Electronic Supplementary Material (ESI) for Dalton Transactions.

Heteroleptic Iron(II) Complexes of Chiral 2,6-Bis(Oxazolin-2-yl)-pyridine (PyBox) and 2,6-Bis(Thiazolin-2-yl)pyridine Ligands – the Interplay of Two Different Ligands on the Metal Ion Spin State

Namrah Shahid,[a,b] Kay E. Burrows,[a] Christopher M. Pask,[a] Oscar Cespedes,[c] Mark J. Howard,[a] Patrick C. McGowan[a] and Malcolm A. Halcrow[a,*]

[a]*School of Chemistry, University of Leeds, Woodhouse Lane, Leeds LS2 9JT, United Kingdom.*
E-mail: m.a.halcrow@leeds.ac.uk

[b]*Current address: Department of Chemistry, University of Durham, Durham DH1 3LE, United Kingdom.*

[c]*School of Physics and Astronomy, University of Leeds, WH Bragg Building, Leeds LS2 9JT, United Kingdom.*

Supporting Information

Complex synthesis and Characterisation Data

The L^1R,[1] L^2R[2] and bpp[3] ligands were synthesised using literature procedures. Other ligand and metal salt reagents, and organic solvents, were purchased commercially and used as supplied.

Caution. Although we have experienced no problems when using the perchlorate salts in this study, metal–organic perchlorates are potentially explosive and should be handled with care in small quantities.

Complex synthesis. The same protocol was used to synthesise all the complexes, with minor variations as described below. Around 0.25 mmol of the two ligands used was dissolved in acetonitrile (20 cm^3), then an equimolar amount of solid $Fe[ClO_4]_2{\cdot}6H_2O$ was added to the solution. The mixture was stirred at room temperature for the stated length of time, when all the solids had dissoved, then concentrated to *ca* 5 cm^3 volume. Slow diffusion of diethyl ether vapour into the filtered solution yielded the solid complex products, which were purified as described below.

Complexes containing L^2iPr were prepared on a reduced scale, because the challenging synthesis of that ligand meant it was only available in small quantities.[2]

Synthesis of [Fe((*S*)-L^1Ph)((*R*)-L^2Ph)][ClO_4]$_2{\cdot}MeNO_2$ (1·$MeNO_2$). Method as above, using (*S*)-L^1Ph (89 mg, 0.24 mmol), (*R*)-L^2Ph (96 mg, 0.24 mmol) and $Fe[ClO_4]_2{\cdot}6H_2O$ (88 mg, 0.24 mmol). The dark purple solution was stirred for 20 hrs before workup. Recrystallisation of the crude purple powder from nitromethane solution by diethyl ether vapour diffusion afforded single crystals of the complex. Yield 171 mg, 66 %. Found: C, 51.8; H, 3.67; N, 8.87 %. Calcd for $C_{46}H_{38}Cl_2FeN_6O_{10}S_2{\cdot}CH_3NO_2$: C, 51.9; H, 3.80; N, 9.02 %. ^{1}H NMR (CD_3CN) δ 3.6 (2H), 3.8 (2H), 5.0 (2H), 5.2 (2H), 5.4 (2H), 5.7 (4H), 6.0 (2H), 6.5 (4H), 7.0 (4H), 7.3 (8H), 10.1 (1H), 11.4 (1H), 14.7 (2H), 15.0 (2H). Contact-shifted peaks arising from [Fe((*S*)-L^1Ph)$_2$]$^{2+}$ are also resolved,[4] in a ratio of *ca* 0.15:1 compared to the main species (Figure 2).

The presence of one equiv nitromethane in this compound was confirmed crystallographically.

Synthesis of [Fe((*R*)-L^1iPr)((*S*)-L^2iPr)][ClO_4]$_2$ (2). Method as above, using reduced quantities of (*R*)-L^1iPr (18 mg, 0.06 mmol), (*S*)-L^2iPr (22 mg, 0.06 mmol) and $Fe[ClO_4]_2{\cdot}6H_2O$ (22 mg, 0.06 mmol) with the solvent volumes scaled appropriately. Diffusion of diethyl ether vapour into the filtered reaction solution yielded purple crystals of **2**·MeCN, which lost their lattice solvent upon exposure to air. Yield 37 mg, 69 %. Found: C, 45.7; H, 5.01; N, 9.09 %. Calcd for $C_{34}H_{46}Cl_2FeN_6O_{10}S_2$: C, 45.9; H, 5.21; N, 9.45 %. ^{1}H NMR (CD_3CN) δ –10.0 (6H), –8.3 (2H), –4.8 (6H), –1.9 (6H), –1.6 (6H), 6.0 (2H), 9.2 (2H), 14.4 (4H), 15.6 (2H), 16.6 (2H), 20.8 (1H), 27.0 (1H), 60.9 (4H). One more resonance of integral 2H is expected upfield of 2 ppm, corresponding to an *iso*propyl CH environment. However this was not unambiguously identified, and could be masked by solvent peaks (Figure S7). Peaks arising from [Fe((*R*)-L^1iPr)$_2$]$^{2+}$ are also present,[4] in a ratio of *ca* 0.20:1 compared to the main species, along with some uncoordinated ligand which is probably L^2iPr.

Synthesis of [Fe((*R*)-L^1Ph)(bimpy)][ClO_4]$_2{\cdot}$MeCN (3·MeCN). Method as above, using (*R*)-L^1Ph (103 mg, 0.28 mmol), bimpy (87 mg, 0.28 mmol) and $Fe[ClO_4]_2{\cdot}6H_2O$ (102 mg, 0.28 mmol). The purple-red solution was stirred for 20 hrs before workup, which afforded purple single crystals of the product in analytical purity. Yield 228 mg, 83 %. Found: C, 53.9; H, 3.54; N, 12.8 %. Calcd for $C_{42}H_{32}Cl_2FeN_8O_{10}{\cdot}CH_3CN$: C, 54.1; H, 3.61; N, 12.9 %. ^{1}H NMR (CD_3CN) δ 3.8 (2H), 4.1 (2H), 4.3 (2H), 5.5 (4H), 5.9 (2H), 6.0 (2H), 6.5 (2H), 6.8 (2H), 7.5 (2H), 11.8 (1H), 12.1 (2H), 16.6 (2H), 27.8 (1H), 33.1 (2H), 33.9 (2H), 36.3 (2H).

The presence of one equiv acetonitrile in this material was confirmed crystallographically.

Synthesis of [Fe((*R*)-L^2Ph)(bimpy)][ClO_4]$_2{\cdot}H_2O$ (4·H_2O). Method as above, using (*R*)-L^2Ph (112 mg, 0.28 mmol), bimpy (87 mg, 0.28 mmol) and $Fe[ClO_4]_2{\cdot}6H_2O$ (102 mg, 0.28 mmol). The purple solution was stirred for 20 hrs before workup, which afforded violet single crystals of the product. No further purification was required. Yield 126 mg, 46 %. Found: C, 50.9; H, 3.21; N, 11.1 %. Calcd for $C_{42}H_{32}Cl_2FeN_8O_8S_2{\cdot}H_2O$: C, 51.2; H, 3.48; N, 11.4 %. ^{1}H NMR (CD_3CN) δ 2.9 (2H), 3.9 (2H), 4.2 (2H), 5.3 (4H), 6.5 (6H), 7.1 (2H), 7.2 (2H), 7.4 (2H), 8.3 (1H), 8.4 (2H), 10.2 (2H), 10.6 (2H), 10.8 (1H), 13.8 (2H).

Synthesis of [Fe((*S*)-*L*^{1}*i*Pr)(bimpy)][ClO$_4$]$_2$ (5). Method as above, using (*S*)-*L*^{1}*i*Pr (83 mg, 0.28 mmol), bimpy (87 mg, 0.28 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (102 mg, 0.28 mmol). The purple-red solution was stirred for 20 hrs before workup. The crude purple powder gave a dark red crystalline solid after recrystallisation from acetone solution by diethyl ether vapour diffusion. Yield 130 mg, 53 %. Found: C, 49.6; H, 3.86; N, 13.4 %. Calcd for $C_{36}H_{36}Cl_2O_{10}FeN_8$: C, 49.9; H, 4.18; N, 12.9 %. ^{1}H NMR (CD$_3$CN) δ –29.0 (6H), –12.6 (2H), –7.5 (6H), 7.1 (2H), 7.9 (1H), 13.1 (2H), 17.4 (2H), 18.6 (2H), 21.2 (1H), 26.4 (2H), 37.4 (2H), 55.7 (2H), 60.8 (2H), 63.9 (2H). Peaks from [Fe((*R*)-*L*^{1}*i*Pr)$_2$]$^{2+}$ are also present,[4] in a ratio of *ca* 0.25:1 compared to the main species, along with extra peaks in the diamagnetic region which might be uncoordinated bimpy.

Synthesis of [Fe((*S*)-*L*^{2}*i*Pr)(bimpy)][ClO$_4$]$_2$ (6). Method as above, but using half-quantities of (*S*)-*L*^{2}*i*Pr (53 mg, 0.16 mmol), bimpy (47 mg, 0.16 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (58 mg, 0.16 mmol) with the solvent volumes scaled appropriately. The purple solution was stirred for 20 hrs before workup, which afforded purple crystals suitable for X-ray diffraction. Yield 54 mg, 40 %. Found: C, 47.7; H, 3.87; N, 12.2 %. Calcd for $C_{36}H_{36}Cl_2FeN_8O_8S_2$: C, 48.1; H, 4.03; N, 12.5 %. ^{1}H NMR (CD$_3$CN) δ –5.9 (6H), –4.4 (2H), –0.7 (6H), 5.1 (2H), 5.2 (2H), 5.4 (2H), 7.0 (2H), 7.3 (2H), 9.1 (2H), 10.5 (1H), 12.5 (2H), 16.3 (1H), 20.3 (2H), 21.1 (2H), 23.0 (2H).

Synthesis of [Fe((*R*)-*L*^{1}Ph)(bpp)][ClO$_4$]$_2$ (7). Method as above, using (*R*)-*L*^{1}Ph (89 mg, 0.24 mmol), bpp (52 mg, 0.24 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (88 mg, 0.24 mmol). The dark brown solution was stirred for 2 hrs before workup, giving a red-brown polycrystalline product which was analysed without further purification. Yield 117 mg, 59 %. Found: C, 48.6; H, 3.38; N, 13.0 %. Calcd for $C_{34}H_{28}Cl_2FeN_8O_{10}$: C, 48.9; H, 3.38; N, 13.4 ^{1}H NMR (CD$_3$CN) δ 0.7 (4H), 3.8 (2H), 5.4 (4H), 6.2 (2H), 7.4 (1H), 9.1 (2H), 9.4 (2H), 20.8 (2H), 23.8 (2H), 26.8 (1H), 34.0 (2H), 38.5 (2H), 40.0 (2H).

Synthesis of [Fe((*R*)-*L*^{2}Ph)(bpp)][ClO$_4$]$_2$·MeCN·H$_2$O (8·MeCN·H$_2$O). Method as above, using (*R*)-*L*^{2}Ph (96 mg, 0.24 mmol), bpp (52 mg, 0.24 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (88 mg, 0.24 mmol). The dark brown solution was stirred for 2 hrs before workup. The reaction mixture yielded the product as brown single crystals, after the manual removal of a small quantity of yellow [Fe(bpp)$_2$][ClO$_4$]$_2$.[5] Yield 185 mg, 89 %. Found: C, 46.7; H, 3.28; N, 13.9 %. Calcd for $C_{34}H_{28}Cl_2FeN_8O_8S_2$·CH$_3$CN·H$_2$O: C, 46.7; H, 3.59; N, 13.6 %. C^{1}H NMR (CD$_3$CN) δ 2.2 (2H), 4.2 (4H), 5.4 (2H), 5.8 (1H), 6.3 (4H), 6.7 (4H), 12.4 (2H), 12.7 (2H), 13.1 (1H), 14.9 (2H), 15.5 (2H), 15.7 (2H). Peaks from [Fe(bpp)$_2$]$^{2+}$ are also present in a ratio of *ca* 0.10:1 compared to the main species.[6]

The crystals of this complex contain two equiv acetonitrile, so the microanalysis implies partial replacement of that solvent by atmospheric moisture.

Synthesis of [Fe((*S*)-*L*^{1}*i*Pr)(bpp)][ClO$_4$]$_2$·MeNO$_2$ (9·MeNO$_2$) Method as above, using (*S*)-*L*^{1}*i*Pr (69 mg, 0.23 mmol), bpp (49 mg, 0.23 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (87 mg, 0.23 mmol). The bright red solution was stirred for 2 hrs before workup. The crude product was recrystallised from nitromethane solution by diethyl ether vapour diffusion, giving a red polycrystalline solid containing a small quantity of yellow [Fe(bpp)$_2$][ClO$_4$]$_2$,[5] which was removed manually. Recrystallised yield 66 mg, 37 %. Found: C, 42.4; H, 3.88; N, 15.0 %. Calcd for $C_{28}H_{32}Cl_2FeN_8O_{10}$·CH$_3NO_2$: C, 42.1; H, 4.26; N, 15.2 ^{1}H NMR (CD$_3$CN) δ –36.1 (6H), –13.7 (2H), –6.0 (6H), 3.4 (1H), 10.2 (2H), 15.8 (2H), 24.2 (2H), 33.7 (2H), 39.4 (2H), 59.0 (2H), 67.7 (2H), 68.9 (2H). One more resonance expected from the molecule could not be unambiguously identified (Figure S25). Peaks from [Fe(bpp)$_2$]$^{2+}$ are also present in a ratio of *ca* 0.15:1 compared to the main species,[6] along with weak resonances in the diamagnetic region which may be uncoordinated *L*^{1}*i*Pr.

Synthesis of [Fe((*S*)-*L*^{2}*i*Pr)(bpp)][ClO$_4$]$_2$·2H$_2$O (10·2H$_2$O). Method as above, but using half-quantities of (*S*)-*L*^{2}*i*Pr (39 mg, 0.12 mmol), bpp (25 mg, 0.12 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (44 mg, 0.12 mmol) with the solvent volumes scaled appropriately. The red-brown solution was stirred for 3 hrs before workup. The product was a brown powder, containing a small quantity of yellow [Fe(bpp)$_2$][ClO$_4$]$_2$[5] which was removed manually. Yield 53 mg, 56 %. Found: C, 40.3; H, 3.99; N, 13.1 %. Calcd for $C_{28}H_{32}Cl_2FeN_8O_8S_2$·2H$_2$O: C, 40.3; H, 4.34; N, 13.4. ^{1}H NMR (CD$_3$CN) δ –8.2 (6H), –5.2 (2H), –1.4 (6H), 2.9 (1H), 7.6 (2H), 8.2 (2H), 10.7 (2H), 18.5 (1H), 21.5 (2H), 21.8 (2H), 28.9 (2H), 31.7 (2H), 33.2 (2H). Peaks from [Fe(bpp)$_2$]$^{2+}$ are also

present in a ratio of *ca* 0.20:1 compared to the main species,[6] along with another weak paramagnetic molecule whose identity is unclear (Figure S26).

Synthesis of [Fe((*R*)-*L*^{1}Ph)(terpy)][ClO$_4$]$_2$·H$_2$O (11·H$_2$O). Method as above, using (*R*)-*L*^{1}Ph (103 mg, 0.28 mmol), terpy (66 mg, 0.28 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (102 mg, 0.28 mmol). The dark purple solution was stirred for 20 hrs before workup, giving a purple polycrystalline product. Yield 174 mg, 74 %. Found: C, 51.9; H, 3.45; N, 9.62 %. Calcd for $C_{38}H_{30}FeCl_2N_6O_{10}\cdot H_2O$: C, 52.1; H, 3.68; N, 9.60 %.

This material contains a mixture of diamagnetic species by ^{1}H NMR, including $[Fe(terpy)_2]^{2+}$ (Figure S30).[7] Recrystallisation of the product from by nitromethane/diethyl ether vapour diffusion yielded a mixture of powder and dark purple crystals, which proved to be a solvate of $[Fe(terpy)_2][ClO_4]_2$ (Figure S29). Hence, despite its good microanalysis, **11**·H$_2$O is evidently a mixture of species.

Synthesis of [Fe((*S*)-*L*^{1}*i*Pr)(terpy)][ClO$_4$]$_2$ (12). Method as above, using (*S*)-*L*^{1}*i*Pr (86 mg, 0.28 mmol), terpy (66 mg, 0.28 mmol) and Fe[ClO$_4$]$_2$·6H$_2$O (102 mg, 0.28 mmol). The dark purple solution was stirred for 20 hrs before workup, giving a purple polycrystalline product. Yield 129 mg, 74 %. Found: C, 48.5; H, 4.10; N, 10.6 %. Calcd for $C_{32}H_{34}FeCl_2N_6O_{10}$: C, 48.7; H, 4.34; N, 10.7 %.

The comments about the composition of **11**·H$_2$O also apply to this material.

Single Crystal Structure Analyses

All crystals were grown by slow diffusion of diethyl ether vapour into concentrated solutions of the complexes. Nitromethane was used as the crystallisation solvent for **1**·MeNO$_2$, while all the other crystals were obtained from acetonitrile solution.

Diffraction data for **4** were collected at station I19 of the Diamond synchrotron (λ = 0.6889 Å). The other crystals were measured with an Agilent Supernova dual-source diffractometer using monochromated Cu-K_α (λ = 1.5418 Å) radiation. The diffractometer was fitted with an Oxford Cryostream low-temperature device. Experimental details of the structure determinations in this study are given in Tables S1-S2. All the structures were solved by direct methods *(SHELXS*[8]), and developed by full least-squares refinement on F^2 (*SHELXL-2018*[8]). Crystallographic figures were prepared using *XSEED*,[9] and octahedral coordination volumes (V_{Oh}) were calculated with *Olex2*.[10]

Unless otherwise stated, the following protocols were used. All crystallographically ordered non-H atoms in these refinements were refined anisotropically. Disordered anions were modelled with refined Cl–O and O···O distance restraints, and disordered lattice solvent molecules were modelled using fixed bond length and angle restraints. All H atoms were placed in calculated positions and refined using a riding model.

Structure refinement of [Fe((*S*)-*L*^{1}Ph)((*R*)-*L*^{2}Ph)][ClO$_4$]$_2$·MeNO$_2$ (1·MeNO$_2$) Phenyl substituent C(13)-C(18) is disordered over two half-occupied orientations, which were refined with all C–C bond distances constrained to be the same (*SHELXL SADI* instruction). The O atoms of one perchlorate ion are also disordered over two equally occupied sites.

Structure refinement of [Fe((*R*)-*L*^{1}*i*Pr)((*S*)-*L*^{1}*i*Pr)][ClO$_4$]$_2$·MeCN (2·MeCN). The asymmetric unit contains two formula units of the compound, that is: two complex dications, four perchlorate ions and two acetonitrile molecules on general crystallographic sites. All four anions and both solvent molecules are disordered over two or three sites, which were treated as described above. All crystallographically ordered non-H atoms, plus Cl atoms from the major orientations of two of the anions, were refined anisotropically.

ADDSYM notes pseudo-inversion symmetry in the crystal,[11] but the Flack parameter of 0.010(2) confirms this is not true inversion symmetry. An attempted refinement in the suggested alternative space group $P2_1/c$ gave much higher residuals (R_1 = 0.19, wR_2 = 0.43). Hence, we are confident our choice of the $P2_1$ space group is correct.

Structure refinement of [Fe((*R*)-*L*^{1}Ph)(bimpy)][ClO$_4$]$_2$·MeCN (3·MeCN). A minor twin domain in the dataset was noted by *CheckCif*, and was accounted for in the final refinement using *Olex2*.[10] The twin law is 0 1 0 1 0 0 0 0 –1, and the ratio of the twin domains refined to 0.98:0.02. The refinement has low precision, but this is likely to reflect the effect of the highly anisotropic unit cell (a = b = 10.6 Å, c = 73.8 Å) on the data rather than this very minor twinning.

The asymmetric unit contains two formula units of the compound, with two complex dications, four ClO_4^- anions and two solvent molecules on general crystallographic sites. No disorder is present in the model, which was refined without distance restraints. However, four atoms in the model required a *SHELXL ISOR* restraint to stop them becoming prolate or non-positive definite. All non-H atoms were refined anisotropically, and H atoms were fixed in calculated positions and refined using a riding model.

The highest residual Fourier peak of +1.0 e Å^{-3} is 0.8 Å from Fe(1A).

Structure refinement of [Fe((*R*)-*L*^{2}Ph)(bimpy)][ClO$_4$]$_2$ (4). Minor disorder in one anion was included in the final model, to mop up a residual Fourier peak. Two orientations of that anion were refined with a 0.90:0.10 occupancy ratio, and refined distance restraints were applied to the minor anion site. All non-H atoms except the minor anion disorder site were refined anisotropically.

Structure refinement of [Fe((*S*)-*L*^{1}*i*Pr)(bimpy)][ClO$_4$]$_2$ (5). Crystals of this compound were consistently twinned. After several attempted data collections, this dataset was successfully deconvoluted into two twin domains using the twin law –1 0 0 0 0 1 0 1 0, in a refined ratio of 0.36:0.64. While the refinement residuals are good, the model has relatively low precision because of this twinning.

*Iso*propyl group C(21)-C(23) is disordered over two equally occupied sites, and was modelled with the refined restraints C–C = 1.53(2) and 1,3-C...C = 2.50(2) Å. All crystallographically ordered non-H atoms were refined anisotropically.

Structure refinement of [Fe((*S*)-*L*^{2}*i*Pr)(bimpy)][ClO$_4$]$_2$·MeCN·Et$_2$O (6·MeCN·Et$_2$O). The diethyl ether molecule is disordered over two equally occupied sites, which were treated with fixed distance restraints. All crystallographically ordered non-H atoms were refined anistropically.

Structure refinement of [Fe((*R*)-*L*^{2}Ph)(1-bpp)][ClO$_4$]$_2$·2MeCN (8·2MeCN). One perchlorate ion in this structure is disordered over two sites, with refined occupancies of 0.73 and 0.27. These were treated with refined distance restraints, as described above. All non-H atoms except the minor anion disorder site were refined anisotropically.

Structure refinement of [Fe(terpy)$_2$][ClO$_4$]$_2$·2MeCN. The asymmetric unit contains two forumla units of the compound; that is, two complex dicatioons, four perchlorate anions and four acetonitrile molecules. Two of the ClO_4^- ions were refined over two disorder sites, with refined occupancy ratios of 0.65:0.35 and 0.75:0.25. The U_{iso} parameters of the O atoms in the minor disorder site of each anion were also constrained to be equal. One MeCN molecule is also disordered, and was modelled over two half-occupied orientations.

CCDC 2132824-2132830 contain the supplementary crystallographic data for this paper (Table S1). These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* **www.ccdc.cam.ac.uk/data_request/cif**.

Table S1 Experimental data for the crystal structures in this work. Data were collected using Cu-K_α radiation unless otherwise stated.

	1·$MeNO_2$	**2**·MeCN	**3**·MeCN	**4**
molecular formula	$C_{47}H_{41}Cl_2FeN_7O_{12}S_2$	$C_{36}H_{49}Cl_2FeN_7O_{10}S_2$	$C_{44}H_{35}Cl_2FeN_9O_{10}$	$C_{42}H_{32}Cl_2FeN_8O_8S_2$
M_r	1086.74	930.69	976.56	967.62
crystal class	monoclinic	monoclinic	tetragonal	monoclinic
space group	$P2_1$	$P2_1$	$P4_1$	$P2_1$
a / Å	11.9689(2)	11.3515(1)	10.6379(1)	9.9525(1)
b / Å	12.0094(1)	18.6328(3)	10.6379(1)	18.2692(1)
c / Å	16.2339(2)	20.5925(3)	73.8154(8)	11.2555(1)
α / °	90	90	90	90
β / °	94.775(1)	102.246(1)	90	90.601(1)
γ / °	90	90	90	90
V / Å^3	2325.35(5)	4256.42(10)	8353.31(18)	2046.41(3)
Z	2	4	8	2
T / K	125(2)	130(2)	130(2)	100(2)
μ{Cu-K_α} / mm^{-1}	5.120	5.445	4.698	0.617[c]
D_c / gcm^{-3}	1.552	1.452	1.553	1.570
measured reflections	20842	37789	32362	32540
independent reflections	8622	15763	16045	17281
R_{int}	0.037	0.036	0.053	0.027
parameters	632	1067	1192	589
restraints	52	98	25	11
R_1 [$F_0 > 4\sigma(F_0)$][a]	0.036	0.059	0.071	0.029
wR_2, all data[b]	0.092	0.157	0.159	0.074
goodness of fit	1.036	1.064	1.131	1.040
$\Delta\rho_{min/max}$ / eÅ^{-3}	–0.43/0.66	–0.72/0.81	–0.56/0.98	–0.33/0.34
Flack parameter	–0.005(2)	0.009(2)	–0.002(3)	0.022(4)
CCDC	2132824	2132825	2132826	2132827

[a] $R = \Sigma[||F_o| - |F_c||] / \Sigma|F_o|$ [b] $wR = [\Sigma w(F_o^2 - F_c^2) \ / \ \Sigma wF_o^4]^{1/2}$ [c] Collected with synchrotron radiation.

Table S1 continued.

	5	**6**·MeCN·Et_2O	**8**·2MeCN	$[Fe(terpy)_2][ClO_4]_2$·2MeCN
molecular formula	$C_{36}H_{36}Cl_2FeN_8O_{10}$	$C_{42}H_{49}Cl_2FeN_9O_9S_2$	$C_{38}H_{34}Cl_2FeN_{10}O_8S_2$	$C_{34}H_{28}Cl_2FeN_8O_8$
M_r	867.48	1014.77	949.62	803.39
crystal class	orthorhombic	monoclinic	orthorhombic	tetragonal
space group	$P2_12_12_1$	$P2_1$	$P2_12_12_1$	$P4_3$
a / Å	10.1310(5)	9.0025(3)	8.8452(1)	12.2320(1)
b / Å	19.1776(10)	24.0613(9)	20.3285(3)	12.2320(1)
c / Å	19.2647(10)	11.2550(5)	22.9238(4)	47.2452(6)
α / °	90	90	90	90
β / °	90	106.649(4)	90	90
γ / °	90	90	90	90
V / Å^3	3742.9(3)	2335.75(16)	4121.92(11)	7068.91(15)
Z	4	2	4	8
T / K	120(2)	130(2)	130(2)	130(2)
μ{Cu-K_α} / mm^{-1}	5.147	5.011	5.630	5.361
D_c / gcm^{-3}	1.539	1.443	1.530	1.510
measured reflections	9691	21424	15685	27682
independent reflections	6463	8331	7950	13607
R_{int}	0.037	0.076	0.046	0.039
parameters	515	586	573	948
restraints	12	15	14	44
R_1 [$F_0 > 4\sigma(F_0)$][a]	0.053	0.052	0.041	0.051
wR_2, all data[b]	0.143	0.132	0.095	0.129
goodness of fit	1.044	1.058	1.031	1.034
$\Delta\rho_{min/max}$ / eÅ^{-3}	–0.95/0.50	–0.70/0.43	–0.35/0.33	–0.73/0.52
Flack parameter	0.003(3)	–0.009(5)	–0.005(4)	–0.005(3)
CCDC	2132828	2132829	2132830	2134550

[a] $R = \Sigma[\,|F_o| - |F_c|\,] / \Sigma|F_o|$ [b] $wR = [\Sigma w(F_o^2 - F_c^2) \;/\; \Sigma wF_o^4]^{1/2}$ [c] Collected with synchrotron radiation.

Definitions of the Structural Parameters Tabulated for the Complexes

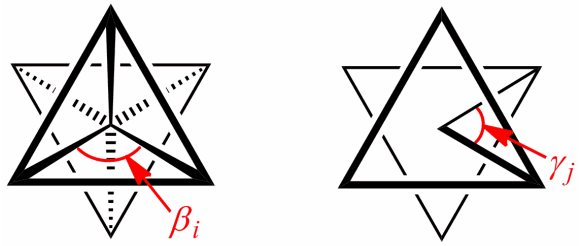
V_{Oh} is the volume (in Å^3) of the FeN_6 coordination octahedron in the complex,[12] which is typically <10 Å^3 in low-spin complexes of meridional *tris*-heterocyclic ligands and ≥11.5 Å^3 in their high-spin form.[13]

Σ and Θ are defined as follows:

$$\Sigma = \sum_{i=1}^{12} |90 - \beta_i| \qquad \Theta = \sum_{j=1}^{24} |60 - \gamma_j|$$

where β_i are the twelve *cis*-N–Fe–N angles about the iron atom and γ_i are the 24 unique N–Fe–N angles measured on the projection of two triangular faces of the octahedron along their common pseudo-threefold axis (Scheme S1). Σ is a general measure of the deviation of a metal ion from an ideal octahedral geometry, while Θ more specifically indicates its distortion towards a trigonal prismatic structure. A perfectly octahedral complex gives $\Sigma = \Theta = 0$.[12,14]

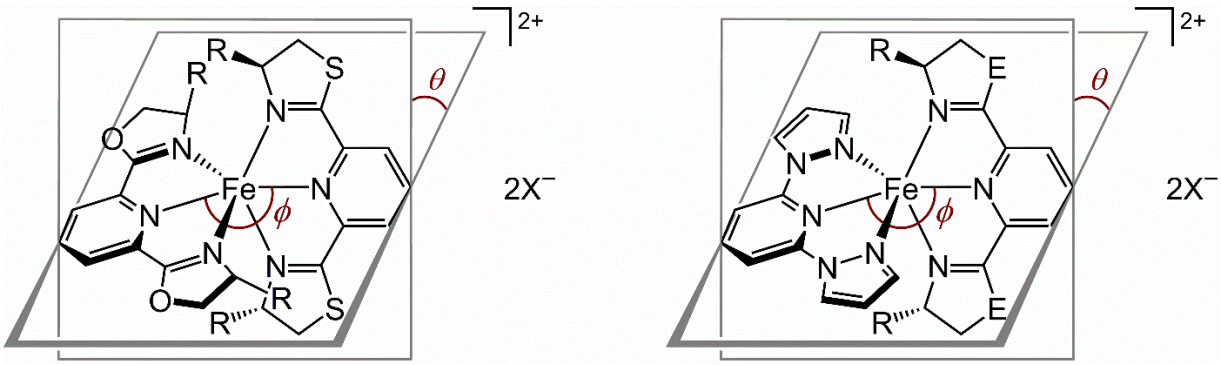
Because the high-spin state of a complex has a more plastic structure than the low-spin, this is reflected in Σ and Θ which are usually much larger in the high-spin state. The absolute values of these parameters depend on the metal/ligand combination in the compound under investigation, however. Typical values of these parameters for complexes related to $[Fe(L^1R)_2]^{2+}$ and $[Fe(L^2R)_2]^{2+}$ are given in ref. 15.



Scheme S1. Angles used in the definitions of the coordination distortion parameters Σ and Θ.

The parameters in Scheme S2 define the relative disposition of the two tridentate ligands around the iron atom.[16] These should be close to their ideal values ($\theta \approx 90°$, $\phi \approx 180°$) in a low-spin complex, but high-spin compounds can show a lot more variation. Significant deviations of θ and ϕ from ideality are associated with an angular Jahn-Teller distortion of the ^5T high-spin configuration in a high-spin complex of this type.[6] This distortion is often observed in high-spin complexes of *tris*-heterocyclic chelates,[2,4-6,17-19] including PyBox and ThioPyBox derivatives.[2,4,19]

Spin-crossover can be inhibited if θ and ϕ deviate significantly from their ideal values, because the associated rearrangement to a more regular low-spin coordination geometry ($\theta \approx 90°$, $\phi \approx 180°$) cannot be accommodated by a rigid solid lattice.[20]



Scheme S2. Definition of the Jahn-Teller distortion parameters θ and ϕ, for two of the families of complexes in this work (E = O or S, R = Ph or *i*Pr).

NB ϕ is often calculated using all the non-H atoms from each tridentate ligand, which works well if the azoline rings are essentially planar. However, since the thiazoline rings in L^2R are puckered, only the coplanar pyridyl and azoline C=N groups of each ligand are used to calculate ϕ in this study.[2]

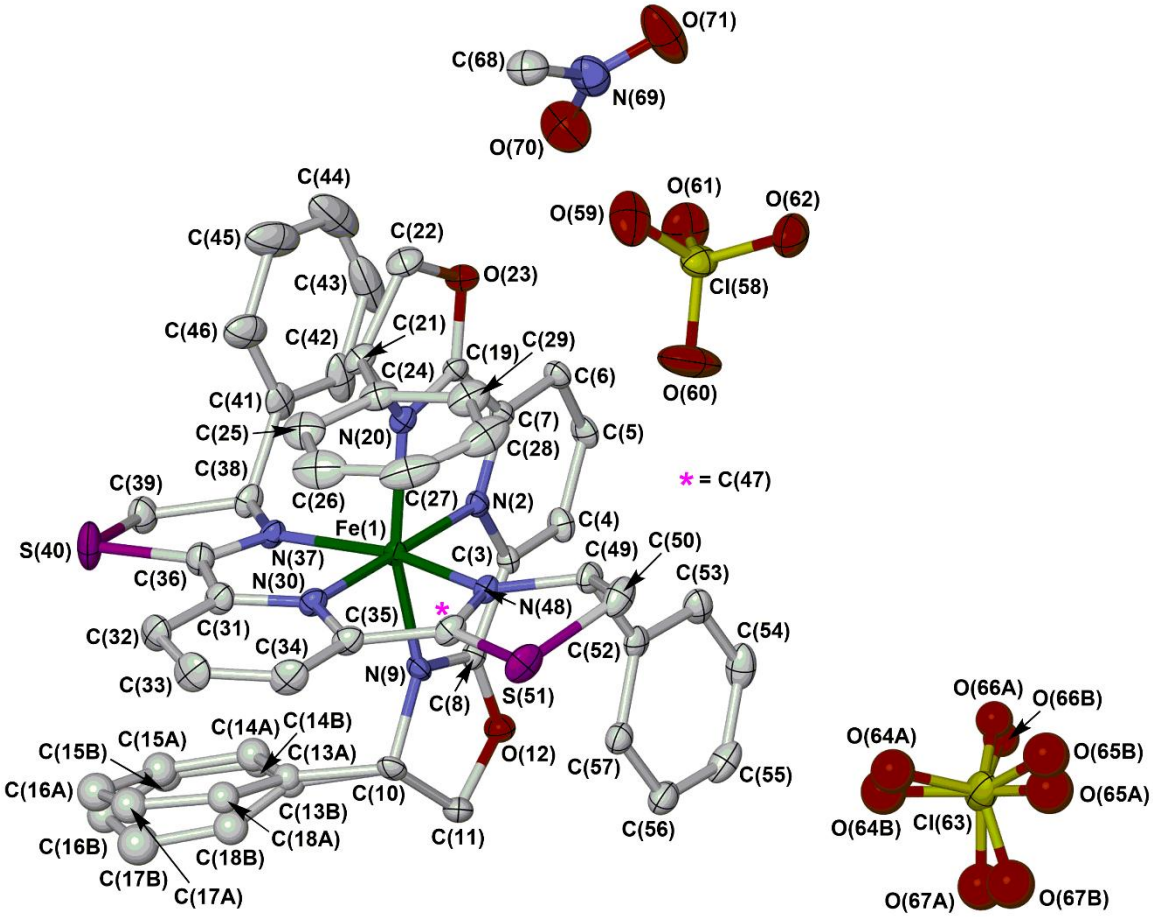


Figure S1 The asymmetric unit of **1**·$MeNO_2$, showing the full atom numbering scheme. Both orientations of the disordered residues in the model are included in the Figure. Displacement ellipsoids are at the 50 % probability level, and H atoms are omitted for clarity. Colour code: C, white; Cl, yellow; Fe, green; N, blue; O, red; S, purple.

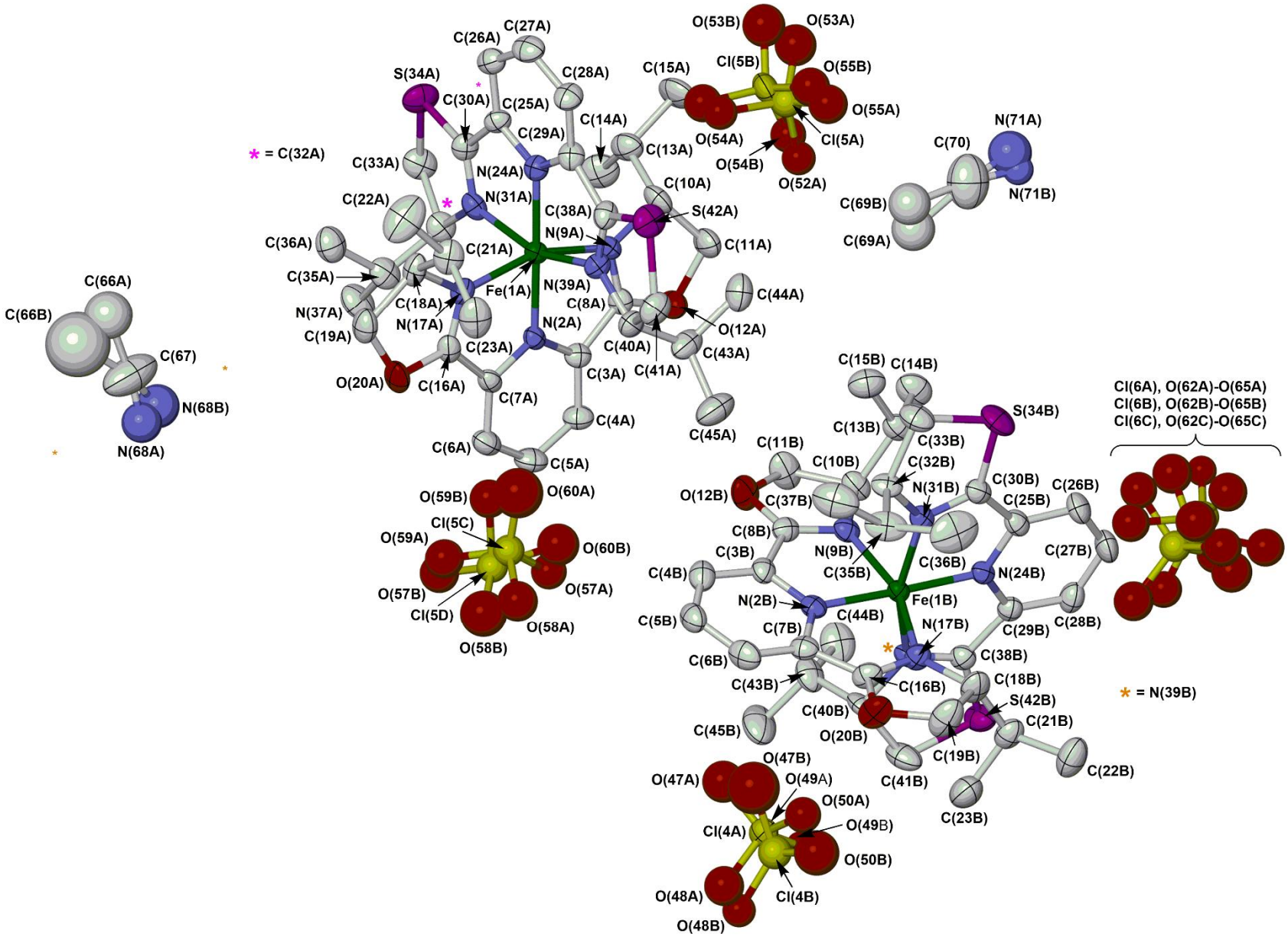
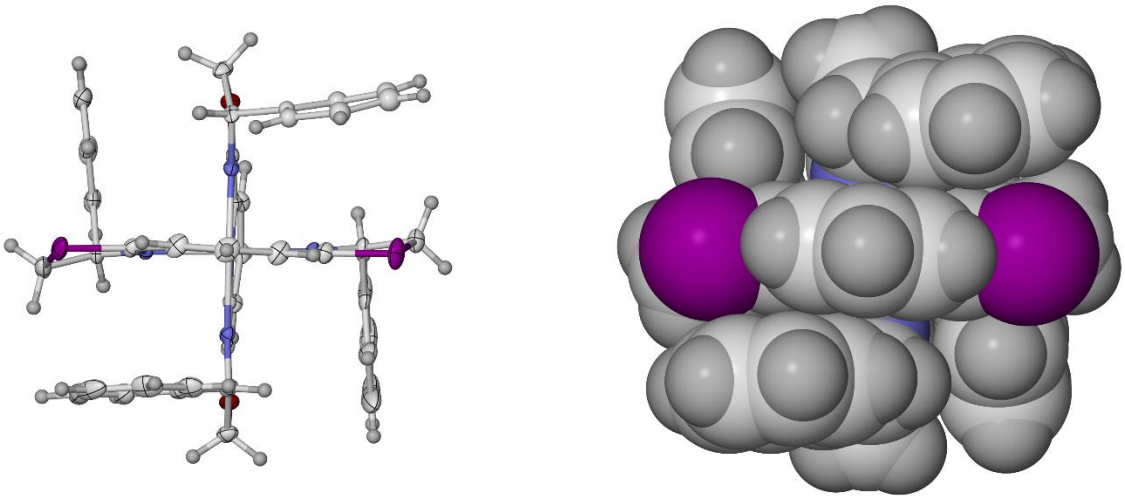


Figure S2 The asymmetric unit of **2**·MeCN. Details as for Figure S1. Colour code: C, white; Cl, yellow; Fe, green; N, blue; O, red; S, purple.

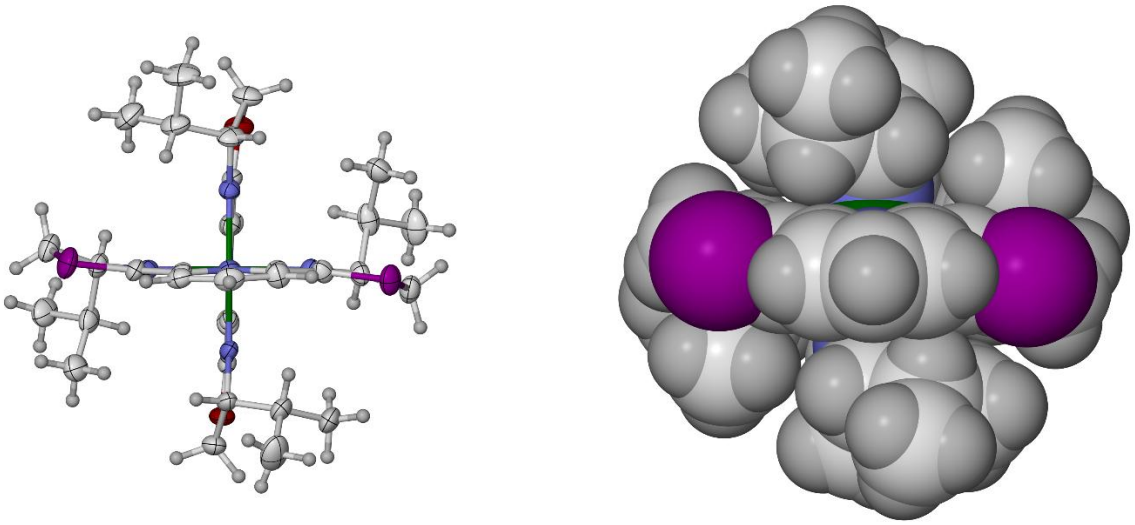
Table S2 Selected bond lengths, angles and other structural parameters (Å , °, Å^3) for the heterochiral [Fe(L^1R)(L^2R)][ClO_4]$_2$ crystals. See Figures S1 and S2 for the atom numbering scheme, while definitions of V_{Oh}, Σ, Θ, φ and θ are given on page S9.

1·$MeNO_2$		**2**·MeCN		
			Molecule A	Molecule B
Fe(1)–N(2)	1.915(3)	Fe(1)–N(2)	1.923(5)	1.907(5)
Fe(1)–N(9)	1.995(3)	Fe(1)–N(9)	1.995(5)	2.007(5)
Fe(1)–N(20)	1.994(3)	Fe(1)–N(17)	1.999(5)	2.000(5)
Fe(1)–N(30)	1.884(3)	Fe(1)–N(24)	1.903(5)	1.888(5)
Fe(1)–N(37)	1.995(3)	Fe(1)–N(31)	2.025(5)	2.003(5)
Fe(1)–N(48)	1.985(3)	Fe(1)–N(39)	2.014(5)	2.008(5)
N(2)–Fe(1)–N(9)	79.45(13)	N(2)–Fe(1)–N(9)	78.9(2)	79.8(2)
N(2)–Fe(1)–N(20)	79.20(13)	N(2)–Fe(1)–N(17)	79.3(2)	79.2(2)
N(2)–Fe(1)–N(30)	179.49(15)	N(2)–Fe(1)–N(24)	178.5(2)	177.2(2)
N(2)–Fe(1)–N(37)	99.73(12)	N(2)–Fe(1)–N(31)	100.7(2)	97.3(2)
N(2)–Fe(1)–N(48)	100.81(12)	N(2)–Fe(1)–N(39)	100.4(2)	103.5(2)
N(9)–Fe(1)–N(20)	158.64(12)	N(9)–Fe(1)–N(17)	158.2(2)	159.0(2)
N(9)–Fe(1)–N(30)	100.20(13)	N(9)–Fe(1)–N(24)	102.6(2)	100.5(2)
N(9)–Fe(1)–N(37)	90.65(12)	N(9)–Fe(1)–N(31)	92.7(2)	90.3(2)
N(9)–Fe(1)–N(48)	93.43(12)	N(9)–Fe(1)–N(39)	92.3(2)	93.0(2)
N(20)–Fe(1)–N(30)	101.15(13)	N(17)–Fe(1)–N(24)	99.3(2)	100.5(2)
N(20)–Fe(1)–N(37)	92.95(12)	N(17)–Fe(1)–N(31)	91.4(2)	92.2(2)
N(20)–Fe(1)–N(48)	90.56(13)	N(17)–Fe(1)–N(39)	91.6(2)	92.1(2)
N(30)–Fe(1)–N(37)	79.90(13)	N(24)–Fe(1)–N(31)	79.4(2)	79.9(2)
N(30)–Fe(1)–N(48)	79.57(13)	N(24)–Fe(1)–N(39)	79.4(2)	79.3(2)
N(37)–Fe(1)–N(48)	159.46(13)	N(31)–Fe(1)–N(39)	158.8(2)	159.2(2)
V_{Oh}	9.720(10)	V_{Oh}	9.928(16)	9.819(16)
Σ	91.4(5)	Σ	94.0(7)	91.2(7)
Θ	300	Θ	308	300
φ	179.49(15)	φ	178.5(2)	177.2(2)
θ	89.67(6)	θ	88.81(9)	87.08(9)

1·$MeNO_2$



2·MeCN, molecule A



2·MeCN, molecule B

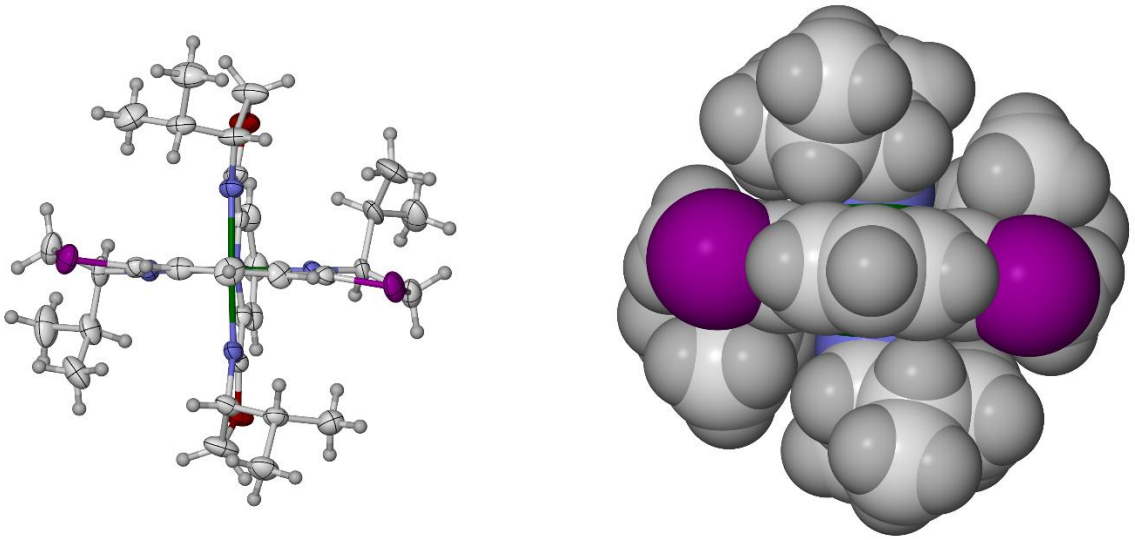


Figure S3 Displacement ellipsoid (left) and space-filling plots (right) of the heterochiral $[Fe(L^1R)(L^2R)]^{2+}$ complex cations in the crystals of **1** and **2**. The view is down the Fe–N{pyridyl} bond to the L^2R ligand.

Only one orientation of the disordered phenyl group in **1** is shown in the Figure. The L^1R and L^2R ligands in **1** and **2** have opposite chirality.

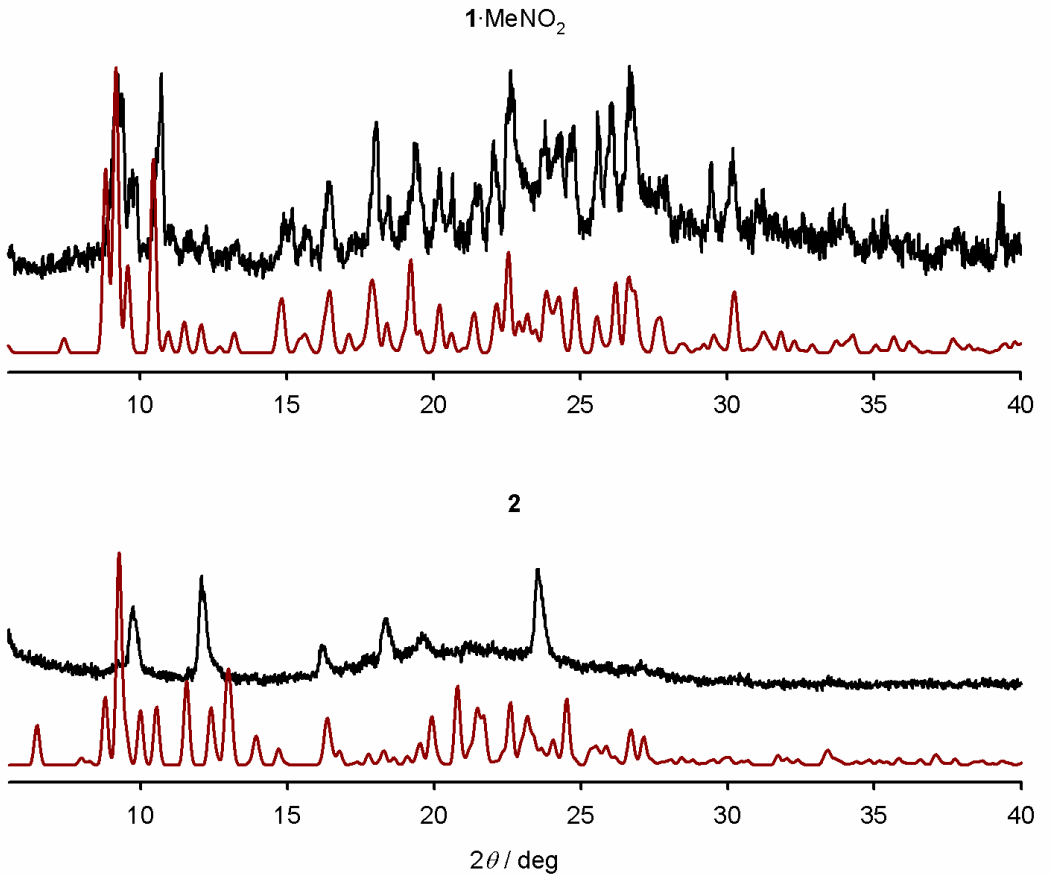


Figure S4 Room temperature X-ray powder diffraction data for **1**·$MeNO_2$ (top) and **2** (bottom). The measured powder patterns are shown in black, and crystallographic simulations are shown in red.

Although the diffraction is weak and the peaks are broadened, the powder pattern of **1**·$MeNO_2$ agrees well with the simulation. However, **2** shows just a few peaks which do not match the simulation, and a broad amorphous hump around $2\theta = 22°$. Hence, solvent loss from **2**·MeCN on exposure to air leads to decomposition of its crystal lattice.

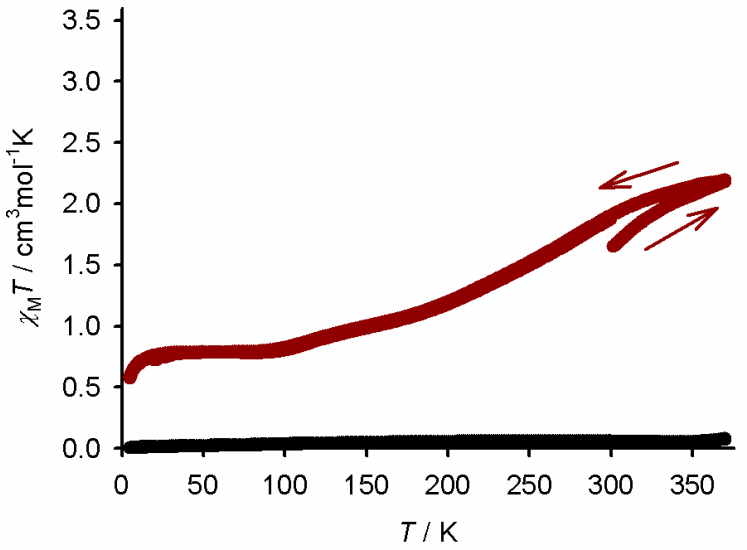


Figure S5 Magnetic susceptibility data for **1**·$MeNO_2$ (black) and **2** (red). Data were measured with a 300⟶370⟶5⟶300 K temperature cycle at a scan rate 5 K min^{-1}.

The low-spin nature of **1** is consistent with its homoleptic counterparts [Fe((*R*)-L^1Ph)((*S*)-L^1Ph)][ClO_4]$_2$ and [Fe((*R*)-L^2Ph)((*S*)-L^2Ph)][ClO_4]$_2$, which are also low-spin in the solid state.[2,4]

Compound **2** has a mixed spin-state population at room temperature, and exhibits an almost continuous gradual SCO on heating and re-cooling. The SCO is incomplete at 80 K and, is quenched at lower temperatures where the residual high-spin population is frozen into the sample.

The ill-defined spin state properties and gradual SCO in **2** are consistent with its poorly crystalline and partially amorphous composition (Figure S4), while the small changes observed during the initial heating and recooling probably reflect loss of a small quantity of residual solvent.[21]

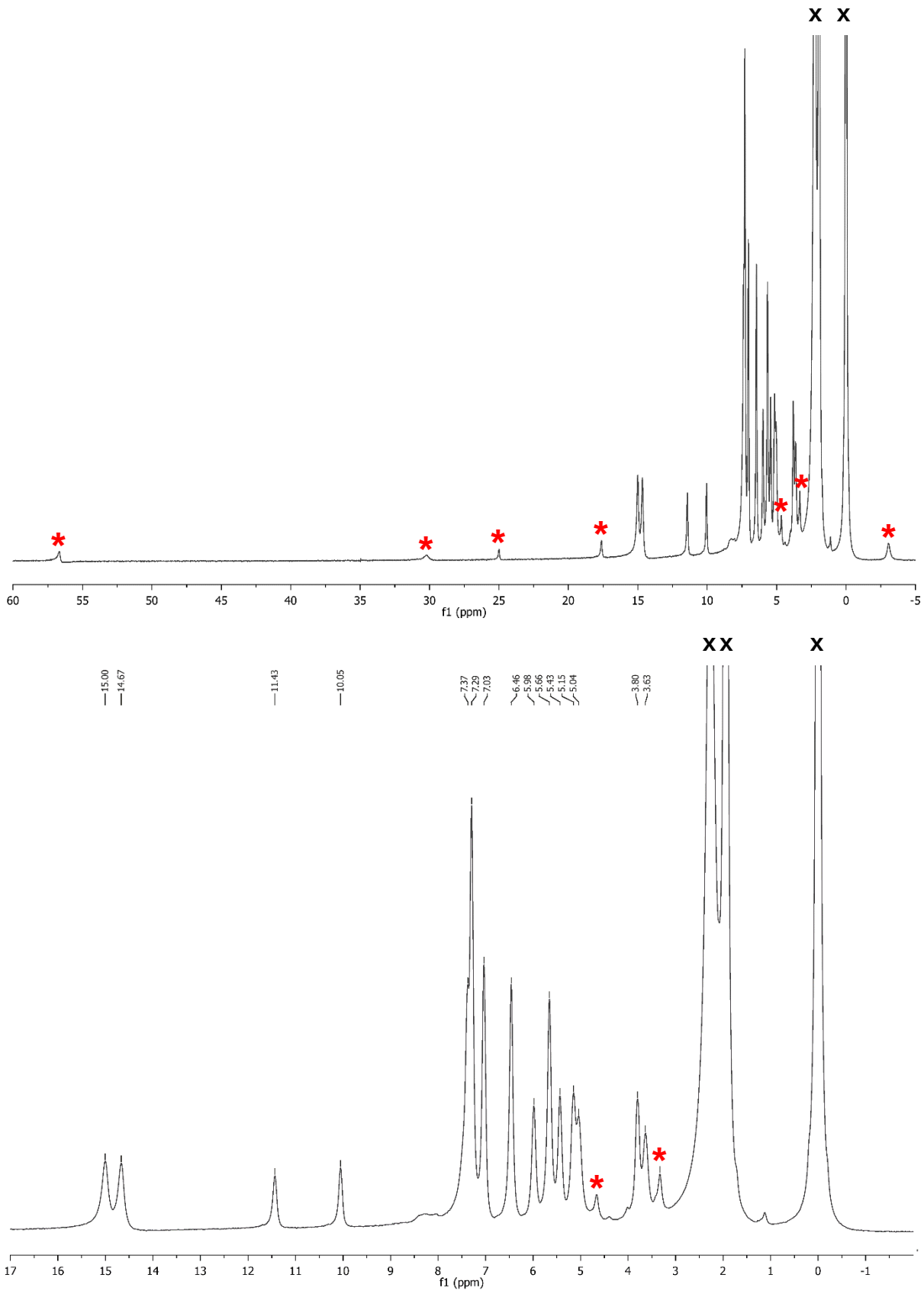


Figure S6 ^{1}H NMR spectrum of preformed **1** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the main peaks assigned to the heteroleptic complex **1**.

A molecule of **1** has 38 protons in 16 unique environments, which are all resolved in the spectrum. The weak contact shifting of the peaks is consistent with its magnetic measurements, which show only a small paramagnetism of $\chi_M T$ = 0.8 cm^3 mol^{-1} K at room temperature (Figure 3, main article). The starred peaks are from $[Fe((R)\text{-}L^1Ph)_2]^{2+}$,[4] which is present in a ratio of *ca* 0.15:1 compared to the main species.

