Influence of Ligand Substituent Conformation on the Spin State of an Iron(II)/Di(pyrazol-1-yl)pyridine Complex

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Supporting Information

Experimental

The iron(II) complexes of 4-(methylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine (bpp^{SMe}),[1] 4-(*iso*-propylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine (bpp^{SiPr})[2] and 4-(*tert*-butylsulfanyl)-2,6-di(pyrazol-1-yl)pyridine (bpp^{StBu})[3] have been reported previously. The same of $[Fe(bpp^{StBu})_2][BF_4]_2$ (**3[BF$_4$]$_2$**) used for the solution magnetic measurement was prepared by our published procedure.[3]

The magnetic susceptibility measurement of **3[BF$_4$]$_2$** in solution has not been published before, and was obtained by Evans method using a Bruker Avance 500 FT spectrometer operating at 500.1 MHz.[4] Tetramethylsilane was added to all the solutions as an internal standard. A diamagnetic correction for the sample,[5] and a correction for the variation of the density of the solvent with temperature,[6] were applied to these data. Thermodynamic parameters were derived by fitting these data to eq 1 and 2:*

$$\ln[(1-n\mathrm{HS}(T))/n\mathrm{HS}(T)] = \Delta H/RT - \Delta S/R \quad (1)$$

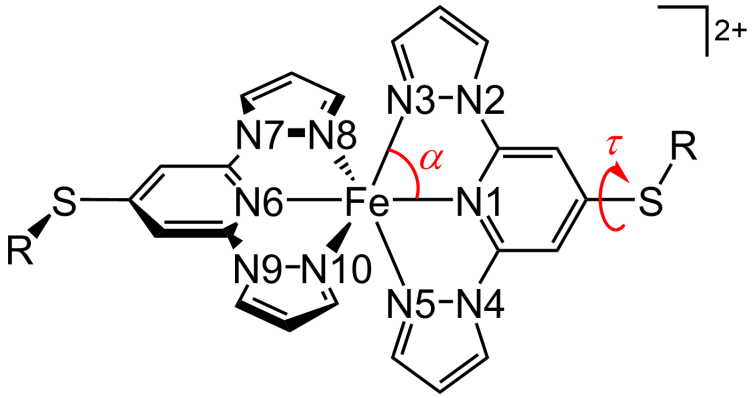
$$\Delta S = \Delta H/T_{½} \quad (2)$$

DFT calculations were performed using *SPARTAN'18* for Windows,[7] with the B86PW91 functional and def2-SVP basis set. Low-spin systems were treated as spin-restricted, and high-spin systems were treated as spin-unrestricted. The calculations were performed in the gas phase, since a solvent gradient for iron is not implemented in *SPARTAN'18* at the time of writing.

Published atomic coordinates for high-spin and low-spin $[Fe(bpp)_2]^{2+}$, minimised under the same protocol, were used as the starting point for the geometry minimisations,[8] with the appropriate alkylsulfanyl substituents appended for each complex. The resultant minimum structures were then reminimised in the perpendicular alkylsulfanyl substituent conformation (Scheme 2), with the C{pyridyl}– C{pyridyl}–S–C{R} torsions fixed at ±90°. This was necessary to prevent the molecules relaxing back toward their parallel alkylsulfanyl conformations, which are the global minimum structures in this computational protocol.

Starting structures for the metal-free ligands were produced from the minimised complexes, and were minimised freely and with fixed C{pyridyl}– C{pyridyl}–S–C{R} torsions as described above.

*Equation 1 is a rearrangement of $\Delta G = -RT\ln K$, where K is the ratio of high-spin and low-spin molecules in the sample at temperature T, and $\Delta G = \Delta H - T\Delta S$. Equation 2 reflects that, at $T_{½}$, the SCO is at equilibrium so that $\Delta G = 0$ and $\Delta H = T_{½}\Delta S$.



Scheme S1 Atom numbering scheme and structural parameters discussed in the energy-minimised structures of the compounds (Table S1).

α is the average bite angle of the tridentate ligands, while τ is the average of the magnitude of the C{pyridyl}–C{pyridyl}–S–C{R} torsion angles in the molecule.

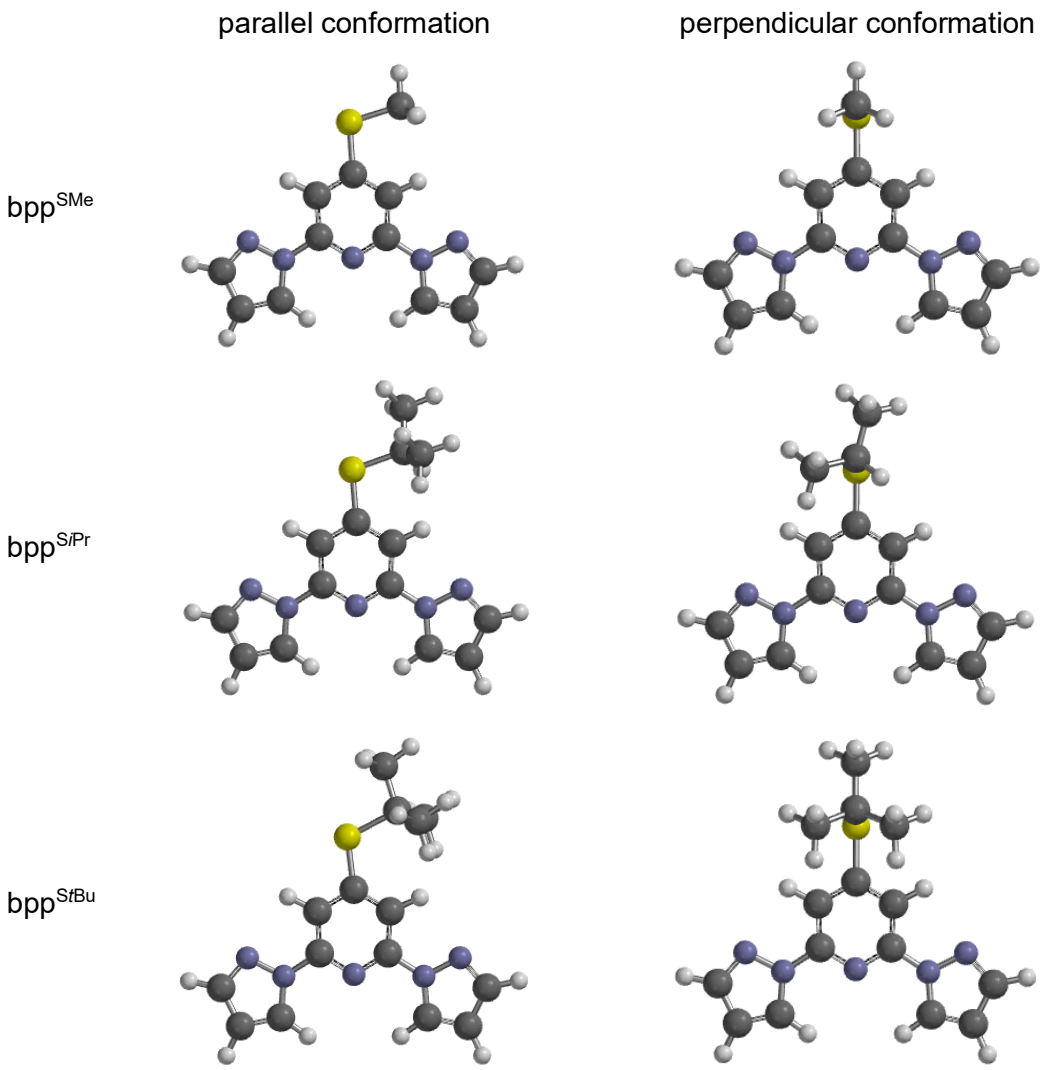


Figure S1 DFT energy-minimised structures of the organic ligands in this work, with parallel and perpendicular substituent conformations.

Colour code: C, dark grey; H, white; N, blue; S, yellow.

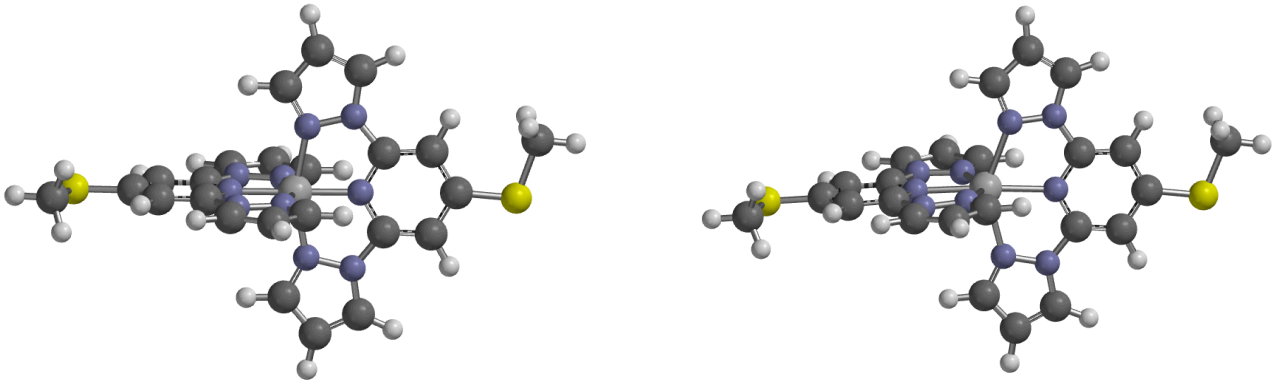
As usual for *tris*-heterocycles of this type, the ligands minimised with a *transoid* disposition of pyridyl and pyrazolyl N donor atoms.[9] The pyrazolyl rings must rotate by *ca* 180° to adopt a *cisoid* conformation suitable for metal binding. This should have a minimal effect on the relative energies of the sulfanyl substituent conformations however, which are the main interest of this calculation.

Table S1 Energies of the minimised organic ligands (Figure S1). ΔE{conf} is the energy difference between the parallel and perpendicular sulfanyl conformations. The average C{pyridyl}–C{pyridyl}–S–C{R} torsion (τ, Scheme 1) in the parallel conformations is also given; τ was fixed at ±90° in the perpendicular conformations.

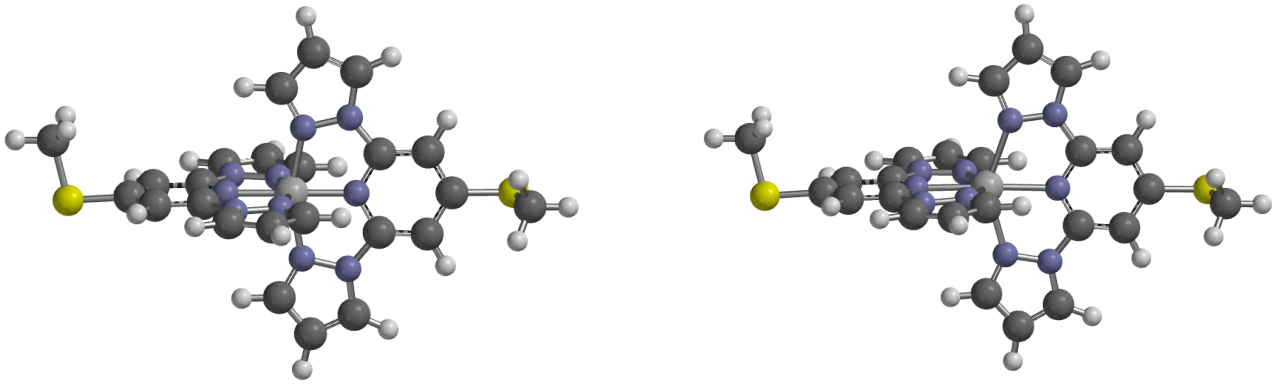
	τ{parallel} / deg	E{parallel} / Ha	E{perpendicular} / Ha	ΔE{conf} / Ha	ΔE{conf} / kcal mol^{-1}
bpp^{SMe}	0.10	-1135.477292	-1135.470042	0.007250	4.5
bpp^{SiPr}	3.20	-1214.073111	-1214.067814	0.005297	3.3
bpp^{StBu}	0.05	-1253.366196	-1253.365016	0.001180	0.7

