SUPPORTING INFORMATION

Spin-State Energies of Heme-Related Models from Spin-Flip TDDFT Calculations

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Table of contents

Spin-state energies

Table S1.

SF-TDDFT calculated excitation energies (in eV) with def2-TZVP basis set with different functionals (SVWN5-LC-BLYP).

		SVWN5	BLYP	B3LYP	BHandHLYP	CAM-B3LYP	LC-BLYP
FeA_2SH	D-Q	-0.15	0.22	0.09	-0.15	0.06	-0.38
	Q-S	0.75	1.13	0.56	-0.28	0.47	1.03
FeL_2SH	D-Q	0.93	1.21	0.88	0.38	0.75	1.15
	Q-S	1.23	1.34	-0.43	0.55	1.17	1.00
FeA_2Cl	D-Q	-0.28	0.10	-0.13	-0.46	-0.19	-0.12
	Q-S	0.73	1.10	0.54	-0.27	0.46	0.99
FeL_2Cl	D-Q	0.45	0.68	0.26	-0.23	0.13	0.60
	Q-S	1.45	1.75	1.20	0.33	1.11	1.73
FePCl	D-Q	0.18	0.10	0.02	-0.21	0.01	0.08
	Q-S	0.90	1.26	0.65	-0.46	0.55	1.21
FeA_2	S0-S1	0.89	0.63	-0.33	-0.29	-0.31	0.63
	S0-T	0.09	-0.17	-1.25	-1.32	-1.26	-0.27
	S-T	0.09	-0.17	-0.92	-1.03	-0.95	-0.27
	T-Q	0.20	0.41	0.55	-0.08	0.42	0.06
FeL_2	S0-S1	1.74	0.32	-0.12	-0.55	-0.29	0.45
	S0-T	0.90	-0.56	-1.24	-1.83	-1.48	-0.30
	S-T	0.90	-0.56	-1.11	-1.28	-1.20	-0.75
	T-Q	1.43	2.02	1.43	0.68	1.32	0.64
FeA_2CN^-	S0-S1	0.78	0.94	1.05	1.00	1.05	0.56
	S0-T	0.32	0.42	0.35	0.15	0.30	0.19
	S-T	0.32	0.42	0.35	0.15	0.30	0.19
	T-Q	0.38	0.72	0.18	-0.42	0.05	0.60
FeL_2CN^-	S0-S1	1.28	1.41	1.56	1.41	1.51	0.93
	S0-T	0.98	1.00	0.84	0.55	0.75	0.82
	S-T	0.98	1.00	0.84	0.55	0.75	0.82
	T-Q	1.61	1.74	1.53	0.72	1.39	1.55
FeA_2NH_3	S0-S1	0.56	0.75	0.81	0.75	0.81	0.29
	S0-T	-0.09	0.06	-0.02	-0.19	-0.06	-0.22
	S-T	-0.09	0.06	-0.02	-0.19	-0.06	-0.22
	T-Q	0.62	0.98	0.45	-0.14	0.32	0.87
FeL_2NH_3	S0-S1	0.70	0.84	0.91	0.86	0.90	0.44
	S0-T	0.07	0.16	0.08	-0.10	0.03	-0.02

	S-T	0.07	0.16	0.08	-0.10	0.03	-0.02
	T-Q	1.83	2.01	1.69	0.89	1.58	1.67
FeP	S0-S1	0.57	0.53	-0.04	-0.08	-2.32	0.65
	S0-T	-0.03	-0.33	-1.05	-1.12	-2.63	-0.09
	S-T	-0.03	-0.33	-1.00	-1.05	-0.31	-0.09
	T-Q	-0.18	0.94	1.00	0.33	0.76	-1.67
$FeOL_2Cl$	D-Q	-0.07	-0.29	-0.06	-0.06	0.03	-0.18
	Q-S	1.75	2.42	1.91	2.13	1.86	2.38
FeL_2OH_2	S0-S1	0.49	0.27	-0.90	0.48	-1.05	-0.99
	S0-T	-0.13	-0.48	-1.95	-0.12	-2.18	-2.07
	S-T	-0.62	-0.74	-1.05	-0.60	-1.13	-1.08
	T-Q	1.69	1.96	1.34	1.73	1.23	1.55

Table S2

The ΔSCF calculated spin-state energies (in eV) with 6-311++g (d,p) basis set with various functionals (SVWN5-LC-BLYP).

		SVWN5	BLYP	B3LYP	BHHLYP	CAM-B3LYP	LC-BLYP
FeA_2SH	D-Q	-0.30	-0.40	-0.86	-1.02	-0.91	-0.56
	Q-S	0.45	0.13	-0.25	-0.90	-0.25	-0.03
FeL_2SH	D-Q	0.95	0.50	0.02	-0.57	0.56	0.62
	Q-S	1.06	0.55	0.14	-0.56	-0.47	-0.24
FeA_2Cl	D-Q	-0.55	-0.58	-0.78	-1.07	-2.74	-1.94
	Q-S	0.49	0.19	-0.17	-0.82	-0.18	0.04
FeL_2Cl	D-Q	0.29	-0.02	-0.39	-0.81	0.28	-1.66
	Q-S	1.09	0.59	0.13	-0.61	-0.60	0.39
FePCl	D-Q	-0.15	-0.31	-0.56	-0.89	-0.58	-0.25
	Q-S	0.69	0.37	-0.05	-0.74	-0.07	-0.60
FeA_2	S1-T	-0.57	-0.39	-0.48	-0.47	-1.78	-6.17
	T-Q	0.34	0.02	0.06	-0.57	-0.32	-0.18
FeL_2	S1-T	-0.45	-0.34	-0.50	-0.56	-1.56	-0.59
	T-Q	1.59	1.03	0.51	-0.24	0.47	-0.41
FeA_2CN^-	S1-T	0.11	-0.13	-0.39	-0.69	-0.49	-0.48
	T-Q	0.28	-0.26	-0.82	-1.51	-0.86	-0.71
FeL_2CN^-	S1-T	0.63	0.24	-0.11	-0.61	-0.19	-0.17
	T-Q	1.30	0.54	-0.13	-1.04	-0.21	-0.06
FeA_2NH_3	S1-T	-0.29	-0.45	-0.53	-0.60	-0.84	-0.45
	T-Q	0.37	0.07	-0.43	-1.10	-0.48	-0.33

FeL_2NH_3	S1-T	-0.22	-0.48	-0.58	-0.68	-0.68	-0.47
	T-Q	1.50	0.81	0.19	-0.68	0.11	0.27
FeP	S1-T	-0.65	-0.52	-0.57	-0.58	-2.04	-0.30
	T-Q	1.12	0.69	0.58	-0.07	2.01	-0.05
$FeOL_2Cl$	D-Q	0.20	-0.02	-0.65	--*	-0.03	-0.22
	Q-S	1.68	1.04	0.71	-0.37	0.09	0.47
FeL_2OH_2	S1-T	--*	-1.11	-1.12	-1.14	-2.53	-2.56
	T-Q	1.46	0.88	0.31	-0.48	0.24	0.40

*The calculations failed to converge.

