	0.113530	2.296156
H	-4.516901	0.406732	2.298009
C	-2.996116	1.029236	0.000000
H	-4.077198	1.198631	0.000000
H	-2.480011	1.999967	0.000000
C	-3.473904	0.113530	-2.296156
H	-4.516901	0.406732	-2.298009
C	-2.712187	-0.477089	-3.254836
H	-2.966834	-0.798183	-4.258026
C	-0.364113	-1.196321	-3.576429
H	-0.245609	-0.509936	-4.427626
H	-0.725891	-2.157046	-3.967873
C	0.975344	-1.453063	-2.907931
H	0.863752	-2.097186	-2.022299
H	1.622042	-1.957134	-3.635702
C	2.726769	0.400137	-3.091067
H	3.134630	0.064260	-4.037208
C	3.105242	1.431662	-2.279715
H	3.897790	2.162797	-2.386739
C	2.288905	2.247665	0.000000
H	1.425832	2.928076	0.000000
H	3.214459	2.831209	0.000000
C	3.105242	1.431662	2.279715
H	3.897790	2.162797	2.386739
C	2.726769	0.400137	3.091067
H	3.134630	0.064260	4.037208
C	0.975344	-1.453063	2.907931

H	1.622042	-1.957134	3.635702
H	0.863752	-2.097186	2.022299
C	-0.364113	-1.196321	3.576429
H	-0.725891	-2.157046	3.967873
H	-0.245609	-0.509936	4.427626

^{3}9 optimized with BP86-D3BJ/def2-TZVP

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FE	0.043713	0.043073	-0.008543
C	0.698248	0.160150	3.034949
H	1.480852	0.046762	3.803062
H	-0.170769	-0.435728	3.324570
H	0.364716	1.198355	2.974441
N	1.145791	1.827546	-0.239104
N	1.218949	-0.297835	1.724962
C	0.416736	3.125362	-0.225233
H	-0.336444	3.161574	-1.013832
H	1.135767	3.947110	-0.372953
C	2.089853	1.860413	0.926659
H	1.589419	2.408030	1.734552
H	2.994318	2.429823	0.657663
C	1.918970	1.735010	-1.517749
H	2.578305	2.619094	-1.569358
H	2.535995	0.830515	-1.461375
C	1.050180	1.685891	-2.770618
H	1.733272	1.767770	-3.629670

H	0.401116	2.570044	-2.840928
C	0.268439	0.395059	-2.967471
H	-0.213273	0.400813	-3.960101
H	0.965240	-0.448534	-2.918692
C	-1.943952	1.026512	-2.178974
H	-2.322035	0.888472	-3.205392
H	-1.639311	2.067141	-2.047167
H	-2.738404	0.831384	-1.456613
N	-1.219602	-1.562710	0.342791
N	-0.793525	0.121479	-1.948248
S	-1.602572	1.292605	1.022781
C	-2.195422	-1.334427	1.459244
H	-1.643093	-1.388484	2.399880
H	-2.928559	-2.162253	1.454444
C	-2.861123	0.019355	1.358069
H	-3.364806	0.251272	2.305970
H	-3.638547	0.045409	0.578677
C	-1.222323	-1.298720	-2.126476
C	-2.005189	-1.759751	-0.922869
H	-2.937051	-1.191875	-0.832426
H	-2.280941	-2.821017	-1.023990
C	-0.423997	-2.797921	0.629837
H	-1.135967	-3.634770	0.736404
H	0.206043	-2.978392	-0.249165
C	0.450883	-2.727367	1.878251
C	1.607342	-1.740175	1.816114
H	-0.092340	3.254761	0.734300

C	2.453357	0.469988	1.380990
H	2.959178	-0.078800	0.579594
H	3.125682	0.517941	2.254589
H	2.205692	-1.953804	0.924644
H	2.244271	-1.861132	2.709167
H	0.901678	-3.724992	1.993214
H	-0.151902	-2.587776	2.785994
H	-0.309577	-1.893027	-2.239634
H	-1.828962	-1.401753	-3.041768
O	1.215679	-0.917469	-0.757462