Low-spin **High-spin**

1^{2+}, parallel conformation



1^{2+}, perpendicular conformation



2^{2+}, parallel conformation

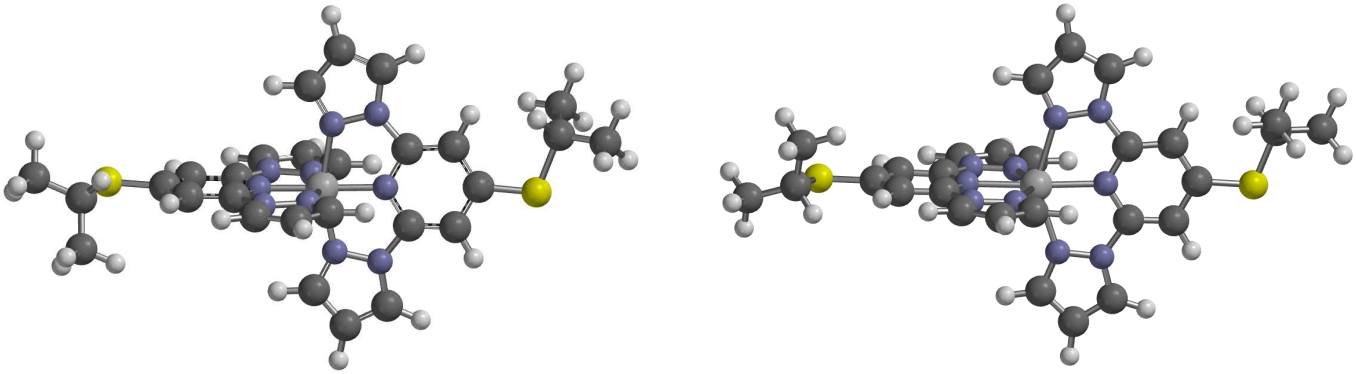
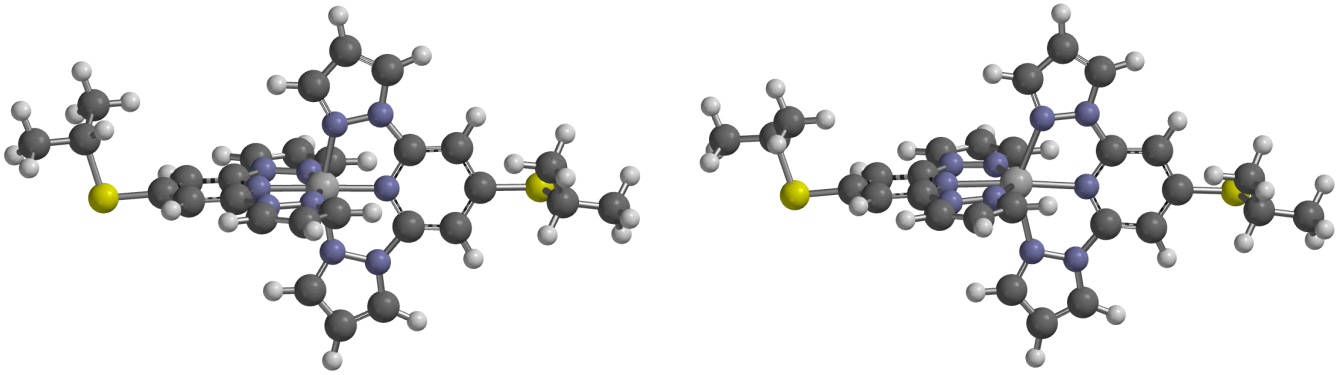


Figure S2 DFT energy-minimised structures of the compounds in this work, with parallel and perpendicular ligand conformations.

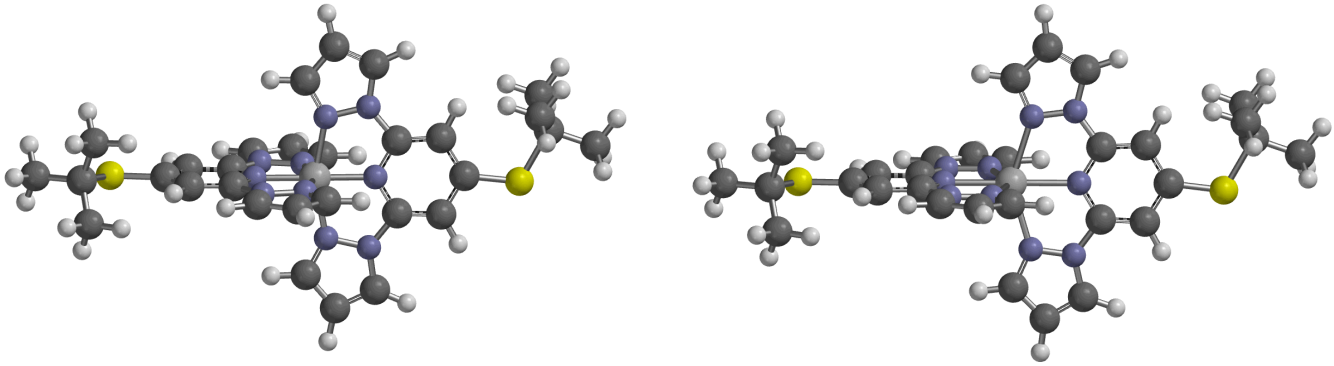
Colour code: C, dark grey; H, white; Fe, pale grey; N, blue; S, yellow.

Low-spin **High-spin**

2^{2+}, perpendicular conformation



3^{2+}, parallel conformation



3^{2+}, perpendicular conformation

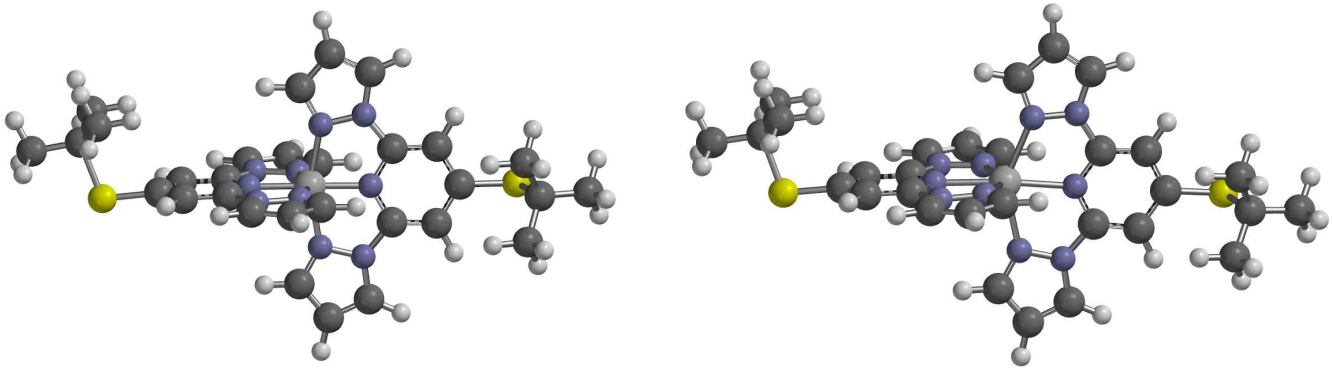


Figure S2 continued. The low-spin **3**$^{2+}$ molecules are the same as in Figure 2 of the main article.

Table S2 Computed metric parameters for the energy-minimise d complexes (Å, °; Figure S42). Experimental crystallographic data are also included in square brackets for comparison, where this is available. The atom numbering in the table is shown in Scheme S1. α is the average bite angle of the tridentate ligands, while τ is the average of the magnitude of the C{pyridyl}–C{pyridyl}–S–C{R} torsion angles in the molecule (Scheme S1).

	$[Fe(bpp)_2]^{2+}$ [a]		$\mathbf{1}^{2+}$ (R = SMe)			
Conformation			parallel[b]		perpendicular	
	HS	LS	HS	LS	HS	LS
Fe–N1	2.155 [2.1390(14)]	1.906 [1.9049(15)]	2.141 [2.118(4)]	1.904 [1.901(5)]	2.153	1.903
Fe–N3	2.202 [2.2063(17)]	1.980 [1.9913(17)]	2.206 [2.168(5)]	1.978 [1.972(5)]	2.203	1.980
Fe–N5	2.201 [2.1865(19)]	1.979 [1.9751(17)]	2.210 [2.160(5)]	1.980 [1.965(5)]	2.206	1.979
Fe–N6	2.157 [2.1402(15)]	1.904 [1.9097(16)]	2.147 [2.103(4)]	1,906 [1.901(4)]	2.153	1.903
Fe–N8	2.205 [2.203(2)]	1.980 [1.9760(18)]	2.205 [2.161(5)]	1.980 [1.975(5)]	2.203	1.979
Fe–N10	2.200 [2.1964(19)]	1.979 [1.9912(18)]	2.210 [2.167(5)]	1.981 [1.980(5)]	2.206	1.980
Fe–N{pyridyl}$_{av}$	2.156 [2.140(2)]	1.905 [1.907(2)]	2.144 [2.111(6)]	1.905 [1.901(7)]	2.153	1.903
Fe–N{pyrazolyl}$_{av}$	2.202 [2.198(4)]	1.980 [1.983(4)]	2.208 [2.128(10)]	1.980 [1.973(10)]	2.205	1.980
N1–Fe–N3	73.3 [73.68(6)]	80.1 [79.97(7)]	73.3 [73.58(18)]	80.0 [80.19(19)]	73.2	80.1
N1–Fe–N5	73.4 [73.23(6)]	80.2 [80.23(7)]	73.3 [73.20(18)]	79.9 [79.7(2)]	73.2	80.1
N1–Fe–N6	179.5 [172.98(7)]	179.6 [178.15(8)]	173.7 [168.3(2)]	179.9 [175.2(2)]	176.1	179.3
N1–Fe–N8	106.5 [100.15(7)]	100.0 [98.08(7)]	111.5 [113.08(19)]	100.1 [102.6(2)]	104.0	100.4
N1–Fe–N10	106.9 [113.16(7)]	99.7 [101.77(7)]	102.4 [100.74(18)]	100.2 [98.0(2)]	109.6	99.3
N3–Fe–N5	146.7 [146.88(7)]	160.3 [160.19(7)]	146.6 [146.57(18)]	159.9 [159.88(19)]	146.4	160.2
N3–Fe–N6	107.0 [104.33(6)]	100.3 [100.80(7)]	111.4 [96.42(19)]	99.9 [95.64(19)]	109.6	100.4
N3–Fe–N8	91.8 [93.03(7)]	91.7 [92.15(7)]	91.5 [97.4(2)]	91.4 [92.8(2)]	97.8	91.7
N3–Fe–N10	97.4 [98.35(7)]	91.6 [93.10(7)]	97.3 [93.8(2)]	91.8 [92.2(2)]	91.4	91.7
N5–Fe–N6	106.3 [108.32(6)]	99.4 [98.99(7)]	102.2 [117.01(19)]	100.3 [104.5(2)]	104.0	99.3
N5–Fe–N8	97.7 [91.23(7)]	91.7 [90.23(7)]	97.7 [92.12(19)]	91.8 [91.1(2)]	92.3	91.7
N5–Fe–N10	92.1 [95.93(7)]	91.7 [91.30(7)]	92.9 [95.97(19)]	92.1 [91.0(2)]	97.8	91.7
N6–Fe–N8	73.2 [73.10(7)]	80.1 [80.22(7)]	73.1 [73.53(18)]	80.0 [79.8(2)]	73.2	80.1
N6–Fe–N10	73.4 [73.68(7)]	80.2 [79.91(7)]	73.1 [73.49(18)]	79.8 [79.76(19)]	73.2	80.1
N8–Fe–N10	146.6 [146.60(7)]	160.3 [160.06(6)]	146.0 [146.12(18)]	159.7 [159.34(19)]	146.4	160.2
α	73.3 [73.42(13)]	80.2 [80.08(14)]	73.2 [73.5(4)]	79.9 [79.9(4)]	73.2	80.1
τ	–	–	0.6	2.3	90[f]	90[f]

[a]Data from ref. 8. [b]Crystallographic data from phase 1 of **1[BF$_4$]$_2$**, ref. 1. [c]Crystallographic data from **2[BF$_4$]$_2$**·MeCN, ref. 2. [d]Crystallographic data from **3[ClO$_4$]$_2$**·MeNO$_2$, ref. 3. [e]Low-spin crystallographic data from phase 1 of **3[BF$_4$]$_2$**·*x*MeNO$_2$, ref. 3. There is no known high-spin salt of $\mathbf{3}^{2+}$ where both ligands are in the perpendicular conformation. [f]Fixed during the calculation.

Table S2 continued.