Cartesian Coordinates

Table S3

Structure of FeP, singlet, atomic coordinates in Å

Fe	0.00000000	0.00000000	0.00000000
N	1.40803810	-1.40803810	0.00000000
N	1.40803810	1.40803810	0.00000000
N	-1.40803810	-1.40803810	0.00000000
N	-1.40803810	1.40803810	0.00000000
C	-2.78142160	1.22776210	0.00000000
C	-1.22776210	2.78142160	0.00000000
C	-2.49789700	3.46184160	0.00000000
C	-3.46184160	2.49789700	0.00000000
C	-3.42456330	0.00000000	0.00000000
C	-2.78142160	-1.22776210	0.00000000
C	-3.46184160	-2.49789700	0.00000000
C	-2.49789700	-3.46184160	0.00000000
C	-1.22776210	-2.78142160	0.00000000
C	0.00000000	-3.42456330	0.00000000
C	1.22776210	-2.78142160	0.00000000
C	2.49789700	-3.46184160	0.00000000
C	3.46184160	-2.49789700	0.00000000
C	2.78142160	-1.22776210	0.00000000
C	3.42456330	0.00000000	0.00000000
C	2.78142160	1.22776210	0.00000000
C	3.46184160	2.49789700	0.00000000
C	2.49789700	3.46184160	0.00000000
C	1.22776210	2.78142160	0.00000000
C	0.00000000	3.42456330	0.00000000
H	0.00000000	4.51485170	0.00000000
H	-2.61822570	4.54198370	0.00000000

H	-4.54198370	2.61822570	0.00000000
H	-4.51485170	0.00000000	0.00000000
H	-4.54198370	-2.61822570	0.00000000
H	-2.61822570	-4.54198370	0.00000000
H	0.00000000	-4.51485170	0.00000000
H	2.61822570	-4.54198370	0.00000000
H	4.54198370	-2.61822570	0.00000000
H	4.51485170	0.00000000	0.00000000
H	4.54198370	2.61822570	0.00000000
H	2.61822570	4.54198370	0.00000000

Table S4

Structure of FeP, triplet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.00000000
N	1.40400810	-1.41060290	0.00000000
N	1.40400810	1.41060290	0.00000000
N	-1.40400810	-1.41060290	0.00000000
N	-1.40400810	1.41060290	0.00000000
C	-2.77665270	1.22789640	0.00000000
C	-1.22641460	2.78646090	0.00000000
C	-2.49565100	3.46412030	0.00000000
C	-3.45730420	2.49600860	0.00000000
C	-3.41997990	0.00000000	0.00000000
C	-2.77665270	-1.22789640	0.00000000
C	-3.45730420	-2.49600860	0.00000000
C	-2.49565100	-3.46412030	0.00000000
C	-1.22641460	-2.78646090	0.00000000
C	0.00000000	-3.43160010	0.00000000
C	1.22641460	-2.78646090	0.00000000
C	2.49565100	-3.46412030	0.00000000
C	3.45730420	-2.49600860	0.00000000
C	2.77665270	-1.22789640	0.00000000
C	3.41997990	0.00000000	0.00000000
C	2.77665270	1.22789640	0.00000000
C	3.45730420	2.49600860	0.00000000
C	2.49565100	3.46412030	0.00000000
C	1.22641460	2.78646090	0.00000000
C	0.00000000	3.43160010	0.00000000
H	0.00000000	4.52168330	0.00000000
H	-2.61900550	4.54373500	0.00000000
H	-4.53775780	2.61482080	0.00000000
H	-4.51022020	0.00000000	0.00000000
H	-4.53775780	-2.61482080	0.00000000

H	-2.61900550	-4.54373500	0.00000000
H	0.00000000	-4.52168330	0.00000000
H	2.61900550	-4.54373500	0.00000000
H	4.53775780	-2.61482080	0.00000000
H	4.51022020	0.00000000	0.00000000
H	4.53775780	2.61482080	0.00000000
H	2.61900550	4.54373500	0.00000000

Table S5

Structure of FePCl, doublet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.02843460
N	1.40706740	-1.39682670	0.23866330
N	1.40706740	1.39682670	0.23866330
N	-1.40706740	-1.39682670	0.23866330
N	-1.40706740	1.39682670	0.23866330
C	-2.77974980	1.22393950	0.31160540
C	-1.22650610	2.76674740	0.16131150
C	-2.49199390	3.45154560	0.20045650
C	-3.45697680	2.49334000	0.30272550
C	-3.42459980	0.00000000	0.35850790
C	-2.77974980	-1.22393950	0.31160540
C	-3.45697680	-2.49334000	0.30272550
C	-2.49199390	-3.45154560	0.20045650
C	-1.22650610	-2.76674740	0.16131150
C	0.00000000	-3.40709300	0.10282020
C	1.22650610	-2.76674740	0.16131150
C	2.49199390	-3.45154560	0.20045650
C	3.45697680	-2.49334000	0.30272550
C	2.77974980	-1.22393950	0.31160540
C	3.42459980	0.00000000	0.35850790
C	2.77974980	1.22393950	0.31160540
C	3.45697680	2.49334000	0.30272550
C	2.49199390	3.45154560	0.20045650
C	1.22650610	2.76674740	0.16131150
C	0.00000000	3.40709300	0.10282020
H	0.00000000	4.49576350	0.04480170
H	-2.60970140	4.53129280	0.16236970
H	-4.53460080	2.61813640	0.36485160
H	-4.51343170	0.00000000	0.41038720
H	-4.53460080	-2.61813640	0.36485160
H	-2.60970140	-4.53129280	0.16236970
H	0.00000000	-4.49576350	0.04480170
H	2.60970140	-4.53129280	0.16236970

