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Structure:Function Relationships for Thermal and Light-Induced Spin-Crossover in Isomorphous Molecular Materials

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Supporting Information

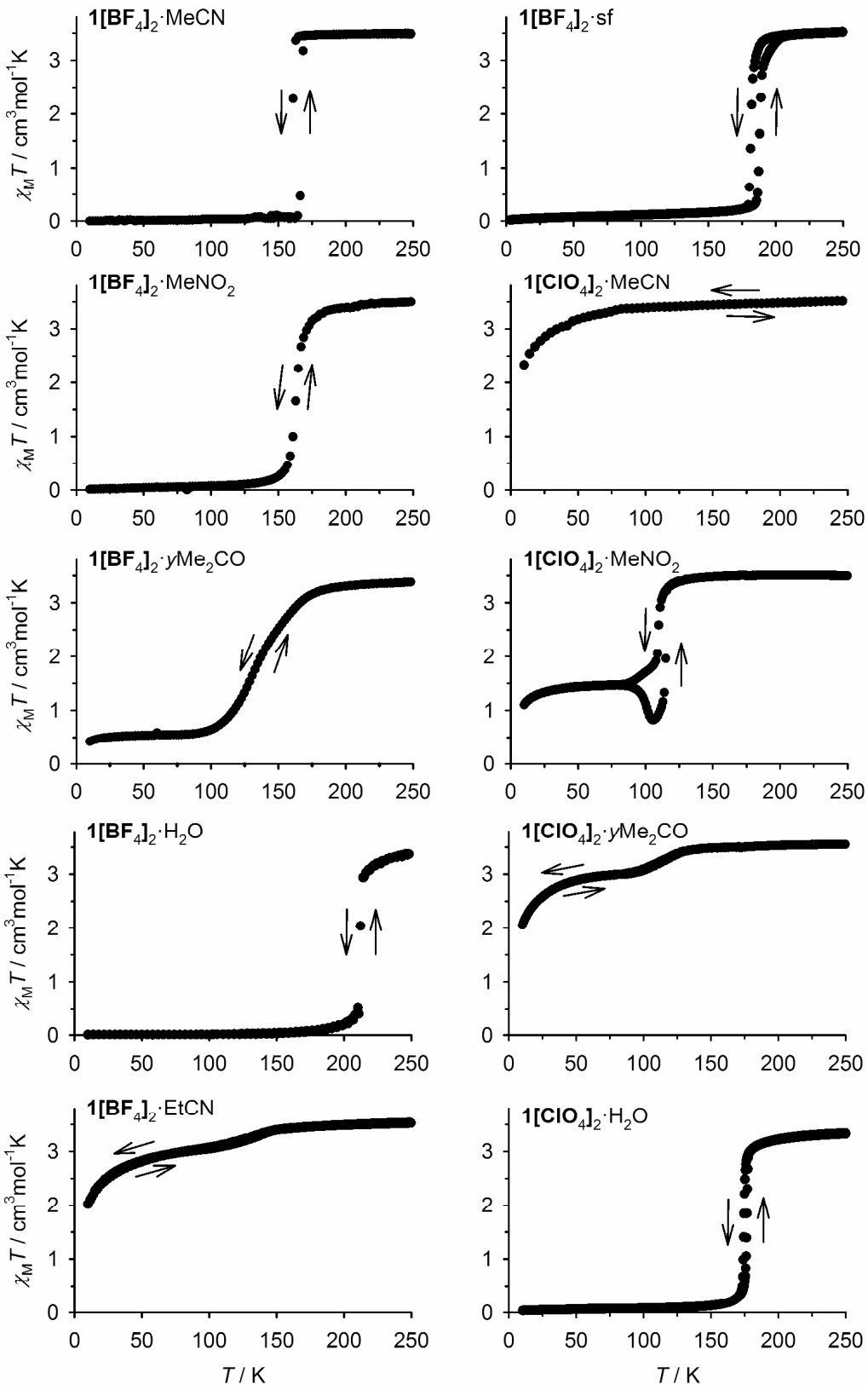


Figure S1 Variable temperature magnetic susceptibility data for ten **1X₂**·solv compounds, at a scan rate of 0.4 Kmin^{-1} or (for **1[BF₄]₂**·EtCN, **1[BF₄]₂**·sf and **1[ClO₄]₂**·H₂O) 5 Kmin^{-1}. Data are taken from refs 1 and 2.

Solvent-free **1[ClO₄]₂**·sf can also be prepared on the diffractometer, by annealing **1[ClO₄]₂**·H₂O *in situ*.[2] Any fraction of the samples that is high-spin near 100 K remains frozen in below that temperature. That is commonly found in complexes of this type,[2,3] when thermal trapping of the high-spin state occurs near $T_{½}$.[3-5]

The unusual form of the SCO in **1[ClO₄]₂**·MeNO₂ similarly reflects a kinetic inhibition of this low temperature spin transition. Poising the sample at 102 K for 80 mins allows it to fully transform to its low-spin state.[2]

Crystallographic refinement details – ligand *L*

The crystallographic equipment and software used for this study are listed in the main article. Experimental data for this structure determination are listed in Table S1.

The dataset is only 89.5 % complete to $\theta = 72°$, which reflects incomplete data collection in the hk*0* and *0*kl zones. That's a consequence of the long unit cell *b* axis, and the crystal's needle morphology. Despite that limitation, the observed data:parameter ratio is 12.3:1, which is easily enough for a precise refinement.

No disorder is present in the final model. All non-H atoms were refined anisotropically, and H atoms were placed in calculated positions and refined using a riding model. CCDC 1978280.

Table S1 Experimental data for the crystal structure determination of ligand *L*.

Formula	$C_{14}H_{15}N_5S$	Z	4
M_r	285.37	T / K	120(2)
Crystal system	monoclinic	$\mu\{\text{Cu-}K_\alpha\}$ / mm^{-1}	2.040
Space group	$P2_1/n$	D_{calc} / gcm^{-3}	1.361
a / Å	4.2184(2)	Measured reflections	4056
b / Å	32.4625(16)	Independent reflections	2468
c / Å	10.1791(4)	R_{int}	0.025
β / °	92.362(4)	R_1, $I > 2\sigma(I)$[a]	0.045
V / Å^3	1392.74(11)	wR_2, all data[b]	0.114

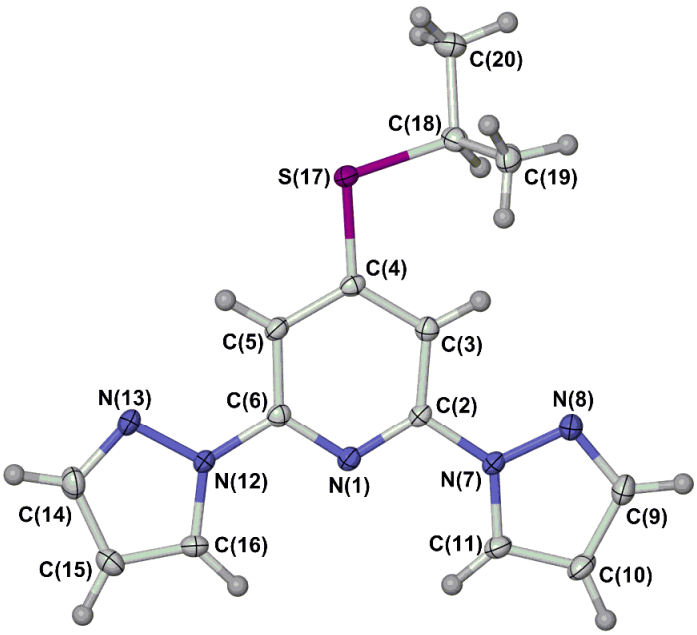


Figure S2. View of the molecule in the asymmetric unit of *L*. Displacement ellipsoids are at the 50 % probability level, except for H atoms which have arbitrary radii. Colour code: C, white; H, pale grey; N, blue; S, purple.

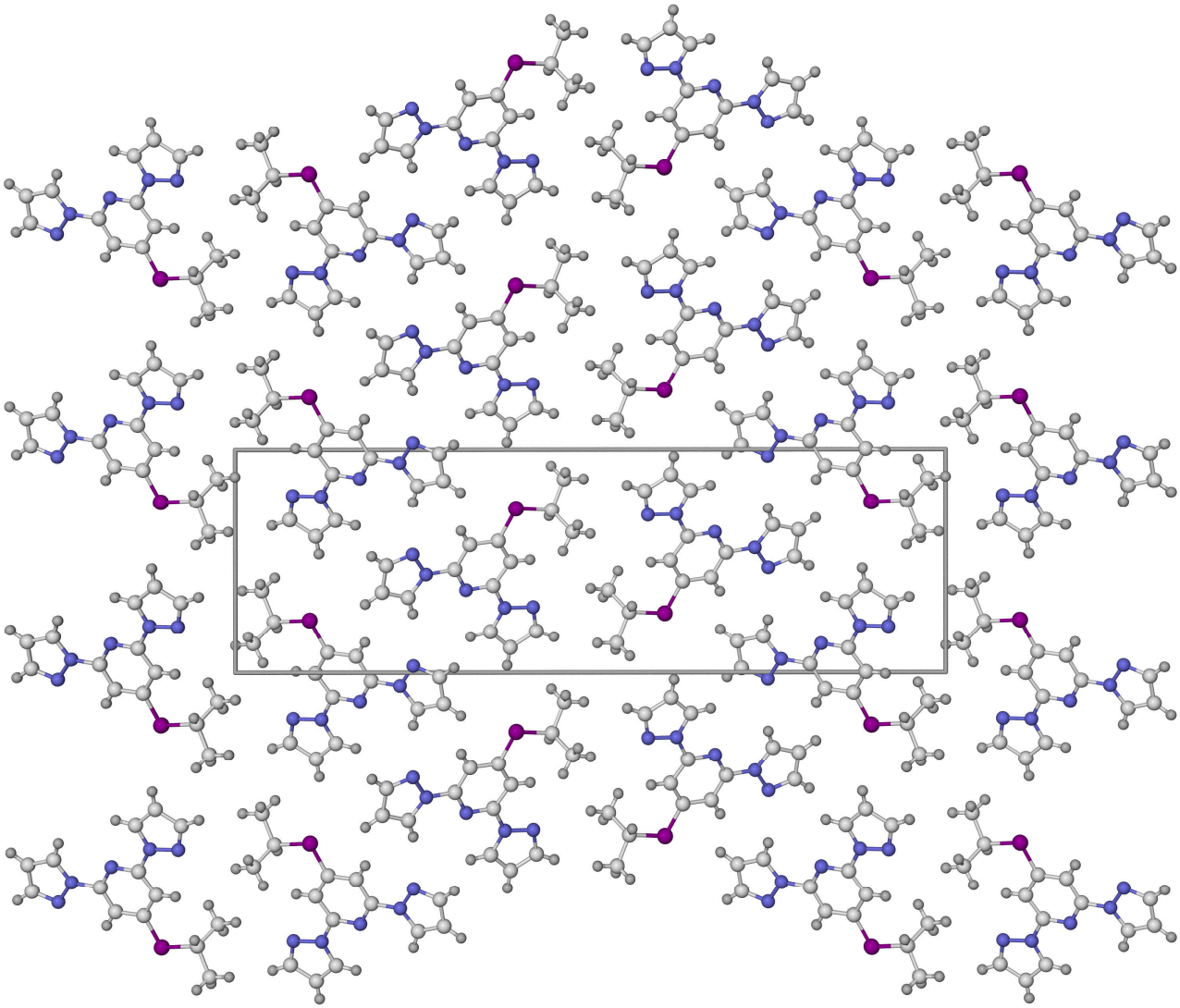


Figure S3. Packing diagram of *L*, viewed parallel to the [100] vector with the unit cell *b* axis horizontal. Colour code: C, white; H, pale grey; N, blue; S, purple.

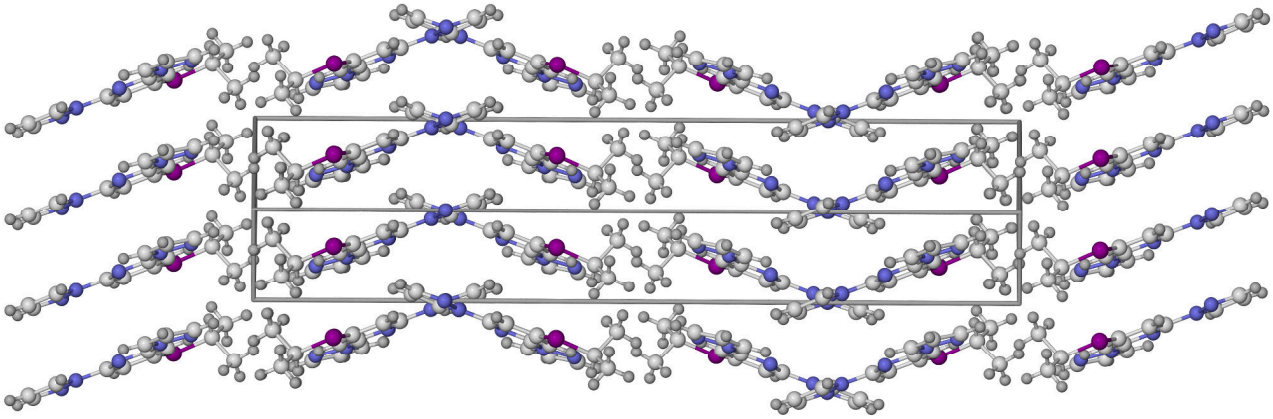


Figure S4. Packing diagrams of *L*, viewed parallel to [$\bar{1}$01] with the unit cell *b* axis horizontal. Other details as for Figure S3.

Molecules of *L* are associated into canted stacks by translation along *a*. The heterocyclic cores of adjacent molecules within the stacks are coplanar by symmetry, and separated by 3.386(8) Å.

Crystallographic refinement details - complexes

The crystallographic equipment and software used for this study are listed in the main article. Experimental data for these structure determinations are listed in Tables S2-S6.

Unless otherwise stated, the following procedures were used to model disordered residues. For disordered *iso*propylsulfanyl groups, fixed restraints were applied: C(pyridyl)–S = 1.75(2), C(alkyl)–S = 1.82(2), C–C = 1.52(2), 1,3-C–C–C = 2.48(2) and 1,3-C–S–C = 2.83(2) Å. In contrast, refined B–F and F…F distance restraints were applied to disordered anions. Unless otherwise stated all non-H atoms with occupancy >0.5 were refined anisotropically, and H atoms were placed in calculated positions and refined using a riding model. Anions were modelled as disordered if two of their F or O atoms exhibited $U_{iso} \geq 0.07$ above 100 K, or $U_{iso} \geq 0.04$ in the photocrystallographic studies at helium temperatures. Similar criteria were used for peripheral atoms in the solvent molecules and for *iso*propylmethyl groups.

Structure refinements of 1[BF_4]$_2$·$MeNO_2$. Thirteen datasets of this compound were determined, at temperatures between 120-230 K (Table S1). Spin-crossover in the crystal occurs between 150 and 190 K, with $T_{½} \approx 165$ K.

Between 210 and 230 K, one of the *iso*propyl substituents on the complex cation is disordered over two equally occupied orientations, which modelled successfully without restraints. Both BF_4^- ions were also disordered, one over two half-occupied sites and the other over three equally occupied orientations that share a common fully occupied B atom. Finally, the nitromethane molecule was also disordered and was refined with three sites with occupancies of 0.50, 0.35 and 0.15. These were modelled with the fixed restraints C–N = 1.45(2), N–O = 1.22(2), O...O = 2.09(2) and C...O = 2.32(2) Å.

At 170-200 K one of the BF_4^- ions became crystallographically ordered, but the other disordered residues were refined as above. Between 130-165 K the remaining anion and solvent disorder was less pronounced, and was modelled using just two rather than three disorder orientations in each case. The disordered *iso*propyl group was treated as before. At 120 K, the *iso*propyl group disorder was crystallographically ordered, and the remaining anion and solvent disorder was modelled over two sites, as above.

CCDC 1976560-1976565, 1976567-1976572 and 1976574.

Structure refinements of 1[BF_4]$_2$·*y*Me_2CO (*y* ≈ 0.75). Twelve datasets of this compound were determined, at temperatures between 110-220 K (Table S2). Spin-crossover in the crystal occurs gradually on cooling between 170 and 110 K, and the crystal may still not be fully low spin at the lowest temperature based on its metric parameters.

The following disorder was present at all temperatures. One isopropyl substituent is disordered over three equally occupied orientations, two of which share a common S atom. The acetone solvent molecule was refined over three sites, whose occupancies vary slightly between temperatures but sum consistently to 0.75. The fixed restraints C–O = 1.22(2), C–C = 1.51(2), 1,3-C...C = 2.62(2) and 1,3-C...O = 2.37(2) Å were applied to the partial solvent molecules.

Between 140-210 K, both BF_4^- ions were also disordered, one over two half-occupied sites and the other over three equally occupied orientations that share a common fully occupied B atom. At 110-130 K, the former anion was crystallographically ordered, while the latter refined reasonably over just two orientations.

CCDC 1976575-1976582 and 1976586-1976589.

Structure refinements of 1[BF_4]$_2$·MeCN. This compound undergoes spin-crossover abruptly and with thermal hysteresis, with $T_{½}\downarrow$ =162±3 K and $T_{½}\uparrow$ =167±3 K. Twenty-five datasets were measured from the same crystal, between 120-230 K on cooling and warming temperature ramps (Table S3). These included two measurements at 165 K, inside the spin-crossover thermal hysteresis loop.

The disorder in this crystal was very consistent, and correlated with its spin state. At temperatures where the crystal was high-spin ($T \geq 165$ K in cooling mode and $T \geq 170$ K in warming mode), the following disorder was present. One *iso*propyl substituent is disordered over two equally occupied orientations, which were modelled as described above. Both BF_4^- ions are also disordered over two sites, one of which was modelled using a common, fully occupied B atom. The MeCN molecule is also disordered across three sites with occupancies of 0.40, 0.40 and 0.20. These were modelled with the fixed restraints C–C = 1.48(2), C–N = 1.15(2) and 1,3-C–C–N = 2.63(2) Å.

Where the crystal was low-spin, the *iso*propyl group and solvent were apparently crystallographically ordered. The displacement ellipsoids of the intra-bilayer anion decrease more gradually on cooling; this was modelled as disordered at $T \geq 150$ K, but was ordered at lower temperatures by the criteria listed above. The inter-bilayer anion remained disordered at all these temperatures, and was refined over two sites in the low-spin structures.

CCDC 1976590-1976612 and 1976614-1976615.

Structure refinements of 1[BF_4]$_2$·H_2O. This crystal undergoes spin-crossover abruptly, at $T_{½} \approx 210$ K. Eleven datasets of this compound were measured, at temperatures between 150 and 260 K (Table S4).

Between 220-260 K, one of the *iso*propylsulfanyl substituents on the complex cation is disordered over three orientations, with occupancies of 0.50, 0.35 and 0.15. Both BF_4^- ions are also disordered, one over two half-occupied sites and the other over three equally occupied orientations with a common fully occupied B atom. Lastly, the water molecule was also refined over three different sites.

At 210 K, the disordered *iso*propylsulfanyl group and water molecule were successfully treated with two disorder sites, rather than three. The anion disorder continued as above.

At 190 and 200 K, the *iso*propylsulfanyl group was now crystallographically ordered. The other disorder in the model continued as above.

At 180 K, the more disordered anion was slightly improved, and was treated with two rather than three disorder sites. The other anion and the lattice water were treated as above.

Between 150-170 K, one anion and the lattice water were now crystallographically ordered. Disorder in the other anion was refined over two orientations, as before. This anion disorder is retained in our published structure of this crystal at 20 K.

The H atoms on the crystallographically ordered lattice water were located in the Fourier map at low temperatures, and refined positionally using the fixed restraints O–H = 0.90(2) and H...H = 1.47(2) Å, and with U_{iso} constrained to 1.5xU_{eq}{O}. Disordered water H atoms could not be located and are not included in the model at these temperatures, but are accounted for in the molecular weight and density calculations.

CCDC 1976616-1976626.

Single crystal X-ray structure determinations at very low temperature, or under irradiation

Unless otherwise stated, all fully occupied non-H atoms were refined anisotropically, and H atoms were placed in calculated positions and refined using a riding model. Disordered anions were modelled using refined B–F or Cl–O distance restraints. Refinement details for the structures from ref 2 are described there.

Structure refinement of 1[BF_4]$_2$·CH_3NO_2, phase 2 at 40 K. This asymmetric unit of this phase contains three formula units of the compound.[2] That is, three complex dications, six BF_4^- ions and three nitromethane molecules, all on general crystallographic sites. No disorder is present in the model. CCDC 1976613.

Structure refinements of 1[BF_4]$_2$·$(CH_3)_2CO$ at 20 K. A similar amount of disorder was found both before and after irradiation of the crystal, although the relative occupancies of the different disorder sites differed slightly in the two structures. One of the isopropyl substitutents on the complex cation is disordered over three orientations, which were modelled with the fixed restraints C(pyridyl) –S = 1.75(2), C(alkyl)–S = 1.82(2), C–C = 1.52(2), 1,3-C–C–C = 2.48(2) and 1,3-C–S–C = 2.83(2) Å. One BF_4^- ion is also disordered over three orientations. Finally, the partial acetone solvent molecule is also disordered over three sites whose occupancies sum to 0.75. The fixed restraints C–O = 1.22(2), C–C = 1.51(2), 1,3-C...C = 2.62(2) and 1,3-C...O = 2.37(2) Å were applied to these sites. All non-H atoms with occupancy >0.5 were refined anisotropically. CCDC 1976566 and 1976573.

Structure refinements of 1[ClO_4]$_2$·CH_3NO_2 at 10 K. In agreement with its magnetic data, this crystal was not fully low-spin at the temperature of measurement, and retained a significant residual high-spin fraction from its metric parameters. The nitromethane molecule in the low-spin 'dark' structure is disordered over two sites, with occupancies of 0.75 and 0.25, which share common wholly occupied C atom and one O atom. The fixed restraints C–N = 1.45(2), N–O = 1.22(2), O...O = 2.09(2) and C...O = 2.32(2) Å were applied to those residues. No disorder is present in the high-spin crystal following irradiation. CCDC 1976559 and 1976585.

Structure refinements of 1[ClO_4]$_2$·H_2O at 10 K. No disorder is present in the low-spin 'dark' structure, but after irradiation one ClO_4^- ion is disordered over two equally occupied sites. The water H atoms were located in the Fourier map and allowed to refine, with U_{iso} constrained to 1.5x U_{eq}(O). CCDC 1976583 and 1976584.

Table S2 Experimental data for the variable temperature crystal structures of **1[BF$_4$]$_2$**·CH_3NO_2 ($C_{29}H_{33}B_2F_8FeN_{11}O_2S_2$, M_r 861.25, monoclinic, $P2_1/c$, $Z = 4$). Datasets were measured in the order of their listing in the Table.

T / K	120(2)	130(2)	140(2)	150(2)	160(2)	165(2)	170(2)
a / Å	19.7604(2)	19.7618(3)	19.7747(3)	19.7876(3)	19.8385(3)	19.9696(4)	20.1147(3)
b / Å	11.9415(2)	11.9423(2)	11.9407(2)	11.9435(2)	11.9496(2)	11.9655(3)	11.9790(2)
c / Å	16.0710(3)	16.0888(3)	16.1117(3)	16.1240(3)	16.1083(3)	16.0392(4)	15.9689(3)
β / °	100.996(1)	100.998(1)	101.035(2)	101.031(2)	100.972(2)	100.959(2)	101.023(2)
V / Å^3	3722.63(10)	3727.24(11)	3734.01(11)	3740.23(11)	3748.86(11)	3762.61(15)	3776.78(11)
μ{Cu-K_α} / mm^{-1}	5.066	5.060	5.051	5.042	5.031	5.012	4.994
D_{calc} / gcm^{-3}	1.537	1.535	1.532	1.529	1.526	1.520	1.515
Measured reflections	16022	16040	16078	16095	16121	16161	16248
Independent reflections	7248	7257	7272	7278	7295	7322	7345
R_{int}	0.044	0.041	0.041	0.044	0.044	0.049	0.048
R_1, $I > 2\sigma(I)$[a]	0.052	0.052	0.051	0.054	0.056	0.055	0.054
wR_2, all data[b]	0.135	0.135	0.129	0.140	0.146	0.148	0.142
CCDC	1976561	1976560	1976563	1976562	1976565	1976564	1976567
T / K	180(2)	190(2)	200(2)	210(2)	220(2)	230(2)	
a / Å	20.1945(3)	20.2133(3)	20.2249(3)	20.2251(4)	20.2365(4)	20.2322(4)	
b / Å	11.9830(2)	11.9863(2)	11.9882(2)	11.9925(3)	11.9924(3)	11.9984(3)	
c / Å	15.9553(4)	15.9773(3)	16.0062(4)	16.0231(4)	16.0676(4)	16.1007(5)	
β / °	101.061(2)	101.083(2)	101.112(2)	101.158(2)	101.180(2)	101.199(3)	
V / Å^3	3789.31(13)	3798.83(11)	3808.11(13)	3812.93(15)	3825.35(15)	3834.09(17)	
μ{Cu-K_α} / mm^{-1}	4.977	4.965	4.952	4.946	4.930	4.919	
D_{calc} / gcm^{-3}	1.510	1.506	1.502	1.500	1.495	1.492	
Measured reflections	16312	16327	16352	16458	16498	16490	
Independent reflections	7371	7385	7402	7407	7420	7439	
R_{int}	0.046	0.044	0.045	0.047	0.047	0.050	
R_1, $I > 2\sigma(I)$[a]	0.052	0.053	0.053	0.059	0.062	0.063	
wR_2, all data[b]	0.138	0.138	0.144	0.164	0.171	0.172	
CCDC	1976568	1976569	1976571	1976570	1976574	1976572	

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

Table S3 Experimental data for the variable temperature crystal structures of **1[BF$_4$]$_2$**·*y*$(CH_3)_2CO$ (*y* ≈ 0.75; $C_{30.25}H_{34.50}B_2F_8FeN_{10}O_{0.75}S_2$, M_r 843.77, monoclinic, $P2_1/c$, $Z = 4$). Datasets were measured in the order of their listing in the Table.

T / K	110(2)	120(2)	130(2)	140(2)	150(2)	160(2)
a / Å	19.8506(2)	19.8690(2)	19.9120(3)	20.0287(6)	20.1820(5)	20.2576(3)
b / Å	11.7392(2)	11.7488(2)	11.7601(2)	11.7606(3)	11.7579(4)	11.7763(2)
c / Å	16.2839(2)	16.2777(2)	16.2542(3)	16.1962(4)	16.1413(3)	16.1018(2)
β / °	101.050(1)	101.090(1)	101.143(2)	101.201(2)	101.2718(19)	101.2296(14)
V / Å^3	3724.29(9)	3728.86(9)	3734.44(11)	3742.32(17)	3756.39(16)	3767.68(10)
μ{Cu-K_α} / mm^{-1}	5.016	5.010	5.003	4.992	4.974	4.959
D_{calc} / gcm^{-3}	1.505	1.503	1.501	1.498	1.492	1.488
Measured reflections	12061	12059	12044	12041	12134	12185
Independent reflections	7173	7182	7180	7184	7212	7240
R_{int}	0.028	0.028	0.030	0.032	0.031	0.028
R_1, $I > 2\sigma(I)$[a]	0.065	0.067	0.072	0.078	0.069	0.066
wR_2, all data[b]	0.183	0.186	0.203	0.201	0.188	0.181
CCDC	1976578	1976579	1976575	1976576	1976577	1976586
T / K	170(2)	180(2)	190(2)	200(2)	210(2)	220(2)
a / Å	20.3009(3)	20.3264(3)	20.3390(2)	20.3429(2)	20.3565(2)	20.3561(3)
b / Å	11.7872(2)	11.7990(2)	11.8032(2)	11.8179(2)	11.8296(2)	11.8436(2)
c / Å	16.0867(2)	16.0878(2)	16.1023(2)	16.1193(2)	16.1440(2)	16.1674(2)
β / °	101.2045(14)	101.227(1)	101.234(1)	101.260(1)	101.298(1)	101.322(1)
V / Å^3	3776.02(10)	3784.52(10)	3791.54(9)	3800.65(9)	3812.29(9)	3821.94(10)
μ{Cu-K_α} / mm^{-1}	4.948	4.937	4.928	4.916	4.901	4.888
D_{calc} / gcm^{-3}	1.484	1.481	1.478	1.475	1.470	1.466
Measured reflections	12204	12272	12325	12339	12385	12427
Independent reflections	7247	7270	7266	7288	7314	7320
R_{int}	0.028	0.022	0.024	0.023	0.023	0.024
R_1, $I > 2\sigma(I)$[a]	0.063	0.060	0.062	0.065	0.066	0.068
wR_2, all data[b]	0.174	0.168	0.177	0.188	0.192	0.199
CCDC	1976587	1976588	1976589	1976580	1976581	1976582

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

Table S4 Experimental data for the variable temperature crystal structures of **1[BF$_4$]$_2$**·CH$_3$CN ($C_{30}H_{33}B_2F_8FeN_{11}S_2$, M_r 841.26, monoclinic, $P2_1/c$, $Z = 4$). Datasets were measured in the order of their listing in the Table.

T / K	120(2) (warming)	130(2) (warming)	140(2) (warming)	150(2) (warming)	160(2) (warming)	165(2) (warming)	170(2) (warming)
a / Å	19.6218(2)	19.6277(2)	19.6351(2)	19.6439(2)	19.6500(2)	19.6561(2)	20.1829(3)
b / Å	12.2678(1)	12.2556(1)	12.2474(1)	12.2378(2)	12.2308(2)	12.2276(2)	11.9583(2)
c / Å	15.7743(2)	15.8045(2)	15.8336(2)	15.8626(2)	15.8907(2)	15.9009(2)	15.8165(2)
β / °	100.653(1)	100.662(1)	100.671(1)	100.707(1)	100.721(1)	100.742(1)	99.624(1)
V / Å^3	3731.69(7)	3736.13(7)	3741.80(7)	3746.95(9)	3752.43(9)	3754.76(9)	3763.64(10)
μ{Cu-K_α} / mm^{-1}	4.998	4.992	4.985	4.978	4.970	4.967	4.956
D_{calc} / gcm^{-3}	1.497	1.496	1.493	1.491	1.489	1.488	1.485
Measured reflections	15015	15077	15079	15077	15135	15149	15188
Independent reflections	7187	7194	7203	7208	7222	7233	7258
R_{int}	0.032	0.031	0.030	0.032	0.032	0.032	0.032
R_1, $I > 2\sigma(I)$[a]	0.043	0.044	0.045	0.049	0.050	0.050	0.055
wR_2, all data[b]	0.108	0.110	0.110	0.125	0.130	0.132	0.147
CCDC	1976598	1976607	1976600	1976601	1976605	1976603	1976602
T / K	180(2) (warming)	190(2) (warming)	200(2) (warming)	210(2) (warming)	220(2) (warming)	230(2)	220(2) (cooling)
a / Å	20.1798(3)	20.1810(3)	20.1820(3)	20.1801(3)	20.1796(3)	20.1794(3)	20.1813(3)
b / Å	11.9656(2)	11.9729(2)	11.9797(2)	11.9865(2)	11.9961(2)	12.0018(2)	11.9949(2)
c / Å	15.8427(2)	15.8706(2)	15.8987(2)	15.9254(2)	15.9538(3)	15.9842(2)	15.9557(2)
β / °	99.664(1)	99.712(1)	99.755(1)	99.798(1)	99.864(2)	99.917(1)	99.865(1)
V / Å^3	3771.15(10)	3779.78(10)	3788.32(10)	3795.99(10)	3804.95(11)	3813.36(10)	3805.33(10)
μ{Cu-K_α} / mm^{-1}	4.946	4.935	4.923	4.913	4.902	4.891	4.901
D_{calc} / gcm^{-3}	1.482	1.478	1.475	1.472	1.469	1.465	1.468
Measured reflections	15228	15239	15331	15289	15351	15419	15368
Independent reflections	7276	7287	7304	7318	7344	7355	7330
R_{int}	0.034	0.032	0.032	0.038	0.034	0.034	0.035
R_1, $I > 2\sigma(I)$[a]	0.057	0.057	0.059	0.066	0.062	0.065	0.064
wR_2, all data[b]	0.150	0.153	0.159	0.185	0.171	0.178	0.176
CCDC	1976614	1976606	1976615	1976604	1976608	1976611	1976599

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

Table S4 continued

T / K	210(2) (cooling)	200(2) (cooling)	190(2) (cooling)	180(2) (cooling)	170(2) (cooling)	165(2) (cooling)
a / Å	20.1805(3)	20.1813(3)	20.1809(3)	20.1826(3)	20.1826(3)	20.1812(2)
b / Å	11.9884(2)	11.9817(2)	11.9732(2)	11.9634(2)	11.9558(2)	11.9527(2)
c / Å	15.9276(3)	15.9009(2)	15.8717(2)	15.8477(2)	15.8221(2)	15.8089(2)
β / °	99.813(2)	99.771(1)	99.728(1)	99.674(1)	99.635(1)	99.613(1)
V / Å^3	3797.02(11)	3789.16(10)	3779.93(10)	3772.05(10)	3764.00(10)	3759.87(9)
μ{Cu-K_α} / mm^{-1}	4.912	4.922	4.934	4.945	4.955	4.961
D_{calc} / gcm^{-3}	1.472	1.475	1.478	1.481	1.485	1.486
Measured reflections	15319	15314	15257	15242	15219	15175
Independent reflections	7319	7307	7294	7278	7264	7258
R_{int}	0.033	0.032	0.032	0.034	0.034	0.032
R_1, $I > 2\sigma(I)$[a]	0.061	0.059	0.058	0.058	0.055	0.056
wR_2, all data[b]	0.169	0.160	0.157	0.155	0.147	0.145
CCDC	1976612	1976610	1976595	1976597	1976596	1976594
T / K	160(2) (cooling)[c]	150(2) (cooling)	140(2) (cooling)	130(2) (cooling)	120(2) (cooling)	
a / Å	19.6553(9)	19.6492(2)	19.6387(2)	19.6366(2)	19.6371(2)	
b / Å	12.2266(6)	12.2304(2)	12.2380(1)	12.2391(2)	12.2394(2)	
c / Å	15.8871(8)	15.8719(2)	15.8419(2)	15.8323(2)	15.8325(2)	
β / °	100.681(5)	100.714(1)	100.684(1)	100.662(1)	100.670(1)	
V / Å^3	3751.8(3)	3747.80(9)	3741.41(7)	3739.35(9)	3739.49(9)	
μ{Cu-K_α} / mm^{-1}	4.971	4.977	4.985	4.988	4.988	
D_{calc} / gcm^{-3}	1.489	1.491	1.494	1.494	1.494	
Measured reflections	14435	15050	15080	15046	15051	
Independent reflections	7229	7208	7200	7193	7192	
R_{int}	0.092	0.033	0.031	0.031	0.034	
R_1, $I > 2\sigma(I)$[a]	0.107	0.051	0.046	0.047	0.047	
wR_2, all data[b]	0.320	0.130	0.116	0.119	0.120	
CCDC	1976592	1976593	1976590	1976591	1976609	

[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] This refinement is lower quality because the temperature of measurement corresponds to the SCO $T_{½}$ value.