	$\mathbf{2}^{2+}$ (R = S*i*Pr)				$\mathbf{3}^{2+}$ (R = S*t*Bu)			
Conformation	parallel[c]		perpendicular		parallel[d]		perpendicular[e]	
	HS	LS	HS	LS	HS	LS	HS	LS
Fe–N1	2.140 [2.128(3)]	1.905 [1.900(2)]	2.152	1.903	2.140 [2.102(3)]	1.906 [1.899(4)]	2.151	1.903 [1.904(4)]
Fe–N3	2.212 [2.208(3)]	1.979 [1.972(2)]	2.211	1.980	2.210 [2.180(3)]	1.981 [1.967(4)]	2.214	1.979 [1.990(4)]
Fe–N5	2.205 [2.174(3)]	1.979 [1.986(2)]	2.200	1.979	2.209 [2.171(3)]	1.980 [1.986(4)]	2.199	1.980 [1.978(4)]
Fe–N6	2.140 [2.120(2)]	1.905 [1.901(2)]	2.152	1.904	2.135 [2.116(3)]	1.903 [1.900(4)]	2.151	1.903 [1.902(4)]
Fe–N8	2.209 [2.171(3)]	1.979 [1.967(2)]	2.211	1.981	2.212 [2.165(3)]	1.980 [1.977(4)]	2.214	1.979 [1.966(4)]
Fe–N10	2.208 [2.173(3)]	1.979 [1.971(2)]	2.200	1.980	2.206 [2.169(3)]	1.978 [1.980(4)]	2.199	1.980 [1.986(4)]
Fe–N{pyridyl}$_{av}$	2.140 [2.124(4)]	1.905 [1.901(3)]	2.152	1.904	2.138 [2.109(4)]	1.905 [1.903(6)]	2.151	1.903 [1.903(6)]
Fe–N{pyrazolyl}$_{av}$	2.209 [2.182(7)]	1.979 [1.974(5)]	2.206	1.980	2.209 [2.171(6)]	1.980 [1.978(8)]	2.207	1.980 [1.980(8)]
N1–Fe–N3	73.2 [72.95(10)]	79.9 [79.95(9)]	73.1	80.1	73.2 [73.67(11)]	79.8 [79.96(15)]	73.1	80.2 [79.92(16)]
N1–Fe–N5	73.3 [73.34(10)]	80.0 [79.49(9)]	73.3	80.2	73.2 [73.91(11)]	79.9 [79.86(15)]	73.3	80.1 [79.90(15)]
N1–Fe–N6	177.3 [167.64(10)]	179.2 [174.30(9)]	172.2	178.7	179.9 [173.83(11)]	179.7 [177.01(19)]	171.5	178.6 [175.75(15)]
N1–Fe–N8	108.5 [98.41(10)]	99.6 [96.62(9)]	101.3	99.0	106.8 [100.93(11)]	100.4 [98.36(15)]	100.8	98.9 [95.74(15)]
N1–Fe–N10	104.5 [115.21(10)]	100.6 [103.73(9)]	112.5	100.8	106.6 [111.95(11)]	99.7 [101.77(15)]	113.0	100.9 [104.36(15)]
N3–Fe–N5	146.4 [146.24(10)]	159.8 [159.43(9)]	146.2	160.2	146.6 [147.54(12)]	159.7 [159.81(15)]	146.2	160.2 [159.70(16)]
N3–Fe–N6	104.7 [98.11(10)]	96.0 [95.53(9)]	101.3	101.0	106.7 [103.36(11)]	100.1 [97.47(15)]	100.8	98.9 [99.90(16)]
N3–Fe–N8	97.3 [94.99(11)]	92.0 [91.94(10)]	98.2	91.7	97.2 [94.07(14)]	92.2 [91.06(16)]	91.7	91.6 [93.04(16)]
N3–Fe–N10	92.6 [95.41(10)]	91.7 [92.44(10)]	91.7	91.6	92.5 [96.45(13)]	91.8 [91.91(15)]	98.0	91.9 [89.48(15)]
N5–Fe–N6	108.9 [115.47(10)]	100.6 [105.03(9)]	112.5	98.8	106.6 [109.07(11)]	100.2 [102.72(15)]	113.0	100.9 [100.39(15)]
N5–Fe–N8	92.2 [91.53(11)]	91.7 [90.87(10)]	91.3	91.7	92.2 [93.52(13)]	91.7 [92.76(15)]	98.0	91.9 [91.15(16)]
N5–Fe–N10	97.0 [97.25(10)]	91.7 [91.97(9)]	98.2	91.8	97.2 [94.10(13)]	91.4 [91.29(16)]	91.8	91.4 [93.38(15)]
N6–Fe–N8	73.2 [73.47(10)]	79.9 [79.99(9)]	73.1	80.1	73.2 [73.69(11)]	79.9 [80.09(15)]	73.1	80.2 [80.02(15)]
N6–Fe–N10	73.3 [73.45(10)]	80.0 [79.80(9)]	73.3	80.1	73.5 [73.55(11)]	80.0 [79.79(15)]	73.3	80.1 [79.87(15)]
N8–Fe–N10	146.5 [146.38(10)]	159.8 [159.64(9)]	146.2	160.2	146.7 [147.08(11)]	159.8 [159.87(14)]	146.2	160.2 [159.87(16)]
α	73.3 [73.3(2)]	80.0 [79.8(2)]	73.2	80.1	73.3 [73.7(2)]	79.9 [79.9(3)]	73.2	80.2 [79.9(3)]
τ	5.2	4.1	90[f]	90[f]	3.2	5.6	90[f]	90[f]

[a]Data from ref. 8. [b]Crystallographic data from phase 1 of **1[BF$_4$]$_2$**, ref. 1. [c]Crystallographic data from **2[BF$_4$]$_2$**·MeCN, ref. 2. [d]Crystallographic data from **3[ClO$_4$]$_2$**·MeNO$_2$, ref. 3. [e]Low-spin crystallographic data from phase 1 of **3[BF$_4$]$_2$**·*x*MeNO$_2$, ref. 3. There is no known high-spin salt of $\mathbf{3}^{2+}$ where both ligands are in the perpendicular conformation. [f]Fixed during the calculation.

The agreement between the computed and measured low-spin structures is excellent, but the computed high-spin Fe−N distances are up to 1.8 % longer than the experimental values. That's a typical level of agreement for this level of DFT calculation. The computed high-spin Fe−N{pyridyl} bond lengths are 0.013±0.01 Å longer in the perpendicular ligand conformation than in the parallel form, but unfortunately there are no relevant crystallographic data available for comparison. The minimised coordination geometries of the low-spin complexes in both ligand conformations are identical within experimental error.

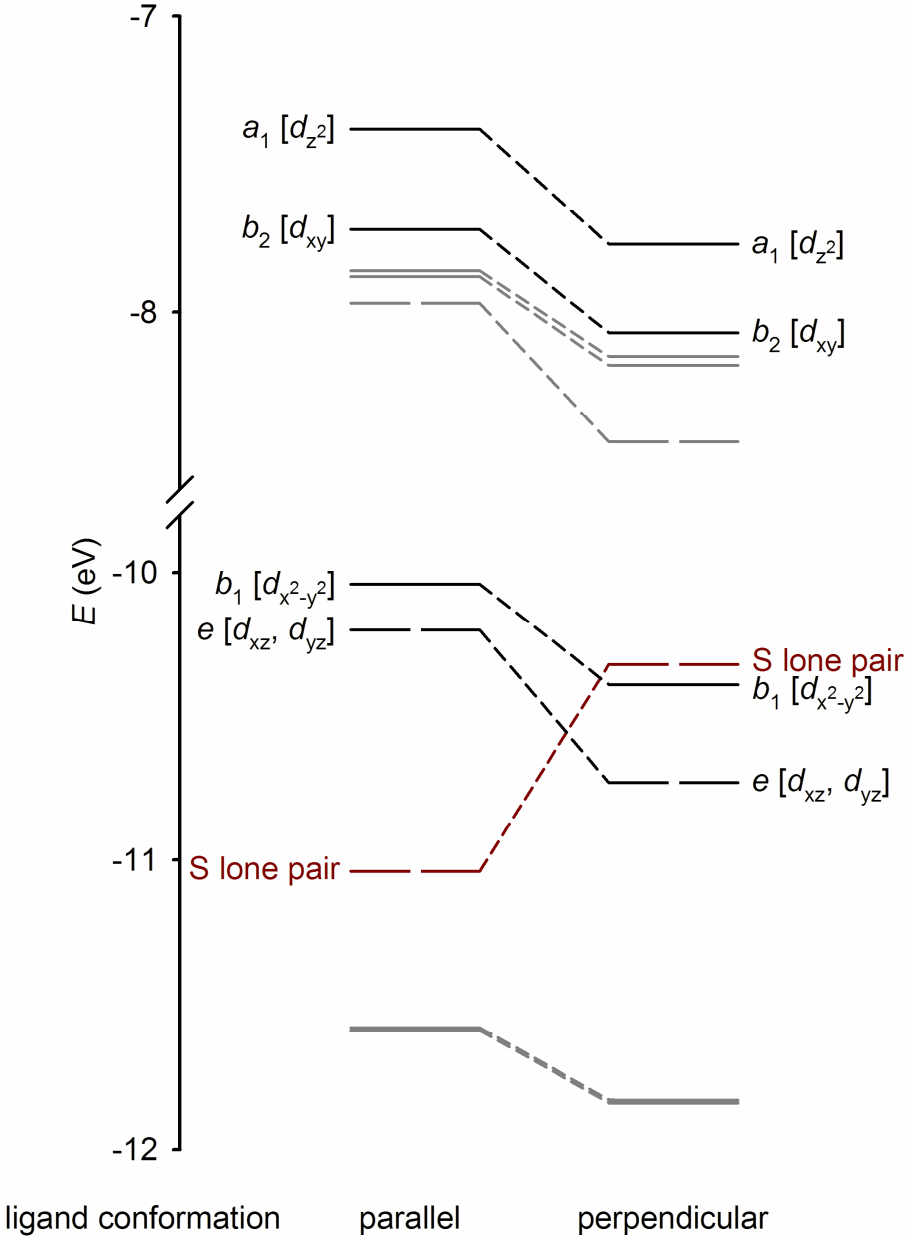


Figure S3 Computed frontier orbital energies for the parallel and perpendicular conformations of low-spin $\mathbf{1}^{2+}$.

Energy levels are colour coded as: metal-based *d*-orbitals (black); sulfur atom lone pair orbitals (red); and ligand-based π or π^* MOs (grey).

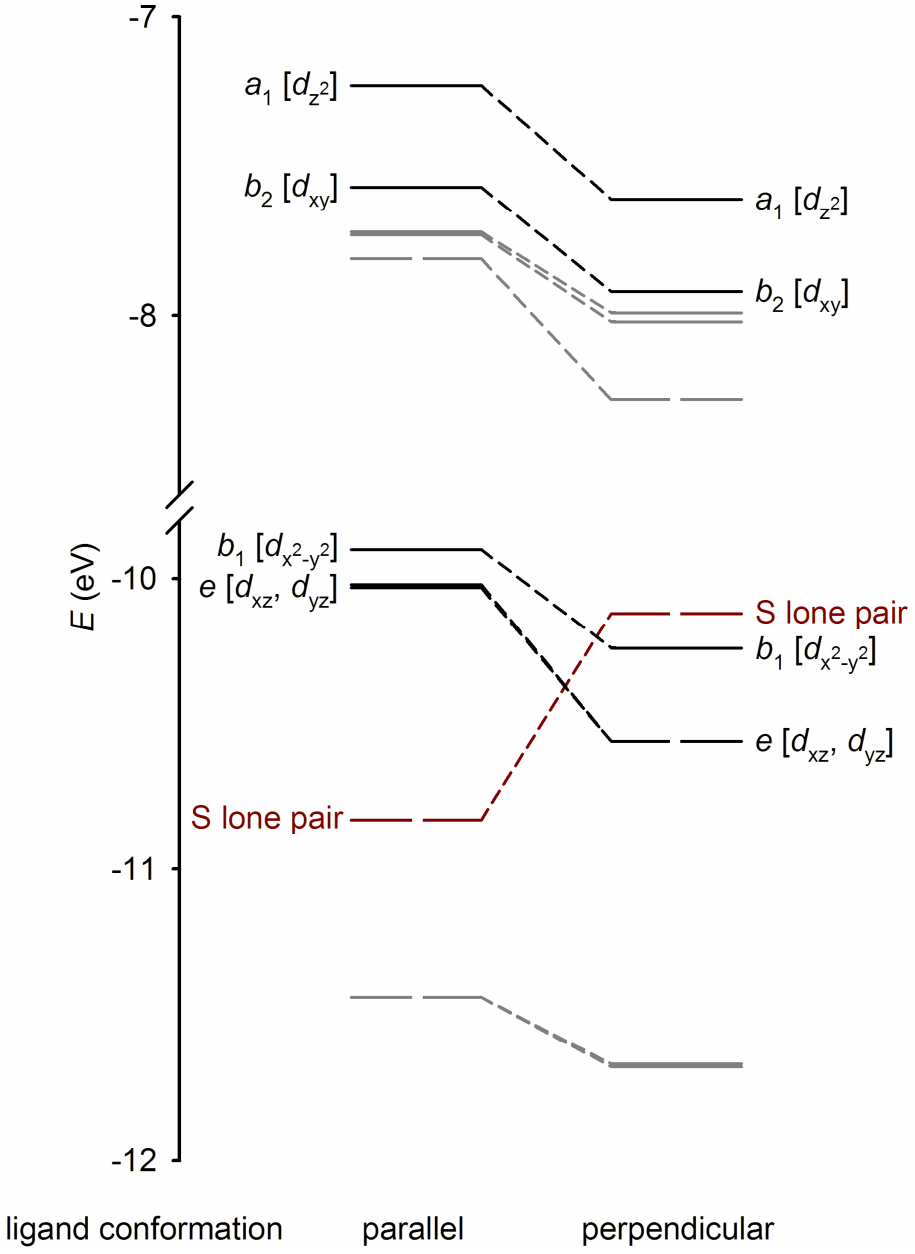


Figure S4 Computed frontier orbital energies for the parallel and perpendicular conformations of low-spin $\mathbf{2}^{2+}$.

Energy levels are colour coded as: metal-based *d*-orbitals (black); sulfur atom lone pair orbitals (red); and ligand-based π or π^* MOs (grey).