H	4.53460080	-2.61813640	0.36485160
H	4.51343170	0.00000000	0.41038720
H	4.53460080	2.61813640	0.36485160
H	2.60970140	4.53129280	0.16236970
Cl	0.00000000	0.00000000	-2.14315810

Table S6

Structure of FePCl, quartet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	-0.04725880
N	1.41113250	-1.41113250	0.24986670
N	1.41113250	1.41113250	0.24986670
N	-1.41113250	-1.41113250	0.24986670
N	-1.41113250	1.41113250	0.24986670
C	-2.77989840	1.22676340	0.26582480
C	-1.22676340	2.77989840	0.26582480
C	-2.49462430	3.45973260	0.29540020
C	-3.45973260	2.49462430	0.29540020
C	-3.42517290	0.00000000	0.26405080
C	-2.77989840	-1.22676340	0.26582480
C	-3.45973260	-2.49462430	0.29540020
C	-2.49462430	-3.45973260	0.29540020
C	-1.22676340	-2.77989840	0.26582480
C	0.00000000	-3.42517290	0.26405080
C	1.22676340	-2.77989840	0.26582480
C	2.49462430	-3.45973260	0.29540020
C	3.45973260	-2.49462430	0.29540020
C	2.77989840	-1.22676340	0.26582480
C	3.42517290	0.00000000	0.26405080
C	2.77989840	1.22676340	0.26582480
C	3.45973260	2.49462430	0.29540020
C	2.49462430	3.45973260	0.29540020
C	1.22676340	2.77989840	0.26582480
C	0.00000000	3.42517290	0.26405080
H	0.00000000	4.51495270	0.27388630
H	-2.61515220	4.53952610	0.31621030
H	-4.53952610	2.61515220	0.31621030
H	-4.51495270	0.00000000	0.27388630
H	-4.53952610	-2.61515220	0.31621030
H	-2.61515220	-4.53952610	0.31621030
H	0.00000000	-4.51495270	0.27388630
H	2.61515220	-4.53952610	0.31621030
H	4.53952610	-2.61515220	0.31621030
H	4.51495270	0.00000000	0.27388630

H	4.53952610	2.61515220	0.31621030
H	2.61515220	4.53952610	0.31621030
Cl	0.00000000	0.00000000	-2.30242370

Table S7

Structure of FeA_2, singlet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.00000000
N	1.09082720	-1.69589260	0.00000000
N	-1.09082720	-1.69589260	0.00000000
N	-1.09082720	1.69589260	0.00000000
N	1.09082720	1.69589260	0.00000000
C	0.00000000	2.43383070	0.00000000
C	0.00000000	-2.43383070	0.00000000
H	-1.99249740	-2.14193710	0.00000000
H	0.00000000	-3.52940160	0.00000000
H	1.99249740	-2.14193710	0.00000000
H	1.99249740	2.14193710	0.00000000
H	0.00000000	3.52940160	0.00000000
H	-1.99249740	2.14193710	0.00000000

Table S8

Structure of FeA_2, triplet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.00000000
N	1.08889980	-1.67280640	0.00000000
N	-1.08889980	-1.67280640	0.00000000
N	-1.08889980	1.67280640	0.00000000
N	1.08889980	1.67280640	0.00000000
C	0.00000000	2.41504980	0.00000000
C	0.00000000	-2.41504980	0.00000000
H	-1.99244650	-2.11507050	0.00000000
H	0.00000000	-3.51028690	0.00000000
H	1.99244650	-2.11507050	0.00000000
H	1.99244650	2.11507050	0.00000000
H	0.00000000	3.51028690	0.00000000
H	-1.99244650	2.11507050	0.00000000

Table S9

Structure of FeA_2NH_3, singlet, atomic coordinates in Å.

Fe	0.00166240	-0.17982270	0.00000000
N	1.09169830	-0.23534450	-1.68777130
N	-1.09153260	-0.24550150	-1.69129640

N	-1.09153260	-0.24550150	1.69129640
N	1.09169830	-0.23534450	1.68777130
C	-0.00014280	-0.24042400	2.44567680
C	-0.00014280	-0.24042400	-2.44567680
H	-2.00196900	-0.25451500	-2.14217150
H	0.00144330	-0.27173710	-3.55159620
H	2.00316410	-0.27755740	-2.13475610
H	2.00316410	-0.27755740	2.13475610
H	0.00144330	-0.27173710	3.55159620
H	-2.00196900	-0.25451500	2.14217150
N	-0.00712520	1.75270450	0.00000000
H	-0.96296810	2.12036320	0.00000000
H	0.48169590	2.09447140	-0.83536570
H	0.48169590	2.09447140	0.83536570

Table S10

Structure of FeA_2NH_3, triplet, atomic coordinates in Å.

Fe	-0.00550810	-0.17717240	0.00000000
N	1.07753470	-0.33578580	-1.65382600
N	-1.09355690	-0.27665870	-1.65791170
N	-1.09355690	-0.27665870	1.65791170
N	1.07753470	-0.33578580	1.65382600
C	-0.00698500	-0.30625020	2.42204090
C	-0.00698500	-0.30625020	-2.42204090
H	-2.00935020	-0.24303260	-2.09577110
H	-0.00537640	-0.31445830	-3.52710290
H	1.99583310	-0.36202430	-2.08685630
H	1.99583310	-0.36202430	2.08685630
H	-0.00537640	-0.31445830	3.52710290
H	-2.00935020	-0.24303260	2.09577110
N	0.05515140	2.06549320	0.00000000
H	-0.89182510	2.44699400	0.00000000
H	0.54009140	2.41327350	-0.82974310
H	0.54009140	2.41327350	0.82974310

Table S11

Structure of FeA_2CN^-, singlet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	-0.23854890
N	-1.67532040	1.09784520	-0.51459880
N	-1.67532040	-1.09784520	-0.51459880
N	1.67532040	-1.09784520	-0.51459880
N	1.67532040	1.09784520	-0.51459880
C	2.41893050	0.00000000	-0.53942920

C	-2.41893050	0.00000000	-0.53942920
H	-2.14712290	-1.98520890	-0.35690950
H	-3.53133990	0.00000000	-0.56089710
H	-2.14712290	1.98520890	-0.35690950
H	2.14712290	1.98520890	-0.35690950
H	3.53133990	0.00000000	-0.56089710
H	2.14712290	-1.98520890	-0.35690950
C	0.00000000	0.00000000	1.57867120
N	0.00000000	0.00000000	2.76444180

Table S12

Structure of FeA_2CN^{-}, triplet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	-0.20911740
N	-1.63895450	1.09388030	-0.60815480
N	-1.63895450	-1.09388030	-0.60815480
N	1.63895450	-1.09388030	-0.60815480
N	1.63895450	1.09388030	-0.60815480
C	2.39333660	0.00000000	-0.63320080
C	-2.39333660	0.00000000	-0.63320080
H	-2.10660630	-1.98191810	-0.43984100
H	-3.50280290	0.00000000	-0.60184090
H	-2.10660630	1.98191810	-0.43984100
H	2.10660630	1.98191810	-0.43984100
H	3.50280290	0.00000000	-0.60184090
H	2.10660630	-1.98191810	-0.43984100
C	0.00000000	0.00000000	1.82339450
N	0.00000000	0.00000000	3.00204280

Table S13

Structure of FeA_2SH, doublet, atomic coordinates in Å.