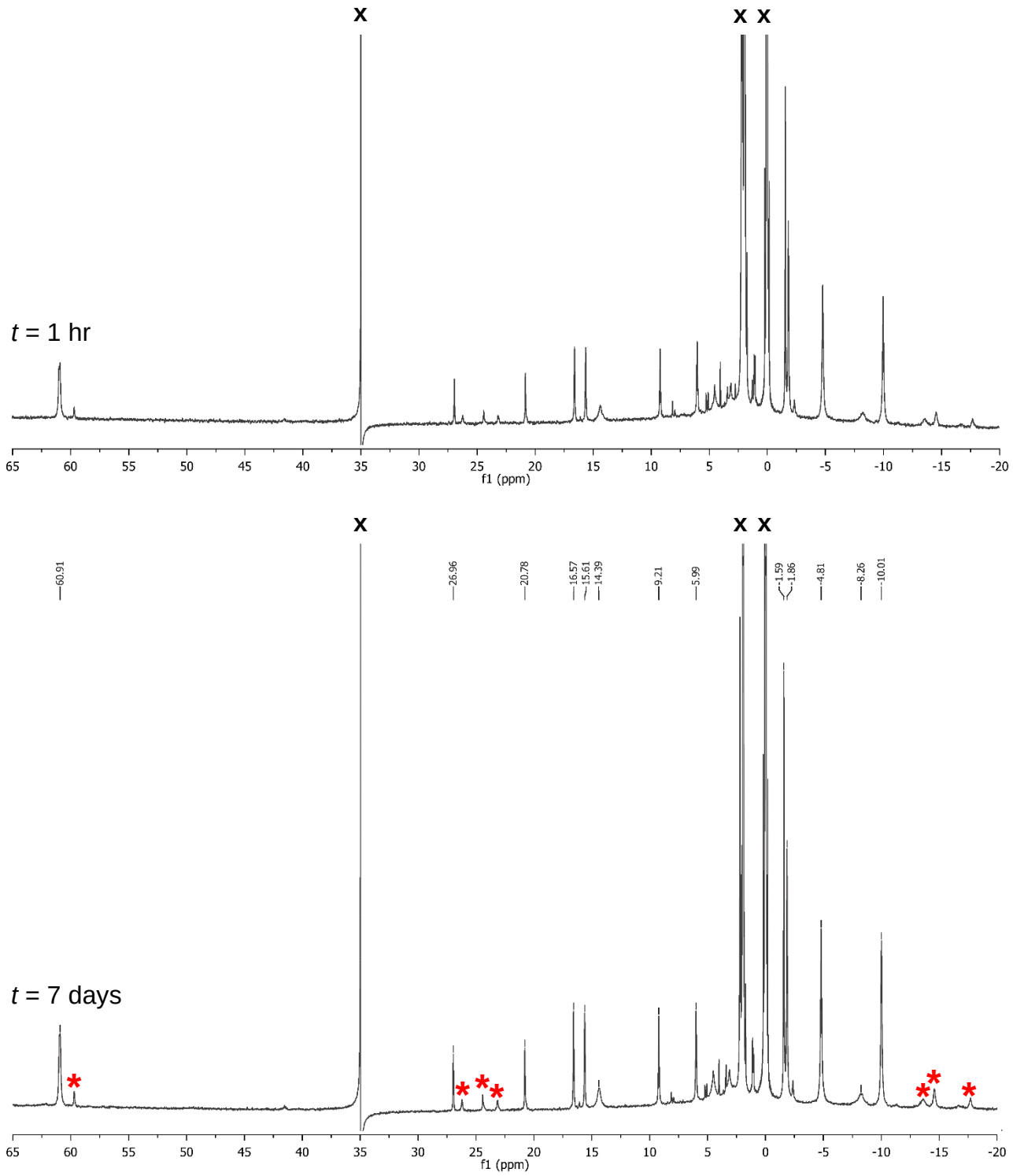


Figure S7 ^{1}H NMR spectrum of **2** (CD_3CN) upon time of mixing (top), and after 7 days (bottom). The feature at 35 ppm is a spectrometer artefact.

In contrast to **1** (Figure 2, main article) there is no change in the composition of the solution over this time.

A molecule of **2** has 46 protons in 16 unique environments, including diastereotopic *iso*propyl groups. The marked peaks in the spectrum correspond to 44 of those H atoms. One more resonance of integral 2H is expected upfield of 2 ppm, from an *iso*propyl C*H* environment, but this could be masked by the solvent peaks. The strongly contact shifted peaks in the spectrum are consistent with its being predominantly high-spin at 298 K from magnetic measurements (Figure 3, main article).

The starred peaks are from $[Fe((R)\text{-}L^1i\text{Pr})_2]^{2+}$,[4] in a ratio of *ca* 0.15:1 compared to the main species. Extra peaks of similar integral in the diamagnetic region may be from uncoordinated L^2iPr.

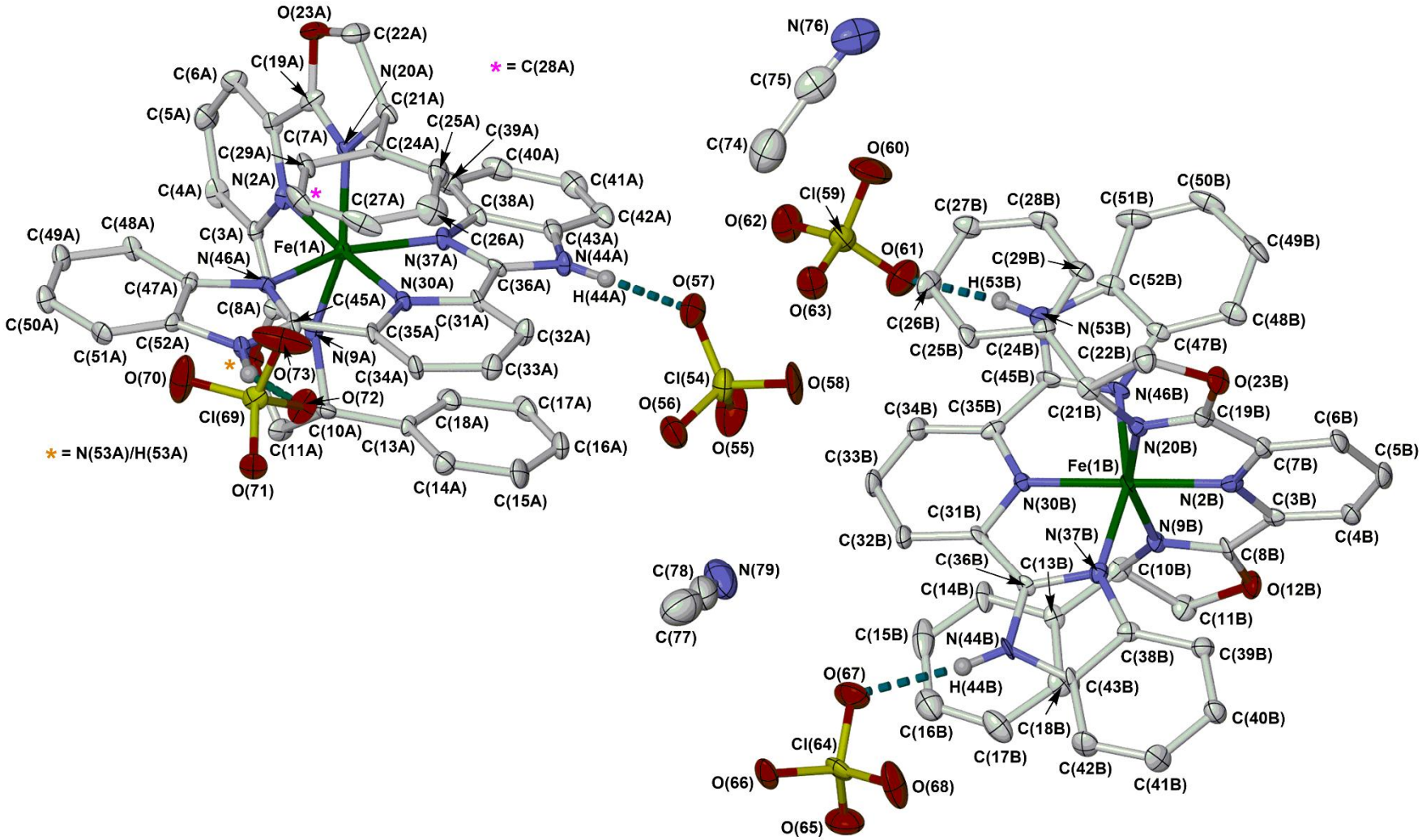


Figure S8 The asymmetric unit of **3**·MeCN. Details as for Figure S1. Colour code: C, white; H, pale grey; Cl, yellow; Fe, green; N, blue; O, red. Atom O(12A) is behind N(53A).

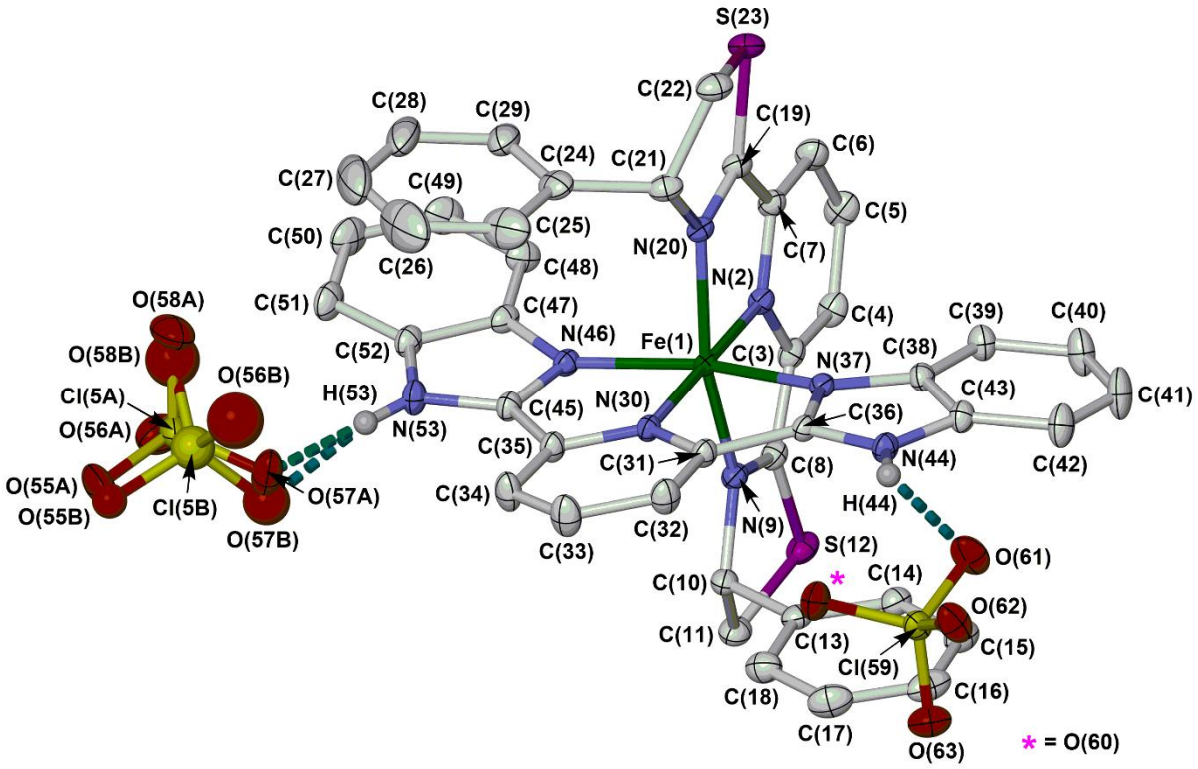


Figure S9 The asymmetric unit of **4**. Details as for Figure S1. Colour code: C, white; H, pale grey; Cl, yellow; Fe, green; N, blue; O, red; S, purple.

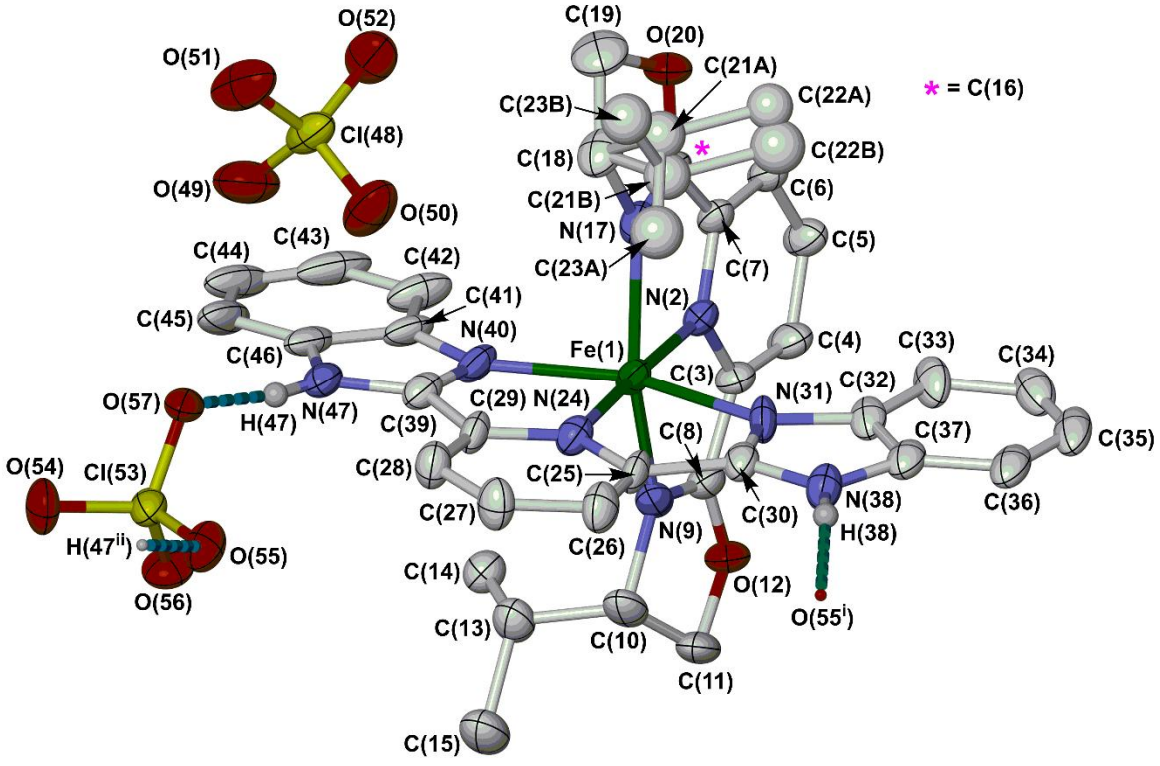


Figure S10 The asymmetric unit of **5**. Details as for Figure S1. Colour code: C, white; H, pale grey; Cl, yellow; Fe, green; N, blue; O, red. Symmetry codes: (i) $-\frac{1}{2}+x, \frac{1}{2}-y, 1-z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, 1-z$.

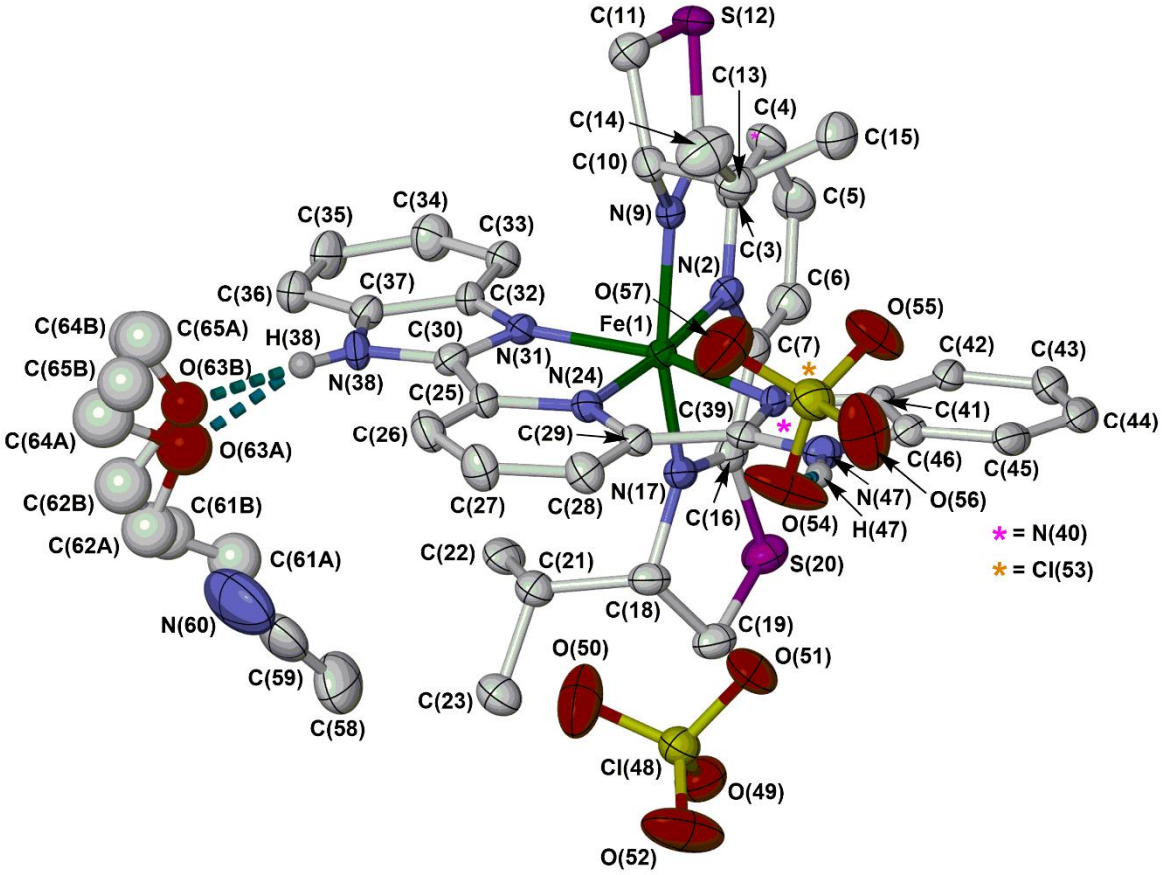


Figure S11 The asymmetric unit of **6**·MeCN·Et_2O. Details as for Figure S1. Colour code: C, white; H, pale grey; Cl, yellow; Fe, green; N, blue; O, red; S, purple.

Atom C(8) is obscured behind C(14).

Table S3 Selected bond lengths, angles and other structural parameters (Å , °, Å^3) for the [Fe(L^1R)(bimpy)][ClO_4]$_2$ and [Fe(L^2R)(bimpy)][ClO_4]$_2$ crystals. See Figures S8-S11 for the atom numbering scheme, while definitions of V_{Oh}, Σ, Θ, φ and θ are given on page S9.

	3·MeCN		**4**		**5**	**6**·MeCN·Et_2O
	Molecule A	Molecule B				
Fe(1)–N(2)	1.900(8)	1.900(8)	1.8795(13)	Fe(1)–N(2)	2.024(6)	1.881(5)
Fe(1)–N(9)	1.983(8)	1.971(8)	1.9739(14)	Fe(1)–N(9)	2.076(8)	1.995(5)
Fe(1)–N(20)	1.979(7)	1.978(8)	1.9574(13)	Fe(1)–N(17)	2.094(8)	2.001(6)
Fe(1)–N(30)	1.934(8)	1.934(8)	1.9322(13)	Fe(1)–N(24)	2.029(7)	1.913(5)
Fe(1)–N(37)	2.035(8)	1.992(8)	1.9813(13)	Fe(1)–N(31)	2.118(7)	1.992(5)
Fe(1)–N(46)	2.006(8)	2.027(8)	1.9937(13)	Fe(1)–N(40)	2.110(7)	1.983(5)
N(2)–Fe(1)–N(9)	79.4(3)	80.3(3)	80.14(6)	N(2)–Fe(1)–N(9)	76.5(3)	80.4(2)
N(2)–Fe(1)–N(20)	79.5(3)	79.3(3)	79.63(6)	N(2)–Fe(1)–N(17)	76.4(3)	79.8(2)
N(2)–Fe(1)–N(30)	177.8(4)	178.0(4)	179.60(6)	N(2)–Fe(1)–N(24)	176.2(3)	175.2(2)
N(2)–Fe(1)–N(37)	99.1(3)	101.5(3)	100.13(6)	N(2)–Fe(1)–N(31)	99.1(3)	96.1(2)
N(2)–Fe(1)–N(46)	102.1(3)	98.9(3)	100.61(6)	N(2)–Fe(1)–N(40)	107.3(3)	103.7(2)
N(9)–Fe(1)–N(20)	158.7(3)	159.6(3)	159.70(6)	N(9)–Fe(1)–N(17)	152.7(3)	160.1(2)
N(9)–Fe(1)–N(30)	102.6(3)	98.1(3)	100.08(6)	N(9)–Fe(1)–N(24)	104.5(3)	96.3(2)
N(9)–Fe(1)–N(37)	92.4(3)	91.7(3)	92.27(5)	N(9)–Fe(1)–N(31)	89.3(3)	90.7(2)
N(9)–Fe(1)–N(46)	90.2(3)	91.3(3)	93.19(6)	N(9)–Fe(1)–N(40)	97.0(3)	93.3(2)
N(20)–Fe(1)–N(30)	98.6(3)	102.3(3)	100.14(5)	N(17)–Fe(1)–N(24)	102.7(3)	103.5(2)
N(20)–Fe(1)–N(37)	92.7(3)	90.7(3)	89.61(5)	N(17)–Fe(1)–N(31)	98.1(3)	93.2(2)
N(20)–Fe(1)–N(46)	92.5(3)	93.4(3)	92.18(6)	N(17)–Fe(1)–N(40)	88.1(3)	89.7(2)
N(30)–Fe(1)–N(37)	79.9(3)	79.7(3)	79.54(5)	N(24)–Fe(1)–N(31)	77.2(3)	80.3(2)
N(30)–Fe(1)–N(46)	78.9(3)	80.0(3)	79.72(5)	N(24)–Fe(1)–N(40)	76.3(3)	79.9(2)
N(37)–Fe(1)–N(46)	158.7(3)	159.7(3)	159.17(5)	N(31)–Fe(1)–N(40)	153.5(3)	160.2(2)
V_{Oh}	9.88(2)	9.82(2)	9.611(4)	V_{Oh}	11.22(2)	9.725(16)
Σ	92.5(10)	88.6(10)	90.0(3)	Σ	124.9(10)	86.7(7)
Θ	305	291	293	Θ	393	284
φ	177.8(4)	178.0(4)	179.60(6)	φ	176.2(3)	175.2(2)
θ	88.21(14)	88.01(13)	88.00(3)	θ	82.44(12)	85.11(8)

Table S4 Hydrogen bond parameters for the bimpy complexes **3**-**6** [Å, °]. See Figures S8-S11 for the atom numbering scheme. Symmetry codes: (i) $-^1/_2+x$, $^1/_2-y$, $1-z$.

	D–H	H···A	D···A	D–H···A
3·MeCN				
N(44A)–H(44A)···O(57)	0.88	2.01	2.875(12)	168.7
N(53A)–H(53A)···O(72)	0.88	2.10	2.928(11)	156.5
N(44B)–H(44B)···O(67)	0.88	2.27	3.056(12)	149.1
N(53B)–H(53B)···O(61)	0.88	2.00	2.871(12)	172.1
4				
N(44)–H(44)···O(61)	0.88	2.02	2.7954(19)	146.0
N(53)–H(53)···O(57A)/O(57B)	0.88	1.93/1.97	2.807(3)/2.84(3)	172.5/170.0
5				
N(38)–H(38)···O(55^i)	0.88	1.96	2.835(10)	172.2
N(47)–H(47)···O(57)	0.88	2.07	2.928(11)	165.4
6·MeCN				
N(38)–H(38)···O(63A)/O(63B)	0.86	1.99/1.90	2.806(16)/2.758(12)	157.9/176.3
N(47)–H(47)···O(54)	0.86	1.99	2.819(9)	162.4

Table S5 Intramolecular $\pi\ldots\pi$ interaction parameters for **3**·MeCN and **4** [Å, °]. See Figures S8 and S9 for the atom numbering scheme. The L^1Ph phenyl groups in **3**·MeCN overlie the C–N bonds linking the pyridyl and imidazolo rings of the bimpy ligand. In contrast, the phenyl substituents in **4** are stacked above the five membered bimpy imidazolo rings.

	Dihedral angle	Interplanar distance[a]	Horizontal offset[b]
3·MeCN			
[C(13A)–C(18A)]···[N(30A)–C(38A), C(43A), N(44A)]	2.9(5)	3.31(3)	0.92
[C(24A)–C(29A)]··· [N(30A)–C(35A), C(45A)–C(47A), C(52A), N(53A)]	4.2(4)	3.29(3)	0.63
[C(13B)–C(18B)]···[N(30B)–C(38B), C(43B), N(44B)]	4.1(5)	3.31(3)	0.67
[C(24B)–C(29B)]··· [N(30B)–C(35B), C(45B)–C(47B), C(52B), N(53B)]	1.1(5)	3.29(3)	0.91
4			
[C(13)–C(18)]···[C(36)–C(38), C(43), N(44)]	3.92(6)	3.342(6)	0.81
[C(24)–C(29)]···[C(45)–C(47), C(52), N(53)]	5.54(10)	3.491(7)	0.68

[a]This is the average distance between each atom in the interacting phenyl ring, and the least squares plane of the stacked benzimidazolyl group. [b]This is calculated from the centroids of the two interacting residues.

There are no intermolecular $\pi\ldots\pi$ interactions in the crystals of **3**-**6**.

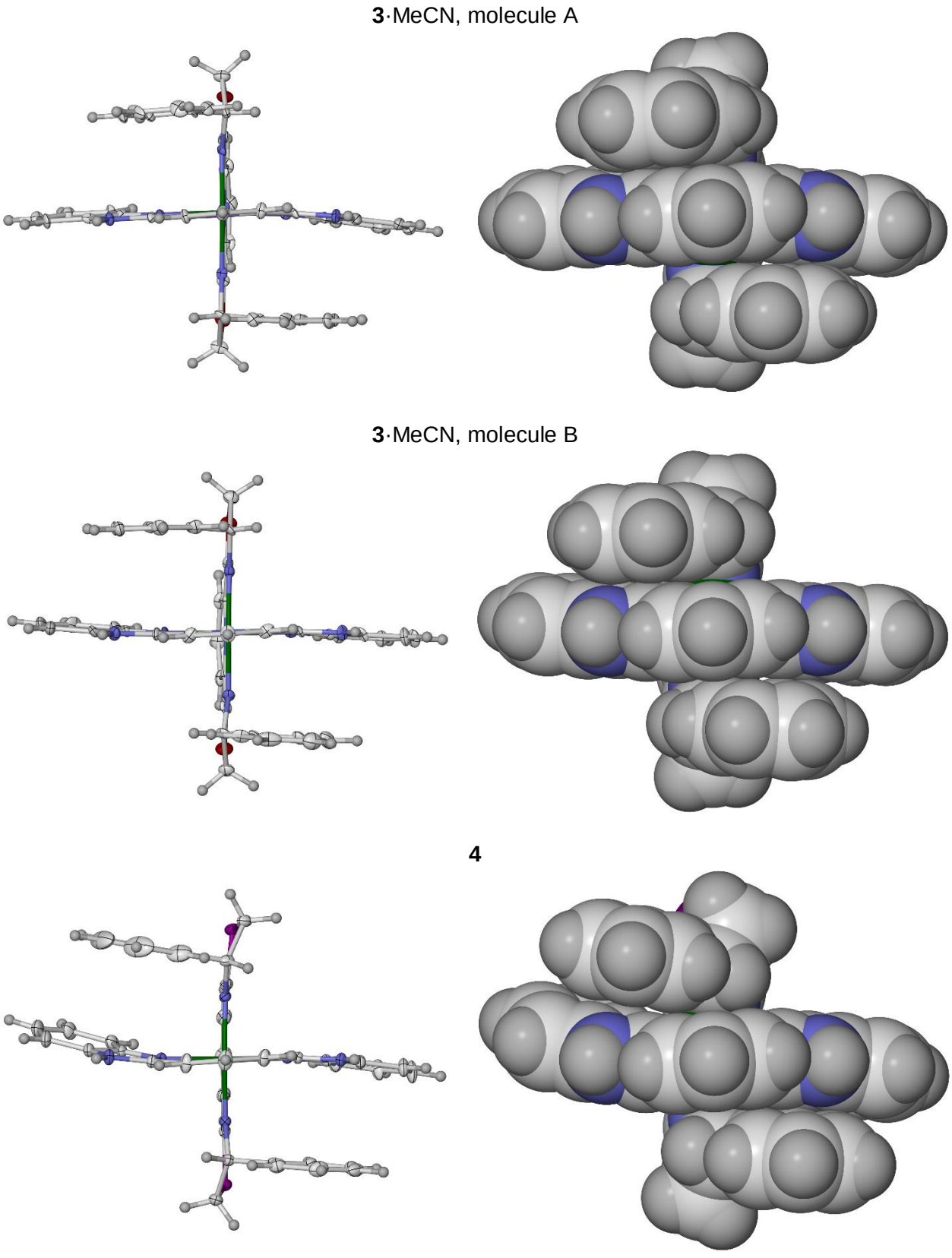
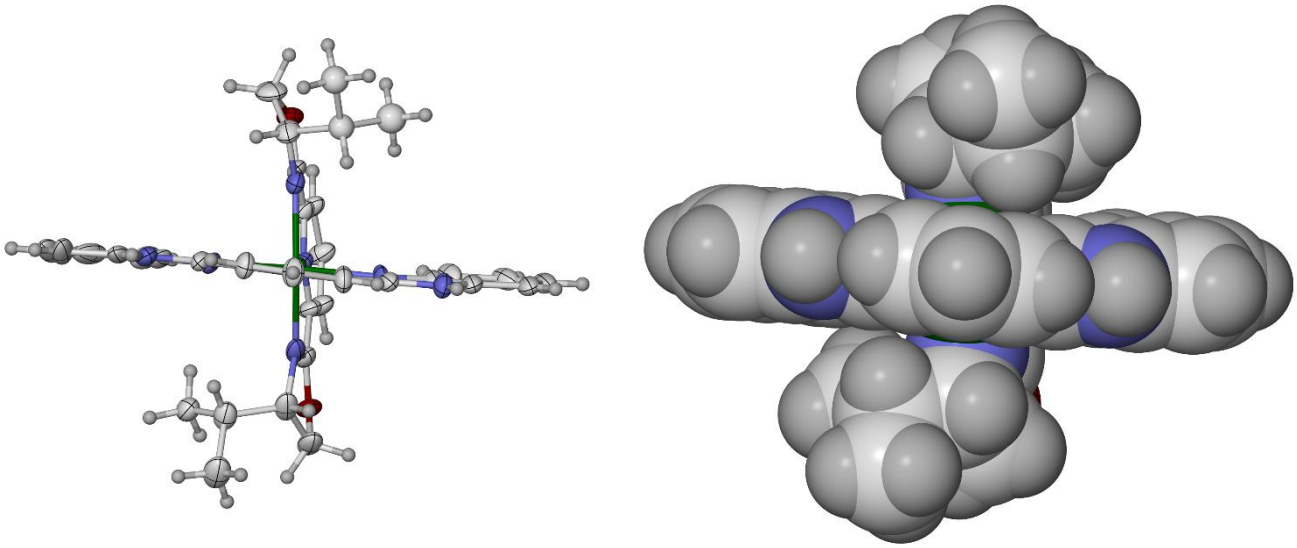


Figure S12 Displacement ellipsoid plots (left) and space-filling views (right) of the $[Fe(L^1R)(bimpy)]^{2+}$ and $[Fe(L^2R)(bimpy)]^{2+}$ complex cations in the crystals of **3**-**6**. The view is down the Fe–N{pyridyl} bond to the bimpy ligand, which highlights the bimpy ligand conformation and its interactions with the L^1R and L^2R 'R' substituents.

Only one orientation of the disordered *iso*propyl group in **5** is shown in the Figure.

5



6·MeCN·Et_2O

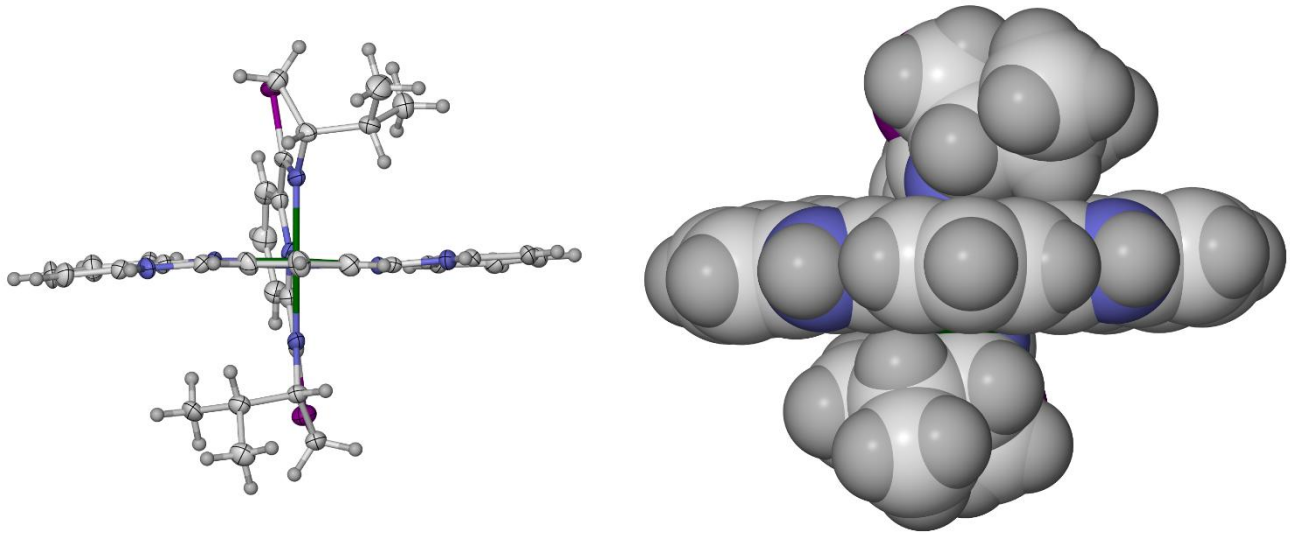


Figure S12 continued.

The S-shaped bimpy conformation in **4** is explained by the steric influence of a short inter-molecular C–H···H–C contact to a benzimidazolyl group in that crystal (Figure S13). This conformational distortion has no obvious effect on the inner coordination sphere of the complex (Table S3), or on its low-spin properties.

The only complex whose structure may be influenced by intramolecular steric interactions is **5**, whose *iso*propyl substituents are oriented to induce the observed canting of the bimpy ligand. This feature is reproduced in the DFT calculations of this molecule (Figure S36), and may contribute to stabilising the high-spin state of that complex.

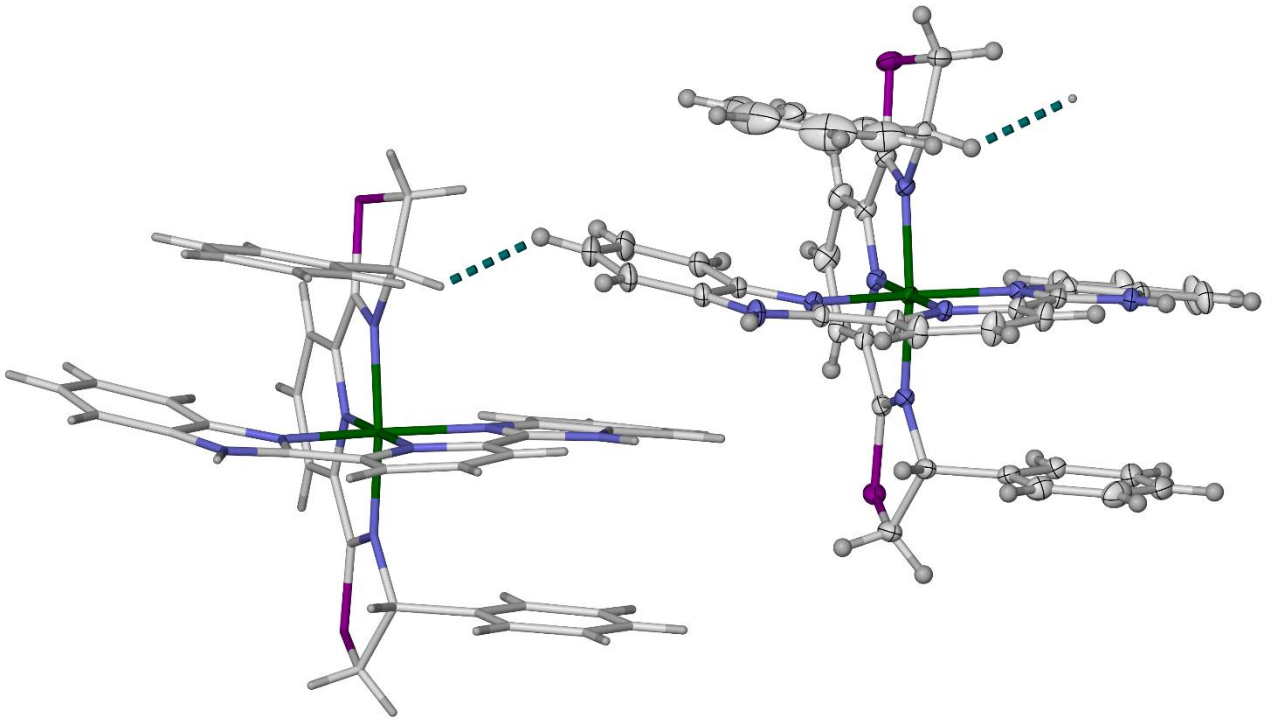


Figure S13 The intermolecular steric clash responsible for the S-shaped conformation of the bimpy ligand in crystals of **4**.

The H···H contact highlighted on the Figure, H(21)···H(50^{iii}), is 2.09 Å [symmetry code: (iii) –1+*x*, *y*, *z*]. While this is *ca* 0.3 Å shorter than the sum of the van der Waals radii of two H atoms,[22] the distance should be interpreted with care since the H atoms in the structure were not refined positionally.

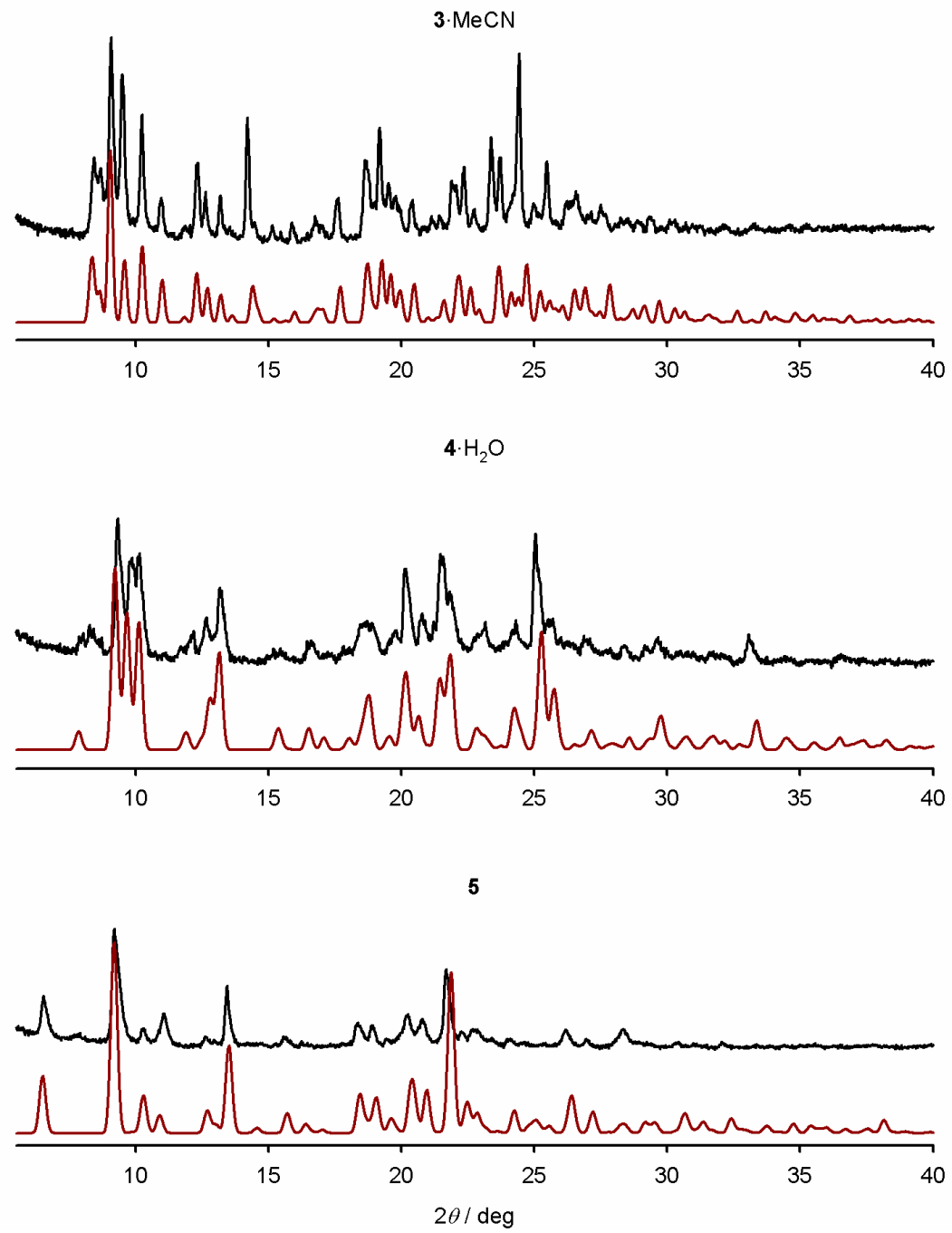


Figure S14 Room temperature X-ray powder diffraction data for **3**·MeCN-**6**. The measured powder patterns are shown in black, and crystallographic simulations are shown in red.

These data are discussed on the following page.

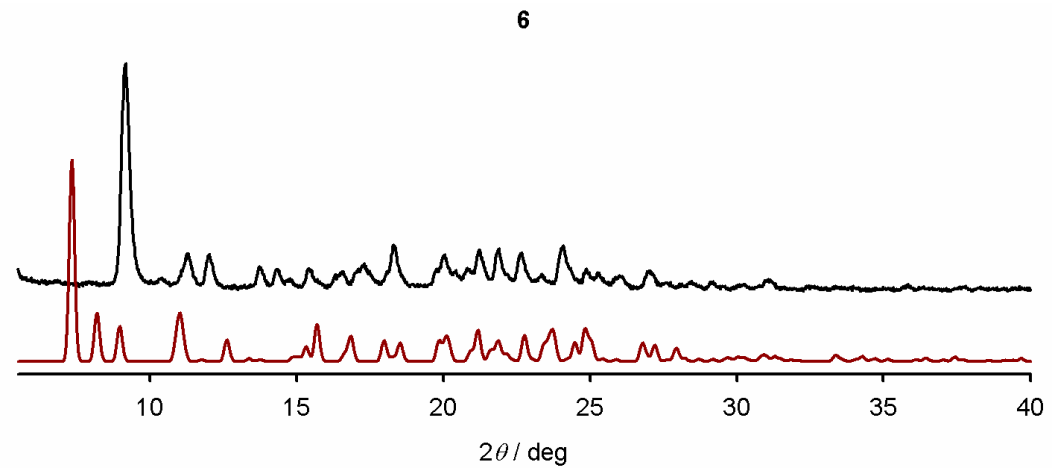


Figure S14 continued.

The powder patterns of **3**·MeCN-**5** on the previous page agree well with their crystallographic simulations. This includes **4**, whose fresh crystals are solvent-free but absorb atmospheric moisture on exposure to air by microanalysis. However, crystals of **6**·MeCN·Et_2O evidently transform to a new phase during solvent loss upon exposure to air.

Magnetic data for these solid materials are shown in Figure 4 of the main article.

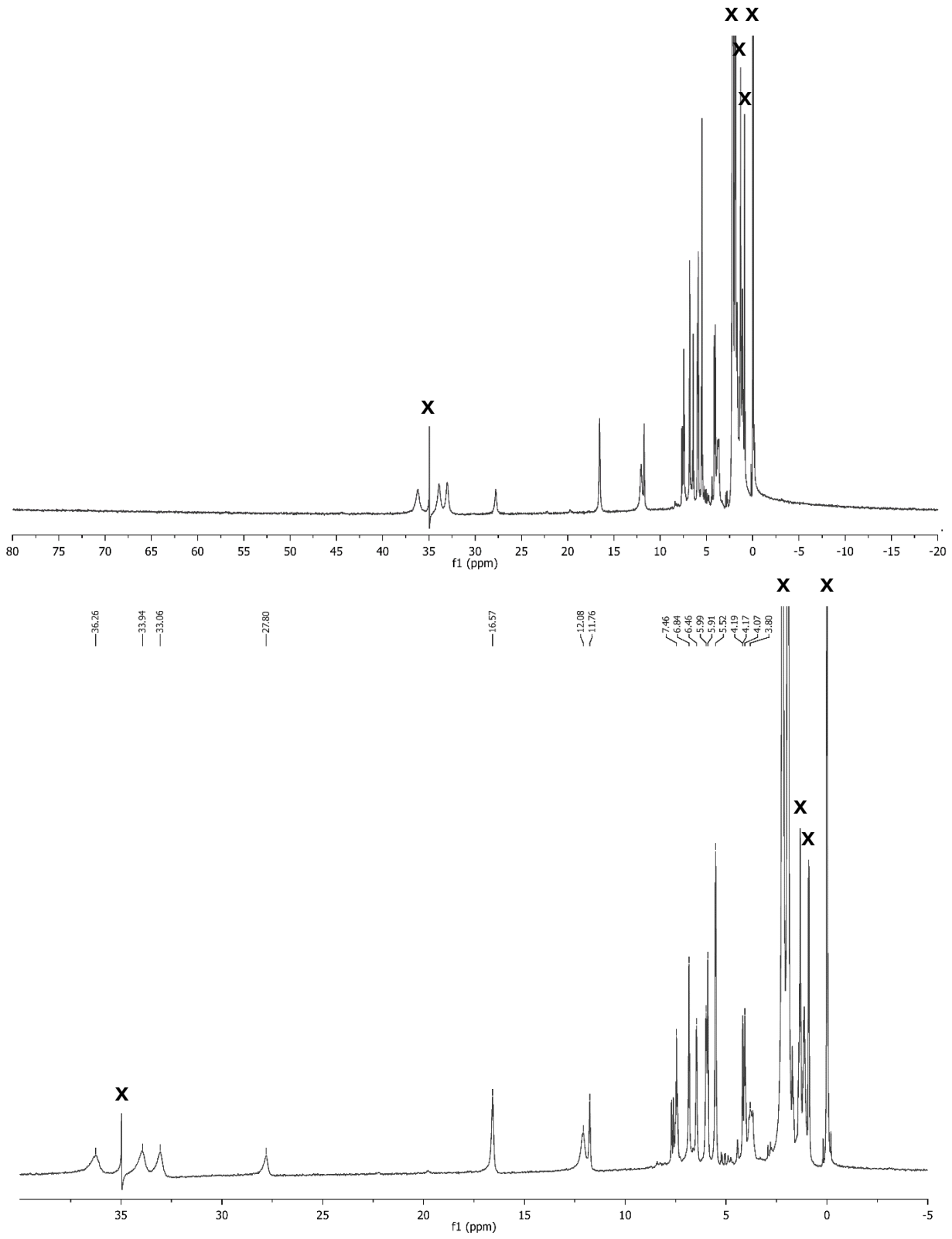


Figure S15 ^{1}H NMR spectrum of **3** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the main peaks assigned to the heteroleptic complex **3**. The feature at 35 ppm is a spectrometer artefact, and the peaks at 0.9 and 1.3 ppm are impurities in the NMR solvent (present in Figures S15-S17, S25, S26, S30 and S31).

A molecule of **3** has 32 protons in 15 unique environments. All these peaks are resolved in the spectrum, and there are no significant iron-containing impurities in the solution.

The moderate contact shifts in the spectrum are consistent with magnetic measurements, which show the solution has a mixed high:low-spin population at 298 K ($\chi_M T$ = 1.8 cm^3 mol^{-1} K; (Figure 5, main article).

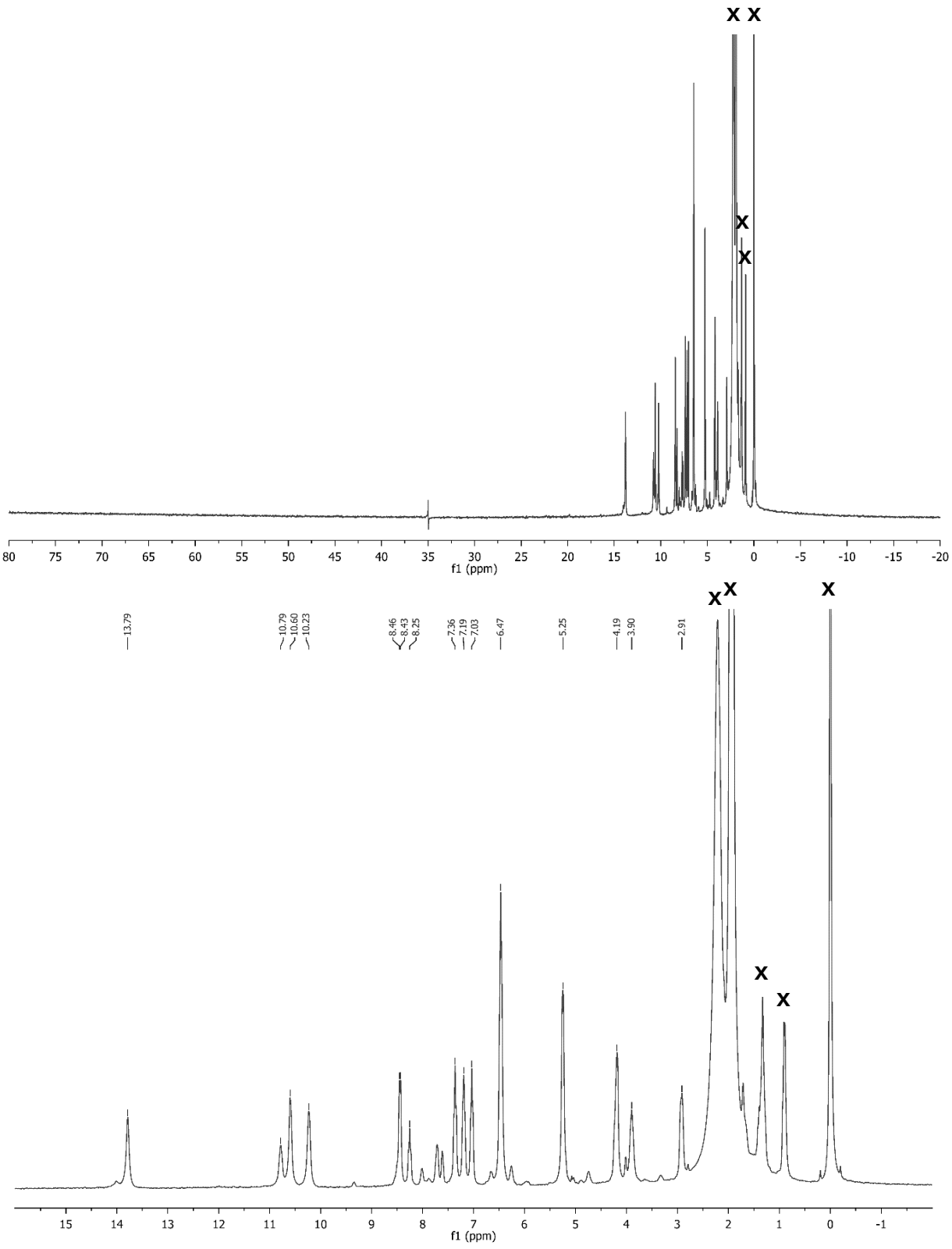


Figure S16 ^{1}H NMR spectrum of **4** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the main peaks assigned to the heteroleptic complex **4**. The feature at 35 ppm is a spectrometer artefact, and the peaks at 0.9 and 1.3 ppm are impurities in the NMR solvent (present in Figures S15-S17, S25, S26, S30 and S31).

A molecule of **4** has 32 protons in 15 unique environments. All these peaks are resolved in the spectrum, and there are no significant iron-containing impurities in the solution.

The small contact shifts in the spectrum support the magnetic measurements, which imply the complex has a small but non-zero paramagnetism at room temperature ($\chi_M T$ = 0.2 cm^3 mol^{-1} K; (Figure 5, main article).

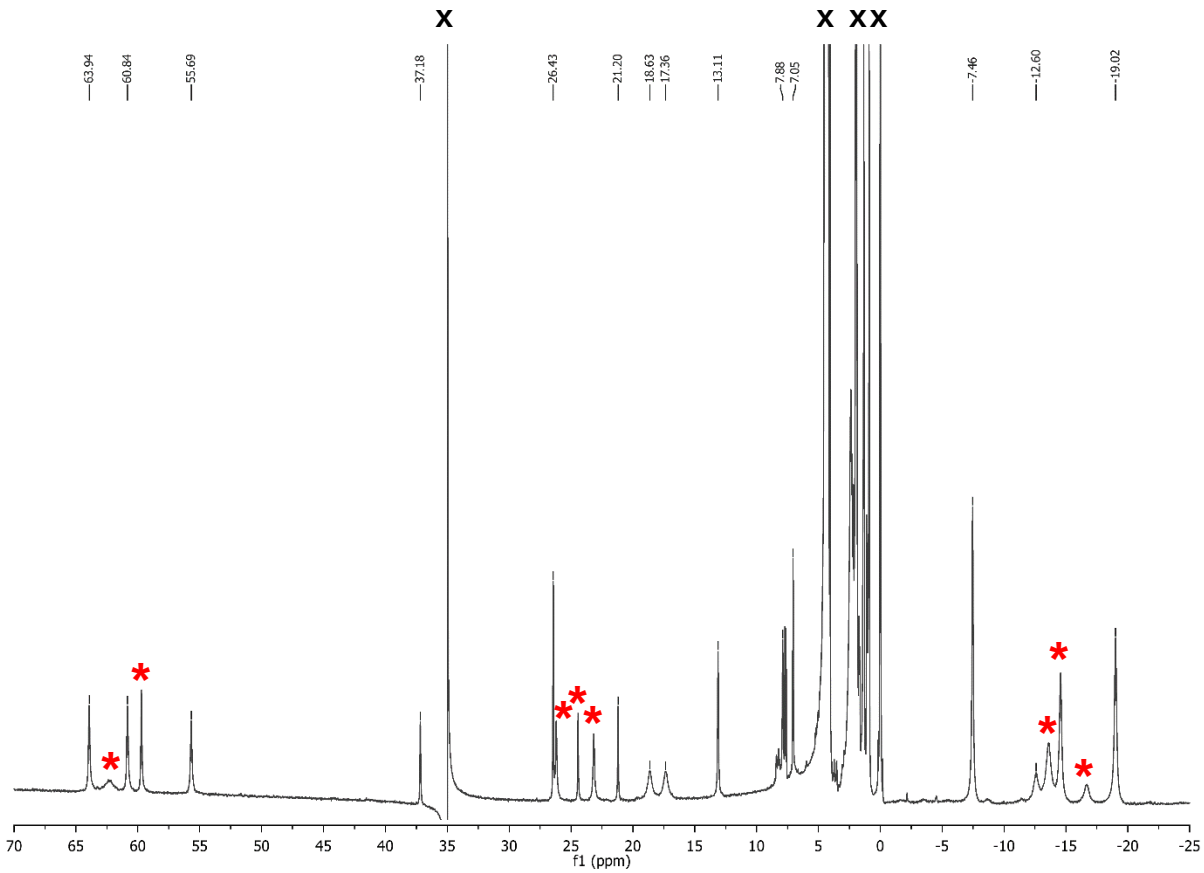


Figure S17 ^{1}H NMR spectrum of **5** (CD_3CN). The feature at 35 ppm is a spectrometer artefact (present in Figures S15-S17, S25, S26, S30 and S31).

A molecule of **5** has 36 protons in 15 unique environments, including diastereotopic *iso*propyl methyl substituents. Only 14 of these environments are clear in the spectrum; we tentatively suggest the peak from the NH protons may not be present.

The starred peaks are from $[Fe((S)\text{-}L^{1}iPr)_2]^{2+}$,[4] in a ratio of *ca* 0.25:1 compared to the main species. There is no $[Fe(bimpy)_2]^{2+}$ in the solution,[23] but extra peaks in the aromatic part of the diamagnetic region may correspond to uncoordinated bimpy.

The large contact shifts in the spectrum are consistent with magnetic measurements in this solvent, which show the complex (and the main impurity $[Fe((R)\text{-}L^{1}iPr)_2]^{2+}$ [4]) are both high-spin at room temperature (Figure 5, main article).

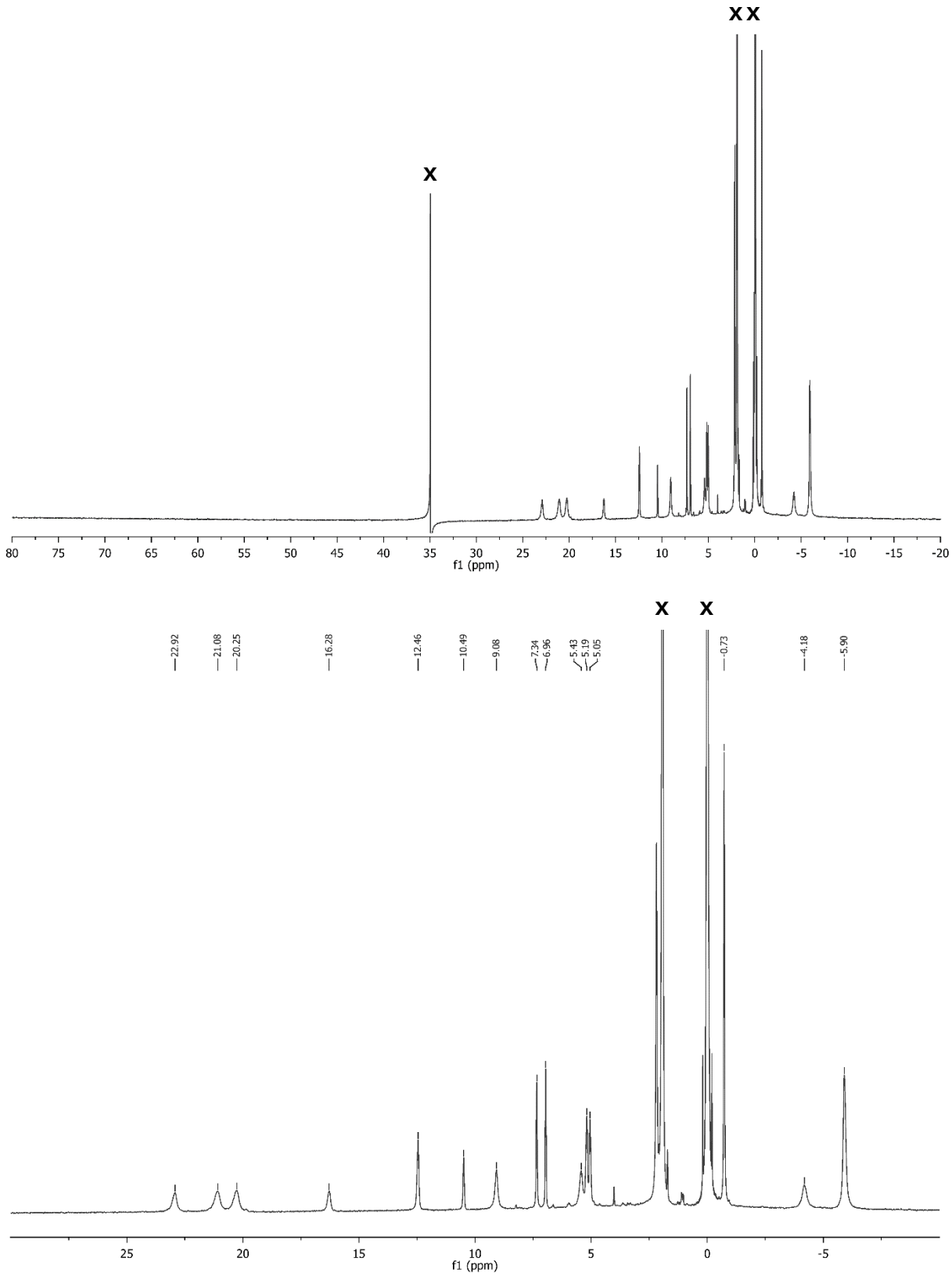


Figure S18 ^{1}H NMR spectrum of **6** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the main peaks assigned to the heteroleptic complex **6**. The feature at 35 ppm is a spectrometer artefact.