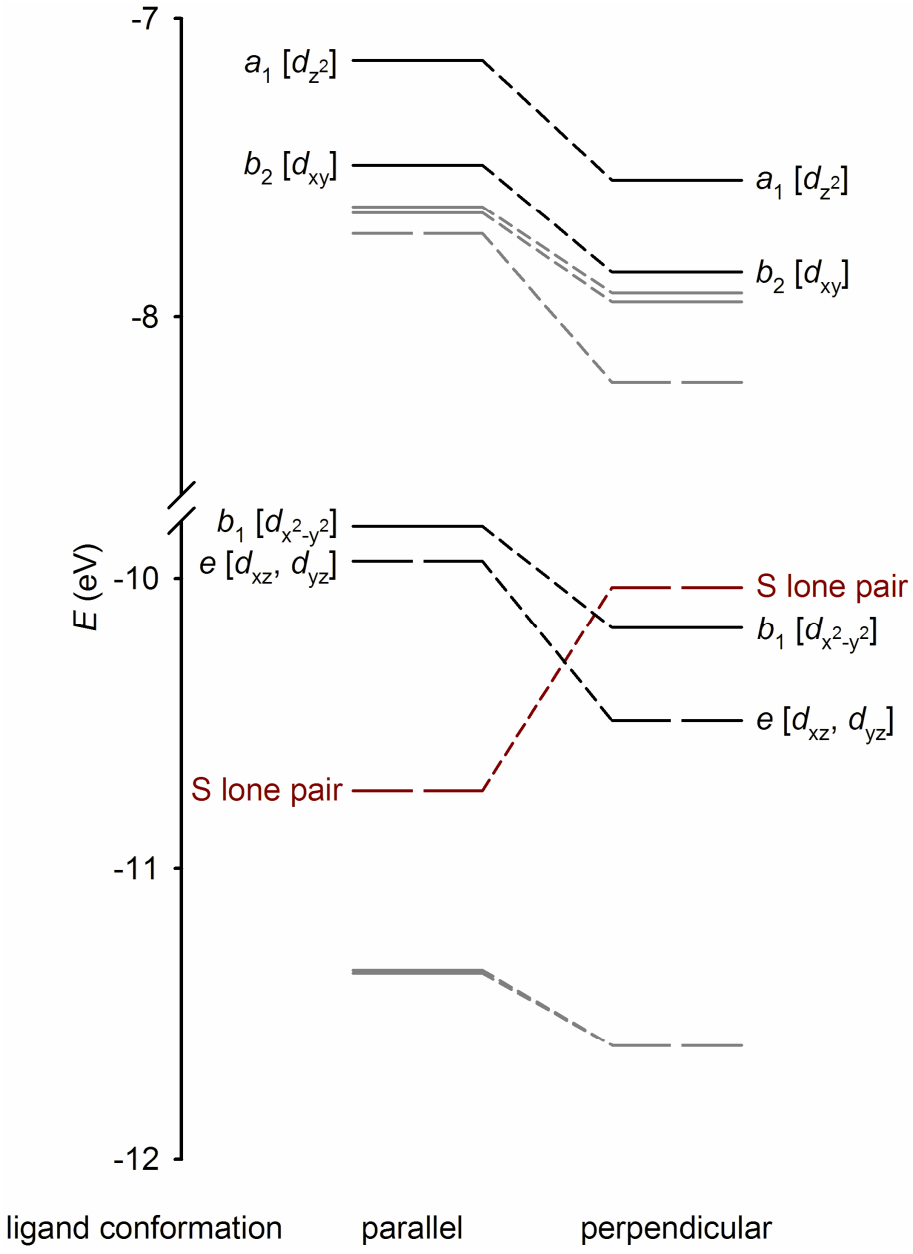


Figure S5 Computed frontier orbital energies for the parallel and perpendicular conformations of low-spin $\mathbf{3}^{2+}$.

Energy levels are colour coded as: metal-based *d*-orbitals (black); sulfur atom lone pair orbitals (red); and ligand-based π or π^* MOs (grey).

These data are also shown in Figure 4 of the main article. They're replotted here to the same scale as Figures S2 and S3, for ease of comparison.

Plots of the *d*-orbital and lone pair MOs for $\mathbf{3}^{2+}$ are shown in Figures S5 and S6.

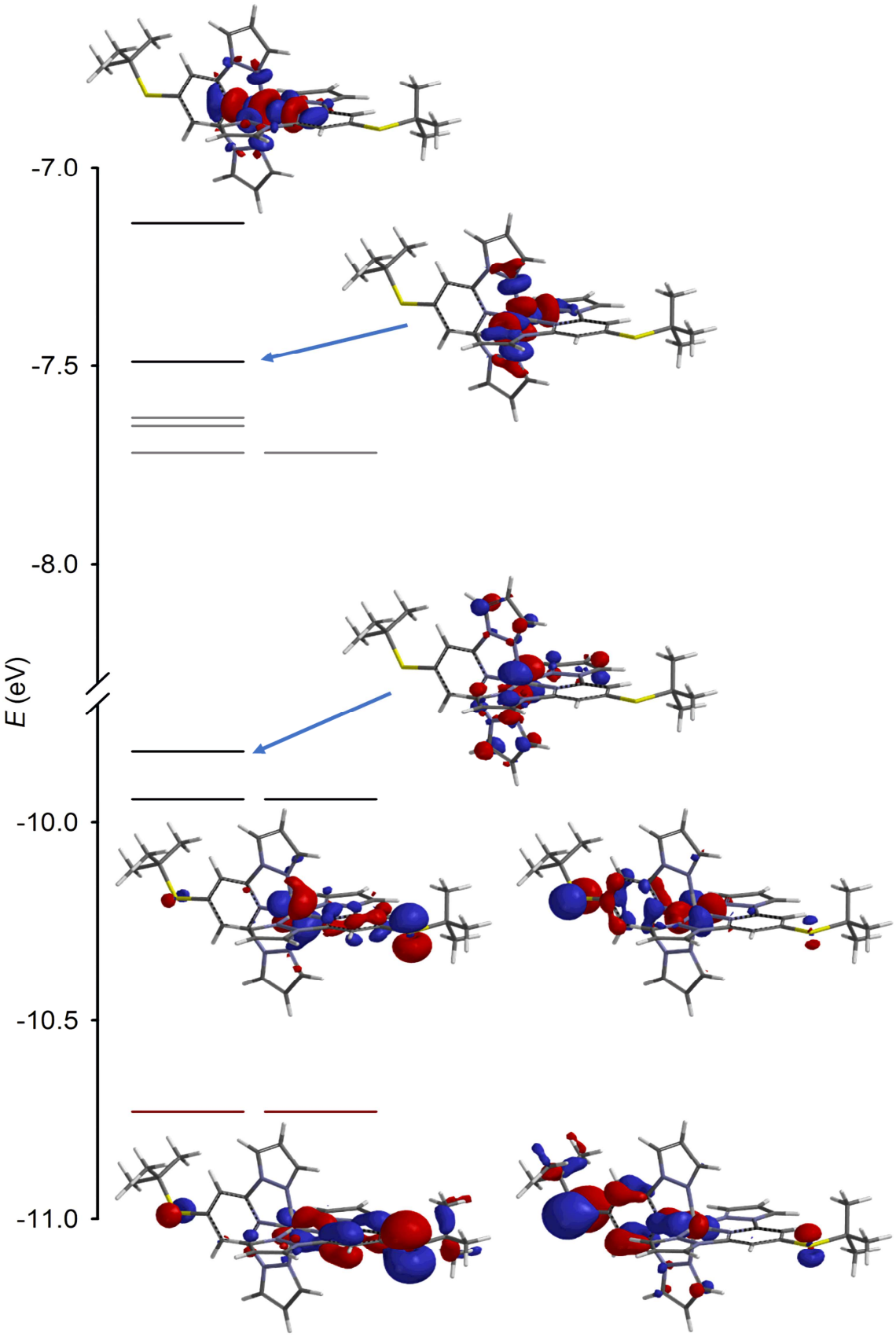


Figure S6 Frontier molecular orbitals for the parallel conformation of low-spin $\mathbf{3}^{2+}$. Plots of the metal-centred *d*-orbitals (black energy levels) and sulfur lone pair orbitals (red) are shown, but ligand-based π^* MOs (grey) are not included, for clarity.

The corresponding orbitals in the parallel conformation of low-spin $\mathbf{1}^{2+}$ and $\mathbf{2}^{2+}$ are visually indistinguishable from those in the Figure.

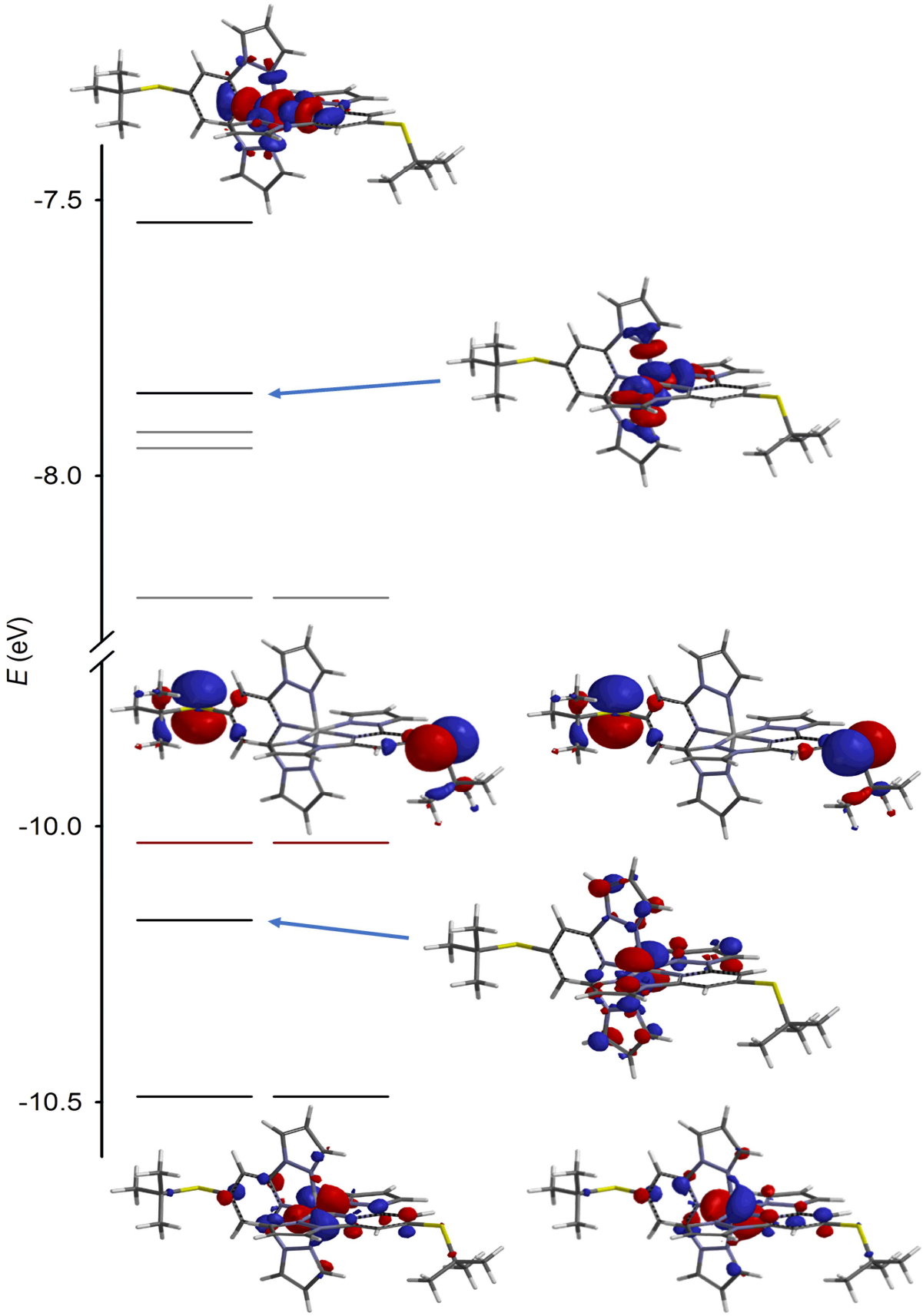


Figure S7 Frontier molecular orbitals for the perpendicular conformation of low-spin $\mathbf{3}^{2+}$. Details as for Figure S5. The energy scale of this Figure is expanded compared to Figure S5. The corresponding orbitals in the perpendicular conformation of low-spin $\mathbf{1}^{2+}$ and $\mathbf{2}^{2+}$ are visually indistinguishable from those in the Figure.

Table S3 Computed atomic coordinates for the energy-minimised organic ligands.

bpp^{SMe}, parallel conformation.

N	0.0990177	0.8203364	0.0554011
C	-0.5190117	-0.0796722	-0.7187504
C	-0.4712988	-1.4735233	-0.5257970
H	-1.0159844	-2.1174014	-1.2225604
C	0.2811064	-1.9507907	0.5679664
C	0.9436217	-1.0190601	1.4015003
C	0.8114150	0.3424845	1.0883530
N	-1.2697099	0.4522252	-1.8051627
N	-1.9621162	-0.3717958	-2.6360308
C	-2.5423564	0.4464645	-3.5189180
H	-3.1711093	0.0259822	-4.3137223
C	-2.2286692	1.8144832	-3.2645094
H	-2.5574474	2.6997391	-3.8174592
C	-1.4038436	1.7807737	-2.1486602
H	-0.9030225	2.5600762	-1.5699757
N	1.4589643	1.3201733	1.8941333
N	2.2218872	0.9453511	2.9552402
C	2.6700644	2.0928829	3.4724753
H	3.3217820	2.0693197	4.3548320
C	2.1971805	3.2263052	2.7464976
H	2.3975913	4.2852312	2.9364549
C	1.4166821	2.6890103	1.7323089
H	0.8411583	3.1375004	0.9195706
H	1.5449248	-1.3175480	2.2680963
S	0.4618227	-3.6575216	0.9923068
C	-0.5129280	-4.5263147	-0.2790554
H	-1.5768372	-4.2230217	-0.2550066
H	-0.4385094	-5.5982704	-0.0173831
H	-0.0943744	-4.3734191	-1.2921455

bpp$^{Si\text{Pr}}$, parallel conformation.