Table S5 Experimental data for the variable temperature crystal structures of **1[BF$_4$]$_2$**·H$_2$O ($C_{28}H_{32}B_2F_8FeN_{10}OS_2$, M_r 818.23, monoclinic, $P2_1/c$, $Z = 4$). Datasets were measured in the order of their listing in the Table.

T / K	150(2)	170(2)	180(2)	190(2)	200(2)	210(2)[c]
a / Å	19.7776(12)	19.8047(5)	19.8157(5)	19.8308(5)	19.8488(6)	19.983(2)
b / Å	11.9368(7)	11.9318(4)	11.9288(4)	11.9218(3)	11.9094(4)	11.8766(10)
c / Å	15.4687(10)	15.5203(6)	15.5408(6)	15.5604(5)	15.5856(6)	15.6253(14)
β / °	102.447(7)	102.448(3)	102.457(3)	102.502(3)	102.562(4)	102.643(10)
V / Å^3	3566.0(4)	3581.3(2)	3587.0(2)	3591.52(18)	3596.0(2)	3618.4(6)
μ{Cu-K_α} / mm^{-1}	5.225	5.202	5.194	5.188	5.181	5.149
D_{calc} / gcm^{-3}	1.524	1.518	1.515	1.513	1.511	1.502
Measured reflections	13285	13479	13498	13580	13624	13504
Independent reflections	7009	7020	7028	7040	7055	7065
R_{int}	0.040	0.037	0.033	0.032	0.034	0.039
R_1, $I > 2\sigma(I)$[a]	0.071	0.069	0.070	0.066	0.069	0.115
wR_2, all data[b]	0.195	0.191	0.197	0.186	0.200	0.302
CCDC	1976616	1976617	1976623	1976624	1976618	1976620
T / K	220(2)	230(2)	240(2)	250(2)	260(2)	
a / Å	20.2764(7)	20.2949(7)	20.3115(7)	20.3054(8)	20.2922(10)	
b / Å	11.7156(5)	11.7133(5)	11.7055(5)	11.6878(6)	11.6992(6)	
c / Å	15.6792(7)	15.7287(7)	15.7741(8)	15.8081(8)	15.8171(9)	
β / °	102.811(4)	102.837(4)	102.832(4)	102.737(5)	102.687(6)	
V / Å^3	3631.9(3)	3645.6(3)	3656.7(3)	3659.3(3)	3663.3(3)	
μ{Cu-K_α} / mm^{-1}	5.130	5.111	5.095	5.092	5.086	
D_{calc} / gcm^{-3}	1.496	1.491	1.486	1.485	1.484	
Measured reflections	13853	13921	13972	13962	14184	
Independent reflections	7112	7128	7146	7161	7142	
R_{int}	0.028	0.027	0.030	0.032	0.039	
R_1, $I > 2\sigma(I)$[a]	0.076	0.080	0.080	0.083	0.081	
wR_2, all data[b]	0.228	0.240	0.239	0.250	0.242	
CCDC	1976619	1976625	1976626	1976621	1976622	

[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] This refinement is lower quality because the temperature of measurement corresponds to the SCO $T_{½}$ value.

Table S6 Experimental data for the crystal structures at very low temperatures, and under irradiation. Data from ref. 2 are also included, for comparison.

		1[BF$_4$]$_2$·CH_3NO_2	
T / K, spin state[a]	40(2), LS (phase 2)	15(2), LS (phase 2)[d]	15(2), HS (phase 3)[d]
Molecular formula	$C_{29}H_{33}B_2F_8FeN_{11}O_2S_2$	$C_{29}H_{33}B_2F_8FeN_{11}O_2S_2$	$C_{29}H_{33}B_2F_8FeN_{11}O_2S_2$
M_r	861.25	861.25	861.25
crystal class, space group	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$	monoclinic, $P2_1$
a / Å	19.7274(3)	19.7255(5)	20.2896(5)
b / Å	35.3821(5)	35.2106(8)	12.0942(3)
c / Å	16.0183(3)	16.0710(4)	15.3831(4)
β / °	100.757(2)	100.706(2)	101.088(2)
V / Å^3	10984.2(3)	10967.8(5)	3704.34(16)
Z	12	12	4
μ{Mo-K_α} / mm^{-1}	0.613	0.614	0.606
D_{calc} / gcm^{-3}	1.562	1.565	1.544
Measured, independent reflections	103313, 24431	53607, 23910	16837, 11529
R_{int}	0.063	0.059	0.027
R_1 [$I > 2\sigma(I)$],[b] wR_2 [all data][c]	0.051, 0.130	0.057, 0.124	0.033, 0.073
Flack parameter	–	–	0.483(15)
CCDC	1976613	1564671	1564672
		1[BF$_4$]$_2$·CH_3CN	
T / K, spin state[a]	85(2), LS[d]	85(2), HS[d]	15(2), HS[d]
Molecular formula	$C_{30}H_{33}B_2F_8FeN_{11}S_2$	$C_{30}H_{33}B_2F_8FeN_{11}S_2$	$C_{30}H_{33}B_2F_8FeN_{11}S_2$
M_r	841.26	841.26	841.26
crystal class, space group	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$
a / Å	19.5906(3)	20.2089(3)	20.2280(5)
b / Å	12.3086(2)	11.8753(2)	11.8526(4)
c / Å	15.6311(2)	15.6161(3)	15.5284(4)
β / °	100.6220(10)	99.4110(10)	99.208(2)
V / Å^3	3704.59(10)	3697.22(11)	3675.03(18)
Z	4	4	4
μ{Mo-K_α} / mm^{-1}	0.600	0.602	0.605
D_{calc} / gcm^{-3}	1.508	1.511	1.520
Measured, independent reflections	34450, 8066	34512, 8048	19748, 7998
R_{int}	0.033	0.034	0.052
R_1 [$I > 2\sigma(I)$],[b] wR_2 [all data][c]	0.034, 0.079	0.038, 0.092	0.051, 0.128
CCDC	1564667	1564668	1564669

[a]HS = high-spin, LS = low-spin, mixed = a mixed high:low-spin population. [b]$R = \Sigma[|F_o| - |F_c|] / \Sigma|F_o|$ [c]$wR = [\Sigma w(F_o^2 - F_c^2) \ / \ \Sigma wF_o^4]^{1/2}$
[d]From ref. 2.

Table S6 continued.

	1[BF$_4$]$_2$·H$_2$O		**1[BF$_4$]$_2$**·*y*(CH$_3$)$_2$CO	
T / K, spin state[a]	20(2), LS[d]	20(2), HS[d]	20(2), LS	20(2), HS
Molecular formula	$C_{28}H_{32}B_2F_8FeN_{10}OS_2$	$C_{28}H_{32}B_2F_8FeN_{10}OS_2$	$C_{30.25}H_{34.50}B_2F_8FeN_{10}O_{0.75}S_2$	$C_{30.25}H_{34.50}B_2F_8FeN_{10}O_{0.75}S_2$
M_r	818.22	818.22	843.77	843.77
crystal class, space group	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$
a / Å	19.7442(10)	20.2276(5)	19.7846(8)	20.2995(4)
b / Å	12.1364(5)	11.8791(3)	11.6554(5)	11.6652(4)
c / Å	15.0558(9)	15.0082(4)	16.2059(5)	15.8730(4)
β / °	103.004(5)	102.531(2)	100.841(4)	100.931(2)
V / Å^3	3515.2(3)	3520.35(16)	3670.3(2)	3690.49(17)
Z	4	4	4	4
μ{Mo-K_α} / mm^{-1}	0.632	0.631	0.607	0.604
D_{calc} / gcm^{-3}	1.546	1.544	1.527	1.519
Measured, independent reflections	18249, 7671	36302, 7685	20126, 8159	25938, 8190
R_{int}	0.070	0.084	0.064	0.069
R_1 [$I > 2\sigma(I)$],[b] wR_2 [all data][c]	0.052, 0.098	0.047, 0.101	0.079, 0.181	0.058, 0.146
CCDC	1564665	1564666	1976573	1976566
	1[ClO$_4$]$_2$·CH$_3$NO$_2$		**1[ClO$_4$]$_2$**·H$_2$O	
T / K, spin state[a]	10(2), mixed	10(2), HS	10(2), LS	10(2), HS
Molecular formula	$C_{29}H_{33}Cl_2FeN_{11}O_{10}S_2$	$C_{29}H_{33}Cl_2FeN_{11}O_{10}S_2$	$C_{28}H_{32}Cl_2FeN_{10}O_9S_2$	$C_{28}H_{32}Cl_2FeN_{10}O_9S_2$
M_r	886.53	886.53	843.51	843.51
crystal class, space group	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$	monoclinic, $P2_1/c$
a / Å	20.1685(10)	20.5362(5)	19.9318(6)	20.4037(4)
b / Å	11.8375(3)	11.8044(3)	12.0905(4)	11.9538(3)
c / Å	15.9452(5)	15.7396(5)	15.2378(6)	14.9788(4)
β / °	102.427(4)	102.257(3)	103.807(3)	103.023(2)
V / Å^3	3717.6(2)	3728.58(18)	3566.0(2)	3559.39(15)
Z	4	4	4	4
μ{Mo-K_α} / mm^{-1}	0.732	0.730	0.756	0.757
D_{calc} / gcm^{-3}	1.584	1.579	1.571	1.574
Measured, independent reflections	28052, 13053	59400, 13139	25643, 12564	25512, 12556
R_{int}	0.084	0.083	0.041	0.046
R_1 [$I > 2\sigma(I)$],[b] wR_2 [all data][c]	0.106, 0.201	0.083, 0.171	0.049, 0.110	0.052, 0.112
CCDC	1976585	1976559	1976583	1976584

[a]HS = high-spin, LS = low-spin, mixed = a mixed high:low-spin population. [b]$R = \Sigma[\,|F_o| - |F_c|\,] / \Sigma|F_o|$ [c]$wR = [\Sigma w(F_o^2 - F_c^2) \;/\; \Sigma wF_o^4]^{1/2}$
[d]From ref. 2.

Definitions of the Structural Parameters in Tables S7-S12

V_{Oh} is the volume (in Å^3) of the FeN_6 coordination octahedron in the complex molecule,[6] which is typically <10 Å^3 in low-spin $[Fe(bpp)_2]^{2+}$ derivatives and ≥11.5 Å^3 in their high-spin form.[7]

θ is the dihedral angle between the least squares planes of the two *L* ligands in a mononuclear $[FeL_2]^{2+}$ complex, while ϕ is the *trans*-N{pyridyl}–Fe–N{pyridyl} bond angle (Scheme S1).[8,9] These parameters can be significantly lower than their ideal values in high-spin $[Fe(bpp)_2]^{2+}$ derivatives (*ie* $\theta < 90$ and/or $\phi < 180°$).[3]

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 S2). 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 $\Sigma = \Theta = 0$.

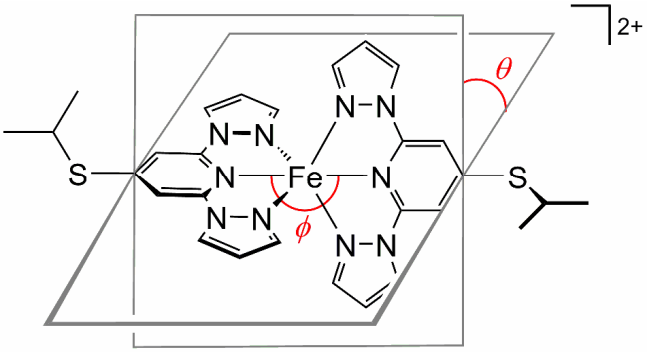
Σ and Θ were originally introduced to quantify small differences in the coordination geometries of high-spin iron(II) complexes of polydentate ligands.[10] More recently, they were popularised by Guionneau *et al.* as a way of confirming the spin state of a metal ion in a crystal structure; and to quantify the magnitude of the structural changes taking place during spin-crossover through $\Delta\Sigma$ and $\Delta\Theta$, the differences in these parameters between the high- and low-spin states of the complex.[6]

Because the high-spin state of a complex has a much 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. [11] Typical values for these parameters for $[Fe(bpp)_2]^{2+}$ complexes are tabulated in ref. 9.

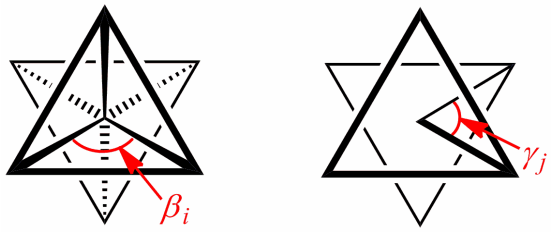
Σ and Θ (and $\Delta\Sigma$ and $\Delta\Theta$) are measures of the change in the metal ion coordination sphere between the spin states. In contrast, θ and ϕ (and $\Delta\theta$ and $\Delta\phi$) quantify the change in shape of the molecule as a whole during spin-crossover, by describing the disposition of the organic ligands with respect to each other.

NB Θ was obtained from the program *OLEX2*[12] in this study, in contrast to our earlier papers on these compounds which calculated Θ by a manual procedure.[1,2] The two methods give identical results for low-spin structures, but Θ values for the high-spin compounds are consistently *ca* 3 % larger by *OLEX2* than by our old method. The difference may arise from the two calculations taking different approaches to account for the more asymmetric coordination geometries typically found in high-spin complexes.

Scheme S1 The parameters θ and ϕ used to discuss the structures of $[Fe(bpp)_2]^{2+}$ derivatives.



Scheme S2 Angles used in the definitions of the distortion parameters Σ and Θ.[6]



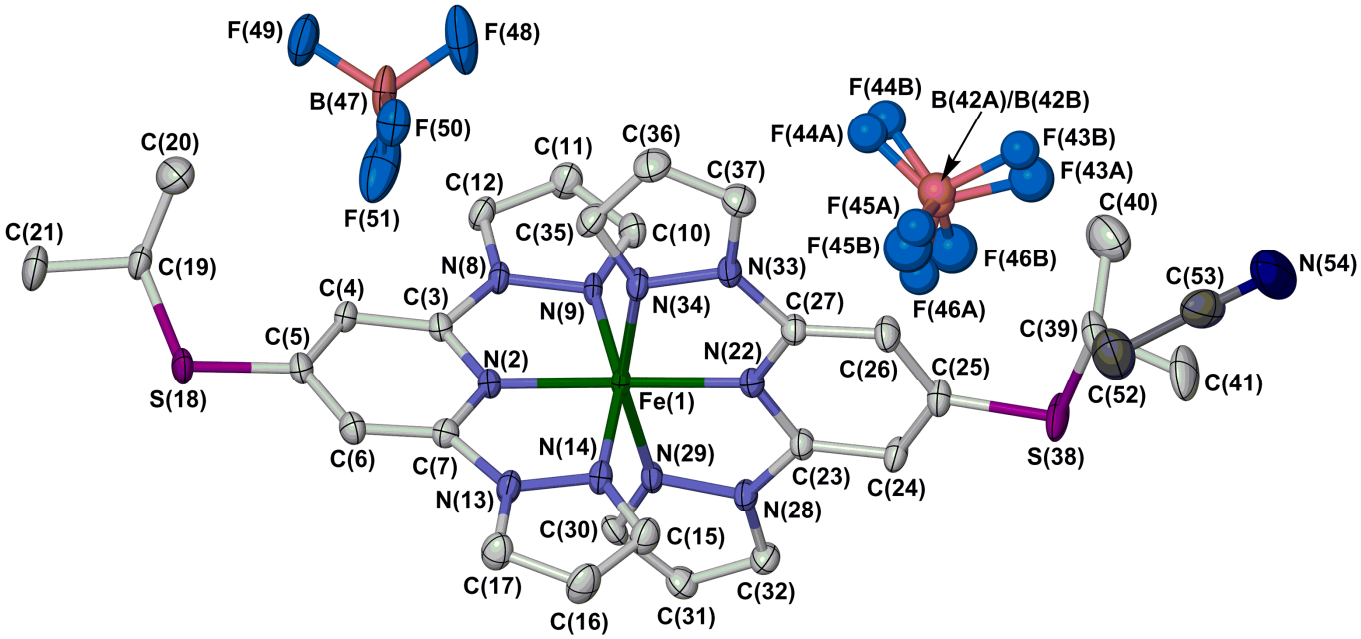


Figure S5. View of the asymmetric unit in **1[BF$_4$]$_2$**·MeCN at 120 K, showing the atom numbering scheme employed in Tables S7-S12. Displacement ellipsoids are at the 50 % probability level, and H atoms have been omitted for clarity. The lattice solvent is shown with dark colouration.

Colour code: C, white or dark grey; Fe, green; N, pale or dark blue; S, purple.

All structure refinements in this study use this atom numbering scheme, with appropriate adjustments for the presence or absence of disorder.

Table S7 Selected bond distances and angular parameters for **1[BF$_4$]$_2$**·CH_3NO_2 at different temperatures (Å, Å^3, °). See Figure S5 for the atom numbering scheme. Definitions of the V_{Oh}, Σ,Φ, φ and θ structural parameters are given on page S15.

T [K]	120(2)	130(2)	140(2)	150(2)	160(2)	165(2)	170(2)
Fe(1)–N(2)	1.905(2)	1.903(2)	1.905(2)	1.910(3)	1.935(3)	2.001(3)	2.067(3)
Fe(1)–N(9)	1.988(3)	1.987(3)	1.989(3)	1.993(3)	2.009(3)	2.058(3)	2.117(3)
Fe(1)–N(14)	1.984(3)	1.983(3)	1.984(3)	1.988(3)	2.006(3)	2.072(3)	2.143(3)
Fe(1)–N(22)	1.905(3)	1.905(2)	1.909(2)	1.911(3)	1.933(3)	1.999(3)	2.064(3)
Fe(1)–N(29)	1.985(3)	1.983(3)	1.986(3)	1.984(3)	1.995(3)	2.054(3)	2.126(3)
Fe(1)–N(34)	1.965(3)	1.966(3)	1.967(3)	1.974(3)	1.992(3)	2.051(3)	2.110(3)
V_{Oh}	9.616(8)	9.601(8)	9.631(8)	9.672(9)	9.893(9)	10.665(10)	11.486(10)
Σ	90.5(4)	90.5(4)	91.2(4)	92.3(4)	98.8(4)	117.5(4)	137.0(4)
Θ	294	294	296	299	319	377	438
ϕ	174.67(11)	174.75(11)	174.72(11)	174.63(12)	173.91(12)	172.52(11)	170.82(11)
θ	87.07(2)	87.03(2)	86.97(2)	86.93(3)	86.95(3)	86.85(3)	86.45(3)

T [K]	180(2)	190(2)	200(2)	210(2)	220(2)	230(2)
Fe(1)–N(2)	2.101(2)	2.112(2)	2.117(2)	2.120(3)	2.121(3)	2.124(3)
Fe(1)–N(9)	2.149(3)	2.157(3)	2.160(3)	2.163(3)	2.161(3)	2.167(4)
Fe(1)–N(14)	2.181(3)	2.193(3)	2.198(3)	2.201(3)	2.202(4)	2.201(4)
Fe(1)–N(22)	2.095(2)	2.107(2)	2.112(2)	2.115(3)	2.117(3)	2.118(3)
Fe(1)–N(29)	2.154(3)	2.163(3)	2.166(3)	2.168(3)	2.169(3)	2.171(3)
Fe(1)–N(34)	2.142(3)	2.152(3)	2.158(3)	2.160(3)	2.163(3)	2.165(4)
V_{Oh}	11.915(10)	12.052(10)	12.109(10)	12.136(12)	12.151(12)	12.181(12)
Σ	146.0(4)	148.9(4)	150.1(4)	151.3(4)	151.6(4)	152.1(5)
Θ	466	475	479	483	484	485
ϕ	170.04(10)	169.82(11)	169.67(11)	169.54(12)	169.50(13)	169.38(13)
θ	86.26(3)	86.13(3)	86.00(3)	85.95(3)	85.77(3)	85.69(3)

Table S8 Selected bond distances and angular parameters for **1[BF$_4$]$_2$**·*y*$(CH_3)_2CO$ at different temperatures (Å, °). See Figure S5 for the atom numbering scheme. Definitions of the V_{Oh}, Σ,Φ, φ and θ structural parameters are given on page S15.

T [K]	110(2)	120(2)	130(2)	140(2)	150(2)	160(2)
Fe(1)–N(2)	1.919(3)	1.922(3)	1.937(3)	1.981(4)	2.046(3)	2.086(3)
Fe(1)–N(9)	1.998(3)	2.003(3)	2.009(4)	2.044(4)	2.095(4)	2.131(3)
Fe(1)–N(14)	1.992(4)	1.998(4)	2.011(4)	2.054(5)	2.124(5)	2.170(4)
Fe(1)–N(22)	1.914(3)	1.916(3)	1.933(3)	1.972(4)	2.035(3)	2.071(3)
Fe(1)–N(29)	1.984(3)	1.987(3)	1.992(4)	2.033(5)	2.102(5)	2.146(4)
Fe(1)–N(34)	1.974(3)	1.976(3)	1.988(4)	2.030(4)	2.090(3)	2.132(3)
V_{Oh}	9.718(10)	9.761(10)	9.902(12)	10.400(14)	11.181(13)	11.696(12)
Σ	92.9(5)	94.0(5)	97.2(5)	110.5(6)	129.9(5)	141.5(4)
Θ	301	305	315	356	417	454
ϕ	174.33(13)	174.24(13)	173.74(14)	172.08(15)	170.12(12)	168.71(11)
θ	86.90(3)	86.96(3)	87.19(4)	87.56(4)	87.41(4)	87.36(4)
T [K]	170(2)	180(2)	190(2)	200(2)	210(2)	220(2)
Fe(1)–N(2)	2.106(3)	2.118(3)	2.124(3)	2.124(3)	2.127(3)	2.129(3)
Fe(1)–N(9)	2.152(3)	2.160(3)	2.164(3)	2.169(3)	2.169(3)	2.173(3)
Fe(1)–N(14)	2.198(4)	2.204(3)	2.206(3)	2.208(3)	2.209(3)	2.210(3)
Fe(1)–N(22)	2.097(3)	2.105(3)	2.109(3)	2.111(3)	2.112(3)	2.113(3)
Fe(1)–N(29)	2.160(3)	2.165(3)	2.164(3)	2.168(3)	2.168(3)	2.169(3)
Fe(1)–N(34)	2.156(3)	2.166(3)	2.172(3)	2.174(3)	2.174(3)	2.173(3)
V_{Oh}	11.969(11)	12.066(11)	12.101(11)	12.139(11)	12.144(11)	12.159(12)
Σ	148.0(4)	150.8(4)	152.2(4)	152.4(4)	153.1(4)	153.4(4)
Θ	474	483	488	489	491	492
ϕ	167.87(11)	167.43(10)	167.15(11)	167.11(11)	167.01(11)	166.93(12)
θ	87.20(3)	87.11(3)	86.95(3)	86.82(3)	86.70(3)	86.59(3)

Table S9 Selected bond distances and angular parameters for **1[BF$_4$]$_2$**·CH$_3$CN at different temperatures (Å, °). See Figure S5 for the atom numbering scheme. Definitions of the V_{Oh}, Σ,Φ, φ and θ structural parameters are given on page S15.

T [K]	120(2) (warming)	130(2) (warming)	140(2) (warming)	150(2) (warming)	160(2) (warming)	165(2) (warming)	170(2) (warming)
Fe(1)–N(2)	1.900(2)	1.900(2)	1.899(2)	1.900(2)	1.899(2)	1.899(2)	2.127(3)
Fe(1)–N(9)	1.984(2)	1.984(2)	1.983(2)	1.984(2)	1.987(2)	1.988(2)	2.173(3)
Fe(1)–N(14)	1.974(2)	1.973(2)	1.972(2)	1.971(2)	1.970(2)	1.972(2)	2.208(3)
Fe(1)–N(22)	1.8984(19)	1.897(2)	1.898(2)	1.898(2)	1.900(2)	1.901(2)	2.120(2)
Fe(1)–N(29)	1.972(2)	1.971(2)	1.972(2)	1.974(2)	1.973(2)	1.972(2)	2.174(3)
Fe(1)–N(34)	1.965(2)	1.966(2)	1.965(2)	1.966(2)	1.968(2)	1.968(2)	2.172(3)
V_{Oh}	9.527(6)	9.521(6)	9.520(6)	9.523(7)	9.531(7)	9.543(7)	12.209(10)
Σ	88.6(3)	88.6(3)	88.5(3)	89.0(3)	89.2(3)	89.0(3)	153.0(4)
Θ	288	288	288	288	289	289	489
ϕ	174.17(8)	174.28(9)	174.35(9)	174.21(9)	174.29(9)	174.30(10)	167.75(10)
θ	89.08(2)	88.97(2)	88.88(2)	88.79(2)	88.69(2)	88.68(2)	87.73(3)
T [K]	180(2) (warming)	190(2) (warming)	200(2) (warming)	210(2) (warming)	220(2) (warming)	230(2)	220(2) (cooling)
Fe(1)–N(2)	2.128(3)	2.129(3)	2.130(3)	2.131(3)	2.130(3)	2.131(3)	2.131(3)
Fe(1)–N(9)	2.174(3)	2.175(3)	2.175(3)	2.174(3)	2.175(3)	2.175(3)	2.173(3)
Fe(1)–N(14)	2.208(3)	2.208(3)	2.209(3)	2.207(4)	2.208(3)	2.206(4)	2.209(4)
Fe(1)–N(22)	2.122(3)	2.120(2)	2.121(3)	2.124(3)	2.122(3)	2.123(3)	2.124(3)
Fe(1)–N(29)	2.172(3)	2.176(3)	2.176(3)	2.178(3)	2.176(3)	2.176(3)	2.174(3)
Fe(1)–N(34)	2.170(3)	2.174(3)	2.173(3)	2.172(3)	2.173(3)	2.174(3)	2.174(3)
V_{Oh}	12.205(10)	12.227(10)	12.231(11)	12.235(12)	12.230(11)	12.235(12)	12.231(12)
Σ	153.1(4)	153.2(4)	153.3(4)	153.5(4)	153.5(4)	153.6(4)	153.7(4)
Θ	490	490	490	491	491	491	492
ϕ	167.54(10)	167.70(10)	167.68(11)	167.61(12)	167.62(12)	167.66(12)	167.59(12)
θ	87.63(3)	87.52(3)	87.43(3)	87.33(3)	87.21(3)	87.11(3)	87.23(3)

Table S9 (continued).

T [K]	210(2) (cooling)	200(2) (cooling)	190(2) (cooling)	180(2) (cooling)	170(2) (cooling)	165(2) (cooling)	160(2) (cooling)
Fe(1)–N(2)	2.130(3)	2.127(3)	2.128(3)	2.129(3)	2.129(2)	2.128(3)	1.900(6)
Fe(1)–N(9)	2.174(3)	2.174(3)	2.174(3)	2.176(3)	2.175(3)	2.174(3)	1.976(8)
Fe(1)–N(14)	2.207(3)	2.210(3)	2.209(3)	2.210(3)	2.208(3)	2.208(3)	1.975(7)
Fe(1)–N(22)	2.124(3)	2.122(3)	2.123(2)	2.122(3)	2.121(2)	2.120(2)	1.904(6)
Fe(1)–N(29)	2.175(3)	2.175(3)	2.175(3)	2.173(3)	2.175(3)	2.173(3)	1.970(7)
Fe(1)–N(34)	2.173(3)	2.170(3)	2.171(3)	2.172(3)	2.172(3)	2.171(3)	1.969(7)
V_{Oh}	12.231(11)	12.218(11)	12.222(10)	12.228(10)	12.225(10)	12.207(10)	9.52(2)
Σ	153.4(4)	153.2(4)	153.2(4)	153.2(4)	152.9(4)	153.2(4)	89.5(10)
Θ	490	490	490	490	489	490	290
ϕ	167.62(11)	167.71(11)	167.75(11)	167.62(10)	167.65(10)	167.64(10)	173.9(3)
θ	87.32(3)	87.45(3)	87.54(3)	87.60(3)	87.70(3)	87.76(3)	88.83(7)
T [K]	150(2) (cooling)	140(2) (cooling)	130(2) (cooling)	120(2) (cooling)			
Fe(1)–N(2)	1.899(2)	1.901(2)	1.903(2)	1.901(2)			
Fe(1)–N(9)	1.986(2)	1.984(2)	1.983(2)	1.983(2)			
Fe(1)–N(14)	1.974(2)	1.973(2)	1.970(2)	1.972(2)			
Fe(1)–N(22)	1.898(2)	1.900(2)	1.899(2)	1.901(2)			
Fe(1)–N(29)	1.974(2)	1.972(2)	1.971(2)	1.972(2)			
Fe(1)–N(34)	1.966(2)	1.965(2)	1.966(2)	1.967(2)			
V_{Oh}	9.536(7)	9.533(7)	9.525(7)	9.537(7)			
Σ	88.7(3)	88.8(3)	88.5(3)	88.5(3)			
Θ	288	288	288	288			
ϕ	174.21(10)	174.31(9)	174.24(9)	174.18(9)			
θ	88.74(2)	88.86(2)	88.86(2)	88.87(2)			

Table S10 Selected bond distances and angular parameters for **1[BF$_4$]$_2$**·H$_2$O at different temperatures (Å, °). See Figure S5 for the atom numbering scheme. Definitions of the V_{Oh}, Σ,Φ, φ and θ structural parameters are given on page S15.

T [K]	150(2)	170(2)	180(2)	190(2)	200(2)	210(2)
Fe(1)–N(2)	1.910(4)	1.909(4)	1.908(4)	1.908(3)	1.916(4)	1.958(6)
Fe(1)–N(9)	1.972(4)	1.978(4)	1.982(4)	1.983(4)	1.990(4)	2.034(7)
Fe(1)–N(14)	1.985(4)	1.983(4)	1.983(4)	1.991(4)	1.993(4)	2.050(7)
Fe(1)–N(22)	1.906(4)	1.904(3)	1.903(4)	1.907(4)	1.910(4)	1.958(6)
Fe(1)–N(29)	1.995(4)	1.993(4)	1.987(4)	1.992(4)	1.994(4)	2.040(8)
Fe(1)–N(34)	1.968(4)	1.970(4)	1.971(4)	1.975(4)	1.978(4)	2.038(6)
V_{Oh}	9.647(12)	9.646(11)	9.636(11)	9.688(11)	9.734(12)	10.36(2)
Σ	87.8(5)	88.4(5)	89.0(5)	89.7(5)	91.0(6)	105.6(10)
Θ	285	287	288	291	295	341
ϕ	175.55(17)	175.76(16)	175.60(16)	175.51(16)	175.32(17)	172.9(3)
θ	88.79(3)	88.73(3)	88.71(4)	88.67(3)	88.58(4)	88.32(7)
T [K]	220(2)	230(2)	240(2)	250(2)	260(2)	
Fe(1)–N(2)	2.108(4)	2.120(4)	2.130(4)	2.131(4)	2.126(4)	
Fe(1)–N(9)	2.143(4)	2.146(4)	2.152(4)	2.154(4)	2.157(5)	
Fe(1)–N(14)	2.188(4)	2.199(4)	2.205(5)	2.208(5)	2.215(5)	
Fe(1)–N(22)	2.089(4)	2.096(4)	2.099(4)	2.104(4)	2.099(4)	
Fe(1)–N(29)	2.178(4)	2.183(4)	2.185(4)	2.185(4)	2.178(5)	
Fe(1)–N(34)	2.142(4)	2.151(5)	2.156(5)	2.155(5)	2.165(5)	
V_{Oh}	11.982(15)	12.080(16)	12.153(16)	12.166(16)	12.163(16)	
Σ	145.3(5)	147.1(6)	148.3(6)	149.1(6)	149.8(6)	
Θ	464	470	474	477	479	
ϕ	169.16(15)	168.63(16)	168.40(16)	168.12(16)	168.01(17)	
θ	86.84(4)	86.66(4)	86.51(5)	86.29(5)	86.20(5)	

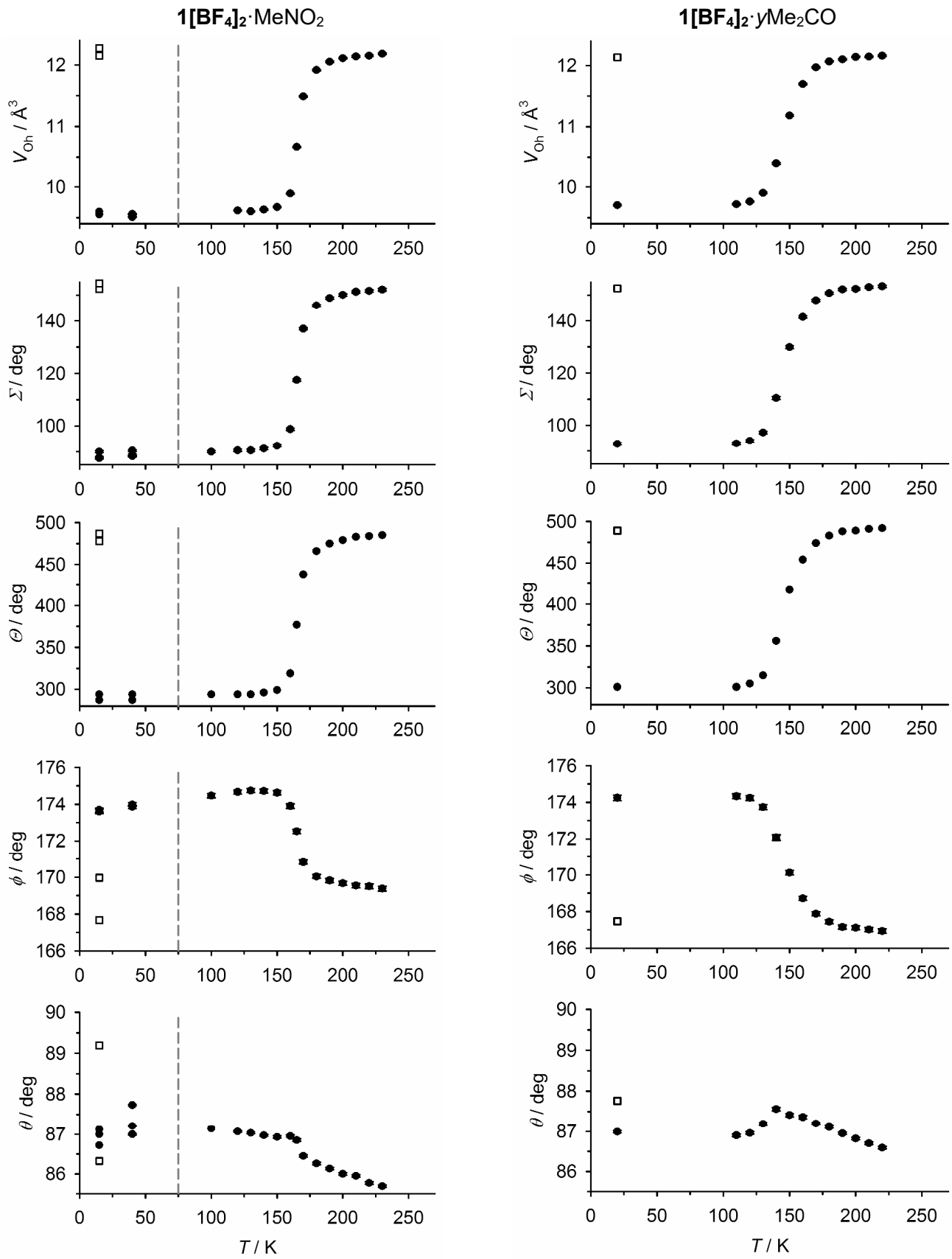


Figure S6 Evolution of the molecular structure of the $[FeL_2]^{2+}$ cation with temperature, as measured by the structural parameters V_{Oh}, Σ, Θ, ϕ and θ (defined on page S15). Error bars are smaller than the symbols in the graphs. Data from the photocrystallographic experiments in this work and ref. 2 are included.