A molecule of **6** has 36 protons in 15 unique environments, including diastereotopic *iso*propyl methyl substituents. All these peaks are resolved in the spectrum, and there are no impurities visible in the solution.

The small contact shifts in the spectrum are consistent with its magnetic measurements, which show only a small paramagnetism of $\chi_M T$ = 1.0 cm^3 mol^{-1} K at room temperature (Figure 5, main article).

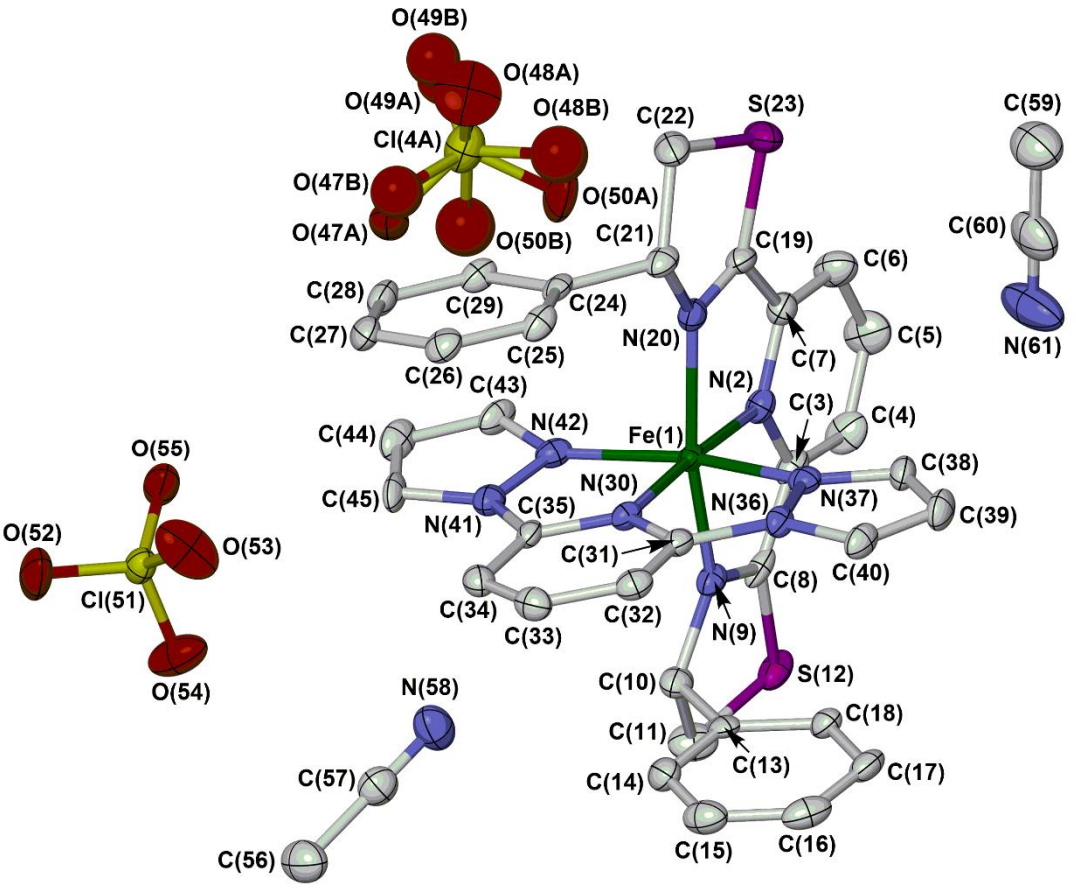


Figure S19 The asymmetric unit of **8**·2MeCN. Details as for Figure S1. Colour code: C, white; Cl, yellow; Fe, green; N, blue; O, red; S, purple.

Partial atom Cl(4B) is obscured behind Cl(4A).

Table S6 Selected bond lengths, angles and other structural parameters (Å , °, Å^3) for homochiral [Fe((*R*)-*L*^{2}Ph)(bpp)][ClO_4]$_2$·2MeCN (**8**·2MeCN). See Figure S19 for the atom numbering scheme, while definitions of V_{Oh}, Σ, Θ, φ and θ are given on page S9.

Fe(1)–N(2)	1.879(4)	Fe(1)–N(30)	1.906(4)
Fe(1)–N(9)	1.978(4)	Fe(1)–N(37)	1.954(4)
Fe(1)–N(20)	1.992(4)	Fe(1)–N(42)	1.961(4)
N(2)–Fe(1)–N(9)	80.40(17)	N(9)–Fe(1)–N(42)	89.62(16)
N(2)–Fe(1)–N(20)	79.76(17)	N(20)–Fe(1)–N(30)	102.54(17)
N(2)–Fe(1)–N(30)	176.77(17)	N(20)–Fe(1)–N(37)	90.14(16)
N(2)–Fe(1)–N(37)	97.99(17)	N(20)–Fe(1)–N(42)	92.99(16)
N(2)–Fe(1)–N(42)	102.29(17)	N(30)–Fe(1)–N(37)	79.81(16)
N(9)–Fe(1)–N(20)	160.10(17)	N(30)–Fe(1)–N(42)	79.94(17)
N(9)–Fe(1)–N(30)	97.34(17)	N(37)–Fe(1)–N(42)	159.72(17)
N(9)–Fe(1)–N(37)	94.22(15)		
V_{Oh}	9.492(12)	φ	176.77(17)
Σ	88.0(6)	θ	85.97(7)
Θ	287		

Table S7 Intramolecular $\pi\ldots\pi$ interaction parameters for **8**·2MeCN (Å, °). See Figure S19 for the atom numbering scheme. The L^2Ph phenyl groups overlie the C–N bonds linking the pyridyl and pyrazolyl rings of the bpp ligand.

	Dihedral angle	Interplanar distance[a]	Horizontal offset[b]
[C(13)–C(18)]···[N(30)–C(40)]	6.0(2)	3.285(13)	0.67
[C(24)–C(29)]···[N(30)–C(35), N(41)–C(45)]	7.6(2)	3.240(13)	0.40

[a]This is the average distance between each atom in the interacting phenyl ring, and the least squares plane of the stacked pyridylpyrazolyl group. [b]This is calculated from the centroids of the two interacting residues.

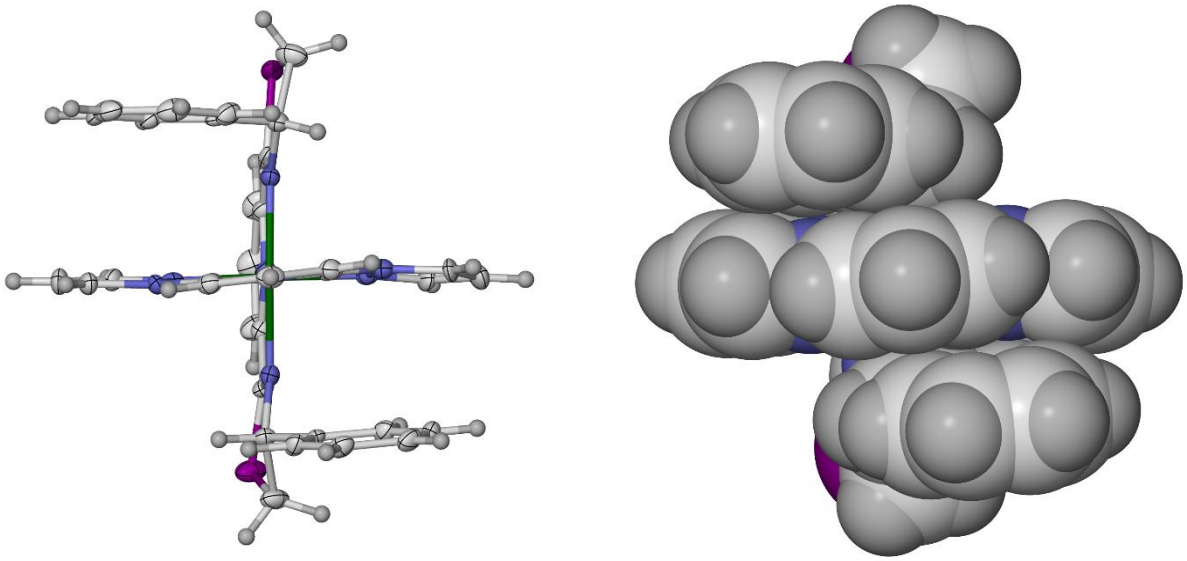


Figure S20 Displacement ellipsoid plot (left) and space-filling view (right) of the $[Fe(L^2Ph)(bpp)]^{2+}$ complex cation in the crystal of **8**·2MeCN. The view is down the Fe–N{pyridyl} bond to the bpp ligand, which highlights the bpp ligand conformation and its interactions with the L^2Ph phenyl groups.

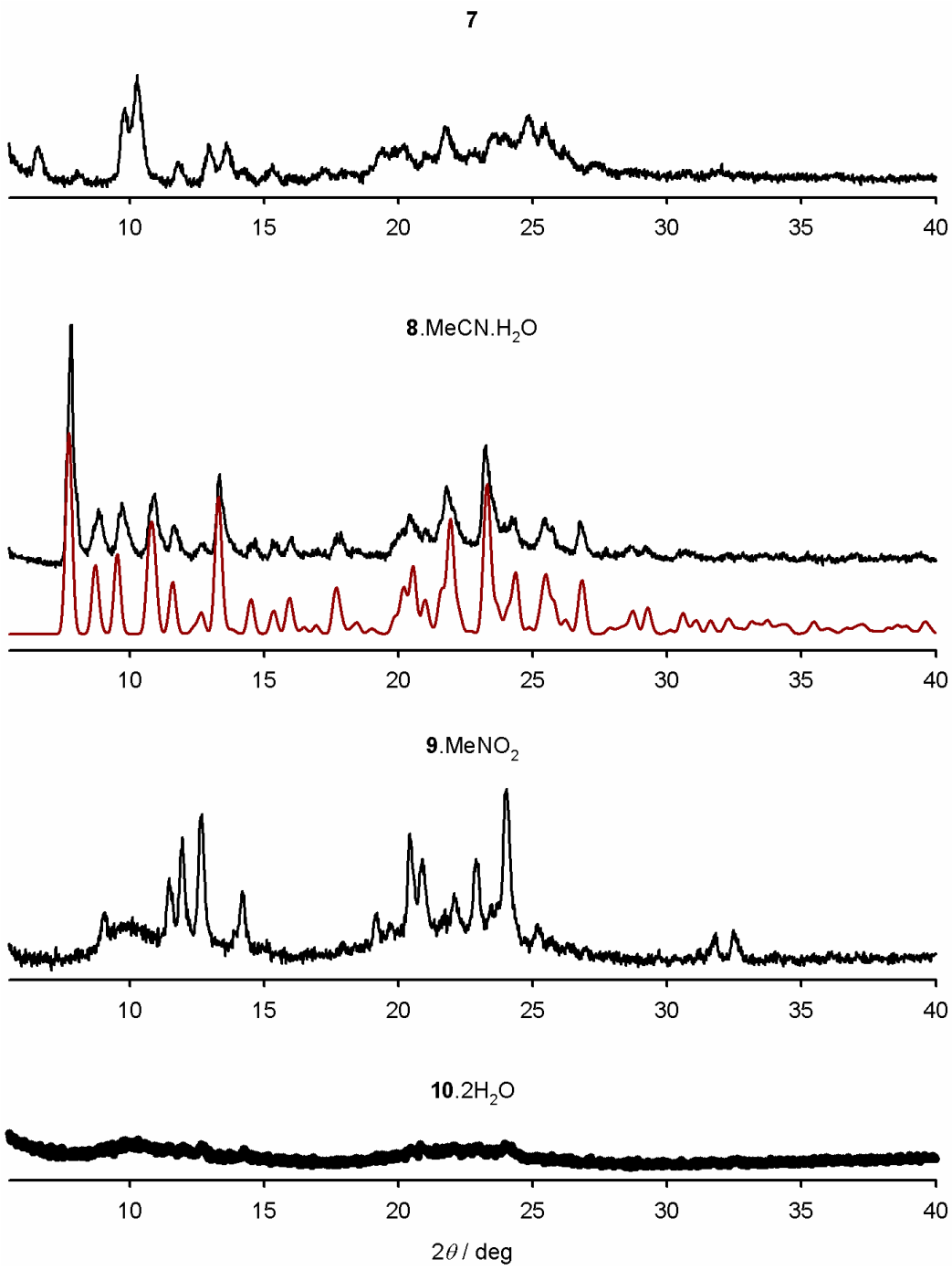


Figure S21 Room temperature X-ray powder diffraction data for **7**-**10**·2H_2O. The measured powder patterns are shown in black, and the crystallographic simulation of **8**·2MeCN is shown in red.

Although the peaks are broadened, the powder pattern of **8**·MeCN·H_2O is a good match for its crystallographic simulation. The peak broadening may be a consequence of partial replacement of the lattice solvent upon exposure to air.

The samples of **7** and **9**·$MeNO_2$ are mixtures of weakly crystalline and amorphous material, while the powder pattern of **10**·2H_2O is almost featureless. No crystal structures are available of these complexes for comparison with these data.

The freshly prepared materials are clearly contaminated by yellow crystals of $[Fe(bpp)_2][ClO_4]_2$, which was removed manually before analysis. There is no evidence for the presence of this phase in these samples.

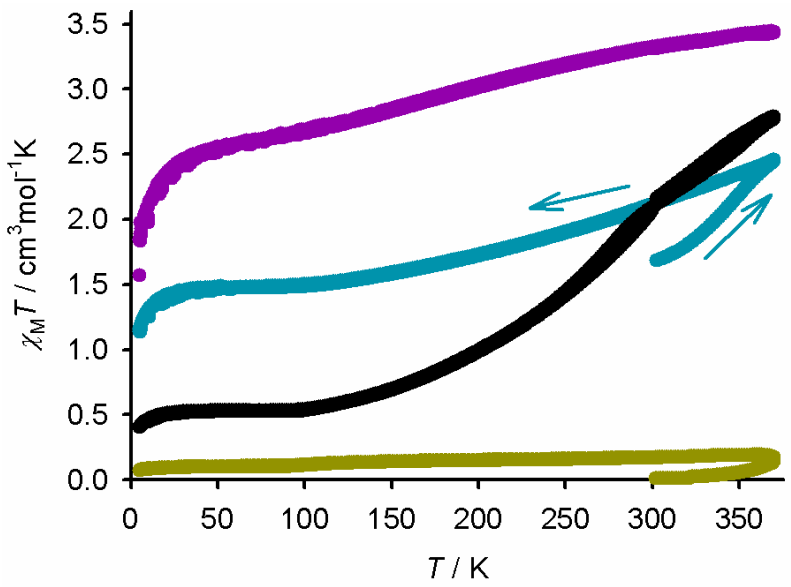


Figure S22 Solid state magnetic data for **7** (black), **8**·MeCN·H_2O (yellow), **9**·$MeNO_2$ (purple) and **10**·$2H_2O$ (cyan), on a 300⟶370⟶5⟶300 K temperature cycle at a scan rate 5 K min^{-1}.

The low-spin nature of **8**·MeCN·H_2O is consistent with the crystal structure of the freshly prepared material, **8**·2MeCN. No crystallographic data are available for the other compounds in the graph, but the gradual and incomplete nature of their SCO is consistent with their poorly crystalline or (for **10**·$2H_2O$) amorphous nature (Figure S21).

The irreversibility in the data for **8**·MeCN·H_2O and **10**·$2H_2O$ above 300 K implies the samples lost lattice solvent on heating inside the magnetometer, which affected their spin-state behaviour.[21]

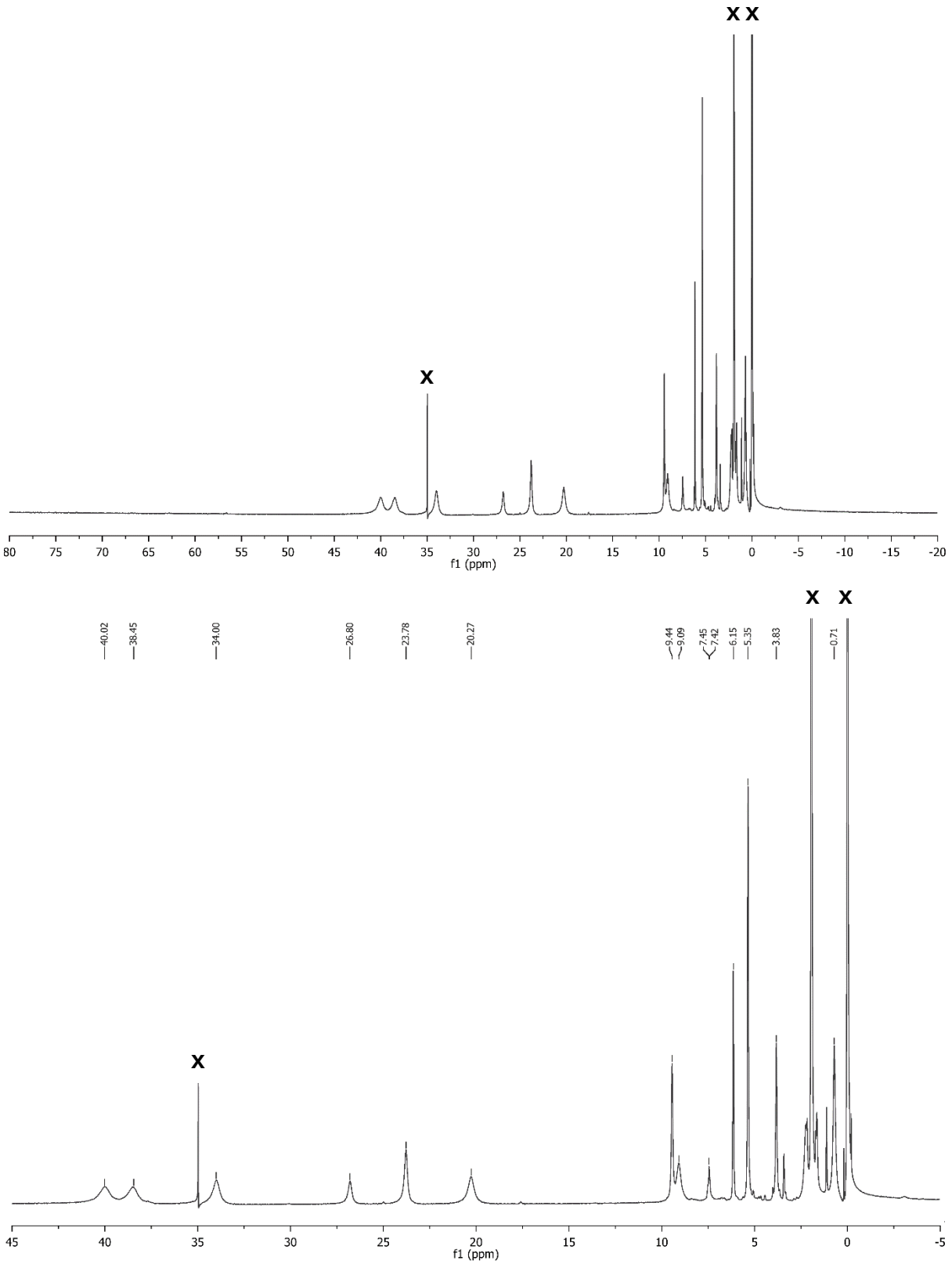


Figure S23 ^{1}H NMR spectrum of **7** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the main peaks assigned to the heteroleptic complex **7**. The feature at 35 ppm is a spectrometer artefact.

A molecule of **7** has 32 protons in 13 unique environments, which are all resolved in the spectrum. There are no significant impurity peaks in the spectrum.

The significant contact shifts in the spectrum are consistent with magnetic measurements, which show the complex adopts a mixed high:low-spin population at room temperature in this solvent ($\chi_M T$ = 2.0 cm^3 mol^{-1} K; Figure 6, main article).

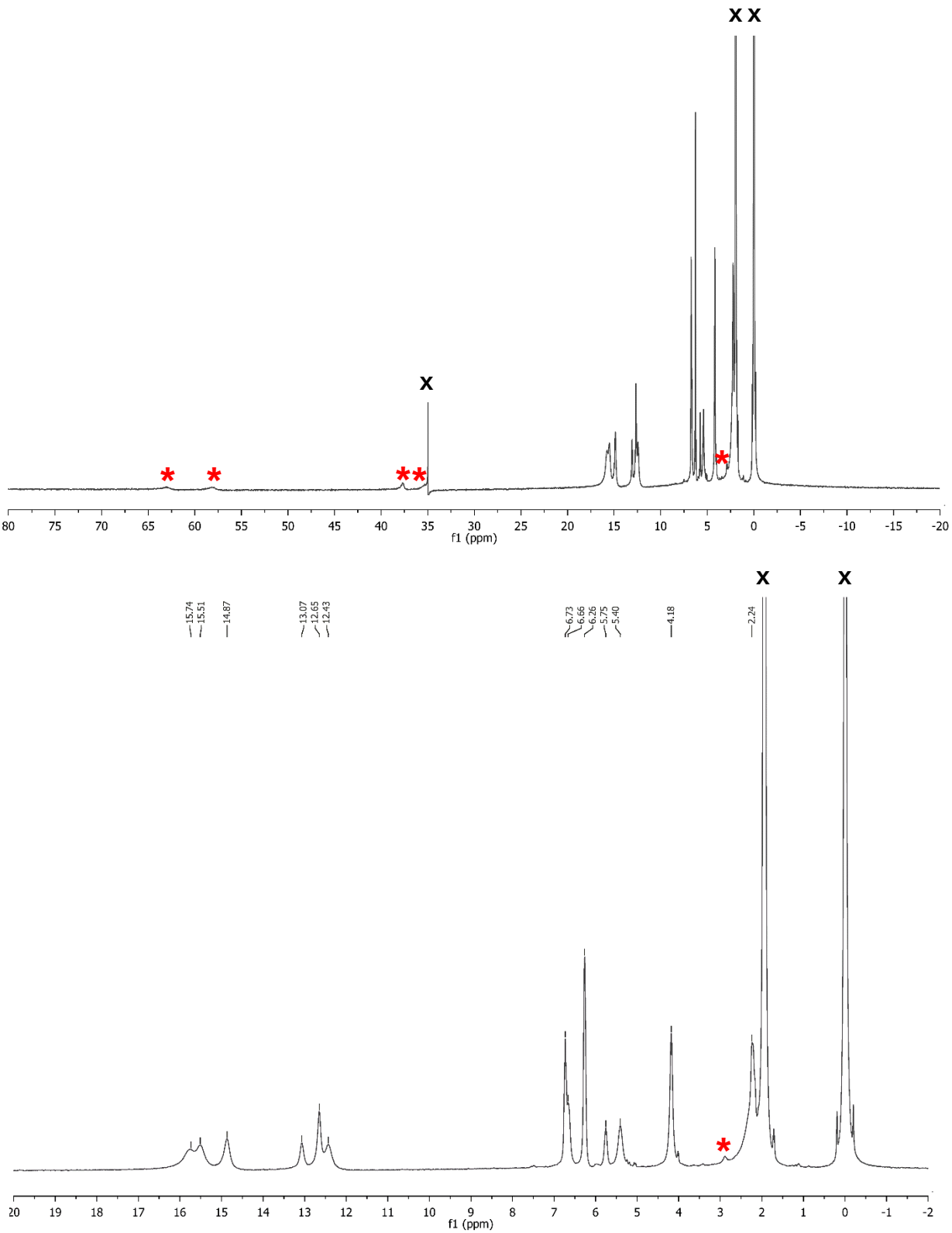


Figure S24 ^{1}H NMR spectrum of **8** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the main peaks assigned to the heteroleptic complex **8**. The feature at 35 ppm is a spectrometer artefact.

A molecule of **8** has 28 protons in 13 unique environments, which are all resolved in the spectrum. The starred peaks are from $[Fe(bpp)_2]^{2+}$,[6] which comprises *ca* 10 % of the sample; there are no peaks attributable to $[Fe((R)\text{-}L^2Ph)_2]^{2+}$.[2]

The small contact shifts in the spectrum are consistent with its solution magnetic measurements, which show only a small paramagnetism of $\chi_M T$ = 0.8 cm^3 mol^{-1} K at room temperature (Figure 6, main article).

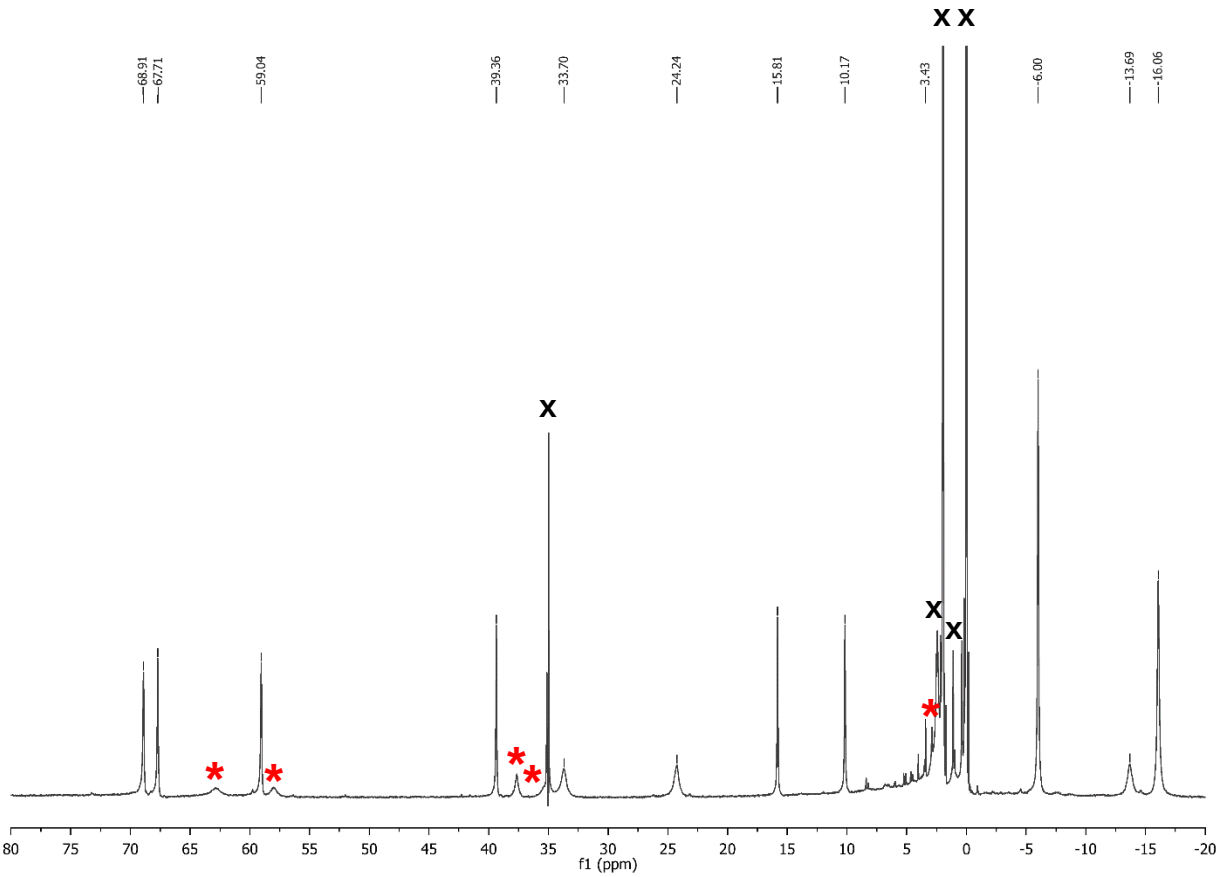


Figure S25 ^{1}H NMR spectrum of **9** (CD_3CN). The feature at 35 ppm is a spectrometer artefact, and the peaks at 0.9 and 1.3 ppm are impurities in the NMR solvent (present in Figures S15-S17, S25, S26, S30 and S31).

A molecule of **9** has 32 protons in 13 unique environments, including diastereotopic *iso*propyl methyl substituents. Only 12 of these are resolved in the spectrum. Another peak is expected between 20-40 ppm, which may be masked by the 35 ppm spectrometer artefact. The starred peaks are from $[Fe(bpp)_2]^{2+}$,[6] which comprises *ca* 15 % of the sample; there are no peaks attributable to $[Fe((S)\text{-}L^1iPr)_2]^{2+}$,[4] but weak resonances in the diamagnetic region might correspond to uncoordinated L^1iPr ligand.

The strongly contact-shifted spectrum is consistent with its solution magnetic measurements, which show the complex is high-spin at room temperature (Figure 6, main article).

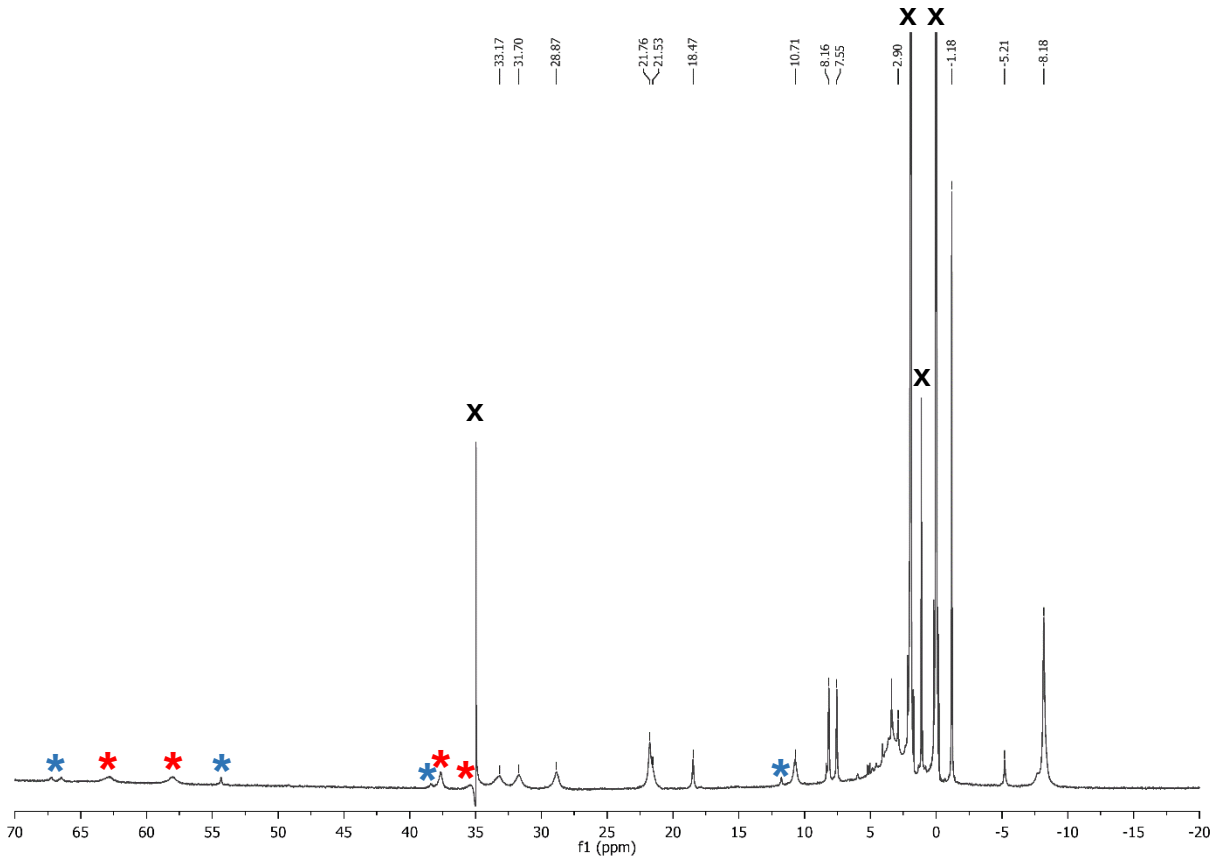


Figure S26 ^{1}H NMR spectrum of **10** (CD_3CN). The feature at 35 ppm is a spectrometer artefact, and the peaks at 0.9 and 1.3 ppm are impurities in the NMR solvent (present in Figures S15-S17, S25, S26, S30 and S31).

A molecule of **10** has 32 protons in 13 unique environments, including diastereotopic *iso*propyl methyl substituents, which are all resolved in the spectrum. The red starred peaks are from $[Fe(bpp)_2]^{2+}$,[6] which comprises *ca* 25 % of the sample, while the blue starred peaks are from another paramagnetic species whose identity is unclear. There are no peaks attributable to $[Fe((S)\text{-}L^2iPr)_2]^{2+}$ in the spectrum.[2]

The moderate contact shifts in the spectrum are consistent with its solution magnetic measurements, which show the complex adopts a mixed high:low-spin population at 298 K ($\chi_M T$ = 2.6 cm^3 mol^{-1} K; Figure 6, main article).

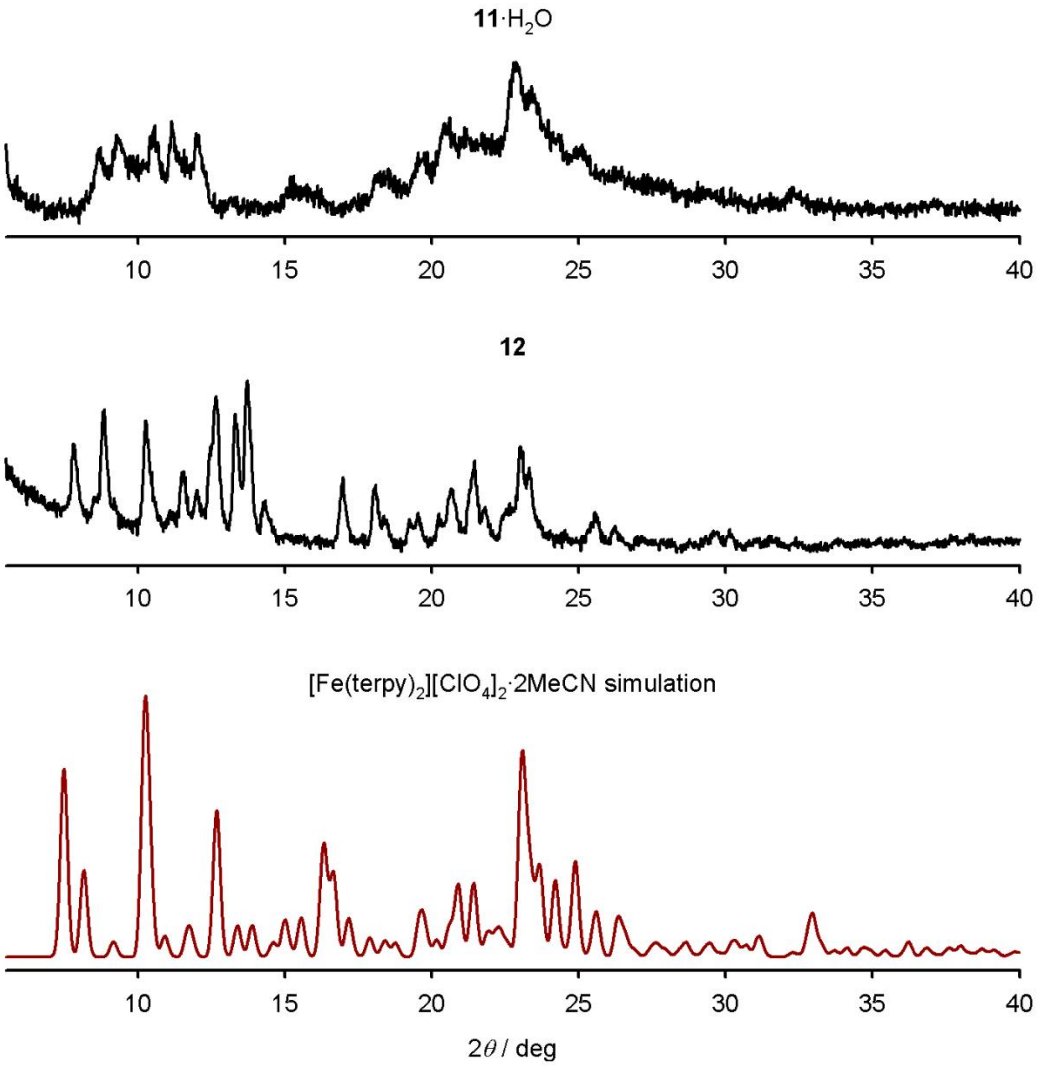


Figure S27 Room temperature X-ray powder diffraction data for **11**·H_2O and **12** (black). A simulation of the solvate of $[Fe(terpy)_2][ClO_4]_2$ isolated from recrystallisations of these compounds is also included (red).

Despite their good microanalyses, these samples contain a mixture of species, which probably includes $[Fe(terpy)_2][ClO_4]_2$ (Figures S30 and S31). Some strong peaks from the simulated powder pattern of $[Fe(terpy)_2][ClO_4]_2$·2MeCN (Figure S29) have counterparts in the data for **11**·H_2O and **12**, which tentatively supports that conclusion.

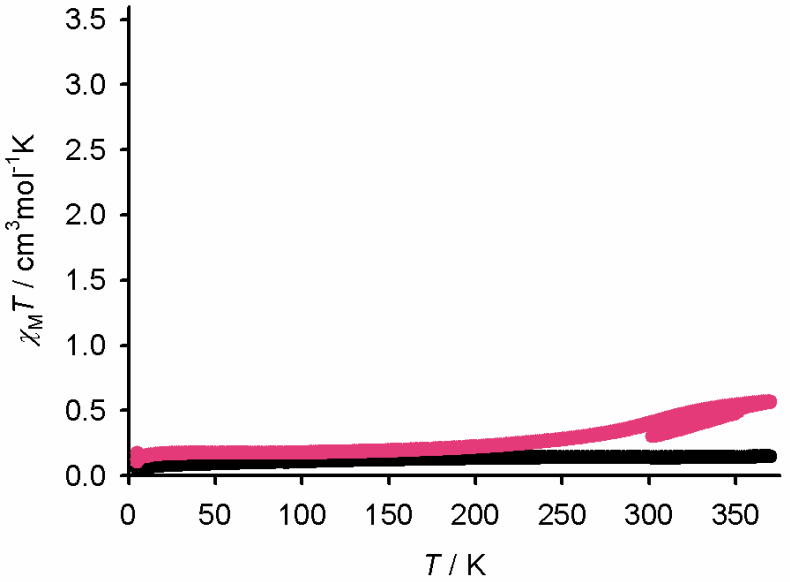


Figure S28 Solid state magnetic data for **11**·H_2O (black) and **12** (pink), on a 300⟶370⟶5⟶300 K temperature cycle at a scan rate 5 K min^{-1}.

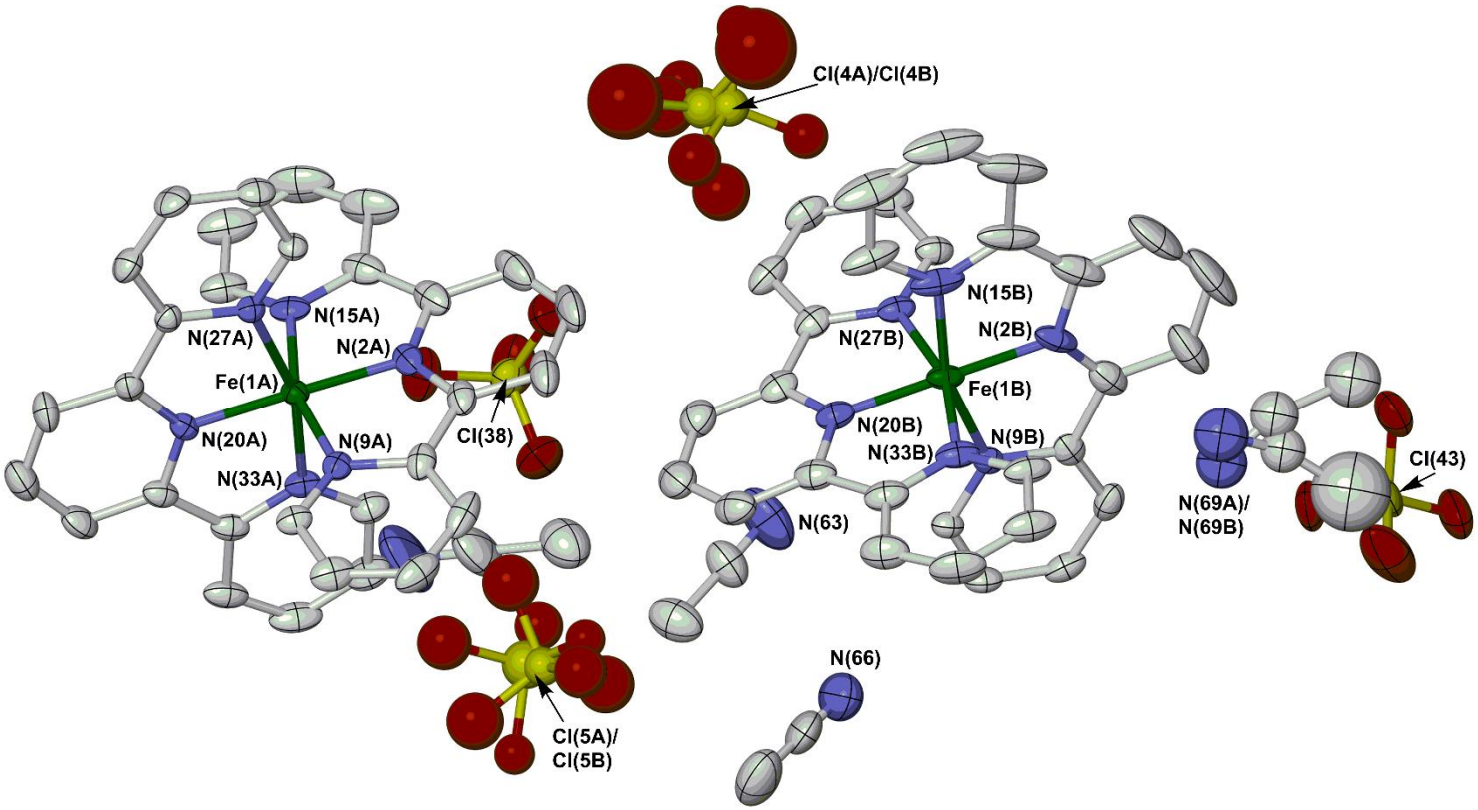


Figure S29 The asymmetric unit of $[Fe(terpy)_2][ClO_4]_2 \cdot 2MeCN$, with selected atom numbering. Other details as for Figure S1.

This crystal was taken from a mixture of crystals and powder, produced by recrystallisation of a material analysing as **11**·H_2O from MeCN/Et_2O. The same crystals also occurred in a recrystallised sample of **12**.

The Fe–N bond lengths and N–Fe–N angles are not tabulated in this ESI, but are typical for low-spin $[Fe(terpy)_2]^{2+}$ derivatives without intramolecular steric hindrance.[24] The crystal is isomorphous with previously published $[Ru(terpy)_2][PF_6]_2 \cdot 2MeCN$.[25]

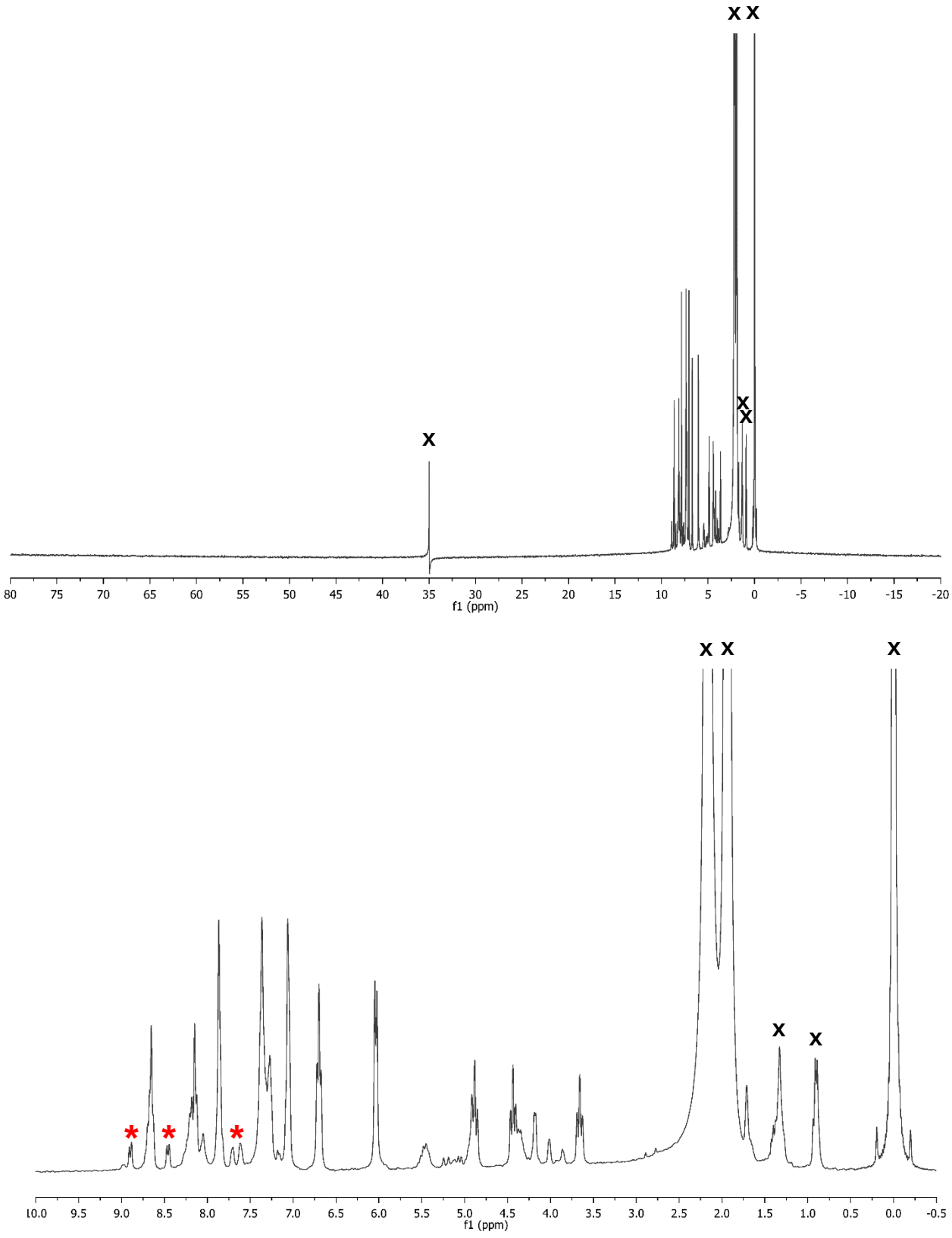


Figure S30 ^{1}H NMR spectrum of **11** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the diamagnetic region. The feature at 35 ppm is a spectrometer artefact and the peaks at 0.9 and 1.3 ppm are impurities in the NMR solvent (present in Figures S15-S17, S25, S26, S30 and S31).

There are at least two diamagnetic species in the spectrum. The starred peaks are a good match for $[Fe(terpy)_2]^{2+}$,[7] which is clearly present since crystals of $[Fe(terpy)_2][ClO_4]_2$ were isolated following recrystallisation of this product. In contrast to **12**, however (Figure S31), there is no evidence for paramagnetic $[Fe((R)\text{-}L^{1}Ph)_2]^{2+}$ in the solution.[4]

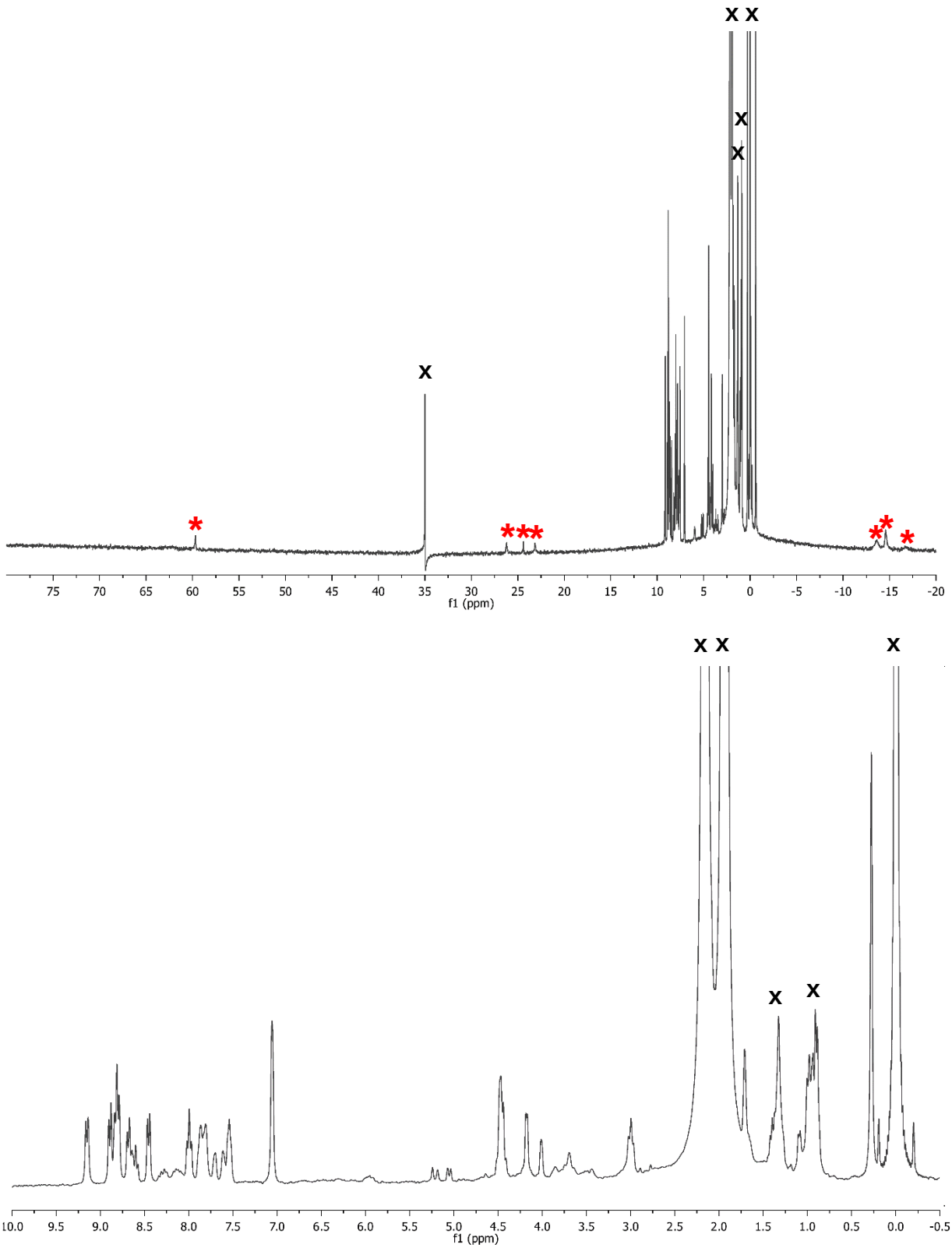


Figure S31 ^{1}H NMR spectrum of **12** (CD_3CN). Top: full paramagnetic range. Bottom: expansion of the diamagnetic region. The feature at 35 ppm is a spectrometer artefact, and peaks at 0.9 and 1.3 ppm are impurities in the NMR solvent (present in Figures S15-S17, S25, S26, S30 and S31).

The starred paramagnetic peaks are from $[Fe((S)\text{-}L^{1}iPr)_2]^{2+}$,[4] which comprises around 10 % of the iron content of the solution. It's less clear whether $[Fe(terpy)_2]^{2+}$ is also a component of this mixture (Figure S30),[7] but the peak integrations imply there are three main diamagnetic species in the solution.

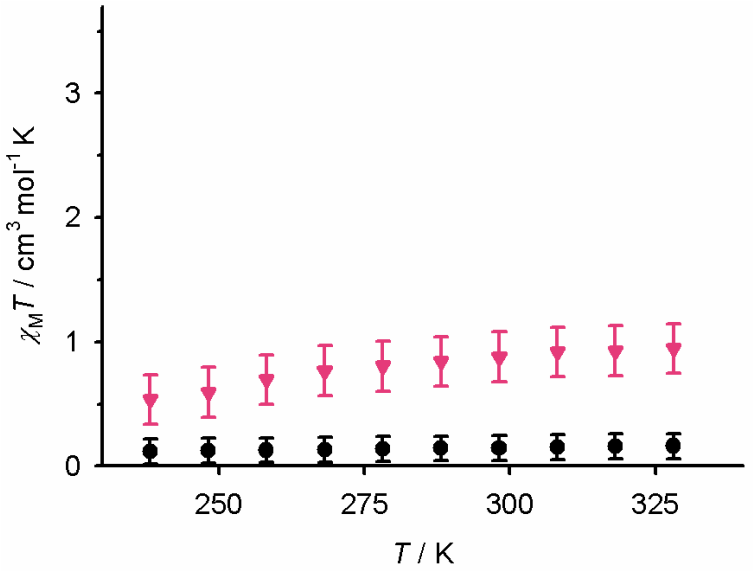


Figure S32 Magnetic data for **11** (black circles) and **12** (pink triangles) in CD_3CN solution.

Although their microanalyses are consistent with the formulae [Fe(L^1R)(terpy)][ClO_4]$_2$ (R = Ph, **11**; R = *i*Pr, **12**) the actual composition of these samples is uncertain. No crystal structures were obtained of these compounds, and their NMR spectra contain a mixture of species (Figures S30-S31).

Both **11**$^{2+}$ and **12**$^{2+}$ are predicted to be low-spin by the DFT calculations, while the ligand exchange product [Fe(terpy)$_2$]$^{2+}$ is also low-spin and diamagnetic. The non-zero magnetic moment for **12** might be explained by the presence of paramagnetic [Fe((*S*)-L^1*i*Pr)$_2$]$^{2+}$,[4] which is clear as a minor component of its NMR spectrum (Figure S31).

Solution magnetic data for compounds **1**-**10** are shown in the main article.

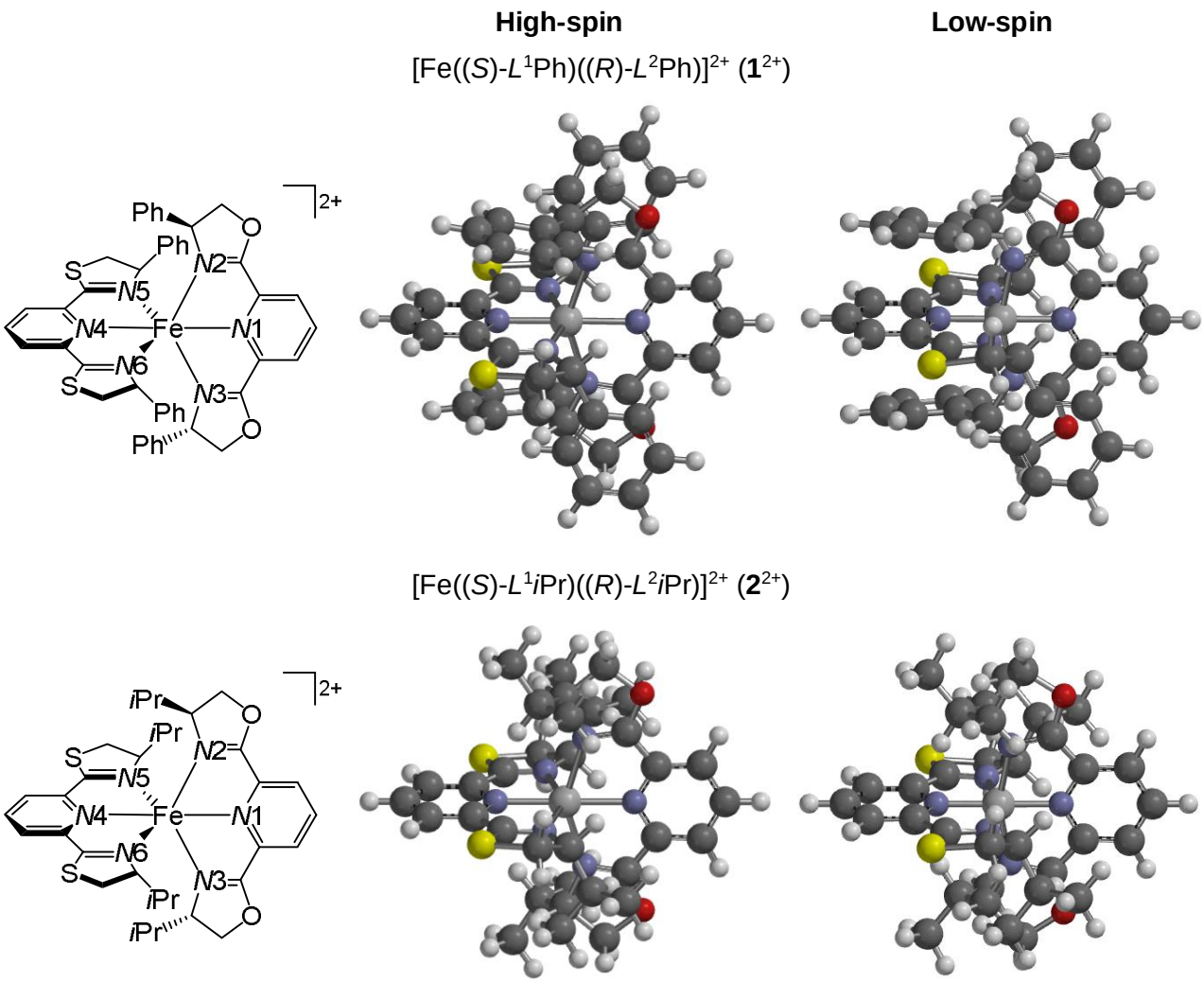


Figure S33 The DFT energy-minimised structures of the heterochiral [Fe((*S*)-*L*^{1}R)((*R*)-*L*^{2}R)]$^{2+}$ (R = Ph or *i*Pr) complexes, showing the atom numbering in Table S8.

Alternative views of these minimised structures are in Figure S34.