N	0.5796491	1.6760207	-0.3306937
C	-0.4633472	0.8871542	-0.6147479
C	-0.5666174	-0.4698084	-0.2564951
H	-1.4672992	-1.0153120	-0.5528213
C	0.5078107	-1.0387439	0.4613825
C	1.6194009	-0.2215497	0.7785199
C	1.5924357	1.1145725	0.3491965
N	-1.5256950	1.5032328	-1.3357143
N	-2.6459123	0.8004473	-1.6518981
C	-3.4156993	1.6694415	-2.3138800
H	-4.3956161	1.3476778	-2.6881541
C	-2.7973552	2.9495944	-2.4293369
H	-3.1874702	3.8497719	-2.9141502
C	-1.5754631	2.8050478	-1.7865806
H	-0.7434821	3.4891466	-1.6052827
N	2.6925158	1.9722739	0.6305788
N	3.7734587	1.5099388	1.3135167
C	4.5999645	2.5570433	1.3884037
H	5.5637320	2.4487347	1.9014836
C	4.0586806	3.7115735	0.7487419
H	4.5061919	4.7053297	0.6502379
C	2.8233972	3.2972726	0.2705627
H	2.0317094	3.8056126	-0.2842636
H	2.4890107	-0.5929830	1.3329507
S	0.6063145	-2.7260074	0.9858238
C	-1.0104856	-3.4914564	0.4792279

C	-0.7717804	-5.0069515	0.3929973
H	-0.4779863	-5.4277301	1.3762311
H	0.0195093	-5.2557291	-0.3397844
H	-1.7074036	-5.5124113	0.0799711
C	-2.1480070	-3.1242482	1.4407408
H	-1.9395881	-3.5023119	2.4612892
H	-3.0999173	-3.5772152	1.0927485
H	-2.2987315	-2.0302550	1.5073841
H	-1.2259240	-3.1071735	-0.5381864

bpp^{S_tBu}, parallel conformation.

N	0.2921652	2.1078049	0.2046889
C	-0.3436654	1.2446887	-0.5956636
C	-0.3336617	-0.1547878	-0.4443652
H	-0.8950016	-0.7521017	-1.1659839
C	0.3999998	-0.6926698	0.6353574
C	1.0787187	0.2054034	1.4969649
C	0.9852445	1.5784106	1.2258811
N	-1.0739005	1.8238752	-1.6731496
N	-1.7790702	1.0394042	-2.5308067
C	-2.3308908	1.8944761	-3.3973592
H	-2.9629709	1.5103614	-4.2077570
C	-1.9853905	3.2468833	-3.1050606
H	-2.2872273	4.1542092	-3.6371931
C	-1.1709351	3.1633256	-1.9839155
H	-0.6554569	3.9148906	-1.3818577
N	1.6560276	2.5130186	2.0639572
N	2.4077574	2.0859007	3.1128145
C	2.8870584	3.2048269	3.6641912
H	3.5371312	3.1367995	4.5454422
C	2.4460386	4.3720010	2.9724172
H	2.6752623	5.4189222	3.1937446
C	1.6526431	3.8864408	1.9420831
H	1.0908942	4.3738774	1.1422136
H	1.6685454	-0.1333873	2.3566816
S	0.5917027	-2.3986229	1.0690092
C	-0.3437463	-3.5156834	-0.1300293
C	-0.0314485	-4.9124346	0.4562459
H	1.0566288	-5.1209719	0.4603326
H	-0.5256721	-5.6857021	-0.1661056
H	-0.4107418	-5.0132938	1.4922200
C	-1.8606575	-3.2574547	-0.0741212
H	-2.1384463	-2.2593878	-0.4582900
H	-2.2391119	-3.3465145	0.9621394
H	-2.3842108	-4.0113889	-0.6989704
C	0.2254050	-3.4137859	-1.5575323
H	1.3150721	-3.6081877	-1.5656358
H	0.0504922	-2.4257663	-2.0202080
H	-0.2645811	-4.1733791	-2.2023801

bpp^{SMe}, perpendicular conformation.

N	-0.0924459	-0.0017716	-0.7927467
C	-0.2782069	-1.1439304	-0.1180897
C	-0.6430850	-1.2053685	1.2428724
H	-0.7826868	-2.1743720	1.7341402
C	-0.8175421	0.0161562	1.9186943
C	-0.6245276	1.2289782	1.2322681
C	-0.2623427	1.1496468	-0.1287091
N	-0.0825723	-2.3405272	-0.8583596
N	-0.2334563	-3.5527515	-0.2598555
C	0.0302743	-4.4399808	-1.2226721

H	-0.0194323	-5.5125297	-0.9969558
C	0.3507914	-3.8063339	-2.4607554
H	0.6062389	-4.2751298	-3.4160121
C	0.2670260	-2.4483189	-2.1888308
H	0.4198246	-1.5565349	-2.8006756
N	-0.0495897	2.3354106	-0.8816452
N	-0.1826793	3.5565073	-0.2970756
C	0.0842114	4.4287767	-1.2728072
H	0.0433006	5.5046102	-1.0614247
C	0.3986476	3.7761711	-2.5026183
H	0.6574012	4.2300588	-3.4641820
C	0.3037222	2.4227042	-2.2126775
H	0.4482155	1.5213192	-2.8123604
H	-0.7499246	2.2039000	1.7154200
S	-1.2873666	0.0249798	3.6603175
C	0.3827260	0.0151935	4.4276834
H	0.9595013	0.9146664	4.1377753
H	0.2133106	0.0297510	5.5213347
H	0.9406666	-0.9012809	4.1579472

bpp$^{S\textit{i}Pr}$, perpendicular conformation.

N	-0.1667382	0.0342871	-1.7339553
C	-0.3978297	-1.0745328	-1.0193553
C	-0.7896437	-1.0734821	0.3365737
H	-0.9700562	-2.0184725	0.8595839
C	-0.9512230	0.1774402	0.9619373
C	-0.7073364	1.3557641	0.2306584
C	-0.3178320	1.2141788	-1.1172807
N	-0.2282227	-2.3044830	-1.7105574
N	-0.4268791	-3.4871199	-1.0685281
C	-0.1859159	-4.4189816	-1.9944630
H	-0.2778277	-5.4797460	-1.7297781
C	0.1719459	-3.8445559	-3.2509031
H	0.4216434	-4.3579495	-4.1845316
C	0.1329030	-2.4750197	-3.0313553
H	0.3238027	-1.6135929	-3.6753334
N	-0.0554757	2.3644975	-1.9093536
N	-0.1861914	3.6108190	-1.3801191
C	0.1344096	4.4373677	-2.3792672
H	0.1081221	5.5215145	-2.2127646
C	0.4786069	3.7291165	-3.5695970
H	0.7822218	4.1378910	-4.5382394
C	0.3452643	2.3906774	-3.2292399
H	0.4922576	1.4626155	-3.7859823
H	-0.8188367	2.3526674	0.6708747
S	-1.4651758	0.2824555	2.6824640
C	0.1873283	0.2676626	3.5674134
C	0.8941355	-1.0894569	3.5038717
H	1.1021081	-1.4074979	2.4643173
H	0.2856884	-1.8776849	3.9910930
H	1.8684259	-1.0291213	4.0337573
C	-0.0982515	0.7127190	5.0093820
H	0.8481123	0.7380668	5.5864900
H	-0.7823268	0.0027702	5.5176787
H	-0.5555819	1.7200781	5.0428641
H	0.8043688	1.0391082	3.0616450

bpp$^{S\textit{t}Bu}$, perpendicular conformation.

N	-0.3006814	0.0000001	-1.9889441
C	-0.4723794	-1.1457420	-1.3168354

C	-0.8237304	-1.2153967	0.0477475
H	-0.9554958	-2.1883582	0.5327281
C	-1.0111646	0.0000002	0.7340942
C	-0.8237302	1.2153969	0.0477475
C	-0.4723792	1.1457421	-1.3168354
N	-0.2761638	-2.3380898	-2.0654078
N	-0.4104655	-3.5546892	-1.4714095
C	-0.1685295	-4.4350792	-2.4463955
H	-0.2178738	-5.5090898	-2.2283795
C	0.1334430	-3.7922595	-3.6841869
H	0.3718490	-4.2537828	-4.6472125
C	0.0579628	-2.4362248	-3.4003661
H	0.2026142	-1.5398430	-4.0072260
N	-0.2761637	2.3380899	-2.0654080
N	-0.4104648	3.5546894	-1.4714096
C	-0.1685291	4.4350793	-2.4463958
H	-0.2178730	5.5090898	-2.2283799
C	0.1334427	3.7922594	-3.6841874
H	0.3718482	4.2537826	-4.6472132
C	0.0579624	2.4362247	-3.4003664
H	0.2026134	1.5398429	-4.0072264
H	-0.9554956	2.1883584	0.5327280
S	-1.4848779	0.0000001	2.4687366
C	0.1728493	-0.0000001	3.3975820
C	-0.2677384	-0.0000005	4.8755179
H	-0.8661851	-0.8989598	5.1218624
H	-0.8661845	0.8989590	5.1218630
H	0.6318048	-0.0000010	5.5245586
C	0.9767019	-1.2686725	3.0719780
H	0.4044423	-2.1825057	3.3214562
H	1.9163800	-1.2749847	3.6636616
H	1.2573342	-1.3142264	2.0022129
C	0.9767017	1.2686727	3.0719785
H	1.9163794	1.2749852	3.6636624
H	0.4044417	2.1825058	3.3214566
H	1.2573344	1.3142268	2.0022135

Table S4 Computed atomic coordinates for the energy-minimised complexes.

1^{2+}, parallel conformation, low-spin

Fe	0.0000474	-0.0451354	0.1551196
N	-0.0424290	-1.8762026	-0.3638387
C	-0.9506803	-2.3087827	-1.2697332
C	-1.0196073	-3.6389410	-1.6944356
C	-0.0916824	-4.5652453	-1.1390625
C	0.8635184	-4.1017610	-0.1825233
H	1.5883649	-4.7971767	0.2598098
C	0.8466750	-2.7549176	0.1669898
N	-1.7747191	-1.2451407	-1.6865977
N	-1.5146971	-0.0104352	-1.1202915
C	-2.4177719	0.8300575	-1.6483332
H	-2.4233143	1.8864001	-1.3584998
C	-3.2685752	0.1492703	-2.5595900
H	-4.0937812	0.5706206	-3.1415130
C	-2.8341718	-1.1691095	-2.5613251
H	-3.1937691	-2.0454577	-3.1088609
N	1.6972826	-2.1022755	1.0805772
N	1.4897324	-0.7463784	1.2502301
C	2.3977389	-0.3493741	2.1557552
H	2.4435708	0.6993935	2.4685317
C	3.1981321	-1.4430074	2.5796760
H	4.0147290	-1.4274657	3.3076847
C	2.7271111	-2.5445142	1.8781559
H	3.0403967	-3.5930367	1.8862107
N	0.0469992	1.7877625	0.6761695
C	0.8155546	2.6715883	-0.0023782
C	0.8997951	4.0228852	0.3457613
H	1.5324369	4.7072967	-0.2292904
C	0.1413631	4.4725463	1.4640692
C	-0.6646966	3.5330635	2.1782282
C	-0.6751834	2.2103211	1.7457139
N	1.4839778	2.0293019	-1.0625402
N	1.2518197	0.6737913	-1.2015456
C	1.9930459	0.2827185	-2.2501870
H	1.9876075	-0.7648100	-2.5706052
C	2.7101352	1.3795392	-2.7978348
H	3.3930631	1.3675135	-3.6525698
C	2.3655757	2.4761130	-2.0195176
H	2.6757726	3.5239331	-2.0738533
N	-1.3952755	1.1385328	2.3082758
N	-1.2280042	-0.0956622	1.7074756
C	-1.9955623	-0.9468169	2.4061066
H	-2.0388926	-2.0056219	2.1288647
C	-2.6648782	-0.2729921	3.4616831
H	-3.3554942	-0.7025337	4.1935695
C	-2.2620051	1.0525069	3.3729322
H	-2.5217284	1.9270596	3.9774791
H	-1.7700397	-3.9508227	-2.4288753
H	-1.2569440	3.8551071	3.0443897
S	-0.0210131	-6.2722312	-1.5180849
S	0.0972763	6.1192612	2.0543809
C	-1.2925786	-6.5230879	-2.7966701
C	1.2505615	7.0317851	0.9805848
H	1.2407818	8.0631241	1.3802874
H	0.8987429	7.0532250	-0.0682859
H	2.2801623	6.6333441	1.0567064
H	-1.2112757	-7.5954050	-3.0562533
H	-1.0834343	-5.9233033	-3.7028186
H	-2.3097660	-6.3304176	-2.4055038