The white square data points are the metastable high-spin structures at low temperatures, generated by irradiation or thermal trapping. The dashed line for **1[BF$_4$]$_2$**·MeNO$_2$ indicates the phase 1→2 transition temperature.

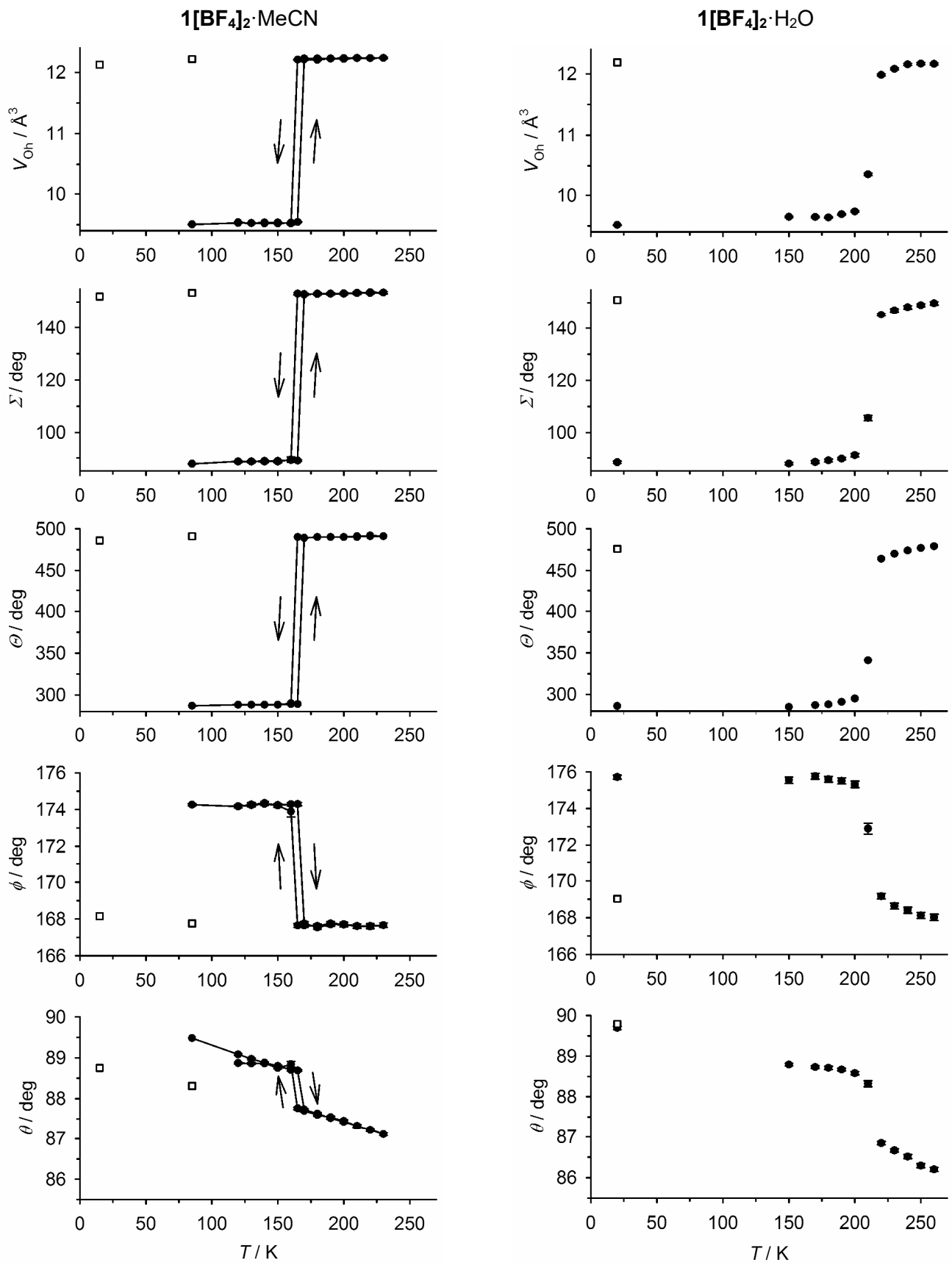


Figure S6 continued.

Data for **1[BF$_4$]$_2$**·MeCN are linked by lines, to distinguish measurements in cooling and warming temperature ramps.

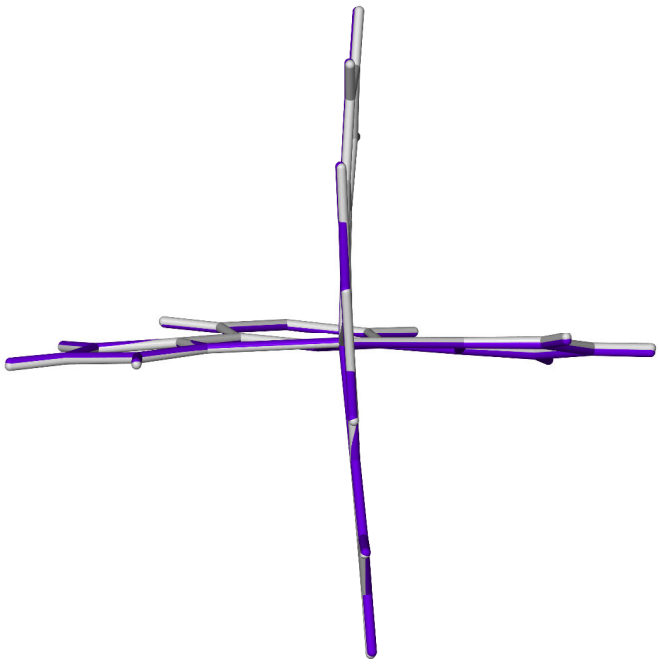


Figure S7 Overlay of the complex cations in high-spin **1[BF$_4$]$_2$**·MeCN at 230 K [white, θ = 87.11(3)°] and 165 K [purple, θ = 87.76(3)°], showing the effect of the temperature dependence of θ in Figure S6 on the molecular structure of the compound. The view is down the N(pyridyl)–Fe–N(pyridyl) vector [N(2)–Fe(1)–N(22), Figure S5] and the *iso*propylsulfanyl ligand substituents are omitted for clarity.

θ is the dihedral angle between the least squares planes of the two heterocyclic *L* ligands (page S15). Although the difference is small, the tridentate ligand geometry is slightly less twisted in the purple, lower temperature structure. This has little effect on the inner coordination sphere of the complex, however, as expressed by the other parameters in Figure S5.

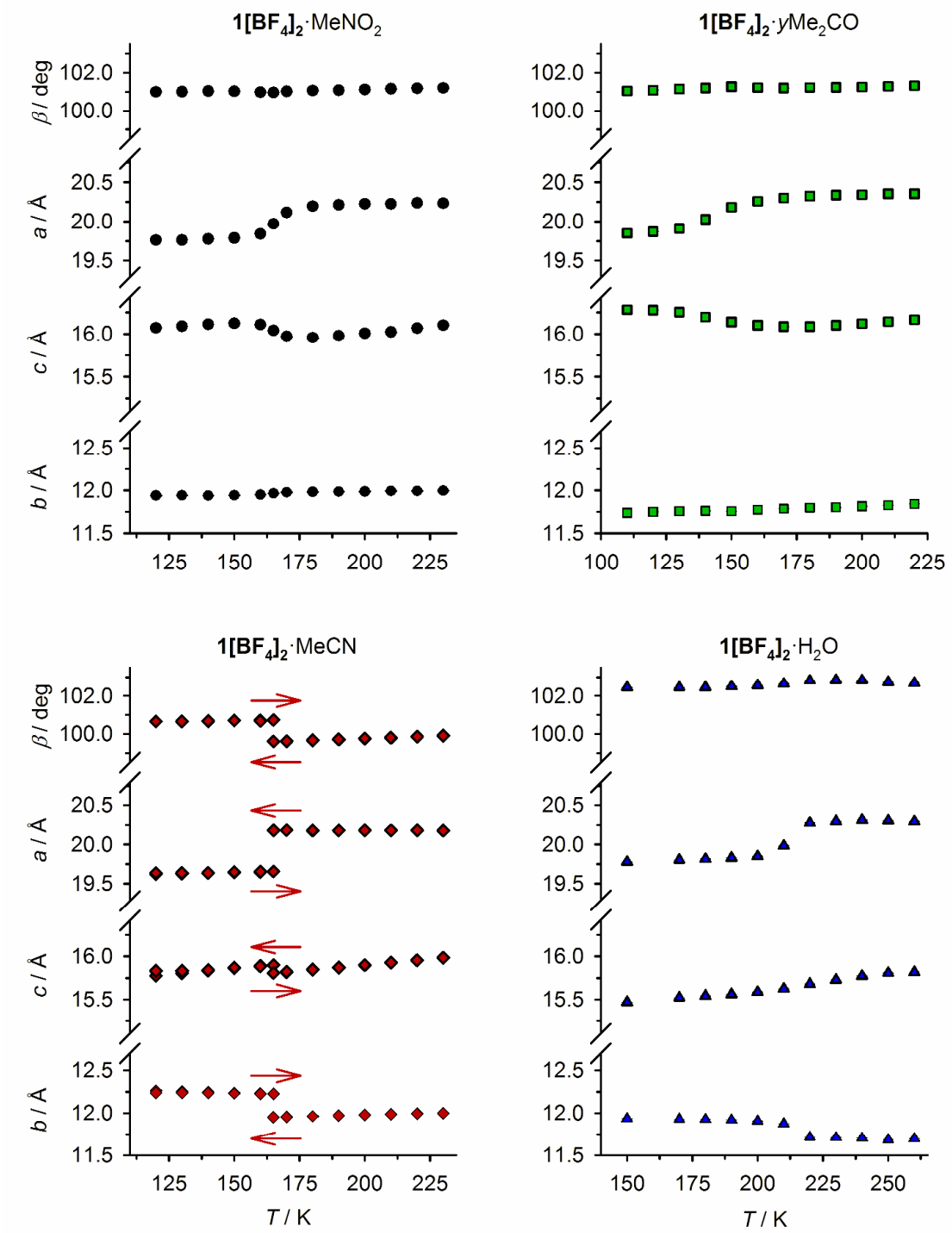


Figure S8 Temperature dependence of the unit cell parameters for the **1[BF$_4$]$_2$**·solv crystals studied in this work (Tables S2-S5). Error bars are shown, but are smaller than the symbols in the graphs. Data for **1[BF$_4$]$_2$**·MeCN are shown in both warming and cooling temperature ramps.

These data follow the same trends as our original study on these compounds.[1] High→low-spin SCO in the less cooperative crystals **1[BF$_4$]$_2$**·MeNO$_2$ and **1[BF$_4$]$_2$**·*y*Me$_2$CO is reflected in a decrease in *a* and an increase in *c*, with *b* and *β* being almost unaffected. Conversely, the more cooperative spin transitions in **1[BF$_4$]$_2$**·MeCN and **1[BF$_4$]$_2$**·H$_2$O lead to significant increases in *b* and *β*, as well as the aforementioned decrease in *a*, but have little effect on *c*. These changes lead to an unusually small 0.1 % contraction of the unit cell volume during the high→low-spin transition in **1[BF$_4$]$_2$**·MeCN. The other solvates show a more typical *ca* 1 % unit cell contraction under the same conditions, where the comparison can be made (Figure S9).[1]

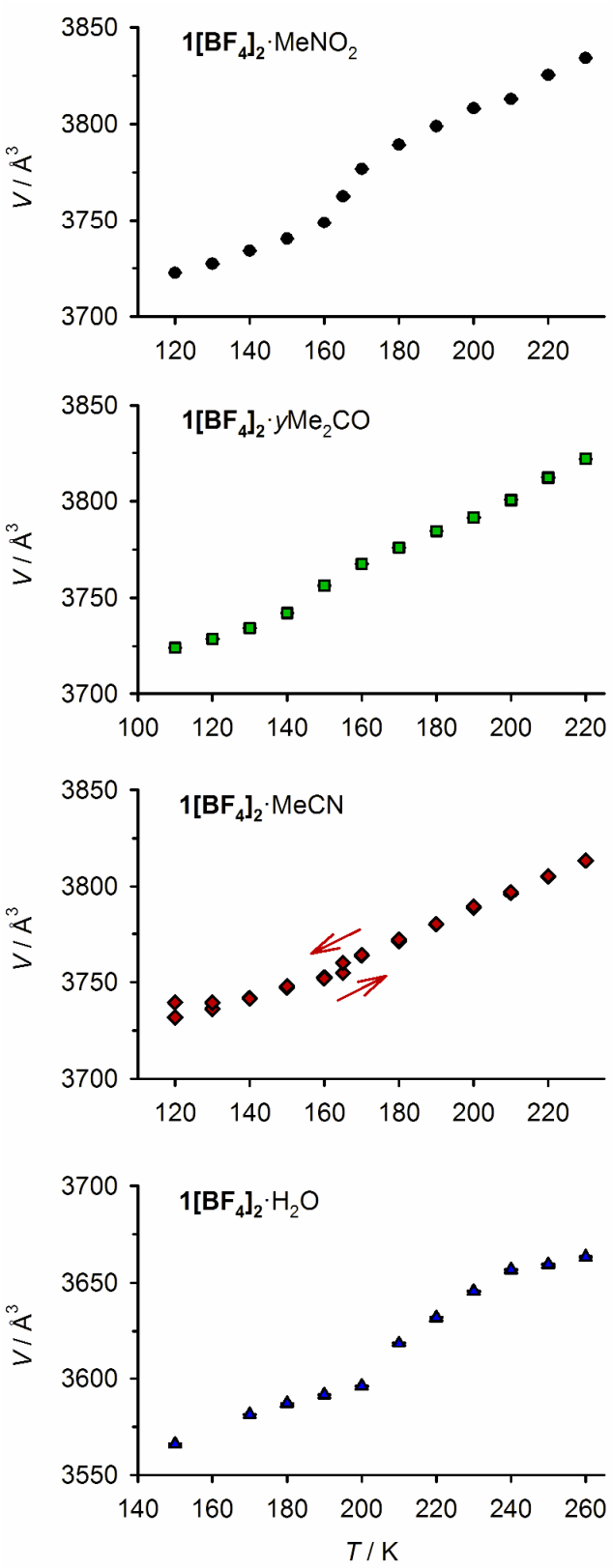
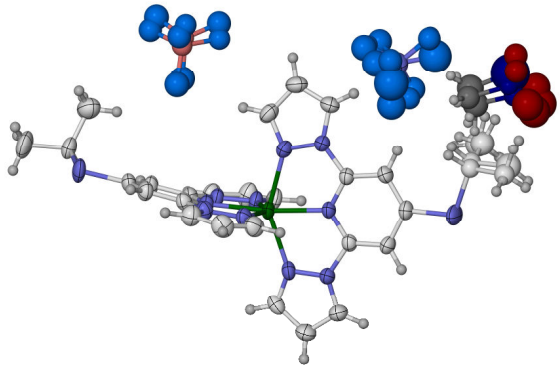
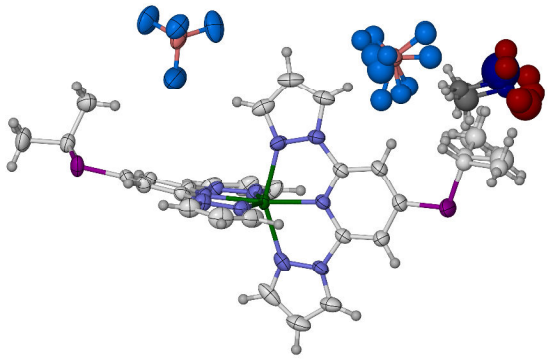


Figure S9 Temperature dependence of the unit cell volumes for the **1[BF$_4$]$_2$**·solv crystals studied in this work (Tables S2-S5). Error bars are shown, but are smaller than the symbols in the graphs. Data for **1[BF$_4$]$_2$**·MeCN are shown in both warming and cooling temperature ramps.

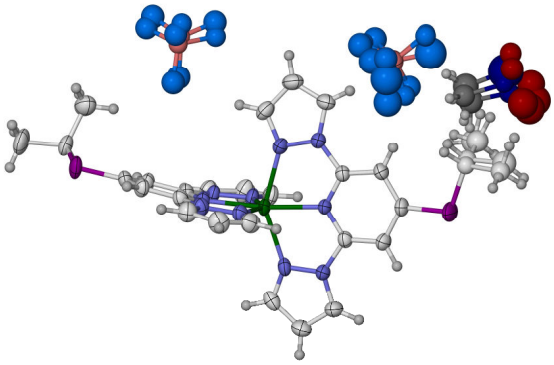
These data follow the same trends as our original study on these compounds.[1] In particular the abrupt, hysteretic spin transition shown by **1[BF$_4$]$_2$**·MeCN around 165 K has almost no effect on its unit cell volume.



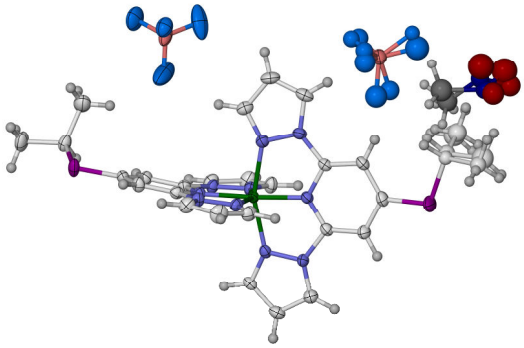
T = 230 K, high-spin



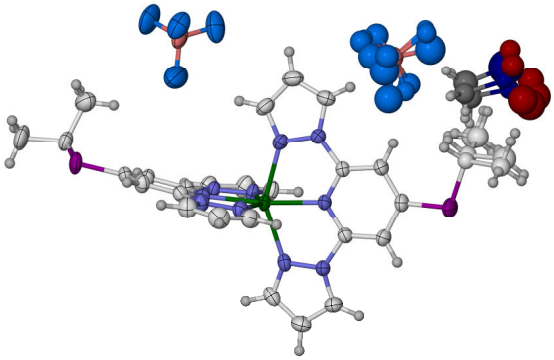
T = 170 K, mixed-spin



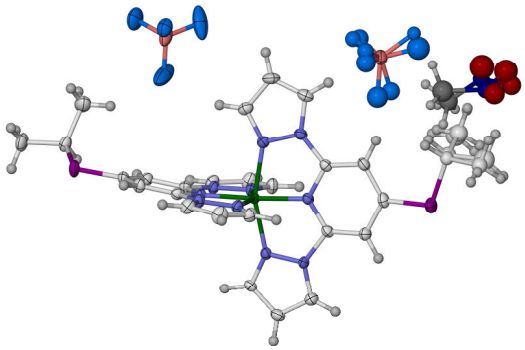
T = 210 K, high-spin



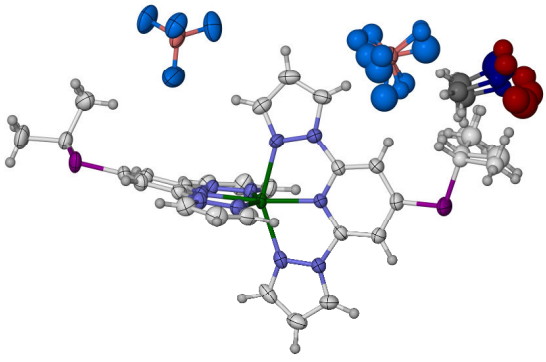
T = 160 K, low-spin



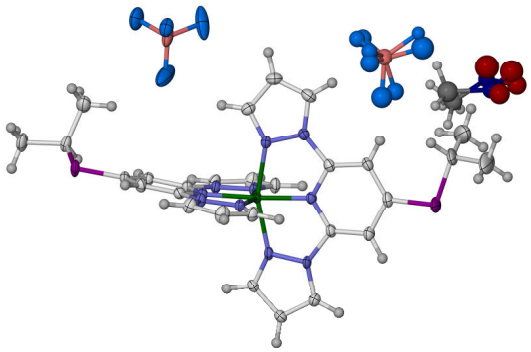
T = 200 K, high-spin



T = 130 K, low-spin



T = 180 K, mixed-spin

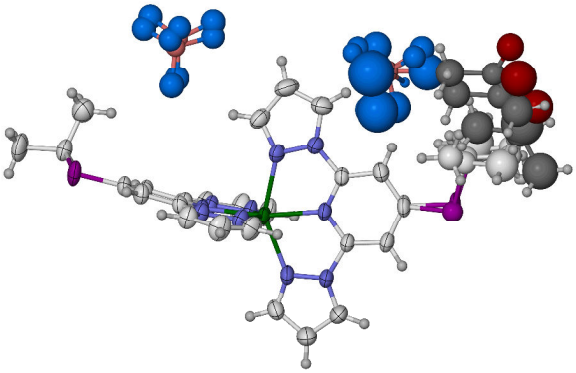


T = 120 K, low-spin

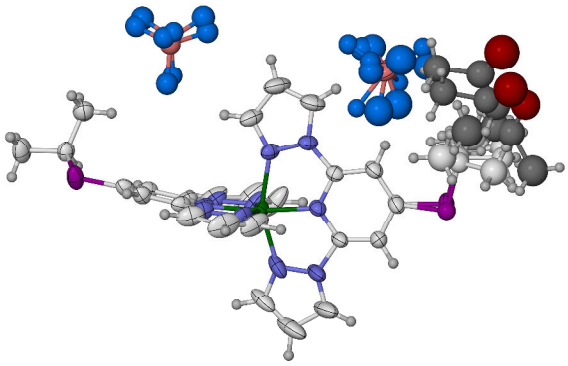
Figure S10 Temperature dependence of the crystallographic disorder in phase 1 of **1[BF$_4$]$_2$**·MeNO$_2$. Displacement ellipsoids are at the 50 % probability level.

Colour code: C, white or dark gray; H, pale gray; Cl, yellow; Fe, green; N, pale or dark blue; O, red; S, purple.

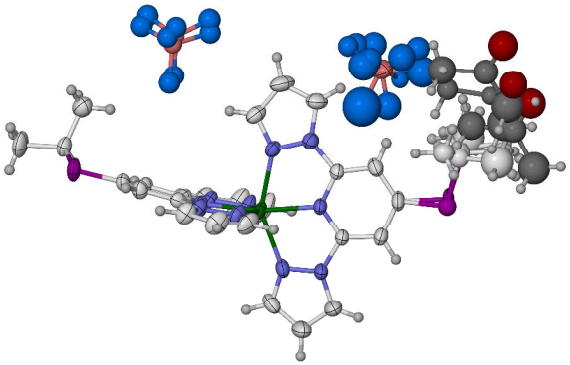
Anions were treated as disordered above 100 K if any two F atoms exhibited $U_{iso} \geq 0.07$. In practise, the displacement parameters of the intrabilayer anion decrease slowly with temperature, and the change from a disordered to an ordered model for that anion at 10 K lower temperature does not imply an abrupt quenching of its libration.



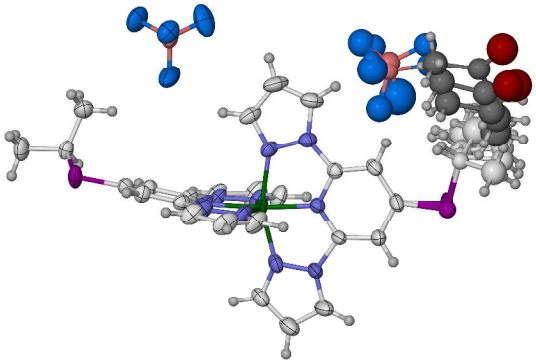
T = 210 K, high-spin



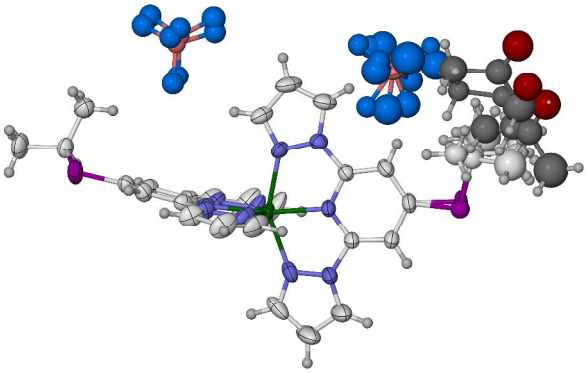
T = 140 K, mixed-spin



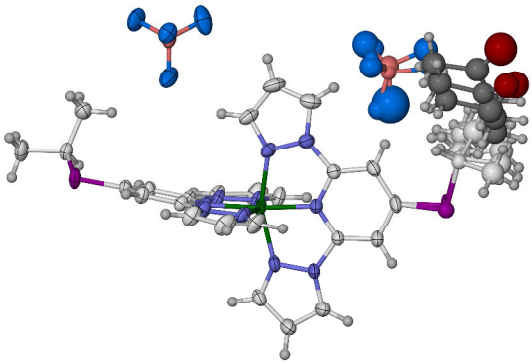
T = 170 K, high-spin



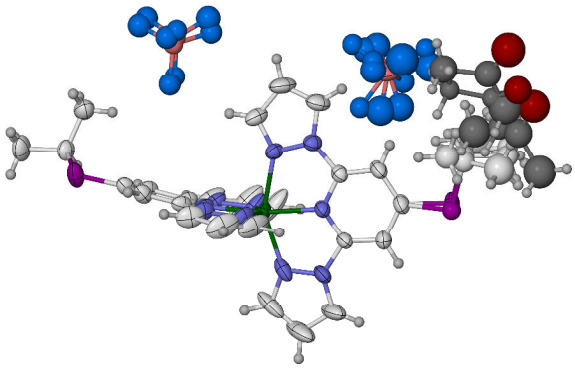
T = 130 K, mixed-spin



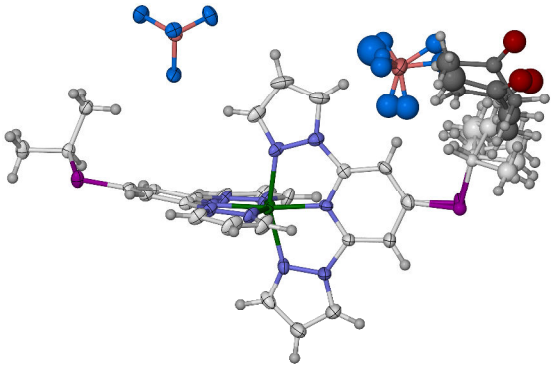
T = 160 K, mixed-spin



T = 110 K, low-spin

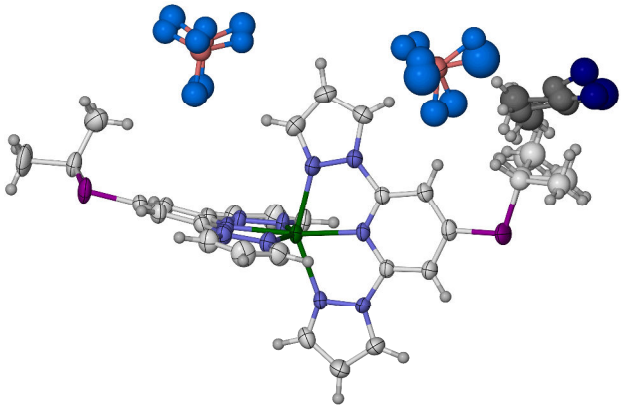


T = 150 K, mixed-spin

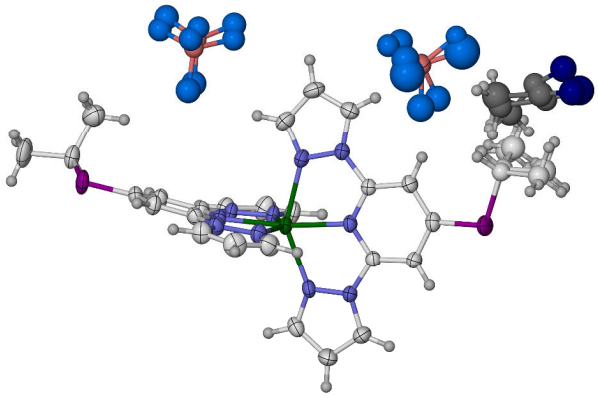


T = 20 K, low-spin

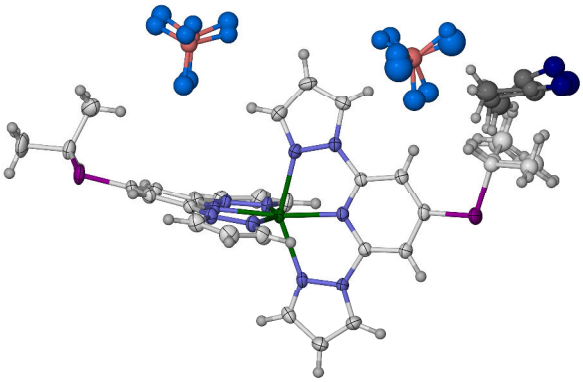
Figure S11 Temperature dependence of the crystallographic disorder in **1[BF$_4$]$_2$**·*y*Me$_2$CO. Details as for Figure S10. The view at 20 K is the same as in Figure S18, below.