Table S8 Computed metric parameters for the heteroleptic, heterochiral [Fe((*S*)-L^1R)((*R*)-L^2R)]$^{2+}$ complexes (Å, °; Figure S33). Experimental crystallographic data are also included in square brackets for comparison, where this is available. α is the average bite angle of the tridentate ligands. Definitions of ϕ and θ are on page S9, and the atom numbering in the Table is shown in Figure S33.

	[Fe((*S*)-L^1Ph)((*R*)-L^2Ph)]$^{2+}$ (**1**$^{2+}$)		[Fe((*S*)-L^1*i*Pr)((*R*)-L^2*i*Pr)]$^{2+}$ (**2**$^{2+}$)	
	High-spin	Low-spin	High-spin	Low-spin[a]
Fe–N1	2.165	1.917 [1.915(3)]	2.141	1.917 [1.923(5)]
Fe–N2	2.251	2.017 [1.995(3)]	2.249	2.021 [1.995(5)]
Fe–N3	2.231	2.017 [1.994(3)]	2.252	2.021 [1.999(5)]
Fe–N4	2.115	1.897 [1.884(3)]	2.132	1.898 [1.903(5)]
Fe–N5	2.228	2.004 [1.985(3)]	2.270	2.021 [2.025(5)]
Fe–N6	2.220	2.004 [1.995(3)]	2.268	2.021 [2.014(5)]
N1–Fe–N2	73.7	79.7 [79.45(13)]	74.2	79.7 [78.9(2)]
N1–Fe–N3	73.8	79.7 [79.20(13)]	74.1	79.7 [79.3(2)]
N1–Fe–N4	178.5	180.0 [179.49(15)]	179.8	179.9 [178.5(2)]
N1–Fe–N5	104.7	99.9 [100.81(12)]	105.6	99.9 [100.7(2)]
N1–Fe–N6	106.4	99.9 [99.73(12)]	105.9	100.0 [100.4(2)]
N2–Fe–N3	147.5	159.3 [158.64(12)]	148.3	159.4 [158.2(2)]
N2–Fe–N4	107.4	100.3 [100.20(13)]	105.8	100.2 [102.6(2)]
N2–Fe–N5	97.0	92.7 [93.43(12)]	92.9	92.9 [92.7(2)]
N2–Fe–N6	92.0	90.9 [90.65(12)]	95.4	90.6 [92.3(2)]
N3–Fe–N4	105.1	100.3 [101.15(13)]	105.8	100.4 [99.3(2)]
N3–Fe–N5	91.8	90.9 [90.56(13)]	95.7	90.7 [91.4(2)]
N3–Fe–N6	96.4	92.7 [92.95(12)]	93.0	92.9 [91.6(2)]
N4–Fe–N5	74.4	80.1 [79.57(13)]	74.2	80.1 [79.4(2)]
N4–Fe–N6	74.6	80.1 [79.90(13)]	74.3	80.1 [79.4(2)]
N5–Fe–N6	149.0	160.2 [159.46(13)]	148.5	160.1 [158.8(2)]
a	74.1	79.9 [79.5(2)]	74.2	79.9 [79.3(4)]
φ	178.5	180.0 [179.49(15)]	179.8	179.9 [178.5(2)]
θ	87.3	88.5 [89.67(6)]	88.8	88.4 [88.81(9)]

[a]Experimental values are from molecule A in the crystal structure of this complex. Experimental bonds and angles involving N5 and N6 have been swapped in the Table, because the crystallographic and computed structures having opposite handedness.

Computed metric parameters for the corresponding homoleptic, heterochiral [Fe((*R*)-L^1R)((*S*)-L^1R)]$^{2+}$ and [Fe((*R*)-L^2R)((*S*)-L^2R)]$^{2+}$ complexes are in ref. 2.

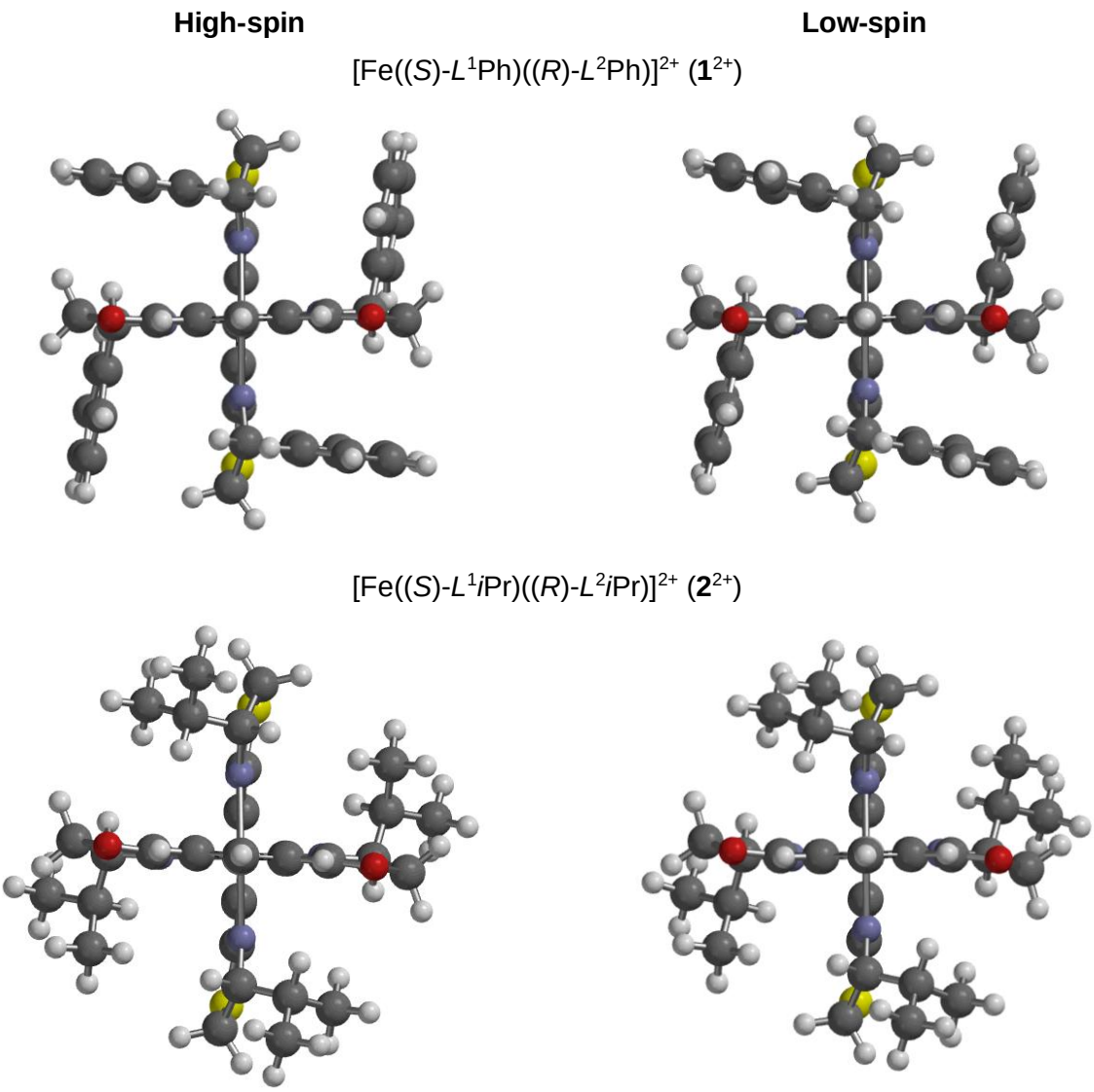


Figure S34 Alternative views of the DFT energy-minimised structures of the heterochiral [Fe((*S*)-L^1R)((*R*)-L^2R)]$^{2+}$ (R = Ph or *i*Pr) complexes, emphasising the conformations and orientations of the heterocyclic ligands. Other details as for Figure S33.

Corresponding views of the minimised structures of homoleptic, heterochiral [Fe((*R*)-L^1R)((*S*)-L^1R)]$^{2+}$ and [Fe((*R*)-L^2R)((*S*)-L^2R)]$^{2+}$ complexes are in ref. 2. The conformations of minimised **1**$^{2+}$ and **2**$^{2+}$ closely resemble their homoleptic counterparts.

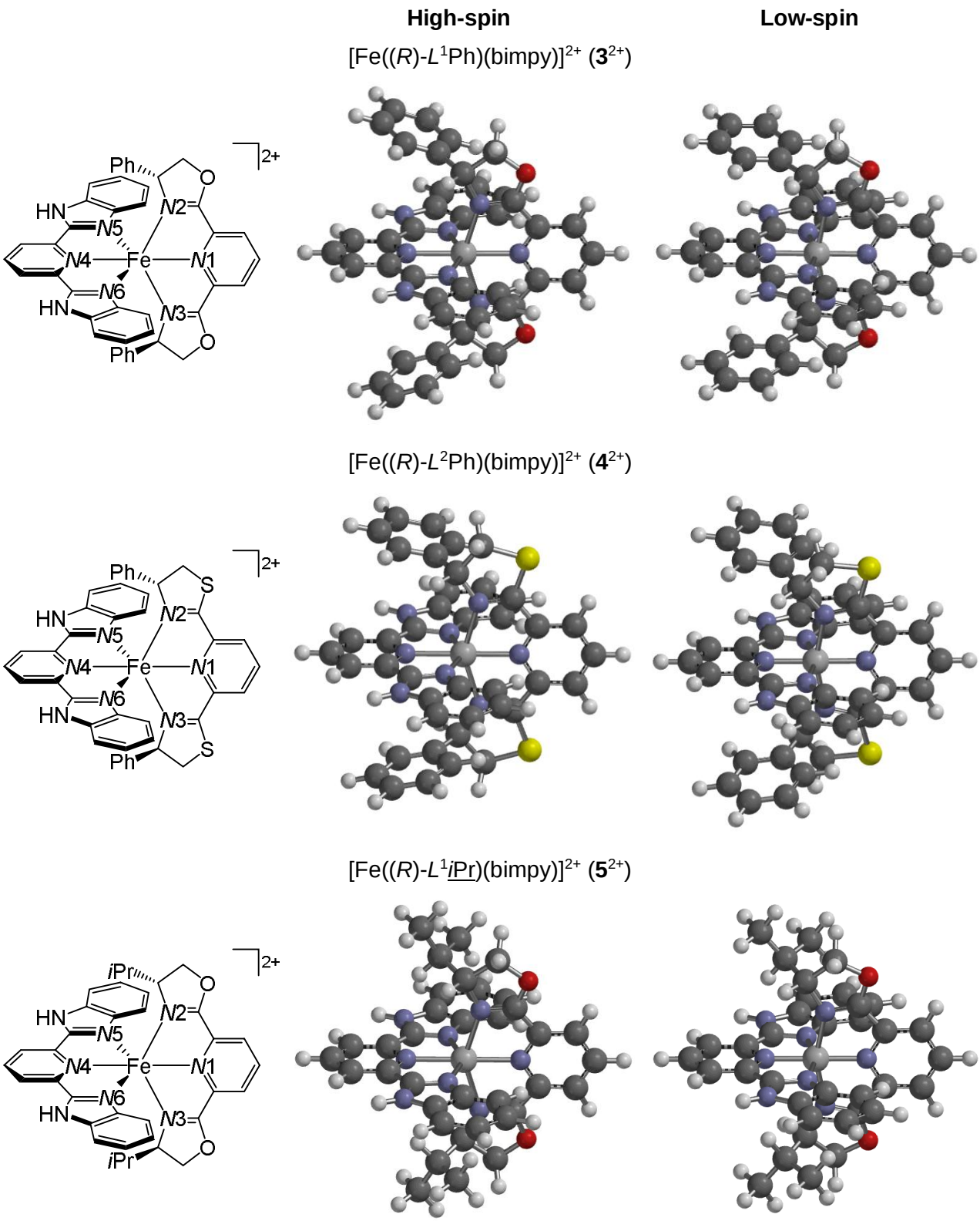


Figure S35 DFT energy-minimised structures of the heteroleptic $[Fe(LR)L]^{2+}$ (L = bimpy, bpp or terpy) complexes, showing the atom numbering in Table S9. Details as for Figure S33.

Alternative views of these minimised structures are in Figure S36.

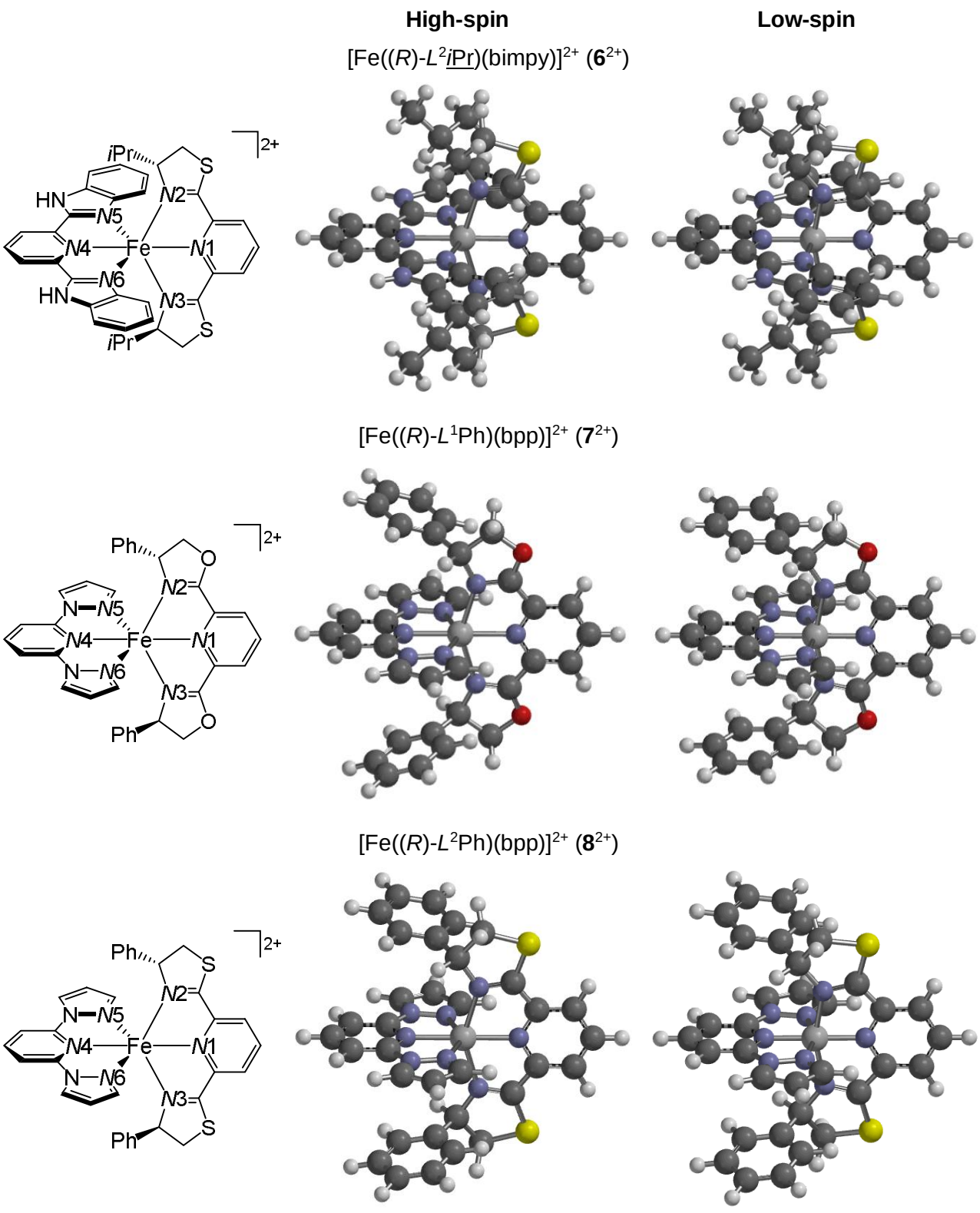


Figure S35 continued.

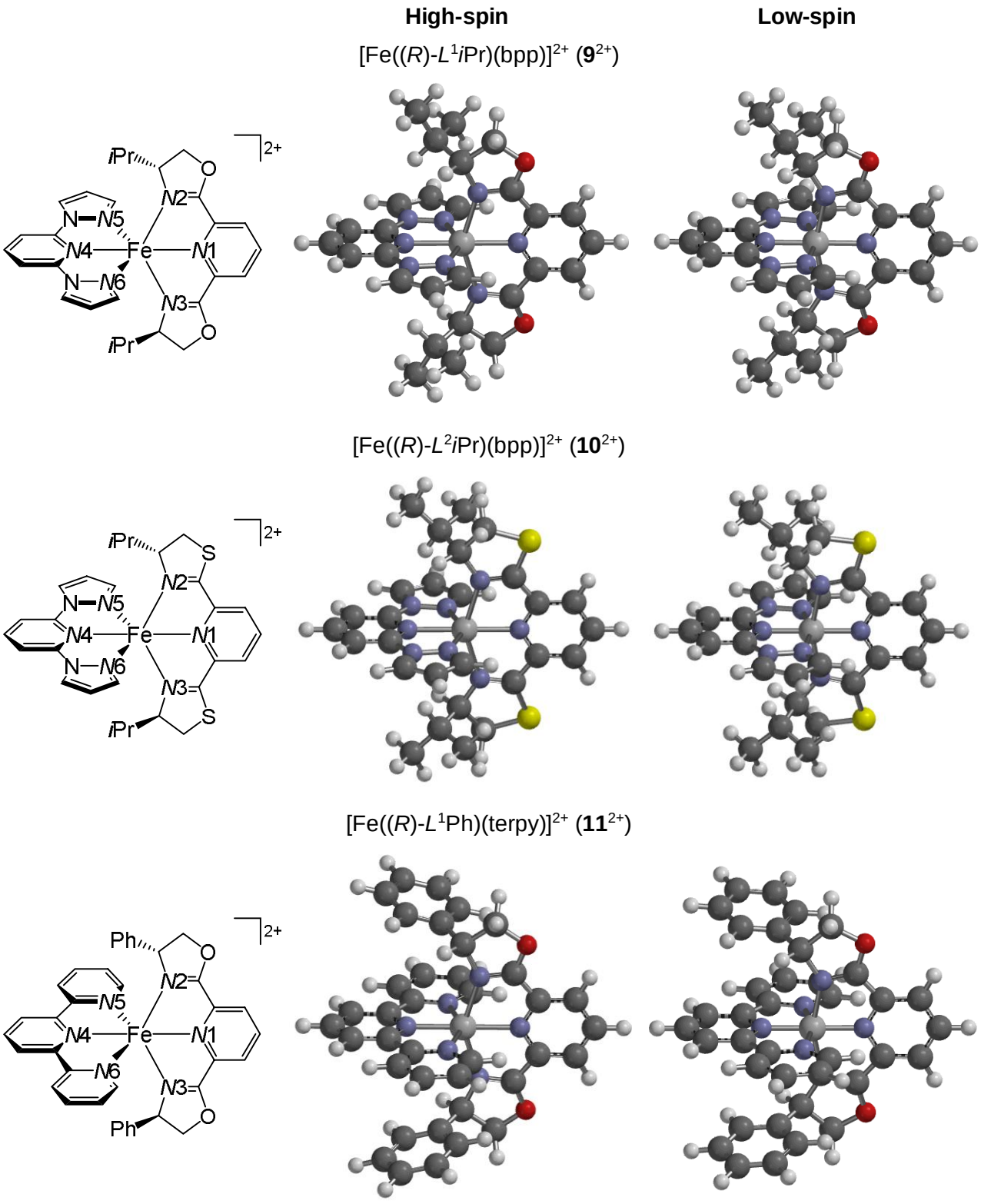


Figure S35 continued.

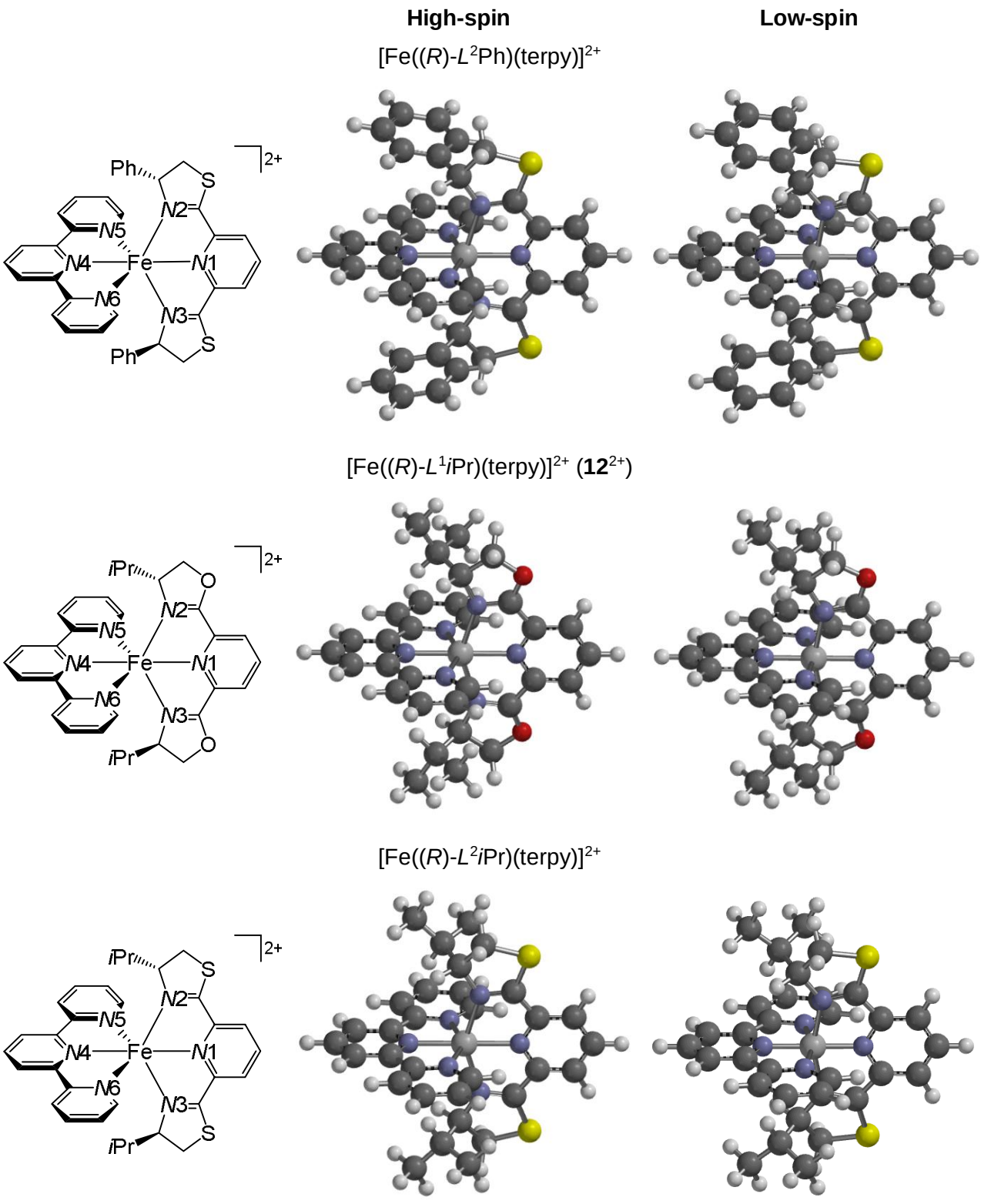


Figure S35 continued.

Table S9 Computed metric parameters for the heteroleptic [Fe(*L*R)L]$^{2+}$ complexes (Å, °; Figure S43). Experimental crystallographic data are also included in square brackets for comparison, where this is available. α is the average bite angle of the tridentate ligands. Definitions of ϕ and θ are on page S9, and the atom numbering in the Table is shown in Figure S35.

	[Fe((*R*)-*L*^{1}Ph)(bimpy)]$^{2+}$ (**3**$^{2+}$)		[Fe((*R*)-*L*^{2}Ph)(bimpy)]$^{2+}$ (**4**$^{2+}$)		[Fe((*R*)-*L*^{1}*i*Pr)(bimpy)]$^{2+}$ (**5**$^{2+}$)	
	High-spin	Low-spin[a]	High-spin	Low-spin	High-spin	Low-spin
Fe–N1	2.128	1.908 [1.900(8)]	2.103	1.891 [1.8795(13)]	2.133	1.911
Fe–N2	2.227	2.006 [1.983(8)]	2.211	1.991 [1.9739(14)]	2.251	2.010
Fe–N3	2.226	2.006 [1.979(7)]	2.212	1.991 [1.9574(13)]	2.250	2.010
Fe–N4	2.182	1.926 [1.934(8)]	2.184	1.928 [1.9322(13)]	2.181	1.925
Fe–N5	2.226	2.008 [2.035(8)]	2.226	2.008 [1.9813(13)]	2.225	2.010
Fe–N6	2.227	2.009 [2.006(8)]	2.226	2.009 [1.9937(13)]	2.227	2.010
N1–Fe–N2	74.2	79.9 [79.4(3)]	74.5	80.3 [80.14(6)]	74.2	79.8
N1–Fe–N3	74.2	79.9 [79.5(3)]	74.5	80.3 [79.63(6)]	74.3	79.9
N1–Fe–N4	179.8	180.0 [177.8(4)]	179.9	179.9 [179.60(6)]	179.7	179.9
N1–Fe–N5	105.8	99.8 [99.1(3)]	105.6	99.7 [100.13(6)]	105.9	99.8
N1–Fe–N6	105.7	99.7 [102.1(3)]	105.9	99.9 [100.61(6)]	105.8	99.7
N2–Fe–N3	148.4	159.8 [158.7(3)]	149.1	160.6 [159.70(6)]	148.4	159.7
N2–Fe–N4	105.6	100.1 [102.6(3)]	105.5	99.8 [100.08(6)]	105.6	100.2
N2–Fe–N5	99.3	92.8 [92.4(3)]	98.1	94.3 [92.27(5)]	100.2	94.1
N2–Fe–N6	89.2	90.5 [90.2(3)]	90.2	89.0 [93.19(6)]	88.1	89.3
N3–Fe–N4	106.0	100.1 [98.6(3)]	105.4	99.7 [100.14(5)]	106.0	100.1
N3–Fe–N5	89.2	90.5 [92.7(3)]	90.2	89.0 [89.61(5)]	88.3	89.3
N3–Fe–N6	99.4	92.9 [92.5(3)]	98.2	94.4 [92.18(6)]	100.5	94.2
N4–Fe–N5	74.3	80.3 [79.9(3)]	74.3	80.2 [79.54(5)]	74.2	80.3
N4–Fe–N6	74.2	80.3 [78.9(3)]	74.2	80.2 [79.72(5)]	74.2	80.3
N5–Fe–N6	148.5	160.5 [158.7(3)]	148.5	160.4 [159.17(5)]	148.4	160.5
a	74.2	80.1 [79.4(6)]	74.4	80.3 [79.75(12)]	74.2	80.1
φ	179.8	180.0 [177.8(4)]	179.9	179.9 [179.60(6)]	179.7	179.9
θ	83.6	88.8 [88.21(14)]	87.2	86.6 [88.00(3)]	82.4	85.4

[a]Experimental values are from molecule A in the crystal structure of this complex. [b]Experimental bonds and angles involving N5 and N6 have been swapped for this compound, because the crystallographic and computed structures having opposite handedness.

Table S9 continued.

	[Fe((*R*)-L^2*i*Pr)(bimpy)]$^{2+}$ (**6**$^{2+}$)		[Fe((*R*)-L^1Ph)(bpp)]$^{2+}$ (**7**$^{2+}$)		[Fe((*R*)-L^2Ph)(bpp)]$^{2+}$ (**8**$^{2+}$)	
	High-spin	Low-spin[b]	High-spin	Low-spin	High-spin	Low-spin
Fe–N1	2.109	1.896 [1.881(5)]	2.126	1.913	2.104	1.896 [1.879(4)]
Fe–N2	2.244	2.001 [1.995(5)]	2.219	2.012	2.205	1.999 [1.978(4)]
Fe–N3	2.241	2.001 [2.001(6)]	2.221	2.012	2.205	2.000 [1.992(4)]
Fe–N4	2.190	1.927 [1.913(5)]	2.169	1.905	2.165	1.905 [1.906(4)]
Fe–N5	2.227	2.011 [1.983(5)]	2.217	1.973	2.214	1.974 [1.954(4)]
Fe–N6	2.229	2.011 [1.992(5)]	2.216	1.973	2.214	1.974 [1.961(4)]
N1–Fe–N2	74.5	80.2 [80.4(2)]	74.3	79.9	74.6	80.3 [80.40(17)]
N1–Fe–N3	74.5	80.2 [79.8(2)]	74.3	79.9	74.6	80.3 [79.76(17)]
N1–Fe–N4	179.6	179.9 [175.2(2)]	179.7	180.0	180.0	179.9 [176.77(17)]
N1–Fe–N5	106.3	99.9 [103.7(2)]	106.7	99.9	106.6	100.1 [97.99(17)]
N1–Fe–N6	105.9	99.8 [96.1(2)]	106.9	100.0	106.6	99.9 [102.29(17)]
N2–Fe–N3	149.0	160.3 [160.1(2)]	148.6	159.9	149.3	160.7 [160.10(17)]
N2–Fe–N4	105.2	99.9 [96.3(2)]	106.0	100.1	105.4	99.6 [97.34(17)]
N2–Fe–N5	100.3	95.1 [93.3(2)]	99.1	92.9	98.6	94.3 [94.22(15)]
N2–Fe–N6	88.3	88.2 [90.7(2)]	90.0	90.6	90.2	89.1 [89.62(16)]
N3–Fe–N4	105.9	99.8 [103.5(2)]	105.5	100.1	105.4	99.7 [102.54(17)]
N3–Fe–N5	88.2	88.2 [89.7(2)]	90.0	90.5	90.2	89.1 [90.14(16)]
N3–Fe–N6	100.3	95.2 [93.2(2)]	99.0	92.9	98.6	94.3 [92.99(16)]
N4–Fe–N5	73.9	80.2 [79.9(2)]	73.2	80.0	73.4	80.0 [79.81(16)]
N4–Fe–N6	73.9	80.2 [80.3(2)]	73.2	80.0	73.4	80.0 [79.94(17)]
N5–Fe–N6	147.8	160.4 [160.2(2)]	146.4	160.1	146.7	160.0 [159.72(17)]
a	74.2	80.2 [80.1(4)]	73.8	80.0	74.0	80.2 [80.0(3)]
φ	179.6	179.9 [175.2(2)]	179.7	180.0	180.0	179.9 [176.77(17)]
θ	81.9	84.4 [85.11(8)]	84.5	88.3	85.3	86.2 [85.97(7)]

[a]Experimental values are from molecule A in the crystal structure of this complex. [b]Experimental bonds and angles involving N5 and N6 have been swapped for this compound, because the crystallographic and computed structures having opposite handedness.

Table S9 continued.

	[Fe((*R*)-*L*^{1}*i*Pr)(bpp)]$^{2+}$ (**9**$^{2+}$)		[Fe((*R*)-*L*^{2}*i*Pr)(bpp)]$^{2+}$ (**10**$^{2+}$)		[Fe((*R*)-*L*^{1}Ph)(terpy)]$^{2+}$ (**11**$^{2+}$)	
	High-spin	Low-spin[a]	High-spin	Low-spin	High-spin	Low-spin
Fe–N1	2.124	1.916	2.106	1.899	2.134	1.916
Fe–N2	2.235	2.019	2.231	2.010	2.227	1.999
Fe–N3	2.235	2.019	2.229	2.010	2.227	1.999
Fe–N4	2.178	1.901	2.183	1.905	2.128	1.892
Fe–N5	2.220	1.975	2.221	1.976	2.226	1.997
Fe–N6	2.220	1.975	2.221	1.976	2.226	1.997
N1–Fe–N2	74.4	79.9	74.6	80.2	74.1	79.8
N1–Fe–N3	74.4	79.9	74.6	80.2	74.1	79.8
N1–Fe–N4	179.7	180.0	179.8	180.0	180.0	180.0
N1–Fe–N5	106.7	99.9	107.3	100.1	104.9	98.9
N1–Fe–N6	107.4	100.0	107.0	100.0	104.9	98.9
N2–Fe–N3	148.8	159.8	149.3	160.5	148.1	159.6
N2–Fe–N4	105.6	100.1	105.3	99.8	105.9	100.2
N2–Fe–N5	99.8	94.2	100.2	94.7	98.0	93.7
N2–Fe–N6	89.3	89.3	88.8	88.7	90.1	89.4
N3–Fe–N4	105.6	100.1	105.5	99.8	105.9	100.2
N3–Fe–N5	89.3	89.2	88.8	88.7	90.1	89.4
N3–Fe–N6	99.7	94.2	100.2	94.7	98.0	93.7
N4–Fe–N5	73.0	80.1	72.8	80.0	75.1	81.1
N4–Fe–N6	73.0	80.1	72.9	80.0	75.1	81.1
N5–Fe–N6	145.9	160.1	145.7	159.9	150.2	162.1
a	73.7	80.0	73.7	80.1	74.6	80.5
φ	179.7	180.0	179.8	180.0	180.0	180.0
θ	83.2	85.1	83.0	84.4	84.5	85.9

[a]Experimental values are from molecule A in the crystal structure of this complex. [b]Experimental bonds and angles involving N5 and N6 have been swapped for this compound, because the crystallographic and computed structures having opposite handedness.

Table S9 continued.

	[Fe((*R*)-*L*^{2}Ph)(terpy)]$^{2+}$		[Fe((*R*)-*L*^{1}*i*Pr)(terpy)]$^{2+}$ (**12**$^{2+}$)		[Fe((*R*)-*L*^{2}*i*Pr)(terpy)]$^{2+}$	
	High-spin	Low-spin[a]	High-spin	Low-spin	High-spin	Low-spin
Fe–N1	2.112	1.900	2.139	1.921	2.124	1.906
Fe–N2	2.221	2.000	2.239	2.007	2.235	2.011
Fe–N3	2.221	2.000	2.239	2.007	2.235	2.011
Fe–N4	2.130	1.895	2.129	1.893	2.136	1.894
Fe–N5	2.227	1.998	2.230	1.995	2.226	1.995
Fe–N6	2.227	1.998	2.230	1.995	2.226	1.995
N1–Fe–N2	74.3	80.1	74.1	79.7	74.2	80.0
N1–Fe–N3	74.3	80.1	74.1	79.7	74.2	80.0
N1–Fe–N4	180.0	180.0	180.0	180.0	180.0	180.0
N1–Fe–N5	105.0	99.0	105.1	99.0	105.3	99.1
N1–Fe–N6	105.0	99.0	105.1	99.0	105.3	99.1
N2–Fe–N3	148.6	160.2	148.3	159.4	148.4	160.0
N2–Fe–N4	105.7	99.9	105.9	100.3	105.8	100.0
N2–Fe–N5	99.1	94.7	99.9	94.3	99.6	95.0
N2–Fe–N6	88.9	88.4	88.3	89.0	88.6	88.1
N3–Fe–N4	105.7	99.9	105.9	100.3	105.8	100.0
N3–Fe–N5	88.9	88.4	88.3	89.0	88.6	88.1
N3–Fe–N6	99.1	94.7	99.9	94.3	99.6	95.0
N4–Fe–N5	75.0	81.0	74.9	81.0	74.7	80.9
N4–Fe–N6	75.0	81.0	74.9	81.0	74.7	80.9
N5–Fe–N6	150.0	162.0	149.9	161.9	149.4	161.9
a	74.7	80.6	74.5	80.4	74.5	80.5
φ	180.0	180.0	180.0	180.0	180.0	180.0
θ	83.4	85.4	82.7	84.8	82.9	84.4

[a]Experimental values are from molecule A in the crystal structure of this complex. [b]Experimental bonds and angles involving N5 and N6 have been swapped for this compound, because the crystallographic and computed structures having opposite handedness.

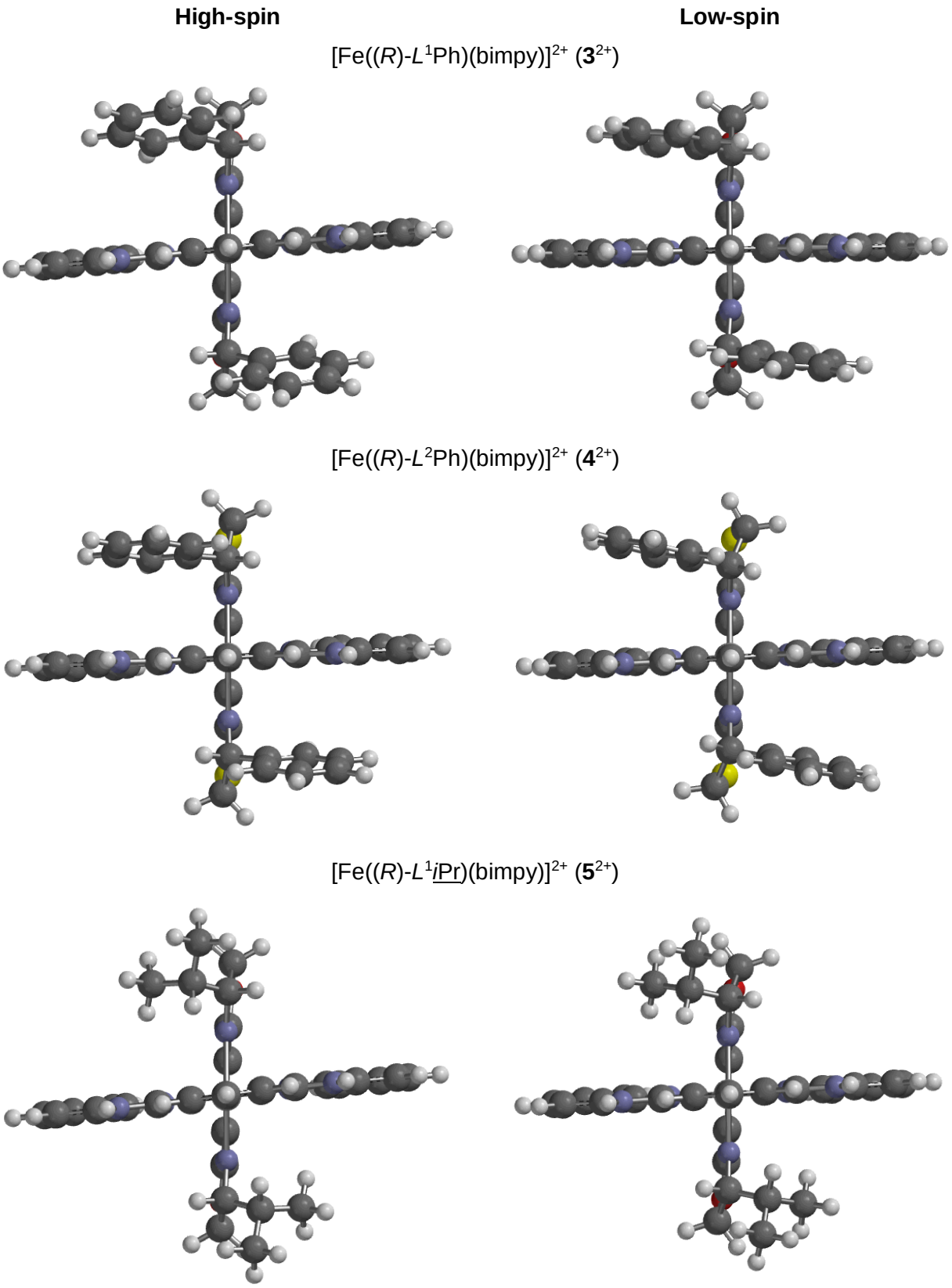
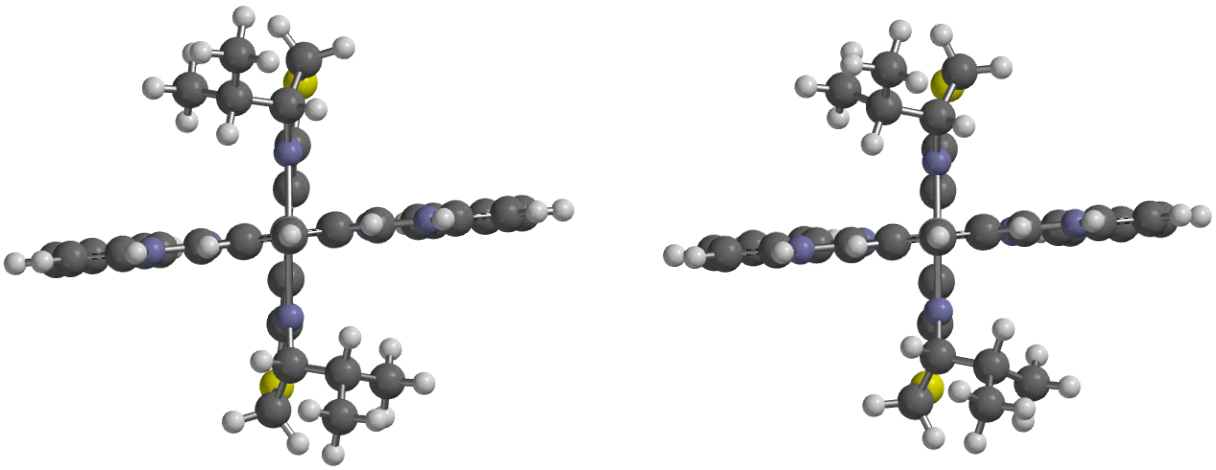


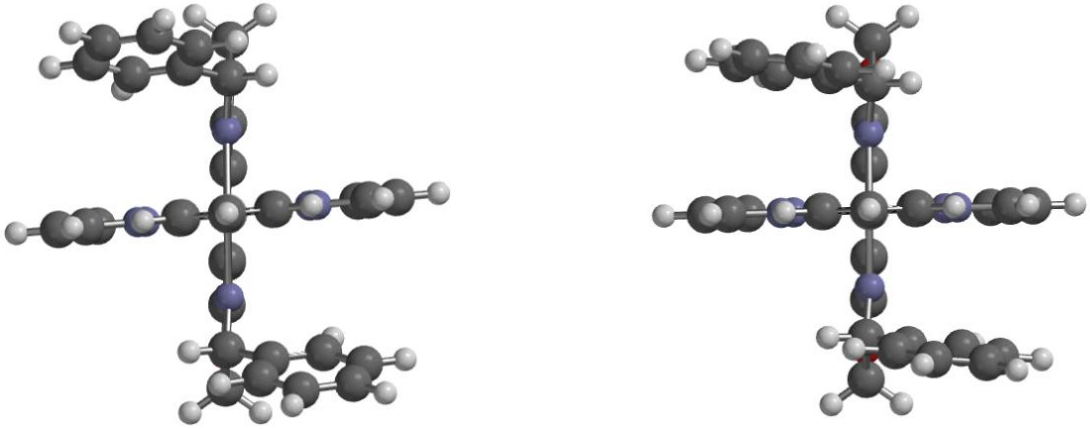
Figure S36 Alternative views of the DFT energy-minimised structures of the heteroleptic $[Fe(LR)L]^{2+}$ (L = bimpy, bpp or terpy) complexes, emphasising the conformations and orientations of the heterocyclic ligands. Other details as for Figure S33.

High-spin **Low-spin**

[Fe((*R*)-*L*^{2}*i*Pr)(bimpy)]$^{2+}$ (**6**$^{2+}$)



[Fe((*R*)-*L*^{1}Ph)(bpp)]$^{2+}$ (**7**$^{2+}$)



[Fe((*R*)-*L*^{2}Ph)(bpp)]$^{2+}$ (**8**$^{2+}$)

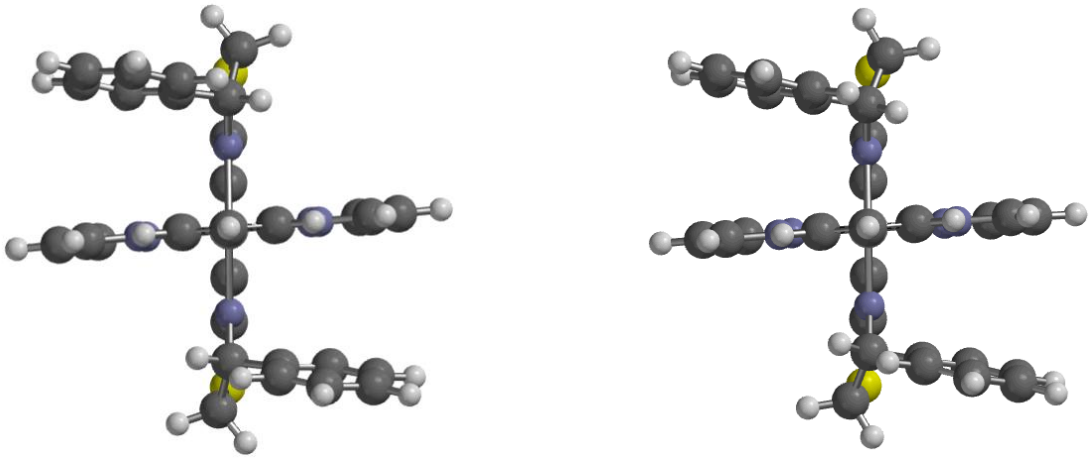
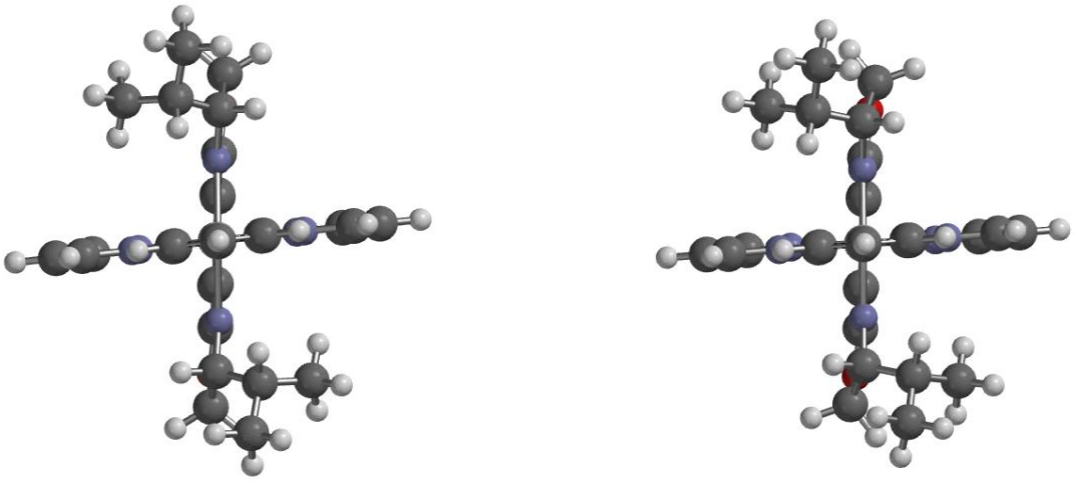


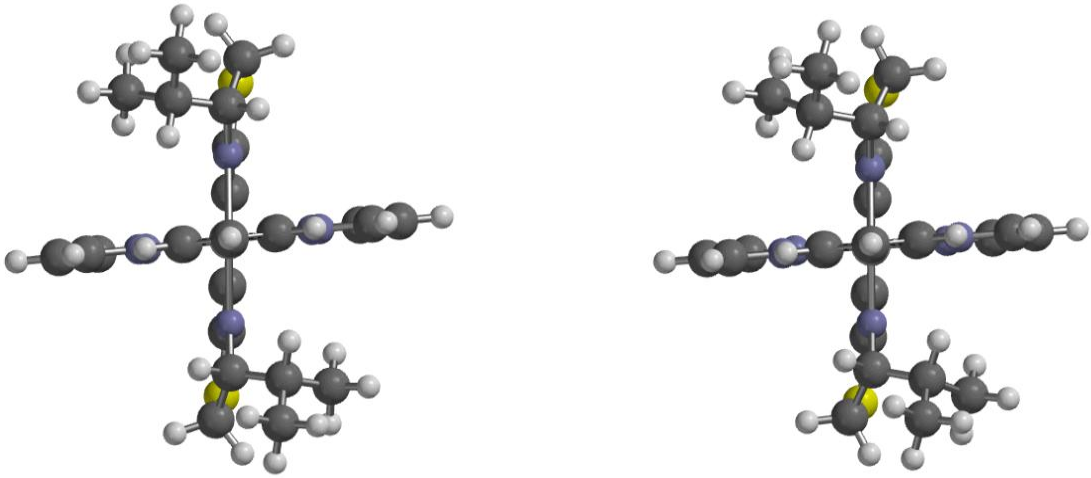
Figure S36 continued.

High-spin **Low-spin**

[Fe((*R*)-*L*^{1}*i*Pr)(bpp)]$^{2+}$ (**9**$^{2+}$)



[Fe((*R*)-*L*^{2}*i*Pr)(bpp)]$^{2+}$ (**10**$^{2+}$)



[Fe((*R*)-*L*^{1}Ph)(terpy)]$^{2+}$ (**11**$^{2+}$)

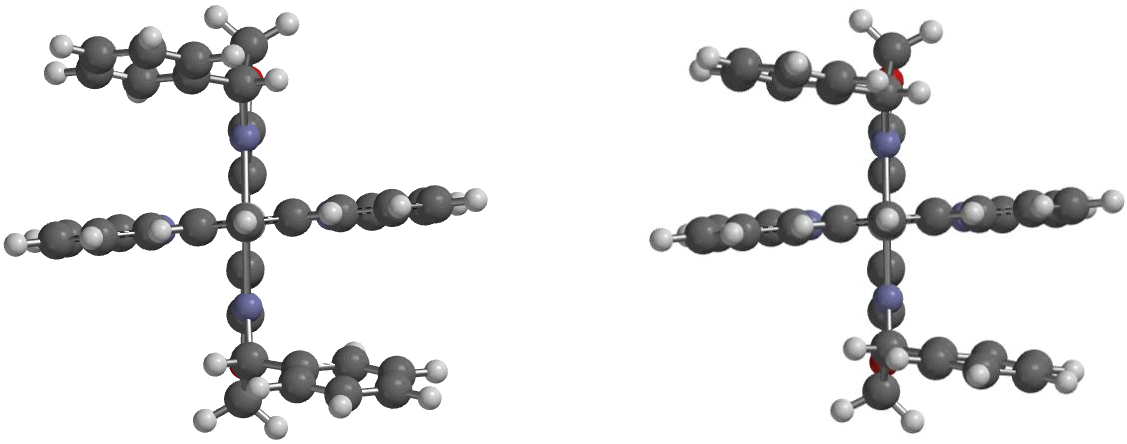
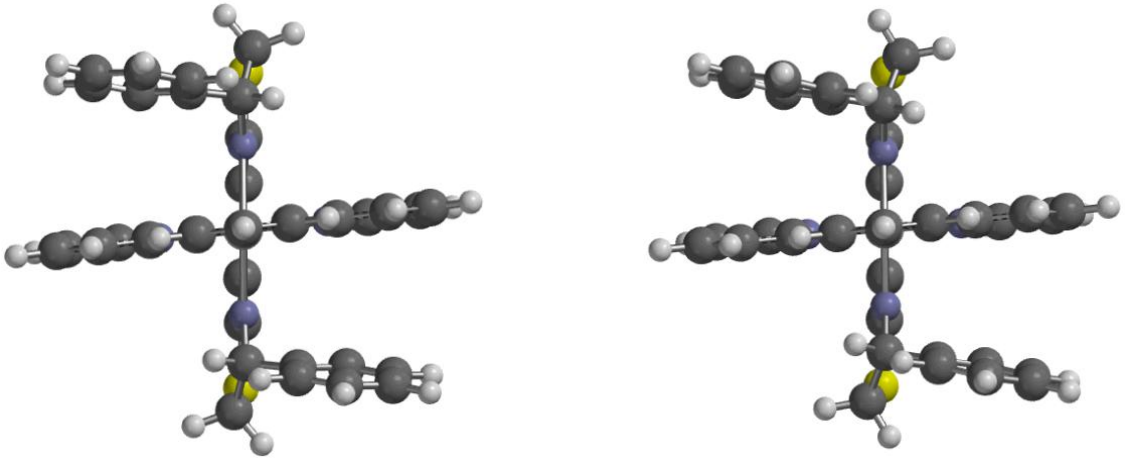


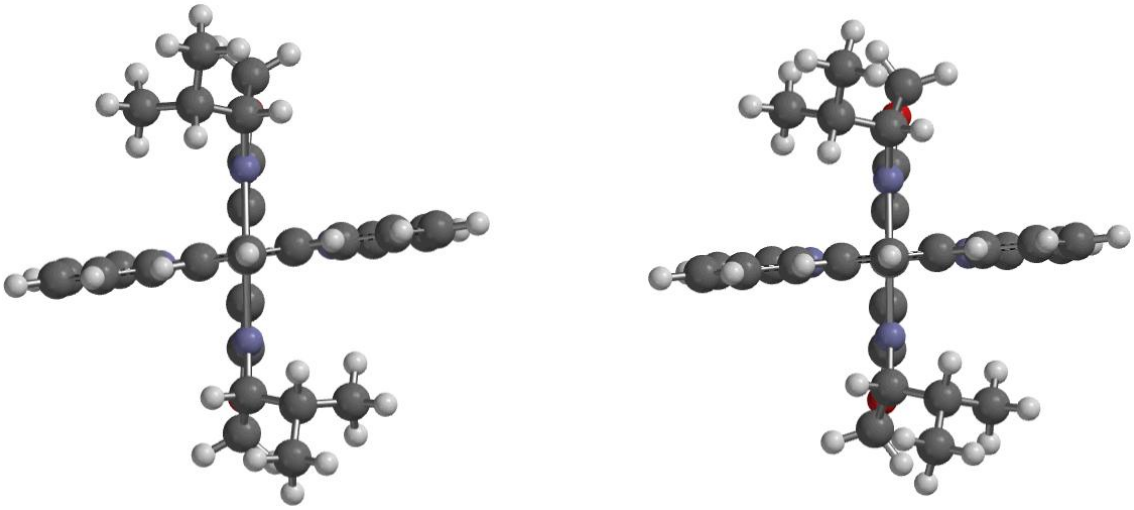
Figure S36 continued.

High-spin **Low-spin**

[Fe((*R*)-*L*^{2}Ph)(terpy)]$^{2+}$



[Fe((*R*)-*L*^{1}*i*Pr)(terpy)]$^{2+}$ (**12**$^{2+}$)



[Fe((*R*)-*L*^{2}*i*Pr)(terpy)]$^{2+}$

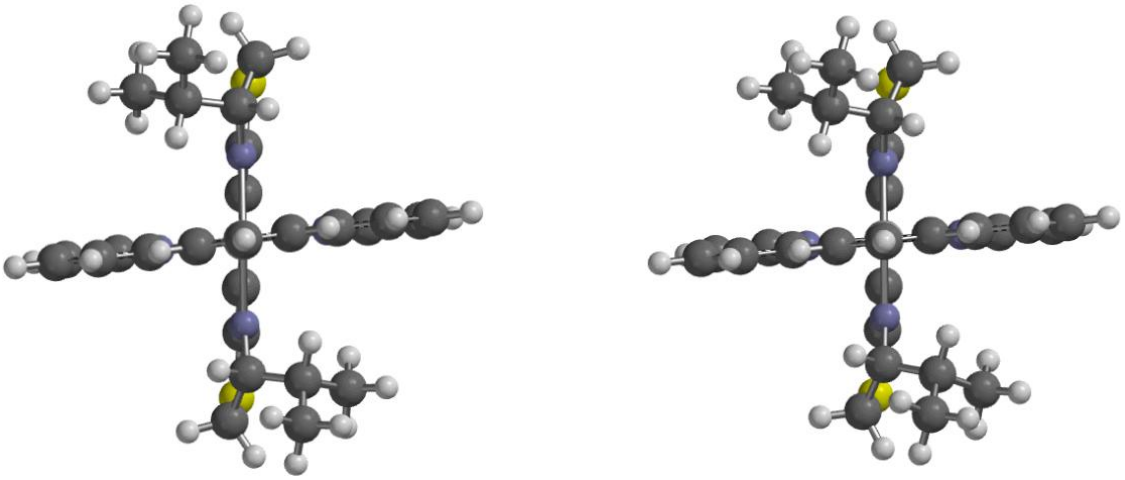


Figure S36 continued.

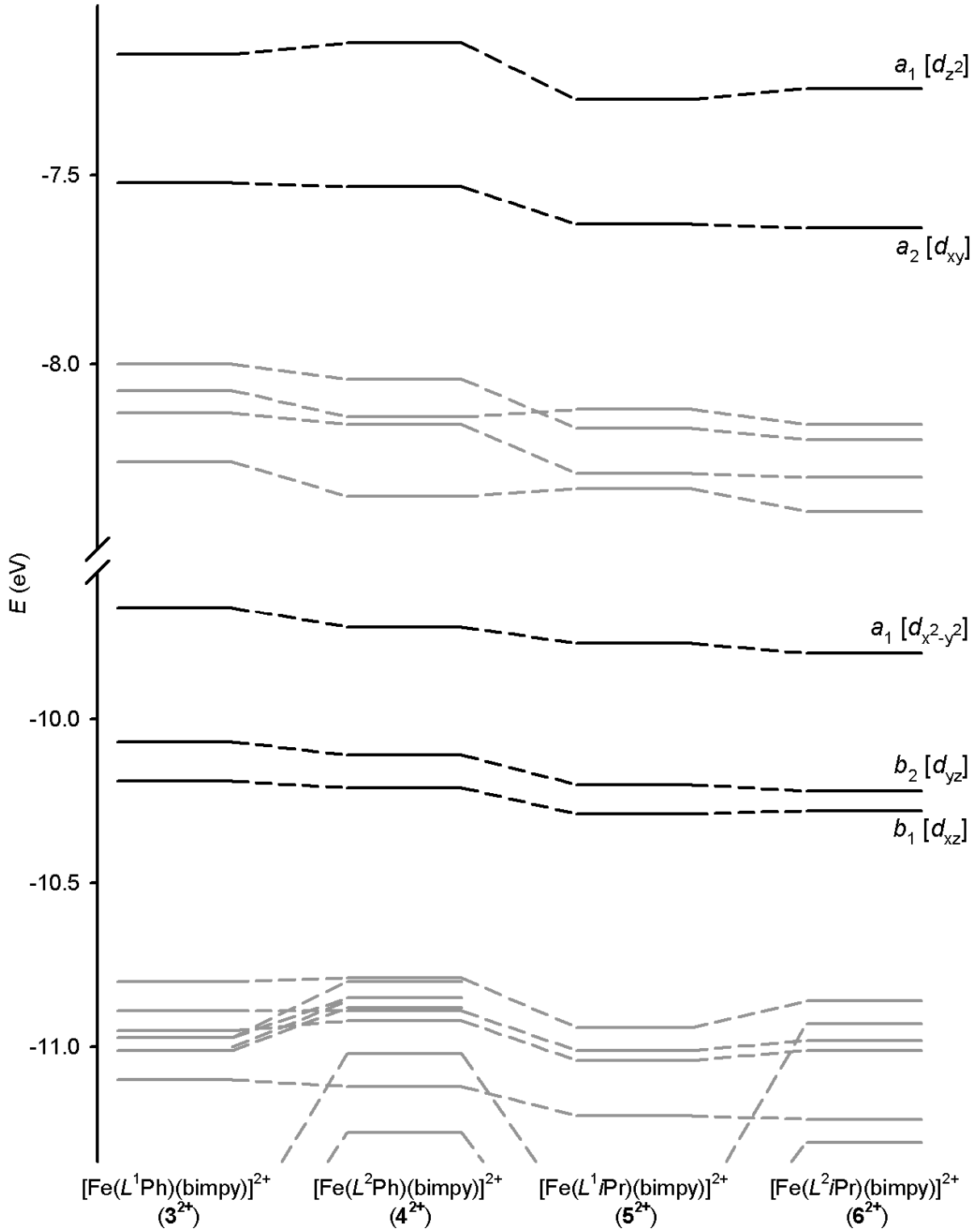


Figure S37 Computed frontier molecular orbital energies of the low-spin [Fe(*L*R)(bimpy)]$^{2+}$ derivatives. The metal-based *d*-orbitals are shown in black, while ligand-centred orbitals are de-emphasised in grey. The *d*-orbitals are given C_{2v} symmetry labels, which is the point group of an idealised [Fe(*L*R)(bimpy)]$^{2+}$ molecule if the 'R' substituents are discounted.

d_{zz} reports on out-of-plane π-bonding to the L^R pyridyl ring.
d_{yz} reports on out-of-plane π-bonding to the bimpy pyridyl ring.
d_{y2-y2} reports on out-of-plane π-bonding to the distal L^R and bimpy azolyl donors.