[5]9 optimized with BP86-D3BJ/def2-TZVP

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FE	0.035978	0.044093	-0.002463
C	0.805722	0.183163	3.107012
H	1.583572	0.058114	3.880218
H	-0.084925	-0.379740	3.402263
H	0.507116	1.232765	3.039068
N	1.206963	1.907676	-0.216253
N	1.298914	-0.299614	1.803388
C	0.486738	3.201577	-0.149082
H	-0.294441	3.249222	-0.912196
H	1.192664	4.035436	-0.300229
C	2.180026	1.860937	0.918880
H	1.736927	2.431362	1.744660
H	3.110154	2.379890	0.631966

C	1.907940	1.793135	-1.532286
H	2.574655	2.669073	-1.631781
H	2.523234	0.885747	-1.497152
C	0.984864	1.737056	-2.754276
H	1.633953	1.884190	-3.630825
H	0.299452	2.596804	-2.769829
C	0.238550	0.426116	-3.003762
H	-0.198368	0.446691	-4.018087
H	0.954715	-0.401791	-2.952456
C	-2.019094	0.979966	-2.264142
H	-2.398310	0.849048	-3.292455
H	-1.740633	2.027195	-2.114441
H	-2.812963	0.753709	-1.548004
N	-1.290717	-1.639473	0.344620
N	-0.851934	0.107281	-2.034807
S	-1.603025	1.262892	1.034229
C	-2.286481	-1.370340	1.422637
H	-1.760458	-1.422708	2.380350
H	-3.054804	-2.166322	1.417838
C	-2.903700	0.005698	1.282362
H	-3.458823	0.255938	2.196159
H	-3.625934	0.055037	0.453402
C	-1.221806	-1.329356	-2.164447
C	-2.003708	-1.833886	-0.957396
H	-2.964599	-1.311685	-0.890237
H	-2.230538	-2.903625	-1.094998
C	-0.454669	-2.831410	0.681113

H	-1.131639	-3.695580	0.808641
H	0.189395	-3.019711	-0.186594
C	0.414643	-2.698082	1.937123
C	1.617883	-1.756581	1.866595
H	0.004739	3.306156	0.828139
C	2.514004	0.450710	1.383659
H	2.978617	-0.118717	0.571239
H	3.232660	0.512784	2.220350
H	2.195838	-1.989440	0.965739
H	2.260627	-1.930512	2.748204
H	0.829882	-3.701965	2.116171
H	-0.197655	-2.492730	2.825902
H	-0.286458	-1.890062	-2.266657
H	-1.827226	-1.488198	-3.073951
O	1.202483	-0.917930	-0.753120

^{3}10 optimized with BP86-D3BJ/def2-TZVP

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FE	0.673487	0.147916	0.145233
O	1.998386	0.792196	0.879804
N	-0.682539	0.865438	1.551035
C	-0.670931	-0.120660	2.695527
H	-0.874907	0.406240	3.639266
H	-1.493746	-0.828753	2.537627
C	0.645280	-0.853188	2.761695
H	1.464652	-0.161690	2.983668

H	0.614976	-1.623635	3.549545
N	0.942122	-1.480584	1.434501
C	2.380317	-1.913431	1.450349
H	2.468060	-2.750438	2.162236
H	2.954294	-1.066329	1.842228
C	2.950255	-2.323849	0.100667
H	2.439750	-3.206191	-0.307948
H	3.980044	-2.661657	0.291243
C	3.047545	-1.208624	-0.932711
H	3.584509	-0.349939	-0.512508
H	3.605348	-1.576892	-1.809384
N	1.724247	-0.699962	-1.431491
C	1.957725	0.395811	-2.443134
H	2.921302	0.235403	-2.948003
H	1.178550	0.312347	-3.210287
C	1.920336	1.750925	-1.786275
H	2.752282	1.867554	-1.084037
H	1.986489	2.550178	-2.542143
N	0.654386	1.896219	-0.994321
C	0.814115	3.110562	-0.126324
H	0.828008	3.993589	-0.786338
H	1.796840	3.020840	0.348855
C	-0.244366	3.300518	0.951247
H	-1.237111	3.484142	0.512886
H	0.000127	4.244548	1.461580
C	-0.293543	2.230552	2.036512
H	0.694783	2.120324	2.499604