Fe	0.00244860	-0.32497540	0.00000000
N	1.08038860	-0.57396900	-1.60459210
N	-1.08760610	-0.43263370	-1.61746600
N	-1.08760610	-0.43263370	1.61746600
N	1.08038860	-0.57396900	1.60459210
C	0.00096790	-0.50359980	2.37894260
C	0.00096790	-0.50359980	-2.37894260
H	-2.00920860	-0.29337640	-2.03459670
H	0.00813890	-0.49561510	-3.49361580
H	2.01681290	-0.49142210	-2.00396060
H	2.01681290	-0.49142210	2.00396060

H	0.00813890	-0.49561510	3.49361580
H	-2.00920860	-0.29337640	2.03459670
S	0.20187100	1.94920740	0.00000000
H	-1.13824660	2.20144540	0.00000000

Table S14

Structure of FeA_2SH, quartet, atomic coordinates in Å.

Fe	0.01218660	-0.11261630	0.00000000
N	1.08122470	-0.63687380	-1.58474000
N	-1.09021340	-0.52968820	-1.59258390
N	-1.09021340	-0.52968820	1.59258390
N	1.08122470	-0.63687380	1.58474000
C	-0.00153730	-0.58342700	2.34961680
C	-0.00153730	-0.58342700	-2.34961680
H	-1.98927860	-0.32808540	-2.02097700
H	0.00440780	-0.54651830	-3.45179150
H	1.99652110	-0.49309630	-2.00257570
H	1.99652110	-0.49309630	2.00257570
H	0.00440780	-0.54651830	3.45179150
H	-1.98927860	-0.32808540	2.02097700
S	0.20180780	2.17627250	0.00000000
H	-1.13118280	2.41616650	0.00000000

Table S15

Structure of FeA_2Cl, doublet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.32986740
N	1.61524170	1.08298890	0.56404040
N	1.61524170	-1.08298890	0.56404040
N	-1.61524170	-1.08298890	0.56404040
N	-1.61524170	1.08298890	0.56404040
C	-2.38082950	0.00000000	0.56404040
C	2.38082950	0.00000000	0.56404040
H	2.01537880	-2.00144210	0.40205510
H	3.48294750	0.00000000	0.54943180
H	2.01537880	2.00144210	0.40205510
H	-2.01537880	2.00144210	0.40205510
H	-3.48294750	0.00000000	0.54943180
H	-2.01537880	-2.00144210	0.40205510
Cl	0.00000000	0.00000000	-1.87015710

Table S16

Structure of FeA_2Cl, quartet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.20285890
N	1.57955780	1.08758720	0.71116930
N	1.57955780	-1.08758720	0.71116930
N	-1.57955780	-1.08758720	0.71116930
N	-1.57955780	1.08758720	0.71116930
C	-2.33934830	0.00000000	0.71116930
C	2.33934830	0.00000000	0.71116930
H	1.99745980	-1.99271480	0.51321210
H	3.44142440	0.00000000	0.67388240
H	1.99745980	1.99271480	0.51321210
H	-1.99745980	1.99271480	0.51321210
H	-3.44142440	0.00000000	0.67388240
H	-1.99745980	-1.99271480	0.51321210
Cl	0.00000000	0.00000000	-2.02199660

Table S17

Structure of FeL_2, singlet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.00000000
N	-1.37805880	1.38660100	0.00000000
N	-1.37805880	-1.38660100	0.00000000
N	1.37805880	-1.38660100	0.00000000
N	1.37805880	1.38660100	0.00000000
C	-1.22499300	2.69535760	0.00000000
C	0.00000000	3.36241280	0.00000000
C	1.22499300	2.69535760	0.00000000
C	-1.22499300	-2.69535760	0.00000000
C	0.00000000	-3.36241280	0.00000000
C	1.22499300	-2.69535760	0.00000000
H	-2.12538910	3.30916670	0.00000000
H	0.00000000	4.44231650	0.00000000
H	2.12538910	3.30916670	0.00000000
H	2.35289510	1.11448570	0.00000000
H	-2.35289510	1.11448570	0.00000000
H	-2.35289510	-1.11448570	0.00000000
H	-2.12538910	-3.30916670	0.00000000
H	0.00000000	-4.44231650	0.00000000
H	2.12538910	-3.30916670	0.00000000
H	2.35289510	-1.11448570	0.00000000

Table S18

Structure of FeL_2, triplet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.00000000
N	-1.37147350	1.38128270	0.00000000
N	-1.37147350	-1.38128270	0.00000000
N	1.37147350	-1.38128270	0.00000000
N	1.37147350	1.38128270	0.00000000
C	-1.22149860	2.69058130	0.00000000
C	0.00000000	3.36074100	0.00000000
C	1.22149860	2.69058130	0.00000000
C	-1.22149860	-2.69058130	0.00000000
C	0.00000000	-3.36074100	0.00000000
C	1.22149860	-2.69058130	0.00000000
H	-2.12277800	3.30412440	0.00000000
H	0.00000000	4.44060240	0.00000000
H	2.12277800	3.30412440	0.00000000
H	2.34934230	1.11483790	0.00000000
H	-2.34934230	1.11483790	0.00000000
H	-2.34934230	-1.11483790	0.00000000
H	-2.12277800	-3.30412440	0.00000000
H	0.00000000	-4.44060240	0.00000000
H	2.12277800	-3.30412440	0.00000000
H	2.34934230	-1.11483790	0.00000000

Table S19

Structure of FeL_2NH_3, singlet, atomic coordinates in Å.