The four MOs near –11 eV for [Fe(*L*Ph)(bimpy)]$^{2+}$ which do not have counterparts in [Fe(*Li*Pr)(bimpy)]$^{2+}$ are two near-degenerate pairs of π-orbitals on the *L*Ph phenyl substituents.

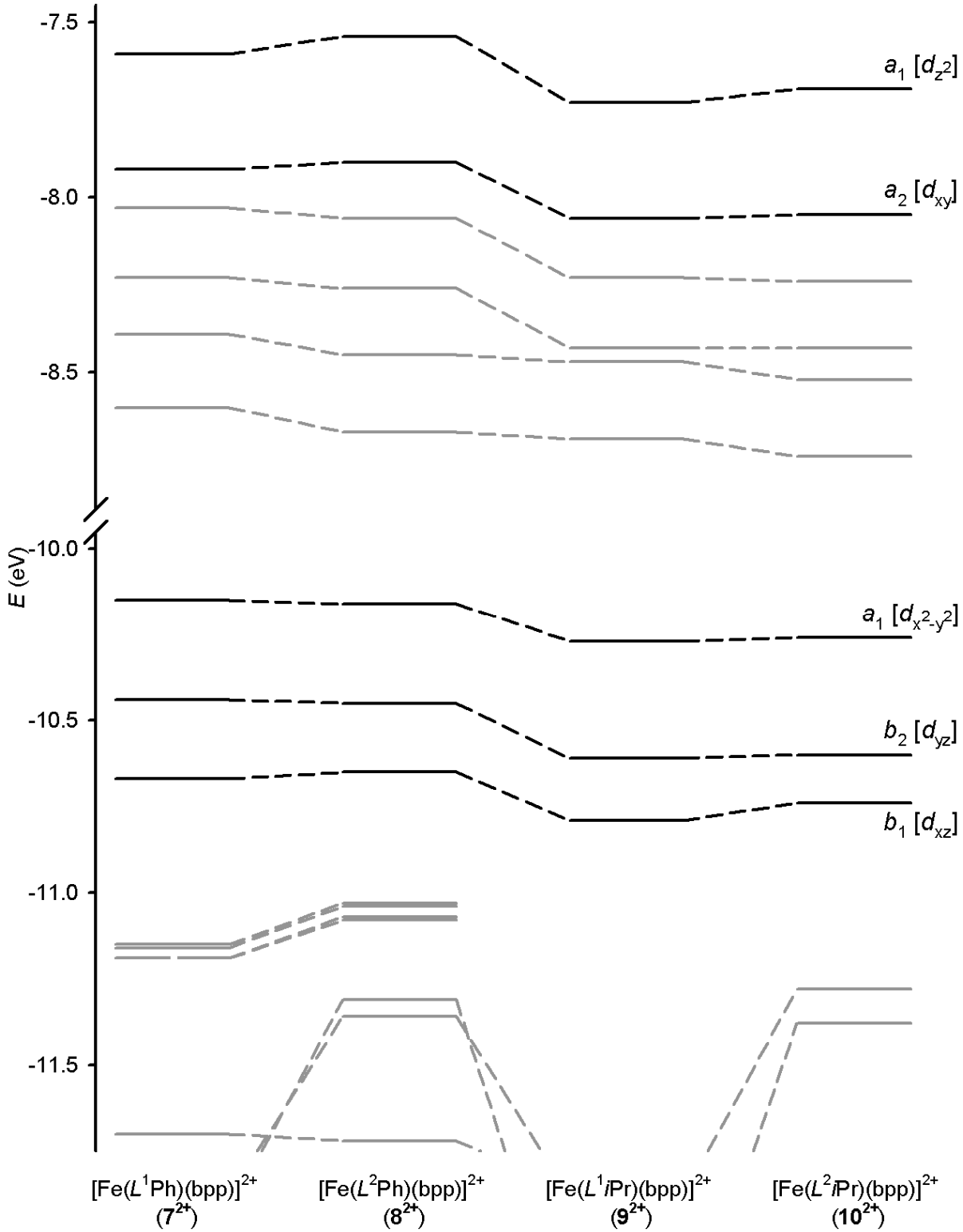


Figure S38 Computed frontier molecular orbital energies of the low-spin [Fe(*L*R)(bpp)]$^{2+}$ derivatives. The energy levels are plotted to the same vertical expansion as Figures S37 and S39, to facilitate comparison. Other details as for Figure S37.

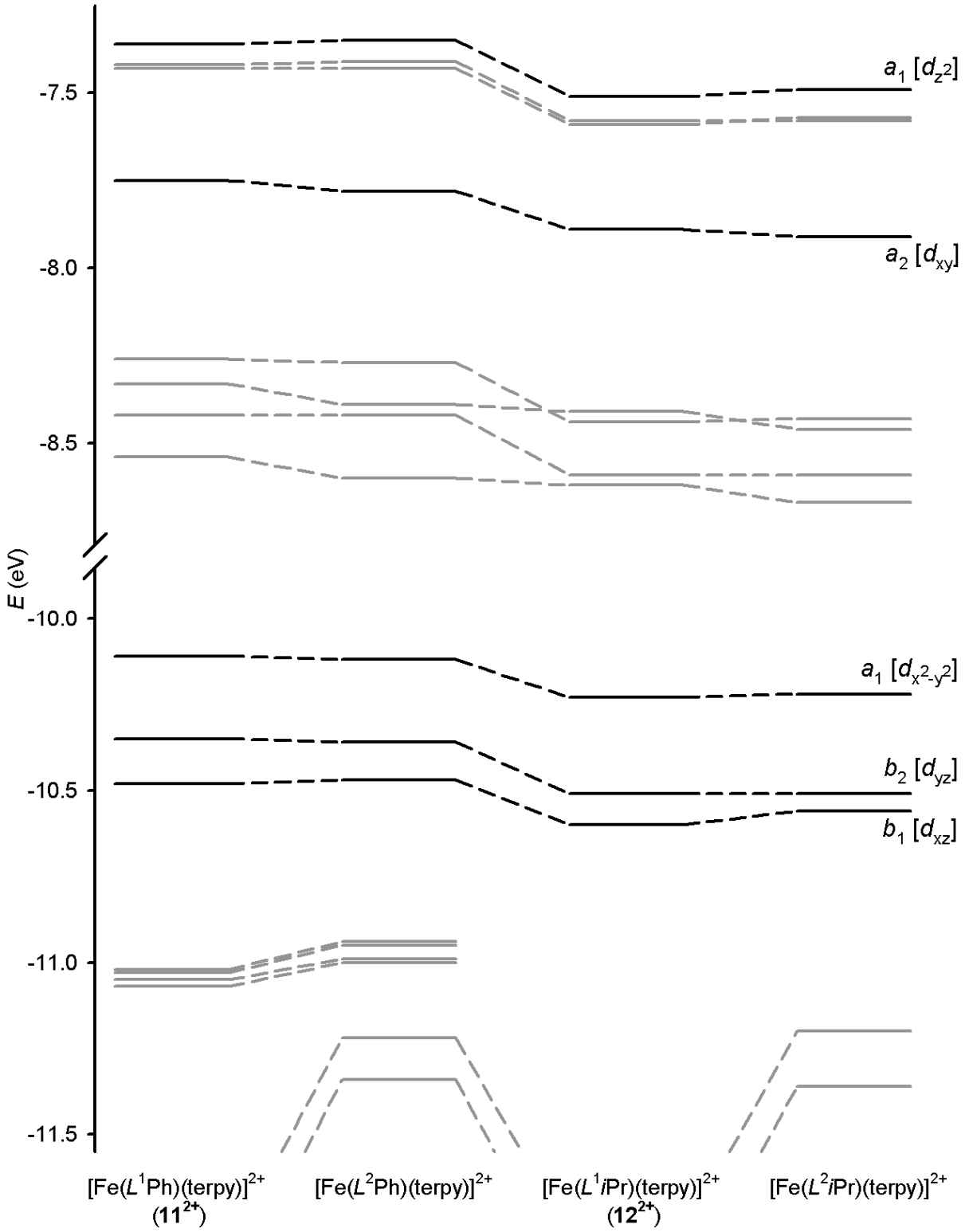


Figure S39 Computed frontier molecular orbital energies of the low-spin [Fe(*L*R)(terpy)]$^{2+}$ derivatives. The energy levels are plotted to the same vertical expansion as Figures S37 and S38, to facilitate comparison. Other details as for Figure S37.

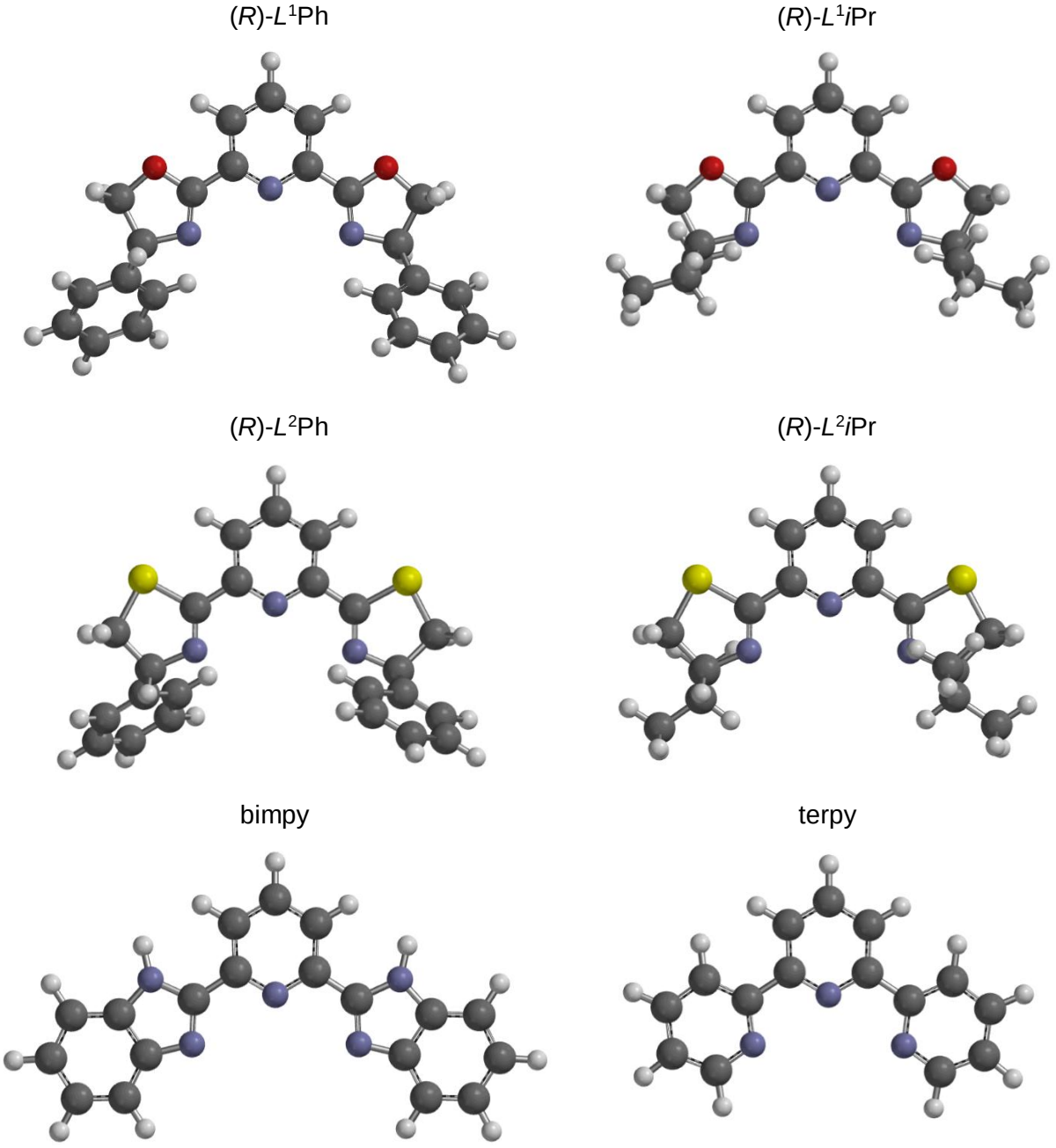


Figure S40 Computed molecular structures for the organic ligands, minimised in the *cisoid* conformation appropriate for metal binding. Colour code: C, dark grey; H, white; N, blue; O, red; S, yellow.

Minimisations of the other ligands in Table S10 by the same protocol are reported in refs. 2 (L^1H and L^2H) and 13 (bpp).

Table S10 Computed energies of the minimised organic ligands, and the energies of their N-donor lone pair combination MOs (Figure S41). The ligands are listed in order of decreasing average energy, E_{av}{lone pair}.

	E / Ha	E{lone pair 1} / eV	E{lone pair 2} / eV	E{lone pair 3} / eV	E_{av}{lone pair} / eV
terpy	–742.197061	–5.11	–5.38	–5.69	–5.40
(*R*)-L^2iPr	–1621.822396	–5.70	–5.89	–6.04	–5.88
L^2H[a]	–1386.035366	–5.74	–5.96	–6.08	–5.93
bimpy	–1005.289103	–5.68	–5.98	–6.14	–5.93
(*R*)-L^1iPr	–975.957011	–5.69	–6.05	–6.16	–5.97
L^1H[a]	–740.165969	–5.71	–6.09	–6.18	–5.99
(*R*)-L^2Ph	–1847.979456	–5.83	–6.01	–6.20	–6.01
(*R*)-L^1Ph	–1202.115052	–5.88	–6.27	–6.36	–6.17
bpp[b]	–698.043540	–5.94	–6.42	–6.82	–6.39

[a]Data from ref 2. [b]Data from ref 13.

Discussion of these data, and the other frontier orbitals in the molecules (Figure S41, next page)

The average E_{av}{lone pair} energy should correlate with the Brønsted basicity of the ligands, with a more positive E_{av} value corresponding to a more strongly σ-donating ligand. In that respect:

- terpy is much more basic than the other ligands in the Table;
- the basicity of bimpy resembles L^1R and L^2R;
- bpp is the least basic ligand.

Each individual L^2R ligand is more basic than its L^1R analogue, by 0.06-0.16 eV, which is consistent with previous work.[2] The *L*H and *Li*Pr ligands within each of those series have similar basicities, but the *L*Ph derivative is less basic.

It is impossible to deconvolute the individual basicities of the different heterocyclic N-donors in more detail from these data, because there is extensive mixing of the N lone pair MOs.

The energies of the π-HOMO and π*-LUMO orbitals for L^2H, bimpy and L^1H mostly mirror each other, with higher energy azolyl π-donor HOMOs being associated with lower energy pyridyl π-acceptor LUMOs, and *vice versa* (Figure S41). That is, the ligands which are better π-donors from their azolyl rings, are also better π-acceptors into their pyridyl rings.

Hence, overall those ligands should have similar π-acidities with respect to metal–ligand bonding. That agrees with our previous computational study of $[Fe(L^1R)_2]^{2+}$ and $[Fe(L^2R)_2]^{2+}$ complexes.[2]

The pyridyl π-HOMO and π*-LUMOs in bpp are all higher energy, implying its pyridyl ring is less π-acidic than the above ligands (Figure S41). Moreover the pyrazolyl π-donor MOs in bpp are lowered in energy by a larger amount, compared to the analogous orbitals in the other azolyl ligands. We conclude bpp should be a worse π-donor and a worse π-acceptor than the other ligands; that is, bpp has a reduced overall metal–ligand π-bonding capability.

Since the π*-LUMO energies for terpy are similar to the other ligands but the corresponding π-donor MOs are much lower energy, terpy is the best π-acceptor ligand in the Table (Figure S41).

Since it contains the strongest σ-donor *and* the best π-acceptor co-ligand, $[Fe(LR)(terpy)]^{2+}$ should be the most strongly low-spin of the complexes in this study, as observed computationally and in preliminary experimental data (Figures S28-S32).

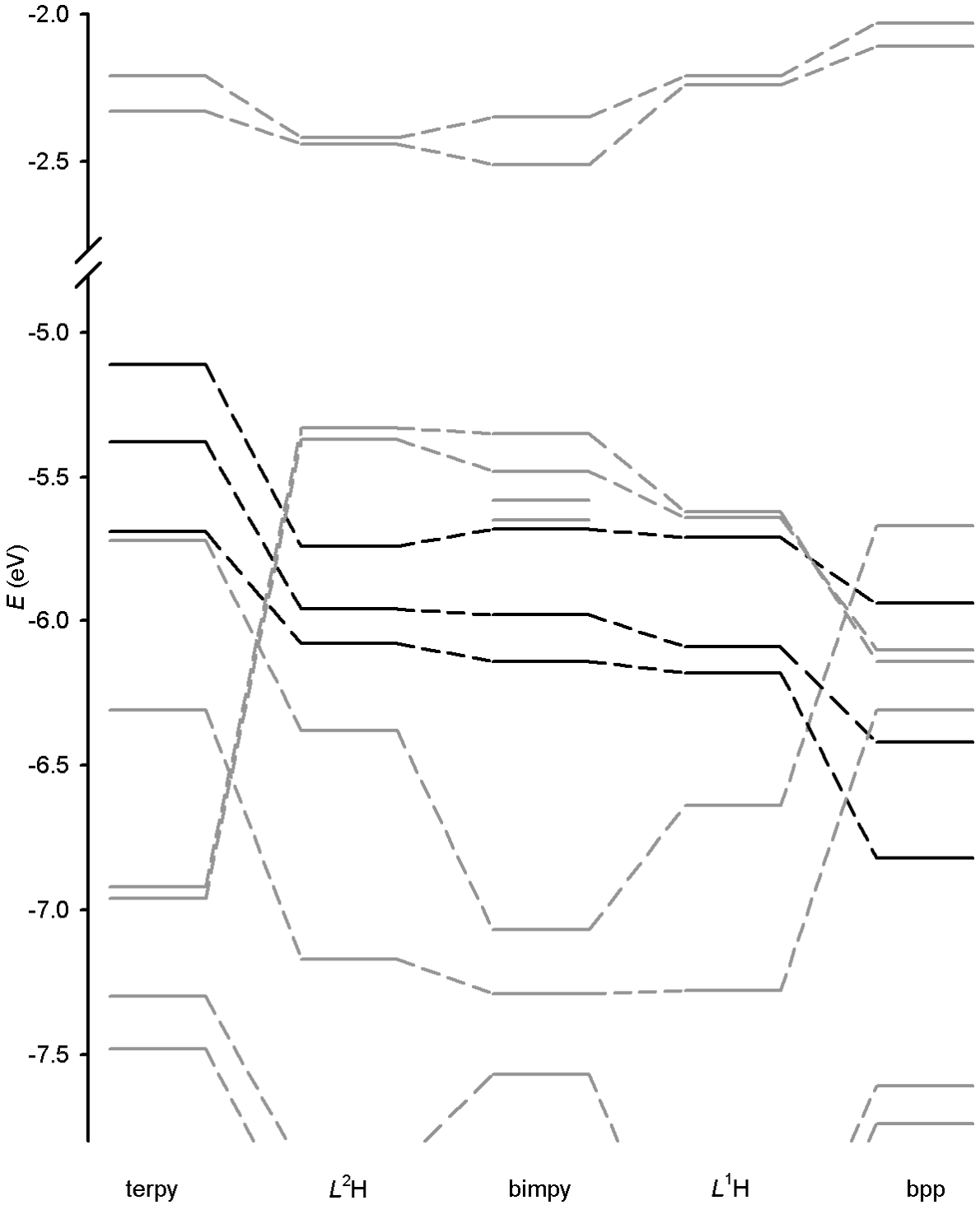


Figure S41 Frontier molecular orbital energies of metal-free ligands from this study. The metal-donor N lone pair MOs are in black, while ligand-centred orbitals are in grey. These data are interpreted on page S65.

The N lone pair MO energies show decreasing Brønsted basicity from left to right in the Figure (Table S10).

The HOMO and HOMO–1 of L^2H, bimpy and L^1H are azole-centred π orbitals, which should contribute to ligand⟶metal π-bonding. These orbitals are the HOMO–2 and HOMO–3 for bpp.

The HOMO for bpp is a pyridyl-centred π-orbital, which is much higher energy in bpp. That implies the pyridyl ring in bpp should be a better π-donor/worse π-acceptor than in the other ligands.

The HOMO–2 and HOMO–3 for bimpy are π orbital combinations centred on the benzimidazolyl benzo groups, which have no counterparts in the other ligands in the Figure.

The LUMO and LUMO+1 are π*-orbitals, which are mostly centered on the central pyridyl ring.

Table S11 Computed energies of the homoleptic complexes, used to calculated $\Delta E\{\text{het}\}$ for the heterochiral molecules (Table 2, main article and Table S12). Their experimental solution-phase SCO mid-point temperatures ($T_{½}$) are also included (HS = high-spin, LS = low-spin).

	$T_{½}$, K	E(HS), Ha	E(LS), Ha	ΔE_{rel}\{HS–LS\}, kcal mol^{-1} [a]	Ref
$[Fe((R)\text{-}L^1Ph)_2]^{2+}$	244	–3667.635387	–3667.660670	–0.1	2
$[Fe((R)\text{-}L^2Ph)_2]^{2+}$	344	–4959.373908	–4959.400465	+0.7	2
$[Fe((R)\text{-}L^1iPr)_2]^{2+}$	HS	–3215.310328	–3215.320134	–9.8	2
$[Fe((R)\text{-}L^2iPr)_2]^{2+}$	277	–4507.045026	–4507.068592	–1.2	2
$[Fe(L^1H)_2]^{2+}$	245	−2743.727948	−2743.753346	0	2
$[Fe(L^2H)_2]^{2+}$	LS	−4035.468705	−4035.503406	+5.8	2
$[Fe(bimpy)_2]^{2+}$	320±15[b]	–3274.011366	–3274.038130	+0.9	this work
$[Fe(bpp)_2]^{2+}$	248[c]	–2659.474752	–2659.500527	+0.2[d]	13
$[Fe(terpy)_2]^{2+}$	LS	–2747.823887	–2747.866679	+10.9	this work

[a]A positive ΔE_{rel}\{HS−LS\} means the low-spin state is more stable than for $[Fe(L^1H)_2]^{2+}$, and *vice versa*. [b]Ref. 23. $T_{½}$ for $[Fe(bimpy)_2]^{2+}$ is solvent-dependent, which may reflect the influence of hydrogen bonding of the solvent to the bimpy N–H groups. [c]Ref. 6. [d]The ΔE_{rel}\{HS–LS\} value for $[Fe(bpp)_2]^{2+}$ in ref. 13 is rescaled relative to $[Fe(L^1H)_2]^{2+}$ in this Table, for consistency with the other compounds in this work.

Note the ligand nomenclature used in ref. 2 is different from this paper.

Table S12 Computed energies of $[Fe(LH)L]^{2+}$ (L = bimpy, bpp or terpy), the unsubstituted analogues of the heteroleptic complexes synthesised in this work.

	E(HS), Ha	E(LS), Ha	ΔE_{rel}\{HS–LS\}, kcal mol^{-1} [a]	ΔE\{het, HS\}, kcal mol^{-1} [b]	ΔE\{het, LS\}, kcal mol^{-1} [b]
$[Fe(L^1H)(bimpy)]^{2+}$	–3008.871965	–3008.897390	0.0	+1.5	+1.0
$[Fe(L^2H)(bimpy)]^{2+}$	–3654.742485	–3654.771662	+2.4	+1.5	+0.6
$[Fe(L^1H)(bpp)]^{2+}$	–2701.602925	–2701.627370	–0.6	+1.0	+0.3
$[Fe(L^2H)(bpp)]^{2+}$	–3347.473716	–3347.501527	+1.5	+1.3	–0.3
$[Fe(L^1H)(terpy)]^{2+}$	–2745.776841	–2745.810779	+5.4	+0.6	+0.5
$[Fe(L^2H)(terpy)]^{2+}$	–3391.647743	–3391.685274	+7.6	+0.9	+0.2

[a]A positive ΔE_{rel}\{HS−LS\} means the low-spin state is more stable than for $[Fe(L^1H)_2]^{2+}$, and *vice versa*. [b]A positive $\Delta E\{\text{het}\}$ means heteroleptic $[Fe(LH)L]^{2+}$ is more stable than an equimolar mixture of homoleptic $[Fe(LH)_2]^{2+}$ and $[FeL_2]^{2+}$ by this protocol.

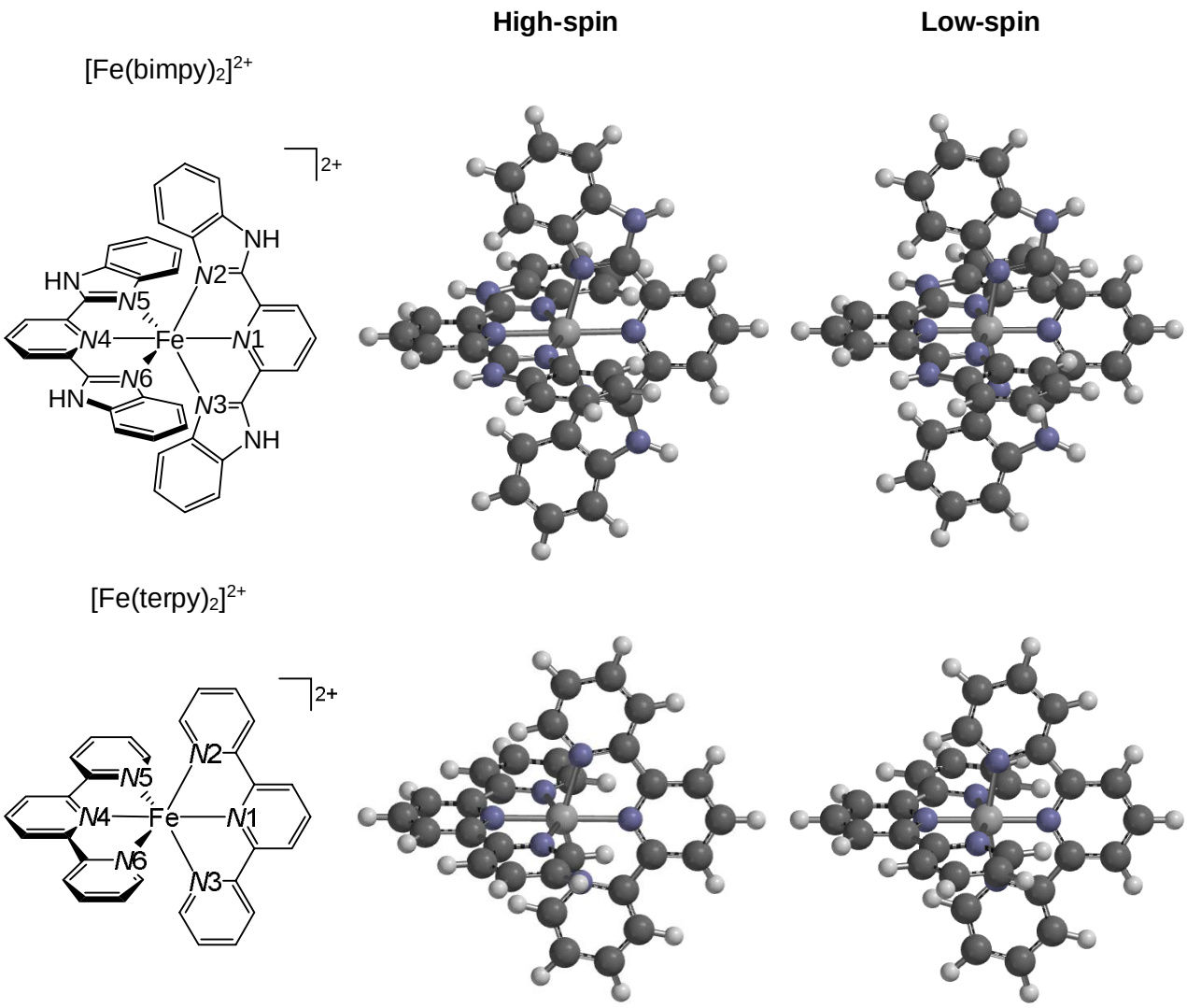


Figure S42 DFT energy-minimised structures of $[Fe(bimpy)_2]^{2+}$ and $[Fe(terpy)_2]^{2+}$ (Table S11), which were produced in this study for the ΔE{het} calculations (Table 2, main article). Other details as for Figure S33.

The minimised structures of the other molecules in Table S11 are reported in refs. 2 and 13.

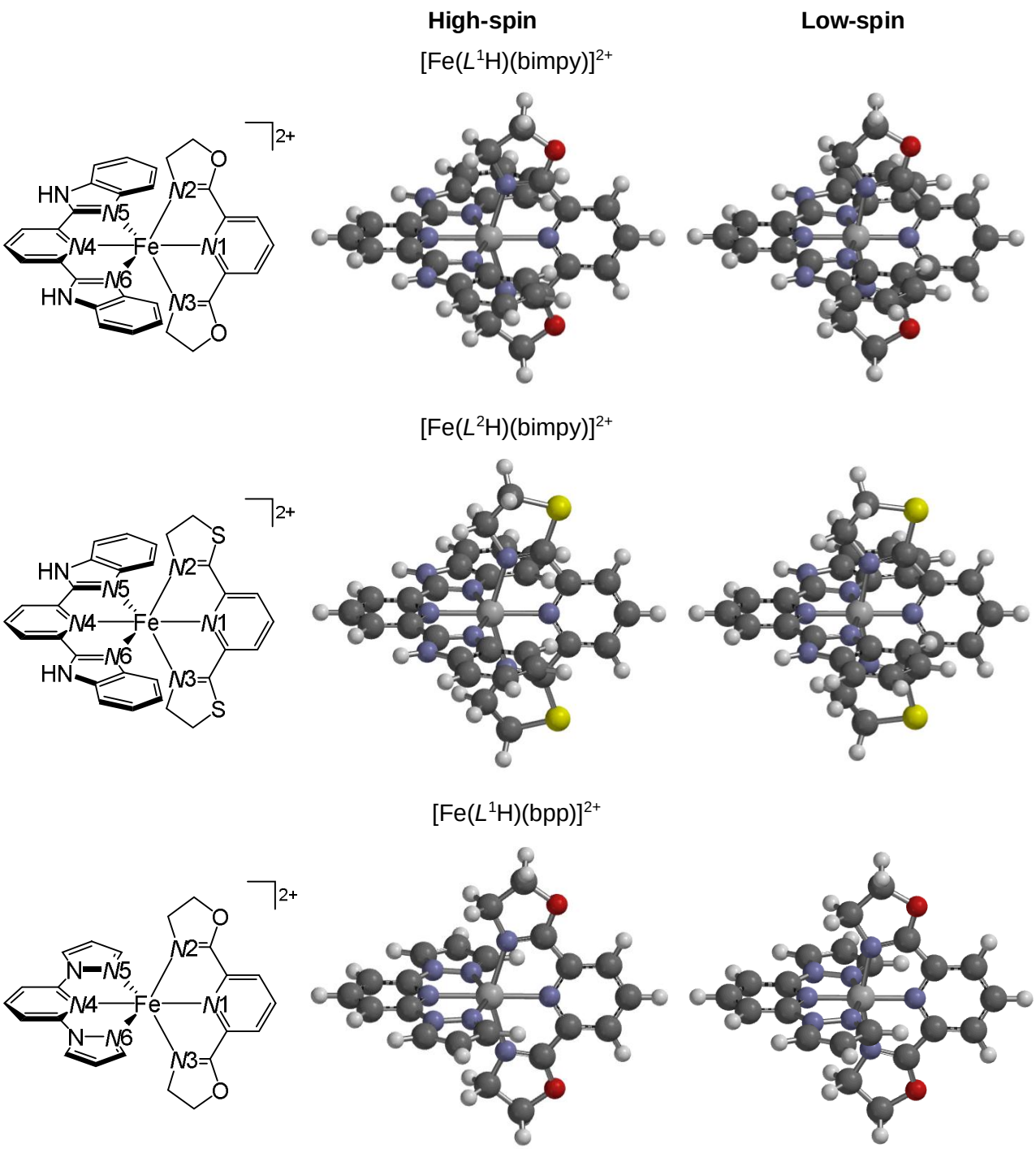


Figure S43 DFT energy-minimised structures of $[Fe(LH)L]^{2+}$ (L = bimpy, bpp or terpy), the unsubstituted analogues of the heteroleptic complexes synthesised in this work (Table S12).

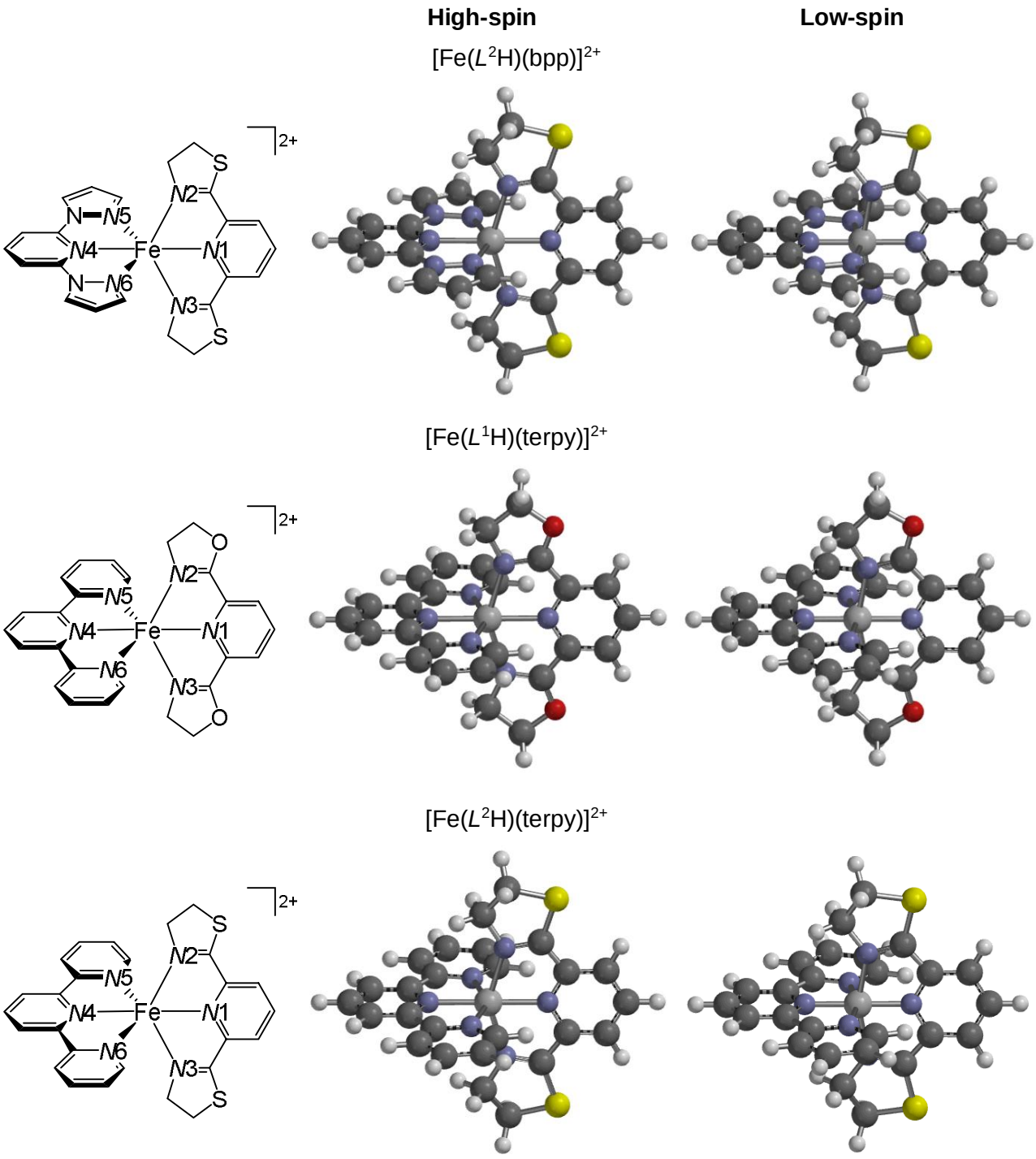


Figure S43 continued.

Table S13 Atomic coordinates for the DFT-minimised molecules in this study.

[Fe((*S*)-*L*^{1}Ph)((*R*)-*L*^{2}Ph)]$^{2+}$ (**1**$^{2+}$), high-spin

1	Fe	0.0440141	-0.0078238	0.0010666
2	N	-2.1173589	-0.1256075	-0.0547602
3	C	-2.7311242	-0.6965912	-1.1124651
4	C	-4.1320321	-0.8053089	-1.1908072
5	C	-4.8947341	-0.3015131	-0.1193241
6	H	-5.9914441	-0.3711197	-0.1444306
7	C	-4.2513197	0.2908249	0.9846544
8	H	-4.8170235	0.6900504	1.8369732
9	C	-2.8458182	0.3595471	0.9715778
10	C	-1.7545408	-1.1482365	-2.1255915
11	N	-0.4744272	-1.0344561	-1.9105958
12	C	0.2215050	-1.6013469	-3.1025434
13	C	-0.9626111	-1.8864734	-4.0854651
14	O	-2.1732549	-1.6638311	-3.2798588
15	C	-1.9846842	0.9305626	2.0285713
16	N	-0.6904568	0.9824461	1.8841633
17	C	-0.1444857	1.6485242	3.1053238
18	C	-1.4086571	1.7721956	4.0213146
19	O	-2.5316888	1.3957227	3.1501968
20	N	2.1580602	0.0584022	0.0333852
21	C	2.8607254	-0.9925525	0.5204712
22	C	4.2682783	-0.9791763	0.5628506
23	H	4.8238428	-1.8460366	0.9469440
24	C	4.9439088	0.1685052	0.1106263
25	H	6.0414033	0.2128234	0.1431391
26	C	4.2060802	1.2597766	-0.3829665
27	C	2.8021478	1.1619830	-0.4185430
28	C	1.9855500	-2.0857008	0.9994301
29	N	0.6893677	-1.9252223	0.9350720
30	C	-0.0730729	-3.0395079	1.5467756
31	C	0.8948736	-4.2585776	1.7146543
32	S	2.6148951	-3.5763699	1.6780852
33	C	1.8716525	2.1903330	-0.9348165
34	N	0.5877850	1.9436665	-0.9065332
35	C	-0.2306942	3.0036106	-1.5415283
36	C	0.6596114	4.2823663	-1.6923961
37	S	2.4202280	3.7198417	-1.5944025
38	H	4.7119430	2.1696016	-0.7354776
39	H	-4.6041973	-1.2716880	-2.0658347
40	H	0.5043747	4.8015737	-2.6553879
41	H	0.5007295	4.9957957	-0.8621815
42	H	-1.0590794	3.2398432	-0.8439828
43	H	-0.8703207	-3.3245330	0.8313014
44	H	0.7443603	-4.7955245	2.6687849
45	H	0.8130241	-4.9746374	0.8754379
46	H	0.8809381	-0.8115362	-3.5135871
47	H	-1.0032973	-1.1751121	-4.9312273
48	H	-0.9951532	-2.9236845	-4.4636399
49	H	-1.4034899	1.0580538	4.8660138
50	H	-1.5987641	2.7952808	4.3918377
51	H	0.5966943	0.9653121	3.5641496
52	C	1.0757928	-2.8176679	-2.7582505
53	C	2.6780397	-5.0934725	-2.2407123
54	C	0.4816454	-4.0430192	-2.3782505
55	C	2.4803552	-2.7473340	-2.8642199
56	C	3.2781632	-3.8773167	-2.6094609
57	C	1.2772385	-5.1730418	-2.1228597
58	H	-0.6141452	-4.1322361	-2.3028484
59	H	2.9546465	-1.8038125	-3.1767227
60	H	4.3704491	-3.8128941	-2.7197989

61	H	0.8014527	-6.1281585	-1.8550456
62	H	3.2980203	-5.9833921	-2.0601021
63	C	-0.7478864	-2.6033915	2.8496060
64	C	-2.0184291	-1.9125623	5.2836361
65	C	0.0137101	-2.1612605	3.9567056
66	C	-2.1500341	-2.6926057	2.9795537
67	C	-2.7835611	-2.3464357	4.1871712
68	C	-0.6179941	-1.8233533	5.1657915
69	H	1.1107579	-2.1057215	3.8882018
70	H	-2.7532054	-3.0606689	2.1346778
71	H	-3.8757673	-2.4365161	4.2785976
72	H	-0.0125982	-1.5076569	6.0284026
73	H	-2.5100609	-1.6627969	6.2351290
74	C	0.5399600	2.9747645	2.7877584
75	C	1.8049922	5.4570468	2.2851105
76	C	1.9189964	3.1407864	3.0316703
77	C	-0.2016912	4.0717591	2.2920948
78	C	0.4258063	5.3047977	2.0454787
79	C	2.5499040	4.3725501	2.7792103
80	H	2.5041374	2.3043104	3.4450602
81	H	-1.2853282	3.9770908	2.1168998
82	H	-0.1678952	6.1585375	1.6860719
83	H	3.6229776	4.4907189	2.9884543
84	H	2.2923585	6.4259851	2.1046090
85	C	-0.8479543	2.5182124	-2.8548229
86	C	-2.0231497	1.7340148	-5.3080662
87	C	-2.2507143	2.4765277	-2.9988726
88	C	-0.0370896	2.1577899	-3.9567496
89	C	-0.6217749	1.7744475	-5.1759304
90	C	-2.8366562	2.0840943	-4.2164106
91	H	-2.8936120	2.7763472	-2.1564405
92	H	1.0598932	2.2033397	-3.8771449
93	H	0.0191320	1.5247403	-6.0344896
94	H	-3.9314456	2.0732904	-4.3198126
95	H	-2.4796990	1.4496885	-6.2673338

[Fe((*S*)-*L*^{1}Ph)((*R*)-*L*^{2}Ph)]$^{2+}$ (**1**$^{2+}$), low-spin

1	Fe	0.0000000	0.0000001	0.0087686
2	N	0.0000000	-0.0000002	1.9253081
3	C	1.1771345	0.0670159	2.6084894
4	C	1.2175920	0.0737081	4.0129441
5	C	0.0000001	-0.0000001	4.7174574
6	H	0.0000002	-0.0000001	5.8162552
7	C	-1.2175919	-0.0737082	4.0129442
8	H	-2.1832890	-0.1285005	4.5327160
9	C	-1.1771344	-0.0670160	2.6084896
10	C	2.2803197	0.0754721	1.6494142
11	N	1.9836825	0.0606052	0.3710306
12	C	3.2747427	0.0195209	-0.3859198
13	C	4.3201576	-0.1577407	0.7678870
14	O	3.5581619	0.0430996	2.0100833
15	C	-2.2803197	-0.0754721	1.6494143
16	N	-1.9836825	-0.0606051	0.3710306
17	C	-3.2747427	-0.0195211	-0.3859198
18	C	-4.3201574	0.1577410	0.7678871
19	O	-3.5581618	-0.0430996	2.0100833
20	N	0.0000003	0.0000003	-1.8880074
21	C	-0.0288937	1.1854079	-2.5638653
22	C	-0.0305571	1.2181383	-3.9702197
23	H	-0.0501121	2.1795523	-4.5012539
24	C	0.0000010	0.0000007	-4.6740602
25	H	0.0000014	0.0000010	-5.7727407

26	C	0.0305587	-1.2181370	-3.9702200
27	C	0.0288946	-1.1854072	-2.5638656
28	C	-0.0125056	2.2998359	-1.6146576
29	N	-0.0285577	1.9742826	-0.3364264
30	C	-0.0164658	3.1564813	0.5686238
31	C	0.4707200	4.3776224	-0.2739511
32	S	0.0850626	3.9932489	-2.0448003
33	C	0.0125060	-2.2998354	-1.6146582
34	N	0.0285576	-1.9742824	-0.3364269
35	C	0.0164654	-3.1564812	0.5686231
36	C	-0.4707203	-4.3776221	-0.2739523
37	S	-0.0850621	-3.9932483	-2.0448012
38	H	2.1832891	0.1285005	4.5327159
39	H	0.0501143	-2.1795509	-4.5012545
40	H	-0.0397648	5.3151881	0.0101759
41	H	1.5656878	4.5206721	-0.2096909
42	H	0.0397641	-5.3151880	0.0101749
43	H	-1.5656881	-4.5206714	-0.2096928
44	H	-4.7420545	1.1789160	0.8125743
45	H	-5.1377772	-0.5844500	0.7503980
46	H	4.7420549	-1.1789156	0.8125744
47	H	5.1377770	0.5844506	0.7503980
48	H	-3.2649831	0.8845791	-1.0254491
49	H	3.2649833	-0.8845795	-1.0254488
50	H	-0.7350973	-2.9559349	1.3576304
51	H	0.7350968	2.9559348	1.3576312
52	C	3.5206876	1.2351563	-1.2738400
53	C	4.1720217	3.4359925	-2.9317834
54	C	3.7854103	2.5059644	-0.7123193
55	C	3.5825452	1.0860346	-2.6747014
56	C	3.9046591	2.1789910	-3.5000757
57	C	4.1120079	3.5972722	-1.5347565
58	H	3.7688845	2.6438687	0.3807739
59	H	3.4041325	0.0978546	-3.1270284
60	H	3.9691143	2.0420568	-4.5893122
61	H	4.3419771	4.5740190	-1.0840144
62	H	4.4438608	4.2862920	-3.5735118
63	C	-1.3612605	3.4102409	1.2520544
64	C	-3.7898172	4.0820666	2.5436044
65	C	-2.5402399	3.6202487	0.4995626
66	C	-1.4171688	3.5423843	2.6564200
67	C	-2.6229598	3.8774148	3.2991430
68	C	-3.7446447	3.9554094	1.1420447
69	H	-2.5137967	3.5610843	-0.5990162
70	H	-0.5031460	3.4015817	3.2549932
71	H	-2.6472456	3.9917867	4.3925606
72	H	-4.6490941	4.1417968	0.5440614
73	H	-4.7299466	4.3572832	3.0429173
74	C	-3.5206877	-1.2351568	-1.2738395
75	C	-4.1720220	-3.4359937	-2.9317821
76	C	-3.5825450	-1.0860358	-2.6747010
77	C	-3.7854107	-2.5059646	-0.7123183
78	C	-4.1120084	-3.5972727	-1.5347552
79	C	-3.9046590	-2.1789925	-3.5000748
80	H	-3.4041318	-0.0978559	-3.1270283
81	H	-3.7688848	-2.6438685	0.3807750
82	H	-4.3419781	-4.5740192	-1.0840125
83	H	-3.9691139	-2.0420589	-4.5893114
84	H	-4.4438613	-4.2862933	-3.5735102
85	C	1.3612601	-3.4102409	1.2520539
86	C	3.7898165	-4.0820664	2.5436042
87	C	1.4171682	-3.5423842	2.6564195

88	C	2.5402396	-3.6202486	0.4995621
89	C	3.7446443	-3.9554092	1.1420445
90	C	2.6229591	-3.8774146	3.2991426
91	H	0.5031452	-3.4015817	3.2549925
92	H	2.5137966	-3.5610843	-0.5990166
93	H	4.6490938	-4.1417965	0.5440613
94	H	2.6472447	-3.9917866	4.3925603
95	H	4.7299459	-4.3572830	3.0429172

[Fe((*S*)-*L*^{1}*i*Pr)((*R*)-*L*^{2}*i*Pr)]$^{2+}$ (**2**$^{2+}$), high-spin

1	Fe	0.0018485	0.0017959	-0.0721019
2	N	0.0261911	0.0001178	2.0690386
3	C	1.2034745	0.0162596	2.7358361
4	C	1.2664842	0.0093276	4.1414143
5	C	0.0558816	0.0014940	4.8606304
6	H	0.0675058	0.0022923	5.9596258
7	C	-1.1697276	-0.0078146	4.1672920
8	H	-2.1310381	-0.0143432	4.6985681
9	C	-1.1367592	-0.0163873	2.7607931
10	C	2.3530344	0.0396081	1.8088184
11	N	2.1716908	0.1139390	0.5186793
12	C	3.5213785	0.1531991	-0.1076106
13	C	4.4725617	-0.1212064	1.1008530
14	O	3.5947179	-0.0374401	2.2806440
15	C	-2.3058978	-0.0435242	1.8587414
16	N	-2.1515448	-0.1187819	0.5652279
17	C	-3.5133879	-0.1606490	-0.0335964
18	C	-4.4411083	0.1055055	1.1950548
19	O	-3.5376558	0.0297681	2.3562326
20	N	-0.0221353	0.0098197	-2.2037383
21	C	-0.0782606	1.1856459	-2.8720994
22	C	-0.0950702	1.2308179	-4.2797251
23	H	-0.1444512	2.1922829	-4.8098045
24	C	-0.0502093	0.0187399	-4.9908294
25	H	-0.0612346	0.0222792	-6.0897992
26	C	0.0086183	-1.1978327	-4.2885889
27	C	0.0203116	-1.1616840	-2.8806648
28	C	-0.0950644	2.3640542	-1.9707670
29	N	-0.1802202	2.1816835	-0.6801885
30	C	-0.2112082	3.4447531	0.0915818
31	C	0.2137294	4.6188005	-0.8504610
32	S	0.0631559	3.9986938	-2.5860314
33	C	0.0534914	-2.3460607	-1.9877320
34	N	0.1624864	-2.1725723	-0.6977526
35	C	0.2005319	-3.4404594	0.0656789
36	C	-0.2410939	-4.6076690	-0.8773254
37	S	-0.1207511	-3.9760896	-2.6110663
38	H	2.2391598	0.0156581	4.6515004
39	H	0.0465773	-2.1559493	-4.8256163
40	H	-0.4282465	5.5125739	-0.7458806
41	H	1.2656586	4.9251803	-0.6987655
42	H	0.4025347	-5.5021374	-0.7895891
43	H	-1.2901742	-4.9152583	-0.7090155
44	H	-4.8960733	1.1146154	1.2048881
45	H	-5.2334921	-0.6497210	1.3430254
46	H	4.9185044	-1.1344598	1.1010713
47	H	5.2751874	0.6262989	1.2321177
48	H	-3.5901258	0.6715734	-0.7628214
49	H	-0.5496431	-3.3468699	0.8785169
50	C	3.7881618	1.4797904	-0.8760965
51	H	2.9203577	1.5938906	-1.5612026
52	C	5.0596052	1.3552270	-1.7360894

53	H	5.9651545	1.2109691	-1.1116288
54	H	5.2218879	2.2761747	-2.3285478
55	H	4.9991951	0.5053098	-2.4446318
56	C	3.8399621	2.7203038	0.0335886
57	H	4.7542905	2.7423948	0.6601167
58	H	2.9657298	2.7878249	0.7118230
59	H	3.8621322	3.6429342	-0.5788235
60	C	-1.5854837	3.6537814	0.8039017
61	H	-1.7632681	2.7068552	1.3576411
62	C	-2.7623182	3.8649447	-0.1648501
63	H	-2.8447556	3.0538866	-0.9152438
64	H	-2.6856188	4.8244682	-0.7143866
65	H	-3.7167738	3.9013972	0.3965717
66	C	-1.4900641	4.7839397	1.8466486
67	H	-0.6814453	4.5999947	2.5818166
68	H	-2.4404211	4.8725030	2.4074460
69	H	-1.3020831	5.7715168	1.3790458
70	C	1.5830345	-3.6598366	0.7585536
71	H	1.7727710	-2.7174693	1.3160139
72	C	2.7457023	-3.8706104	-0.2271339
73	H	3.7074026	-3.9175924	0.3210220
74	H	2.8233019	-3.0541509	-0.9722764
75	H	2.6553226	-4.8252555	-0.7830956
76	C	1.4958258	-4.7960996	1.7953682
77	H	2.4537522	-4.8938869	2.3415252
78	H	1.2950365	-5.7795115	1.3243268
79	H	0.6991724	-4.6120223	2.5434754
80	C	-3.7897290	-1.4852107	-0.8022643
81	H	-2.9297302	-1.5971175	-1.4975677
82	C	-5.0714503	-1.3597370	-1.6466784
83	H	-5.2391599	-2.2789726	-2.2403217
84	H	-5.0213360	-0.5073087	-2.3530468
85	H	-5.9696897	-1.2194600	-1.0108076
86	C	-3.8303266	-2.7281107	0.1047081
87	H	-2.9530646	-2.7918913	0.7793799
88	H	-3.8499548	-3.6495483	-0.5095592
89	H	-4.7419451	-2.7571139	0.7348602
90	H	0.5502288	3.3492945	0.8936869
91	H	3.5804489	-0.6763620	-0.8415267

[Fe((*S*)-*L*^{1}*i*Pr)((*R*)-*L*^{2}*i*Pr)]$^{2+}$ (**2**$^{2+}$), low-spin

1	Fe	0.0014106	-0.0001668	-0.0718399
2	N	0.0199835	-0.0040503	1.8446915
3	C	1.2023107	0.0893854	2.5173617
4	C	1.2565588	0.0882385	3.9217344
5	C	0.0471347	-0.0055460	4.6381167
6	H	0.0577661	-0.0059910	5.7368761
7	C	-1.1759565	-0.0989739	3.9452058
8	H	-2.1349911	-0.1707092	4.4756860
9	C	-1.1490689	-0.0986435	2.5401351
10	C	2.2948325	0.1345790	1.5453727
11	N	1.9868515	0.1627522	0.2694874
12	C	3.2709835	0.1726034	-0.4925571
13	C	4.3137858	-0.1332338	0.6268559
14	O	3.5770608	0.0744924	1.8876957
15	C	-2.2604058	-0.1419523	1.5897331
16	N	-1.9767782	-0.1660773	0.3081593
17	C	-3.2749636	-0.1727890	-0.4293970
18	C	-4.2963919	0.1292104	0.7106944
19	O	-3.5359917	-0.0828128	1.9565902
20	N	-0.0213705	0.0046398	-1.9697237
21	C	-0.0829442	1.1900455	-2.6439500

22	C	-0.0992283	1.2268645	-4.0505721
23	H	-0.1441307	2.1889861	-4.5795049
24	C	-0.0587946	0.0117237	-4.7592296
25	H	-0.0737371	0.0144891	-5.8578198
26	C	0.0004077	-1.2069763	-4.0580496
27	C	0.0223041	-1.1773629	-2.6513652
28	C	-0.0929419	2.3047994	-1.6932764
29	N	-0.1282526	1.9873987	-0.4136631
30	C	-0.1479661	3.1748007	0.4831227
31	C	0.3148098	4.4066313	-0.3508733
32	S	0.0316760	3.9922783	-2.1346532
33	C	0.0558842	-2.2969599	-1.7068090
34	N	0.1223375	-1.9859741	-0.4268699
35	C	0.1589614	-3.1771689	0.4639893
36	C	-0.3222256	-4.4051966	-0.3652229
37	S	-0.0806929	-3.9822602	-2.1532851
38	H	2.2258129	0.1594405	4.4333355
39	H	0.0302676	-2.1664008	-4.5929335
40	H	-0.2575456	5.3210849	-0.1130687
41	H	1.3909246	4.6279309	-0.2281899
42	H	0.2563643	-5.3203699	-0.1460336
43	H	-1.3951188	-4.6276404	-0.2188188
44	H	-4.6497867	1.1780322	0.7244194
45	H	-5.1663644	-0.5494514	0.7340324
46	H	4.6674213	-1.1820523	0.6304326
47	H	5.1843695	0.5450590	0.6366288
48	H	-3.2535993	0.6608777	-1.1600040
49	H	-0.5750269	-2.9871975	1.2739526
50	C	3.5310595	1.4925336	-1.2768660
51	H	2.6121950	1.6737611	-1.8736043
52	C	4.6977711	1.2949356	-2.2641744
53	H	5.6498428	1.0723443	-1.7400689
54	H	4.8653782	2.2134006	-2.8588967
55	H	4.5020208	0.4665349	-2.9736074
56	C	3.7597211	2.7155627	-0.3707570
57	H	4.7312829	2.6670286	0.1602113
58	H	2.9661130	2.8323209	0.3932993
59	H	3.7832170	3.6398105	-0.9799520
60	C	-1.5230730	3.3840540	1.1965005
61	H	-1.7672914	2.4094470	1.6644120
62	C	-2.6755568	3.7522859	0.2450437
63	H	-2.8095013	3.0096029	-0.5656494
64	H	-2.5274722	4.7422566	-0.2300008
65	H	-3.6273759	3.8122030	0.8086017
66	C	-1.3792493	4.4084396	2.3397035
67	H	-0.5845046	4.1223956	3.0578019
68	H	-2.3275731	4.4897695	2.9048916
69	H	-1.1440723	5.4244915	1.9636218
70	C	1.5469781	-3.3907050	1.1504567
71	H	1.8004580	-2.4179023	1.6171250
72	C	2.6805803	-3.7558574	0.1753992
73	H	3.6429697	-3.8212430	0.7201194
74	H	2.8004741	-3.0085904	-0.6332291
75	H	2.5208559	-4.7425500	-0.3025358
76	C	1.4237584	-4.4191679	2.2923300
77	H	2.3832399	-4.5048016	2.8376537
78	H	1.1783446	-5.4331027	1.9171908
79	H	0.6445928	-4.1336889	3.0274301
80	C	-3.5503165	-1.4902453	-1.2129679
81	H	-2.6396244	-1.6737761	-1.8212307
82	C	-4.7287555	-1.2856708	-2.1846676
83	H	-4.9125315	-2.2042272	-2.7744090

84	H	-4.5356921	-0.4607002	-2.8988094
85	H	-5.6710036	-1.0532035	-1.6473301
86	C	-3.7730960	-2.7146613	-0.3068846
87	H	-2.9754923	-2.8335176	0.4527904
88	H	-3.8004902	-3.6380125	-0.9173158
89	H	-4.7416346	-2.6668801	0.2296483
90	H	0.6020040	2.9832806	1.2778361
91	H	3.2355037	-0.6583415	-1.2257091