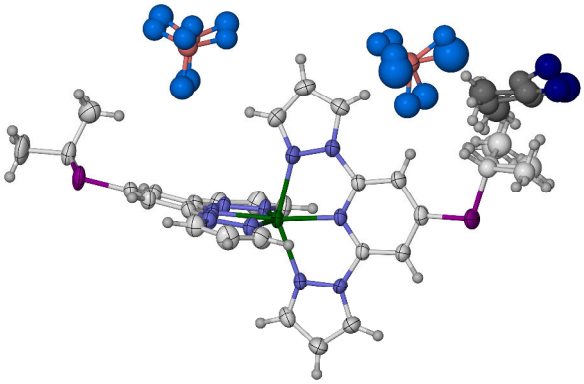
T = 230 K, high-spin



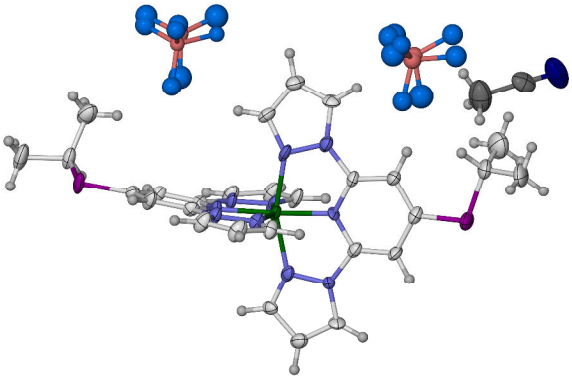
T = 220 K {warming}, high-spin



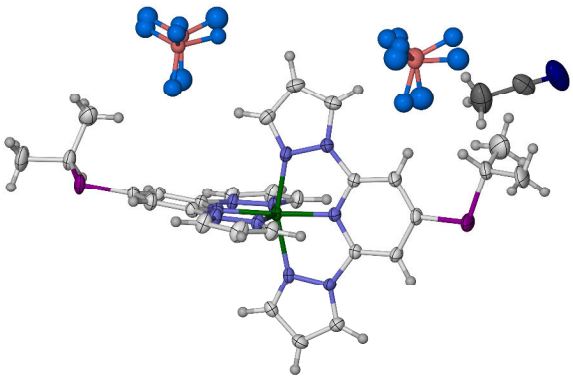
T = 165 K {cooling}, high-spin



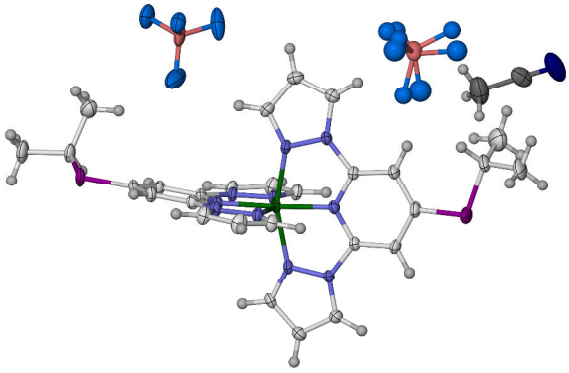
T = 170 K {warming}, high-spin



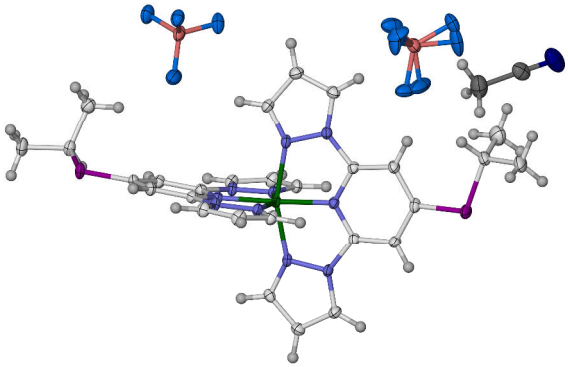
T = 160 K {cooling}, low-spin



T = 165 K {warming}, low-spin

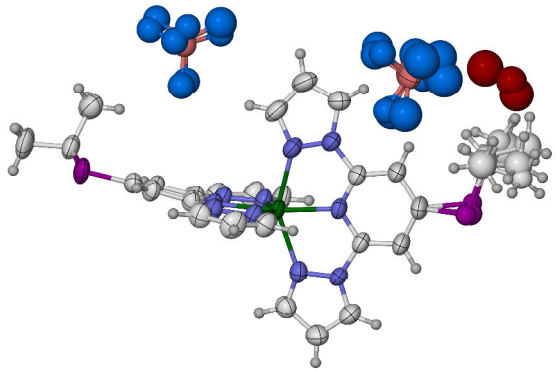


T = 120 K {cooling}, low-spin

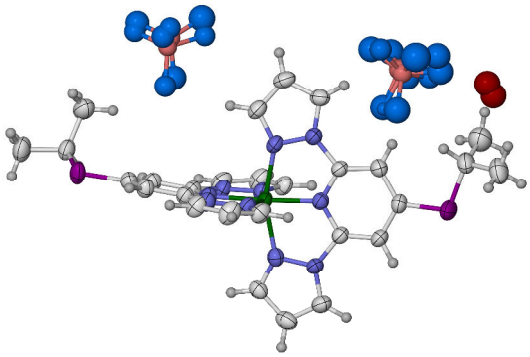


T = 85 K, low-spin

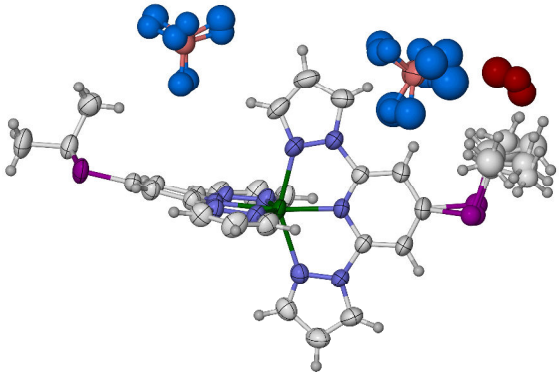
Figure S12 Temperature dependence of the crystallographic disorder in **1[BF$_4$]$_2$**·MeCN. Data measured in both cooling (left) and warming (right) temperature ramps are included. Other details as for Figure S10. The view at 85 K is the same as in Figure S18, and is taken from ref. 2.



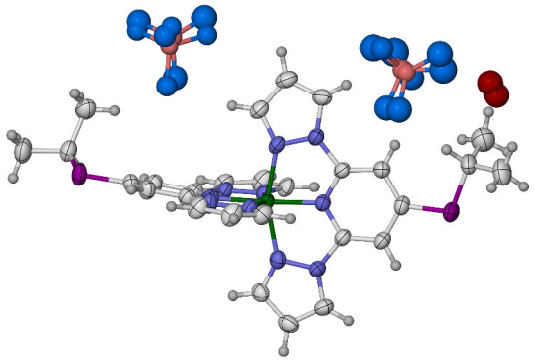
T = 260 K, high-spin



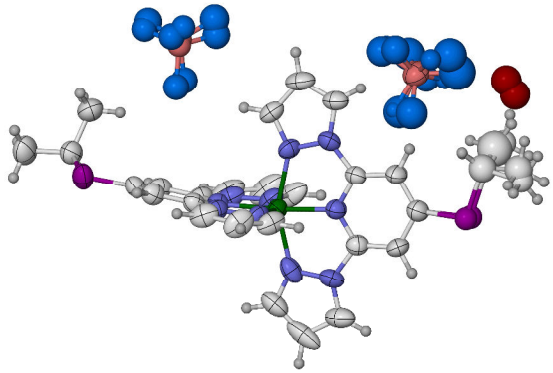
T = 190 K, low-spin



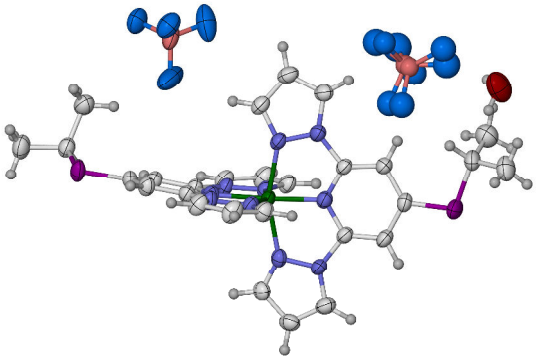
T = 220 K, high-spin



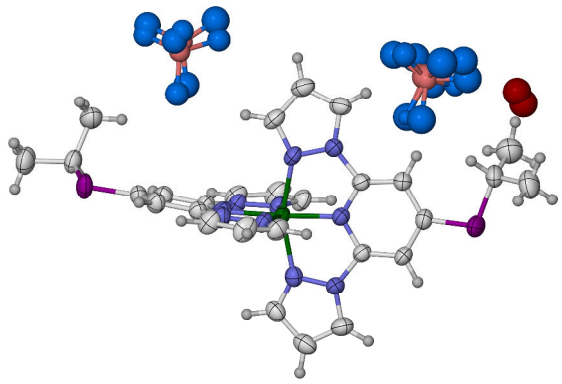
T = 180 K, low-spin



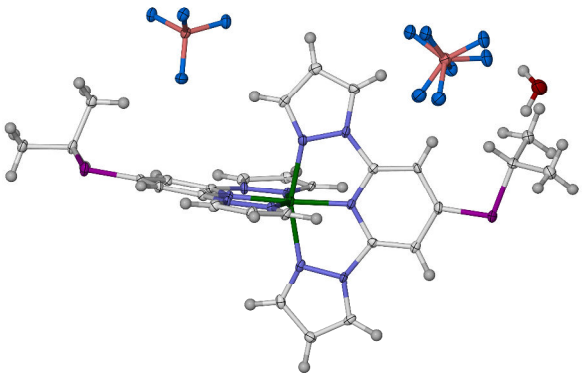
T = 210 K, mixed-spin



T = 170 K, low-spin

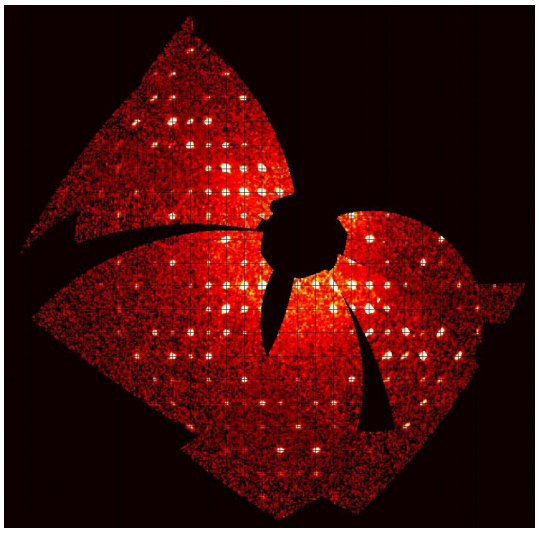


T = 200 K, low-spin

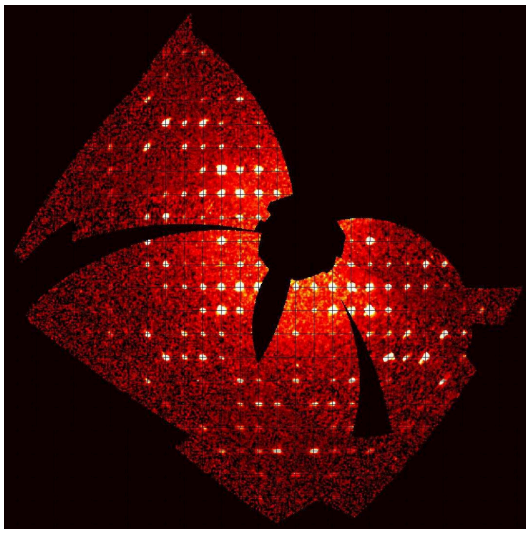


T = 20 K, low-spin

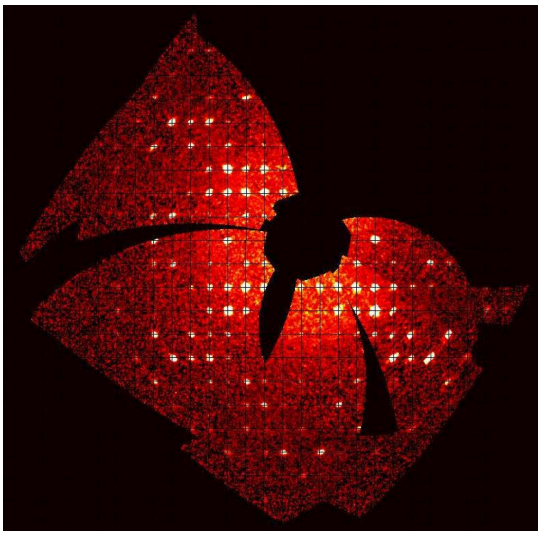
Figure S13 Temperature dependence of the crystallographic disorder in **1[BF$_4$]$_2$**·H$_2$O. Details as for Figure S10. The view at 20 K is the same as in Figure S18, and is taken from ref. 2.



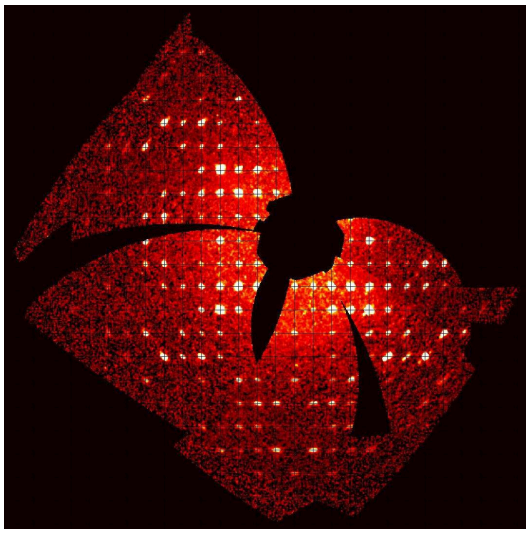
90 K



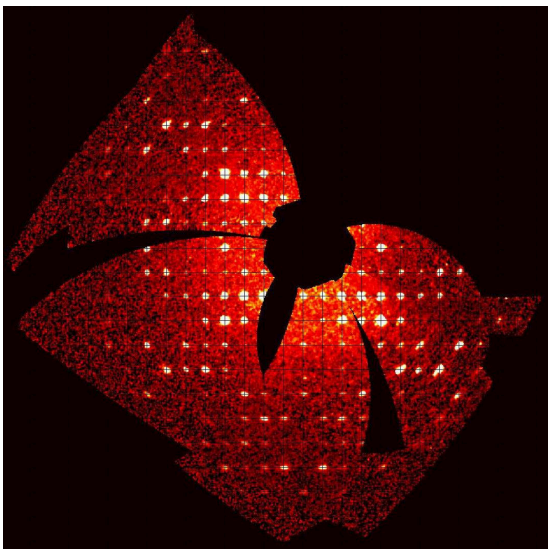
70 K



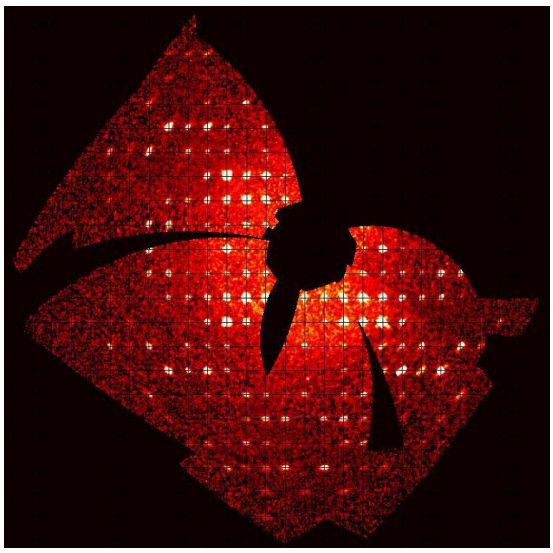
80 K



45 K



75 K



15 K

Figure S14 Diffraction images from a single crystal of **1[BF$_4$]$_2$**·MeNO$_2$ in the *hk*0 zone, on cooling from 90-15 K. Additional reflections associated with the phase 1→2 transition appear between 80 and 75 K.

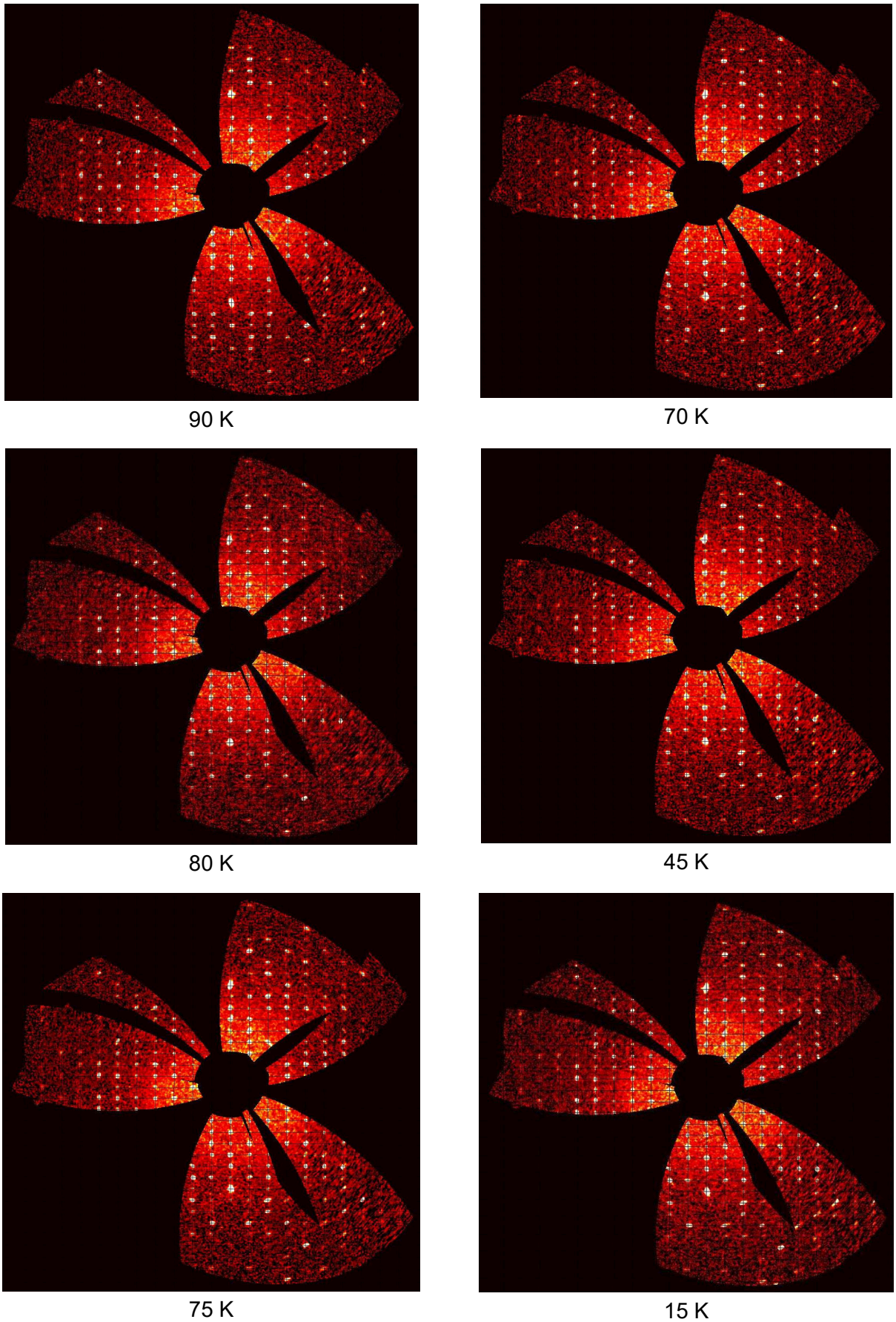


Figure S15 Diffraction images from a single crystal of **1[BF$_4$]$_2$**·MeNO$_2$ in the 0*k*l zone, on cooling from 90-15 K. Additional reflections associated with the phase 1→2 transition appear between 80 and 75 K.

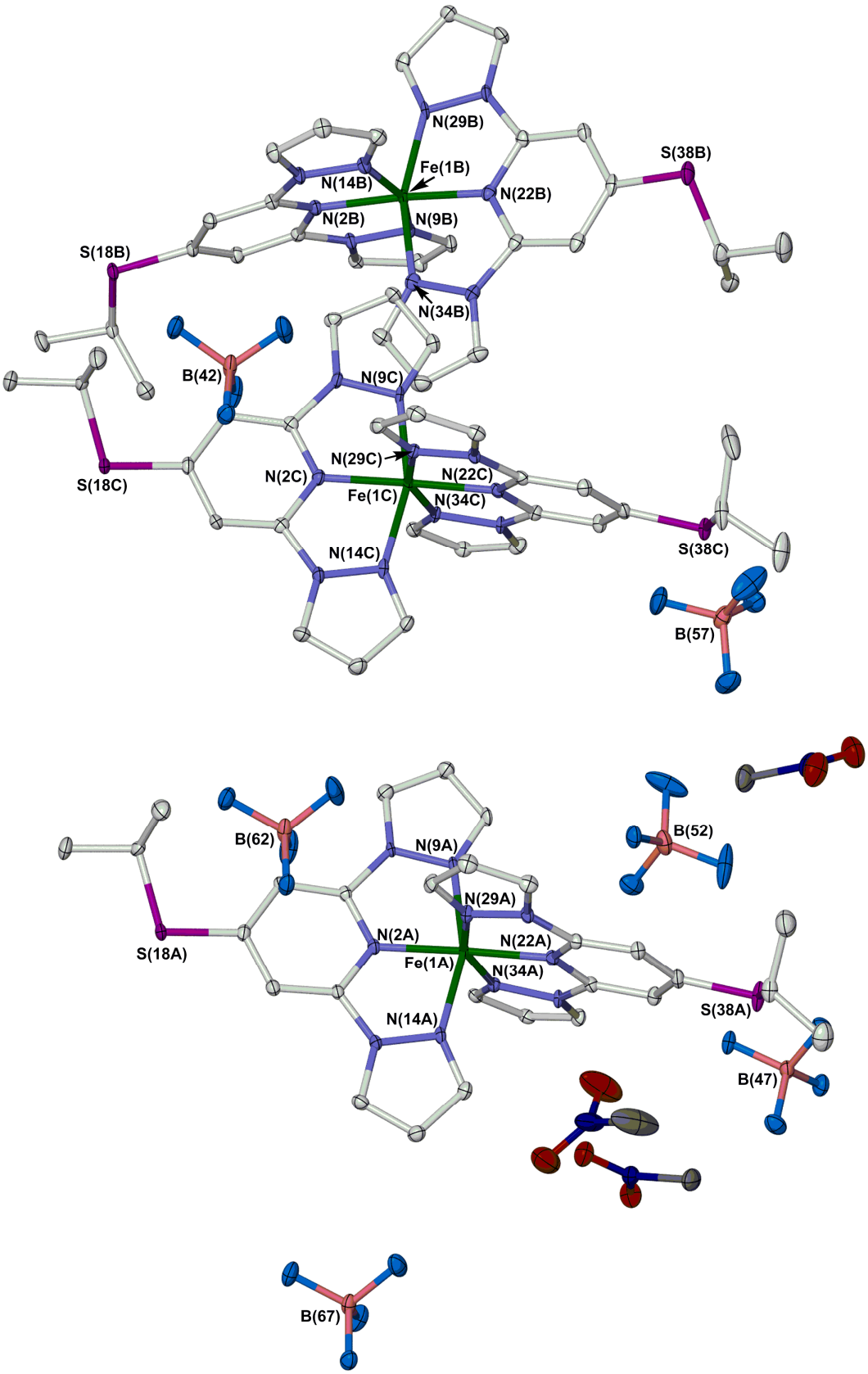


Figure S16 The asymmetric unit in phase 2 of **1[BF_4]$_2$**·$MeNO_2$ at 40 K, with partial atom numbering. Other details as in Figure S5.

The numbering of the other atoms in cations A-C follows that in Figure S5, with A, B or C suffixes as appropriate. The crystal packing in this phase and its relationship to phases 1 and 3 of this material are discussed in ref. 2.

Table S11 Selected bond distances and angular parameters for phase 2 of **1[BF$_4$]$_2$**·MeNO$_2$ at 40 K. See Figure S16 for the atom numbering scheme. Corresponding values from the previously published structure at 15 K are given in square brackets, for comparison.[2] Definitions of the V_{Oh}, Σ, Φ, φ and θ structural parameters are given on page S15.

	Molecule A	Molecule B	Molecule C
Fe(1)–N(2)	1.899(2) [1.905(2)]	1.903(2) [1.903(2)]	1.894(2) [1.900(3)]
Fe(1)–N(9)	1.986(2) [1.986(3)]	1.982(2) [1.986(3)]	1.983(2) [1.982(3)]
Fe(1)–N(14)	1.978(2) [1.978(3)]	1.980(2) [1.982(3)]	1.987(2) [1.992(3)]
Fe(1)–N(22)	1.902(2) [1.904(2)]	1.894(2) [1.896(2)]	1.901(2) [1.901(2)]
Fe(1)–N(29)	1.965(2) [1.962(3)]	1.975(2) [1.977(3)]	1.965(2) [1.965(3)]
Fe(1)–N(34)	1.980(2) [1.978(3)]	1.952(2) [1.959(3)]	1.969(2) [1.970(3)]
V_{Oh}	9.552(7) [9.559]	9.508(7) [9.553]	9.560(7) [9.595]
Σ	90.4(3) [90.0(4)]	88.3(3) [87.5(4)]	88.7(3) [87.7(4)]
Θ	294 [294[a]]	287 [287[a]]	287 [287[a]]
ϕ	173.86(9) [173.69(11)]	173.99(10) [173.61(12)]	176.63(9) [176.74(12)]
θ	87.21(2) [86.72]	87.00(2) [87.00]	87.73(2) [87.12]

[a]These are slightly different values from those in ref. 2. See page S15 for details.

Table S12 Variable temperature unit cell data for phase 3 of **1[BF$_4$]$_2$**·MeNO$_2$, including its relaxation to phase 1 at 70±5 K (Figure S17).

T / K	a / Å	b / Å	c / Å	β / °	V / Å^3
15	20.2510(14)	12.0672(9)	15.3539(11)	101.039(7)	3682.6(5)
25	20.2518(14)	12.0625(9)	15.3675(11)	101.032(7)	3684.7(5)
35	20.2499(13)	12.0572(10)	15.3886(11)	101.018(6)	3688.0(5)
45	20.2545(12)	12.0485(9)	15.4207(12)	100.999(6)	3694.1(5)
55	20.2577(13)	12.0426(10)	15.4498(12)	101.019(6)	3699.6(5)
60	20.2575(12)	12.0377(10)	15.4662(11)	100.100(6)	3702.2(4)
65	20.2570(12)	12.0349(10)	15.4813(11)	100.984(7)	3705.1(5)
70	20.2556(13)	12.0268(10)	15.5034(12)	101.010(7)	3707.3(5)
75	20.2529(13)	12.0161(10)	15.5325(13)	101.005(7)	3710.5(5)
80	20.231(2)	11.9838(16)	15.616(2)	100.961(14)	3717.0(9)
85	19.897(5)	11.929(3)	15.942(4)	100.95(2)	3714.9(15)
92	19.7407(12)	11.9285(8)	16.0053(12)	100.962(7)	3700.1(4)

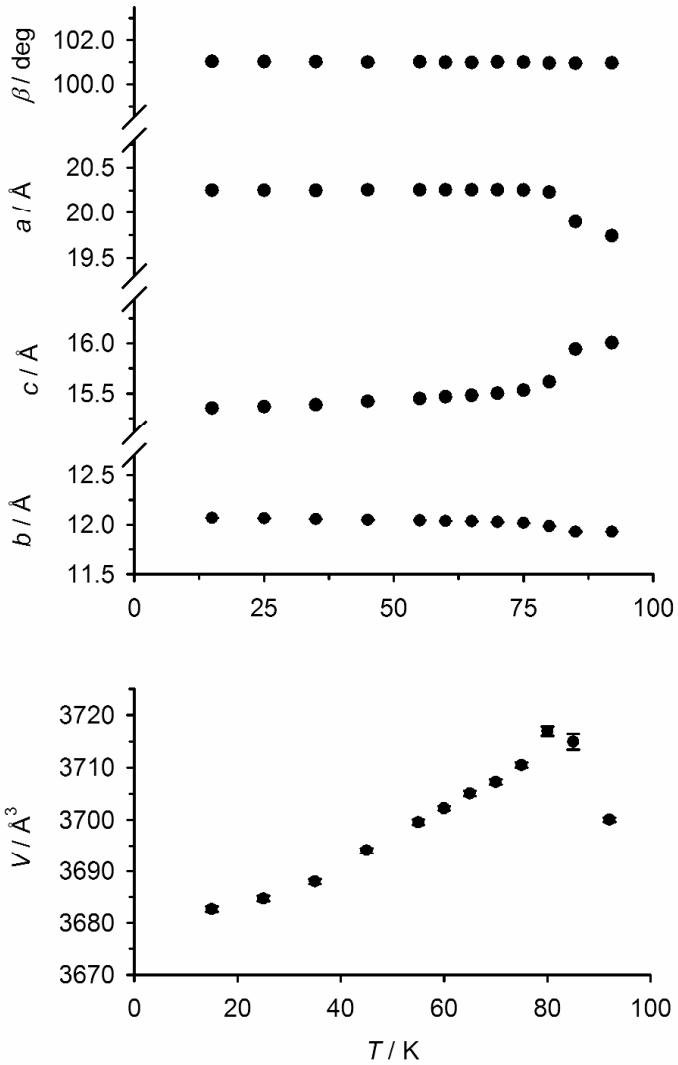


Figure S17 Variable temperature unit cell parameters (top) and unit cell volume (bottom) showing the LIESST relaxation of **1[BF_4]$_2$**·$MeNO_2$.

The phase 3→1 transformation at 70±5 K has no clear impact on the unit cell parameters.

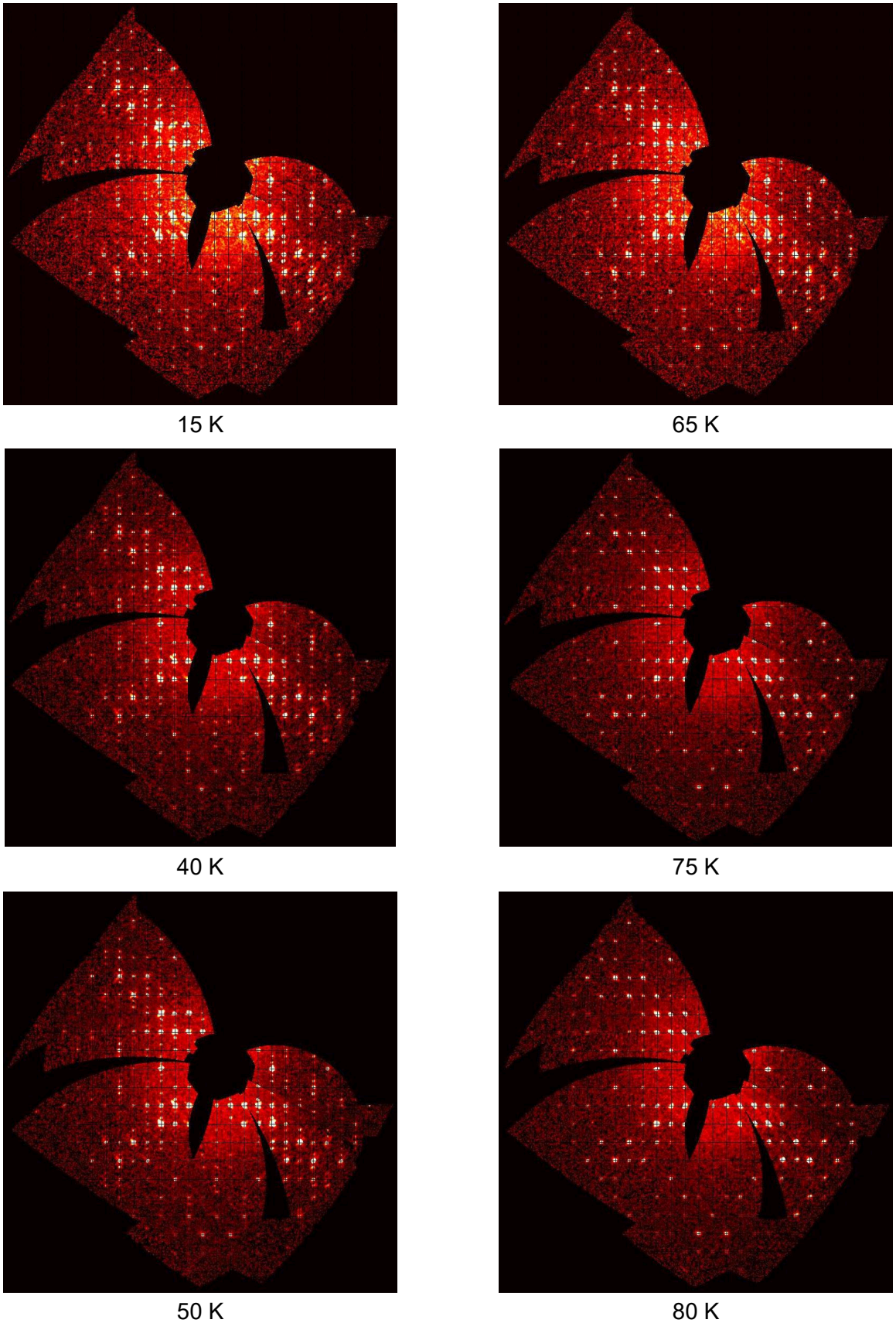


Figure S18 Diffraction images from a single crystal of **1[BF$_4$]$_2$**·MeNO$_2$ in the *hk*0 zone, on warming from 15-80 K under continuous irradiation. The 65 K and 75 K images are the same as those in Figure 4 of the main article.

The phase 3→phase 1 transformation occurs between 65 and 75 K, which is slightly below the onset of LIESST relaxation (Figure S17). The transformation is less clear in the *h*0*l* and 0*kl* zone images.

Table S13 Selected bond distances and angular parameters for the **1[BF$_4$]$_2$**·solv or **1[ClO$_4$]$_2$**·solv crystals, in phase 1, before and after irradiation at low temperature (Å, Å^3, °). See Figure S5 for the atom numbering scheme. Data for the previously published examples are included in the Table, for comparison. Definitions of the V_{Oh}, Σ, Φ, φ and θ structural parameters are given on page S15.