1^{2+}, parallel conformation, high-spin

Fe	0.0001916	0.0030391	-0.0044885
N	-0.0071318	-2.1206646	-0.3165015
C	-1.0679182	-2.7303052	-0.8828257
C	-1.1216058	-4.1043924	-1.1431074
C	0.0080643	-4.8929410	-0.7938541
C	1.1297525	-4.2486708	-0.1926687
H	2.0146137	-4.8333406	0.0881112
C	1.0636184	-2.8739212	0.0234749
N	-2.1257048	-1.8326829	-1.1780221
N	-1.9802452	-0.5165011	-0.8234411
C	-3.1071246	0.0931778	-1.2227588
H	-3.2426175	1.1661396	-1.0442219
C	-3.9943684	-0.8246179	-1.8417383
H	-4.9841072	-0.6231243	-2.2625562
C	-3.3372474	-2.0470996	-1.7940212
H	-3.6416083	-3.0354658	-2.1501612
N	2.1054085	-2.1156455	0.6174420
N	1.9279020	-0.7651067	0.7566435
C	3.0398072	-0.3133882	1.3578403
H	3.1483836	0.7540492	1.5815943
C	3.9485094	-1.3713946	1.6143794
H	4.9322007	-1.3136388	2.0900540
C	3.3203549	-2.5105136	1.1267439
H	3.6467511	-3.5545654	1.1093193
N	0.2268142	2.1200904	0.2192453
C	0.7944611	2.8622640	-0.7591911
C	1.0157619	4.2330362	-0.6466391
H	1.4879034	4.8075610	-1.4533208
C	0.6176819	4.8855523	0.5576456
C	0.0110486	4.1094953	1.5820892
C	-0.1541785	2.7382924	1.3559180
N	1.1421385	2.0971236	-1.9022512
N	0.9097070	0.7477018	-1.8764393
C	1.3138779	0.2872847	-3.0709094
H	1.2357972	-0.7810566	-3.3028630
C	1.8116243	1.3384256	-3.8822736
H	2.2089175	1.2733180	-4.8997068
C	1.6882493	2.4825270	-3.1040183
H	1.9428847	3.5243739	-3.3201155
N	-0.7463388	1.8535376	2.2929164
N	-0.8799939	0.5338648	1.9471610
C	-1.4586968	-0.0608020	3.0015544
H	-1.6820825	-1.1334900	2.9709136
C	-1.7040507	0.8701929	4.0435416
H	-2.1643033	0.6829143	5.0184144
C	-1.2396318	2.0849171	3.5567792
H	-1.2276472	3.0790402	4.0128808
H	-0.3197084	4.5681717	2.5190757
H	-2.0095176	-4.5549497	-1.5973905
S	0.1476612	-6.6188480	-1.0330709
S	0.9264582	6.6038114	0.6399282
C	0.3361188	7.1103982	2.2872828
C	-1.4248608	-7.1165992	-1.8073585
H	-1.5535774	-6.6518911	-2.8031688
H	-2.2865774	-6.9095733	-1.1452205
H	-1.3339752	-8.2112904	-1.9366473
H	-0.7533638	6.9516031	2.3945988
H	0.5418292	8.1962429	2.3319963
H	0.9036899	6.6083345	3.0934072

1^{2+}, perpendicular conformation, low-spin

Fe	0.0000001	-0.0000001	0.1435057
N	-1.9015907	0.0726083	0.1559028
C	-2.5504936	0.9422845	-0.6561707
C	-3.9466974	1.0587466	-0.6544127
C	-4.6817301	0.2464658	0.2444789
C	-3.9999494	-0.6746560	1.0778440
H	-4.5645151	-1.3074306	1.7744628
C	-2.6014759	-0.7188621	1.0050738
N	-1.6354374	1.6686416	-1.4392483
N	-0.2968387	1.3893283	-1.2352694
C	0.3747542	2.1950195	-2.0725153
H	1.4693363	2.1695062	-2.1062337
C	-0.5213684	3.0008995	-2.8241448
H	-0.2676851	3.7488260	-3.5814582
C	-1.7930092	2.6427368	-2.3988907
H	-2.7827836	2.9999922	-2.7000481
N	-1.7348323	-1.5290099	1.7601438
N	-0.3827586	-1.3673151	1.5226145
C	0.2378110	-2.2241180	2.3482439
H	1.3311530	-2.2923600	2.3564565
C	-0.7060502	-2.9468324	3.1260559
H	-0.4991233	-3.7111197	3.8812905
C	-1.9522404	-2.4822375	2.7291912
H	-2.9613925	-2.7517567	3.0562086
N	1.9015907	-0.0726085	0.1559030
C	2.5504937	-0.9422847	-0.6561706
C	3.9466974	-1.0587467	-0.6544125
H	4.4698092	-1.7724379	-1.3035009
C	4.6817300	-0.2464658	0.2444790
C	3.9999493	0.6746559	1.0778441
C	2.6014759	0.7188620	1.0050739
N	1.6354375	-1.6686418	-1.4392482
N	0.2968388	-1.3893284	-1.2352693
C	-0.3747541	-2.1950196	-2.0725153
H	-1.4693362	-2.1695063	-2.1062337
C	0.5213686	-3.0008997	-2.8241447
H	0.2676853	-3.7488262	-3.5814581
C	1.7930093	-2.6427370	-2.3988906
H	2.7827837	-2.9999923	-2.7000480
N	1.7348322	1.5290097	1.7601439
N	0.3827586	1.3673150	1.5226145
C	-0.2378111	2.2241178	2.3482438
H	-1.3311531	2.2923598	2.3564563
C	0.7060499	2.9468322	3.1260559
H	0.4991229	3.7111195	3.8812905
C	1.9522402	2.4822374	2.7291913
H	2.9613923	2.7517566	3.0562087
H	-4.4698091	1.7724379	-1.3035010
H	4.5645151	1.3074306	1.7744629
S	-6.4705232	0.3841471	0.3269481
S	6.4705232	-0.3841470	0.3269482
C	-6.9630905	-0.8620923	-0.9353167
C	6.9630906	0.8620931	-0.9353172
H	8.0692406	0.8371586	-0.9329001
H	6.6251027	1.8767588	-0.6547960
H	6.5987397	0.5847222	-1.9417637
H	-6.6251028	-1.8767580	-0.6547956
H	-8.0692405	-0.8371578	-0.9328997
H	-6.5987396	-0.5847216	-1.9417632

1^{2+}, perpendicular conformation, high-spin

Fe	0.0000001	-0.0000008	0.0767623
N	-2.1515008	0.0372765	0.1497734
C	-2.8449660	0.8706352	-0.6523272
C	-4.2452929	0.9568933	-0.6265282
C	-4.9422649	0.1435536	0.2963937
C	-4.2177444	-0.7425945	1.1263784
H	-4.7526969	-1.3777128	1.8430651
C	-2.8187147	-0.7509564	1.0167584
N	-2.0180716	1.6347553	-1.5103830
N	-0.6632460	1.4309472	-1.4614744
C	-0.1373265	2.2819833	-2.3564552
H	0.9468748	2.3098451	-2.5153935
C	-1.1491455	3.0465381	-2.9925415
H	-1.0276053	3.8146576	-3.7623946
C	-2.3403584	2.6065109	-2.4304488
H	-3.3748885	2.9115344	-2.6146481
N	-1.9658173	-1.5695788	1.7959143
N	-0.6118842	-1.4685505	1.6055986
C	-0.0617142	-2.3542353	2.4510694
H	1.0277854	-2.4657539	2.4983166
C	-1.0564245	-3.0394409	3.1949738
H	-0.9135212	-3.8130121	3.9556568
C	-2.2630671	-2.5130240	2.7529728
H	-3.2928086	-2.7382595	3.0465214
N	2.1515009	-0.0372766	0.1497730
C	2.8449663	-0.8706352	-0.6523274
C	4.2452931	-0.9568928	-0.6265285
H	4.8020544	-1.6415262	-1.2782081
C	4.9422647	-0.1435526	0.2963933
C	4.2177440	0.7425952	1.1263782
C	2.8187145	0.7509564	1.0167583
N	2.0180721	-1.6347558	-1.5103828
N	0.6632463	-1.4309486	-1.4614740
C	0.1373277	-2.2819853	-2.3564549
H	-0.9468735	-2.3098481	-2.5153934
C	1.1491473	-3.0465394	-2.9925412
H	1.0276077	-3.8146592	-3.7623942
C	2.3403598	-2.6065110	-2.4304489
H	3.3748902	-2.9115333	-2.6146485
N	1.9658169	1.5695785	1.7959142
N	0.6118839	1.4685500	1.6055991
C	0.0617139	2.3542347	2.4510701
H	-1.0277857	2.4657528	2.4983175
C	1.0564241	3.0394403	3.1949742
H	0.9135208	3.8130113	3.9556574
C	2.2630666	2.5130241	2.7529723
H	3.2928082	2.7382601	3.0465204
H	-4.8020539	1.6415268	-1.2782080
H	4.7526963	1.3777137	1.8430647
S	-6.7331565	0.2359258	0.4128198
S	6.7331564	-0.2359238	0.4128190
C	-7.2184078	-1.0429271	-0.8196748
C	7.2184062	1.0429288	-0.8196752
H	8.3247608	1.0350509	-0.8015263
H	6.8601822	2.0471997	-0.5264369
H	6.8728995	0.7779153	-1.8361539
H	-6.8601844	-2.0471983	-0.5264363
H	-8.3247624	-1.0350482	-0.8015253
H	-6.8729011	-0.7779139	-1.8361535

2^{2+}, parallel conformation, low-spin

Fe	0.0000002	0.3446272	0.0000001
N	1.8981659	0.3309615	-0.1568477
C	2.6408709	-0.5069113	0.6038677
C	4.0329467	-0.5808696	0.5102499
C	4.6878382	0.2592062	-0.4378688
C	3.8942086	1.1471949	-1.2312195
H	4.3719678	1.8092265	-1.9647587
C	2.5143027	1.1421681	-1.0541500
N	1.8098494	-1.2622643	1.4560390
N	0.4510210	-1.0302168	1.3499543
C	-0.1297136	-1.8506336	2.2391686
H	-1.2191856	-1.8582694	2.3524909
C	0.8456792	-2.6199794	2.9274161
H	0.6746878	-3.3690465	3.7063029
C	2.0696669	-2.2221498	2.4063959
H	3.0897758	-2.5430983	2.6375088
N	1.5653198	1.9279328	-1.7382629
N	0.2409731	1.7232000	-1.3991978
C	-0.4666827	2.5662252	-2.1678866
H	-1.5586904	2.5997143	-2.0895862
C	0.3918370	3.3219408	-3.0090484
H	0.1053534	4.0847980	-3.7390745
C	1.6783971	2.8927721	-2.7118135
H	2.6507715	3.1973632	-3.1109201
N	-1.8981659	0.3309618	0.1568476
C	-2.6408709	-0.5069110	-0.6038679
C	-4.0329467	-0.5808692	-0.5102502
H	-4.5958401	-1.2742233	-1.1434229
C	-4.6878381	0.2592066	0.4378686
C	-3.8942085	1.1471953	1.2312192
C	-2.5143026	1.1421684	1.0541498
N	-1.8098494	-1.2622641	-1.4560392
N	-0.4510210	-1.0302168	-1.3499546
C	0.1297136	-1.8506337	-2.2391689
H	1.2191856	-1.8582696	-2.3524911
C	-0.8456793	-2.6199792	-2.9274164
H	-0.6746880	-3.3690462	-3.7063033
C	-2.0696670	-2.2221495	-2.4063962
H	-3.0897759	-2.5430978	-2.6375093
N	-1.5653197	1.9279332	1.7382628
N	-0.2409730	1.7232002	1.3991980
C	0.4666827	2.5662255	2.1678867
H	1.5586905	2.5997145	2.0895864
C	-0.3918370	3.3219412	3.0090482
H	-0.1053536	4.0847986	3.7390743
C	-1.6783971	2.8927725	2.7118133
H	-2.6507715	3.1973638	3.1109197
H	4.5958402	-1.2742236	1.1434227
H	-4.3719677	1.8092269	1.9647586
S	6.4041620	0.2862821	-0.7684963
S	-6.4041619	0.2862822	0.7684964
C	-7.2158024	-0.8724149	-0.4542817
H	-6.5825306	-1.7835511	-0.4801251
C	7.2158024	-0.8724148	0.4542821
H	6.5825307	-1.7835510	0.4801256
C	8.5768587	-1.2333436	-0.1612471
H	9.1063264	-1.9295846	0.5184662
H	9.2189701	-0.3388732	-0.2863653
H	8.4690212	-1.7292716	-1.1444453
C	-7.3299983	-0.2329709	-1.8423733
H	-7.9623539	0.6752873	-1.8073782

H	-7.8068733	-0.9506420	-2.5406465
H	-6.3476212	0.0517235	-2.2670696
C	-8.5768586	-1.2333437	0.1612477
H	-9.2189699	-0.3388732	0.2863659
H	-8.4690210	-1.7292716	1.1444459
H	-9.1063264	-1.9295846	-0.5184655
C	7.3299981	-0.2329705	1.8423736
H	7.8068732	-0.9506416	2.5406469
H	6.3476210	0.0517237	2.2670697
H	7.9623537	0.6752876	1.8073784