$[Fe((R)\text{-}L^1Ph)(bimpy)]^{2+}$ ($\mathbf{3}^{2+}$), high-spin

1	Fe	0.0005098	-0.0004836	-0.3908866
2	N	0.0110065	0.0039114	1.7910219
3	C	-1.1615046	-0.0767542	2.4624197
4	C	-1.1951435	-0.0762657	3.8730548
5	C	0.0230129	0.0161292	4.5675327
6	H	0.0277367	0.0212150	5.6666299
7	C	1.2350943	0.1021097	3.8617819
8	H	2.1857187	0.1756869	4.4069806
9	C	1.1892501	0.0900712	2.4514872
10	C	-2.3122803	-0.1538477	1.5550695
11	N	-2.1341138	-0.1405711	0.2230816
12	C	-3.4004807	-0.2057487	-0.3393386
13	C	-4.3742594	-0.2649369	0.7075473
14	N	-3.6395832	-0.2318443	1.8869087
15	C	2.3321039	0.1597636	1.5336616
16	N	2.1425061	0.1397454	0.2033175
17	C	3.4043058	0.1988160	-0.3701019
18	C	4.3870827	0.2611080	0.6682304
19	N	3.6623772	0.2364205	1.8538977
20	N	-0.0080937	0.0022323	-2.5186677
21	C	-0.0842259	-1.1659485	-3.2043936
22	C	-0.0976403	-1.2106619	-4.6099377
23	H	-0.1642765	-2.1754925	-5.1306487
24	C	-0.0197803	0.0052033	-5.3165004
25	H	-0.0242865	0.0063642	-6.4153497
26	C	0.0636229	1.2195792	-4.6080271
27	C	0.0618719	1.1719039	-3.2025011
28	C	-0.1404689	-2.3197399	-2.2902050
29	N	-0.0675958	-2.1410518	-0.9988974
30	C	-0.1601308	-3.4804841	-0.3584466
31	C	-0.2615451	-4.4471556	-1.5912513
32	O	-0.2750280	-3.5575174	-2.7622579
33	C	0.1245265	2.3238088	-2.2863002
34	N	0.0616938	2.1423301	-0.9948684
35	C	0.1547482	3.4806063	-0.3523129
36	C	0.2529840	4.4496173	-1.5837115
37	O	0.2536361	3.5626906	-2.7568057
38	H	-2.1409399	-0.1444451	4.4272988
39	H	0.1255167	2.1855571	-5.1271835
40	H	0.6122573	-5.1178189	-1.6941965
41	H	-1.1908231	-5.0450737	-1.6175260
42	H	-0.6175795	5.1254638	-1.6792346
43	H	1.1855520	5.0422558	-1.6149728
44	H	1.0970931	3.5092895	0.2335846
45	H	-1.1015032	-3.5092654	0.2291150
46	C	0.9983066	-3.7877213	0.5828274
47	C	3.1347641	-4.4865601	2.2982615
48	C	2.3373774	-3.6309373	0.1597597
49	C	0.7438544	-4.2935123	1.8750302
50	C	1.8059116	-4.6419364	2.7286945
51	C	3.3984505	-3.9778119	1.0123752
52	H	2.5591314	-3.2431701	-0.8467153

53	H	-0.2949875	-4.4342447	2.2125809
54	H	1.5933268	-5.0500244	3.7275086
55	H	4.4364377	-3.8659356	0.6662166
56	H	3.9652841	-4.7746185	2.9590786
57	C	-1.0024239	3.7854374	0.5914865
58	C	-3.1366234	4.4818967	2.3108313
59	C	-0.7462140	4.2918080	1.8831207
60	C	-2.3421272	3.6269373	0.1710179
61	C	-3.4020626	3.9727376	1.0254905
62	C	-1.8071421	4.6389796	2.7387262
63	H	0.2930496	4.4339536	2.2187746
64	H	-2.5653566	3.2388991	-0.8350156
65	H	-4.4405284	3.8596116	0.6812061
66	H	-1.5931888	5.0475379	3.7370614
67	H	-3.9662637	4.7691033	2.9731228
68	H	6.5157851	0.3722963	1.2043685
69	C	5.7671604	0.3261027	0.4016981
70	C	3.8065585	0.2010382	-1.7242635
71	H	3.0659565	0.1523640	-2.5330598
72	H	7.2080176	0.3753060	-1.2074271
73	C	6.1411670	0.3263262	-0.9474711
74	C	5.1776369	0.2646360	-1.9921190
75	H	5.5259369	0.2669808	-3.0346155
76	H	-3.0798633	-0.1698328	-2.5050906
77	C	-3.8138223	-0.2162816	-1.6900612
78	C	-5.7563124	-0.3352166	0.4527816
79	H	-6.4981245	-0.3792155	1.2618817
80	C	-6.1415278	-0.3437783	-0.8932077
81	H	-7.2103817	-0.3971826	-1.1439088
82	H	-5.5438326	-0.2937364	-2.9857837
83	C	-5.1869334	-0.2850238	-1.9462232
84	H	-4.0297100	-0.2444655	2.8296700
85	H	4.0603893	0.2524807	2.7932934

$[Fe((R)\text{-}L^{1}Ph)(bimpy)]^{2+}$ ($\mathbf{3}^{2+}$), low-spin

1	Fe	-0.0001629	-0.0003339	-0.4630921
2	N	0.0093152	-0.0002129	1.4633337
3	C	-1.1722176	-0.0322150	2.1482099
4	C	-1.1981330	-0.0349805	3.5557329
5	C	0.0230384	-0.0000341	4.2515611
6	H	0.0284033	0.0003033	5.3501679
7	C	1.2373446	0.0344200	3.5438242
8	H	2.1941160	0.0616094	4.0818683
9	C	1.1975269	0.0313720	2.1365398
10	C	-2.2741195	-0.0527500	1.2045165
11	N	-1.9770424	-0.0487711	-0.1138575
12	C	-3.1933694	-0.0544878	-0.7923991
13	C	-4.2498040	-0.0614983	0.1753367
14	N	-3.6245422	-0.0632353	1.4155724
15	C	2.2900130	0.0526012	v
16	N	1.9805978	0.0490698	-0.1336129
17	C	3.1907109	0.0554939	-0.8234711
18	C	4.2560444	0.0635531	0.1344957
19	N	3.6423188	0.0652267	1.3804811
20	N	-0.0082774	-0.0006660	-2.3708558
21	C	-0.0125972	-1.1814453	-3.0543476
22	C	-0.0210550	-1.2216983	-4.4593741
23	H	-0.0287548	-2.1886702	-4.9798804
24	C	-0.0198747	-0.0012276	-5.1639513
25	H	-0.0246634	-0.0014396	-6.2626800
26	C	-0.0125828	1.2195265	-4.4598675
27	C	-0.0092791	1.1798724	-3.0548097

28	C	-0.0245412	-2.2804668	-2.0914747
29	N	0.0043804	-1.9757468	-0.8145698
30	C	-0.0926306	-3.2523671	-0.0466307
31	C	-0.1151177	-4.3278020	-1.1891899
32	O	-0.0971752	-3.5598839	-2.4428468
33	C	0.0113117	2.2792063	-2.0923741
34	N	-0.0099581	1.9748029	-0.8152506
35	C	0.0909782	3.2516472	-0.0481669
36	C	0.1096158	4.3266488	-1.1911022
37	O	0.0847476	3.5584248	-2.4444345
38	H	-2.1494843	-0.0618673	4.1033516
39	H	-0.0092567	2.1862830	-4.9808186
40	H	0.7758295	-4.9827292	-1.1873662
41	H	-1.0284956	-4.9499635	-1.1935676
42	H	-0.7804291	4.9827677	-1.1851470
43	H	1.0238268	4.9475094	-1.2000675
44	H	1.0654511	3.2433291	0.4822637
45	H	-1.0653356	-3.2439579	0.4871014
46	C	1.0132747	-3.4551026	0.9819767
47	C	3.0299923	-3.9289088	2.9103504
48	C	2.3700977	-3.5414179	0.5947148
49	C	0.6830627	-3.6092837	2.3447163
50	C	1.6834466	-3.8460322	3.3044753
51	C	3.3711277	-3.7729499	1.5531264
52	H	2.6569460	-3.4416583	-0.4637556
53	H	-0.3711373	-3.5584769	2.6586630
54	H	1.4069694	-3.9862803	4.3596072
55	H	4.4208884	-3.8549515	1.2352518
56	H	3.8116928	-4.1363346	3.6556282
57	C	-1.0118660	3.4545515	0.9838258
58	C	-3.0234544	3.9280284	2.9176929
59	C	-0.6781367	3.6073032	2.3458472
60	C	-2.3696588	3.5420303	0.6001083
61	C	-3.3680982	3.7733341	1.5612080
62	C	-1.6759537	3.8439051	3.3083194
63	H	0.3767303	3.5549315	2.6572701
64	H	-2.6595582	3.4429920	-0.4576050
65	H	-4.4185756	3.8561862	1.2459513
66	H	-1.3966988	3.9830038	4.3628699
67	H	-3.8031843	4.1353279	3.6650701
68	H	6.4185134	0.0753979	0.5069487
69	C	5.6118479	0.0680365	-0.2385688
70	C	3.4938042	0.0538751	-2.2042685
71	H	2.7025649	0.0507263	-2.9625904
72	H	6.9299691	0.0663743	-1.9511010
73	C	5.8850712	0.0634160	-1.6111662
74	C	4.8420928	0.0568198	-2.5760774
75	H	5.1062572	0.0551726	-3.6429732
76	H	-2.7238545	-0.0500029	-2.9351689
77	C	-3.5085198	-0.0526748	-2.1703879
78	C	-5.6089351	-0.0649971	-0.1856622
79	H	-6.4090793	-0.0716019	0.5671776
80	C	-5.8942869	-0.0601659	-1.5557579
81	H	-6.9424087	-0.0621980	-1.8864020
82	H	-5.1339370	-0.0523938	-3.5943444
83	C	-4.8601114	-0.0544006	-2.5301155
84	H	-4.0917841	-0.0405968	2.3218113
85	H	4.1182182	0.0437992	2.2822211

$[Fe((R)\text{-}L^2Ph)(bimpy)]^{2+}$ (**4**$^{2+}$), high-spin

1	Fe	-0.0017266	-0.0004788	-0.4414498
2	N	0.0050189	0.0001407	1.7425618

3	C	-1.1722567	0.0115664	2.4095003
4	C	-1.2081266	0.0078844	3.8202487
5	C	0.0131514	0.0004974	4.5158480
6	H	0.0163452	0.0006223	5.6150375
7	C	1.2303342	-0.0069711	3.8131311
8	H	2.1826178	-0.0076783	4.3601877
9	C	1.1861413	-0.0110152	2.4025908
10	C	-2.3229014	0.0154957	1.4988833
11	N	-2.1418565	-0.0517972	0.1691337
12	C	-3.4074898	-0.0358223	-0.3970628
13	C	-4.3842477	0.0454850	0.6453324
14	N	-3.6522559	0.0704348	1.8259561
15	C	2.3312381	-0.0146714	1.4850403
16	N	2.1421123	0.0530612	0.1564168
17	C	3.4043745	0.0380364	-0.4173736
18	C	4.3874119	-0.0430799	0.6191159
19	N	3.6625655	-0.0691660	1.8040828
20	N	-0.0118889	-0.0024629	-2.5446329
21	C	-0.0803117	-1.1783962	-3.2241317
22	C	-0.0985846	-1.2171766	-4.6309950
23	H	-0.1643776	-2.1776664	-5.1614260
24	C	-0.0313059	-0.0047142	-5.3414879
25	H	-0.0389961	-0.0056178	-6.4401233
26	C	0.0456665	1.2088992	-4.6339815
27	C	0.0470631	1.1724283	-3.2269478
28	C	-0.1393079	-2.3454033	-2.3194919
29	N	-0.1103202	-2.1300823	-1.0291577
30	C	-0.1425479	-3.3584952	-0.2095365
31	C	-0.4397797	-4.5858500	-1.1483098
32	S	-0.2526923	-3.9982847	-2.8931486
33	C	0.1176974	2.3408537	-2.3249004
34	N	0.1033920	2.1272920	-1.0340554
35	C	0.1453111	3.3567114	-0.2164881
36	C	0.4346075	4.5823617	-1.1598552
37	S	0.2261964	3.9929198	-2.9018272
38	H	-2.1570723	0.0088331	4.3731037
39	H	0.1034838	2.1685290	-5.1668858
40	H	0.2655061	-5.4207418	-0.9838306
41	H	-1.4720731	-4.9653071	-1.0308362
42	H	-0.2672898	5.4186874	-0.9883254
43	H	1.4689432	4.9599112	-1.0547807
44	H	0.9989166	3.2512367	0.4844505
45	H	-0.9894790	-3.2533580	0.4995027
46	C	1.1305696	-3.5316346	0.6193301
47	C	3.4591003	-4.0240877	2.1492634
48	C	2.4071763	-3.4893112	0.0151313
49	C	1.0360230	-3.8241550	1.9964363
50	C	2.1923536	-4.0741075	2.7576980
51	C	3.5630043	-3.7290115	0.7765844
52	H	2.5040787	-3.2778574	-1.0603193
53	H	0.0461596	-3.8858731	2.4755267
54	H	2.1007643	-4.3242195	3.8248601
55	H	4.5499671	-3.7002466	0.2922022
56	H	4.3637693	-4.2345910	2.7383595
57	C	-1.1196185	3.5320524	0.6244598
58	C	-3.4328353	4.0268613	2.1763337
59	C	-1.0113889	3.8257891	2.0002483
60	C	-2.4020206	3.4899079	0.0325926
61	C	-3.5503350	3.7306548	0.8050332
62	C	-2.1601986	4.0769703	2.7724400
63	H	-0.0168705	3.8870518	2.4696443
64	H	-2.5090878	3.2777631	-1.0417326

65	H	-4.5419878	3.7021930	0.3302900
66	H	-2.0582645	4.3279635	3.8384552
67	H	-4.3315975	4.2383472	2.7740746
68	H	6.5180794	-0.1392004	1.1515064
69	C	5.7681927	-0.0802566	0.3507340
70	C	3.8052740	0.0844679	-1.7708909
71	H	3.0626102	0.1472063	-2.5767055
72	H	7.2088831	-0.0587350	-1.2591400
73	C	6.1414113	-0.0341609	-0.9977684
74	C	5.1768142	0.0465884	-2.0404954
75	H	5.5251799	0.0813531	-3.0823793
76	H	-3.0788412	-0.1446939	-2.5585324
77	C	-3.8165533	-0.0814773	-1.7481320
78	C	-5.7665973	0.0837805	0.3852074
79	H	-6.5115401	0.1429711	1.1904326
80	C	-6.1479799	0.0385045	-0.9610234
81	H	-7.2168907	0.0639907	-1.2159204
82	H	-5.5442390	-0.0767885	-3.0494391
83	C	-5.1896923	-0.0425552	-2.0095304
84	H	-4.0435739	0.1467769	2.7651745
85	H	4.0594955	-0.1458823	2.7409081

[Fe((*R*)-*L*^{2}Ph)(bimpy)]$^{2+}$ (**4**$^{2+}$), low-spin

1	Fe	-0.0014927	-0.0011096	-0.3736787
2	N	0.0039591	0.0003063	1.5542311
3	C	-1.1796997	-0.0311655	2.2368227
4	C	-1.2082001	-0.0394804	3.6445742
5	C	0.0117364	0.0000981	4.3429808
6	H	0.0147868	-0.0000657	5.4416158
7	C	1.2277595	0.0399089	3.6378135
8	H	2.1830292	0.0702819	4.1784710
9	C	1.1913872	0.0317952	2.2301779
10	C	-2.2799008	-0.0409812	1.2907363
11	N	-1.9797313	-0.0198688	-0.0268820
12	C	-3.1936169	-0.0193531	-0.7088056
13	C	-4.2523066	-0.0413604	0.2561308
14	N	-3.6308299	-0.0556848	1.4977899
15	C	2.2861484	0.0422544	1.2777865
16	N	1.9787650	0.0202854	-0.0381973
17	C	3.1889326	0.0213047	-0.7266479
18	C	4.2528432	0.0451438	0.2325030
19	N	3.6381598	0.0590343	1.4774795
20	N	-0.0104178	-0.0036063	-2.2650736
21	C	-0.0679672	-1.1911820	-2.9384415
22	C	-0.0853573	-1.2243515	-4.3453113
23	H	-0.1422544	-2.1845203	-4.8763759
24	C	-0.0316187	-0.0067427	-5.0503830
25	H	-0.0402113	-0.0079566	-6.1490459
26	C	0.0325749	1.2124805	-4.3489252
27	C	0.0367265	1.1824512	-2.9419109
28	C	-0.1362357	-2.2977813	-1.9818574
29	N	-0.0770914	-1.9625836	-0.7067234
30	C	-0.1293598	-3.1293186	0.2114851
31	C	-0.6931456	-4.3360190	-0.6044438
32	S	-0.3372210	-3.9884217	-2.3909488
33	C	0.1167047	2.2913255	-1.9887845
34	N	0.0715153	1.9593278	-0.7123059
35	C	0.1348557	3.1281645	0.2025784
36	C	0.6889526	4.3332138	-0.6226456
37	S	0.3149910	3.9805954	-2.4044234
38	H	-2.1604060	-0.0699957	4.1906242
39	H	0.0800454	2.1714904	-4.8829993

40	H	-0.2151472	-5.2920218	-0.3247650
41	H	-1.7907095	-4.4362181	-0.5022307
42	H	0.2129186	5.2895054	-0.3405697
43	H	1.7873937	4.4348959	-0.5320479
44	H	0.8700768	2.8837343	0.9951076
45	H	-0.8551909	-2.8832806	1.0121160
46	C	1.2167273	-3.4234272	0.8757905
47	C	3.6477671	-4.1332997	2.1368239
48	C	2.3938627	-3.6003742	0.1137622
49	C	1.2754942	-3.6003319	2.2753531
50	C	2.4824700	-3.9575932	2.9031569
51	C	3.6003522	-3.9526433	0.7416971
52	H	2.3701204	-3.4850610	-0.9798472
53	H	0.3640449	-3.4723194	2.8807335
54	H	2.5084090	-4.1117160	3.9918222
55	H	4.5055979	-4.1039730	0.1358136
56	H	4.5894026	-4.4268808	2.6231845
57	C	-1.2033842	3.4238585	0.8817911
58	C	-3.6194121	4.1377333	2.1695103
59	C	-1.2472738	3.5980987	2.2822336
60	C	-2.3880245	3.6051725	0.1324887
61	C	-3.5869556	3.9594340	0.7736287
62	C	-2.4466656	3.9574625	2.9232822
63	H	-0.3300488	3.4662965	2.8779987
64	H	-2.3762085	3.4919826	-0.9615572
65	H	-4.4980324	4.1141521	0.1774134
66	H	-2.4607501	4.1096778	4.0124304
67	H	-4.5551210	4.4329828	2.6661764
68	H	6.4145990	0.0665236	0.6071861
69	C	5.6090147	0.0484240	-0.1389690
70	C	3.4929272	-0.0014638	-2.1068552
71	H	2.7018435	-0.0202728	-2.8648905
72	H	6.9284579	0.0279419	-1.8499168
73	C	5.8834142	0.0258731	-1.5110041
74	C	4.8414195	0.0008795	-2.4769744
75	H	5.1070224	-0.0163165	-3.5433633
76	H	-2.7181763	0.0207086	-2.8493088
77	C	-3.5049465	0.0031591	-2.0873613
78	C	-5.6104797	-0.0430434	-0.1081262
79	H	-6.4123557	-0.0600809	0.6426346
80	C	-5.8921885	-0.0208373	-1.4786544
81	H	-6.9394295	-0.0218953	-1.8121025
82	H	-5.1266384	0.0194175	-3.5147994
83	C	-4.8554288	0.0023551	-2.4502556
84	H	-4.1012257	-0.0431458	2.4027152
85	H	4.1136479	0.0480132	2.3797585

[Fe((*R*)-*L*^{1}*i*Pr)(bimpy)]$^{2+}$ (**5**$^{2+}$), high-spin

1	Fe	-0.0013707	-0.0005398	-0.1201137
2	N	0.0081155	0.0075004	2.0612178
3	C	-1.1628740	-0.1028834	2.7354820
4	C	-1.1956828	-0.1055218	4.1463243
5	C	0.0189398	0.0224376	4.8419016
6	H	0.0231935	0.0286823	5.9409440
7	C	1.2280695	0.1428472	4.1355509
8	H	2.1758376	0.2471659	4.6809446
9	C	1.1842992	0.1247095	2.7250805
10	C	-2.3116190	-0.1964045	1.8288243
11	N	-2.1325199	-0.1719531	0.4961565
12	C	-3.3977267	-0.2553072	-0.0685987
13	C	-4.3715648	-0.3309251	0.9775116
14	N	-3.6388877	-0.2920515	2.1581973

15	C	2.3256617	0.2120903	1.8086226
16	N	2.1359207	0.1795650	0.4775945
17	C	3.3970190	0.2514630	-0.0978647
18	C	4.3791417	0.3343688	0.9399191
19	N	3.6555530	0.3100206	2.1266384
20	N	-0.0083437	0.0008752	-2.2529873
21	C	-0.0885420	-1.1665520	-2.9350303
22	C	-0.1030570	-1.2133117	-4.3407693
23	H	-0.1751083	-2.1785203	-4.8598281
24	C	-0.0182480	0.0013583	-5.0479199
25	H	-0.0221236	0.0015410	-6.1468939
26	C	0.0714145	1.2157716	-4.3409796
27	C	0.0669821	1.1685783	-2.9351689
28	C	-0.1547651	-2.3239768	-2.0237774
29	N	-0.0729449	-2.1641080	-0.7321259
30	C	-0.1827231	-3.5121964	-0.1161659
31	C	-0.3787014	-4.4510720	-1.3525171
32	O	-0.3187263	-3.5510547	-2.5137705
33	C	0.1387969	2.3255765	-2.0238760
34	N	0.0651412	2.1647749	-0.7318719
35	C	0.1797880	3.5118379	-0.1148196
36	C	0.3633682	4.4526954	-1.3514895
37	O	0.2995383	3.5532022	-2.5133809
38	H	-2.1391781	-0.2028907	4.7003547
39	H	0.1394529	2.1811510	-4.8602699
40	H	0.4213855	-5.2035698	-1.4804163
41	H	-1.3605892	-4.9583212	-1.3814631
42	H	-0.4410902	5.2014543	-1.4738790
43	H	1.3425591	4.9646415	-1.3868313
44	H	1.1021806	3.5165157	0.5044878
45	H	6.5069130	0.4615647	1.4751045
46	C	5.7583847	0.4111506	0.6726585
47	C	3.7986281	0.2490025	-1.4522737
48	H	3.0588564	0.1836460	-2.2605868
49	H	7.1985145	0.4568789	-0.9364483
50	C	6.1318470	0.4052067	-0.6764020
51	C	5.1687787	0.3269757	-1.7205318
52	H	5.5171174	0.3248230	-2.7629946
53	H	-3.0754724	-0.2187709	-2.2345411
54	C	-3.8093967	-0.2703902	-1.4198815
55	C	-5.7522452	-0.4195673	0.7215720
56	H	-6.4941524	-0.4747851	1.5298193
57	C	-6.1358757	-0.4293713	-0.6246339
58	H	-7.2037716	-0.4947776	-0.8764171
59	H	-5.5377000	-0.3667561	-2.7165036
60	C	-5.1812020	-0.3565608	-1.6768624
61	H	-4.0302033	-0.3213913	3.1002908
62	H	4.0542131	0.3467182	3.0653826
63	C	-1.0062598	3.8627548	0.8258804
64	H	-1.0101886	3.0576537	1.5936437
65	H	-1.0976750	-3.5183632	0.5135857
66	C	1.0128532	-3.8657651	0.8115426
67	H	1.0236696	-3.0635464	1.5821916
68	C	2.3760322	-3.8547482	0.0993966
69	H	3.1882439	-4.0246194	0.8326936
70	H	2.5775290	-2.8896181	-0.4052171
71	H	2.4619002	-4.6629047	-0.6554589
72	C	0.7523877	-5.2003805	1.5359586
73	H	1.5579435	-5.4067339	2.2663953
74	H	0.7302148	-6.0581239	0.8329954
75	H	-0.2086507	-5.1914408	2.0881250
76	C	-0.7377808	5.1943368	1.5531643

77	H	0.2300664	5.1828772	2.0932766
78	H	-1.5340807	5.3972963	2.2946277
79	H	-0.7241660	6.0554253	0.8541077
80	C	-2.3766115	3.8545400	0.1271978
81	H	-2.4702995	4.6652683	-0.6240015
82	H	-3.1813175	4.0215364	0.8693364
83	H	-2.5830160	2.8912956	-0.3791359

[Fe((*R*)-*L*^{1}*i*Pr)(bimpy)]$^{2+}$ (**5**$^{2+}$), low-spin

1	Fe	-0.0006365	0.0011677	-0.0939862
2	N	0.0063784	0.0030681	1.8305391
3	C	-1.1759383	-0.0542524	2.5166006
4	C	-1.2026438	-0.0571430	3.9249483
5	C	0.0165774	0.0094225	4.6228358
6	H	0.0206015	0.0117453	5.7214507
7	C	1.2306538	0.0732250	3.9157747
8	H	2.1853787	0.1273783	4.4561182
9	C	1.1936318	0.0641640	2.5076345
10	C	-2.2770211	-0.0914738	1.5718979
11	N	-1.9798515	-0.0457377	0.2537126
12	C	-3.1948965	-0.0899867	-0.4264534
13	C	-4.2509146	-0.1624143	0.5394315
14	N	-3.6272362	-0.1599185	1.7809686
15	C	2.2876838	0.0983404	1.5546386
16	N	1.9810982	0.0473179	0.2387601
17	C	3.1913851	0.0865633	-0.4501813
18	C	4.2542572	0.1618012	0.5079779
19	N	3.6394001	0.1660292	1.7538335
20	N	-0.0098987	0.0010804	-2.0053850
21	C	-0.0719749	-1.1781800	-2.6875171
22	C	-0.0885596	-1.2177879	-4.0924849
23	H	-0.1483076	-2.1829195	-4.6130639
24	C	-0.0261126	0.0011865	-4.7969075
25	H	-0.0324825	0.0012313	-5.8956844
26	C	0.0443300	1.2201149	-4.0931898
27	C	0.0441589	1.1803898	-2.6881332
28	C	-0.1303484	-2.2751538	-1.7233839
29	N	-0.0421190	-1.9768714	-0.4481158
30	C	-0.0944107	-3.2575358	0.3089539
31	C	-0.4882898	-4.2796480	-0.8039779
32	O	-0.2963829	-3.5476853	-2.0681727
33	C	0.1133396	2.2773883	-1.7247585
34	N	0.0381789	1.9793831	-0.4486348
35	C	0.1003941	3.2599908	0.3078409
36	C	0.4806021	4.2824054	-0.8097336
37	O	0.2764506	3.5497248	-2.0715630
38	H	-2.1533991	-0.1083855	4.4725489
39	H	0.0976630	2.1853156	-4.6143299
40	H	0.1546685	-5.1765683	-0.8406205
41	H	-1.5499127	-4.5906465	-0.7681222
42	H	-0.1643763	5.1781533	-0.8398001
43	H	1.5419074	4.5955628	-0.7853886
44	H	0.9165465	3.1844389	1.0552602
45	H	-0.9011758	-3.1827078	1.0665014
46	H	6.4144317	0.2653529	0.8815900
47	C	5.6094209	0.2112669	0.1359470
48	C	3.4961623	0.0564617	-1.8303780
49	H	2.7068412	-0.0043758	-2.5880597
50	H	6.9288065	0.2178080	-1.5752664
51	C	5.8841285	0.1818129	-1.2358653
52	C	4.8437068	0.1051496	-2.2009914
53	H	5.1099199	0.0826056	-3.2671180

54	H	-2.7246331	-0.0122004	-2.5678210
55	C	-3.5088680	-0.0708788	-1.8047125
56	C	-5.6085005	-0.2167730	0.1767763
57	H	-6.4084186	-0.2690263	0.9279899
58	C	-5.8923650	-0.1980429	-1.1933599
59	H	-6.9391493	-0.2388383	-1.5256624
60	H	-5.1316594	-0.1196851	-3.2306545
61	C	-4.8586644	-0.1264561	-2.1660277
62	H	-4.0966554	-0.2047610	2.6857085
63	H	4.1154798	0.2141054	2.6549178
64	C	-1.2192780	3.5823966	1.0694444
65	H	-1.4123085	2.6913281	1.7042859
66	C	1.2347872	-3.5798718	1.0540267
67	H	1.4370391	-2.6878034	1.6847948
68	C	-1.0095901	4.7867348	2.0068756
69	H	-0.1783419	4.6137973	2.7192503
70	H	-1.9241263	4.9835356	2.5986836
71	H	-0.7842152	5.7161085	1.4452981
72	C	-2.4317430	3.7766247	0.1417746
73	H	-2.3317277	4.6806290	-0.4920317
74	H	-3.3531044	3.9142810	0.7402470
75	H	-2.5958534	2.9075522	-0.5245992
76	C	2.4346485	-3.7778578	0.1109416
77	H	3.3626733	-3.9216287	0.6975564
78	H	2.5952494	-2.9082661	-0.5555985
79	H	2.3216637	-4.6797502	-0.5237066
80	C	1.0350569	-4.7826681	1.9956042
81	H	1.9579422	-4.9828558	2.5731030
82	H	0.7973528	-5.7113551	1.4379530
83	H	0.2154948	-4.6060284	2.7204443

[Fe((*R*)-*L*^{2}*i*Pr)(bimpy)]$^{2+}$ (**6**$^{2+}$), high-spin

1	Fe	-0.0036018	0.0009486	-0.1669874
2	N	-0.0127289	0.0116144	2.0229534
3	C	0.0530797	-1.1621684	2.6987914
4	C	0.0515619	-1.1945880	4.1095431
5	C	-0.0325286	0.0240418	4.8047581
6	H	-0.0408548	0.0289055	5.9037776
7	C	-0.1056609	1.2364023	4.0975978
8	H	-0.1759484	2.1876984	4.6422363
9	C	-0.0864509	1.1914359	2.6872326
10	C	0.1091909	-2.3142924	1.7938262
11	N	0.1053744	-2.1332472	0.4611586
12	C	0.1411181	-3.3999057	-0.1047341
13	C	0.1702679	-4.3770217	0.9405894
14	N	0.1510745	-3.6446915	2.1221055
15	C	-0.1254659	2.3357029	1.7715165
16	N	-0.1068478	2.1432671	0.4405587
17	C	-0.1240876	3.4055731	-0.1361116
18	C	-0.1558668	4.3916653	0.9007790
19	N	-0.1590290	3.6691448	2.0883527
20	N	-0.0084722	-0.0008303	-2.2764009
21	C	1.1571755	-0.1465381	-2.9561376
22	C	1.1920726	-0.1634942	-4.3634891
23	H	2.1445345	-0.2912622	-4.8968861
24	C	-0.0136022	-0.0048366	-5.0697366
25	H	-0.0156433	-0.0061580	-6.1685500
26	C	-1.2167470	0.1550103	-4.3594483
27	C	-1.1767268	0.1415918	-2.9521798
28	C	2.3271729	-0.2686980	-2.0590790
29	N	2.1497046	-0.1399803	-0.7700991
30	C	3.4025965	-0.2030966	0.0108193

31	C	4.5468980	-0.7301266	-0.9167064
32	S	3.9421261	-0.5892375	-2.6591830
33	C	-2.3440113	0.2625203	-2.0513969
34	N	-2.1626851	0.1338672	-0.7630296
35	C	-3.4140212	0.1922934	0.0209589
36	C	-4.5636677	0.7124805	-0.9040334
37	S	-3.9615408	0.5776180	-2.6476088
38	H	0.1138859	-2.1408441	4.6638696
39	H	-2.1712874	0.2804530	-4.8896765
40	H	5.4776352	-0.1400282	-0.8289636
41	H	4.7904581	-1.7932145	-0.7334292
42	H	-5.4899757	0.1156000	-0.8150409
43	H	-4.8145044	1.7735572	-0.7189032
44	H	-3.2563556	0.9362105	0.8301583
45	H	3.2427657	-0.9452707	0.8212094
46	H	-0.1853775	6.5244328	1.4324715
47	C	-0.1708891	5.7727089	0.6315571
48	C	-0.1109092	3.8042177	-1.4912702
49	H	-0.0847183	3.0602963	-2.2978491
50	H	-0.1598850	7.2105192	-0.9804408
51	C	-0.1555039	6.1431169	-0.7182186
52	C	-0.1275080	5.1759852	-1.7612415
53	H	-0.1159698	5.5225010	-2.8042370
54	H	0.1359760	-3.0715981	-2.2693372
55	C	0.1535156	-3.8091845	-1.4566324
56	C	0.2086497	-5.7597964	0.6827804
57	H	0.2287288	-6.5046580	1.4899616
58	C	0.2186055	-6.1410519	-0.6640692
59	H	0.2480703	-7.2102128	-0.9173626
60	H	0.2084398	-5.5371941	-2.7555057
61	C	0.1926696	-5.1827117	-1.7152620
62	H	0.1600990	-4.0379745	3.0638169
63	H	-0.1738022	4.0702087	3.0266934
64	C	3.7072180	1.1641693	0.7032980
65	H	2.7737370	1.4151173	1.2530975
66	C	-3.7106265	-1.1755821	0.7156666
67	H	-2.7756316	-1.4200852	1.2656679
68	C	-4.8349621	-1.0236210	1.7575224
69	H	-4.6117067	-0.2267026	2.4950978
70	H	-4.9754220	-1.9695422	2.3154545
71	H	-5.8101129	-0.7835773	1.2874315
72	C	-3.9900102	-2.3228789	-0.2706351
73	H	-4.9278504	-2.1639982	-0.8402754
74	H	-4.1090691	-3.2770889	0.2788123
75	H	-3.1664868	-2.4615921	-0.9979105
76	C	3.9934962	2.3082783	-0.2847181
77	H	4.1173541	3.2627206	0.2632544
78	H	3.1712816	2.4502747	-1.0128218
79	H	4.9309242	2.1432225	-0.8532901
80	C	4.8311955	1.0070690	1.7447497
81	H	4.9780186	1.9531031	2.3008381
82	H	5.8043019	0.7601895	1.2739499
83	H	4.6037787	0.2128483	2.4839743

[Fe((*R*)-*L*^{2}*i*Pr)(bimpy)]$^{2+}$ (**6**$^{2+}$), low-spin

1	Fe	-0.0000630	0.0010986	-0.1728377
2	N	0.0066676	0.0028492	1.7544654
3	C	-1.1757315	-0.0574620	2.4408252
4	C	-1.2024493	-0.0620228	3.8491213
5	C	0.0165596	0.0080688	4.5471952
6	H	0.0204451	0.0101052	5.6457890
7	C	1.2305930	0.0756336	3.8402692

8	H	2.1849974	0.1318189	4.3809736
9	C	1.1939007	0.0658827	2.4321725
10	C	-2.2767548	-0.0895742	1.4957344
11	N	-1.9795269	-0.0360491	0.1773863
12	C	-3.1946735	-0.0601226	-0.5030869
13	C	-4.2513404	-0.1305830	0.4623838
14	N	-3.6276807	-0.1469924	1.7039094
15	C	2.2882097	0.0943344	1.4791845
16	N	1.9819921	0.0367826	0.1630321
17	C	3.1926340	0.0559923	-0.5256446
18	C	4.2558696	0.1275503	0.4325496
19	N	3.6405843	0.1498200	1.6780994
20	N	-0.0083390	0.0010242	-2.0690262
21	C	-0.0931064	-1.1832381	-2.7441328
22	C	-0.1094470	-1.2149198	-4.1509264
23	H	-0.1881073	-2.1732830	-4.6825011
24	C	-0.0244362	0.0012884	-4.8550865
25	H	-0.0310276	0.0014027	-5.9538021
26	C	0.0688545	1.2173457	-4.1517601
27	C	0.0689751	1.1853833	-2.7448802
28	C	-0.1881426	-2.2904609	-1.7902632
29	N	-0.0884183	-1.9684931	-0.5148477
30	C	-0.1620525	-3.1409683	0.3916796
31	C	-0.8168193	-4.3027342	-0.4087587
32	S	-0.4968153	-3.9614002	-2.2038916
33	C	0.1741100	2.2924995	-1.7919993
34	N	0.0851666	1.9708067	-0.5157086
35	C	0.1655416	3.1441117	0.3894446
36	C	0.8166910	4.3041237	-0.4161786
37	S	0.4811439	3.9629729	-2.2085434
38	H	-2.1529951	-0.1159146	4.3968283
39	H	0.1408228	2.1758202	-4.6840689
40	H	-0.3887947	-5.2902828	-0.1583091
41	H	-1.9141193	-4.3494279	-0.2745817
42	H	0.3928025	5.2926615	-0.1626293
43	H	1.9151579	4.3482025	-0.2909273
44	H	0.8473097	2.8672688	1.2202357
45	H	-0.8393692	-2.8639223	1.2260481
46	H	6.4174099	0.2013681	0.8063195
47	C	5.6117850	0.1550789	0.0608435
48	C	3.4970203	0.0121254	-1.9054824
49	H	2.7065077	-0.0435417	-2.6622637
50	H	6.9314136	0.1254396	-1.6499007
51	C	5.8862092	0.1103564	-1.3105295
52	C	4.8450553	0.0411678	-2.2756175
53	H	5.1114140	0.0079398	-3.3414152
54	H	-2.7218660	0.0234499	-2.6430907
55	C	-3.5078615	-0.0248860	-1.8811334
56	C	-5.6094595	-0.1664437	0.0993435
57	H	-6.4099638	-0.2182723	0.8499550
58	C	-5.8927413	-0.1291620	-1.2704448
59	H	-6.9399207	-0.1536786	-1.6031462
60	H	-5.1312872	-0.0349849	-3.3068237
61	C	-4.8581086	-0.0604151	-2.2425391
62	H	-4.0979156	-0.1908304	2.6082877
63	H	4.1171232	0.1964261	2.5790305
64	C	1.2274203	-3.4829726	1.0211992
65	H	1.5949582	-2.5243913	1.4432216
66	C	-1.2201501	3.4882124	1.0262488
67	H	-1.5872627	2.5301558	1.4497679
68	C	-2.2713352	3.9870295	0.0182946
69	H	-1.9896670	4.9621920	-0.4258845

70	H	-3.2426176	4.1361673	0.5292963
71	H	-2.4412713	3.2719207	-0.8098824
72	C	-1.0450308	4.4719700	2.1996122
73	H	-0.3314673	4.0935352	2.9594025
74	H	-2.0144852	4.6423451	2.7065462
75	H	-0.6844570	5.4653527	1.8639773
76	C	2.2738065	-3.9794596	0.0071568
77	H	3.2476971	-4.1296124	0.5128683
78	H	2.4392831	-3.2620982	-0.8199352
79	H	1.9899611	-4.9535813	-0.4379420
80	C	1.0598991	-4.4673283	2.1951105
81	H	2.0321119	-4.6357352	2.6973855
82	H	0.6998333	-5.4613831	1.8609178
83	H	0.3491409	-4.0904533	2.9583106

[Fe((*R*)-*L*^{1}Ph)(bpp)]$^{2+}$ (**7**$^{2+}$), high-spin

1	Fe	-0.0002286	-0.0033862	-0.6694911
2	N	0.0109077	0.0030036	1.4991994
3	C	-1.1502813	-0.0655934	2.1756026
4	C	-1.2008554	-0.0617794	3.5797187
5	C	0.0237179	0.0178586	4.2643702
6	H	0.0287941	0.0240035	5.3635553
7	C	1.2418963	0.0898313	3.5675787
8	H	2.1932315	0.1531107	4.1088518
9	C	1.1782913	0.0783559	2.1639935
10	N	-2.2906729	-0.1457264	1.3410784
11	N	-2.1136388	-0.1420660	-0.0189011
12	C	-3.3454373	-0.2207121	-0.5422923
13	C	-4.3344339	-0.2779163	0.4743378
14	C	-3.6259911	-0.2265144	1.6669736
15	N	2.3108631	0.1494048	1.3180937
16	N	2.1210881	0.1367128	-0.0401825
17	C	3.3482263	0.2081063	-0.5754714
18	C	4.3468937	0.2690496	0.4315270
19	C	3.6494642	0.2283978	1.6309962
20	N	-0.0084233	0.0005831	-2.7953061
21	C	-0.0593242	-1.1678145	-3.4816423
22	C	-0.0696595	-1.2127322	-4.8873531
23	H	-0.1147428	-2.1787051	-5.4083375
24	C	-0.0187000	0.0044283	-5.5934594
25	H	-0.0227164	0.0059472	-6.6923405
26	C	0.0373240	1.2196342	-4.8843681
27	C	0.0373290	1.1708540	-3.4787403
28	C	-0.1016008	-2.3212404	-2.5662844
29	N	-0.0453005	-2.1376644	-1.2735460
30	C	-0.1449982	-3.4778470	-0.6295612
31	C	-0.2061321	-4.4481547	-1.8617449
32	O	-0.2154607	-3.5603256	-3.0346909
33	C	0.0855790	2.3218053	-2.5604996
34	N	0.0374832	2.1347491	-1.2679954
35	C	0.1379552	3.4733468	-0.6210987
36	C	0.1975099	4.4467554	-1.8511403
37	O	0.1958264	3.5621682	-3.0264714
38	H	-2.1470641	-0.1186715	4.1306233
39	H	0.0783813	2.1870811	-5.4029347
40	H	0.6816935	-5.1024567	-1.9486812
41	H	-1.1230143	-5.0638221	-1.9036401
42	H	-0.6871290	5.1061068	-1.9314934
43	H	1.1175828	5.0574925	-1.8963359
44	H	1.0965856	3.5048683	-0.0622766
45	H	-1.1031933	-3.5102740	-0.0699538
46	C	0.9857697	-3.7752883	0.3468630

47	C	3.0718522	-4.4586436	2.1288622
48	C	2.3366953	-3.6378615	-0.0449003
49	C	0.6938737	-4.2553241	1.6410851
50	C	1.7311867	-4.5959550	2.5279276
51	C	3.3726737	-3.9767912	0.8408517
52	H	2.5860144	-3.2742314	-1.0540010
53	H	-0.3543099	-4.3850711	1.9534438
54	H	1.4900701	-4.9852475	3.5277377
55	H	4.4203133	-3.8806980	0.5203508
56	H	3.8832613	-4.7405983	2.8154170
57	C	-0.9922306	3.7684597	0.3568543
58	C	-3.0772941	4.4500296	2.1408040
59	C	-0.6995766	4.2481142	1.6510649
60	C	-2.3434124	3.6306558	-0.0339300
61	C	-3.3788643	3.9687751	0.8527524
62	C	-1.7363786	4.5877768	2.5388995
63	H	0.3487622	4.3783145	1.9627199
64	H	-2.5934399	3.2673161	-1.0429647
65	H	-4.4266941	3.8723702	0.5329737
66	H	-1.4946812	4.9768216	3.5386714
67	H	-3.8883220	4.7313266	2.8280810
68	H	5.4313712	0.3353415	0.3012364
69	H	3.4688378	0.2164610	-1.6650415
70	H	-3.4759121	-0.2371280	-1.6306376
71	H	-5.4198597	-0.3485488	0.3546177
72	H	-3.9727374	-0.2401357	2.7046219
73	H	4.0054055	0.2495070	2.6653740

[Fe((*R*)-*L*^{1}Ph)(bpp)]$^{2+}$ (**7**$^{2+}$), low-spin

1	Fe	-0.0010785	-0.0004421	-0.8095780
2	N	0.0071669	0.0000346	1.0949697
3	C	-1.1648883	-0.0312023	1.7729054
4	C	-1.2102345	-0.0340018	3.1732092
5	C	0.0187586	0.0022509	3.8587341
6	H	0.0233391	0.0032824	4.9574760
7	C	1.2419956	0.0372761	3.1629038
8	H	2.1977374	0.0652257	3.7000022
9	C	1.1848649	0.0321622	1.7629804
10	N	-2.2533998	-0.0591827	0.8855373
11	N	-1.9422921	-0.0435024	-0.4596815
12	C	-3.1170778	-0.0653370	-1.1086076
13	C	-4.1979793	-0.0950778	-0.1874520
14	C	-3.6162065	-0.0866502	1.0731281
15	N	2.2657555	0.0591445	0.8662737
16	N	1.9433394	0.0428749	-0.4762748
17	C	3.1126558	0.0644181	-1.1350413
18	C	4.2013130	0.0946061	-0.2229714
19	C	3.6300897	0.0866602	1.0424492
20	N	-0.0105387	-0.0004772	-2.7225580
21	C	-0.0201293	-1.1809004	-3.4036616
22	C	-0.0292061	-1.2212570	-4.8088192
23	H	-0.0400278	-2.1877934	-5.3303002
24	C	-0.0241838	-0.0005469	-5.5125972
25	H	-0.0295631	-0.0005709	-6.6114183
26	C	-0.0122706	1.2201986	-4.8089507
27	C	-0.0075069	1.1799156	-3.4037695
28	C	-0.0338813	-2.2823586	-2.4390749
29	N	-0.0011991	-1.9814976	-1.1614352
30	C	-0.0980588	-3.2621105	-0.3962464
31	C	-0.1046811	-4.3333146	-1.5420534
32	O	-0.1117086	-3.5587064	-2.7940013
33	C	0.0158661	2.2814122	-2.4393874

34	N	-0.0047708	1.9805956	-1.1614964
35	C	0.0967684	3.2612584	-0.3970218
36	C	0.0999829	4.3323692	-1.5431834
37	O	0.0901333	3.5577353	-2.7950784
38	H	-2.1613836	-0.0607565	3.7184825
39	H	-0.0066325	2.1867078	-5.3305623
40	H	0.8014036	-4.9671581	-1.5498268
41	H	-1.0033045	-4.9761350	-1.5443979
42	H	-0.8016466	4.9724818	-1.5425236
43	H	1.0030805	4.9688753	-1.5540937
44	H	1.0767153	3.2589418	0.1238985
45	H	-1.0762093	-3.2602116	0.1281531
46	C	0.9993952	-3.4589164	0.6416437
47	C	3.0016714	-3.9239546	2.5870386
48	C	2.3596184	-3.5427200	0.2655801
49	C	0.6583402	-3.6102517	2.0024833
50	C	1.6519427	-3.8426339	2.9704470
51	C	3.3533681	-3.7702812	1.2323955
52	H	2.6555774	-3.4458156	-0.7906900
53	H	-0.3987051	-3.5655061	2.3081881
54	H	1.3675131	-3.9823095	4.0235220
55	H	4.4060620	-3.8494722	0.9243418
56	H	3.7784020	-4.1264786	3.3386480
57	C	-0.9972906	3.4587335	0.6444415
58	C	-2.9939978	3.9246125	2.5952886
59	C	-0.6524105	3.6093396	2.0043758
60	C	-2.3584884	3.5436089	0.2720878
61	C	-3.3494717	3.7716556	1.2415513
62	C	-1.6432897	3.8420961	2.9750489
63	H	0.4053754	3.5635252	2.3073345
64	H	-2.6573090	3.4472511	-0.7834397
65	H	-4.4029297	3.8516823	0.9363536
66	H	-1.3559446	3.9811757	4.0274106
67	H	-3.7685483	4.1274383	3.3490632
68	H	5.2685484	0.1193832	-0.4627757
69	H	3.1308934	0.0590981	-2.2303631
70	H	-5.2671980	-0.1202534	-0.4181940
71	H	-3.1443839	-0.0607677	-2.2037295
72	H	-4.0585620	-0.0989679	2.0736885
73	H	4.0809145	0.0994922	2.0392209

[Fe((*R*)-L^2Ph)(bpp)]$^{2+}$ (**8**$^{2+}$), high-spin

1	Fe	0.0000005	0.0000000	-0.6791717
2	N	-0.0000003	0.0000001	1.4862920
3	C	0.4805845	1.0639989	2.1550842
4	C	0.5036548	1.1160180	3.5594199
5	C	-0.0000016	0.0000008	4.2498691
6	H	-0.0000024	0.0000011	5.3491101
7	C	-0.5036573	-1.1160169	3.5594199
8	H	-0.8948746	-1.9826764	4.1050198
9	C	-0.4805855	-1.0639984	2.1550842
10	N	0.9378945	2.1058246	1.3143085
11	N	0.8498970	1.9436702	-0.0450697
12	C	1.3259930	3.0793764	-0.5737166
13	C	1.7285292	3.9902704	0.4382978
14	C	1.4674008	3.3366362	1.6340561
15	N	-0.9378948	-2.1058245	1.3143085
16	N	-0.8498955	-1.9436711	-0.0450695
17	C	-1.3259910	-3.0793774	-0.5737164
18	C	-1.7285286	-3.9902707	0.4382979
19	C	-1.4674013	-3.3366359	1.6340562
20	N	0.0000001	0.0000005	-2.7831568

21	C	-1.0382712	0.5528796	-3.4619401
22	C	-1.0709472	0.5741384	-4.8692718
23	H	-1.9168223	1.0317449	-5.4015158
24	C	-0.0000002	0.0000002	-5.5777699
25	H	-0.0000005	-0.0000002	-6.6764846
26	C	1.0709469	-0.5741377	-4.8692719
27	C	1.0382712	-0.5528785	-3.4619402
28	C	-2.0613697	1.1155199	-2.5559544
29	N	-1.8753190	1.0026440	-1.2639024
30	C	-2.9649749	1.5861650	-0.4483043
31	C	-3.8952648	2.4319205	-1.3912196
32	S	-3.4932157	1.9456190	-3.1295592
33	C	2.0613696	-1.1155188	-2.5559544
34	N	1.8753183	-1.0026432	-1.2639023
35	C	2.9649747	-1.5861646	-0.4483049
36	C	3.8952638	-2.4319207	-1.3912202
37	S	3.4932161	-1.9456173	-3.1295593
38	H	0.8948715	1.9826779	4.1050197
39	H	1.9168218	-1.0317446	-5.4015159
40	H	-4.9675811	2.2342208	-1.2109872
41	H	-3.7133906	3.5193114	-1.2986125
42	H	4.9675803	-2.2342225	-1.2109872
43	H	3.7133881	-3.5193113	-1.2986140
44	H	2.4956408	-2.2803600	0.2784855
45	H	-2.4956413	2.2803606	0.2784858
46	C	-3.7221918	0.5233089	0.3461744
47	C	-5.2953766	-1.3176579	1.8092786
48	C	-4.3135726	-0.5862833	-0.2996723
49	C	-3.9216816	0.6928754	1.7328094
50	C	-4.7039154	-0.2218467	2.4614142
51	C	-5.0966496	-1.4982486	0.4272919
52	H	-4.1830077	-0.7298802	-1.3831402
53	H	-3.4886267	1.5659630	2.2460271
54	H	-4.8690766	-0.0648469	3.5374232
55	H	-5.5678107	-2.3467734	-0.0898944
56	H	-5.9233716	-2.0226203	2.3729983
57	C	3.7221922	-0.5233091	0.3461738
58	C	5.2953781	1.3176569	1.8092782
59	C	3.9216815	-0.6928755	1.7328089
60	C	4.3135741	0.5862826	-0.2996728
61	C	5.0966517	1.4982475	0.4272916
62	C	4.7039157	0.2218462	2.4614137
63	H	3.4886259	-1.5659627	2.2460266
64	H	4.1830097	0.7298794	-1.3831407
65	H	5.5678138	2.3467716	-0.0898948
66	H	4.8690766	0.0648464	3.5374228
67	H	5.9233734	2.0226190	2.3729981
68	H	1.6219495	3.6519328	2.6701385
69	H	-1.6219513	-3.6519320	2.6701385
70	H	-1.3627977	-3.2023037	-1.6624285
71	H	-2.1528855	-4.9909921	0.3126211
72	H	2.1528863	4.9909917	0.3126209
73	H	1.3628011	3.2023023	-1.6624286

[Fe((*R*)-*L*^{2}Ph)(bpp)]$^{2+}$ (**8**$^{2+}$), low-spin

1	Fe	-0.0028520	-0.0019881	-0.7076393
2	N	0.0034798	-0.0018077	1.1978451
3	C	-1.1699540	-0.0346650	1.8750114
4	C	-1.2158980	-0.0429288	3.2762276
5	C	0.0122836	-0.0013991	3.9635340
6	H	0.0157547	-0.0010153	5.0622182
7	C	1.2360960	0.0392959	3.2684254

8	H	2.1911904	0.0705762	3.8068362
9	C	1.1812305	0.0301236	1.8674682
10	N	-2.2570870	-0.0549251	0.9872146
11	N	-1.9456069	-0.0215486	-0.3577471
12	C	-3.1200550	-0.0343769	-1.0075599
13	C	-4.2017396	-0.0747715	-0.0872876
14	C	-3.6209551	-0.0864676	1.1732035
15	N	2.2626134	0.0483842	0.9725827
16	N	1.9424504	0.0179289	-0.3704730
17	C	3.1126596	0.0345501	-1.0277359
18	C	4.2001305	0.0755768	-0.1143772
19	C	3.6274923	0.0851072	1.1498356
20	N	-0.0118834	-0.0038956	-2.6033348
21	C	-0.0697338	-1.1911414	-3.2747691
22	C	-0.0863160	-1.2243287	-4.6817435
23	H	-0.1429792	-2.1839947	-5.2139576
24	C	-0.0304322	-0.0067794	-5.3862704
25	H	-0.0377806	-0.0079228	-6.4850046
26	C	0.0345645	1.2122409	-4.6851105
27	C	0.0366865	1.1819272	-3.2779903
28	C	-0.1362491	-2.3012223	-2.3172406
29	N	-0.0761136	-1.9718951	-1.0409995
30	C	-0.1303183	-3.1436650	-0.1259627
31	C	-0.6772078	-4.3531903	-0.9508857
32	S	-0.3364999	-3.9873317	-2.7367035
33	C	0.1145194	2.2940627	-2.3237122
34	N	0.0676572	1.9677630	-1.0461667
35	C	0.1326110	3.1416273	-0.1343701
36	C	0.6702891	4.3495249	-0.9681348
37	S	0.3123623	3.9788091	-2.7494997
38	H	-2.1675145	-0.0742172	3.8207864
39	H	0.0833600	2.1708182	-5.2200742
40	H	-0.1809452	-5.3028749	-0.6814703
41	H	-1.7721043	-4.4756289	-0.8446610
42	H	0.1758869	5.2995551	-0.6963991
43	H	1.7660460	4.4733987	-0.8730366
44	H	0.8788498	2.9051964	0.6503420
45	H	-0.8677658	-2.9057468	0.6665690
46	C	1.2091916	-3.4298008	0.5534789
47	C	3.6247423	-4.1491519	1.8379640
48	C	2.3885642	-3.6313342	-0.1994475
49	C	1.2577768	-3.5867746	1.9559127
50	C	2.4577369	-3.9479321	2.5952187
51	C	3.5873826	-3.9883406	0.4400782
52	H	2.3701252	-3.5359677	-1.2953900
53	H	0.3433521	-3.4453413	2.5539718
54	H	2.4765485	-4.0874831	3.6859449
55	H	4.4948303	-4.1578695	-0.1575517
56	H	4.5605690	-4.4448697	2.3338150
57	C	-1.1992701	3.4298964	0.5589931
58	C	-3.5996992	4.1555251	1.8684607
59	C	-1.2335035	3.5852755	1.9620203
60	C	-2.3855466	3.6360839	-0.1818095
61	C	-3.5767127	3.9963964	0.4700524
62	C	-2.4258817	3.9494125	2.6137511
63	H	-0.3136418	3.4405145	2.5508616
64	H	-2.3785623	3.5422452	-1.2780326
65	H	-4.4894321	4.1697991	-0.1183768
66	H	-2.4332446	4.0877571	3.7047703
67	H	-4.5295380	4.4537623	2.3739696
68	H	-4.0637937	-0.0982918	2.1736515
69	H	4.0762925	0.1186305	2.1470980

70	H	-3.1463488	-0.0082583	-2.1023465
71	H	-5.2710700	-0.0770236	-0.3187224
72	H	5.2674173	0.1064250	-0.3531433
73	H	3.1314938	0.0299776	-2.1229748

[Fe((*R*)-L^1*i*Pr)(bpp)]$^{2+}$ (**9**$^{2+}$), high-spin

1	Fe	-0.0028224	0.0020143	-0.3595998
2	N	-0.0070229	-0.0031200	1.8186920
3	C	1.1575291	0.0477959	2.4929488
4	C	1.2118205	0.0497372	3.8972441
5	C	-0.0116567	-0.0149215	4.5861103
6	H	-0.0134536	-0.0200085	5.6853578
7	C	-1.2327994	-0.0734292	3.8926034
8	H	-2.1829915	-0.1270987	4.4372063
9	C	-1.1738239	-0.0591945	2.4885333
10	N	2.2974567	0.0949744	1.6550305
11	N	2.1169308	0.0808081	0.2947943
12	C	3.3497835	0.1160911	-0.2319339
13	C	4.3427162	0.1533223	0.7822276
14	C	3.6365851	0.1383842	1.9769205
15	N	-2.3108201	-0.0985065	1.6463573
16	N	-2.1254816	-0.0763570	0.2867723
17	C	-3.3565465	-0.1045094	-0.2444096
18	C	-4.3531637	-0.1452329	0.7660237
19	C	-3.6512654	-0.1398404	1.9632554
20	N	0.0139692	0.0055813	-2.4833893
21	C	0.1302715	1.1709549	-3.1648660
22	C	0.1554611	1.2191793	-4.5703759
23	H	0.2568902	2.1829080	-5.0875202
24	C	0.0443829	0.0087938	-5.2806095
25	H	0.0563755	0.0100483	-6.3794939
26	C	-0.0824200	-1.2032196	-4.5757885
27	C	-0.0879629	-1.1581510	-3.1699970
28	C	0.2258994	2.3203266	-2.2482075
29	N	0.1292890	2.1512583	-0.9566663
30	C	0.3056164	3.4864440	-0.3239952
31	C	0.5030091	4.4344967	-1.5526339
32	O	0.4376623	3.5438146	-2.7221785
33	C	-0.2044062	-2.3099879	-2.2589063
34	N	-0.1353661	-2.1454198	-0.9650525
35	C	-0.3162455	-3.4842453	-0.3414253
36	C	-0.5134737	-4.4238038	-1.5766399
37	O	-0.4061328	-3.5317832	-2.7416680
38	H	2.1601047	0.0984586	4.4456294
39	H	-0.1727106	-2.1658146	-5.0970696
40	H	-0.2970905	5.1882184	-1.6739636
41	H	1.4848499	4.9411431	-1.5804110
42	H	0.2693689	-5.1972419	-1.6850267
43	H	-1.5072006	-4.9056723	-1.6234302
44	H	-1.2499256	-3.4490643	0.2598963
45	H	1.2392030	3.4475885	0.2776526
46	H	-5.4396814	-0.1751577	0.6388953
47	H	-3.4811066	-0.0974198	-1.3336180
48	H	3.4781372	0.1165845	-1.3207195
49	H	5.4295646	0.1875452	0.6590514
50	H	3.9869377	0.1555909	3.0134655
51	H	-4.0052695	-0.1622864	2.9984498
52	C	-0.8489704	3.8758896	0.6406433
53	H	-0.8629298	3.0718995	1.4103047
54	C	0.8390395	-3.8834924	0.6188991
55	H	0.8530798	-3.0900435	1.3993475
56	C	-2.2324644	3.9122797	-0.0299366