Fe	-0.00218310	0.06079870	0.00000000
N	-1.36904410	0.18675890	1.33896730
N	-1.36904410	0.18675890	-1.33896730
N	1.36059840	0.21857860	-1.34234400
N	1.36059840	0.21857860	1.34234400
C	-1.23948680	0.21866990	2.66355940
C	-0.00809750	0.20262360	3.33632500
C	1.22448910	0.23669100	2.66780800
C	-1.23948680	0.21866990	-2.66355940
C	-0.00809750	0.20262360	-3.33632500
C	1.22448910	0.23669100	-2.66780800
H	-2.15249060	0.28460800	3.27008650
H	-0.00975670	0.23556610	4.42421860
H	2.13434600	0.31011100	3.27841670
H	2.34532590	0.27409840	1.05972010
H	-2.35350200	0.22972950	1.05248810
H	-2.35350200	0.22972950	-1.05248810

H	-2.15249060	0.28460800	-3.27008650
H	-0.00975670	0.23556610	-4.42421860
H	2.13434600	0.31011100	-3.27841670
H	2.34532590	0.27409840	-1.05972010
N	0.05505820	-1.88893400	0.00000000
H	-0.88619230	-2.29006730	0.00000000
H	0.54967830	-2.22240210	-0.83399670
H	0.54967830	-2.22240210	0.83399670

Table S20

Structure of FeL_2NH_3, triplet, atomic coordinates in Å.

Fe	-0.00222990	0.10499610	0.00000000
N	-1.36100430	0.21775360	1.33365260
N	-1.36100430	0.21775360	-1.33365260
N	1.35557320	0.23452920	-1.33424610
N	1.35557320	0.23452920	1.33424610
C	-1.23179330	0.24514410	2.66090170
C	-0.00340210	0.22613710	3.33254170
C	1.22501410	0.26029570	2.66194880
C	-1.23179330	0.24514410	-2.66090170
C	-0.00340210	0.22613710	-3.33254170
C	1.22501410	0.26029570	-2.66194880
H	-2.14605930	0.30434210	3.26510540
H	-0.00395150	0.25243660	4.42064680
H	2.13812890	0.33107510	3.26671340
H	2.33698360	0.31422170	1.04850160
H	-2.34321610	0.28494230	1.04734710
H	-2.34321610	0.28494230	-1.04734710
H	-2.14605930	0.30434210	-3.26510540
H	-0.00395150	0.25243660	-4.42064680
H	2.13812890	0.33107510	-3.26671340
H	2.33698360	0.31422170	-1.04850160
N	0.02928950	-2.23223390	0.00000000
H	-0.90461460	-2.64614190	0.00000000
H	0.52548890	-2.56577400	-0.82852770
H	0.52548890	-2.56577400	0.82852770

Table S21

Structure of FeL_2CN^-, singlet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.18214820
N	1.35699070	1.33536960	0.36003930
N	1.35699070	-1.33536960	0.36003930

N	-1.35699070	-1.33536960	0.36003930
N	-1.35699070	1.33536960	0.36003930
C	1.23136980	2.65852020	0.36363940
C	0.00000000	3.33350890	0.33922450
C	-1.23136980	2.65852020	0.36363940
C	1.23136980	-2.65852020	0.36363940
C	0.00000000	-3.33350890	0.33922450
C	-1.23136980	-2.65852020	0.36363940
H	2.14765370	3.26710810	0.39701040
H	0.00000000	4.42300160	0.35980820
H	-2.14765370	3.26710810	0.39701040
H	-2.34107800	1.04429280	0.32381920
H	2.34107800	1.04429280	0.32381920
H	2.34107800	-1.04429280	0.32381920
H	2.14765370	-3.26710810	0.39701040
H	0.00000000	-4.42300160	0.35980820
H	-2.14765370	-3.26710810	0.39701040
H	-2.34107800	-1.04429280	0.32381920
C	0.00000000	0.00000000	-1.65491640
N	0.00000000	0.00000000	-2.83570620

Table S22

Structure of FeL_2CN^-, triplet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.19416790
N	1.35724050	1.33573210	0.40296040
N	1.35724050	-1.33573210	0.40296040
N	-1.35724050	-1.33573210	0.40296040
N	-1.35724050	1.33573210	0.40296040
C	1.22975670	2.65974030	0.42268400
C	0.00000000	3.33392990	0.38214280
C	-1.22975670	2.65974030	0.42268400
C	1.22975670	-2.65974030	0.42268400
C	0.00000000	-3.33392990	0.38214280
C	-1.22975670	-2.65974030	0.42268400
H	2.14436060	3.26750700	0.48272160
H	0.00000000	4.42330370	0.40157580
H	-2.14436060	3.26750700	0.48272160
H	-2.33906960	1.04190090	0.43987740
H	2.33906960	1.04190090	0.43987740
H	2.33906960	-1.04190090	0.43987740
H	2.14436060	-3.26750700	0.48272160
H	0.00000000	-4.42330370	0.40157580
H	-2.14436060	-3.26750700	0.48272160

H	-2.33906960	-1.04190090	0.43987740
C	0.00000000	0.00000000	-1.95862640
N	0.00000000	0.00000000	-3.13510650

Table S23

Structure of FeL_2SH, doublet, atomic coordinates in Å.

Fe	-0.00352460	-0.17590940	0.00000000
N	-1.35286510	-0.37903260	1.31916590
N	-1.35286510	-0.37903260	-1.31916590
N	1.33550720	-0.42014390	-1.31458180
N	1.33550720	-0.42014390	1.31458180
C	-1.23112600	-0.40865700	2.64258980
C	-0.00552840	-0.39963640	3.31562340
C	1.21654790	-0.44630950	2.63948820
C	-1.23112600	-0.40865700	-2.64258980
C	-0.00552840	-0.39963640	-3.31562340
C	1.21654790	-0.44630950	-2.63948820
H	-2.14857330	-0.47004900	3.24002060
H	-0.00445560	-0.42946980	4.40310140
H	2.13371590	-0.53817470	3.23335520
H	2.31470870	-0.48245160	1.01843410
H	-2.33402480	-0.40480740	1.02530440
H	-2.33402480	-0.40480740	-1.02530440
H	-2.14857330	-0.47004900	-3.24002060
H	-0.00445560	-0.42946980	-4.40310140
H	2.13371590	-0.53817470	-3.23335520
H	2.31470870	-0.48245160	-1.01843410
S	-0.00309900	2.01947150	0.00000000
H	1.33272060	2.26720190	0.00000000

Table S24

Structure of FeL_2SH, quartet, atomic coordinates in Å.