2^{2+}, parallel conformation, high-spin

Fe	-0.0672642	-0.4495442	-0.1272230
N	-2.1685685	-0.0683385	-0.2649238
C	-2.6474921	0.8823749	-1.0936718
C	-4.0069174	1.1833104	-1.2224115
H	-4.3480304	1.9505946	-1.9236219
C	-4.9327800	0.4549823	-0.4237081
C	-4.4247124	-0.5548214	0.4485534
H	-5.1148317	-1.1312268	1.0770876
C	-3.0497377	-0.7755944	0.4794159
N	-1.6250326	1.5397363	-1.8269934
N	-0.3289712	1.1359807	-1.6430594
C	0.4130146	1.9216466	-2.4388189
H	1.5006091	1.7907200	-2.4776066
C	-0.3985749	2.8449568	-3.1462502
H	-0.0812669	3.6061722	-3.8653256
C	-1.6963840	2.5717021	-2.7335492
H	-2.6473806	3.0320419	-3.0162922
N	-2.4235931	-1.7535669	1.2951375
N	-1.0576996	-1.8502856	1.2632800
C	-0.7455633	-2.8536472	2.0984608
H	0.3031044	-3.1314165	2.2550745
C	-1.9102870	-3.4174308	2.6782746
H	-1.9741087	-4.2437076	3.3926658
C	-2.9661517	-2.6893453	2.1444815
H	-4.0452772	-2.7720713	2.3041688
S	-6.6675867	0.6541574	-0.4254566
C	-7.0568287	2.1200645	-1.5194800
H	-6.4690393	1.9743973	-2.4501818
C	-6.7041251	3.4463002	-0.8376176
H	-6.9436432	4.2859231	-1.5214644
H	-5.6318510	3.5223374	-0.5716319
H	-7.2933440	3.5868100	0.0894116
C	-8.5509245	1.9900416	-1.8550550
H	-9.1783388	2.0428980	-0.9432790
H	-8.7765017	1.0449555	-2.3842633
H	-8.8472294	2.8305181	-2.5128989
N	2.0263099	-0.8241112	0.1103016
C	2.6577850	-1.7368320	-0.6633292
C	4.0128669	-2.0355606	-0.5419247
H	4.4982679	-2.7738710	-1.1921312
C	4.7747293	-1.3530727	0.4544051
C	4.1090887	-0.3947417	1.2689985
H	4.6447297	0.1499145	2.0522908
C	2.7460965	-0.1749626	1.0485511
N	1.7955111	-2.3436893	-1.6132745
N	0.4883044	-1.9361535	-1.6576142
C	-0.0882911	-2.6694864	-2.6225419
H	-1.1485005	-2.5256841	-2.8606643
C	0.8428806	-3.5627054	-3.2109939
H	0.6696128	-4.2814110	-4.0176251

C	2.0383887	-3.3272254	-2.5434004
H	3.0255526	-3.7832863	-2.6633541
N	1.9709744	0.7517771	1.7944041
N	0.6328717	0.8494909	1.5211168
C	0.1615111	1.7960791	2.3473966
H	-0.9020348	2.0602233	2.3278545
C	1.1942197	2.3220057	3.1650126
H	1.1162647	3.0992704	3.9311425
C	2.3381235	1.6308236	2.7861949
H	3.3686439	1.7049267	3.1449488
S	6.4556642	-1.8095976	0.5732287
C	7.2443697	-0.6867748	1.8448538
H	6.5387462	-0.6469064	2.7008391
C	7.5054243	0.7114834	1.2743537
H	6.5787040	1.2167333	0.9387767
H	8.1979545	0.6665256	0.4115316
H	7.9750192	1.3456683	2.0536913
C	8.5229000	-1.4113478	2.2922586
H	8.3041619	-2.3969747	2.7447675
H	9.0412574	-0.7923915	3.0507526
H	9.2252014	-1.5597618	1.4479539

2^{2+}, perpendicular conformation, low-spin

Fe	-0.0119133	-0.0829535	0.3199271
N	-1.9033235	0.1318631	0.3178423
C	-2.4789255	1.0511017	-0.4945487
C	-3.8591070	1.2877931	-0.4876964
C	-4.6595890	0.5541755	0.4261630
C	-4.0535396	-0.4268360	1.2532377
H	-4.6679342	-1.0032413	1.9563117
C	-2.6657141	-0.5947271	1.1715823
N	-1.5068261	1.6988405	-1.2789223
N	-0.1949805	1.3210320	-1.0649346
C	0.5413186	2.0710300	-1.9001786
H	1.6309674	1.9622105	-1.9254075
C	-0.2867170	2.9388609	-2.6601639
H	0.0272795	3.6626004	-3.4182841
C	-1.5844807	2.6791034	-2.2414236
H	-2.5426655	3.1084915	-2.5501139
N	-1.8677756	-1.4738825	1.9266416
N	-0.5066589	-1.4206339	1.6938247
C	0.0396580	-2.3302065	2.5159159
H	1.1239160	-2.4867576	2.5260843
C	-0.9619821	-2.9783437	3.2867409
H	-0.8204255	-3.7617689	4.0373594
C	-2.1651358	-2.4114139	2.8887844
H	-3.1943074	-2.6004488	3.2094937
N	1.8789312	-0.2933356	0.3662906
C	2.4774141	-1.2138913	-0.4283786
C	3.8576293	-1.4438168	-0.3875381
H	4.3393784	-2.2004208	-1.0193657
C	4.6355951	-0.6954964	0.5341037
C	4.0063657	0.2875889	1.3411179
C	2.6185005	0.4425637	1.2313216
N	1.5262258	-1.8675968	-1.2334428
N	0.2088703	-1.4890903	-1.0561181
C	-0.5043037	-2.2405915	-1.9097252
H	-1.5928680	-2.1318248	-1.9649405
C	0.3441291	-3.1095021	-2.6456916
H	0.0509705	-3.8343995	-3.4110194
C	1.6301349	-2.8487900	-2.1925165
H	2.5964714	-3.2783639	-2.4744072

N	1.7988622	1.3178758	1.9675867
N	0.4436162	1.2554807	1.7048187
C	-0.1276686	2.1573577	2.5182501
H	-1.2129828	2.3058849	2.5049838
C	0.8518055	2.8095161	3.3138249
H	0.6877634	3.5881557	4.0648429
C	2.0676613	2.2528920	2.9406967
H	3.0878007	2.4474422	3.2860050
H	-4.3199092	2.0462155	-1.1320224
H	4.5990447	0.8713817	2.0560730
S	-6.4182419	0.8591405	0.5389898
S	6.3922914	-1.0021680	0.6639114
C	-7.1516311	-0.3442354	-0.7259444
C	-8.6675852	-0.2380128	-0.5181580
H	-8.9615610	-0.4800838	0.5208017
H	-9.1759048	-0.9559829	-1.1923043
H	-9.0406577	0.7763315	-0.7631951
C	-6.7100988	-0.0443988	-2.1560346
H	-7.1815913	-0.7745351	-2.8458883
H	-5.6138683	-0.1354102	-2.2865348
H	-7.0220195	0.9704692	-2.4729815
C	7.1234485	0.1971306	-0.6063663
C	8.5814311	-0.2486469	-0.7704990
H	8.6572487	-1.3003305	-1.1057420
H	9.1510294	-0.1385813	0.1738845
H	9.0707465	0.3901117	-1.5327388
C	6.9768530	1.6568999	-0.1835338
H	7.4268522	2.3115785	-0.9584728
H	7.5002205	1.8530169	0.7727998
H	5.9171126	1.9620077	-0.0758539
H	-6.8013448	-1.3494749	-0.4122851
H	6.5666946	0.0040501	-1.5468390

2^{2+}, perpendicular conformation, high-spin

Fe	-0.0000001	-0.0000001	0.2117178
N	-2.1423257	0.1412081	0.3573111
C	-2.8220775	0.9998141	-0.4294259
C	-4.2127065	1.1644146	-0.3503664
C	-4.9186132	0.4142231	0.6213750
C	-4.2081335	-0.5093376	1.4255473
H	-4.7482107	-1.1044150	2.1719649
C	-2.8192423	-0.6040505	1.2546043
N	-1.9884995	1.7075248	-1.3301522
N	-0.6452005	1.4343530	-1.3267825
C	-0.1097278	2.2430882	-2.2551620
H	0.9678578	2.2123201	-2.4535927
C	-1.1035621	3.0498674	-2.8663274
H	-0.9716203	3.7987761	-3.6531493
C	-2.2940888	2.6813607	-2.2528762
H	-3.3178780	3.0362988	-2.4044151
N	-1.9843744	-1.4736253	1.9986427
N	-0.6367254	-1.4527038	1.7521364
C	-0.1061907	-2.3791307	2.5660181
H	0.9754639	-2.5566853	2.5661719
C	-1.1086090	-3.0094076	3.3470531
H	-0.9816052	-3.7981399	4.0948074
C	-2.2984437	-2.4058843	2.9605505
H	-3.3271260	-2.5718364	3.2942118
N	2.1423255	-0.1412083	0.3573112
C	2.8220773	-0.9998142	-0.4294258
C	4.2127065	-1.1644146	-0.3503663
H	4.7537546	-1.8731111	-0.9885119

C	4.9186133	-0.4142232	0.6213751
C	4.2081336	0.5093373	1.4255475
C	2.8192422	0.6040503	1.2546045
N	1.9884994	-1.7075249	-1.3301521
N	0.6452005	-1.4343532	-1.3267825
C	0.1097277	-2.2430882	-2.2551621
H	-0.9678579	-2.2123198	-2.4535929
C	1.1035620	-3.0498673	-2.8663275
H	0.9716202	-3.7987761	-3.6531493
C	2.2940887	-2.6813607	-2.2528762
H	3.3178779	-3.0362987	-2.4044153
N	1.9843744	1.4736254	1.9986429
N	0.6367253	1.4527041	1.7521366
C	0.1061906	2.3791311	2.5660182
H	-0.9754639	2.5566857	2.5661720
C	1.1086091	3.0094078	3.3470531
H	0.9816054	3.7981403	4.0948073
C	2.2984439	2.4058843	2.9605507
H	3.3271262	2.5718361	3.2942120
H	-4.7537546	1.8731112	-0.9885119
H	4.7482107	1.1044146	2.1719652
S	-6.6822695	0.6249601	0.8354868
S	6.6822696	-0.6249603	0.8354867
C	-7.4177599	-0.6478052	-0.3595210
C	-8.9285369	-0.5840941	-0.1018938
H	-9.1774632	-0.7895546	0.9566307
H	-9.4319229	-1.3509117	-0.7240761
H	-9.3480605	0.4035365	-0.3786090
C	-7.0348242	-0.3915363	-1.8145676
H	-7.5231055	-1.1523066	-2.4579900
H	-5.9434936	-0.4747760	-1.9838932
H	-7.3729356	0.6069957	-2.1557623
C	7.4177599	0.6478051	-0.3595211
C	8.9285369	0.5840943	-0.1018938
H	9.3480606	-0.4035363	-0.3786089
H	9.1774631	0.7895550	0.9566308
H	9.4319229	1.3509118	-0.7240762
C	7.0348243	0.3915361	-1.8145677
H	7.3729362	-0.6069957	-2.1557625
H	7.5231052	1.1523066	-2.4579900
H	5.9434936	0.4747753	-1.9838932
H	-7.0249581	-1.6288845	-0.0212971
H	7.0249578	1.6288843	-0.0212971

3^{2+}, parallel conformation, low-spin

Fe	0.0083313	0.1303610	0.4583019
N	0.0802360	1.9615636	-0.0529943
C	0.9973838	2.3859640	-0.9528179
C	1.0839913	3.7133392	-1.3788809
C	0.1598955	4.6571536	-0.8411263
C	-0.8030546	4.1965279	0.1145835
H	-1.5293344	4.8979454	0.5451090
C	-0.7997012	2.8524526	0.4718324
N	1.8128727	1.3122659	-1.3651653
N	1.5302261	0.0790988	-0.8079259
C	2.4274887	-0.7713151	-1.3307012
H	2.4150874	-1.8288808	-1.0457470
C	3.2960520	-0.0981216	-2.2301689
H	4.1211607	-0.5276196	-2.8060738
C	2.8793627	1.2263826	-2.2292196
H	3.2562114	2.1012759	-2.7672076
N	-1.6637076	2.2095592	1.3815691

N	-1.4738338	0.8513035	1.5505886
C	-2.3910051	0.4639471	2.4513235
H	-2.4501738	-0.5846751	2.7621759
C	-3.1792826	1.5668940	2.8730561
H	-3.9988903	1.5609650	3.5977098
C	-2.6913680	2.6633956	2.1744010
H	-2.9903789	3.7160159	2.1822033
N	-0.0742498	-1.7026668	0.9724447
C	-0.8537800	-2.5718830	0.2889964
C	-0.9713526	-3.9201152	0.6355957
H	-1.6285137	-4.5801598	0.0635733
C	-0.2281686	-4.3979515	1.7556157
C	0.5972798	-3.4680470	2.4683247
C	0.6348987	-2.1445036	2.0423595
N	-1.5058810	-1.9136287	-0.7734814
N	-1.2494962	-0.5623081	-0.9063098
C	-1.9744163	-0.1555730	-1.9606628
H	-1.9479355	0.8928823	-2.2768866
C	-2.7050322	-1.2380943	-2.5177702
H	-3.3800030	-1.2122348	-3.3783976
C	-2.3856198	-2.3426979	-1.7393629
H	-2.7121931	-3.3851184	-1.7993621
N	1.3720637	-1.0870325	2.6130694
N	1.2297439	0.1516712	2.0163091
C	2.0084057	0.9873573	2.7217480
H	2.0706108	2.0460981	2.4480681
C	2.6601165	0.2981303	3.7780041
H	3.3540151	0.7126940	4.5152913
C	2.2343450	-1.0201568	3.6818286
H	2.4753258	-1.9016159	4.2840367
H	1.8541381	4.0140292	-2.0942376
H	1.1825859	-3.8035913	3.3340295
S	0.0566013	6.3681577	-1.1960373
S	-0.2109897	-6.0194921	2.4128728
C	1.2117485	6.8866401	-2.6177735
C	2.6919505	6.7235324	-2.2354012
H	2.9177826	7.1987707	-1.2623591
H	3.3151353	7.2211098	-3.0064279
H	3.0225774	5.6689799	-2.1931688
C	0.8328482	6.1531166	-3.9142215
H	1.4466286	6.5551947	-4.7460425
H	-0.2313277	6.3111000	-4.1728330
H	1.0205260	5.0635833	-3.8655112
C	0.8542113	8.3872336	-2.7225144
H	1.0941428	8.9358515	-1.7911366
H	-0.2160345	8.5407568	-2.9609390
H	1.4502748	8.8360051	-3.5417527
C	-1.2396997	-7.2366053	1.3726741
C	-0.9669908	-8.5503851	2.1398763
H	-1.3075291	-8.4933705	3.1918521
H	0.1061897	-8.8217132	2.1283171
H	-1.5285946	-9.3692729	1.6482305
C	-2.7348401	-6.8825431	1.4348250
H	-3.0961686	-6.8279965	2.4792771
H	-3.3142944	-7.6742075	0.9173952
H	-2.9773936	-5.9236250	0.9387598
C	-0.6892069	-7.3361056	-0.0594237
H	-1.2156551	-8.1567153	-0.5885534
H	0.3916062	-7.5728285	-0.0601805
H	-0.8379549	-6.4164545	-0.6574531