57	H	-3.0181532	4.0937121	0.7289946
58	H	-2.4743053	2.9598183	-0.5415272
59	H	-2.3196058	4.7324571	-0.7716902
60	C	-0.5211100	5.1985565	1.3601148
61	H	-1.2949265	5.4311088	2.1166552
62	H	-0.4926511	6.0569600	0.6579806
63	H	0.4563134	5.1563190	1.8812298
64	C	2.2205344	-3.9082373	-0.0560623
65	H	2.2990375	-4.7067246	-0.8222412
66	H	3.0081172	-4.1155516	0.6941681
67	H	2.4650546	-2.9424538	-0.5407685
68	C	0.5137110	-5.2164914	1.3198485
69	H	-0.4645663	-5.1839672	1.8400569
70	H	1.2869616	-5.4573118	2.0744109
71	H	0.4888591	-6.0653032	0.6060496

[Fe((*R*)-*L*^{1}*i*Pr)(bpp)]$^{2+}$ (**9**$^{2+}$), low-spin

1	Fe	-0.0010475	0.0000469	-0.3777457
2	N	0.0055196	0.0003662	1.5237218
3	C	-1.1681849	0.0045592	2.2032745
4	C	-1.2142780	0.0006473	3.6041252
5	C	0.0148738	-0.0004156	4.2917429
6	H	0.0185662	-0.0007504	5.3905400
7	C	1.2393666	-0.0010902	3.5958746
8	H	2.1950237	-0.0015107	4.1346604
9	C	1.1837962	-0.0042262	2.1953209
10	N	-2.2569792	0.0215713	1.3155215
11	N	-1.9441578	0.0578531	-0.0300620
12	C	-3.1193365	0.0658049	-0.6788917
13	C	-4.2017626	0.0409621	0.2414686
14	C	-3.6218706	0.0125896	1.5022576
15	N	2.2665356	-0.0210852	1.3001127
16	N	1.9447207	-0.0574111	-0.0433526
17	C	3.1155817	-0.0657647	-0.6999456
18	C	4.2041544	-0.0412818	0.2131731
19	C	3.6326432	-0.0126018	1.4777795
20	N	-0.0090724	-0.0011369	-2.2942220
21	C	-0.1362014	-1.1754776	-2.9728420
22	C	-0.1533759	-1.2154128	-4.3781118
23	H	-0.2650928	-2.1758191	-4.8991998
24	C	-0.0216254	-0.0023248	-5.0825570
25	H	-0.0265528	-0.0027750	-6.1814419
26	C	0.1163916	1.2113428	-4.3804048
27	C	0.1119336	1.1725630	-2.9750338
28	C	-0.2504342	-2.2706040	-2.0068050
29	N	-0.1504699	-1.9819293	-0.7301525
30	C	-0.2532666	-3.2649685	0.0221089
31	C	-0.6840006	-4.2659970	-1.0963592
32	O	-0.4721735	-3.5310478	-2.3573181
33	C	0.2344886	2.2686405	-2.0111915
34	N	0.1454286	1.9817419	-0.7333503
35	C	0.2546001	3.2658142	0.0164151
36	C	0.6729479	4.2660816	-1.1077811
37	O	0.4531696	3.5284430	-2.3656615
38	H	-2.1662429	0.0006653	4.1494263
39	H	0.2232991	2.1713551	-4.9032382
40	H	-0.0693248	-5.1821351	-1.1403954
41	H	-1.7545208	-4.5439687	-1.0609255
42	H	0.0540128	5.1796499	-1.1491261
43	H	1.7427903	4.5477133	-1.0814172
44	H	1.0680748	3.1676663	0.7639839
45	H	-1.0589481	-3.1655958	0.7778621

46	H	5.2720023	-0.0447288	-0.0256435
47	H	3.1356081	-0.0932459	-1.7949416
48	H	-5.2711817	0.0440789	0.0098020
49	H	-3.1465263	0.0932979	-1.7737236
50	H	-4.0665414	-0.0147725	2.5018983
51	H	4.0840465	0.0148597	2.4744021
52	C	1.0612055	-3.6437547	0.7675893
53	H	1.2894414	-2.7718365	1.4180745
54	C	-1.0523956	3.6450988	0.7748407
55	H	-1.2750684	2.7734252	1.4275895
56	C	0.8163021	-4.8554369	1.6875728
57	H	1.7305447	-5.0970453	2.2626817
58	H	0.5484843	-5.7652755	1.1131921
59	H	0.0021030	-4.6640375	2.4146954
60	C	2.2575607	-3.8675393	-0.1737866
61	H	3.1763294	-4.0576385	0.4137212
62	H	2.4525821	-2.9920012	-0.8232164
63	H	2.1128099	-4.7514980	-0.8263581
64	C	-0.7987996	4.8570117	1.6921980
65	H	0.0224019	4.6662780	2.4115490
66	H	-1.7075554	5.0984278	2.2760705
67	H	-0.5369755	5.7668204	1.1150306
68	C	-2.2575635	3.8699460	-0.1550141
69	H	-2.1179149	4.7542177	-0.8086174
70	H	-3.1707364	4.0601413	0.4410943
71	H	-2.4591629	2.9944596	-0.8025375

[Fe((*R*)-*L*^{2}*i*Pr)(bpp)]$^{2+}$ (**10**$^{2+}$), high-spin

1	Fe	0.0030290	0.0000404	-0.4179830
2	N	-0.0028265	0.0066003	1.7647294
3	C	0.4690081	1.0749336	2.4349091
4	C	0.4817811	1.1348756	3.8389683
5	C	-0.0145692	0.0178290	4.5331441
6	H	-0.0194022	0.0223958	5.6323478
7	C	-0.5049049	-1.1048952	3.8439085
8	H	-0.8875182	-1.9746156	4.3911009
9	C	-0.4802351	-1.0562518	2.4395180
10	N	0.9446607	2.1086232	1.5930796
11	N	0.8688577	1.9391707	0.2333972
12	C	1.3872927	3.0562228	-0.2976441
13	C	1.8089208	3.9596858	0.7133599
14	C	1.5120345	3.3239095	1.9105536
15	N	-0.9488803	-2.0964293	1.6017106
16	N	-0.8625001	-1.9367756	0.2413008
17	C	-1.3757970	-3.0582500	-0.2853543
18	C	-1.8049907	-3.9544847	0.7289067
19	C	-1.5177962	-3.3098000	1.9236502
20	N	0.0068701	-0.0006845	-2.5238899
21	C	-0.9879529	0.6236993	-3.2044157
22	C	-1.0125489	0.6528746	-4.6119084
23	H	-1.8214085	1.1710277	-5.1460981
24	C	0.0152119	0.0030843	-5.3181644
25	H	0.0186078	0.0048276	-6.4169513
26	C	1.0386671	-0.6488126	-4.6075490
27	C	1.0055149	-0.6236355	-3.2001245
28	C	-1.9883700	1.2391525	-2.3063679
29	N	-1.8547262	1.0819355	-1.0132341
30	C	-2.9509079	1.6924118	-0.2258870
31	C	-3.7769904	2.6310479	-1.1644589
32	S	-3.3348757	2.1848587	-2.9031171
33	C	2.0003409	-1.2414900	-2.2973527
34	N	1.8609080	-1.0834481	-1.0049943

35	C	2.9479908	-1.7002547	-0.2106983
36	C	3.7882910	-2.6300224	-1.1465489
37	S	3.3464883	-2.1914275	-2.8873690
38	H	0.8596342	2.0090214	4.3824117
39	H	1.8509144	-1.1650757	-5.1384160
40	H	-4.8689419	2.5052867	-1.0474050
41	H	-3.5331775	3.7004628	-1.0226439
42	H	4.8781446	-2.4876758	-1.0262677
43	H	3.5593544	-3.7025568	-1.0042925
44	H	2.4670411	-2.3352209	0.5632372
45	H	-2.4792456	2.3213635	0.5584764
46	H	1.6620641	3.6439206	2.9460894
47	H	-1.6758764	-3.6220929	2.9603472
48	H	-1.4187568	-3.1821615	-1.3738361
49	H	-2.2627670	-4.9407606	0.6054474
50	H	2.2685605	4.9446322	0.5862430
51	H	1.4395496	3.1716925	-1.3866408
52	C	3.7798736	-0.6171754	0.5449934
53	H	3.0229863	-0.0135150	1.0930039
54	C	-3.7895167	0.6024897	0.5130593
55	H	-3.0364800	-0.0027880	1.0647545
56	C	4.7018326	-1.2672624	1.5943342
57	H	5.4877571	-1.8946997	1.1273886
58	H	4.1390729	-1.9075302	2.3035231
59	H	5.2251507	-0.4894591	2.1833818
60	C	4.5498059	0.3321513	-0.3893121
61	H	5.3545608	-0.1894582	-0.9456040
62	H	5.0395604	1.1328003	0.1984191
63	H	3.8858299	0.8188035	-1.1301973
64	C	-4.5482352	-0.3438463	-0.4332375
65	H	-3.8769411	-0.8208449	-1.1736947
66	H	-5.3533002	0.1767684	-0.9898223
67	H	-5.0365853	-1.1520732	0.1452982
68	C	-4.7232037	1.2437142	1.5574510
69	H	-4.1697502	1.8821566	2.2755911
70	H	-5.2490508	0.4604320	2.1369429
71	H	-5.5071390	1.8705719	1.0865030

[Fe((*R*)-*L*^{2}*i*Pr)(bpp)]$^{2+}$ (**10**$^{2+}$), low-spin

1	Fe	-0.0011356	-0.0008340	-0.4716884
2	N	0.0070784	0.0008145	1.4330715
3	C	-1.1643308	-0.0562231	2.1142299
4	C	-1.2089791	-0.0619479	3.5151555
5	C	0.0189993	0.0033318	4.2017195
6	H	0.0237050	0.0044294	5.3004796
7	C	1.2410406	0.0671404	3.5045146
8	H	2.1959023	0.1183891	4.0422969
9	C	1.1843565	0.0587576	2.1039888
10	N	-2.2535341	-0.0897139	1.2273674
11	N	-1.9454585	-0.0263227	-0.1189726
12	C	-3.1215563	-0.0457978	-0.7652131
13	C	-4.2004231	-0.1190003	0.1568155
14	C	-3.6173366	-0.1419384	1.4161476
15	N	2.2658623	0.0907226	1.2076533
16	N	1.9463432	0.0252717	-0.1358892
17	C	3.1169029	0.0443982	-0.7921271
18	C	4.2035717	0.1193609	0.1205686
19	C	3.6311950	0.1435917	1.3847856
20	N	-0.0102542	-0.0019909	-2.3710829
21	C	-0.1052619	-1.1855565	-3.0430139
22	C	-0.1240403	-1.2181544	-4.4498056
23	H	-0.2118724	-2.1755554	-4.9819192

24	C	-0.0259087	-0.0033898	-5.1541757
25	H	-0.0321355	-0.0039395	-6.2529600
26	C	0.0800889	1.2120858	-4.4522024
27	C	0.0771415	1.1809544	-3.0452495
28	C	-0.1923352	-2.2962651	-2.0877193
29	N	-0.0846487	-1.9799586	-0.8113828
30	C	-0.1306297	-3.1596662	0.0902389
31	C	-0.7639193	-4.3314685	-0.7142699
32	S	-0.4824227	-3.9656724	-2.5110270
33	C	0.1743153	2.2926204	-2.0920325
34	N	0.0783717	1.9776563	-0.8143975
35	C	0.1313436	3.1587897	0.0851494
36	C	0.7603846	4.3283506	-0.7256242
37	S	0.4618253	3.9614178	-2.5194813
38	H	-2.1591450	-0.1122173	4.0613093
39	H	0.1615481	2.1689520	-4.9862766
40	H	-0.3070731	-5.3103200	-0.4815325
41	H	-1.8571724	-4.4109095	-0.5639799
42	H	0.3076493	5.3083905	-0.4896787
43	H	1.8551382	4.4053264	-0.5851612
44	H	0.8195924	2.9029934	0.9175939
45	H	-0.8139703	-2.9029717	0.9264555
46	H	-4.0589098	-0.1924629	2.4162876
47	H	4.0813319	0.1963750	2.3809917
48	H	-3.1517267	-0.0057297	-1.8595640
49	H	-5.2698297	-0.1485588	-0.0730078
50	H	5.2709352	0.1497374	-0.1184813
51	H	3.1378876	0.0032378	-1.8866650
52	C	1.2643391	-3.4759079	0.7208191
53	H	1.6052148	-2.5172370	1.1640793
54	C	-1.2596493	3.4774272	0.7234006
55	H	-1.5997829	2.5195763	1.1689851
56	C	-2.3305085	3.9257847	-0.2875326
57	H	-2.0715417	4.8903448	-0.7667572
58	H	-3.2984929	4.0737030	0.2295386
59	H	-2.4955240	3.1781669	-1.0876974
60	C	-1.1043349	4.4884086	1.8765432
61	H	-0.3668693	4.1506057	2.6325488
62	H	-2.0727895	4.6313446	2.3933013
63	H	-0.7856825	5.4873782	1.5169246
64	C	2.3300178	-3.9230793	-0.2960683
65	H	3.3006348	-4.0719376	0.2157886
66	H	2.4911245	-3.1742401	-1.0958822
67	H	2.0682876	-4.8869609	-0.7751946
68	C	1.1170577	-4.4865593	1.8752762
69	H	2.0883369	-4.6266317	2.3874757
70	H	0.7993735	-5.4865750	1.5177042
71	H	0.3822881	-4.1501412	2.6345076

$[Fe((R)\text{-}L^1Ph)(terpy)]^{2+}$ (**11**$^{2+}$), high-spin

1	Fe	0.0000001	-0.0000004	-0.5273675
2	N	-0.0000005	0.0000008	1.6002067
3	C	0.6792125	0.9693364	2.2599025
4	C	0.6950490	0.9974074	3.6696485
5	C	-0.0000012	0.0000022	4.3714899
6	H	-0.0000017	0.0000028	5.4707103
7	C	-0.6950509	-0.9974039	3.6696492
8	H	-1.2386644	-1.7762143	4.2183950
9	C	-0.6792137	-0.9693342	2.2599031
10	C	1.3816870	1.9546423	1.3864673
11	N	1.2556643	1.7471848	0.0450092
12	C	1.8730293	2.5808931	-0.8141132

13	C	2.1375168	3.0343229	1.8871336
14	C	-1.3816876	-1.9546413	1.3864686
15	N	-1.2556640	-1.7471853	0.0450103
16	C	-1.8730282	-2.5808947	-0.8141115
17	C	-2.1375174	-3.0343215	1.8871357
18	N	0.0000002	0.0000004	-2.6610204
19	C	-0.8724577	0.7808333	-3.3465937
20	C	-0.9016384	0.8179821	-4.7521889
21	H	-1.6179639	1.4690873	-5.2712894
22	C	0.0000012	0.0000024	-5.4604493
23	H	0.0000016	0.0000033	-6.5592787
24	C	0.9016402	-0.8179785	-4.7521894
25	C	0.8724583	-0.7808317	-3.3465943
26	C	-1.7495445	1.5320452	-2.4316469
27	N	-1.6417139	1.3755356	-1.1389696
28	C	-2.6998026	2.2112675	-0.5016136
29	C	-3.3231797	2.9664815	-1.7271480
30	O	-2.6662395	2.3748591	-2.9021423
31	C	1.7495449	-1.5320447	-2.4316480
32	N	1.6417140	-1.3755365	-1.1389705
33	C	2.6998026	-2.2112688	-0.5016149
34	C	3.3231797	-2.9664820	-1.7271498
35	O	2.6662399	-2.3748582	-2.9021438
36	H	1.2386624	1.7762183	4.2183939
37	H	1.6179660	-1.4690830	-5.2712905
38	H	-4.4113941	2.8073081	-1.8371677
39	H	-3.1055543	4.0510814	-1.7394688
40	H	4.4113942	-2.8073090	-1.8371692
41	H	3.1055538	-4.0510818	-1.7394718
42	H	2.2073256	-2.9277854	0.1858467
43	H	-2.2073256	2.9277835	0.1858486
44	C	-3.6969693	1.3845062	0.3037573
45	C	-5.6231568	-0.0647150	1.7814855
46	C	-4.4348958	0.3452236	-0.3063401
47	C	-3.9336119	1.6852723	1.6613258
48	C	-4.8919628	0.9650076	2.3975297
49	C	-5.3927928	-0.3734004	0.4275585
50	H	-4.2768925	0.0991392	-1.3681297
51	H	-3.3747997	2.5025742	2.1440381
52	H	-5.0793089	1.2213288	3.4503797
53	H	-5.9749448	-1.1680182	-0.0615970
54	H	-6.3844204	-0.6178229	2.3505101
55	C	3.6969692	-1.3845079	0.3037565
56	C	5.6231563	0.0647127	1.7814857
57	C	3.9336115	-1.6852744	1.6613250
58	C	4.4348958	-0.3452252	-0.3063404
59	C	5.3927926	0.3733985	0.4275588
60	C	4.8919621	-0.9650101	2.3975293
61	H	3.3747990	-2.5025765	2.1440369
62	H	4.2768928	-0.0991405	-1.3681300
63	H	5.9749446	1.1680166	-0.0615963
64	H	5.0793081	-1.2213317	3.4503793
65	H	6.3844198	0.6178203	2.3505107
66	H	-1.7453022	-2.3622706	-1.8854443
67	H	1.7453038	2.3622678	-1.8854458
68	H	2.2356563	3.1998630	2.9672732
69	H	-2.2356576	-3.1998603	2.9672754
70	C	2.7700874	3.9062222	0.9878703
71	H	3.3592527	4.7553563	1.3627176
72	H	3.1214396	4.3334644	-1.1290618
73	C	2.6405964	3.6768649	-0.3910814
74	C	-2.7700871	-3.9062221	0.9878730

75	H	-3.3592523	-4.7553558	1.3627208
76	H	-3.1214377	-4.3334668	-1.1290588
77	C	-2.6405952	-3.6768664	-0.3910789

[Fe((*R*)-*L*^{1}Ph)(terpy)]$^{2+}$ (**11**$^{2+}$), low-spin

1	Fe	-0.0000001	-0.0000003	-0.6390389
2	N	-0.0000002	0.0000000	1.2529053
3	C	0.7078237	0.9564512	1.9198275
4	C	0.7210322	0.9798531	3.3266421
5	C	-0.0000010	0.0000007	4.0302919
6	H	-0.0000015	0.0000013	5.1290110
7	C	-0.7210335	-0.9798522	3.3266423
8	H	-1.2889879	-1.7473828	3.8678247
9	C	-0.7078243	-0.9564510	1.9198276
10	C	1.3952611	1.8746670	0.9975507
11	N	1.2045524	1.5620193	-0.3291140
12	C	1.7886832	2.3389305	-1.2702378
13	C	2.1703006	2.9830376	1.3849145
14	C	-1.3952613	-1.8746673	0.9975509
15	N	-1.2045524	-1.5620197	-0.3291139
16	C	-1.7886831	-2.3389312	-1.2702375
17	C	-2.1703005	-2.9830379	1.3849148
18	N	0.0000000	0.0000000	-2.5546409
19	C	-0.8928873	0.7739906	-3.2369871
20	C	-0.9197884	0.8034555	-4.6424517
21	H	-1.6464454	1.4398145	-5.1653265
22	C	0.0000009	0.0000011	-5.3463460
23	H	0.0000014	0.0000017	-6.4450926
24	C	0.9197895	-0.8034541	-4.6424517
25	C	0.8928876	-0.7739903	-3.2369872
26	C	-1.7238943	1.4914349	-2.2687958
27	N	-1.5104640	1.2612634	-0.9929328
28	C	-2.4931153	2.0739386	-0.2162945
29	C	-3.1803638	2.9197741	-1.3454850
30	O	-2.6634569	2.3658094	-2.6090138
31	C	1.7238944	-1.4914348	-2.2687958
32	N	1.5104639	-1.2612638	-0.9929329
33	C	2.4931151	-2.0739390	-0.2162947
34	C	3.1803635	-2.9197745	-1.3454852
35	O	2.6634572	-2.3658091	-2.6090140
36	H	1.2889861	1.7473841	3.8678246
37	H	1.6464470	-1.4398126	-5.1653266
38	H	-4.2801857	2.8189759	-1.3609786
39	H	-2.9062286	3.9913102	-1.3227242
40	H	4.2801855	-2.8189769	-1.3609785
41	H	2.9062277	-3.9913105	-1.3227249
42	H	1.9309760	-2.7367179	0.4710203
43	H	-1.9309761	2.7367175	0.4710204
44	C	-3.4562155	1.2294472	0.6116893
45	C	-5.3373840	-0.2169010	2.1494546
46	C	-4.3476749	0.3261796	-0.0103020
47	C	-3.5156854	1.3941731	2.0112471
48	C	-4.4525651	0.6765242	2.7771459
49	C	-5.2807315	-0.3934312	0.7538005
50	H	-4.3307777	0.1915594	-1.1033403
51	H	-2.8344042	2.1041972	2.5061891
52	H	-4.5034938	0.8305401	3.8648134
53	H	-5.9795183	-1.0822540	0.2572981
54	H	-6.0824627	-0.7650618	2.7440509
55	C	3.4562155	-1.2294476	0.6116889
56	C	5.3373841	0.2169010	2.1494537
57	C	3.5156854	-1.3941730	2.0112468

58	C	4.3476750	-0.3261803	-0.0103028
59	C	5.2807316	0.3934306	0.7537994
60	C	4.4525652	-0.6765240	2.7771452
61	H	2.8344041	-2.1041969	2.5061890
62	H	4.3307778	-0.1915604	-1.1033411
63	H	5.9795187	1.0822531	0.2572968
64	H	4.5034939	-0.8305395	3.8648128
65	H	6.0824629	0.7650618	2.7440497
66	H	-1.6221094	-2.0557877	-2.3183121
67	H	1.6221097	2.0557868	-2.3183122
68	H	2.3047305	3.2143395	2.4495001
69	H	-2.3047305	-3.2143397	2.4495004
70	C	2.7642558	3.7880333	0.4022884
71	H	3.3693352	4.6600735	0.6873616
72	H	3.0178339	4.0554757	-1.7547069
73	C	2.5705987	3.4572497	-0.9491574
74	C	-2.7642557	-3.7880338	0.4022888
75	H	-3.3693347	-4.6600742	0.6873619
76	H	-3.0178336	-4.0554767	-1.7547065
77	C	-2.5705985	-3.4572504	-0.9491571

[Fe((*R*)-*L*^{2}Ph)(terpy)]$^{2+}$, high-spin

1	Fe	0.0000001	-0.0000010	-0.6120387
2	N	-0.0000003	-0.0000007	1.5176862
3	C	0.6023782	1.0188772	2.1776722
4	C	0.6146331	1.0489026	3.5875689
5	C	-0.0000008	-0.0000002	4.2895013
6	H	-0.0000008	-0.0000001	5.3887424
7	C	-0.6146346	-1.0489032	3.5875691
8	H	-1.0961747	-1.8679716	4.1357195
9	C	-0.6023790	-1.0188785	2.1776722
10	C	1.2236460	2.0573947	1.3050394
11	N	1.1208862	1.8367491	-0.0362453
12	C	1.6648931	2.7201272	-0.8956016
13	C	1.8824826	3.1985445	1.8059676
14	C	-1.2236466	-2.0573962	1.3050395
15	N	-1.1208871	-1.8367502	-0.0362452
16	C	-1.6648948	-2.7201277	-0.8956015
17	C	-1.8824827	-3.1985462	1.8059678
18	N	0.0000003	-0.0000006	-2.7243646
19	C	-0.9279561	0.7232533	-3.4058425
20	C	-0.9517502	0.7547357	-4.8131536
21	H	-1.7029299	1.3555536	-5.3451745
22	C	-0.0000003	0.0000002	-5.5223723
23	H	-0.0000008	0.0000005	-6.6210427
24	C	0.9517498	-0.7547359	-4.8131550
25	C	0.9279563	-0.7232542	-3.4058438
26	C	-1.8599937	1.4316743	-2.5048369
27	N	-1.7102147	1.2829164	-1.2123522
28	C	-2.7304942	1.9931138	-0.4069654
29	C	-3.5185274	2.9713494	-1.3501921
30	S	-3.1495620	2.4644581	-3.0899297
31	C	1.8599956	-1.4316761	-2.5048405
32	N	1.7102155	-1.2829180	-1.2123545
33	C	2.7304964	-1.9931166	-0.4069658
34	C	3.5185302	-2.9713498	-1.3501951
35	S	3.1495638	-2.4644575	-3.0899309
36	H	1.0961728	1.8679712	4.1357191
37	H	1.7029292	-1.3555533	-5.3451764
38	H	-4.6111575	2.9171674	-1.1928145
39	H	-3.1949231	4.0229179	-1.2333952
40	H	4.6111604	-2.9171668	-1.1928167

41	H	3.1949270	-4.0229189	-1.2333983
42	H	2.1922624	-2.6033172	0.3464113
43	H	-2.1922608	2.6033132	0.3464110
44	C	-3.6372538	1.0230810	0.3510454
45	C	-5.4493388	-0.6309932	1.7569818
46	C	-4.3608120	0.0158713	-0.3274249
47	C	-3.8277059	1.1851076	1.7396662
48	C	-4.7285589	0.3632203	2.4406493
49	C	-5.2630535	-0.8026184	0.3721918
50	H	-4.2415461	-0.1171835	-1.4136291
51	H	-3.2854824	1.9803685	2.2753175
52	H	-4.8815752	0.5133255	3.5192817
53	H	-5.8375777	-1.5695608	-0.1676377
54	H	-6.1687725	-1.2625226	2.2981514
55	C	3.6372548	-1.0230812	0.3510446
56	C	5.4493372	0.6309976	1.7569821
57	C	3.8277063	-1.1851056	1.7396661
58	C	4.3608139	-0.0158711	-0.3274254
59	C	5.2630535	0.8026208	0.3721923
60	C	4.7285580	-0.3632158	2.4406492
61	H	3.2854829	-1.9803671	2.2753180
62	H	4.2415494	0.1171823	-1.4136306
63	H	5.8375771	1.5695633	-0.1676373
64	H	4.8815726	-0.5133198	3.5192819
65	H	6.1687689	1.2625283	2.2981518
66	H	1.9619630	3.3743231	2.8860359
67	H	1.5591771	2.4901768	-1.9668662
68	H	-1.5591793	-2.4901770	-1.9668661
69	H	-1.9619626	-3.3743252	2.8860361
70	C	2.4401431	4.1202757	0.9068025
71	H	2.9527777	5.0176119	1.2818164
72	H	2.7580625	4.5730738	-1.2102717
73	C	2.3342716	3.8786116	-0.4720309
74	C	-2.3342730	-3.8786125	-0.4720311
75	H	-2.7580641	-4.5730744	-1.2102719
76	C	-2.4401434	-4.1202773	0.9068024
77	H	-2.9527777	-5.0176139	1.2818162

$[Fe((R)\text{-}L^2Ph)(terpy)]^{2+}$, low-spin

1	Fe	0.0000000	0.0000001	-0.6697074
2	N	0.0000001	0.0000002	1.2252677
3	C	0.5963865	1.0302524	1.8922222
4	C	0.6015700	1.0580664	3.2990646
5	C	0.0000002	0.0000004	4.0023153
6	H	0.0000001	0.0000005	5.1010682
7	C	-0.6015696	-1.0580656	3.2990648
8	H	-1.0770656	-1.8859818	3.8403238
9	C	-0.5963862	-1.0302520	1.8922224
10	C	1.1993931	2.0057993	0.9704010
11	N	1.0531281	1.6689306	-0.3563077
12	C	1.5917515	2.4798702	-1.2959974
13	C	1.8746649	3.1772280	1.3584382
14	C	-1.1993928	-2.0057989	0.9704014
15	N	-1.0531278	-1.6689306	-0.3563074
16	C	-1.5917511	-2.4798705	-1.2959968
17	C	-1.8746645	-3.1772276	1.3584388
18	N	-0.0000001	0.0000002	-2.5696647
19	C	-0.9633837	0.6942020	-3.2459793
20	C	-0.9861700	0.7175739	-4.6531376
21	H	-1.7608068	1.2866950	-5.1853857
22	C	-0.0000001	0.0000004	-5.3567527
23	H	0.0000001	0.0000005	-6.4554692

24	C	0.9861699	-0.7175733	-4.6531377
25	C	0.9633835	-0.6942017	-3.2459794
26	C	-1.8536788	1.3608382	-2.2916684
27	N	-1.6049546	1.1424662	-1.0133864
28	C	-2.5528795	1.8425399	-0.1023461
29	C	-3.2801542	2.9443158	-0.9404928
30	S	-3.1609701	2.4404210	-2.7200586
31	C	1.8536787	-1.3608379	-2.2916686
32	N	1.6049546	-1.1424661	-1.0133866
33	C	2.5528794	-1.8425400	-0.1023463
34	C	3.2801541	-2.9443158	-0.9404932
35	S	3.1609701	-2.4404206	-2.7200590
36	H	1.0770660	1.8859826	3.8403234
37	H	1.7608067	-1.2866944	-5.1853859
38	H	-4.3473149	3.0377557	-0.6703129
39	H	-2.7969532	3.9356128	-0.8463219
40	H	4.3473147	-3.0377558	-0.6703133
41	H	2.7969530	-3.9356128	-0.8463226
42	H	1.9441773	-2.3457270	0.6749664
43	H	-1.9441777	2.3457267	0.6749669
44	C	-3.5142758	0.8879450	0.6056254
45	C	-5.4046895	-0.7258473	1.9536649
46	C	-4.3410513	-0.0017940	-0.1185774
47	C	-3.6467004	0.9568808	2.0092952
48	C	-4.5869471	0.1557229	2.6813923
49	C	-5.2795429	-0.8022658	0.5536619
50	H	-4.2740158	-0.0553218	-1.2157164
51	H	-3.0184096	1.6578336	2.5816653
52	H	-4.6912551	0.2317939	3.7734489
53	H	-5.9291688	-1.4800756	-0.0192265
54	H	-6.1509981	-1.3435141	2.4739506
55	C	3.5142756	-0.8879454	0.6056255
56	C	5.4046891	0.7258466	1.9536656
57	C	3.6467001	-0.9568816	2.0092952
58	C	4.3410512	0.0017938	-0.1185769
59	C	5.2795427	0.8022654	0.5536625
60	C	4.5869467	-0.1557237	2.6813927
61	H	3.0184094	-1.6578345	2.5816652
62	H	4.2740157	0.0553219	-1.2157159
63	H	5.9291686	1.4800754	-0.0192256
64	H	4.6912545	-0.2317950	3.7734492
65	H	6.1509976	1.3435133	2.4739515
66	H	1.9766057	3.4256601	2.4227878
67	H	1.4672873	2.1751883	-2.3437790
68	H	-1.4672869	-2.1751888	-2.3437785
69	H	-1.9766052	-3.4256595	2.4227885
70	C	2.4181517	4.0186704	0.3772989
71	H	2.9468337	4.9386210	0.6636969
72	H	2.6899608	4.2832202	-1.7781736
73	C	2.2765462	3.6600356	-0.9735699
74	C	-2.2765458	-3.6600359	-0.9735691
75	H	-2.6899605	-4.2832207	-1.7781726
76	C	-2.4181514	-4.0186702	0.3772997
77	H	-2.9468334	-4.9386207	0.6636980

[Fe((*R*)-*L*^{1}*i*Pr)(terpy)]$^{2+}$ (**12**$^{2+}$), high-spin

1	Fe	-0.0000009	-0.0000008	-0.3094465
2	N	0.0000006	-0.0000011	1.8194212
3	C	0.3044164	1.1435564	2.4834594
4	C	0.3048266	1.1757307	3.8933872
5	C	0.0000031	-0.0000021	4.5967526
6	H	0.0000041	-0.0000025	5.6958889

7	C	-0.3048218	-1.1757344	3.8933870
8	H	-0.5425131	-2.0957119	4.4414776
9	C	-0.3044141	-1.1435589	2.4834592
10	C	0.6449315	2.3055409	1.6127303
11	N	0.6102040	2.0649483	0.2704754
12	C	0.9389332	3.0525749	-0.5861936
13	C	1.0004583	3.5745699	2.1150422
14	C	-0.6449311	-2.3055426	1.6127298
15	N	-0.6102053	-2.0649488	0.2704751
16	C	-0.9389359	-3.0525747	-0.5861940
17	C	-1.0004577	-3.5745721	2.1150413
18	N	0.0000000	-0.0000009	-2.4481939
19	C	-1.0685167	0.4794098	-3.1295364
20	C	-1.1093064	0.5035000	-4.5354658
21	H	-1.9905955	0.9034461	-5.0548834
22	C	0.0000004	-0.0000011	-5.2424270
23	H	0.0000006	-0.0000009	-6.3414100
24	C	1.1093069	-0.5035022	-4.5354654
25	C	1.0685168	-0.4794119	-3.1295360
26	C	-2.1277484	0.9453431	-2.2140391
27	N	-1.9869691	0.8319228	-0.9213941
28	C	-3.2223370	1.3716204	-0.2943675
29	C	-4.0382941	1.8947624	-1.5220193
30	O	-3.2359650	1.5029394	-2.6934141
31	C	2.1277486	-0.9453446	-2.2140388
32	N	1.9869694	-0.8319239	-0.9213939
33	C	3.2223378	-1.3716201	-0.2943661
34	C	4.0382956	-1.8947625	-1.5220173
35	O	3.2359659	-1.5029403	-2.6934126
36	H	0.5425186	2.0957080	4.4414781
37	H	1.9905962	-0.9034481	-5.0548827
38	H	-5.0340457	1.4282983	-1.6376289
39	H	-4.1478700	2.9946148	-1.5553453
40	H	5.0340468	-1.4282978	-1.6376271
41	H	4.1478718	-2.9946148	-1.5553427
42	H	2.9265056	-2.2211738	0.3567727
43	H	-2.9265041	2.2211745	0.3567703
44	H	-0.8999306	-2.8056085	-1.6583275
45	H	0.8999266	2.8056093	-1.6583271
46	H	1.0220149	3.7655755	3.1953152
47	H	-1.0220128	-3.7655783	3.1953142
48	C	1.3350130	4.6011143	1.2186433
49	H	1.6139417	5.5955600	1.5953730
50	H	1.5692697	5.1096885	-0.8972572
51	C	1.3102720	4.3371059	-0.1604385
52	C	-1.3350138	-4.6011158	1.2186425
53	H	-1.6139423	-5.5955616	1.5953718
54	H	-1.5692735	-5.1096882	-0.8972581
55	C	-1.3102747	-4.3371062	-0.1604390
56	C	3.9537642	-0.3316286	0.6019339
57	H	3.1965357	-0.0145288	1.3531118
58	C	-3.9537651	0.3316309	0.6019333
59	H	-3.1965376	0.0145306	1.3531118
60	C	5.1117419	-1.0015944	1.3654342
61	H	5.5773753	-0.2853524	2.0693778
62	H	5.9147774	-1.3496966	0.6834322
63	H	4.7678488	-1.8754347	1.9547449
64	C	4.4140875	0.9199236	-0.1643093
65	H	4.8248314	1.6725243	0.5366303
66	H	3.5820604	1.3987208	-0.7181617
67	H	5.2219373	0.6929100	-0.8898519
68	C	-4.4140905	-0.9199213	-0.1643085

69	H	-3.5820639	-1.3987216	-0.7181589
70	H	-5.2219389	-0.6929068	-0.8898525
71	H	-4.8248377	-1.6725195	0.5366318
72	C	-5.1117419	1.0015996	1.3654326
73	H	-4.7678477	1.8754405	1.9547417
74	H	-5.5773761	0.2853594	2.0693775
75	H	-5.9147771	1.3497018	0.6834301

[Fe((*R*)-*L*^{1}*i*Pr)(terpy)]$^{2+}$ (**12**$^{2+}$), low-spin

1	Fe	0.0000001	-0.0000001	-0.3561786
2	N	-0.0000002	0.0000003	1.5370562
3	C	0.4002546	1.1208128	2.2061608
4	C	0.4045537	1.1472632	3.6133485
5	C	-0.0000016	0.0000012	4.3176914
6	H	-0.0000022	0.0000015	5.4163874
7	C	-0.4045561	-1.1472613	3.6133489
8	H	-0.7216455	-2.0475841	4.1551989
9	C	-0.4002555	-1.1208119	2.2061612
10	C	0.8044575	2.1944110	1.2836265
11	N	0.7235770	1.8327152	-0.0430560
12	C	1.0757135	2.7407071	-0.9833864
13	C	1.2383256	3.4759960	1.6709006
14	C	-0.8044576	-2.1944106	1.2836272
15	N	-0.7235766	-1.8327154	-0.0430556
16	C	-1.0757126	-2.7407078	-0.9833857
17	C	-1.2383256	-3.4759956	1.6709015
18	N	-0.0000001	-0.0000001	-2.2773404
19	C	-1.0620436	0.5178762	-2.9588928
20	C	-1.0962282	0.5388289	-4.3643459
21	H	-1.9627913	0.9657355	-4.8870363
22	C	0.0000000	0.0000009	-5.0677561
23	H	0.0000002	0.0000014	-6.1665963
24	C	1.0962281	-0.5388276	-4.3643462
25	C	1.0620434	-0.5178759	-2.9588932
26	C	-2.0455216	1.0061949	-1.9912031
27	N	-1.8003211	0.8121195	-0.7152760
28	C	-2.9541009	1.3692255	0.0470106
29	C	-3.7395921	2.1318549	-1.0642176
30	O	-3.1521127	1.6567071	-2.3306155
31	C	2.0455217	-1.0061948	-1.9912037
32	N	1.8003214	-0.8121201	-0.7152765
33	C	2.9541013	-1.3692263	0.0470097
34	C	3.7395927	-2.1318548	-1.0642192
35	O	3.1521129	-1.6567065	-2.3306166
36	H	0.7216428	2.0475863	4.1551983
37	H	1.9627913	-0.9657337	-4.8870368
38	H	-4.8197593	1.9041493	-1.0932307
39	H	-3.6002560	3.2296477	-1.0370019
40	H	4.8197598	-1.9041486	-1.0932323
41	H	3.6002573	-3.2296477	-1.0370040
42	H	2.5595177	-2.0813793	0.8000897
43	H	-2.5595172	2.0813777	0.8000913
44	H	-1.0031165	-2.4225374	-2.0321766
45	H	1.0031177	2.4225364	-2.0321772
46	H	1.2918909	3.7394982	2.7353122
47	H	-1.2918913	-3.7394974	2.7353132
48	C	1.5981024	4.4101698	0.6888879
49	H	1.9373455	5.4160526	0.9734512
50	H	1.7910237	4.7267397	-1.4679127
51	C	1.5167866	4.0322298	-0.6620750
52	C	-1.5981019	-4.4101698	0.6888891
53	H	-1.9373449	-5.4160525	0.9734528

54	H	-1.7910223	-4.7267407	-1.4679113
55	C	-1.5167857	-4.0322305	-0.6620739
56	C	-3.7719994	0.2811379	0.8021610
57	H	-3.0303838	-0.2576360	1.4286393
58	C	3.7719996	-0.2811391	0.8021609
59	H	3.0303838	0.2576340	1.4286398
60	C	-4.7863239	0.9496222	1.7500965
61	H	-4.2890919	1.6121287	2.4867592
62	H	-5.3536706	0.1842253	2.3135364
63	H	-5.5301231	1.5593314	1.1974169
64	C	-4.4435654	-0.7436343	-0.1297607
65	H	-3.7231124	-1.2104460	-0.8303899
66	H	-5.2599067	-0.2918802	-0.7286502
67	H	-4.9036056	-1.5562252	0.4649986
68	C	4.4435652	0.7436340	-0.1297600
69	H	4.9036036	1.5562255	0.4649997
70	H	3.7231124	1.2104447	-0.8303901
71	H	5.2599079	0.2918810	-0.7286485
72	C	4.7863243	-0.9496239	1.7500957
73	H	5.3536705	-0.1842272	2.3135365
74	H	5.5301240	-1.5593320	1.1974157
75	H	4.2890926	-1.6121314	2.4867578

$[Fe((R)\text{-}L^2i\text{Pr})(terpy)]^{2+}$, high-spin

1	Fe	-0.0000003	0.0000001	-0.3520055
2	N	0.0000002	0.0000003	1.7840169
3	C	0.1413320	1.1752286	2.4485814
4	C	0.1411504	1.2064707	3.8584749
5	C	0.0000018	0.0000005	4.5617444
6	H	0.0000025	0.0000006	5.6608674
7	C	-0.1411477	-1.2064697	3.8584753
8	H	-0.2538280	-2.1498025	4.4070087
9	C	-0.1413309	-1.1752280	2.4485818
10	C	0.3089094	2.3735800	1.5764341
11	N	0.3024046	2.1257645	0.2346784
12	C	0.4849702	3.1457768	-0.6274863
13	C	0.4867585	3.6811884	2.0730355
14	C	-0.3089092	-2.3735796	1.5764349
15	N	-0.3024054	-2.1257644	0.2346790
16	C	-0.4849717	-3.1457770	-0.6274854
17	C	-0.4867580	-3.6811876	2.0730367
18	N	-0.0000001	0.0000003	-2.4763776
19	C	-1.1303330	0.3262369	-3.1538572
20	C	-1.1646011	0.3474037	-4.5614048
21	H	-2.0854292	0.6250726	-5.0934171
22	C	0.0000004	0.0000019	-5.2694794
23	H	0.0000005	0.0000026	-6.3683300
24	C	1.1646016	-0.3474009	-4.5614049
25	C	1.1303331	-0.3262357	-3.1538573
26	C	-2.2626005	0.6356882	-2.2522011
27	N	-2.0870329	0.5207884	-0.9602100
28	C	-3.3170999	0.7684334	-0.1762245
29	C	-4.3445109	1.4991211	-1.0966425
30	S	-3.8245408	1.1669024	-2.8419985
31	C	2.2626004	-0.6356879	-2.2522011
32	N	2.0870327	-0.5207886	-0.9602098
33	C	3.3170993	-0.7684342	-0.1762241
34	C	4.3445102	-1.4991219	-1.0966422
35	S	3.8245407	-1.1669020	-2.8419983
36	H	0.2538316	2.1498035	4.4070080
37	H	2.0854299	-0.6250692	-5.0934172
38	H	-5.3802519	1.1355747	-0.9635751

39	H	-4.3408786	2.5963288	-0.9544921
40	H	5.3802513	-1.1355761	-0.9635743
41	H	4.3408772	-2.5963297	-0.9544924
42	H	3.0474521	-1.4538318	0.6546203
43	H	-3.0474530	1.4538308	0.6546201
44	H	0.4864057	3.8776662	3.1525655
45	H	0.4733451	2.8892889	-1.6978340
46	H	-0.4733476	-2.8892893	-1.6978331
47	H	-0.4864044	-3.8776652	3.1525667
48	C	0.6706256	4.7407835	1.1708833
49	H	0.8092488	5.7659233	1.5430900
50	H	0.8215975	5.2695794	-0.9477082
51	C	0.6767638	4.4709290	-0.2074555
52	C	-0.6767652	-4.4709290	-0.2074543
53	H	-0.8215996	-5.2695795	-0.9477066
54	C	-0.6706260	-4.7407830	1.1708847
55	H	-0.8092489	-5.7659228	1.5430919
56	C	3.8336388	0.5520721	0.4812446
57	H	2.9450042	0.9693027	1.0036697
58	C	-3.8336391	-0.5520733	0.4812438
59	H	-2.9450045	-0.9693035	1.0036693
60	C	-4.3211565	-1.6076657	-0.5274358
61	H	-3.5658670	-1.8335941	-1.3058054
62	H	-5.2546168	-1.2971490	-1.0377216
63	H	-4.5482418	-2.5558022	-0.0018953
64	C	-4.9029252	-0.2491953	1.5474952
65	H	-4.5419482	0.4739331	2.3064103
66	H	-5.1939255	-1.1760225	2.0786048
67	H	-5.8291648	0.1658917	1.1003394
68	C	4.9029243	0.2491935	1.5474963
69	H	5.1939247	1.1760203	2.0786063
70	H	5.8291639	-0.1658939	1.1003409
71	H	4.5419466	-0.4739350	2.3064110
72	C	4.3211570	1.6076646	-0.5274347
73	H	4.5482424	2.5558009	-0.0018938
74	H	3.5658678	1.8335935	-1.3058044
75	H	5.2546174	1.2971476	-1.0377201

[Fe((*R*)-*L*^{2}*i*Pr)(terpy)]$^{2+}$, low-spin

1	Fe	0.0000001	0.0000002	-0.4524618
2	N	0.0000003	0.0000003	1.4418778
3	C	0.1651058	1.1791177	2.1113995
4	C	0.1656450	1.2053041	3.5185984
5	C	0.0000007	0.0000004	4.2222886
6	H	0.0000010	0.0000004	5.3210058
7	C	-0.1656439	-1.2053034	3.5185985
8	H	-0.3010067	-2.1497562	4.0613447
9	C	-0.1651051	-1.1791171	2.1113997
10	C	0.3515291	2.3108239	1.1886046
11	N	0.3528719	1.9385347	-0.1384019
12	C	0.5437944	2.8926233	-1.0794969
13	C	0.5325893	3.6521148	1.5733864
14	C	-0.3515290	-2.3108233	1.1886049
15	N	-0.3528718	-1.9385343	-0.1384017
16	C	-0.5437947	-2.8926229	-1.0794965
17	C	-0.5325895	-3.6521143	1.5733867
18	N	-0.0000001	0.0000002	-2.3585142
19	C	-1.1467676	0.3029367	-3.0342912
20	C	-1.1771094	0.3169733	-4.4415952
21	H	-2.1045301	0.5701228	-4.9737590
22	C	-0.0000001	0.0000002	-5.1456185
23	H	-0.0000001	0.0000002	-6.2443681

24	C	1.1771093	-0.3169729	-4.4415952
25	C	1.1467675	-0.3029364	-3.0342912
26	C	-2.2178638	0.6099235	-2.0817352
27	N	-1.9227988	0.4746338	-0.8019622
28	C	-3.0627303	0.7973781	0.0965870
29	C	-4.0969625	1.6135737	-0.7350701
30	S	-3.7980652	1.2084209	-2.5194993
31	C	2.2178638	-0.6099232	-2.0817352
32	N	1.9227987	-0.4746337	-0.8019622
33	C	3.0627301	-0.7973784	0.0965869
34	C	4.0969624	-1.6135739	-0.7350703
35	S	3.7980651	-1.2084206	-2.5194995
36	H	0.3010079	2.1497569	4.0613444
37	H	2.1045300	-0.5701223	-4.9737590
38	H	-5.1436771	1.3566143	-0.4920291
39	H	-3.9697193	2.7067625	-0.6212009
40	H	5.1436769	-1.3566143	-0.4920294
41	H	3.9697193	-2.7067626	-0.6212013
42	H	2.6663538	-1.4548694	0.8974288
43	H	-2.6663541	1.4548689	0.8974292
44	H	0.5234674	3.9268520	2.6364702
45	H	0.5451627	2.5602756	-2.1261926
46	H	-0.5451631	-2.5602754	-2.1261923
47	H	-0.5234673	-3.9268514	2.6364706
48	C	0.7243280	4.6336295	0.5902562
49	H	0.8667560	5.6856940	0.8744971
50	H	0.8844564	4.9758657	-1.5651416
51	C	0.7325584	4.2446694	-0.7595501
52	C	-0.7325590	-4.2446690	-0.7595495
53	H	-0.8844573	-4.9758654	-1.5651410
54	C	-0.7243286	-4.6336291	0.5902568
55	H	-0.8667567	-5.6856936	0.8744979
56	C	3.6464369	0.4683991	0.8006152
57	H	2.7704690	0.9694550	1.2617020
58	C	-3.6464370	-0.4683997	0.8006148
59	H	-2.7704689	-0.9694556	1.2617014
60	C	4.5861819	0.0499572	1.9481528
61	H	4.9310659	0.9412467	2.5063472
62	H	5.4944156	-0.4675223	1.5781111
63	H	4.0823926	-0.6259595	2.6681445
64	C	4.3178642	1.4718424	-0.1532014
65	H	4.6226704	2.3780363	0.4056519
66	H	3.6451298	1.7995009	-0.9701330
67	H	5.2358782	1.0580412	-0.6161411
68	C	-4.3178640	-1.4718429	-0.1532023
69	H	-3.6451294	-1.7995009	-0.9701340
70	H	-5.2358780	-1.0580416	-0.6161421
71	H	-4.6226700	-2.3780370	0.4056506
72	C	-4.5861823	-0.0499585	1.9481523
73	H	-4.0823931	0.6259581	2.6681443
74	H	-4.9310660	-0.9412483	2.5063465
75	H	-5.4944159	0.4675209	1.5781108

Table S14 Atomic coordinates for the DFT-minimised metal-free ligands. Other minimised ligands in Table S11 are taken from ref. 2 and 13.

L^1Ph

1	N	0.0000000	0.0000001	1.7009392
2	C	1.1222450	0.2657104	2.3907377
3	C	1.1767054	0.2730672	3.8065004
4	H	2.1226235	0.4910608	4.3180646
5	C	0.0000001	0.0000000	4.5171908
6	H	0.0000001	0.0000000	5.6168732
7	C	-1.1767053	-0.2730672	3.8065005
8	C	-1.1222450	-0.2657104	2.3907377
9	C	2.3444953	0.5769299	1.5972593
10	N	2.4440199	0.5916648	0.3156683
11	C	3.8163545	1.0153128	0.0046995
12	C	4.5467703	0.9845421	1.3902539
13	O	3.4614732	0.8793451	2.3445946
14	C	-2.3444954	-0.5769298	1.5972593
15	N	-2.4440199	-0.5916647	0.3156683
16	C	-3.8163545	-1.0153128	0.0046995
17	C	-4.5467704	-0.9845421	1.3902538
18	O	-3.4614732	-0.8793451	2.3445946
19	H	-2.1226234	-0.4910608	4.3180647
20	H	5.2034317	0.0954229	1.4997882
21	H	5.1299196	1.8964614	1.6197701
22	H	-5.2034316	-0.0954229	1.4997882
23	H	-5.1299196	-1.8964614	1.6197700
24	H	-3.7574704	-2.0654679	-0.3665231
25	H	3.7574704	2.0654679	-0.3665231
26	C	4.4935236	0.1896039	-1.0823569
27	C	5.7928575	-1.3145608	-3.0968491
28	C	5.7703766	0.5685830	-1.5535568
29	C	3.8723280	-0.9480565	-1.6360921
30	C	4.5197696	-1.6939658	-2.6374590
31	C	6.4182103	-0.1790807	-2.5505645
32	H	6.2621413	1.4661718	-1.1456957
33	H	2.8704716	-1.2270308	-1.2807490
34	H	4.0217025	-2.5772731	-3.0646623
35	H	7.4117286	0.1303162	-2.9080280
36	H	6.2952239	-1.8983445	-3.8823017
37	C	-4.4935236	-0.1896039	-1.0823569
38	C	-5.7928576	1.3145608	-3.0968491
39	C	-5.7703766	-0.5685830	-1.5535568
40	C	-3.8723281	0.9480565	-1.6360921
41	C	-4.5197696	1.6939659	-2.6374590
42	C	-6.4182102	0.1790806	-2.5505646
43	H	-6.2621412	-1.4661719	-1.1456958
44	H	-2.8704717	1.2270309	-1.2807490
45	H	-4.0217026	2.5772731	-3.0646622
46	H	-7.4117285	-0.1303163	-2.9080280
47	H	-6.2952240	1.8983445	-3.8823017

L^1*i*Pr

1	N	0.0000001	-0.0000001	1.0856665
2	C	1.1356937	0.2055958	1.7742872
3	C	1.1890854	0.2165795	3.1898707
4	H	2.1433996	0.3921364	3.7024918
5	C	-0.0000002	0.0000007	3.8998861
6	H	-0.0000004	0.0000011	4.9998364
7	C	-1.1890857	-0.2165785	3.1898706
8	C	-1.1356938	-0.2055956	1.7742870
9	C	2.3755668	0.4262015	0.9769113

10	N	2.4621594	0.4697031	-0.3045022
11	C	3.8777413	0.6971412	-0.6312776
12	C	4.5968770	0.7501117	0.7575976
13	O	3.5224919	0.5962790	1.7199123
14	C	-2.3755667	-0.4262016	0.9769110
15	N	-2.4621592	-0.4697031	-0.3045025
16	C	-3.8777411	-0.6971414	-0.6312780
17	C	-4.5968767	-0.7501127	0.7575972
18	O	-3.5224918	-0.5962794	1.7199119
19	H	-2.1434001	-0.3921351	3.7024915
20	H	5.3245615	-0.0731434	0.9147814
21	H	5.1080572	1.7126268	0.9569064
22	H	-5.3245620	0.0731418	0.9147811
23	H	-5.1080562	-1.7126281	0.9569057
24	H	-3.9534316	-1.6845720	-1.1398594
25	H	3.9534320	1.6845720	-1.1398586
26	C	4.4087605	-0.3640355	-1.6369638
27	H	3.7582372	-0.2511619	-2.5307616
28	C	5.8557557	-0.0584656	-2.0624609
29	H	6.5695854	-0.1798201	-1.2203110
30	H	5.9618712	0.9769574	-2.4465902
31	H	6.1845531	-0.7481117	-2.8654791
32	C	4.2438586	-1.8065474	-1.1310376
33	H	4.8683780	-2.0119490	-0.2355842
34	H	4.5503873	-2.5308934	-1.9119673
35	H	3.1881545	-2.0127819	-0.8686588
36	C	-4.4087603	0.3640356	-1.6369637
37	H	-3.7582372	0.2511625	-2.5307616
38	C	-5.8557556	0.0584657	-2.0624609
39	H	-6.5695853	0.1798205	-1.2203110
40	H	-5.9618713	-0.9769574	-2.4465899
41	H	-6.1845530	0.7481117	-2.8654791
42	C	-4.2438588	1.8065473	-1.1310368
43	H	-4.8683773	2.0119481	-0.2355826
44	H	-4.5503888	2.5308936	-1.9119659
45	H	-3.1881545	2.0127821	-0.8686591

L^2Ph

1	N	-1.6136305	-0.0150330	0.1921035
2	C	-2.3944337	0.5546040	-0.7422866
3	C	-3.8056098	0.6014832	-0.6297429
4	H	-4.4184947	1.0648512	-1.4160122
5	C	-4.4053312	0.0424310	0.5068460
6	H	-5.4975281	0.0670844	0.6307842
7	C	-3.5912621	-0.5458088	1.4842353
8	C	-2.1898471	-0.5576878	1.2793659
9	C	-1.6971072	1.1409653	-1.9300166
10	N	-0.4220020	1.1709798	-2.0596168
11	C	0.0395907	1.8813198	-3.2417322
12	C	-1.1671268	2.1405912	-4.2269546
13	S	-2.6951974	1.9124480	-3.2318335
14	C	-1.2710345	-1.1726746	2.2876615
15	N	0.0072654	-1.1536809	2.1882925
16	C	0.6918305	-1.9150666	3.2233776
17	C	-0.3048159	-2.2287913	4.4034132
18	S	-1.9915132	-2.0602635	3.6967409
19	H	-4.0300936	-0.9812706	2.3932131
20	H	-1.1575892	3.1636160	-4.6465579
21	H	-1.1779865	1.4127012	-5.0614950
22	H	-0.1818067	-3.2504596	4.8071002
23	H	-0.1967389	-1.5032510	5.2333174
24	H	1.5062623	-1.2759544	3.6297993

25	H	0.7667084	1.2222400	-3.7654537
26	C	0.8003125	3.1617299	-2.8638349
27	C	2.2160878	5.5306721	-2.2285184
28	C	0.8980936	3.6001881	-1.5281635
29	C	1.4350330	3.9164959	-3.8758404
30	C	2.1349329	5.0927502	-3.5629838
31	C	1.5985966	4.7789317	-1.2150322
32	H	0.4331536	2.9994978	-0.7343821
33	H	1.3864854	3.5787325	-4.9234495
34	H	2.6237036	5.6672974	-4.3641000
35	H	1.6645994	5.1083446	-0.1671594
36	H	2.7643518	6.4517267	-1.9808227
37	C	1.3665394	-3.1665301	2.6378317
38	C	2.6342672	-5.4829461	1.6116380
39	C	1.2131754	-3.5265863	1.2837455
40	C	2.1780178	-3.9727193	3.4669830
41	C	2.8044741	-5.1230446	2.9608742
42	C	1.8407059	-4.6788323	0.7768406
43	H	0.6087004	-2.8866635	0.6262930
44	H	2.3300865	-3.6963117	4.5223582
45	H	3.4328934	-5.7382662	3.6222943
46	H	1.7086360	-4.9462983	-0.2823335
47	H	3.1246457	-6.3835413	1.2132130

L^2*i*Pr

1	N	-1.2546341	0.0045804	0.1637382
2	C	-2.0407906	0.5569695	-0.7768307
3	C	-3.4501845	0.6245422	-0.6481588
4	H	-4.0677524	1.0718282	-1.4400624
5	C	-4.0411467	0.1113921	0.5140599
6	H	-5.1312948	0.1533485	0.6513409
7	C	-3.2211049	-0.4549287	1.4995193
8	C	-1.8226305	-0.4945429	1.2757199
9	C	-1.3533380	1.1168161	-1.9826942
10	N	-0.0815045	1.1449927	-2.1319358
11	C	0.3702410	1.7995480	-3.3514618
12	C	-0.8483080	2.0837756	-4.3080094
13	S	-2.3706077	1.8263546	-3.3106769
14	C	-0.9017542	-1.1115942	2.2810347
15	N	0.3733043	-1.1356206	2.1616698
16	C	1.0694091	-1.8429995	3.2272775
17	C	0.0724564	-2.2086527	4.3920902
18	S	-1.6222640	-1.8924433	3.7556167
19	H	-3.6549193	-0.8579893	2.4256930
20	H	-0.8506094	3.1171981	-4.7051283
21	H	-0.8663384	1.3868227	-5.1677740
22	H	0.1427057	-3.2691129	4.7022441
23	H	0.2352820	-1.5790244	5.2874832
24	H	1.8359132	-1.1465856	3.6330947
25	H	1.0581338	1.0932938	-3.8660961
26	C	1.2307966	3.0527963	-2.9913547
27	H	1.9741857	2.6716968	-2.2587133
28	C	2.0000976	3.5769990	-4.2158803
29	H	2.6083029	2.7793967	-4.6893218
30	H	2.6898821	4.3947982	-3.9260855
31	H	1.3194327	3.9878379	-4.9913943
32	C	0.4278083	4.1665675	-2.2971100
33	H	1.1053148	4.9744419	-1.9546354
34	H	-0.1089376	3.7831333	-1.4080137
35	H	-0.3161192	4.6314543	-2.9762085
36	C	1.8566290	-3.0545055	2.6328207
37	H	2.4589923	-2.6131700	1.8104732

38	C	2.8330674	-3.6559814	3.6594627
39	H	3.5270961	-2.8911691	4.0643035
40	H	3.4459876	-4.4509226	3.1901739
41	H	2.3045544	-4.1185764	4.5184357
42	C	0.9403110	-4.1221548	2.0117129
43	H	1.5449084	-4.9399426	1.5711095
44	H	0.3162167	-3.6899532	1.2064089
45	H	0.2632095	-4.5807149	2.7620632

bimpy

1	N	0.0000000	0.0000000	0.6166300
2	C	-1.1622556	-0.0019720	1.2954017
3	C	-1.2077964	-0.0044103	2.7151712
4	C	0.0000000	0.0000000	3.4236008
5	H	0.0000000	0.0000000	4.5231928
6	C	1.2077964	0.0044103	2.7151712
7	H	2.1570400	0.0104528	3.2695011
8	C	1.1622557	0.0019721	1.2954017
9	C	-2.4013163	-0.0001150	0.4844911
10	N	-2.4579934	-0.0067528	-0.8409254
11	C	-3.8025879	-0.0036945	-1.1528298
12	C	-4.5971454	0.0075171	0.0409746
13	N	-3.6718166	0.0105412	1.0676437
14	C	2.4013163	0.0001150	0.4844911
15	N	2.4579934	0.0067528	-0.8409254
16	C	3.8025879	0.0036945	-1.1528298
17	C	4.5971454	-0.0075171	0.0409746
18	N	3.6718166	-0.0105412	1.0676437
19	H	-2.1570400	-0.0104527	3.2695011
20	H	6.6063691	-0.0224685	0.9355531
21	C	6.0040235	-0.0135757	0.0155746
22	C	4.4413988	0.0090880	-2.4144795
23	H	3.8396248	0.0176653	-3.3337458
24	H	7.7075930	-0.0127822	-1.3179762
25	C	6.6097576	-0.0081038	-1.2497599
26	C	5.8407739	0.0030352	-2.4447293
27	H	6.3626931	0.0066565	-3.4128731
28	H	-3.8396248	-0.0176652	-3.3337458
29	C	-4.4413988	-0.0090880	-2.4144796
30	C	-6.0040235	0.0135757	0.0155746
31	H	-6.6063691	0.0224684	0.9355531
32	C	-6.6097576	0.0081038	-1.2497599
33	H	-7.7075930	0.0127821	-1.3179762
34	H	-6.3626931	-0.0066566	-3.4128731
35	C	-5.8407739	-0.0030353	-2.4447293
36	H	-3.8900654	0.0239535	2.0612959
37	H	3.8900654	-0.0239535	2.0612959

terpy

1	N	-0.0001994	-0.0009588	0.0870561
2	C	1.1480550	-0.2103486	0.7561340
3	C	1.1880726	-0.2258352	2.1737789
4	C	-0.0013767	-0.0080019	2.8804540
5	H	-0.0018648	-0.0109048	3.9804373
6	C	-1.1901900	0.2136120	2.1738852
7	H	-2.1238235	0.3845335	2.7250250
8	C	-1.1489583	0.2053872	0.7562175
9	C	2.3898048	-0.4178383	-0.0754176
10	N	2.2418344	-0.3434779	-1.4165485
11	C	3.3159042	-0.5201986	-2.1950729
12	C	3.6523243	-0.6816444	0.5138604
13	C	-2.3898943	0.4175412	-0.0753804

14	N	-2.2407205	0.3499856	-1.4167340
15	C	-3.3139455	0.5313975	-2.1953413
16	C	-3.6527548	0.6793404	0.5140795
17	H	2.1212446	-0.3994135	2.7248677
18	H	-3.1403075	0.4645502	-3.2848170
19	H	3.1432361	-0.4478729	-3.2843523
20	H	3.7736385	-0.7464011	1.6030974
21	H	-3.7749646	0.7388435	1.6035153
22	C	4.7708156	-0.8667560	-0.3116325
23	H	5.7570156	-1.0726385	0.1305460
24	H	5.4562453	-0.9224661	-2.3902278
25	C	4.6086696	-0.7851732	-1.7030844
26	C	-4.7703324	0.8695367	-0.3115043
27	H	-5.7567663	1.0740561	0.1307845
28	H	-5.4537992	0.9362939	-2.3904202
29	C	-4.6069631	0.7948520	-1.7032056

Table S15 Atomic coordinates for the other DFT-minimised molecules used to calculate $\Delta E\{\text{het}\}$ (Tables S11-S12).