Fe	0.01496160	-0.13001700	0.00000000
N	-1.32235060	-0.55063110	1.34386540
N	-1.32235060	-0.55063110	-1.34386540
N	1.38207460	-0.38409340	-1.35001410
N	1.38207460	-0.38409340	1.35001410
C	-1.19019630	-0.57240620	2.66048600
C	0.02572970	-0.46761670	3.34356580
C	1.24797670	-0.43515190	2.66679230
C	-1.19019630	-0.57240620	-2.66048600
C	0.02572970	-0.46761670	-3.34356580

C	1.24797670	-0.43515190	-2.66679230
H	-2.10111510	-0.69939500	3.25936070
H	0.02451850	-0.49709400	4.43022300
H	2.16510920	-0.46925460	3.26865630
H	2.36220250	-0.39542300	1.05847580
H	-2.29460480	-0.66651080	1.04911100
H	-2.29460480	-0.66651080	-1.04911100
H	-2.10111510	-0.69939500	-3.25936070
H	0.02451850	-0.49709400	-4.43022300
H	2.16510920	-0.46925460	-3.26865630
H	2.36220250	-0.39542300	-1.05847580
S	-0.18658070	2.24152760	0.00000000
H	1.14391570	2.48999840	0.00000000

Table S25

Structure of FeL_2Cl, doublet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.20584840
N	-1.34023150	1.31934600	0.41897910
N	-1.34023150	-1.31934600	0.41897910
N	1.34023150	-1.31934600	0.41897910
N	1.34023150	1.31934600	0.41897910
C	-1.22337780	2.64321530	0.43943430
C	0.00000000	3.31887360	0.41897910
C	1.22337780	2.64321530	0.43943430
C	-1.22337780	-2.64321530	0.43943430
C	0.00000000	-3.31887360	0.41897910
C	1.22337780	-2.64321530	0.43943430
H	-2.14282400	3.23717550	0.49972000
H	0.00000000	4.40638740	0.44340860
H	2.14282400	3.23717550	0.49972000
H	2.32047310	1.02222080	0.43115170
H	-2.32047310	1.02222080	0.43115170
H	-2.32047310	-1.02222080	0.43115170
H	-2.14282400	-3.23717550	0.49972000
H	0.00000000	-4.40638740	0.44340860
H	2.14282400	-3.23717550	0.49972000
H	2.32047310	-1.02222080	0.43115170
Cl	0.00000000	0.00000000	-1.99686980

Table S26

Structure of FeL_2Cl, quartet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	0.14919470

N	-1.35416770	1.34526690	0.47332310
N	-1.35416770	-1.34526690	0.47332310
N	1.35416770	-1.34526690	0.47332310
N	1.35416770	1.34526690	0.47332310
C	-1.22564200	2.66671410	0.49975670
C	0.00000000	3.35488900	0.47332310
C	1.22564200	2.66671410	0.49975670
C	-1.22564200	-2.66671410	0.49975670
C	0.00000000	-3.35488900	0.47332310
C	1.22564200	-2.66671410	0.49975670
H	-2.15170060	3.27161680	0.56407040
H	0.00000000	4.45176220	0.49753540
H	2.15170060	3.27161680	0.56407040
H	2.33806680	1.04728730	0.50425320
H	-2.33806680	1.04728730	0.50425320
H	-2.33806680	-1.04728730	0.50425320
H	-2.15170060	-3.27161680	0.56407040
H	0.00000000	-4.45176220	0.49753540
H	2.15170060	-3.27161680	0.56407040
H	2.33806680	-1.04728730	0.50425320
Cl	0.00000000	0.00000000	-2.13078090

Table S27

Structure of $FeOL_2Cl$, doublet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	-0.32978040
N	-1.37723900	1.37667510	-0.18354550
N	-1.37723900	-1.37667510	-0.18354550
N	1.37723900	-1.37667510	-0.18354550
N	1.37723900	1.37667510	-0.18354550
C	-1.22397680	2.68304150	-0.16226720
C	0.00000000	3.35902250	-0.18354550
C	1.22397680	2.68304150	-0.16226720
C	-1.22397680	-2.68304150	-0.16226720
C	0.00000000	-3.35902250	-0.18354550
C	1.22397680	-2.68304150	-0.16226720
H	-2.13836460	3.28704490	-0.10475360
H	0.00000000	4.44545390	-0.16674390
H	2.13836460	3.28704490	-0.10475360
H	2.34293440	1.06122070	-0.09968920
H	-2.34293440	1.06122070	-0.09968920
H	-2.34293440	-1.06122070	-0.09968920
H	-2.13836460	-3.28704490	-0.10475360
H	0.00000000	-4.44545390	-0.16674390

H	2.13836460	-3.28704490	-0.10475360
H	2.34293440	-1.06122070	-0.09968920
O	0.00000000	0.00000000	-1.93858390
Cl	0.00000000	0.00000000	2.06142120

Table S28

Structure of $FeOL_2Cl$, quartet, atomic coordinates in Å.

Fe	0.00000000	0.00000000	-0.25597740
N	-1.37014370	1.37252750	-0.21043360
N	-1.37014370	-1.37252750	-0.21043360
N	1.37014370	-1.37252750	-0.21043360
N	1.37014370	1.37252750	-0.21043360
C	-1.23381330	2.68103110	-0.21243980
C	0.00000000	3.35018080	-0.21043360
C	1.23381330	2.68103110	-0.21243980
C	-1.23381330	-2.68103110	-0.21243980
C	0.00000000	-3.35018080	-0.21043360
C	1.23381330	-2.68103110	-0.21243980
H	-2.14457050	3.29190390	-0.21013060
H	0.00000000	4.43784060	-0.20615330
H	2.14457050	3.29190390	-0.21013060
H	2.34732990	1.07100110	-0.21257000
H	-2.34732990	1.07100110	-0.21257000
H	-2.34732990	-1.07100110	-0.21257000
H	-2.14457050	-3.29190390	-0.21013060
H	0.00000000	-4.43784060	-0.20615330
H	2.14457050	-3.29190390	-0.21013060
H	2.34732990	-1.07100110	-0.21257000
O	0.00000000	0.00000000	-1.95448820
Cl	0.00000000	0.00000000	2.10809950

Table S29

Structure of FeL_2OH_2, singlet, atomic coordinates in Å.