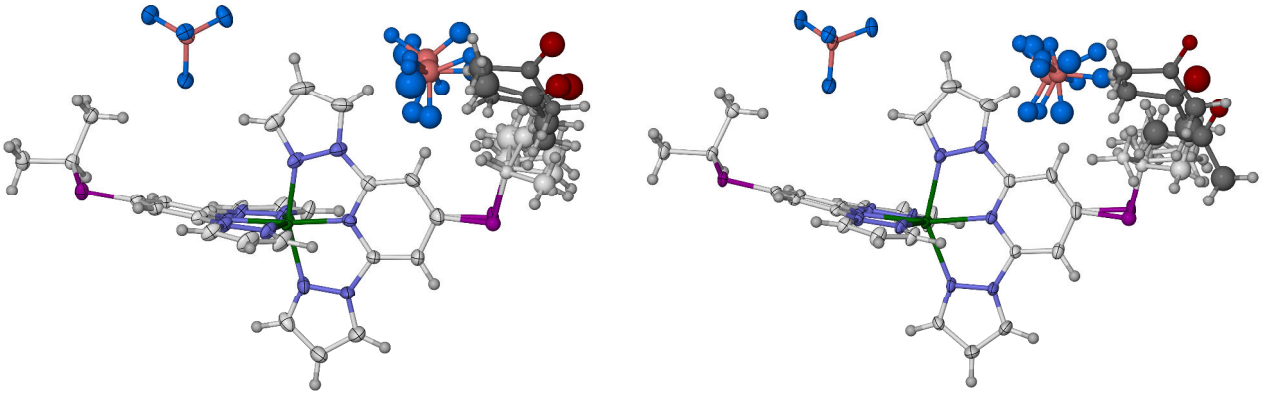
	1[BF$_4$]$_2$·*y*(CH$_3$)$_2$CO		**1[ClO$_4$]$_2$**·CH$_3$NO$_2$		**1[ClO$_4$]$_2$**·H$_2$O	
T / K	20	20	10	10	10	10
Spin state[a]	LS	HS	mixed[b]	HS	LS	HS
Fe(1)–N(2)	1.918(4)	2.129(2)	1.961(4)	2.130(3)	1.9014(17)	2.1271(17)
Fe(1)–N(9)	1.999(4)	2.161(3)	2.032(4)	2.172(3)	1.9854(18)	2.1628(18)
Fe(1)–N(14)	1.992(4)	2.203(3)	2.028(4)	2.204(3)	1.9770(18)	2.2088(18)
Fe(1)–N(22)	1.912(4)	2.115(3)	1.962(4)	2.122(3)	1.8979(17)	2.1102(17)
Fe(1)–N(29)	1.980(4)	2.164(3)	2.003(5)	2.168(3)	1.9839(18)	2.1842(18)
Fe(1)–N(34)	1.973(4)	2.179(3)	2.021(4)	2.169(3)	1.9617(17)	2.1712(18)
V_{Oh}	9.703(13)	12.135(10)	10.147(13)	12.192(10)	9.568(5)	12.238(7)
Σ	92.8(5)	152.6(4)	108.1(5)	154.0(4)	89.3(2)	151.9(2)
Θ	301	489	349	491	290	480
ϕ	174.25(15)	167.46(10)	172.23(15)	169.09(11)	175.86(7)	169.45(6)
θ	86.99(3)	87.76(3)	86.30(3)	86.02(3)	89.53(2)	89.91(2)
	1[BF$_4$]$_2$·CH$_3$CN[2]			**1[BF$_4$]$_2$**·H$_2$O[2]		
T / K	85	85	15	20	20	
Spin state[a]	LS	HS	HS	LS	HS	
Fe(1)–N(2)	1.9845(15)	2.1745(17)	2.197(3)	1.976(3)	2.154(2)	
Fe(1)–N(9)	1.8987(14)	2.1289(16)	2.122(3)	1.894(3)	2.123(2)	
Fe(1)–N(14)	1.9673(15)	2.2073(17)	2.169(3)	1.975(3)	2.202(2)	
Fe(1)–N(22)	1.9706(15)	2.1721(17)	2.171(3)	1.957(3)	2.175(2)	
Fe(1)–N(29)	1.8986(14)	2.1246(16)	2.117(2)	1.893(3)	2.098(2)	
Fe(1)–N(34)	1.9619(15)	2.1726(17)	2.166(2)	1.984(3)	2.190(2)	
V_{Oh}	9.504(5)	12.217(6)	12.126(9)	9.513(8)	12.187(8)	
Σ	87.7(2)	153.5(2)	152.1(3)	88.3(4)	151.1(3)	
Θ	287[c]	491[c]	486[c]	286[c]	476[c]	
ϕ	174.26(6)	167.76(6)	168.15(9)	175.72(11)	169.02(8)	
θ	89.48	88.31	88.75	89.69	89.79	

[a]HS = high-spin, LS = low-spin, mixed = a mixture of high- and low-spin populations. [b]The metric parameters show the crystal is predominantly low-spin under these conditions, but that a fully low-spin population was not achieved upon cooling this crystal in the helium cryostat. [c]These are slightly different values from those in ref. 2. See page S15 for details.

Table S14 Hydrogen bond parameters for the crystal structures of **1[ClO$_4$]$_2$**·H$_2$O at 10 K (Å, °). See Figure S5 for the atom numbering scheme. Symmetry code: (i) 1–*x*, 1–*y*, 1–*z*.

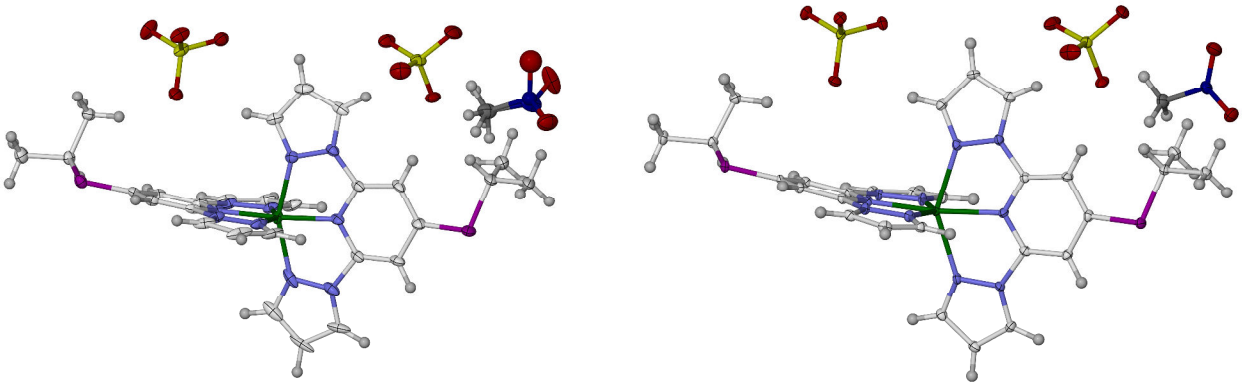
	D−H	H…A	D…A	D−H…A
Low-spin				
O(52)–H(52A)…O(43)	0.91(3)	2.07(3)	2.976(3)	172(3)
O(52)–H(52B)…O(46^{i})	0.94(3)	2.14(3)	3.072(3)	172(3)
High-spin				
O(52)–H(52A)…O(43A)/O(43B)	0.873(17)	2.115(19)/2.019(19)	2.976(4)/2.883(5)	169(3)/170(3)
O(52)–H(52B)…O(46A^{i})/O(46B^{i})	0.919(17)	2.35(2)/2.09(2)	3.233(4)/2.991(5)	160(3)/165(3)

1[BF$_4$]$_2$·*y*Me$_2$CO



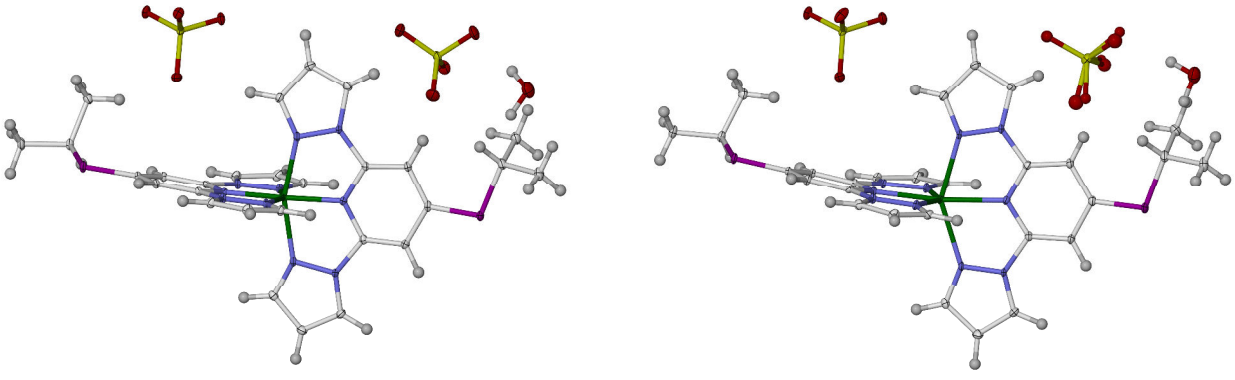
T = 20 K, low-spin | *T* = 20 K, high-spin

1[ClO$_4$]$_2$·MeNO$_2$



T = 10 K, mixed-spin | *T* = 10 K, high-spin

1[ClO$_4$]$_2$·H$_2$O



T = 10 K, low-spin | *T* = 10 K, high-spin

Figure S19 The asymmetric units of **1[BF$_4$]$_2$**·*y*Me$_2$CO, **1[ClO$_4$]$_2$**·MeNO$_2$ and **1[ClO$_4$]$_2$**·H$_2$O at 10 or 20 K, before and after irradiation. Atomic displacement ellipsoids are drawn at the 50 % probability level.

Colour code: C{complex}, white; C{solvent}, dark gray; H, pale gray; B, pink; Cl, yellow; F, cyan; Fe, green; N{complex}, pale blue; N{solvent}, dark blue; O, red; S, purple.

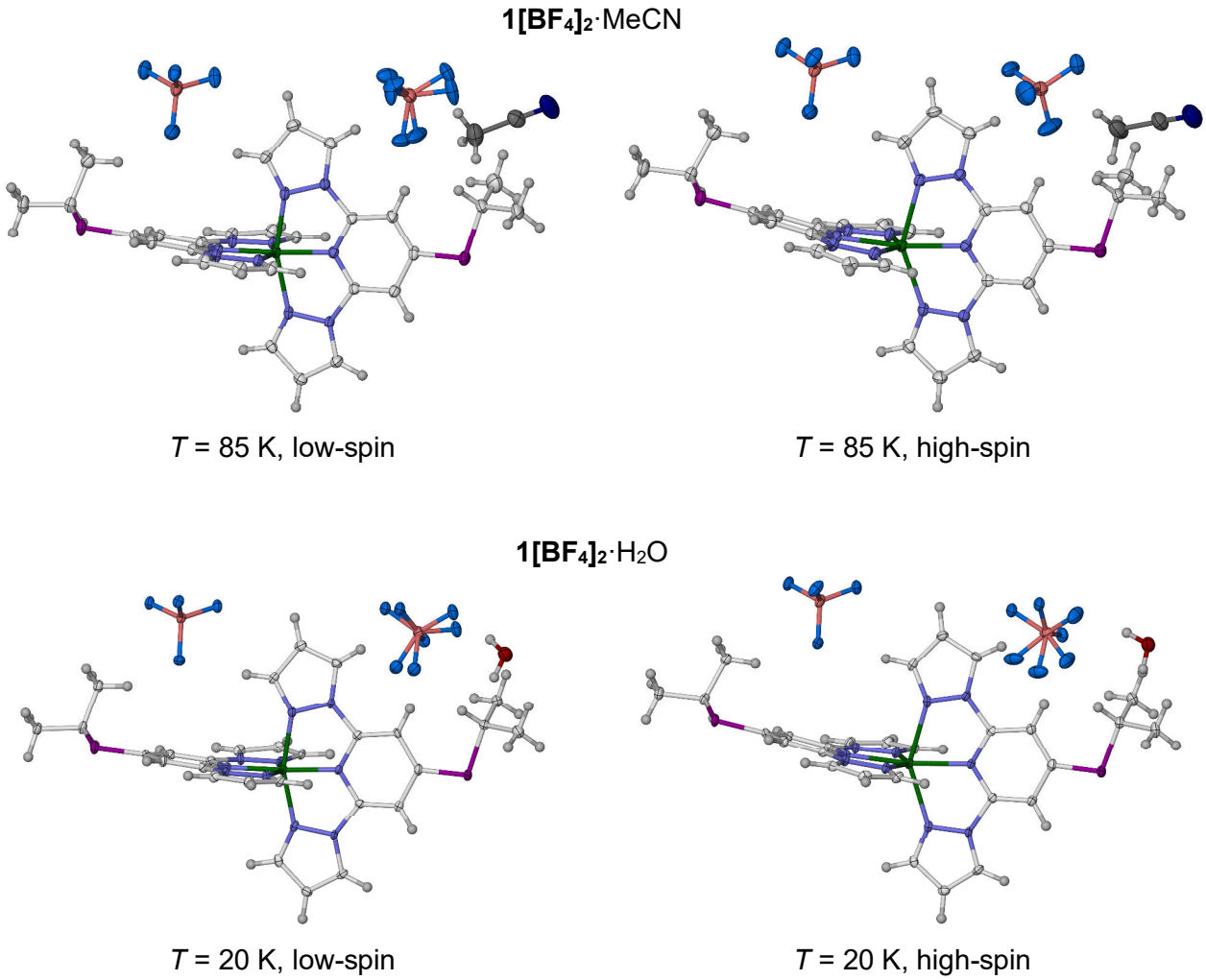


Figure S20 The asymmetric units of **1[BF$_4$]$_2$**·MeCN and **1[BF$_4$]$_2$**·H$_2$O, before and after isothermal photoexcitation. Data are taken from ref. 2. Other details as for Figure S19.

High-spin **1[BF$_4$]$_2$**·MeCN was also characterised at 15 K by thermal trapping of its high-spin state, and is visually indistinguishable from the 85 K high-spin structure in this view (Figure S36).[2]

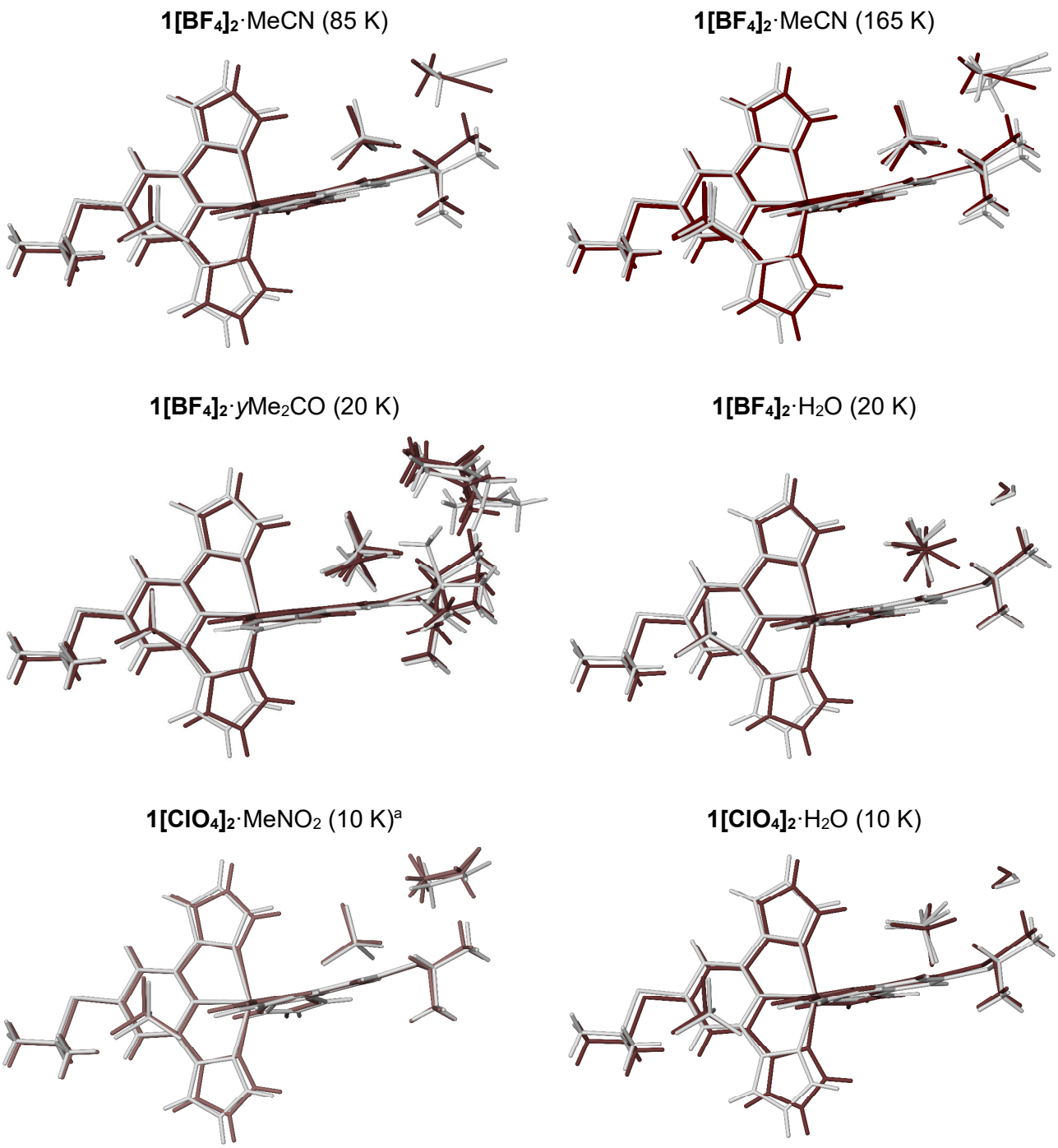


Figure S21 Overlays of the isothermal, phase 1 high-spin (white) and low-spin (brown) asymmetric units for the compounds in this work. Disordered residues are included in the figure.

[a]A fully low-spin structure of this solvate was not achieved; the pale brown structure has a mixed spin state population.

The view is different from Figures S10-S13, S19 and S20, and is chosen to highlight the structural changes in the inter-bilayer space between the spin states.

Discussion of the Hirshfeld surface analyses

A Hirshfeld surface is the boundary surrounding a molecule in a crystal, where the electron density from the enclosed molecule is equal to that from its nearest neighbours.[13] The surface can be plotted in various ways, including interaction (or fingerprint) maps which show intermolecular distances from each atom inside the surface (d_i, i = internal) and its nearest neighbours in the lattice (d_e, e = external). These are scaled according to their distance from the Hirshfeld surface about the residue of interest.[14] Intermolecular contacts between different elements are plotted separately, chosen to highlight relevant C–H...X (X = O or F), C–H...π, anion...π, or O–H...X hydrogen bonding intermolecular interactions.[15]

Each graph is marked with the Pauling Van der Waals radii of the elements plotted. Only data points with d_i and d_e less than the relevant Van der Waals radius are significant intermolecular contacts. Strong interactions like O–H...X hydrogen bonds afford characteristic sharp lines on the donor X...H and acceptor X...H maps, extending well below the Van der Waals radii of each element. Weaker interactions like C–H...X or anion...π appear broader in the maps, and extend only slightly below the Van der Waals radii limits.

A limitation is that the technique does not distinguish irrelevant steric clashes between disorder orientations of nearest neighbour residues. This is often tractable where only one of the atoms involved in a datapoint is disordered, but if both atoms are disordered artefacts manifesting as unreasonably short intermolecular contacts appear in the maps. Thus Hirshfeld maps for **1[BF$_4$]$_2$**·*y*Me$_2$CO could not be interpreted meaningfully because of the extensive disorder in that crystal (Figure S11), and are not included in this SI.

Interaction maps for the cation, intra-bilayer anion, inter-bilayer anion and solvent molecules are plotted separately, for isothermal pairs of high-spin and low-spin structures in **1[BF$_4$]$_2$**·MeCN, **1[BF$_4$]$_2$**·H$_2$O, **1[ClO$_4$]$_2$**·MeNO$_2$ and **1[ClO$_4$]$_2$**·H$_2$O (Figures S21-S32). No analysis for **1[BF$_4$]$_2$**·MeNO$_2$ was undertaken, because its low temperature low-spin (phase 2) and high-spin (phase 3) forms are not isostructural.

To probe the influence of temperature on these maps, data for two compounds are plotted at different temperatures. Low- and high-spin data for **1[BF$_4$]$_2$**·MeCN are plotted at 85 K and 165 K, together with the 15 K high-spin structure. Additional disorder in the 165 K high-spin crystal complicates the comparison a little. However, the Hirshfeld fingerprints near the van der Waals radii for each spin state at different temperatures are essentially the same (Figures S22-S24). We conclude that SCO has a much greater effect on the Hirshfeld interaction fingerprints than the background contraction or expansion on the lattice between temperatures.

Two pairs of structures are also plotted for **1[BF$_4$]$_2$**·H$_2$O: the isothermal structures at 20 K; and the near-isothermal high- and low-spin structures at 220 and 200 K, respectively, which lie either side of its abrupt spin transition (Figures S25-S27). There is more disorder in those structures, including the lattice water during the thermal spin transition. None-the-less, the statements in the previous paragraph are also supported by these data.

More detailed interpretations of the intermolecular interactions in each structure are given beside the relevant Figure. The most important conclusion in the context of this study, is that there are no short intermolecular interactions unique to **1[BF$_4$]$_2$**·MeCN, at any temperature, that could lead to its SCO hysteresis and anomalous LIESST properties.

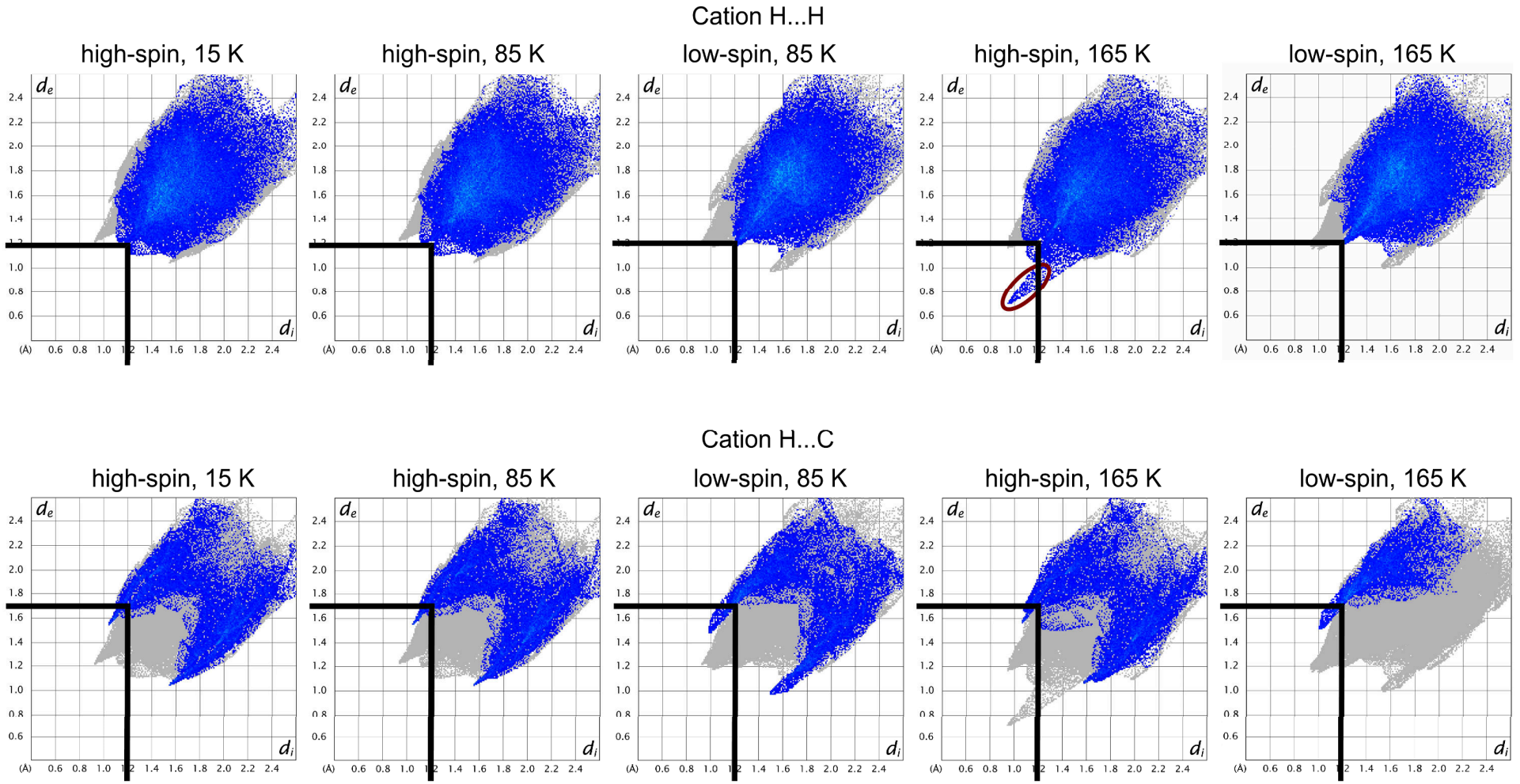


Figure S22 Hirshfeld surface maps of **1[BF$_4$]$_2$**·MeCN in its isothermal high- and low-spin states, showing intermolecular contacts surrounding the complex cation. Data from the 15 K high-spin structure are also included. See page S42 for more details.

Datapoints symmetrically distributed about the central diagonal of the graphs are contacts between nearest neighbour cations. Points that are not symmetrically distributed involve the cation and an anion or solvent residue. The highlighted short H...H contacts in the high-spin 165 K structure are artefacts involving the disordered solvent molecule in that refinement. There are no other noteworthy H...H contacts in these analyses

The short H...C contacts are C–H...π interactions between neighbouring cations, which are clearly shorter in the low-spin structures.

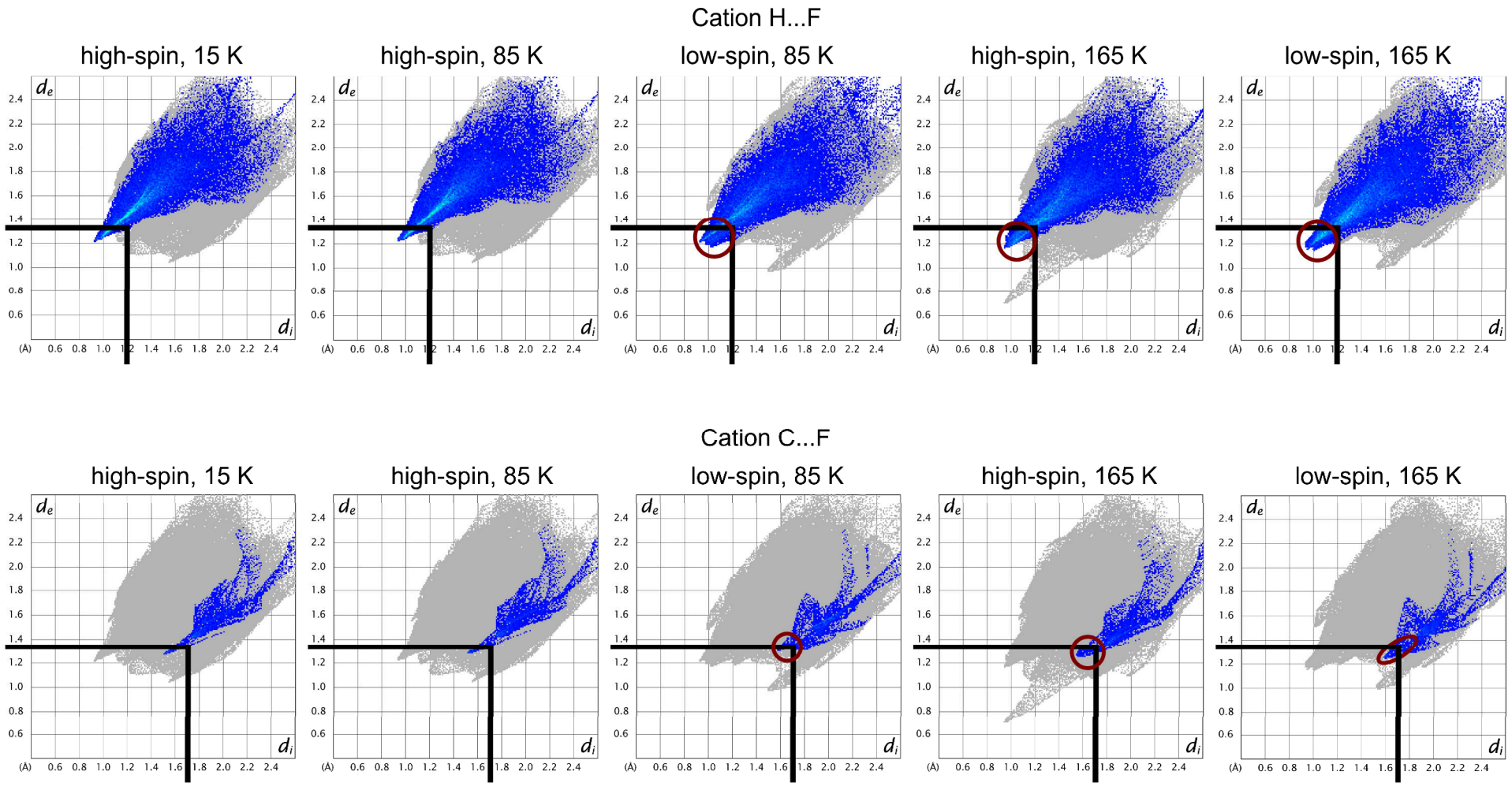


Figure S22 continued.

These H...F maps contain weak C–H...F interactions between the cation and neighbouring anions, while the C...F plots imply a directional anion...π contact to the inter-bilayer anion. These are shown more clearly in the interaction maps from the individual anions, plotted in the next Figure.

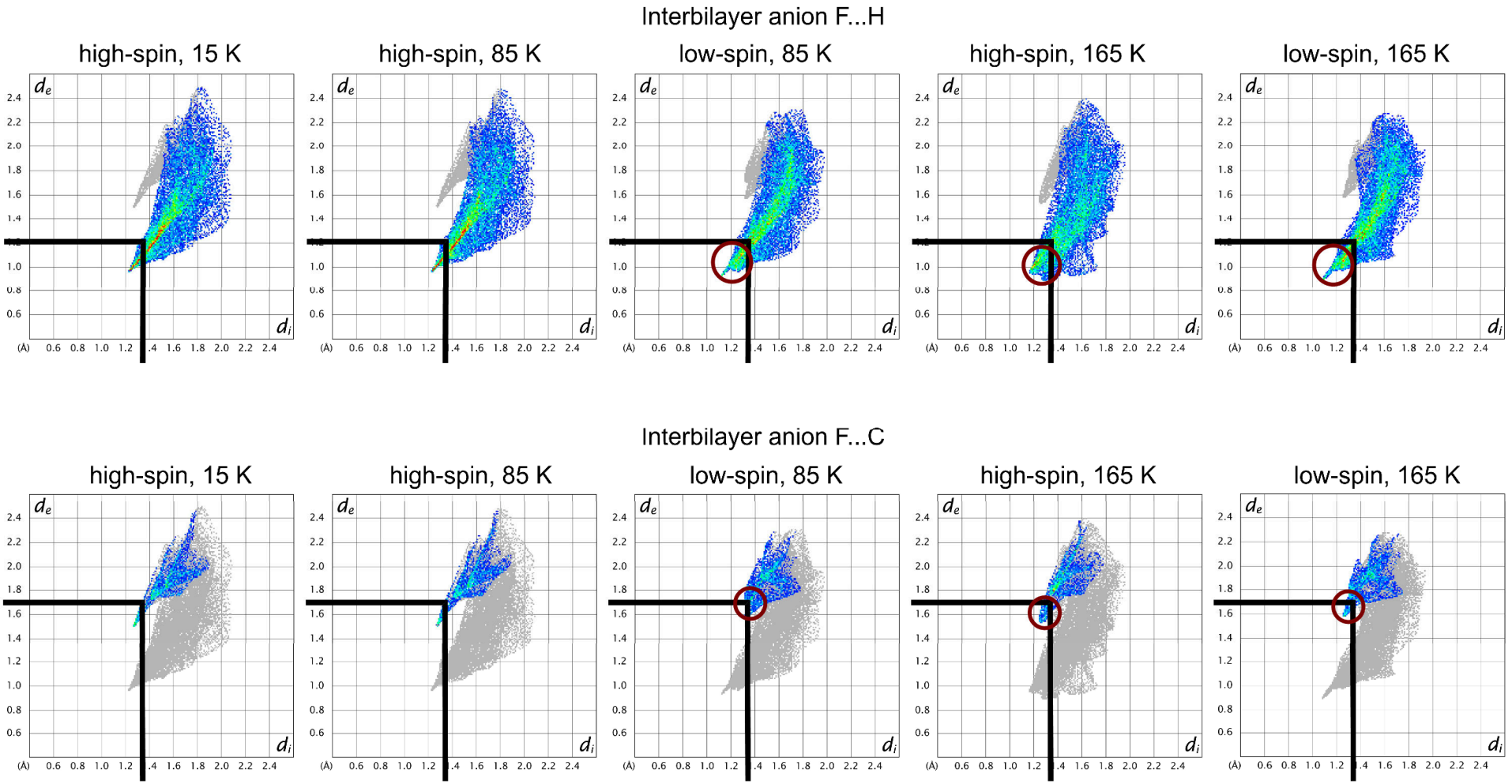


Figure S23 Hirshfeld surface maps of **1[BF$_4$]$_2$**·MeCN in its isothermal high- and low-spin states, showing intermolecular contacts surrounding the BF_4^- anions. See page S42 for more details.

The inter-bilayer anion [B(42)-F(46), Figure S5] is in the region between the cation bilayers, and is close to the lattice solvent. That anion is disordered in both low-spin structures, and in the high-spin analysis at 165 K. That accounts for the wider spread of short F...H and F...C contacts in those structures.

The anion forms a typical distribution of C–H...F contacts to neighbour cations. A weak directional anion...π contact to the inter-bilayer anion is also evident in most of the F...C analyses (see also the previous page).