$[Fe(bimpy)_2]^{2+}$, high-spin

1	Fe	0.0000003	0.0000011	-0.0284933
2	N	-0.0000001	0.0000001	2.1596401
3	C	-0.8344271	-0.8340029	2.8226546
4	C	-0.8623816	-0.8619058	4.2342726
5	C	0.0000009	-0.0000004	4.9338439
6	H	0.0000015	-0.0000007	6.0330500
7	C	0.8623829	0.8619053	4.2342723
8	H	1.5349351	1.5340847	4.7839424
9	C	0.8344272	0.8340029	2.8226545
10	C	-1.6484349	-1.6478089	1.9113448
11	N	-1.5262859	-1.5256916	0.5786055
12	C	-2.4251122	-2.4246335	0.0245729
13	C	-3.1114651	-3.1109641	1.0772421
14	N	-2.5879141	-2.5872912	2.2515999
15	C	1.6484348	1.6478087	1.9113439
16	N	1.5262847	1.5256903	0.5786047
17	C	2.4251112	2.4246333	0.0245736
18	C	3.1114647	3.1109634	1.0772432
19	N	2.5879144	2.5872903	2.2516000
20	N	0.0000010	0.0000010	-2.1634776
21	C	0.8335269	-0.8331706	-2.8455202
22	C	0.8597019	-0.8593034	-4.2545797
23	H	1.5346378	-1.5339282	-4.7988801
24	C	0.0000004	0.0000003	-4.9612478
25	H	0.0000001	0.0000000	-6.0598368
26	C	-0.8597011	0.8593041	-4.2545798
27	C	-0.8335256	0.8331718	-2.8455203
28	C	1.6441517	-1.6436272	-1.9386504
29	N	1.5090960	-1.5086541	-0.6066238
30	C	2.4033275	-2.4029448	-0.0302585
31	C	3.0982786	-3.0978026	-1.0699824
32	N	2.5866119	-2.5860262	-2.2564244
33	C	-1.6441523	1.6436264	-1.9386502
34	N	-1.5090982	1.5086512	-0.6066237
35	C	-2.4033277	2.4029444	-0.0302590
36	C	-3.0982800	3.0978009	-1.0699831
37	N	-2.5866151	2.5860228	-2.2564247
38	H	-1.5349332	-1.5340858	4.7839428
39	H	-1.5346377	1.5339281	-4.7988802
40	H	4.6131287	4.6127354	1.6450549
41	C	4.0909451	4.0905510	0.8317532
42	C	2.7240029	2.7236559	-1.3238975
43	H	2.2075245	2.2072138	-2.1433187
44	H	5.1265630	5.1264000	-0.7550630
45	C	4.3687441	4.3684824	-0.5114388
46	C	3.6968188	3.6965804	-1.5707671
47	H	3.9542089	3.9540841	-2.6078700
48	H	-2.2075259	-2.2072122	-2.1433191
49	C	-2.7240041	-2.7236550	-1.3238983
50	C	-4.0909455	-4.0905516	0.8317518
51	H	-4.6131287	-4.6127365	1.6450534
52	C	-4.3687450	-4.3684822	-0.5114403
53	H	-5.1265640	-5.1263996	-0.7550649
54	H	-3.9542103	-3.9540823	-2.6078714
55	C	-3.6968201	-3.6965794	-1.5707684
56	H	-2.8611765	-2.8605661	3.1959251
57	H	2.8611765	2.8605646	3.1959254
58	H	2.8684919	-2.8678645	-3.1954649

59	H	-2.8684960	2.8678597	-3.1954653
60	C	4.0750318	-4.0745835	-0.8066773
61	H	4.6037043	-4.6032000	-1.6116102
62	C	2.6910735	-2.6908099	1.3222639
63	H	2.1697999	-2.1696231	2.1358164
64	H	5.0985829	-5.0982899	0.7968920
65	C	4.3427335	-4.3424070	0.5413259
66	H	3.9097122	-3.9095752	2.6294821
67	C	3.6623304	-3.6620941	1.5875486
68	C	-4.0750324	4.0745827	-0.8066782
69	H	-4.6037058	4.6031981	-1.6116112
70	C	-2.6910717	2.6908120	1.3222633
71	H	-2.1697975	2.1696260	2.1358161
72	H	-3.9097083	3.9095796	2.6294812
73	C	-3.6623278	3.6620970	1.5875478
74	H	-5.0985810	5.0982919	0.7968909
75	C	-4.3427320	4.3424084	0.5413249

$[Fe(bimpy)_2]^{2+}$, low-spin

1	Fe	-0.0000005	0.0000007	-0.0000002
2	N	-0.0000002	0.0000001	1.9196186
3	C	-0.8391322	-0.8391321	2.6004315
4	C	-0.8617694	-0.8617693	4.0091715
5	C	-0.0000001	-0.0000001	4.7125966
6	H	-0.0000001	-0.0000001	5.8112137
7	C	0.8617691	0.8617692	4.0091716
8	H	1.5374997	1.5374998	4.5506894
9	C	0.8391319	0.8391321	2.6004316
10	C	-1.6145218	-1.6145213	1.6499321
11	N	-1.3972745	-1.3972735	0.3334279
12	C	-2.2527713	-2.2527707	-0.3544993
13	C	-3.0056680	-3.0056675	0.6041210
14	N	-2.5714650	-2.5714645	1.8499261
15	C	1.6145212	1.6145216	1.6499322
16	N	1.3972733	1.3972743	0.3334280
17	C	2.2527707	2.2527712	-0.3544990
18	C	3.0056675	3.0056678	0.6041214
19	N	2.5714643	2.5714648	1.8499263
20	N	0.0000000	0.0000001	-1.9196187
21	C	0.8391320	-0.8391321	-2.6004317
22	C	0.8617689	-0.8617695	-4.0091717
23	H	1.5374993	-1.5375002	-4.5506895
24	C	-0.0000006	-0.0000004	-4.7125967
25	H	-0.0000010	-0.0000005	-5.8112137
26	C	-0.8617697	0.8617690	-4.0091716
27	C	-0.8391321	0.8391320	-2.6004317
28	C	1.6145215	-1.6145214	-1.6499324
29	N	1.3972741	-1.3972737	-0.3334282
30	C	2.2527712	-2.2527705	0.3544991
31	C	3.0056678	-3.0056675	-0.6041212
32	N	2.5714646	-2.5714647	-1.8499263
33	C	-1.6145213	1.6145213	-1.6499320
34	N	-1.3972732	1.3972734	-0.3334279
35	C	-2.2527703	2.2527707	0.3544990
36	C	-3.0056673	3.0056674	-0.6041212
37	N	-2.5714646	2.5714643	-1.8499261
38	H	-1.5374999	-1.5374999	4.5506893
39	H	-1.5375005	1.5374994	-4.5506893
40	H	4.5349063	4.5349063	0.9767778
41	C	3.9644809	3.9644809	0.2310524
42	C	2.4666888	2.4666888	-1.7350923
43	H	1.9060618	1.9060617	-2.4918610

44	H	4.8967454	4.8967446	-1.4808159
45	C	4.1576051	4.1576047	-1.1413286
46	C	3.4200906	3.4200901	-2.1068373
47	H	3.6071864	3.6071855	-3.1736219
48	H	-1.9060617	-1.9060616	-2.4918613
49	C	-2.4666888	-2.4666886	-1.7350927
50	C	-3.9644810	-3.9644808	0.2310519
51	H	-4.5349065	-4.5349063	0.9767772
52	C	-4.1576049	-4.1576049	-1.1413291
53	H	-4.8967448	-4.8967452	-1.4808165
54	H	-3.6071856	-3.6071861	-3.1736224
55	C	-3.4200902	-3.4200903	-2.1068378
56	H	-2.9088870	-2.9088865	2.7515062
57	H	2.9088863	2.9088868	2.7515065
58	H	2.9088865	-2.9088868	-2.7515064
59	H	-2.9088867	2.9088863	-2.7515062
60	C	3.9644809	-3.9644806	-0.2310521
61	H	4.5349063	-4.5349063	-0.9767773
62	C	2.4666890	-2.4666883	1.7350925
63	H	1.9060620	-1.9060610	2.4918611
64	H	4.8967451	-4.8967446	1.4808164
65	C	4.1576050	-4.1576045	1.1413290
66	H	3.6071861	-3.6071852	3.1736223
67	C	3.4200905	-3.4200898	2.1068376
68	C	-3.9644805	3.9644805	-0.2310520
69	H	-4.5349062	4.5349059	-0.9767773
70	C	-2.4666880	2.4666886	1.7350925
71	H	-1.9060608	1.9060617	2.4918611
72	H	-3.6071850	3.6071857	3.1736222
73	C	-3.4200895	3.4200901	2.1068376
74	H	-4.8967445	4.8967446	1.4808164
75	C	-4.1576044	4.1576046	1.1413290

$[Fe(terpy)_2]^{2+}$, high-spin

1	Fe	-0.0000001	0.0000001	0.0120580
2	N	-0.0000001	-0.0000001	2.1242061
3	C	0.8363594	0.8361441	2.8019652
4	C	0.8570990	0.8568516	4.2110838
5	C	-0.0000001	0.0000001	4.9194277
6	H	-0.0000001	0.0000002	6.0180873
7	C	-0.8570991	-0.8568514	4.2110839
8	H	-1.5309227	-1.5304830	4.7550087
9	C	-0.8363595	-0.8361441	2.8019652
10	C	1.6867715	1.6864646	1.9315400
11	N	1.5035698	1.5033920	0.5901674
12	C	2.2312810	2.2311948	-0.2840398
13	C	2.6243265	2.6239355	2.4130746
14	C	-1.6867715	-1.6864646	1.9315400
15	N	-1.5035699	-1.5033919	0.5901674
16	C	-2.2312810	-2.2311947	-0.2840398
17	C	-2.6243265	-2.6239355	2.4130745
18	N	-0.0000001	0.0000000	-2.1313071
19	C	-0.8382030	0.8379624	-2.7904052
20	C	-0.8600154	0.8597339	-4.2009844
21	H	-1.5311615	1.5306657	-4.7510469
22	C	0.0000000	-0.0000001	-4.9026483
23	H	0.0000001	-0.0000001	-6.0018848
24	C	0.8600154	-0.8597340	-4.2009843
25	C	0.8382028	-0.8379624	-2.7904052
26	C	-1.6954279	1.6950994	-1.9148893
27	N	-1.5237562	1.5235615	-0.5725098
28	C	-2.2566834	2.2565903	0.2869163

29	C	-3.2035586	3.2034464	-0.1364533
30	C	1.6954278	-1.6950994	-1.9148893
31	N	1.5237561	-1.5235614	-0.5725098
32	C	2.2566834	-2.2565902	0.2869163
33	C	3.2035587	-3.2034464	-0.1364536
34	H	1.5309225	1.5304832	4.7550087
35	H	1.5311615	-1.5306658	-4.7510468
36	H	-2.0440351	-2.0440310	-1.3527606
37	H	2.0440351	2.0440311	-1.3527606
38	H	2.7681223	2.7676182	3.4914367
39	H	-2.7681222	-2.7676182	3.4914367
40	C	3.3771889	3.3768864	1.5009977
41	H	4.1112465	4.1108752	1.8629350
42	H	3.7479630	3.7479086	-0.6254021
43	C	3.1794219	3.1792996	0.1229601
44	C	-3.3771889	-3.3768864	1.5009976
45	H	-4.1112465	-4.1108753	1.8629348
46	H	-3.7479629	-3.7479086	-0.6254022
47	C	-3.1794219	-3.1792996	0.1229600
48	C	3.3889943	-3.3887038	-1.5153193
49	C	-3.3889940	3.3887036	-1.5153191
50	C	2.6267707	-2.6263738	-2.4156579
51	C	-2.6267705	2.6263737	-2.4156579
52	H	3.7786612	-3.7786281	0.6020058
53	H	2.0755334	-2.0755209	1.3576084
54	H	4.1195594	-4.1192163	-1.8912752
55	H	2.7632820	-2.7627758	-3.4959253
56	H	-2.0755334	2.0755208	1.3576084
57	H	-3.7786610	3.7786281	0.6020061
58	H	-4.1195591	4.1192162	-1.8912749
59	H	-2.7632820	2.7627758	-3.4959252

$[Fe(terpy)_2]^{2+}$, low-spin

1	Fe	0.0000000	0.0000001	0.0000000
2	N	0.0000000	0.0000000	1.8962563
3	C	0.8423658	0.8423658	2.5658139
4	C	0.8605570	0.8605569	3.9729797
5	C	0.0000001	-0.0000001	4.6772647
6	H	0.0000001	-0.0000001	5.7759632
7	C	-0.8605570	-0.8605570	3.9729797
8	H	-1.5355081	-1.5355082	4.5147087
9	C	-0.8423658	-0.8423658	2.5658139
10	C	1.6531518	1.6531518	1.6413260
11	N	1.3930011	1.3930011	0.3130839
12	C	2.0804896	2.0804896	-0.6290354
13	C	2.6101927	2.6101927	2.0275347
14	C	-1.6531518	-1.6531518	1.6413260
15	N	-1.3930011	-1.3930011	0.3130839
16	C	-2.0804896	-2.0804896	-0.6290354
17	C	-2.6101927	-2.6101927	2.0275346
18	N	0.0000000	-0.0000001	-1.8962563
19	C	-0.8423659	0.8423658	-2.5658139
20	C	-0.8605571	0.8605569	-3.9729797
21	H	-1.5355082	1.5355080	-4.5147087
22	C	-0.0000001	-0.0000001	-4.6772647
23	H	-0.0000002	-0.0000001	-5.7759632
24	C	0.8605569	-0.8605570	-3.9729797
25	C	0.8423658	-0.8423659	-2.5658139
26	C	-1.6531518	1.6531518	-1.6413260
27	N	-1.3930011	1.3930011	-0.3130839
28	C	-2.0804897	2.0804897	0.6290354
29	C	-3.0451676	3.0451677	0.3079319

30	C	1.6531518	-1.6531518	-1.6413259
31	N	1.3930011	-1.3930011	-0.3130838
32	C	2.0804896	-2.0804896	0.6290355
33	C	3.0451677	-3.0451676	0.3079321
34	H	1.5355081	1.5355080	4.5147087
35	H	1.5355080	-1.5355082	-4.5147087
36	H	-1.8474583	-1.8474583	-1.6766599
37	H	1.8474583	1.8474584	-1.6766598
38	H	2.8005573	2.8005572	3.0919377
39	H	-2.8005572	-2.8005573	3.0919376
40	C	3.3163531	3.3163531	1.0436945
41	H	4.0670933	4.0670932	1.3277464
42	H	3.5729268	3.5729267	-1.1140432
43	C	3.0451676	3.0451676	-0.3079319
44	C	-3.3163531	-3.3163531	1.0436944
45	H	-4.0670932	-4.0670933	1.3277462
46	H	-3.5729267	-3.5729267	-1.1140434
47	C	-3.0451676	-3.0451676	-0.3079321
48	C	3.3163532	-3.3163531	-1.0436944
49	C	-3.3163531	3.3163532	-1.0436945
50	C	2.6101927	-2.6101927	-2.0275346
51	C	-2.6101928	2.6101928	-2.0275347
52	H	3.5729268	-3.5729267	1.1140433
53	H	1.8474584	-1.8474583	1.6766599
54	H	4.0670934	-4.0670932	-1.3277463
55	H	2.8005573	-2.8005573	-3.0919376
56	H	-1.8474584	1.8474585	1.6766598
57	H	-3.5729268	3.5729269	1.1140432
58	H	-4.0670932	4.0670934	-1.3277464
59	H	-2.8005573	2.8005572	-3.0919377

[Fe(L^1H)(bimpy)]$^{2+}$, high-spin

1	Fe	0.0003589	-0.0014698	0.1339029
2	N	0.0103445	0.0038650	2.3192921
3	C	-1.1643113	-0.0610134	2.9902754
4	C	-1.1975400	-0.0619900	4.4013717
5	C	0.0221705	0.0161888	5.0955243
6	H	0.0268325	0.0212256	6.1946791
7	C	1.2358926	0.0880804	4.3903669
8	H	2.1866363	0.1521166	4.9366291
9	C	1.1906436	0.0744574	2.9796260
10	C	-2.3156291	-0.1217884	2.0818183
11	N	-2.1367470	-0.1033410	0.7486835
12	C	-3.4034409	-0.1544110	0.1849709
13	C	-4.3779422	-0.2171098	1.2313650
14	N	-3.6439158	-0.1957627	2.4116034
15	C	2.3340923	0.1277953	2.0609277
16	N	2.1437933	0.1016271	0.7295098
17	C	3.4058160	0.1455750	0.1547609
18	C	4.3893047	0.2129881	1.1924589
19	N	3.6652972	0.2014384	2.3789788
20	N	-0.0088193	0.0018094	-1.9927284
21	C	-0.0620094	-1.1673824	-2.6785356
22	C	-0.0741753	-1.2123611	-4.0840075
23	H	-0.1211949	-2.1779222	-4.6055641
24	C	-0.0213492	0.0052344	-4.7900498
25	H	-0.0262048	0.0065719	-5.8888924
26	C	0.0375778	1.2210991	-4.0815291
27	C	0.0380331	1.1726831	-2.6761084
28	C	-0.0939155	-2.3206997	-1.7629906
29	N	-0.0343447	-2.1374318	-0.4707918
30	C	-0.1051896	-3.4730371	0.1547929

31	C	-0.1570190	-4.4532220	-1.0551188
32	O	-0.1813775	-3.5636986	-2.2307626
33	C	0.0777421	2.3236962	-1.7579352
34	N	0.0296168	2.1369499	-0.4658134
35	C	0.1033793	3.4708945	0.1627391
36	C	0.1485502	4.4542787	-1.0449273
37	O	0.1602874	3.5679960	-2.2231777
38	H	-2.1435128	-0.1206325	4.9564774
39	H	0.0797202	2.1879740	-4.6010547
40	H	0.7369280	-5.0978031	-1.1497947
41	H	-1.0655189	-5.0818626	-1.0980371
42	H	-0.7437675	5.1022916	-1.1306125
43	H	1.0589508	5.0798181	-1.0934795
44	H	1.0053262	3.5394406	0.8056180
45	H	-1.0039415	-3.5427914	0.8020362
46	H	6.5187047	0.3234132	1.7272840
47	C	5.7694908	0.2741168	0.9254339
48	C	3.8070091	0.1380221	-1.1996965
49	H	3.0658667	0.0855885	-2.0077434
50	H	7.2088290	0.3112663	-0.6846937
51	C	6.1421095	0.2655129	-0.4236941
52	C	5.1778025	0.1988417	-1.4678815
53	H	5.5262309	0.1950880	-2.5103238
54	H	-3.0817360	-0.1080511	-1.9806551
55	C	-3.8159614	-0.1569929	-1.1660701
56	C	-5.7601624	-0.2835412	0.9763490
57	H	-6.5024784	-0.3294023	1.7847939
58	C	-6.1441399	-0.2850224	-0.3696261
59	H	-7.2129100	-0.3352275	-0.6212378
60	H	-5.5459337	-0.2268491	-2.4618309
61	C	-5.1888222	-0.2229434	-1.4223402
62	H	-4.0359088	-0.2228157	3.3536696
63	H	4.0652222	0.2329251	3.3175581
64	H	-0.7783475	3.6378004	0.8135432
65	H	0.7797068	-3.6420938	0.8006643

$[Fe(L^1H)(bimpy)]^{2+}$, low-spin

1	Fe	-0.0018498	-0.0000804	0.2216461
2	N	-0.0103550	-0.0004372	2.1486370
3	C	1.1728038	-0.0055388	2.8347670
4	C	1.1987702	-0.0076215	4.2434134
5	C	-0.0225635	-0.0008508	4.9405172
6	H	-0.0273603	-0.0009737	6.0391220
7	C	-1.2377511	0.0061016	4.2327676
8	H	-2.1944797	0.0127178	4.7721581
9	C	-1.1994377	0.0043913	2.8243486
10	C	2.2755839	-0.0055093	1.8908008
11	N	1.9771222	-0.0001771	0.5715132
12	C	3.1932227	-0.0006228	-0.1084277
13	C	4.2507693	-0.0063100	0.8586185
14	N	3.6269529	-0.0098223	2.1000124
15	C	-2.2938038	0.0050731	1.8705886
16	N	-1.9841878	0.0003445	0.5538310
17	C	-3.1946014	0.0009509	-0.1362267
18	C	-4.2602120	0.0067045	0.8219705
19	N	-3.6468549	0.0099801	2.0684918
20	N	0.0095810	0.0000620	-1.6872933
21	C	0.0184736	1.1818327	-2.3691183
22	C	0.0290335	1.2217661	-3.7739355
23	H	0.0372724	2.1879555	-4.2959050
24	C	0.0288997	0.0002366	-4.4772346
25	H	0.0366519	0.0003088	-5.5760377

26	C	0.0191118	-1.2213825	-3.7741715
27	C	0.0099022	-1.1816276	-2.3693437
28	C	0.0122789	2.2777093	-1.4015662
29	N	-0.0017968	1.9603170	-0.1269874
30	C	0.0092996	3.2217252	0.6395644
31	C	-0.0258372	4.3182529	-0.4677326
32	O	0.0206610	3.5631801	-1.7351527
33	C	0.0035630	-2.2776793	-1.4019700
34	N	0.0017367	-1.9605213	-0.1272563
35	C	-0.0179690	-3.2220192	0.6389605
36	C	0.0265842	-4.3185010	-0.4680517
37	O	-0.0005881	-3.5630811	-1.7358466
38	H	2.1507084	-0.0143326	4.7912380
39	H	0.0186383	-2.1875041	-4.2963300
40	H	-0.9575187	4.9142346	-0.4768530
41	H	0.8443029	4.9997682	-0.4583249
42	H	0.9556082	-4.9186433	-0.4653650
43	H	-0.8466287	-4.9961857	-0.4699376
44	H	-0.9362927	-3.2780360	1.2584540
45	H	0.9218085	3.2782650	1.2676091
46	H	-6.4229836	0.0131999	1.1953432
47	C	-5.6162173	0.0089731	0.4496624
48	C	-3.4975676	-0.0021269	-1.5171444
49	H	-2.7068561	-0.0060669	-2.2759661
50	H	-6.9339491	0.0066775	-1.2627602
51	C	-5.8888585	0.0053151	-0.9227007
52	C	-4.8457281	0.0000023	-1.8880759
53	H	-5.1105021	-0.0023714	-2.9548017
54	H	2.7227037	0.0066667	-2.2518233
55	C	3.5073656	0.0026730	-1.4867777
56	C	5.6098151	-0.0083396	0.4973371
57	H	6.4104674	-0.0125351	1.2495722
58	C	5.8936263	-0.0044722	-0.8727515
59	H	6.9414665	-0.0055995	-1.2042745
60	H	5.1320632	0.0034467	-2.9112010
61	C	4.8585122	0.0008199	-1.8466955
62	H	4.0975431	-0.0094669	3.0054521
63	H	-4.1251441	0.0096303	2.9698868
64	H	0.8527595	-3.2736134	1.3226592
65	H	-0.8677686	3.2727669	1.3150973

$[Fe(L^2H)(bimpy)]^{2+}$, high-spin

1	Fe	-0.0010424	-0.0003122	0.0541279
2	N	-0.0077112	0.0006882	2.2551082
3	C	1.1698120	-0.0325074	2.9220857
4	C	1.2056857	-0.0336641	4.3334794
5	C	-0.0152552	0.0037011	5.0290568
6	H	-0.0182208	0.0049312	6.1283095
7	C	-1.2324136	0.0392777	4.3268058
8	H	-2.1835131	0.0703175	4.8752789
9	C	-1.1888421	0.0350046	2.9156184
10	C	2.3202695	-0.0646525	2.0104476
11	N	2.1382197	-0.0675641	0.6775468
12	C	3.4049804	-0.0898732	0.1122621
13	C	4.3831086	-0.1044254	1.1573677
14	N	3.6509259	-0.0885538	2.3386136
15	C	-2.3342348	0.0631607	1.9975702
16	N	-2.1446819	0.0623490	0.6657579
17	C	-3.4080276	0.0841928	0.0929654
18	C	-4.3921900	0.0993527	1.1323556
19	N	-3.6668449	0.0855344	2.3179513
20	N	0.0101407	0.0026909	-2.0506639

21	C	0.0166802	1.1803632	-2.7310121
22	C	0.0350535	1.2202874	-4.1379324
23	H	0.0547050	2.1831148	-4.6678640
24	C	0.0312731	0.0059589	-4.8486288
25	H	0.0398328	0.0072521	-5.9472346
26	C	0.0166119	-1.2100113	-4.1409493
27	C	0.0133869	-1.1733953	-2.7338175
28	C	0.0141832	2.3441557	-1.8243679
29	N	0.0297597	2.1230767	-0.5321894
30	C	-0.0772765	3.3627649	0.2508478
31	C	0.3146038	4.5627249	-0.6419327
32	S	-0.0318150	4.0098545	-2.3779478
33	C	0.0017721	-2.3393469	-1.8301208
34	N	-0.0299717	-2.1213766	-0.5376948
35	C	0.0632693	-3.3632037	0.2436333
36	C	-0.3213038	-4.5595841	-0.6570456
37	S	0.0503018	-4.0038559	-2.3871052
38	H	2.1536956	-0.0638121	4.8873427
39	H	0.0056101	-2.1716016	-4.6733719
40	H	-0.2762280	5.4727372	-0.4322780
41	H	1.3918270	4.8112520	-0.5789788
42	H	0.2630193	-5.4724560	-0.4416290
43	H	-1.4002487	-4.8039708	-0.6091389
44	H	-0.5987446	-3.3075192	1.1304629
45	H	0.5735833	3.3069345	1.1458732
46	H	-6.5238077	0.1335755	1.6695140
47	C	-5.7739134	0.1228160	0.8668600
48	C	-3.8091994	0.0930365	-1.2614116
49	H	-3.0662662	0.0818862	-2.0692841
50	H	-7.2143675	0.1486846	-0.7422312
51	C	-6.1465638	0.1307326	-0.4821428
52	C	-5.1812553	0.1163198	-1.5278115
53	H	-5.5303078	0.1237576	-2.5700173
54	H	3.0762517	-0.0898985	-2.0521214
55	C	3.8142110	-0.1003817	-1.2397142
56	C	5.7663576	-0.1290593	0.8999878
57	H	6.5115085	-0.1393454	1.7070572
58	C	6.1469548	-0.1386999	-0.4467656
59	H	7.2162607	-0.1577032	-0.7005207
60	H	5.5428520	-0.1338381	-2.5382181
61	C	5.1877921	-0.1248606	-1.4980637
62	H	4.0452849	-0.0927779	3.2801073
63	H	-4.0665593	0.0905560	3.2571757
64	H	1.1077246	-3.4569309	0.6172917
65	H	-1.1267028	3.4521391	0.6113431

$[Fe(L^2H)(bimpy)]^{2+}$, low-spin

1	Fe	0.0014850	-0.0000840	0.1517768
2	N	0.0071905	0.0017187	2.0818411
3	C	-1.1770316	0.0283128	2.7666321
4	C	-1.2047442	0.0302999	4.1753560
5	C	0.0154111	0.0031280	4.8742280
6	H	0.0186392	0.0036456	5.9728369
7	C	1.2314283	-0.0247086	4.1682244
8	H	2.1869863	-0.0477370	4.7092875
9	C	1.1954230	-0.0241581	2.7596452
10	C	-2.2783416	0.0530395	1.8213780
11	N	-1.9786785	0.0529009	0.5022844
12	C	-3.1933248	0.0739146	-0.1797038
13	C	-4.2518681	0.0881524	0.7862117
14	N	-3.6298130	0.0759606	2.0285730
15	C	2.2910486	-0.0500595	1.8078167

16	N	1.9837672	-0.0516918	0.4904426
17	C	3.1945057	-0.0731383	-0.1984422
18	C	4.2585791	-0.0858437	0.7614192
19	N	3.6436897	-0.0723326	2.0072901
20	N	-0.0068318	-0.0021715	-1.7418385
21	C	-0.0462481	-1.1907122	-2.4150681
22	C	-0.0627116	-1.2239164	-3.8218864
23	H	-0.1055606	-2.1845323	-4.3535742
24	C	-0.0249155	-0.0050696	-4.5262408
25	H	-0.0322022	-0.0061990	-5.6249710
26	C	0.0218653	1.2152493	-3.8249585
27	C	0.0237936	1.1849749	-2.4179935
28	C	-0.0715405	-2.2969770	-1.4559483
29	N	-0.0548829	-1.9523146	-0.1810317
30	C	0.0495285	-3.1191679	0.7108290
31	C	-0.4353533	-4.3650059	-0.0563352
32	S	-0.0933328	-4.0029729	-1.8480158
33	C	0.0596997	2.2932882	-1.4615688
34	N	0.0554534	1.9514191	-0.1858042
35	C	-0.0391848	3.1203613	0.7044254
36	C	0.4394431	4.3639640	-0.0702385
37	S	0.0790471	3.9984451	-1.8574965
38	H	-2.1570810	0.0538544	4.7220630
39	H	0.0570414	2.1747611	-4.3592005
40	H	0.1019124	-5.2872830	0.2296039
41	H	-1.5249234	-4.5339633	0.0466016
42	H	-0.0937454	5.2875493	0.2191016
43	H	1.5302123	4.5317293	0.0213629
44	H	0.5646575	2.9592732	1.6185511
45	H	-0.5457784	-2.9565477	1.6302636
46	H	6.4207456	-0.1148726	1.1376228
47	C	5.6149702	-0.1058217	0.3909291
48	C	3.4986146	-0.0822479	-1.5789159
49	H	2.7082698	-0.0749744	-2.3379695
50	H	6.9343861	-0.1272075	-1.3199226
51	C	5.8889893	-0.1126190	-0.9810814
52	C	4.8470016	-0.1014345	-1.9478561
53	H	5.1131717	-0.1083135	-3.0142035
54	H	-2.7190896	0.0731913	-2.3218664
55	C	-3.5051768	0.0815356	-1.5584284
56	C	-5.6103508	0.1081962	0.4233125
57	H	-6.4118939	0.1184219	1.1745269
58	C	-5.8920862	0.1134817	-0.9471282
59	H	-6.9393707	0.1280821	-1.2801033
60	H	-5.1278400	0.1065599	-2.9846061
61	C	-4.8556222	0.1007918	-1.9197796
62	H	-4.1017893	0.0805422	2.9332734
63	H	4.1209464	-0.0755510	2.9092208
64	H	-1.1016780	3.2256890	1.0194531
65	H	1.1150888	-3.2228047	1.0157934

$[Fe(L^1H)(bpp)]^{2+}$, high-spin

1	Fe	0.0000386	-0.0059329	-0.1017630
2	N	0.0097020	0.0017227	2.0703456
3	C	-1.1553095	0.0064047	2.7458876
4	C	-1.2061569	0.0156257	4.1502781
5	C	0.0210544	0.0164254	4.8356799
6	H	0.0255422	0.0223366	5.9349772
7	C	1.2425908	0.0100309	4.1402767
8	H	2.1950617	0.0105118	4.6834845
9	C	1.1801845	0.0042153	2.7362986
10	N	-2.2974488	0.0008085	1.9099744

11	N	-2.1199162	-0.0106011	0.5482502
12	C	-3.3551444	-0.0140203	0.0260637
13	C	-4.3458758	-0.0057256	1.0430214
14	C	-3.6363263	0.0049521	2.2356016
15	N	2.3152705	0.0012795	1.8908712
16	N	2.1264831	0.0013043	0.5305183
17	C	3.3574190	-0.0008851	-0.0017133
18	C	4.3564940	-0.0015416	1.0071096
19	C	3.6568012	-0.0010504	2.2055091
20	N	-0.0117205	-0.0015845	-2.2270135
21	C	-0.0038049	-1.1707173	-2.9134747
22	C	-0.0098637	-1.2158683	-4.3190813
23	H	-0.0014096	-2.1823713	-4.8410904
24	C	-0.0269480	0.0029349	-5.0244035
25	H	-0.0330057	0.0047176	-6.1233111
26	C	-0.0360933	1.2194506	-4.3149819
27	C	-0.0265881	1.1697565	-2.9095491
28	C	0.0077414	-2.3225053	-1.9953760
29	N	0.0186192	-2.1298258	-0.7017735
30	C	0.0093327	-3.4656875	-0.0692407
31	C	0.0230246	-4.4521762	-1.2748060
32	O	0.0033812	-3.5687635	-2.4556568
33	C	-0.0269971	2.3185498	-1.9876264
34	N	-0.0232744	2.1214749	-0.6947383
35	C	-0.0059693	3.4550623	-0.0577958
36	C	-0.0316347	4.4457311	-1.2598020
37	O	-0.0268519	3.5663758	-2.4438041
38	H	-2.1540329	0.0214818	4.7014675
39	H	-0.0501009	2.1876835	-4.8336500
40	H	0.9362902	-5.0720354	-1.3446456
41	H	-0.8668082	-5.1052408	-1.3384946
42	H	-0.9446520	5.0672182	-1.3170847
43	H	0.8584582	5.0976479	-1.3313473
44	H	0.9050016	3.5663715	0.5650959
45	H	-0.8948928	-3.5801136	0.5628318
46	H	5.4432452	-0.0030620	0.8781334
47	H	3.4819840	-0.0012228	-1.0909899
48	H	-3.4884872	-0.0229844	-1.0621359
49	H	-5.4336557	-0.0064826	0.9229898
50	H	-3.9843494	0.0140823	3.2730887
51	H	4.0131308	-0.0016880	3.2401946
52	H	0.8942148	-3.5859814	0.5881233
53	H	-0.8837478	3.5739116	0.6092767

$[Fe(L^1H)(bpp)]^{2+}$, low-spin

1	Fe	0.0003460	0.0000233	-0.0925019
2	N	0.0081872	0.0002799	1.8126906
3	C	-1.1652063	0.0084566	2.4925244
4	C	-1.2102585	0.0101275	3.8936544
5	C	0.0193766	0.0004275	4.5802095
6	H	0.0238019	0.0004756	5.6790519
7	C	1.2434250	-0.0093289	3.8837445
8	H	2.1995372	-0.0179938	4.4216245
9	C	1.1870396	-0.0078044	2.4829816
10	N	-2.2546864	0.0144235	1.6051239
11	N	-1.9431263	0.0091064	0.2581938
12	C	-3.1190095	0.0170441	-0.3895052
13	C	-4.2003610	0.0260558	0.5323656
14	C	-3.6193173	0.0243810	1.7929455
15	N	2.2692095	-0.0139011	1.5866400
16	N	1.9468101	-0.0088274	0.2422704
17	C	3.1174468	-0.0168124	-0.4148248

18	C	4.2062173	-0.0256054	0.4982968
19	C	3.6353140	-0.0237542	1.7635060
20	N	-0.0091367	-0.0003260	-2.0061383
21	C	-0.0212748	-1.1815742	-2.6856533
22	C	-0.0296054	-1.2221728	-4.0907046
23	H	-0.0402355	-2.1882683	-4.6131450
24	C	-0.0241271	-0.0008333	-4.7939149
25	H	-0.0299660	-0.0010342	-5.8928165
26	C	-0.0112648	1.2207630	-4.0912480
27	C	-0.0044912	1.1806797	-2.6861752
28	C	-0.0206893	-2.2806396	-1.7171581
29	N	-0.0118730	-1.9694124	-0.4410374
30	C	-0.0209633	-3.2367681	0.3190759
31	C	-0.0038295	-4.3273471	-0.7945258
32	O	-0.0291367	-3.5618869	-2.0578123
33	C	0.0049967	2.2801010	-1.7181204
34	N	0.0091774	1.9693220	-0.4418689
35	C	0.0247420	3.2369256	0.3177154
36	C	0.0000279	4.3271758	-0.7960809
37	O	0.0097288	3.5612224	-2.0592952
38	H	-2.1619534	0.0188660	4.4393358
39	H	-0.0064633	2.1866673	-4.6141282
40	H	0.9136748	-4.9444354	-0.8055845
41	H	-0.8897993	-4.9882085	-0.7940807
42	H	-0.9152699	4.9475892	-0.7979058
43	H	0.8883601	4.9848388	-0.8050401
44	H	0.9352483	3.2943496	0.9482063
45	H	-0.9268968	-3.2942609	0.9561643
46	H	5.2740209	-0.0323066	0.2590282
47	H	3.1378049	-0.0143424	-1.5102137
48	H	-5.2700618	0.0327756	0.3017306
49	H	-3.1481657	0.0143729	-1.4846878
50	H	-4.0632345	0.0296623	2.7933736
51	H	4.0873007	-0.0288627	2.7603197
52	H	-0.8552727	3.2968654	0.9892107
53	H	0.8638824	-3.2962712	0.9841835

$[Fe(L^2H)(bpp)]^{2+}$, high-spin

1	Fe	-0.0000048	-0.0000001	-0.1911313
2	N	-0.0000031	0.0000002	1.9919829
3	C	-0.2917130	1.1304943	2.6629060
4	C	-0.3048580	1.1856967	4.0674836
5	C	0.0000018	0.0000010	4.7580207
6	H	0.0000039	0.0000014	5.8573745
7	C	0.3048587	-1.1856953	4.0674832
8	H	0.5404416	-2.1067867	4.6137454
9	C	0.2917086	-1.1304936	2.6629056
10	N	-0.5782190	2.2319451	1.8219791
11	N	-0.5278070	2.0554554	0.4614110
12	C	-0.8456679	3.2465471	-0.0664667
13	C	-1.1045001	4.2077582	0.9464030
14	C	-0.9242593	3.5269756	2.1420952
15	N	0.5782114	-2.2319450	1.8219782
16	N	0.5277949	-2.0554556	0.4614101
17	C	0.8456560	-3.2465472	-0.0664680
18	C	1.1044937	-4.2077573	0.9464010
19	C	0.9242553	-3.5269747	2.1420935
20	N	0.0000010	-0.0000002	-2.3017514
21	C	-1.1390790	-0.2918341	-2.9812161
22	C	-1.1790363	-0.2933623	-4.3887472
23	H	-2.1143896	-0.5184780	-4.9205308
24	C	0.0000008	0.0000005	-5.0972745

25	H	0.0000004	0.0000010	-6.1960362
26	C	1.1790384	0.2933626	-4.3887482
27	C	1.1390813	0.2918335	-2.9812178
28	C	-2.2662769	-0.5836410	-2.0728834
29	N	-2.0508991	-0.5241703	-0.7797765
30	C	-3.2249749	-0.9495465	0.0000596
31	C	-4.4861797	-0.8469574	-0.8858052
32	S	-3.8704468	-1.0234039	-2.6270898
33	C	2.2662820	0.5836399	-2.0728894
34	N	2.0509034	0.5241711	-0.7797801
35	C	3.2249842	0.9495494	0.0000621
36	C	4.4861869	0.8469537	-0.8858069
37	S	3.8704500	1.0233986	-2.6270896
38	H	-0.5404393	2.1067881	4.6137463
39	H	2.1143907	0.5184783	-4.9205319
40	H	-5.2240090	-1.6447476	-0.6846339
41	H	-4.9896223	0.1363712	-0.8083900
42	H	5.2240206	1.6447397	-0.6846357
43	H	4.9896246	-0.1363776	-0.8083903
44	H	3.3287355	0.3262479	0.9103266
45	H	-3.3287284	-0.3262449	0.9103211
46	H	-1.0157874	3.8659504	3.1784354
47	H	1.0157869	-3.8659492	3.1784335
48	H	0.8764272	-3.3711905	-1.1552826
49	H	1.3838400	-5.2584235	0.8208469
50	H	-1.3838449	5.2584249	0.8208495
51	H	-0.8764433	3.3711899	-1.1552812
52	H	3.0536752	1.9975086	0.3345483
53	H	-3.0536658	-1.9975020	0.3345523

$[Fe(L^2H)(bpp)]^{2+}$, low-spin

1	Fe	0.0000235	-0.0000650	-0.1773179
2	N	0.0070312	0.0016533	1.7308452
3	C	-1.1659727	0.0457831	2.4107579
4	C	-1.2114472	0.0500217	3.8118951
5	C	0.0170401	0.0029319	4.4990621
6	H	0.0210017	0.0034370	5.5979168
7	C	1.2405281	-0.0447846	3.8030835
8	H	2.1955898	-0.0841821	4.3414805
9	C	1.1849303	-0.0418835	2.4022712
10	N	-2.2546140	0.0862040	1.5234056
11	N	-1.9434534	0.0800793	0.1761386
12	C	-3.1184139	0.1175105	-0.4717134
13	C	-4.1992637	0.1481532	0.4503741
14	C	-3.6188473	0.1266677	1.7109663
15	N	2.2670492	-0.0833534	1.5069715
16	N	1.9461923	-0.0789639	0.1619684
17	C	3.1164866	-0.1169224	-0.4942296
18	C	4.2039708	-0.1461693	0.4200888
19	C	3.6326156	-0.1230578	1.6847940
20	N	-0.0084425	-0.0020206	-2.0756784
21	C	-0.0676499	-1.1891808	-2.7469724
22	C	-0.0839891	-1.2224651	-4.1539008
23	H	-0.1431694	-2.1818251	-4.6865576
24	C	-0.0230633	-0.0047720	-4.8580423
25	H	-0.0288261	-0.0058602	-5.9568491
26	C	0.0451301	1.2143131	-4.1569993
27	C	0.0435595	1.1838325	-2.7499151
28	C	-0.1075365	-2.2989189	-1.7876907
29	N	-0.0852548	-1.9610530	-0.5109015
30	C	0.0135471	-3.1360823	0.3737945
31	C	-0.4801733	-4.3744265	-0.4003916

32	S	-0.1471824	-3.9996263	-2.1913073
33	C	0.0929751	2.2954850	-1.7932889
34	N	0.0823965	1.9601926	-0.5156752
35	C	-0.0076758	3.1370604	0.3675156
36	C	0.4794965	4.3735867	-0.4137243
37	S	0.1296002	3.9953964	-2.2006087
38	H	-2.1625683	0.0899073	4.3572111
39	H	0.0984184	2.1726190	-4.6921703
40	H	0.0561768	-5.3005022	-0.1250907
41	H	-1.5694840	-4.5420787	-0.2932272
42	H	-0.0536673	5.3005581	-0.1352465
43	H	1.5698660	4.5407787	-0.3170696
44	H	0.5941499	2.9812613	1.2839935
45	H	-0.5800672	-2.9786345	1.2953279
46	H	-4.0628123	0.1380807	2.7113218
47	H	4.0838018	-0.1326577	2.6819392
48	H	-3.1469082	0.1212107	-1.5668376
49	H	-5.2683884	0.1825295	0.2195278
50	H	5.2714255	-0.1800906	0.1815829
51	H	3.1371463	-0.1217229	-1.5895290
52	H	1.0788896	-3.2490676	0.6767119
53	H	-1.0701675	3.2511129	0.6799887

$[Fe(L^1H)(terpy)]^{2+}$, high-spin

1	Fe	-0.0000008	-0.0000019	-0.0925732
2	N	-0.0000006	-0.0000003	2.0410695
3	C	1.1270904	-0.3623671	2.7005787
4	C	1.1586593	-0.3678188	4.1108868
5	C	-0.0000002	-0.0000002	4.8127254
6	H	-0.0000002	-0.0000002	5.9119713
7	C	-1.1586598	0.3678185	4.1108868
8	H	-2.0637035	0.6546624	4.6602311
9	C	-1.1270913	0.3623667	2.7005788
10	C	2.2756199	-0.7493037	1.8272215
11	N	2.0409497	-0.6955130	0.4844212
12	C	3.0213213	-1.0466180	-0.3706771
13	C	3.5275005	-1.1556124	2.3319013
14	C	-2.2756206	0.7493042	1.8272216
15	N	-2.0409502	0.6955144	0.4844212
16	C	-3.0213213	1.0466220	-0.3706768
17	C	-3.5275005	1.1556139	2.3319019
18	N	-0.0000005	-0.0000012	-2.2227078
19	C	0.4148854	1.0953377	-2.9085545
20	C	0.4314055	1.1389249	-4.3140602
21	H	0.7730932	2.0441866	-4.8341010
22	C	0.0000005	-0.0000010	-5.0220037
23	H	0.0000011	-0.0000010	-6.1208476
24	C	-0.4314051	-1.1389270	-4.3140605
25	C	-0.4148861	-1.0953398	-2.9085549
26	C	0.8194672	2.1722206	-1.9892852
27	N	0.7486367	1.9905289	-0.6959825
28	C	1.2174165	3.2394044	-0.0605394
29	C	1.5574418	4.1690028	-1.2637171
30	O	1.2594399	3.3406362	-2.4470593
31	C	-0.8194679	-2.1722227	-1.9892853
32	N	-0.7486368	-1.9905310	-0.6959829
33	C	-1.2174159	-3.2394072	-0.0605406
34	C	-1.5574422	-4.1690047	-1.2637186
35	O	-1.2594403	-3.3406378	-2.4470603
36	H	2.0637032	-0.6546624	4.6602309
37	H	-0.7730923	-2.0441888	-4.8341014
38	H	0.9261183	5.0745387	-1.3293516

39	H	2.6219885	4.4614344	-1.3265270
40	H	-0.9261195	-5.0745409	-1.3293539
41	H	-2.6219891	-4.4614357	-1.3265285
42	H	-2.0979072	-3.0325328	0.5815070
43	H	2.0979082	3.0325291	0.5815074
44	H	-2.7809481	0.9857340	-1.4432363
45	H	2.7809482	-0.9857287	-1.4432366
46	H	3.7136659	-1.1935107	3.4125871
47	H	-3.7136657	1.1935116	3.4125878
48	C	4.5458166	-1.5186002	1.4362833
49	H	5.5270649	-1.8387871	1.8149051
50	H	5.0576400	-1.7444066	-0.6792578
51	C	4.2906517	-1.4671194	0.0568419
52	C	-4.5458160	1.5186038	1.4362841
53	H	-5.5270640	1.8387913	1.8149062
54	H	-5.0576388	1.7444139	-0.6792569
55	C	-4.2906510	1.4671246	0.0568425
56	H	0.4241086	3.6584749	0.5911702
57	H	-0.4241075	-3.6584782	0.5911679

$[Fe(L^1H)(terpy)]^{2+}$, low-spin

1	Fe	0.0000006	-0.0000004	-0.0745423
2	N	0.0000005	-0.0000007	1.8205195
3	C	1.1330851	-0.3652552	2.4885305
4	C	1.1585448	-0.3717675	3.8959519
5	C	0.0000003	-0.0000021	4.5997129
6	H	-0.0000002	-0.0000024	5.6984351
7	C	-1.1585439	0.3717643	3.8959520
8	H	-2.0675693	0.6623949	4.4381670
9	C	-1.1330840	0.3652535	2.4885307
10	C	2.2239633	-0.7202042	1.5652408
11	N	1.8714855	-0.6168167	0.2371701
12	C	2.7967292	-0.9183028	-0.7037230
13	C	3.5148528	-1.1245556	1.9527824
14	C	-2.2239621	0.7202036	1.5652414
15	N	-1.8714843	0.6168167	0.2371705
16	C	-2.7967280	0.9183041	-0.7037223
17	C	-3.5148512	1.1245557	1.9527832
18	N	0.0000015	-0.0000010	-1.9929698
19	C	0.3673770	1.1237662	-2.6737260
20	C	0.3792003	1.1618234	-4.0791860
21	H	0.6781422	2.0797390	-4.6031176
22	C	0.0000039	-0.0000023	-4.7819048
23	H	0.0000054	-0.0000030	-5.8807724
24	C	-0.3791942	-1.1618272	-4.0791857
25	C	-0.3673734	-1.1237684	-2.6737257
26	C	0.7069321	2.1653313	-1.7022512
27	N	0.6166271	1.8593607	-0.4272885
28	C	1.0266670	3.0541606	0.3403521
29	C	1.3098831	4.1141653	-0.7644319
30	O	1.1006208	3.3878926	-2.0337230
31	C	-0.7069309	-2.1653324	-1.7022507
32	N	-0.6166268	-1.8593612	-0.4272880
33	C	-1.0266679	-3.0541606	0.3403526
34	C	-1.3098948	-4.1141598	-0.7644304
35	O	-1.1006221	-3.3878930	-2.0337219
36	H	2.0675699	-0.6623991	4.4381668
37	H	-0.6781349	-2.0797435	-4.6031168
38	H	0.6081765	4.9683899	-0.7580915
39	H	2.3473735	4.4934056	-0.7713295
40	H	-0.6082038	-4.9683918	-0.7580879
41	H	-2.3473869	-4.4933830	-0.7713293

42	H	-1.9243511	-2.8245239	0.9495006
43	H	1.9243561	2.8245254	0.9494942
44	H	-2.4844861	0.8292781	-1.7529080
45	H	2.4844874	-0.8292762	-1.7529086
46	H	3.7710213	-1.1990406	3.0177127
47	H	-3.7710196	1.1990399	3.0177136
48	C	4.4678082	-1.4293165	0.9699845
49	H	5.4816731	-1.7436948	1.2550026
50	H	4.8098543	-1.5543367	-1.1875960
51	C	4.0993614	-1.3246318	-0.3817444
52	C	-4.4678064	1.4293181	0.9699857
53	H	-5.4816711	1.7436968	1.2550043
54	H	-4.8098526	1.5543401	-1.1875948
55	C	-4.0993599	1.3246340	-0.3817433
56	H	0.2210433	3.3657544	1.0344805
57	H	-0.2210418	-3.3657597	1.0344733

$[Fe(L^2H)(terpy)]^{2+}$, high-spin

1	Fe	0.0000022	0.0000016	-0.1732304
2	N	0.0000020	0.0000013	1.9685906
3	C	0.7734751	-0.8967999	2.6276896
4	C	0.7977305	-0.9177178	4.0378854
5	C	0.0000006	0.0000010	4.7396713
6	H	0.0000000	0.0000007	5.8389371
7	C	-0.7977287	0.9177197	4.0378849
8	H	-1.4208376	1.6337785	4.5875875
9	C	-0.7734720	0.8968020	2.6276890
10	C	1.5552357	-1.8226546	1.7528639
11	N	1.3918723	-1.6432173	0.4104398
12	C	2.0544848	-2.4414327	-0.4489037
13	C	2.4059151	-2.8287689	2.2539405
14	C	-1.5552330	1.8226552	1.7528624
15	N	-1.3918703	1.6432162	0.4104382
16	C	-2.0544853	2.4414296	-0.4489053
17	C	-2.4059127	2.8287697	2.2539385
18	N	0.0000001	0.0000020	-2.2842491
19	C	0.9034030	0.7541599	-2.9668103
20	C	0.9372465	0.7730698	-4.3740694
21	H	1.6843849	1.3797304	-4.9053040
22	C	-0.0000007	0.0000008	-5.0836247
23	H	-0.0000001	0.0000008	-6.1822831
24	C	-0.9372471	-0.7730669	-4.3740710
25	C	-0.9034041	-0.7541564	-2.9668108
26	C	1.7992205	1.4986028	-2.0607323
27	N	1.6353280	1.3478583	-0.7670522
28	C	2.5189349	2.2286345	0.0139455
29	C	3.7049571	2.6660592	-0.8731841
30	S	3.0631872	2.5836766	-2.6121232
31	C	-1.7992226	-1.4985985	-2.0607372
32	N	-1.6353285	-1.3478561	-0.7670569
33	C	-2.5189386	-2.2286378	0.0139474
34	C	-3.7049589	-2.6660626	-0.8731869
35	S	-3.0631879	-2.5836717	-2.6121241
36	H	1.4208381	-1.6337772	4.5875883
37	H	-1.6843850	-1.3797272	-4.9053052
38	H	4.0472832	3.6960821	-0.6655433
39	H	4.5706942	1.9788596	-0.8046940
40	H	-4.0472831	-3.6960858	-0.6655457
41	H	-4.5706979	-1.9788655	-0.8046935
42	H	-2.8743666	-1.7052465	0.9232418
43	H	2.8743623	1.7052449	0.9232383
44	H	2.5354772	-2.9708859	3.3342871

45	H	1.8874170	-2.2505335	-1.5200448
46	H	-1.8874197	2.2505286	-1.5200464
47	H	-2.5354743	2.9708875	3.3342850
48	C	3.0935938	-3.6590833	1.3542198
49	H	3.7600536	-4.4486758	1.7298341
50	H	3.4346176	-4.0929015	-0.7630386
51	C	2.9164698	-3.4655647	-0.0248147
52	C	-2.9164698	3.4655622	-0.0248167
53	H	-3.4346188	4.0928976	-0.7630409
54	C	-3.0935924	3.6590829	1.3542177
55	H	-3.7600522	4.4486754	1.7298316
56	H	1.9215621	3.1062087	0.3484943
57	H	-1.9215615	-3.1062123	0.3484926

$[Fe(L^2H)(terpy)]^{2+}$, low-spin

1	Fe	0.0000002	-0.0000001	-0.1521551
2	N	0.0000000	0.0000000	1.7451973
3	C	0.7416319	-0.9312773	2.4145121
4	C	0.7586833	-0.9511610	3.8217234
5	C	-0.0000007	-0.0000003	4.5257954
6	H	-0.0000012	-0.0000005	5.6245134
7	C	-0.7586844	0.9511607	3.8217232
8	H	-1.3532175	1.6977999	4.3638658
9	C	-0.7416322	0.9312773	2.4145119
10	C	1.4500150	-1.8347691	1.4926035
11	N	1.2251439	-1.5470681	0.1642192
12	C	1.8246038	-2.3132116	-0.7771658
13	C	2.2797696	-2.9029356	1.8807395
14	C	-1.4500150	1.8347691	1.4926031
15	N	-1.2251437	1.5470680	0.1642188
16	C	-1.8246033	2.3132116	-0.7771663
17	C	-2.2797692	2.9029357	1.8807389
18	N	0.0000000	-0.0000001	-2.0537754
19	C	0.9311972	0.7376209	-2.7290630
20	C	0.9607961	0.7519047	-4.1364171
21	H	1.7212015	1.3398235	-4.6688936
22	C	-0.0000010	0.0000009	-4.8397958
23	H	-0.0000014	0.0000014	-5.9385248
24	C	-0.9607975	-0.7519034	-4.1364170
25	C	-0.9311977	-0.7376206	-2.7290629
26	C	1.7990608	1.4291841	-1.7706470
27	N	1.5313219	1.2174588	-0.4936797
28	C	2.3653678	2.0426525	0.3975614
29	C	3.6200308	2.4909004	-0.3800858
30	S	3.1132206	2.5097329	-2.1708237
31	C	-1.7990609	-1.4291841	-1.7706468
32	N	-1.5313216	-1.2174590	-0.4936795
33	C	-2.3653670	-2.0426532	0.3975617
34	C	-3.6200302	-2.4909009	-0.3800853
35	S	-3.1132206	-2.5097330	-2.1708233
36	H	1.3532159	-1.6978005	4.3638661
37	H	-1.7212032	-1.3398219	-4.6688933
38	H	3.9666423	3.5015741	-0.0984445
39	H	4.4638113	1.7804197	-0.2817939
40	H	-3.9666417	-3.5015745	-0.0984441
41	H	-4.4638107	-1.7804201	-0.2817929
42	H	-2.6402728	-1.4726579	1.3058686
43	H	2.6402739	1.4726570	1.3058681
44	H	2.4415995	-3.1158975	2.9455682
45	H	1.6246840	-2.0556532	-1.8258060
46	H	-1.6246833	2.0556530	-1.8258065
47	H	-2.4415994	3.1158978	2.9455675

48	C	2.8933816	-3.6932082	0.8979870
49	H	3.5418051	-4.5333436	1.1838101
50	H	3.1194496	-3.9811078	-1.2593722
51	C	2.6611159	-3.3908430	-0.4541566
52	C	-2.6611150	3.3908430	-0.4541577
53	H	-3.1194485	3.9811078	-1.2593734
54	C	-2.8933808	3.6932083	0.8979860
55	H	-3.5418039	4.5333440	1.1838089
56	H	1.7573518	2.9165525	0.7222651
57	H	-1.7573508	-2.9165533	0.7222649

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