N	-0.21450000	1.38930000	1.38620000
C	-0.23180000	1.23020000	2.69590000
C	-0.20200000	0.00090000	3.36190000
C	-0.23380000	-1.22830000	2.69590000
N	-0.21680000	-1.38750000	1.38620000
N	-0.21450000	1.38930000	-1.38620000
C	-0.23180000	1.23020000	-2.69590000
C	-0.20200000	0.00090000	-3.36190000
C	-0.23380000	-1.22830000	-2.69590000

N	-0.21680000	-1.38750000	-1.38620000
H	-0.28270000	2.36800000	1.12300000
H	-0.29030000	2.12620000	3.32040000
H	-0.22430000	0.00090000	4.44500000
H	-0.29370000	-2.12420000	3.32040000
H	-0.29030000	2.12620000	-3.32040000
H	-0.22430000	0.00090000	-4.44500000
H	-0.29370000	-2.12420000	-3.32040000
H	-0.28650000	-2.36610000	-1.12300000
H	-0.28270000	2.36800000	-1.12300000
H	-0.28650000	-2.36610000	1.12300000
Fe	-0.08860000	0.00080000	0.00000000
O	1.92970000	0.00000000	0.00000000
H	2.46530000	0.79420000	0.00000000
H	2.46520000	-0.79420000	0.00000000

Table S30

Structure of FeL_2OH_2, triplet, atomic coordinates in Å.

N	-0.23580000	1.37620000	1.37670000
C	-0.25180000	1.22460000	2.68980000
C	-0.22690000	-0.00070000	3.35830000
C	-0.25110000	-1.22610000	2.68980000
N	-0.23530000	-1.37760000	1.37670000
N	-0.23580000	1.37620000	-1.37670000
C	-0.25180000	1.22460000	-2.68980000
C	-0.22690000	-0.00070000	-3.35830000
C	-0.25110000	-1.22610000	-2.68980000
N	-0.23530000	-1.37760000	-1.37670000
H	-0.30690000	2.35240000	1.10770000
H	-0.30390000	2.12550000	3.30620000
H	-0.24330000	-0.00070000	4.44130000
H	-0.30210000	-2.12700000	3.30620000
H	-0.30390000	2.12550000	-3.30620000
H	-0.24330000	-0.00070000	-4.44130000
H	-0.30210000	-2.12700000	-3.30620000
H	-0.30550000	-2.35380000	-1.10770000
H	-0.30690000	2.35240000	-1.10770000
H	-0.30550000	-2.35380000	1.10770000
Fe	-0.13220000	-0.00080000	0.00000000
O	2.21690000	0.00000000	0.00000000
H	2.77520000	0.78240000	0.00000000
H	2.77530000	-0.78240000	0.00000000

Table S31

Structure of FePSH, doublet, atomic coordinates in Å

Fe	-0.00005350	0.00956700	0.00000000
N	-1.40738510	0.21377680	1.39577640
N	1.41244740	0.21024740	1.39688830
N	-1.40738510	0.21377680	-1.39577640
N	1.41244740	0.21024740	-1.39688830
C	1.23031330	0.15333470	-2.76792730
C	2.78495660	0.28401100	-1.22453320
C	3.46162540	0.28775840	-2.49561340
C	2.49580550	0.19930280	-3.45388420
C	0.00286860	0.10583400	-3.40748930
C	-1.22451340	0.15583760	-2.76722530
C	-2.48933350	0.20557400	-3.45344040
C	-3.45601930	0.29693100	-2.49590210
C	-2.78057600	0.29058870	-1.22460710
C	-3.42579860	0.33506040	0.00000000
C	-2.78057600	0.29058870	1.22460710
C	-3.45601930	0.29693100	2.49590210
C	-2.48933350	0.20557400	3.45344040
C	-1.22451340	0.15583760	2.76722530
C	0.00286860	0.10583400	3.40748930
C	1.23031330	0.15333470	2.76792730
C	2.49580550	0.19930280	3.45388420
C	3.46162540	0.28775840	2.49561340
C	2.78495660	0.28401100	1.22453320
C	3.43009160	0.32736760	0.00000000
H	4.51888320	0.38185380	0.00000000
H	4.53915890	0.35209710	-2.62065300
H	2.61245970	0.17686960	-4.53423600
H	0.00234800	0.06498380	-4.49705980
H	-2.60500860	0.18460740	-4.53393190
H	-4.53324650	0.36461670	-2.62193930
H	-4.51448320	0.39261850	0.00000000
H	-4.53324650	0.36461670	2.62193930
H	-2.60500860	0.18460740	4.53393190
H	0.00234800	0.06498380	4.49705980
H	2.61245970	0.17686960	4.53423600
H	4.53915890	0.35209710	2.62065300
S	0.01560540	-2.13877500	0.00000000
H	-1.31995960	-2.40186020	0.00000000

Table S32

Structure of FePSH, quartet, atomic coordinates in Å

Fe	-0.00356330	-0.04286290	0.00000000
N	-1.41461370	0.22781550	1.41170220
N	1.41131280	0.23592380	1.41145480
N	-1.41461370	0.22781550	-1.41170220
N	1.41131280	0.23592380	-1.41145480
C	1.22637420	0.24141560	-2.78078110
C	2.77885630	0.27400730	-1.22793000
C	3.45863820	0.30456070	-2.49685890
C	2.49375250	0.28210560	-3.46182110
C	-0.00121400	0.22856390	-3.42522850
C	-1.22917120	0.23714210	-2.78141900
C	-2.49629030	0.27966270	-3.46221080
C	-3.46165790	0.30093120	-2.49731980
C	-2.78267810	0.26817430	-1.22823310
C	-3.42749000	0.27927130	0.00000000
C	-2.78267810	0.26817430	1.22823310
C	-3.46165790	0.30093120	2.49731980
C	-2.49629030	0.27966270	3.46221080
C	-1.22917120	0.23714210	2.78141900
C	-0.00121400	0.22856390	3.42522850
C	1.22637420	0.24141560	2.78078110
C	2.49375250	0.28210560	3.46182110
C	3.45863820	0.30456070	2.49685890
C	2.77885630	0.27400730	1.22793000
C	3.42368770	0.28445910	0.00000000
H	4.51330030	0.31083570	0.00000000
H	4.53803210	0.34091040	-2.61800130
H	2.61407020	0.29708900	-4.54173480
H	-0.00097350	0.23299980	-4.51515380
H	-2.61646910	0.29786840	-4.54209250
H	-4.54094950	0.33920690	-2.61898800
H	-4.51705260	0.30980360	0.00000000
H	-4.54094950	0.33920690	2.61898800
H	-2.61646910	0.29786840	4.54209250
H	-0.00097350	0.23299980	4.51515380
H	2.61407020	0.29708900	4.54173480
H	4.53803210	0.34091040	2.61800130
S	0.06137420	-2.38624830	0.00000000
H	-1.28240080	-2.55225330	0.00000000