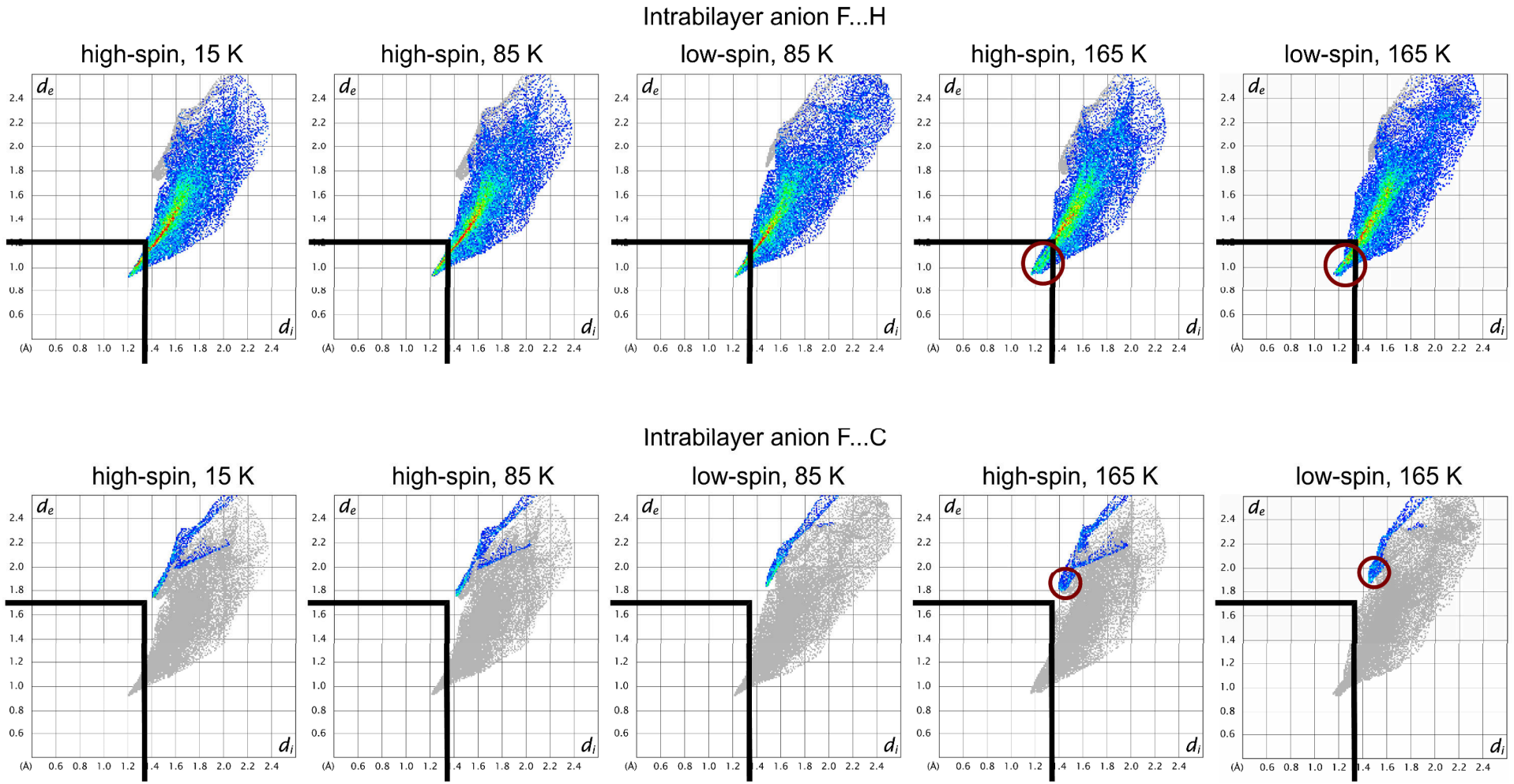


Figure S23 continued.

The intra-bilayer anion [B(47)-F(51), Figure S5] lies within the cation bilayers, and is surrounded by complex cations. It was modelled as disordered in both spin states at 165 K, but is ordered in the other refinements.

This anion participates in a typical distribution of weak C–H...F contacts, but not in anion...π interactions.

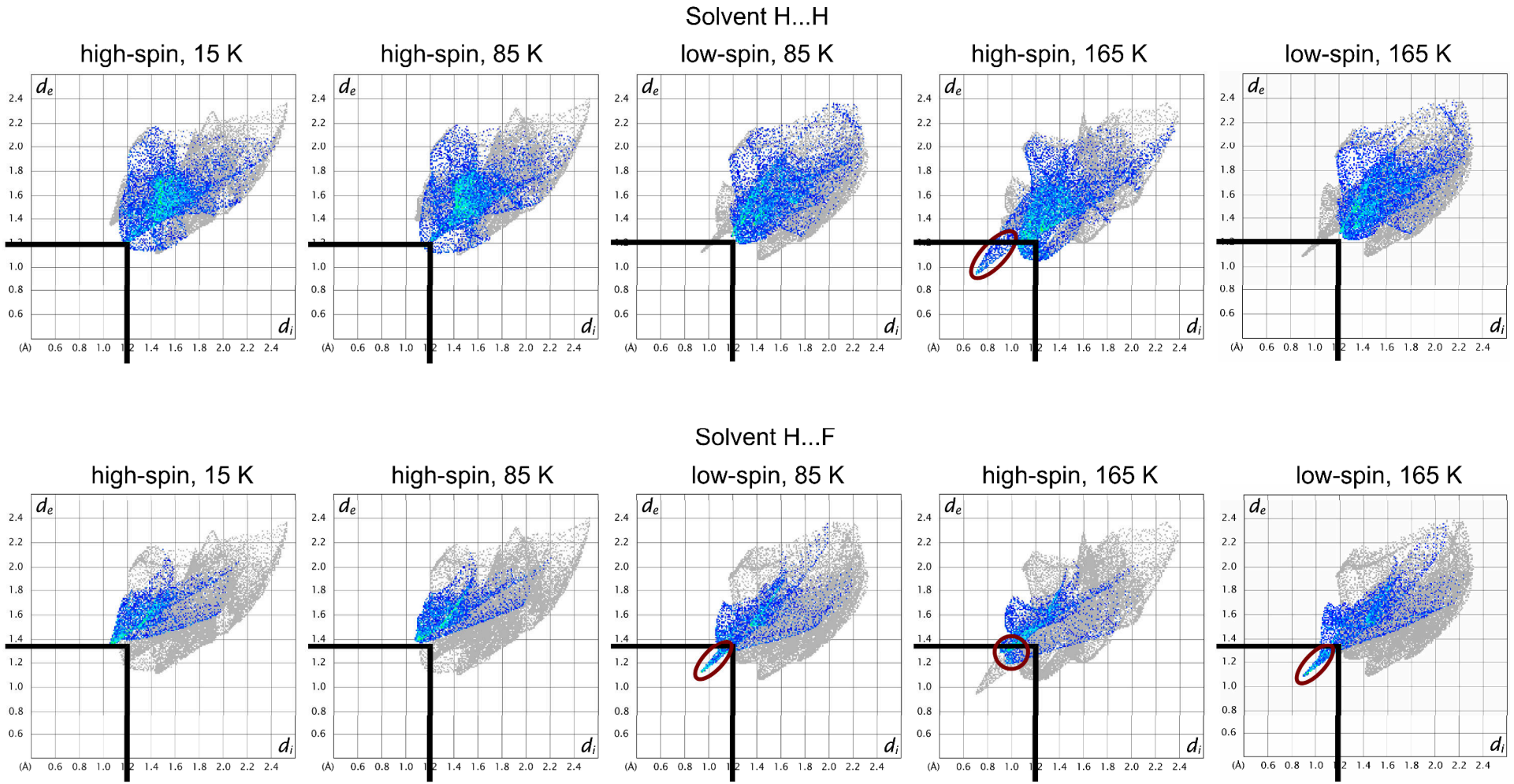


Figure S24 Hirshfeld surface maps of **1[BF$_4$]$_2$**·MeCN in its isothermal high- and low-spin states, showing intermolecular contacts surrounding the acetonitrile solvent molecule. See page S42 for more details.

The acetonitrile molecule and a neighbouring *iso*propyl residue are disordered in the 165 K high-spin analysis (Figures S12 and S21). The highlighted short H...H contacts in that structure involve those disordered groups, and are artefacts of the analysis. These residues are both ordered in the other structures in the Figure.

The significance of the directional C–H...F contact in the low-spin analyses is unclear, because of the crystallographic disorder in the inter-bilayer anion acceptor.

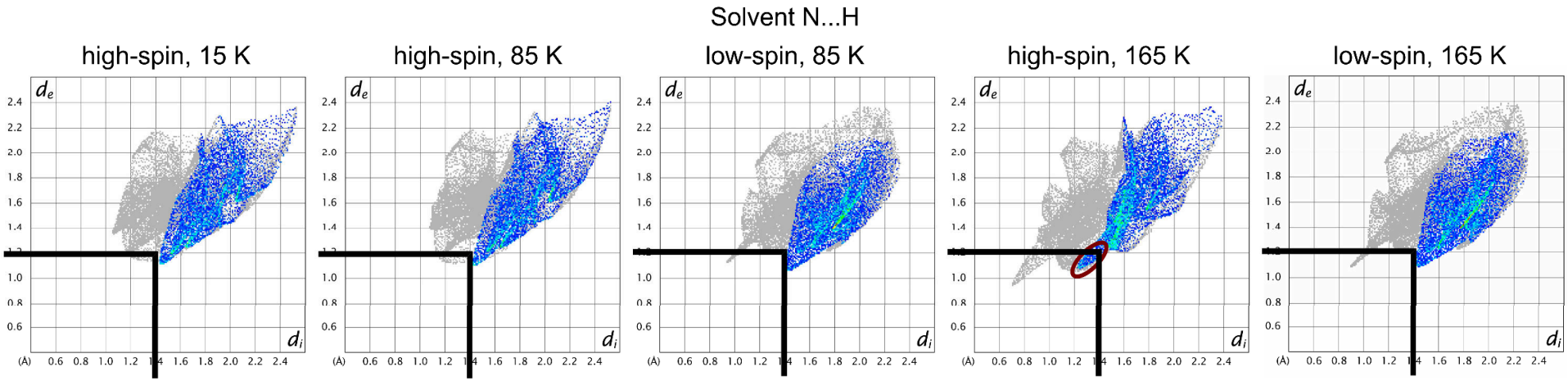


Figure S24 continued.

The apparent C–H...N interaction between the solvent and a neighbouring cation in the high-spin 165 K structure is not matched in the other high-spin refinements, and is probably an artefact reflecting the solvent disorder in that structure.

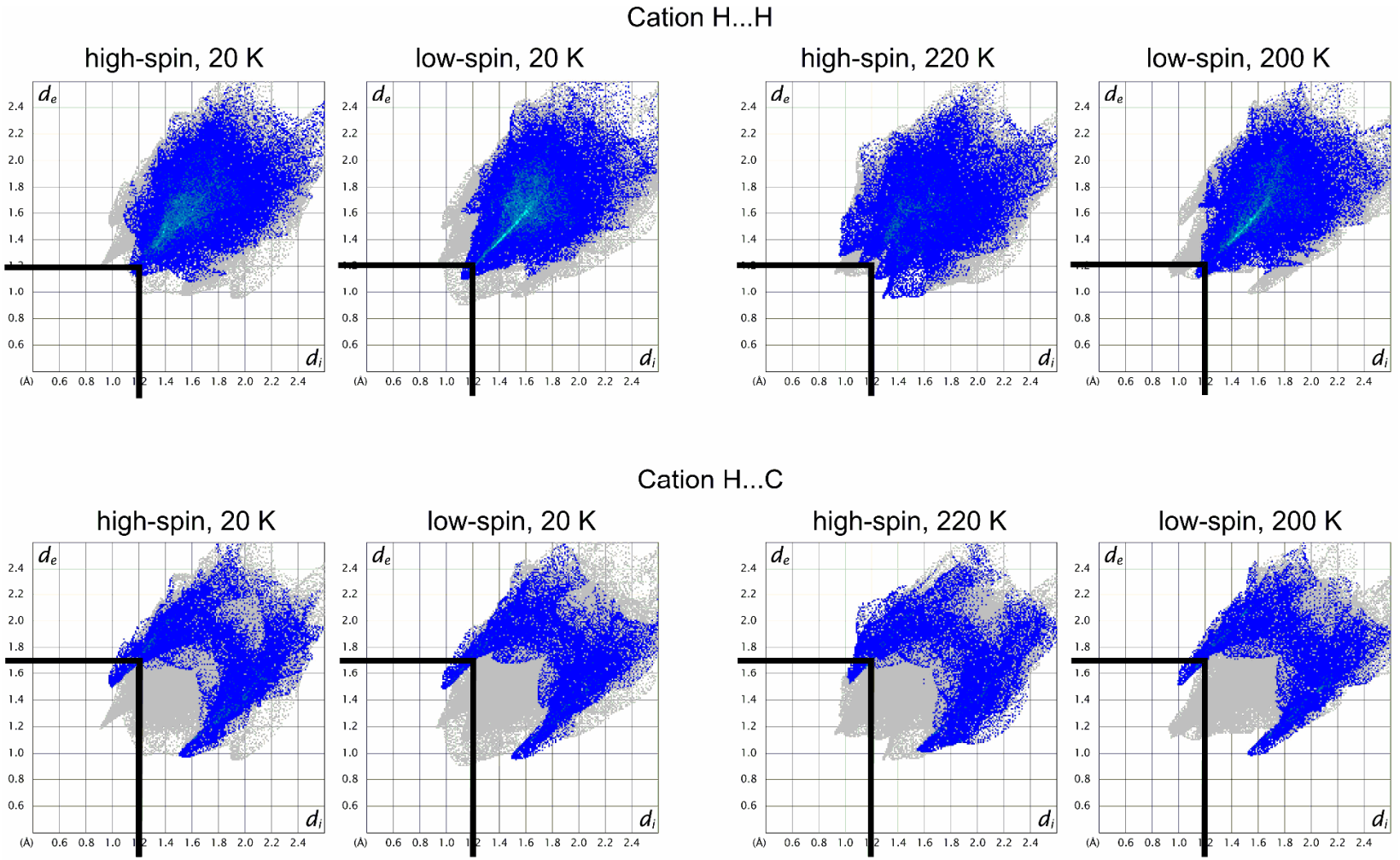


Figure S25 Hirshfeld surface maps of **1[BF$_4$]$_2$**·H$_2$O in its isothermal high- and low-spin states at 20 K, and the near-isothermal analyses either side of its abrupt thermal spin transition at 213 K (Figure S1). The plots show intermolecular contacts surrounding the complex cation. See page S42 for more details.

Datapoints symmetrically distributed about the central diagonal of the graphs are contacts between nearest neighbour cations. Points that are not symmetrically distributed are between the cation and an anion or solvent residue. An *iso*propyl group is disordered at 220 K, but that has little influence on these graphs.

The short H...C contacts are C–H...π interactions between neighbouring cations, which are slightly shorter in the low-spin structures. The shortest H...H datapoints in the low-spin structures are contacts between pyrazolyl goups, reflecting horizontal slippage of molecules within the cation bilayers between the spin states.

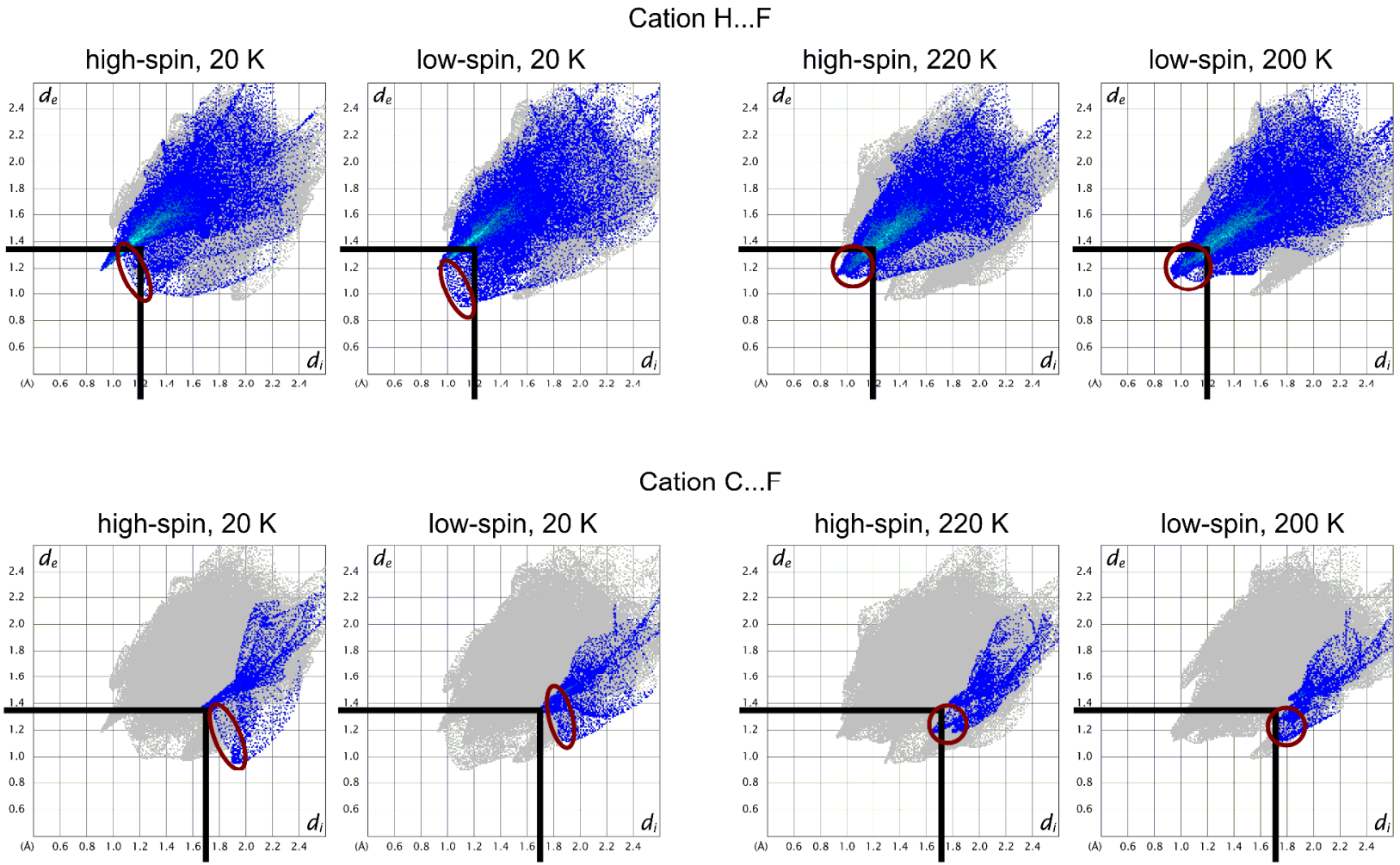


Figure S25 continued.

These are nearest neighbour contacts between the cations and the BF_4^- ions. The inter-bilayer anion is disordered in all these structures, while the intra-bilayer anion is also disordered at the two higher temperatures. For that reason, it's difficult to conclude much from the shorter H...F and C...F contacts in these analyses. The same distances about the individual anions, plotted in the next Figure, are more informative.

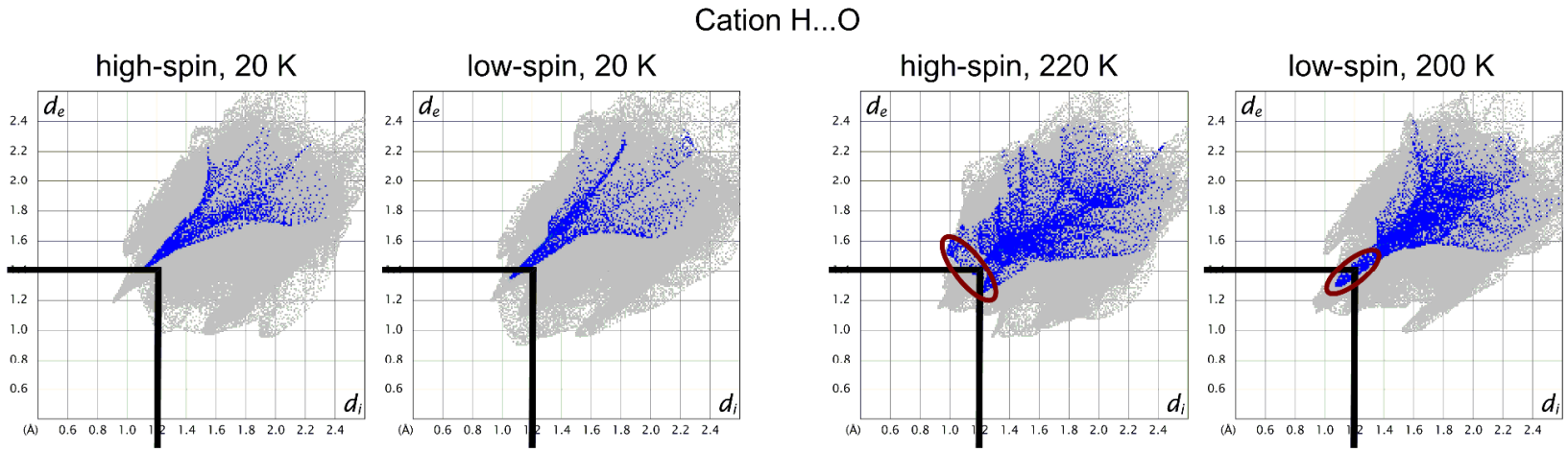


Figure S25 continued.

These are nearest neighbour contacts between the cations and the lattice water. The water molecule is disordered in the 200 and 220 K structures, while a neighbouring *iso*propylgroup is also disordered at 220 K (Figures S13 and S21). That accounts for the much wider spread of shorter H...O contacts at that temperature.

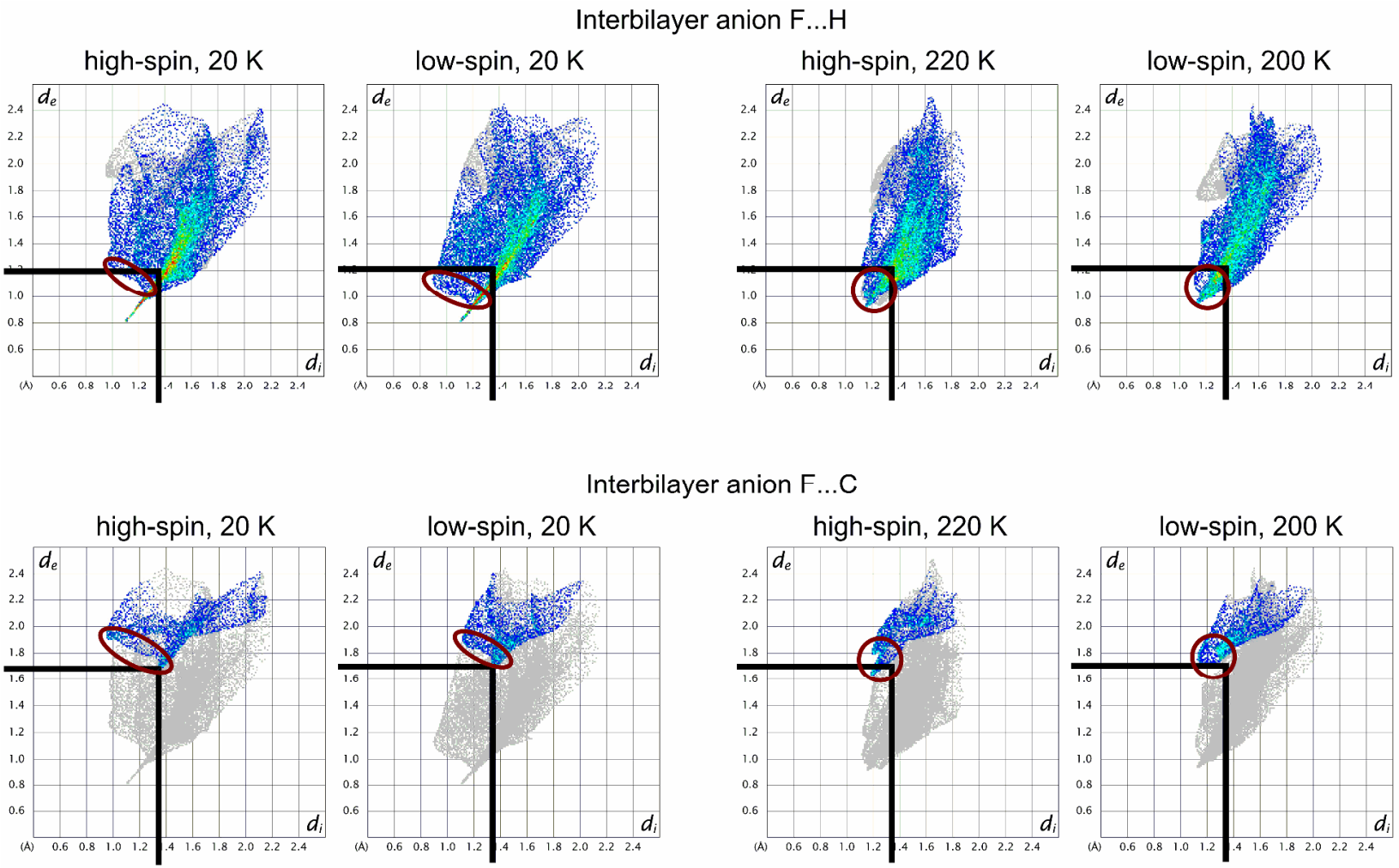


Figure S26 Hirshfeld surface maps of **1[BF$_4$]$_2$**·H$_2$O in its isothermal high- and low-spin states at 20 K, and the near-isothermal analyses either side of its abrupt thermal spin transition at 213 K (Figure S1), showing intermolecular contacts surrounding the BF_4^- anions. See page S42 for more details.

The inter-bilayer anion [B(42)-F(46), Figure S5] lies in the disordered region between the cation bilayers, and is close to the lattice water. That anion is disordered in all these structures, giving a spread of close intermolecular contacts. The directional O–H...F hydrogen bonds do not appear in the higher temperature F...H maps, because the disordered lattice water H atoms are not included in those crystallographic refinements.

An anion...π contact to this anion, which is clear in **1[BF$_4$]$_2$**·MeCN (Figure S23), is not evident in the F...C analyses which may again reflect the anion disorder.

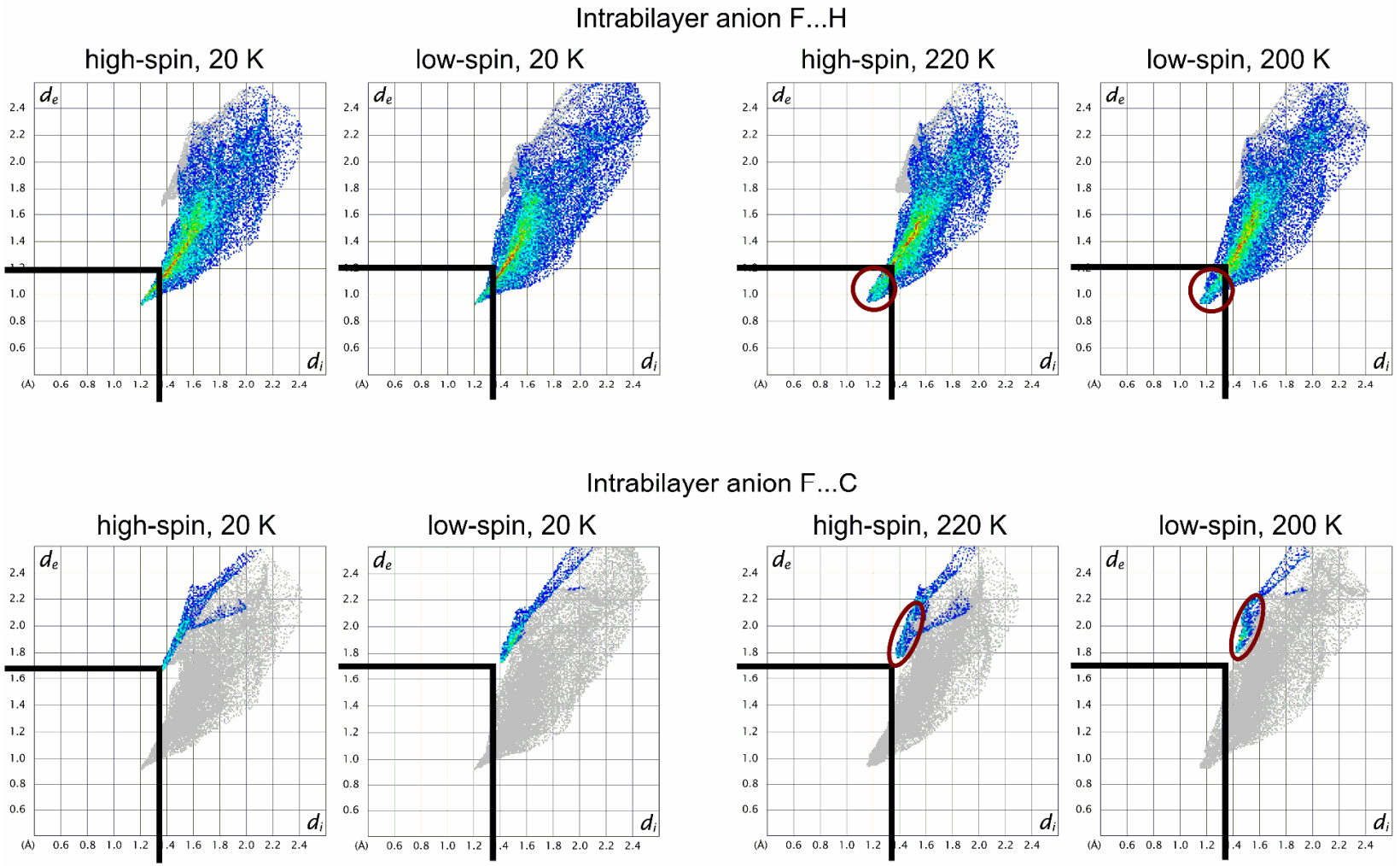


Figure S26 continued.

The intra-bilayer anion [B(47)-F(51), Figure S5] lies within the cation bilayers, and is surrounded by complex cation nearest neighbours. It is crystallographically ordered at 20 K, but disordered in the higher temperature structures. That accounts for the slightly broader spread of short F...H and F...C contacts in those maps.

As for **1[BF$_4$]$_2$**·MeCN, there are a typical number of C–H...F contacts but no anion...π F...C contacts involving this anion.

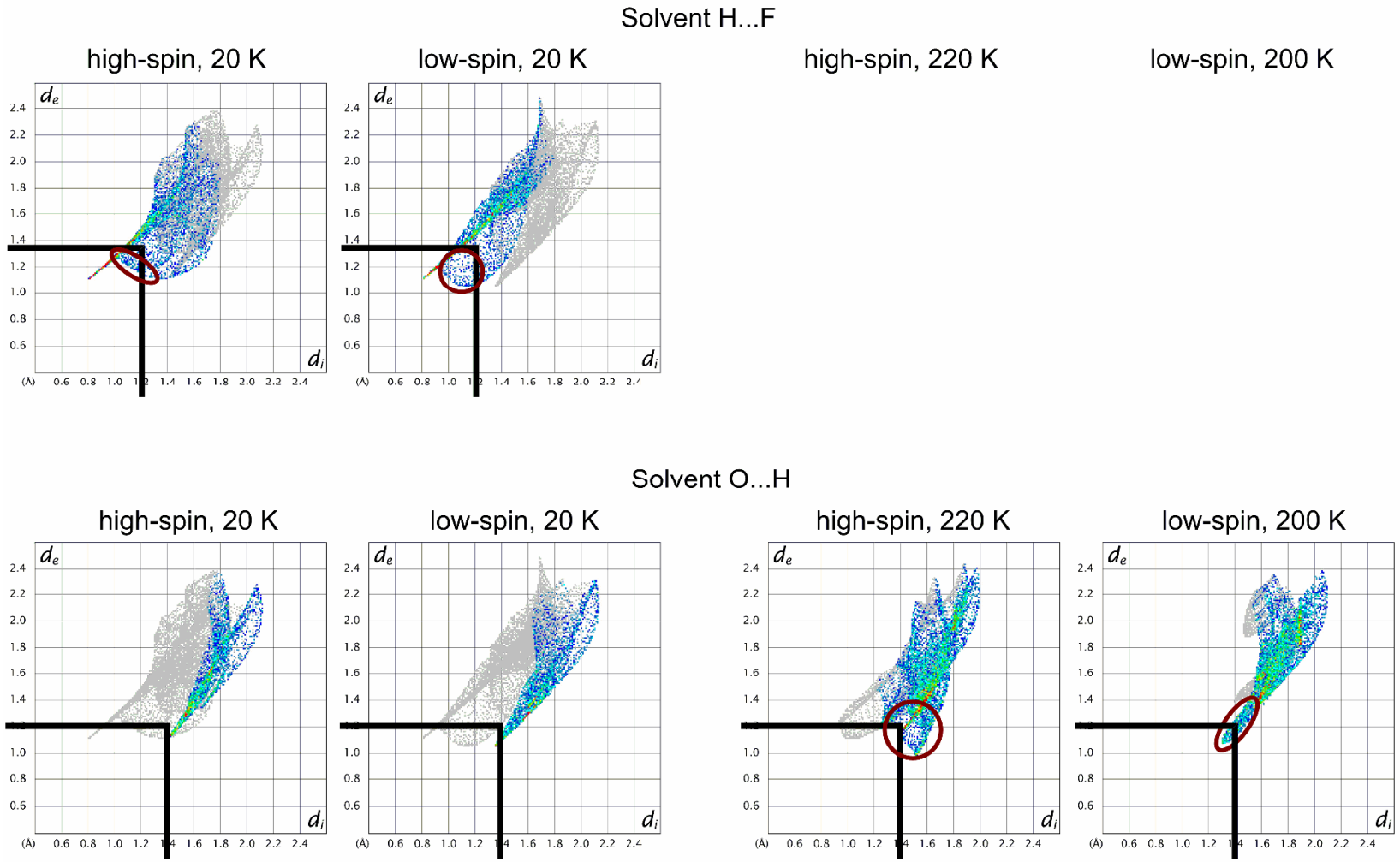


Figure S27 Hirshfeld surface maps of **1[BF_4]$_2$**·H_2O in its isothermal high- and low-spin states at 20 K, and the near-isothermal analyses either side of its abrupt thermal spin transition at 213 K (Figure S1), showing intermolecular contacts surrounding the lattice water. See page S42 for more details.

H...F contact maps are not shown for the higher temperature structures, because the disordered water H atoms could not be included in those refinements.