3^{2+}, parallel conformation, high-spin

Fe	-0.1665550	0.0590024	0.4237895
N	0.0198908	2.1782506	0.1903060
C	1.1237823	2.7222781	-0.3598302
C	1.3064759	4.0969827	-0.5382449
C	0.2666974	4.9765845	-0.1232573
C	-0.9050326	4.3946385	0.4542635
H	-1.7305029	5.0403089	0.7789326
C	-0.9707649	3.0103172	0.5865865
N	2.0882786	1.7492415	-0.7347296
N	1.8168892	0.4318092	-0.4777626
C	2.8724124	-0.2542294	-0.9429924
H	2.9008833	-1.3459426	-0.8497876
C	3.8398915	0.6161163	-1.5067501
H	4.7998491	0.3515317	-1.9601909
C	3.3073086	1.8903445	-1.3553613
H	3.7027676	2.8685408	-1.6431982
N	-2.0812335	2.3194384	1.1387860
N	-2.0417963	0.9510386	1.1762547
C	-3.1987836	0.5698394	1.7400582
H	-3.4150360	-0.4954714	1.8805531
C	-3.9984499	1.6919678	2.0745641
H	-4.9872394	1.6981013	2.5430101
C	-3.2548197	2.7953415	1.6740886
H	-3.4742077	3.8654364	1.7338340
N	-0.3578410	-2.0540448	0.6585272
C	-0.9128085	-2.8155479	-0.3064332
C	-1.0741574	-4.2008610	-0.2059766
H	-1.5482839	-4.7645293	-1.0131130
C	-0.6174352	-4.8496853	0.9764972
C	-0.0284036	-4.0384206	1.9960448
C	0.0701675	-2.6656675	1.7873909
N	-1.3274149	-2.0582841	-1.4344175
N	-1.1612235	-0.6991162	-1.4010562
C	-1.6188953	-0.2476373	-2.5788923
H	-1.6014470	0.8260630	-2.7985794
C	-2.0859651	-1.3143317	-3.3886774
H	-2.5149396	-1.2588607	-4.3936881
C	-1.8866652	-2.4579049	-2.6257328
H	-2.0982204	-3.5083105	-2.8451976
N	0.6377286	-1.7621262	2.7236158
N	0.7118153	-0.4369243	2.3861278
C	1.2720448	0.1759502	3.4409045
H	1.4480981	1.2574830	3.4166828
C	1.5651330	-0.7506114	4.4734284
H	2.0225843	-0.5508909	5.4470567
C	1.1486235	-1.9813792	3.9811325
H	1.1785278	-2.9782383	4.4309075
H	0.3405963	-4.5064396	2.9172690
H	2.2288333	4.4808135	-0.9801410
S	0.2319962	6.7211269	-0.2234028
S	-0.6953949	-6.5510665	1.3671265
C	-1.3498395	-7.5959780	-0.0826675
C	-2.8216919	-7.2656075	-0.3805633
H	-3.4460094	-7.3530039	0.5284258
H	-3.2073750	-7.9895961	-1.1269275
H	-2.9703298	-6.2533351	-0.8016907
C	-1.2354318	-9.0137427	0.5231585
H	-1.8625185	-9.1308196	1.4282540
H	-0.1892490	-9.2694639	0.7795176
H	-1.5886579	-9.7470509	-0.2287060
C	-0.4293027	-7.4672934	-1.3072875

H	-0.7663146	-8.1847518	-2.0832376
H	0.6191698	-7.7138180	-1.0535576
H	-0.4452760	-6.4597628	-1.7649706
C	1.8036702	7.4339009	-1.0324423
C	1.4794125	8.9436171	-0.9753513
H	1.3418002	9.2978240	0.0647403
H	0.5720258	9.1936755	-1.5582589
H	2.3284572	9.5051768	-1.4130903
C	1.9219893	6.9675389	-2.4925343
H	2.7759585	7.4920383	-2.9682584
H	1.0112417	7.2114353	-3.0718728
H	2.1101184	5.8817320	-2.5913353
C	3.0488147	7.1279819	-0.1843968
H	2.9175724	7.4659281	0.8605710
H	3.9139951	7.6755143	-0.6113005
H	3.3200119	6.0558353	-0.1665430

3^{2+}, perpendicular conformation, low-spin

Fe	0.0000005	-0.0000001	0.4045050
N	-1.8915993	0.2029450	0.4270043
C	-2.4858668	1.1100145	-0.3858098
C	-3.8681447	1.3297807	-0.3676440
C	-4.6534160	0.5953695	0.5602992
C	-4.0274435	-0.3805047	1.3801802
H	-4.6250722	-0.9625488	2.0922983
C	-2.6389623	-0.5330751	1.2853426
N	-1.5268787	1.7669055	-1.1797719
N	-0.2095478	1.4012054	-0.9780584
C	0.5124733	2.1618871	-1.8159757
H	1.6029352	2.0641329	-1.8503363
C	-0.3304609	3.0233347	-2.5667927
H	-0.0300158	3.7526537	-3.3250151
C	-1.6222628	2.7487723	-2.1386973
H	-2.5873380	3.1692224	-2.4379875
N	-1.8245897	-1.4037272	2.0334923
N	-0.4670768	-1.3397267	1.7834721
C	0.0979184	-2.2388634	2.6043608
H	1.1835730	-2.3854672	2.6017382
C	-0.8881024	-2.8912986	3.3914397
H	-0.7300948	-3.6685580	4.1451399
C	-2.1013086	-2.3376131	3.0051508
H	-3.1245714	-2.5336368	3.3401430
N	1.8915992	-0.2029451	0.4270044
C	2.4858669	-1.1100145	-0.3858096
C	3.8681448	-1.3297806	-0.3676440
H	4.3446431	-2.0771874	-1.0134874
C	4.6534161	-0.5953695	0.5602992
C	4.0274435	0.3805045	1.3801804
C	2.6389623	0.5330747	1.2853428
N	1.5268789	-1.7669055	-1.1797717
N	0.2095481	-1.4012058	-0.9780578
C	-0.5124731	-2.1618876	-1.8159749
H	-1.6029350	-2.0641336	-1.8503352
C	0.3304610	-3.0233352	-2.5667920
H	0.0300159	-3.7526545	-3.3250142
C	1.6222630	-2.7487725	-2.1386969
H	2.5873381	-3.1692224	-2.4379875
N	1.8245898	1.4037270	2.0334924
N	0.4670769	1.3397266	1.7834719
C	-0.0979184	2.2388632	2.6043605
H	-1.1835730	2.3854670	2.6017379
C	0.8881024	2.8912984	3.3914397

H	0.7300948	3.6685578	4.1451398
C	2.1013086	2.3376128	3.0051509
H	3.1245714	2.5336366	3.3401431
H	-4.3446430	2.0771874	-1.0134875
H	4.6250721	0.9625485	2.0922986
S	-6.4080709	0.9002253	0.6900292
S	6.4080709	-0.9002252	0.6900291
C	-7.2247922	-0.3045597	-0.5657680
C	-8.7109136	0.0766026	-0.4224117
H	-9.0779267	-0.0863656	0.6093277
H	-9.3088728	-0.5658556	-1.0997159
H	-8.8942764	1.1310173	-0.7047999
C	-6.7111357	-0.0278075	-1.9836690
H	-7.2705053	-0.6617127	-2.7027201
H	-5.6375420	-0.2798173	-2.0958720
H	-6.8670696	1.0285405	-2.2754678
C	-6.9771715	-1.7547981	-0.1331888
H	-7.3234460	-1.9307291	0.9028840
H	-5.9076935	-2.0366895	-0.2100072
H	-7.5415438	-2.4379073	-0.8013607
C	7.2247920	0.3045600	-0.5657681
C	8.7109136	-0.0766020	-0.4224118
H	8.8942765	-1.1310167	-0.7047999
H	9.0779267	0.0863664	0.6093275
H	9.3088726	0.5658562	-1.0997163
C	6.7111355	0.0278079	-1.9836690
H	6.8670697	-1.0285400	-2.2754681
H	7.2705049	0.6617134	-2.7027201
H	5.6375418	0.2798174	-2.0958720
C	6.9771711	1.7547983	-0.1331886
H	7.5415433	2.4379077	-0.8013604
H	7.3234456	1.9307292	0.9028842
H	5.9076931	2.0366896	-0.2100071

3^{2+}, perpendicular conformation, high-spin

Fe	0.0001064	0.0002726	0.1843379
N	-2.1304200	0.2475551	0.3438984
C	-2.7719383	1.1424541	-0.4344137
C	-4.1512607	1.3756880	-0.3454451
C	-4.8905981	0.6558058	0.6261176
C	-4.2201242	-0.3063284	1.4210010
H	-4.7817659	-0.8775346	2.1695610
C	-2.8387034	-0.4669720	1.2421066
N	-1.9089206	1.8096187	-1.3395960
N	-0.5818183	1.4674744	-1.3464284
C	-0.0119076	2.2463958	-2.2798784
H	1.0611203	2.1596445	-2.4861051
C	-0.9666558	3.1036909	-2.8834958
H	-0.8020843	3.8450306	-3.6712987
C	-2.1702770	2.7971562	-2.2609556
H	-3.1752534	3.2052061	-2.4044337
N	-2.0447374	-1.3810196	1.9778292
N	-0.6990034	-1.4264629	1.7262616
C	-0.2130876	-2.3832868	2.5332046
H	0.8581345	-2.6154796	2.5276466
C	-1.2431670	-2.9666051	3.3143876
H	-1.1533997	-3.7650244	4.0572002
C	-2.4021575	-2.3011739	2.9359061
H	-3.4368819	-2.4160029	3.2721271
N	2.1305548	-0.2474687	0.3442798
C	2.7720536	-1.1424393	-0.4339708
C	4.1513822	-1.3757098	-0.3450021

H	4.6613656	-2.1115818	-0.9777078
C	4.8907739	-0.6557334	0.6264239
C	4.2203152	0.3063617	1.4213485
C	2.8388877	0.4670269	1.2424768
N	1.9090104	-1.8097253	-1.3390341
N	0.5819255	-1.4675286	-1.3459464
C	0.0119640	-2.2466766	-2.2791695
H	-1.0610692	-2.1599480	-2.4853752
C	0.9666636	-3.1041456	-2.8825911
H	0.8020473	-3.8456854	-3.6701915
C	2.1703150	-2.7974717	-2.2601805
H	3.1752736	-3.2055865	-2.4035843
N	2.0449516	1.3809612	1.9783110
N	0.6992445	1.4264493	1.7267198
C	0.2133196	2.3830350	2.5339367
H	-0.8579033	2.6152023	2.5284556
C	1.2433829	2.9661525	3.3152891
H	1.1535994	3.7643442	4.0583366
C	2.4023785	2.3008855	2.9365923
H	3.4371008	2.4156389	3.2728423
H	-4.6612737	2.1115203	-0.9781741
H	4.7819817	0.8775739	2.1698856
S	-6.6370464	0.9594382	0.8413183
S	6.6372741	-0.9591813	0.8414257
C	-7.4985459	-0.2698126	-0.3643590
C	-8.9819894	0.0878913	-0.1493004
H	-9.2979232	-0.0782486	0.8991609
H	-9.6027153	-0.5650430	-0.7963765
H	-9.1969989	1.1387037	-0.4230211
C	-7.0604362	0.0066930	-1.8075586
H	-7.6436494	-0.6412787	-2.4945502
H	-5.9895426	-0.2264807	-1.9724809
H	-7.2482138	1.0587057	-2.0959840
C	-7.2043987	-1.7121637	0.0645961
H	-7.4973399	-1.8885259	1.1169431
H	-6.1347194	-1.9749728	-0.0607747
H	-7.7861569	-2.4094348	-0.5735394
C	7.4984121	0.2700999	-0.3643963
C	8.9818580	-0.0871891	-0.1495750
H	9.1971618	-1.1379770	-0.4229535
H	9.2978756	0.0794956	0.8986546
H	9.6022014	0.5655669	-0.7969941
C	7.0602304	-0.0066872	-1.8074910
H	7.2483417	-1.0586318	-2.0958866
H	7.6430711	0.6413932	-2.4946022
H	5.9892838	0.2260987	-1.9722588
C	7.2039427	1.7123937	0.0644424
H	7.7853396	2.4096815	-0.5738936
H	7.4970223	1.8890056	1.1166698
H	6.1342170	1.9749066	-0.0607204

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