Table S33

Structure of FePIm, singlet, atomic coordinates in Å

C	-2.77047840	-0.55487600	1.22903880
N	-1.39436540	-0.52079530	1.40419800
C	-1.21636210	-0.52687680	2.77939300
C	-2.48472250	-0.57678430	3.46218460
C	-3.45062860	-0.59354880	2.49980440
Fe	0.00960630	-0.36069210	0.00000000
N	-1.39436540	-0.52079530	-1.40419800
C	-1.21636210	-0.52687680	-2.77939300
C	-2.48472250	-0.57678430	-3.46218460
C	-3.45062860	-0.59354880	-2.49980440
C	-2.77047840	-0.55487600	-1.22903880
C	0.01159970	-0.50650690	-3.42149860
C	1.23916840	-0.50612550	-2.77921160
N	1.41666840	-0.49601050	-1.40386670
C	2.79232830	-0.51516330	-1.22853940
C	3.47347650	-0.54576790	-2.49912210
C	2.50842080	-0.53973370	-3.46192660
C	-3.41352330	-0.56053940	0.00000000
C	3.43536320	-0.51406130	0.00000000
C	2.79232830	-0.51516330	1.22853940
N	1.41666840	-0.49601050	1.40386670
C	1.23916840	-0.50612550	2.77921160
C	2.50842080	-0.53973370	3.46192660
C	3.47347650	-0.54576790	2.49912210
C	0.01159970	-0.50650690	3.42149860
H	-4.50396090	-0.59198480	0.00000000
H	-4.52980550	-0.64256870	-2.62144980
H	-2.60287030	-0.60726620	-4.54240670
H	0.01178590	-0.51658790	-4.51217570
H	2.62731910	-0.56800220	-4.54209090
H	4.55326080	-0.58037010	-2.61993080
H	4.52602620	-0.53158350	0.00000000
H	4.55326080	-0.58037010	2.61993080
H	2.62731910	-0.56800220	4.54209090
H	0.01178590	-0.51658790	4.51217570
H	-2.60287030	-0.60726620	4.54240670
H	-4.52980550	-0.64256870	2.62144980
N	-0.02057780	1.53207710	0.00000000
C	-1.11355330	2.29579360	0.00000000
N	-0.75043320	3.60620740	0.00000000
C	0.62771290	3.68007150	0.00000000
C	1.07268240	2.38270400	0.00000000
H	-2.13640510	1.93853340	0.00000000
H	-1.39216450	4.38961210	0.00000000

H	1.15958390	4.62308300	0.00000000
H	2.08618430	2.00140350	0.00000000

Table S34

Structure of FePIm, triplet, atomic coordinates in Å

C	-2.77832390	-0.64434610	1.22958930
N	-1.40691910	-0.56733250	1.40591750
C	-1.21805760	-0.55721920	2.77649630
C	-2.48305200	-0.62162860	3.46154600
C	-3.45366960	-0.67860640	2.50232810
Fe	0.01414540	-0.41502250	0.00000000
N	-1.40691910	-0.56733250	-1.40591750
C	-1.21805760	-0.55721920	-2.77649630
C	-2.48305200	-0.62162860	-3.46154600
C	-3.45366960	-0.67860640	-2.50232810
C	-2.77832390	-0.64434610	-1.22958930
C	0.01439460	-0.52185330	-3.41487120
C	1.24658530	-0.53124380	-2.77576910
N	1.43539250	-0.53735370	-1.40528790
C	2.80780440	-0.58639100	-1.22900260
C	3.48400220	-0.60716020	-2.50165120
C	2.51301380	-0.56960350	-3.46083150
C	-3.42327330	-0.67658390	0.00000000
C	3.45331050	-0.60657270	0.00000000
C	2.80780440	-0.58639100	1.22900260
N	1.43539250	-0.53735370	1.40528790
C	1.24658530	-0.53124380	2.77576910
C	2.51301380	-0.56960350	3.46083150
C	3.48400220	-0.60716020	2.50165120
C	0.01439460	-0.52185330	3.41487120
H	-4.51192790	-0.74019970	0.00000000
H	-4.53088530	-0.74741330	-2.63012850
H	-2.59965790	-0.63265870	-4.54253510
H	0.01477110	-0.52011790	-4.50563840
H	2.62994400	-0.57660940	-4.54179320
H	4.56247700	-0.65223540	-2.62891740
H	4.54300520	-0.64643280	0.00000000
H	4.56247700	-0.65223540	2.62891740
H	2.62994400	-0.57660940	4.54179320
H	0.01477110	-0.52011790	4.50563840
H	-2.59965790	-0.63265870	4.54253510
H	-4.53088530	-0.74741330	2.63012850
N	-0.01655860	1.81697290	0.00000000

C	-1.11235770	2.56079890	0.00000000
N	-0.78857000	3.88263410	0.00000000
C	0.59064530	3.98464410	0.00000000
C	1.05129720	2.69059840	0.00000000
H	-2.13094480	2.18700000	0.00000000
H	-1.44445610	4.65584180	0.00000000
H	1.09908080	4.94128490	0.00000000
H	2.07382840	2.32990470	0.00000000

Table S35. The singlet-triplet excitation energies of FeA_2 with spin flip up and spin flip down schemes respectively, in eV.

FeA_2	**Spin flip up**		**Spin flip down**	
	S-T gaps	D<S^2>	S-T gaps	D<S^2>
SVWN5	0.09	0	0.05	-0.0007
BLYP	-0.17	0	1.01	-0.5027
B3LYP	-0.92	0	-0.31	-0.0003
BHandHLYP	-1.03	0	-0.21	-0.0001
CAM-B3LYP	-0.95	0	-0.28	-0.0002
LC-BLYP	-0.27	0	0.42	-0.9877
CCSD(T)	-1.54		-1.54	