The directional O–H...F hydrogen bonds are clear in the H...F maps, with the spread of other short H...F distances reflecting disorder in the acceptor inter-bilayer BF_4^- ion. There may be a weak C–H...O interaction between the cation and solvent but, if so, it is less pronounced than in **1[BF_4]$_2$**·MeCN.

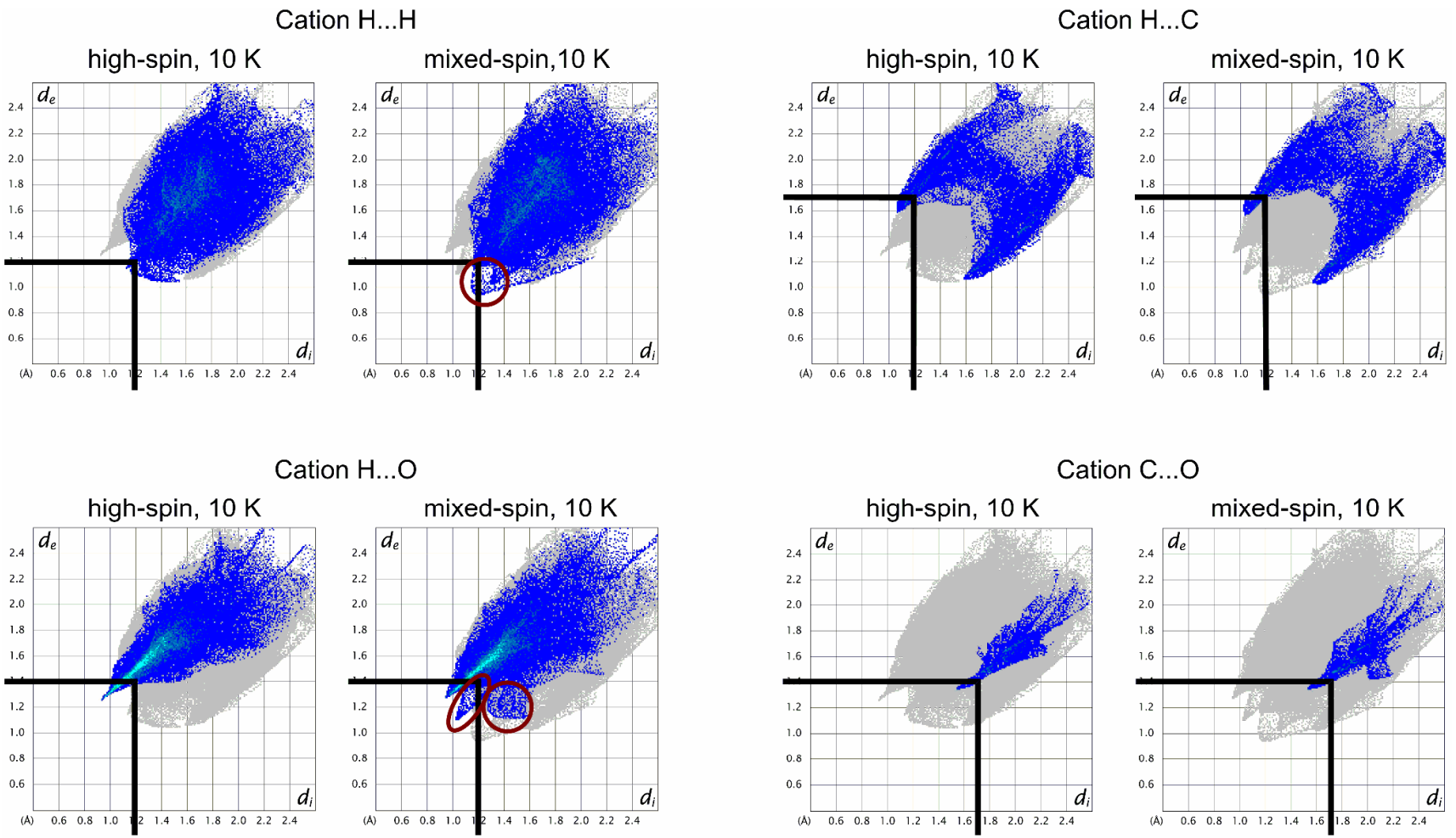


Figure S28 Hirshfeld surface maps of **1[ClO_4]$_2$**·$MeNO_2$ in its isothermal high- and mixed-spin structures at 10 K, showing intermolecular contacts surrounding the complex cation. See page S42 for more details.

Datapoints symmetrically distributed about the central diagonal of the graphs are contacts between nearest neighbour cations. Points that are not symmetrically distributed are between the cation and an anion or solvent residue. The highlighted H...H and H...O distances in the mixed-spin structure involve the lattice solvent, which is disordered in this refinement (Figure S19). There are no noteworthy H...H contacts between crystallographically ordered residues.

The short H...C contacts are C–H...π interactions between neighbouring cations, which are slightly shorter in the mixed-spin structure. Other short H...O datapoints are C–H...O contacts to neighbouring perchlorate ions, while the C...O map shows a weak anion...π interaction with the inter-bilayer anion.

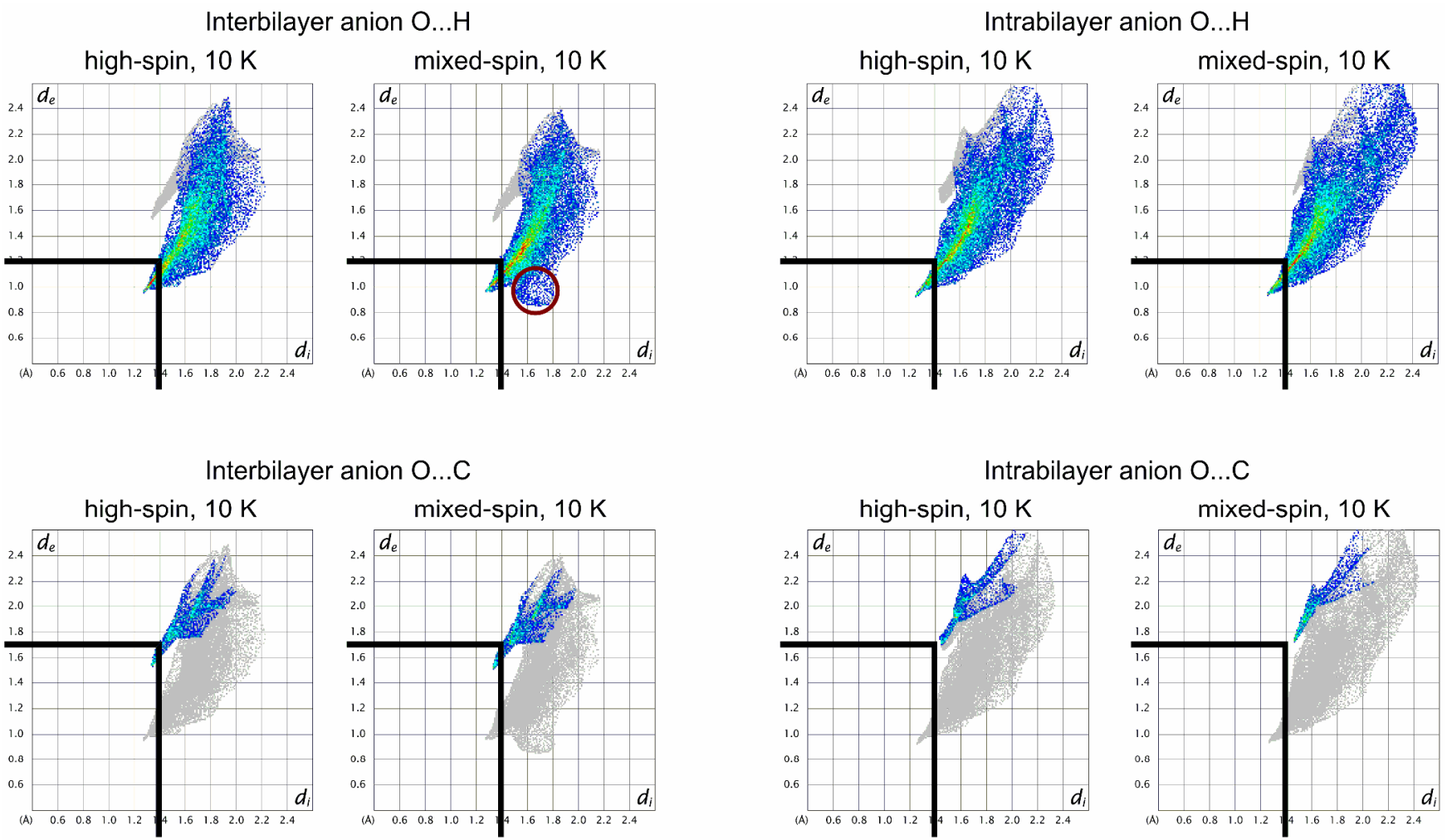


Figure S29 Hirshfeld surface maps of **1[ClO$_4$]$_2$**·MeNO$_2$ in its isothermal high- and mixed-spin structures at 10 K, showing intermolecular contacts surrounding the ClO_4^- anions. See page S42 for more details.

Both anions are crystallographically ordered in each structure. The inter-bilayer anion [Cl(42)-O(46)] lies in the disordered region between the cation bilayers, and is close to the lattice solvent. The highlighted O...H distances to this anion in the mixed-spin structure involve the lattice solvent, which is disordered in this refinement (Figure S17). The intra-bilayer anion [Cl(47)-O(51)] lies within the cation bilayers, and is surrounded by complex cation nearest neighbours.

The plots show typical weak C–H...O interactions between the cation and anion residues, as well as a weak anion...π contact involving the inter-bilayer anion.

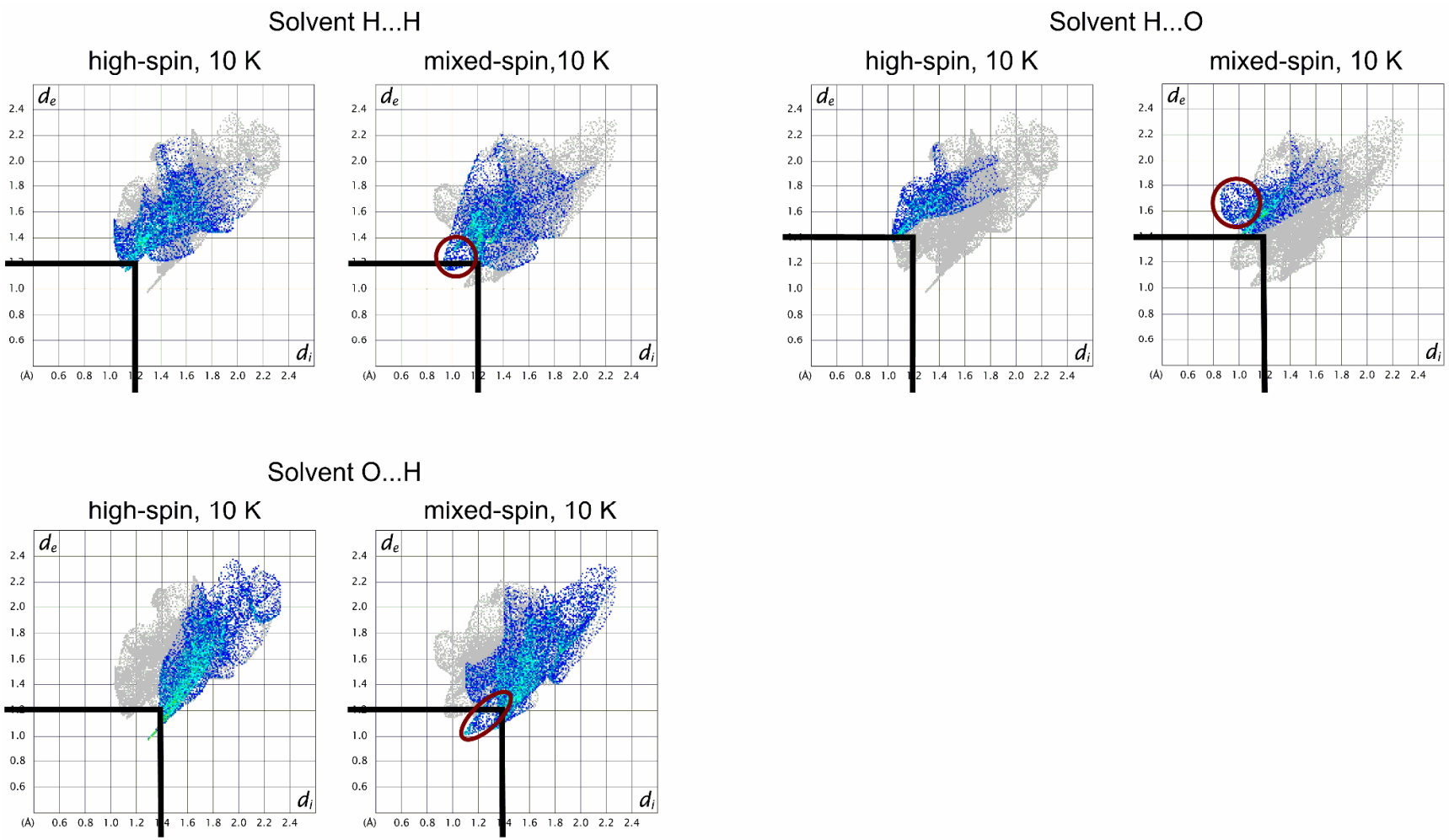


Figure S30 Hirshfeld surface maps of **1[ClO$_4$]$_2$**·MeNO$_2$ in its isothermal high- and mixed-spin structures at 10 K, showing intermolecular contacts surrounding the lattice solvent. See page S42 for more details.

The solvent molecule is disordered in the mixed-spin refinement (Figures S19 and S21), giving rise to the broader spread of highlighted short intermolecular contacts highlighted. A weak directional C–H...O interaction from a cation pyrazolyl C–H group to the solvent is evident in the high-spin structure, but is masked by disorder in the mixed-spin crystal.

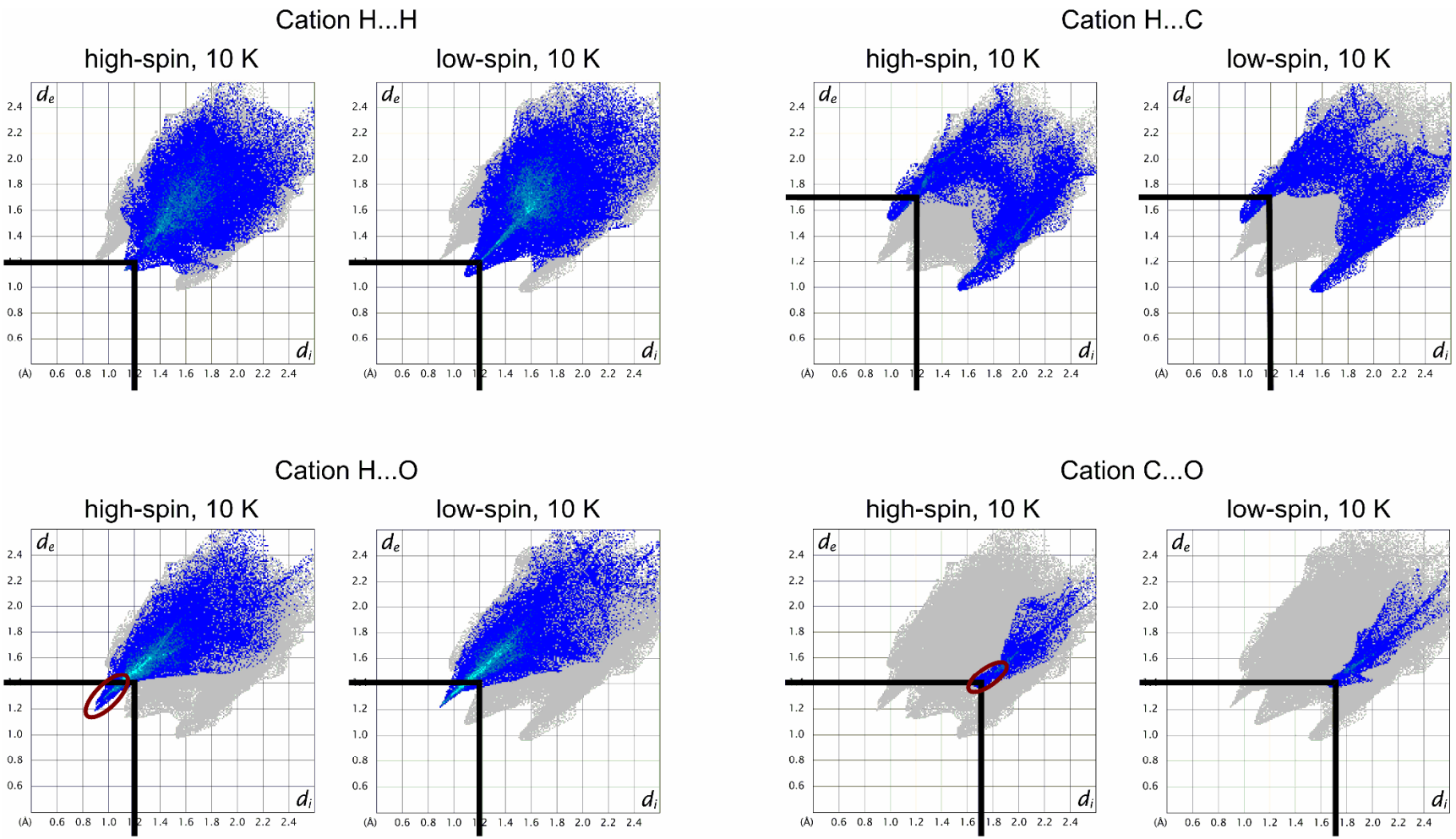


Figure S31 Hirshfeld surface maps of **1[ClO$_4$]$_2$**·H$_2$O in its isothermal high- and low-spin states at 10 K, showing intermolecular contacts surrounding the complex cation. See page S42 for more details.

Datapoints symmetrically distributed about the central diagonal of the graphs are contacts between cations. Points that are not symmetrically distributed involve the cation and an anion or solvent residue. The short, directional H...C contacts are C–H...π interactions between neighbouring cations, which are slightly shorter in the low-spin form. The shortest H...H datapoints in the low-spin structures are contacts between pyrazolyl goups, reflecting horizontal slippage of molecules within the cation bilayers between the spin states. The same pattern of H...H contacts is also shown by **1[BF$_4$]$_2$**·H$_2$O (Figure S25).

The highlighted H...O distances in the high-spin structure involve the inter-bilayer anion, which is disordered in that spin state (Figures S19 and S21).

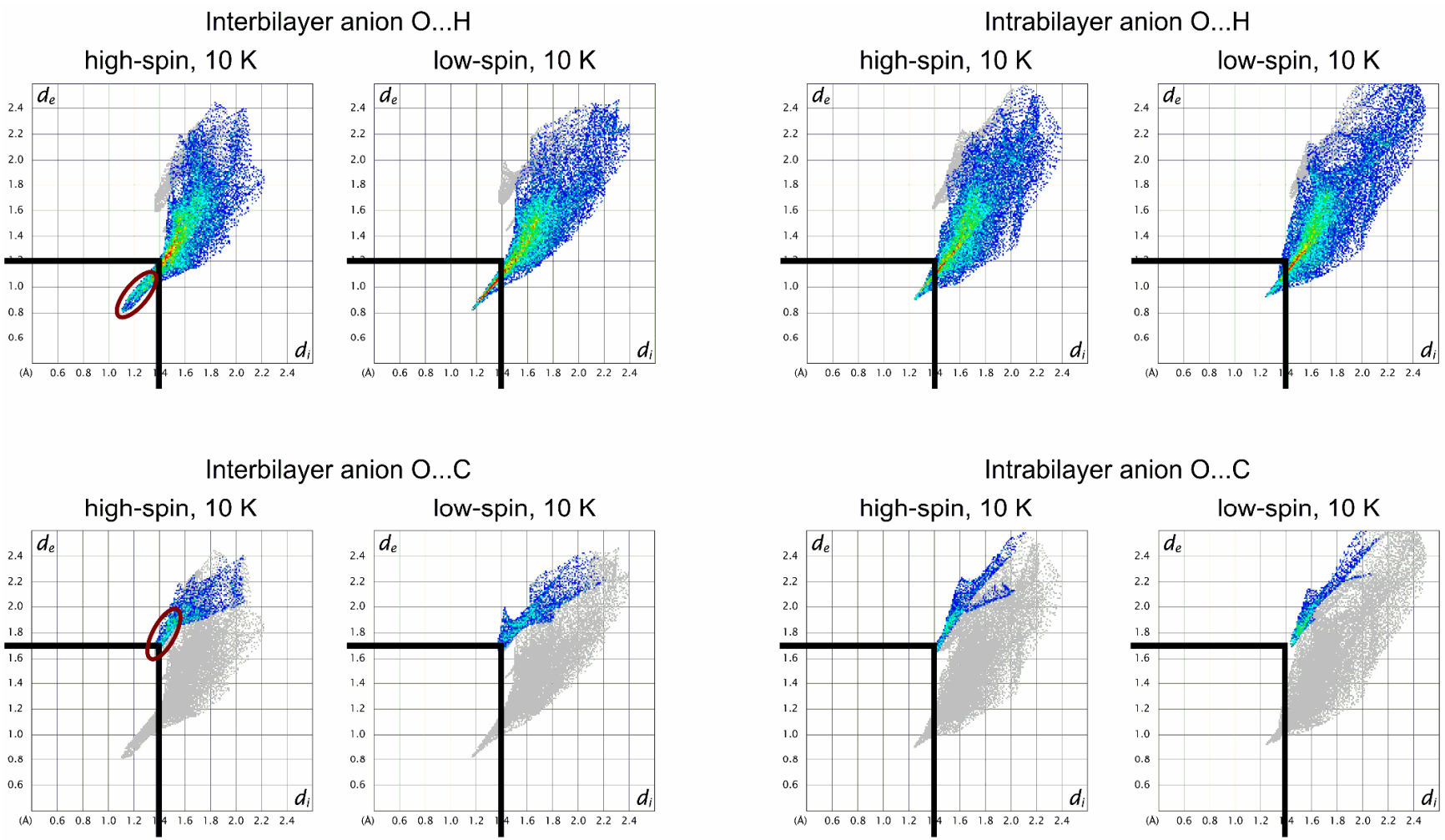


Figure S32 Hirshfeld surface maps of **1[ClO$_4$]$_2$**·H$_2$O in its isothermal high- and low-spin states at 10 K, showing intermolecular contacts surrounding the ClO_4^- anions. See page S42 for more details.

The inter-bilayer anion [Cl(42)-O(46)] lies in the disordered region between the cation bilayers, close to the lattice solvent; the directional O–H...O hydrogen bonds to that anion are clear in the O...H maps. This anion is ordered in the low-spin structure, but disordered in the high-spin crystal (Figures S19 and S21).

The crystallographically ordered intra-bilayer anion [Cl(47)-O(51)] lies within the cation bilayers, and is surrounded by complex cation nearest neighbours through a typical distribution of weak C–H...O interaction. There are no significant anion...π contacts involving either anion.

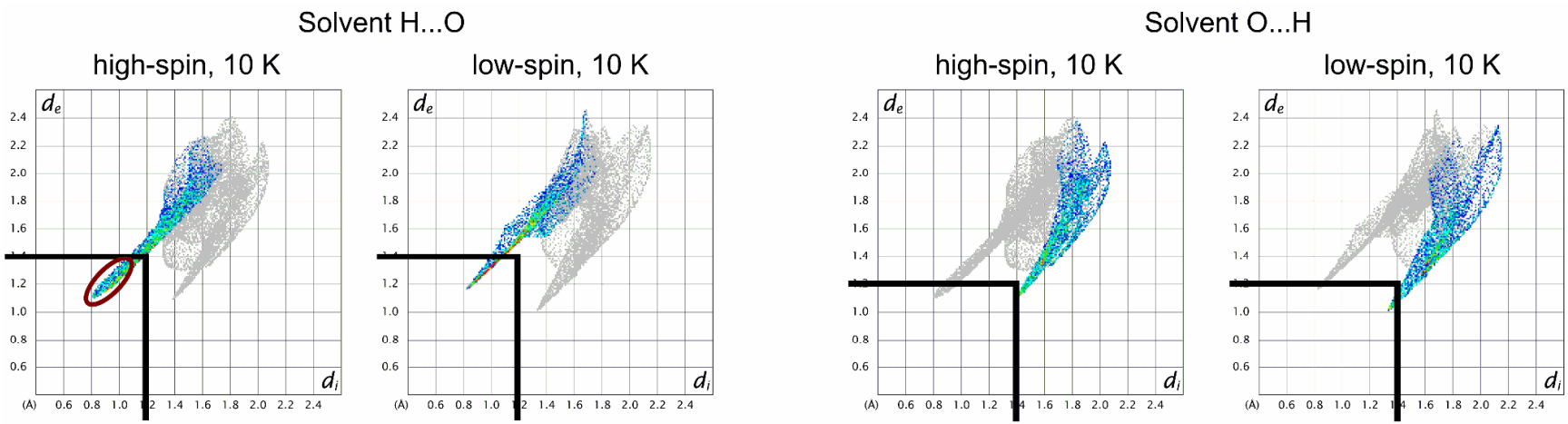


Figure S33 Hirshfeld surface maps of **1[ClO$_4$]$_2$**·H$_2$O in its isothermal high- and low-spin states at 10 K, showing intermolecular contacts surrounding the lattice water. See page S42 for more details.

The directional O–H...O hydrogen bonds to the inter-bilayer anion are clear in the H...O maps. That anion is disordered in the high-spin structure (Figures S19 and S21), explaining the slight broadening of the hydrogen bonding contacts in that spin state. A weak directional C–H...O interaction from the cation to the water molecule is also evident in the low-spin structure.

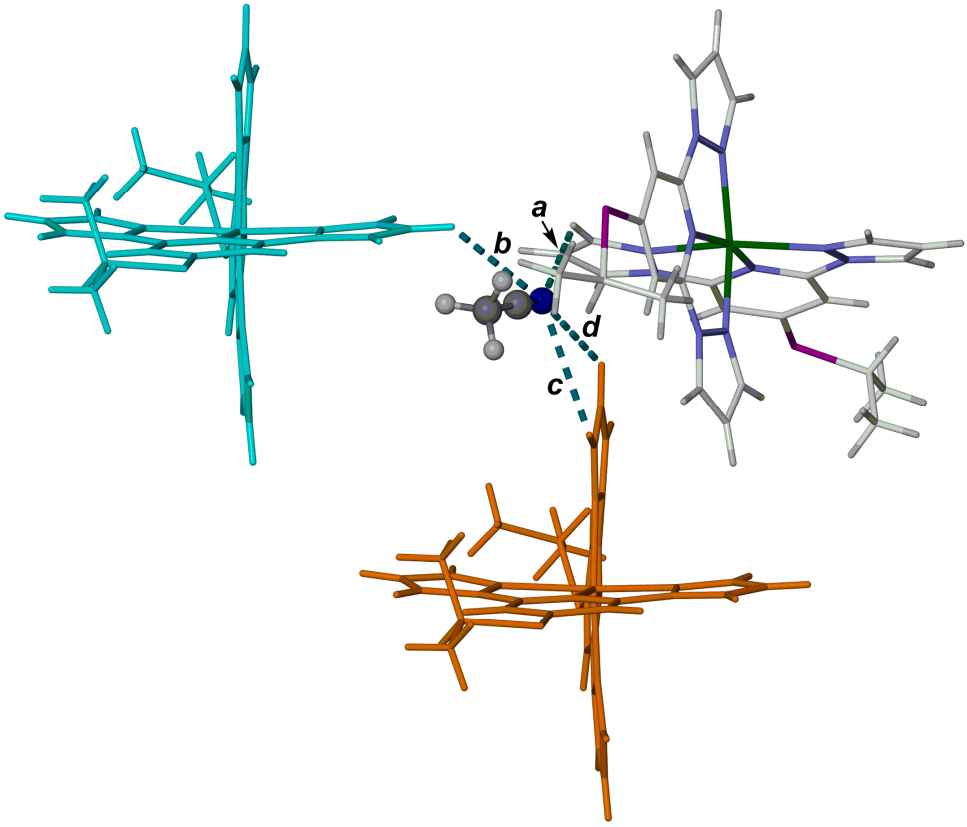


Figure S34 The four intermolecular C–H...N distances in Table S15, involving the acetonitrile molecule in high-spin **1[BF_4]$_2$**·MeCN at 85 K. The atoms involved in these contacts are listed on the next page.

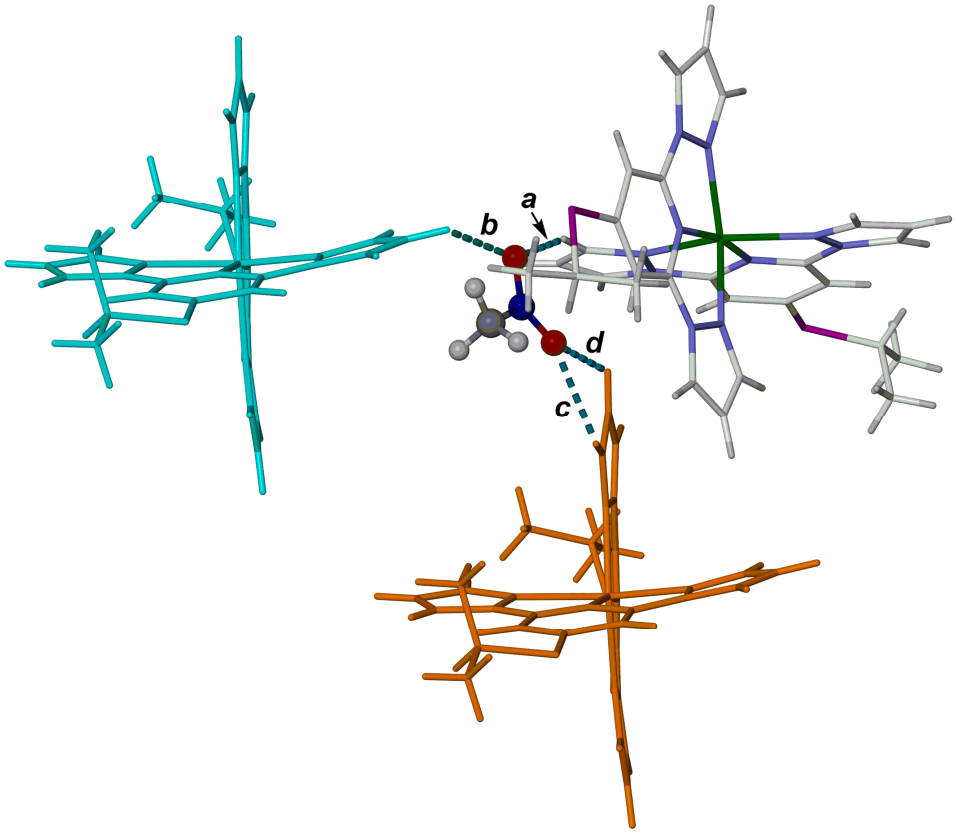


Figure S35 The four intermolecular C–H...O distances in Table S15, involving the nitromethane molecule in high-spin **1[ClO_4]$_2$**·$MeNO_2$ at 10 K. The atoms involved in these contacts are listed on the next page.

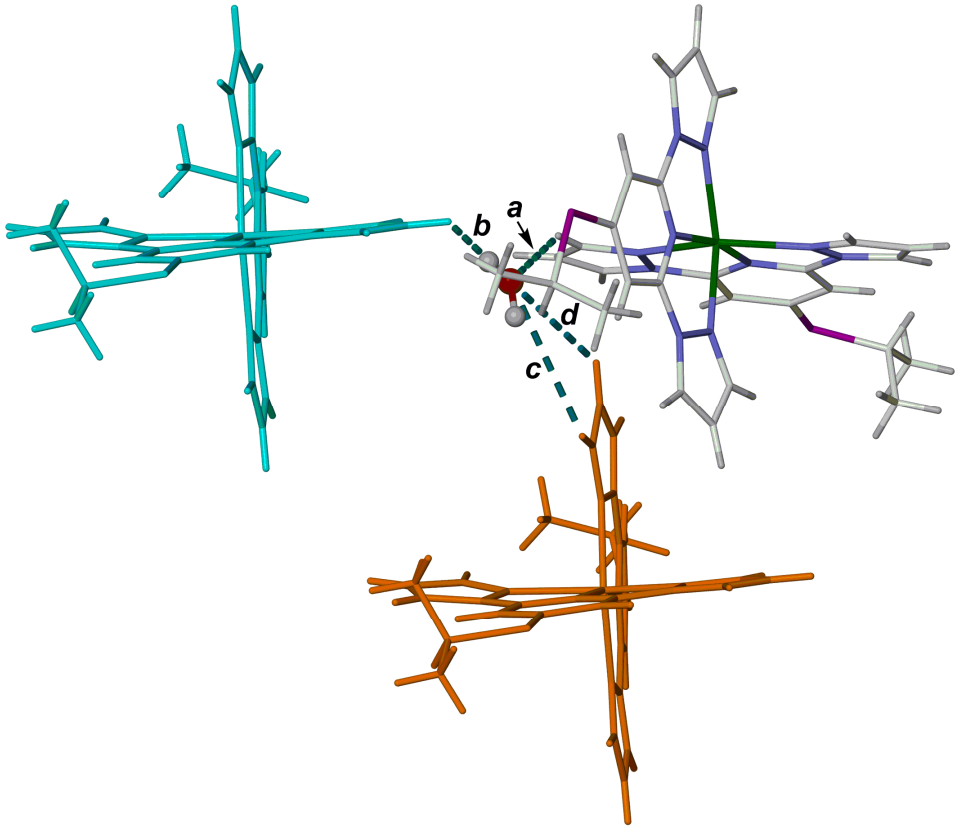


Figure S36 The four intermolecular C–H...O distances in Table S15, involving the lattice water molecule in high-spin **1[ClO$_4$]$_2$**·H$_2$O at 10 K.