H	-1.011316	2.532482	2.817193
C	-2.055076	0.885643	0.976019
H	-2.252307	1.865814	0.524065
H	-2.798731	0.747883	1.772910
C	-2.145366	-0.167425	-0.108231
O	-1.047579	-0.581720	-0.603666
N	-3.319294	-0.614312	-0.538307
C	-4.614767	-0.114538	-0.060325
H	-4.502618	0.801712	0.524156
H	-5.114770	-0.881447	0.547258
H	-5.246246	0.109550	-0.929692
C	-3.390182	-1.641342	-1.586227
H	-4.140076	-2.387422	-1.296002
H	-2.415022	-2.119167	-1.701152
H	-3.695823	-1.185161	-2.537982
C	0.068646	-2.664631	1.233462
H	0.231417	-3.387058	2.047426
H	0.301369	-3.152461	0.284596
H	-0.984454	-2.375622	1.213752
C	1.013326	-1.796984	-2.146912
H	1.639682	-2.151611	-2.979661
H	0.063197	-1.424657	-2.535527
H	0.812347	-2.634103	-1.478140
C	-0.497066	2.071038	-1.915281
H	-0.310922	2.917725	-2.592647
H	-1.407259	2.283732	-1.347638
H	-0.662181	1.164605	-2.503853

[5]10 optimized with BP86-D3BJ/def2-TZVP

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FE	0.697589	0.149572	0.160924
O	2.029749	0.785874	0.881281
N	-0.774255	0.901907	1.664748
C	-0.660110	-0.075868	2.798929
H	-0.788087	0.450641	3.757357
H	-1.495248	-0.782833	2.713906
C	0.662665	-0.837598	2.820193
H	1.497636	-0.154575	3.009578
H	0.633193	-1.580797	3.634740
N	0.937166	-1.516619	1.516493
C	2.373902	-1.951907	1.455753
H	2.497512	-2.792989	2.158212
H	2.972408	-1.110288	1.823533
C	2.881121	-2.374789	0.074688
H	2.304197	-3.222183	-0.320560
H	3.886754	-2.787745	0.246988
C	3.056213	-1.284230	-0.988248
H	3.611541	-0.438074	-0.565041
H	3.646470	-1.699040	-1.823758
N	1.781683	-0.737498	-1.559321
C	2.045111	0.413908	-2.484768
H	3.035916	0.301656	-2.951900
H	1.308614	0.358245	-3.295743
C	1.970749	1.773599	-1.797729

H	2.783944	1.886722	-1.072802
H	2.071870	2.567554	-2.556164
N	0.687879	1.953093	-1.044785
C	0.805451	3.139279	-0.135313
H	0.833305	4.045233	-0.764353
H	1.773012	3.048922	0.371555
C	-0.301536	3.298908	0.910014
H	-1.283664	3.419962	0.428174
H	-0.120189	4.274728	1.386125
C	-0.363612	2.286122	2.058931
H	0.627002	2.193263	2.522260
H	-1.063466	2.657587	2.827461
C	-2.128342	0.853740	1.079251
H	-2.383243	1.836680	0.659251
H	-2.882276	0.636195	1.849201
C	-2.162590	-0.162985	-0.053728
O	-1.052382	-0.543438	-0.556783
N	-3.317571	-0.620416	-0.519938
C	-4.632197	-0.170012	-0.043496
H	-4.556269	0.747949	0.543732
H	-5.106480	-0.957092	0.559076
H	-5.266968	0.033220	-0.915313
C	-3.349676	-1.613470	-1.602234
H	-4.089290	-2.383036	-1.349402
H	-2.363253	-2.067315	-1.716387
H	-3.648891	-1.131372	-2.543189
C	0.035855	-2.674312	1.320192

H	0.221414	-3.431537	2.097956
H	0.208675	-3.125661	0.339175
H	-1.011122	-2.362780	1.367692
C	1.047038	-1.789818	-2.301080
H	1.655072	-2.162223	-3.141486
H	0.108523	-1.379088	-2.684784
H	0.810321	-2.629422	-1.642472
C	-0.452859	2.103110	-1.974741
H	-0.290779	2.964863	-2.640962
H	-1.377403	2.269829	-1.413332
H	-0.577793	1.198653	-2.577556