In the atom numbering in Figure S5, these C–H...Y (Y = N or O) contacts correspond to:

a: C(15)–H(15)...Y^{i} [symmetry code: (i) 1–*x*, 1–*y*, 1–*z*];
b: C(31)–H(31)...Y^{ii} [symmetry code: (ii) 1–*x*, –½+*y*, ½–*z*];
c: C(10)–H(10)...Y^{iii} [symmetry code: (iii) 1–*x*, ½+*y*, ½–*z*].
d: C(11)–H(11)...Y^{iii}.

The atom numbering given is that used in this study. The deposited cif files for these structures from ref. 2 use a different numbering scheme. The corresponding interaction using the atom numbering in ref. 2 would be C(11)–H(11)...N(11).

Interaction ***a*** is the one shown in Figure 4 (main article). This intermolecular contact is very similar in high-spin and low-spin **1[BF$_4$]$_2$**·MeCN but shows more variation in the other crystals, being mostly longer in the high-spin form (Table S15). Since it is retained in both its spin states, this Van der Waals interaction may contribute to coupling the cation spin state and solvent orientation in **1[BF$_4$]$_2$**·MeCN.

The contact is not highlighted by the Hirshfeld analyses of this crystal (Figure S24) because its H...N distances are close to the Van der Waals radii of an H and N atom.[18] Hence, it is best described as a Van der Waals contact, rather than an attractive C–H...N hydrogen bond.

The same C–H group also forms C–H...O contacts to the solvent molecules in **1X$_2$**·MeNO$_2$ and **1X$_2$**·H$_2$O, which are short enough to be considered weak hydrogen bonds in some of the perchlorate salt structures (Table S15; Figures S30 and S33).

Only ***a*** is short enough to be considered a significant Van der Waals contact in the two hydrate crystals. Distances ***b-d*** are included for comparison with the other solvates.

Table S15 Dimensions of the C–H...Y (Y = N or O) contacts between the solvent and cation in **1X**·solv crystals (Figures S34-S36). The C...Y distances for each intermolecular contact are listed (Å); italicised values are too long to be considered as direct Van der Waals contacts between these groups. Data for **1[BF$_4$]$_2$**·*y*Me$_2$CO aren't included, because of the extensive solvent disorder in both spin states of that crystal.

Contact	***a***	***b***	***c***	***d***
1[BF$_4$]$_2$·MeCN (Y = N; ref 2)				
Low-spin, 85 K	3.105(2)	3.244(2)	*4.402(2)*	*3.729(2)*
High-spin, 85 K	3.127(3)	*3.705(3)*	*3.675(3)*	3.439(3)
1[BF$_4$]$_2$·MeNO$_2$ (Y = O)				
Low-spin, 100 K (phase 1)[a]	3.20(1)/3.19(1)	3.14(1)/*4.12(1)*	3.338(4)	3.246(4)
Low-spin, 15 K (phase 2)[b]	3.194(3), 3.223(4), 3.332(4)	3.200(3), *4.549(4), 4.088(4)*	3.351(3), *3.723(4), 3.501(4)*	3.252(3), 3.401(4), 3.244(4)
High-spin, 15 K (phase 3)[c]	3.432(5), 3.332(5)	3.053(5), 3.459(5)	3.210(5), 3.15(1)/3.36(2)	3.185(5), 3.20(1)/3.34(2)
1[BF$_4$]$_2$·H$_2$O (Y = O; ref 2)				
Low-spin, 20 K	3.286(3)	*4.516(3)*	*4.173(3)*	*3.801(3)*
High-spin, 20 K	*3.456(3)*	*3.528(3)*	*4.570(3)*	*4.483(3)*
1[ClO$_4$]$_2$·MeNO$_2$ (Y = O)				
Mixed-spin, 10 K[a,d]	3.246(7)/3.14(2)	3.070(7)/*3.89(2)*	3.208(7)	3.054(7)
High-spin, 10 K	3.284(4)	3.287(4)	3.125(4)	3.182(4)
1[ClO$_4$]$_2$·H$_2$O (Y = O)				
Low-spin, 10 K	3.233(3)	*4.583(3)*	*4.116(3)*	*3.780(3)*
High-spin, 10 K	3.377(3)	*3.616(3)*	*4.511(3)*	*4.405(3)*

[a]The solvent molecule is disordered over two orientations in this refinement. [b]There are three unique formula units in this phase, which are listed separately. [c]There are two unique formula units in this phase, which are listed separately. One of the solvent molecule sites is disordered over two orientations. [d]A fully low-spin structure of this solvate was not achieved.

The Pauling Van der Waals radii of these atoms are N, 1.5 Å; O, 1.4 Å; "radius of a CH$_x$ group", 2.0 Å; "radius of an aromatic ring", 1.7 Å.[16]

In practise the Van der Waals radius of the C–H donor groups will vary between 1.7 Å and 2.0 Å, depending on the relative positions of the C–H and Y moieties. Hence, while distance ***a*** is shortest for **1[BF$_4$]$_2$**·MeCN it is unclear if that implies this contact is stronger for that crystal, or simply reflects the positioning of the solvent molecule over the adjacent pyrazolyl ring. The significance of some other contacts in the range C...Y = 3.3-3.5 Å is also uncertain, for the same reason.

Less ambiguously, distance ***a*** is almost identical in both spin states for **1[BF$_4$]$_2$**·MeCN, despite their different solvent orientations (Figure S37), but is consistently longer in the high-spin forms of the other solvates listed. That Van der Waals contact could provide a mechanism for coupling spin state changes to the reorientation of the solvent molecule in that crystal.

Discussion of the DFT+U+D2 Computational Protocol

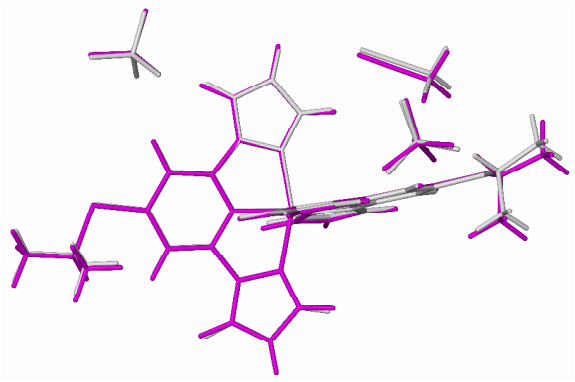
In gradual SCO transitions, the SCO midpoint temperature ($T_{½}$) corresponds to the ratio between the enthalpy and entropy differences (ΔH_{tot} and ΔS_{tot}) involved in the process. Both terms have two major contributions, which are electronic and vibrational (ΔH_{elec}, ΔH_{vibr}, ΔS_{elec} and ΔS_{vibr}).

Computations can evaluate ΔH_{elec} from the structural minima, provided that the electronic structure method of choice is able to capture the HS-LS energetics correctly. Few hybrid DFT functionals are able to do so at an acceptable accuracy, whose cost is prohibitive for solid state computations. For this reason, a common alternative is to dress a cheap DFT functional (PBE or LDA) with a local empirical correction that is applied on the Fe atom. The size of such correction has been benchmarked in the past for the PBE functional and the D2 dispersion[17] and more recently for the D3 and D3BJ dispersion corrections,[18] providing similar accuracy towards ΔH_{elec}.

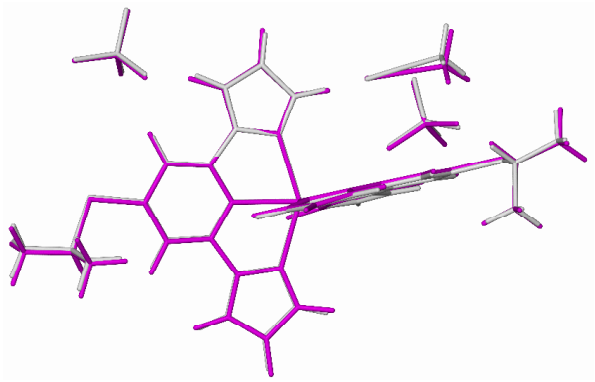
ΔH_{vibr} can be safely modelled using the Harmonic-Oscillator (HO) model, whereas ΔS_{vibr} is better treated combining the HO and Free-Rotor (FR) models.[19] Both models use the vibrational normal modes (ν_i). The computational cost of accurately evaluating ν_i in molecular crystals is large. Moreover, practical restrictions appear associated with the available software. For instance, the computation of phonons in the solid state with DFT+*U* has only become possible recently.[20] Until now, the *U* correction had to be dropped to that purpose. For these reasons, the computational evaluation of ΔH_{vibr} and ΔS_{vibr} has been usually restricted to isolated molecules, for which ν_i can be extracted with more accurate analytical (*vs.* numerical) methods. In our case, all compounds of the **1X₂**·solv serie share the same complex ($\mathbf{1}^{2+}$), so the orthodox way of evaluating of ΔH_{vibr} and ΔS_{vibr} from the gas-phase ν_i of $\mathbf{1}^{2+}$ would lead to exactly the same result for all compounds. For these reasons, we did not pursue the evaluation of ΔH_{vibr} and ΔS_{vibr}. Certainly, these are terms that contribute to the total energy, and hence $T_{½}$. However, there is no reason to believe that they will impact one compound much more than the rest, so it is highly unlikely that the failure of computations to capture **1[BF₄]₂**·MeCN as an outlier, is related to these terms.

Instead, that is probably related to the thermally activated crystallographic disorder. Such effect would manifest in a jump in the vibrational contributions once it activates. Such jump cannot be captured from the vibrational normal modes ν_i obtained from the harmonic approximation at the minima, irrespectively of those being from solid state or gas-phase computations. In other words, this problem is not related to the practical computation ΔH_{vibr} and ΔS_{vibr}, but a more fundamental issue. To estimate its energy contribution, it would be necessary to evaluate the free energy from a series of molecular dynamics simulations conducted at increasing temperatures (encompassing the order-disorder transition). That is an open problem in computational chemistry due to its cost and moderate accuracy.

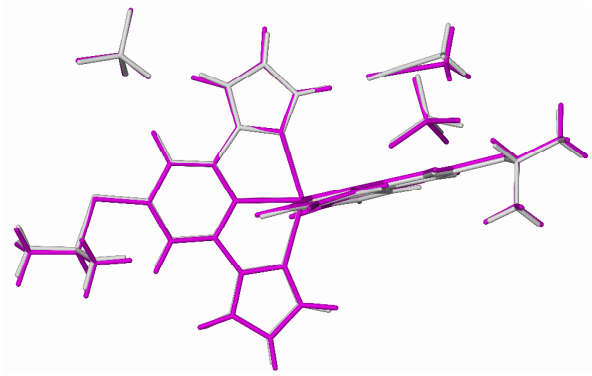
In summary, computations on SCO systems are: (i) strongly reliable at evaluating individual ΔH_{elec} values, and (ii) moderately reliable at evaluating individual ΔH_{vibr} and ΔS_{vibr} values. The reliability of *i* and *ii* increases significantly when relative values (*i.e.* trends) are under discussion, such as in the **1X₂**·solv series studied herein.



Low-spin, 85 K



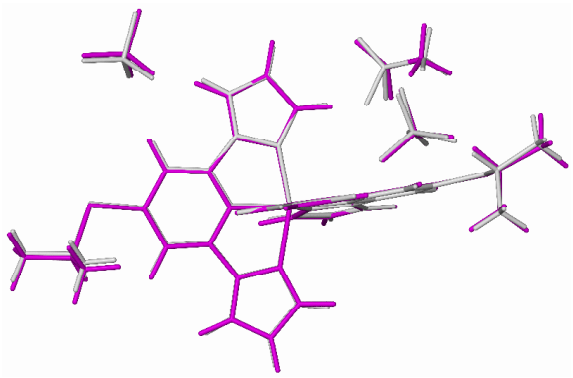
High-spin, 85 K



High-spin, 15 K

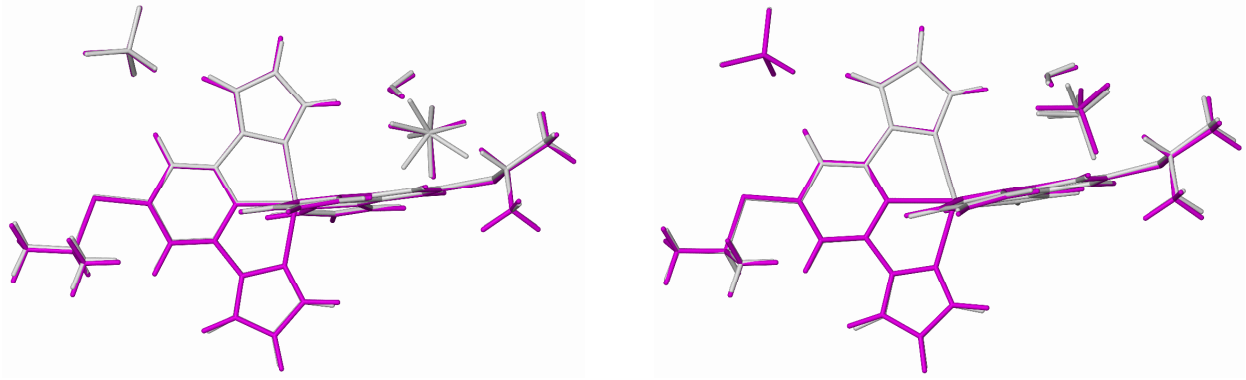
Figure S37 Overlaid isothermal experimental (white) and calculated (pink) asymmetric units of **1[BF$_4$]$_2$**·MeCN in each spin state. The anion disorder in the low-spin crystal structure is included in the figure.

1[BF$_4$]$_2$·MeNO$_2$ (phase 1, 100 K)



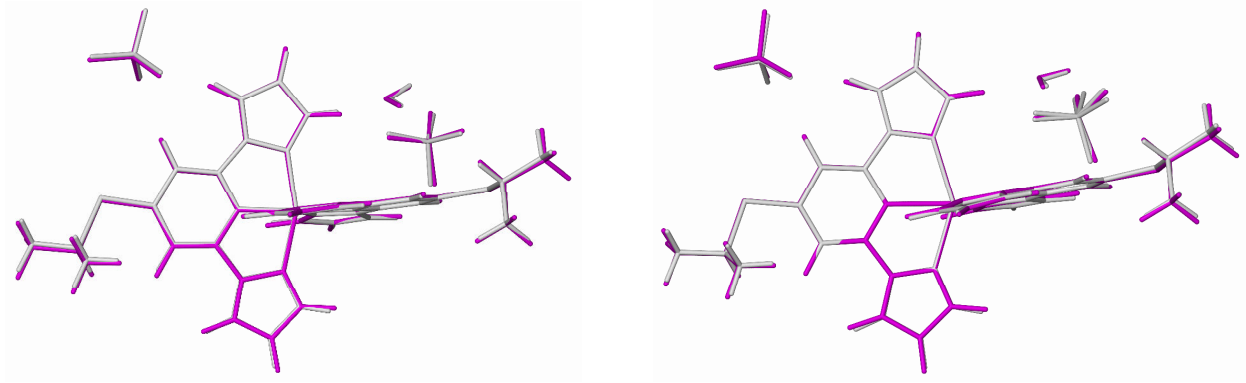
Low-spin

1[BF$_4$]$_2$·H$_2$O (20 K)



Low-spin High-spin

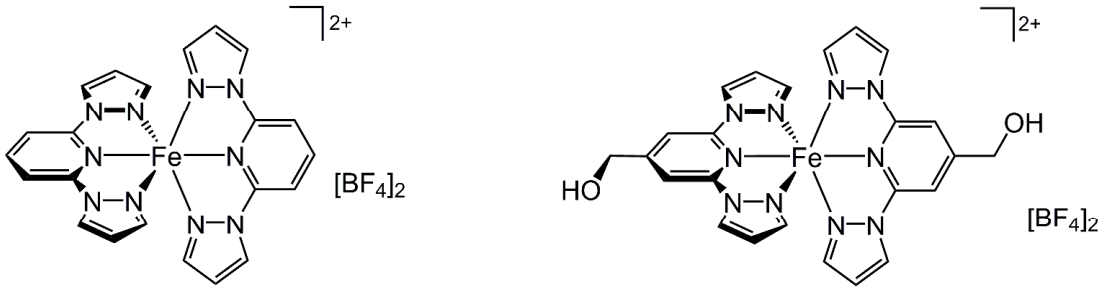
1[ClO$_4$]$_2$·H$_2$O (10 K)



Low-spin High-spin

Figure S38 Overlaid isothermal experimental (white) and calculated (purple) asymmetric units of the other **1X$_2$**·solv compounds in the computational study. Anion or solvent disorder in the experimental structures is included in the figure.

No isothermal high-spin structure of **1[BF$_4$]$_2$**·MeNO$_2$ is available, because of its phase 1→2→3 structural transformations at low temperature.



Scheme S3 Compounds **2** and **3** in the computational study. Both compounds have available crystallographic data in both spin states at 30 K.[21,22]

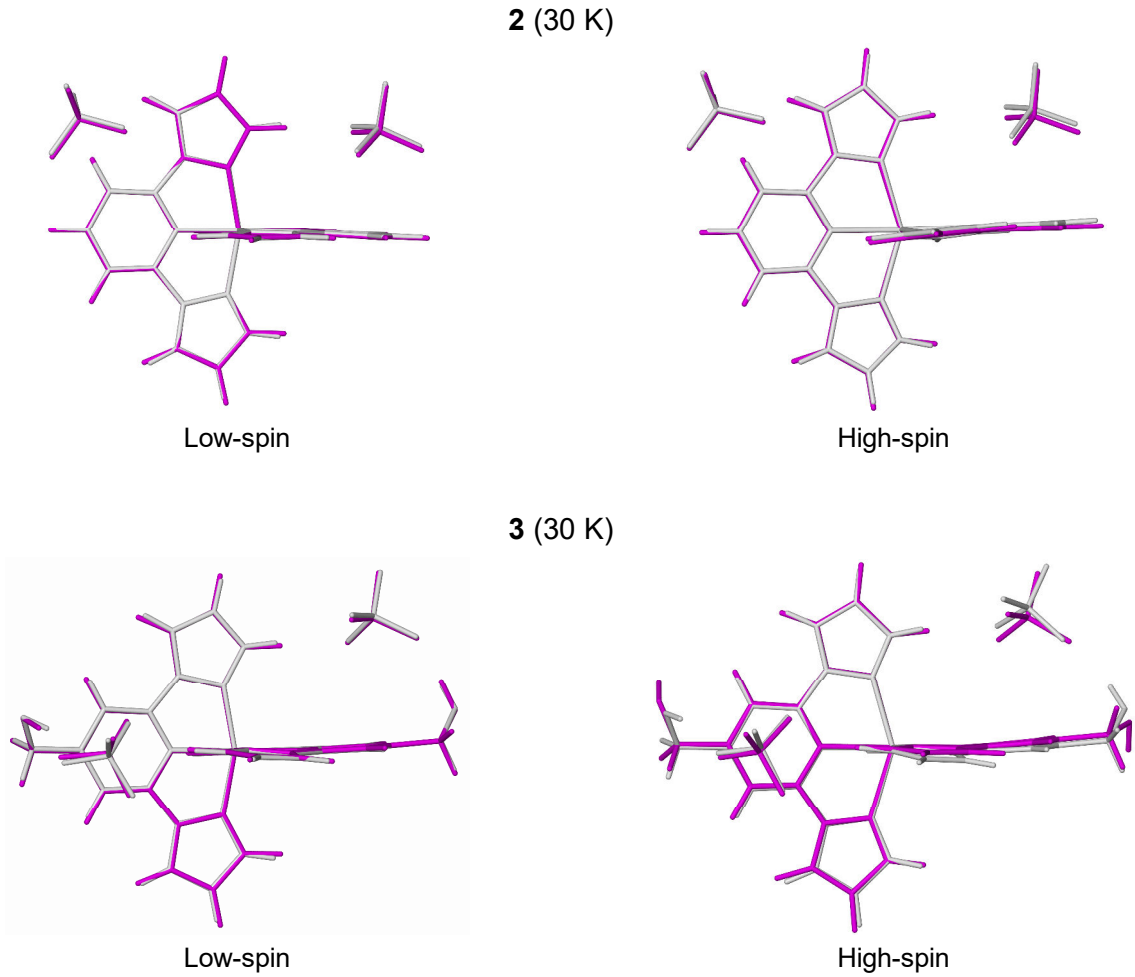


Figure S39 Overlaid isothermal experimental (white) and calculated (purple) asymmetric units of **2** and **3**. Anion or solvent disorder in the experimental structures is included in the figure. Experimental structures are from refs 21 and 22.

The high-spin minimised structure of **3** adopts an alternative conformation of the ligand hydroxymethyl groups, which places them close to different hydrogen-bond acceptor BF_4^- ions in the lattice. That conformational rearrangement doesn't occur experimentally at 30 K, but does manifest as disorder at higher temperatures (Figure S40).

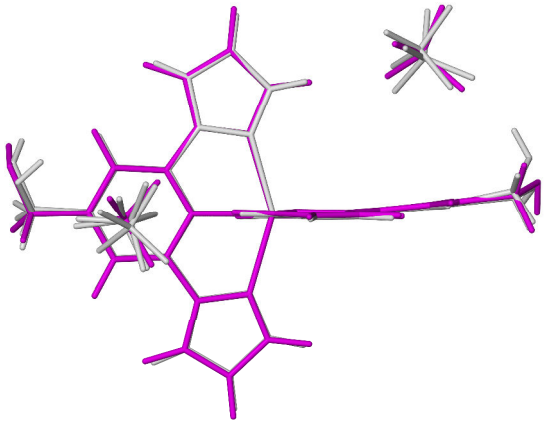


Figure S40 Overlay of the calculated high-spin structure of **3** (purple) and its experimental structure at 300 K (white).[22] Ligand and anion disorder in the experimental structure is included in the figure, which is the same view as in Figure S38.

The alternative hydroxymethyl group and anion orientations in the minimised high-spin structure do not occur experimentally at 30 K (Figure S39), but correspond to one of the disorder sites observed at room temperature.[22]

Table S16 Calculated molecular and intermolecular contributions to the SCO energy ΔH_{elec}, for the compounds in this work in kJmol^{-1} (SCO = cation, X = anion, solv = solvent). The sum of the one-body ($\Sigma\Delta H_i$) and two-body interaction terms ($\Sigma\Delta H_{i-j}$) is also given.

	1[BF$_4$]$_2$·MeNO$_2$ (phase 1)	**1[BF$_4$]$_2$**·MeCN	**1[BF$_4$]$_2$**·H$_2$O	**1[ClO$_4$]$_2$**·H$_2$O	**2**	**3**
ΔH_{SCO}	10.30	10.60	11.70	11.31	17.28	10.12
ΔH_X	–0.23	0.04	–0.05	–0.02	0.21	–0.61
ΔH_{solv}	–0.20	0.04	0.15	0.15	–	–
$\Sigma\Delta H_i$	9.86	10.68	11.80	11.44	17.49	9.51
$\Delta H_{SCO–SCO}$	4.11	9.70	4.89	−8.68	37.58	30.98
$\Delta H_{SCO–X}$	−1.06	−6.29	−4.43	8.19	−25.03	−18.32
$\Delta H_{SCO–solv}$	−0.24	−3.05	−3.99	−4.42	–	–
$\Delta H_{X–X}$	0.11	−2.15	−0.18	1.07	−12.27	−5.24
$\Delta H_{X–solv}$	0.94	−1.55	2.96	3.20	–	–
$\Delta H_{solv–solv}$	0.69	−0.55	−0.20	−0.20	–	–
$\Sigma\Delta H_{i-j}$	4.55	−3.90	−0.94	−0.85	0.27	7.42
Sum	14.41	6.78	10.86	10.59	17.76	16.93
ΔH_{elec}	11.57	8.68	15.48	10.82	18.14	14.92

These data are discussed on the following page.

Discussion of Table S16

The interaction energy terms contributing to ΔH_{elec} were deconvoluted, using the minimised high- and low-spin structures of each compound. Table S16 lists these as the energies of the cations ('SCO'), anions ('X') and solvent ('solv'), which contribute to the conformation and ligand field of the molecules in the crystal; and the intermolecular interaction energies between each of these components. The intermolecular terms include electrostatic, dispersion and Pauli interactions to the overall cohesion of the crystal. The sum of these energies should correspond to ΔH_{elec}. However, discrepancies between the two are often observed, which could reflect that only nearest neighbour intermolecular interactions are considered in the calculation. Errors in the computational treatment of the charged unit cells used to calculate the two body interactions, and truncation of the energy decomposition at the two-body term, might also contribute here.[23]

The individual energies of the cations, anions and solvent in the **1X₂**·solv series show little variation, as expected. This supports the conclusion that conformational differences in the $[FeL_2]^{2+}$ cation do not correlate simply with SCO in these crystals. Therefore, the much larger variations in ΔH_{elec} arise from the intermolecular interactions in the lattice. Within the intermolecular interaction terms, it is striking that $\Delta H_{SCO–SCO}$ and $\Delta H_{SCO–X}$ have opposite signs in **1[ClO₄]₂**·H_2O compared to the three **1[BF₄]₂**·solv materials. The larger ClO_4^- ions separate the cations more effectively, reducing the inter-cation repulsion in the more compact low-spin crystal and giving a more negative $\Delta H_{SCO–SCO}$. The more positive $\Delta H_{SCO–X}$ in the perchlorate salt may reflect the reduced electrostatic interactions to the more diffuse ClO_4^- ion, combined with more efficient packing of the ClO_4^- ions and the larger high-spin cations. These opposing $\Delta H_{SCO–SCO}$ and $\Delta H_{SCO–X}$ terms are similar in magnitude, however, so their contributions to ΔH_{elec} largely cancel. None-the-less, these observations reflect the observed trend for **1[ClO₄]₂**·solv to exhibit lower $T_{½}$ (and ΔH_{elec}) values than **1[BF₄]₂**·solv for a particular lattice solvent.[2] Consistent with that, the remaining intermolecular interactions in **1[BF₄]₂**·H_2O and **1[ClO₄]₂**·H_2O are very similar, as expected.

Two other trends in Table 3 can be noted for the **1X₂**·solv materials. First, is that $\Delta H_{SCO–solv}$ is consistently more negative for smaller solvent molecules. That does not correlate with the solvent polarity, since the polarities of $MeNO_2$ and MeCN are very similar.[24] Rather, it is presumably a packing effect, where smaller solvent molecules interact more favourably with the smaller low-spin cations. Second, $\Delta H_{X–solv}$ is largest, and very similar, for the hydrate crystals reflecting the hydrogen bonding between these residues in the inter-bilayer space.

The individual intermolecular interactions for **2** and **3** are much larger than for **1X₂**·solv, reflecting the closer packing of their cations and ions in the absence of lattice solvent. The lattice contraction associated with the high→low-spin conversion results in strongly unfavourable $\Delta H_{SCO–SCO}$ and favourable $\Delta H_{SCO–X}$. Both aspects are consistent with the electrostatic interactions between these moieties. None-the-less, comparison of the interaction energies in **1X₂**·solv, **2** and **3** highlights the effect of lattice solvent as an inert spacer between SCO centres in a crystal.

Table S17 Computed atomic coordinates for the energy-minimised unit cells of the compounds in this work.

1[BF_4]$_2$·$MeNO_2$ (phase 1), high-spin			
Fe	13.694139990	1.856947612	4.656337128
Fe	3.640729766	7.820673235	10.440064642
Fe	12.274002268	10.176110571	12.114303080
Fe	5.090108351	4.136280477	2.986780595
B	9.004758944	2.728580309	14.449006701
B	8.368426283	8.777740796	0.663051193
B	18.365788146	11.614075893	4.007819496
B	–0.970066830	5.565365663	11.071870291
B	10.239540998	9.420560799	7.052445359
B	7.104650595	3.359648075	8.046243509
B	16.973768268	11.734510870	11.031882762
B	0.383214773	5.700043584	4.046215817
C	12.856229501	4.221928706	6.924258952
C	4.463377569	10.254797087	8.246084430
C	11.647332475	4.759979956	7.420953229
C	5.662998520	10.790791173	7.723144250
C	10.646108954	4.027303239	6.808272474
C	6.676814907	10.064511493	8.321416012
C	10.698080100	2.143378637	5.140095041
C	6.650550787	8.188572631	10.000253817
C	9.347555441	1.850968041	5.121280199
C	8.005973365	7.908494285	10.016376396
C	8.912834835	0.834770300	4.237862209
C	8.452921511	6.894339241	10.892919138
C	9.850090756	0.166604400	3.423841376
C	7.522090756	6.216186298	11.706801127
C	11.182417859	0.544157771	3.550038388
C	6.188241202	6.583705115	11.582496795
C	12.203767123	–1.145780942	1.991878496
C	5.170080822	4.882378734	13.136478561
C	13.510439793	–1.551824013	1.808034352
C	3.863480906	4.466802534	13.311627457
C	14.289504429	–0.701590007	2.625115569
C	3.084194655	5.313510613	12.495055891
C	6.995731667	–1.033279367	3.278141312
C	10.375949920	5.023082498	11.830600714
C	7.568604137	–2.228701981	4.031263242
C	9.795863738	3.837353880	11.067368346
C	5.492895321	–1.180119700	3.033111058
C	11.879697243	4.869325638	12.065729757
C	13.364268668	–0.731662590	6.712041364
C	3.975796813	5.293024624	8.326348238
C	14.202330770	–1.421897535	7.617109152
C	3.118452012	4.605703761	7.437806952
C	15.390735537	–0.721316453	7.631573058
C	1.937693665	5.319284408	7.435496200
C	16.168606742	1.283649899	6.340125139
C	1.189809033	7.332760159	8.728284357
C	17.441613490	1.398303036	6.885814256
C	–0.087210447	7.451289097	8.198029353
C	18.301052788	2.364155947	6.336424537
C	–0.936439849	8.421029354	8.759678177
C	17.851838762	3.156809360	5.250863835

C	–0.473692678	9.212242741	9.840474634
C	16.558717732	2.947046807	4.810335195
C	0.823170542	8.999512646	10.269339952
C	16.549801032	4.489635936	2.812795889
C	0.836196968	10.527898839	12.271830687
C	15.562005102	4.810938637	1.894048897
C	1.821745459	10.841649717	13.192768292
C	14.419608246	4.088809689	2.297675489
C	2.967643126	10.125989423	12.780162414
C	–2.819960553	7.512102954	6.863917174
C	20.174558499	1.441271385	8.240522261
C	–4.045057678	7.986397356	6.083436835
C	21.401621669	1.904362666	9.025148523
C	20.346366509	0.029347689	7.679881003
C	–2.994726429	6.094648602	7.410396576
C	16.978323171	3.315157014	9.948488575
C	0.401853803	9.369469457	5.129990308
C	11.364628545	7.763141434	14.311106117
C	6.008548960	1.706890533	0.806149721
C	10.137989593	7.247967365	14.789055483
C	7.237126736	1.192120943	0.332371900
C	9.159058060	8.031987685	14.203183141
C	8.213595990	1.978194749	0.919533175
C	9.272463412	9.947849490	12.574610685
C	8.093670918	3.896883848	2.544537890
C	7.926940131	10.261816790	12.533777753
C	9.439939787	4.207381087	2.592221875
C	7.523359257	11.275758526	11.635999042
C	9.839982911	5.225456407	3.486715598
C	8.483235189	11.921134370	10.831251821
C	8.877222392	5.877403016	4.282238173
C	9.807923543	11.529107460	10.987510596
C	7.552759434	5.486000585	4.121998604
C	6.478596445	7.114863121	5.709494242
C	10.880084742	13.155796870	9.395787297
C	5.156005140	7.409359162	5.977730210
C	12.202620829	13.444710766	9.120922313
C	4.400902258	6.509838759	5.191096209
C	12.958124720	12.541388580	9.902570189
C	11.684957557	7.131474170	4.479742917
C	5.676874501	13.176467627	10.640495259
C	11.085955298	8.293680395	3.697006297
C	6.285722734	14.342556062	11.409698708
C	13.175955198	7.328073655	4.749598633
C	4.184534332	13.376390530	10.380081969
C	12.901392337	8.072045596	9.637638256
C	4.455639287	2.018669891	5.448594261
C	13.941988212	7.179971768	9.309422207
C	3.416227480	1.121142103	5.765564324
C	14.886467271	7.321706495	10.312799530
C	2.474224817	1.269945937	4.760846856
C	14.981183577	8.812885987	12.338530224
C	2.385290857	2.773389859	2.743252094
C	16.237760251	8.475886101	12.809452498
C	1.132081375	2.436249983	2.262940115
C	16.698815964	9.153094074	13.961984001

C	0.678514464	3.115420616	1.108393067
C	15.891455095	10.141264892	14.557492996
C	1.488622226	4.106094024	0.520923370
C	14.662270522	10.401779614	13.969230623
C	2.714446111	4.364809422	1.116466364
C	3.403786413	6.363594578	–0.248750243
C	13.986476492	12.404292507	15.334940225
C	4.494849337	7.206924257	–0.169185274
C	12.898423776	13.251710718	15.259160332
C	5.319390666	6.664463840	0.840189013
C	12.066466008	12.710662840	14.255081462
C	–1.211936893	3.813903483	–0.891268054
C	18.594343065	9.836549238	15.959673010
C	–2.435042617	3.271914366	–1.633262617
C	19.818183325	9.288775760	16.695614787
C	–1.450621700	5.239457395	–0.402757862
C	18.829718746	11.269568716	15.491611346
C	–0.682900656	1.798664173	11.749754306
C	18.038758512	7.854717821	3.360141053
F	8.043066167	3.720407562	14.070711001
F	9.328340014	9.770085852	1.043547256
F	8.630698729	8.387220814	–0.690712674
F	8.752539976	2.348704993	15.808428646
F	8.894686431	1.594007510	13.609255371
F	8.470608852	7.647339205	1.510914129
F	10.311016925	3.279483703	14.355983518
F	7.062470697	9.330880432	0.742332732
F	0.065182406	6.451217188	11.456825187
F	17.342729912	12.509028551	3.616039292
F	18.661966774	10.743655739	2.906448453
F	–1.266778984	4.699649536	12.176327609
F	–2.149922479	6.291773834	10.737946554
F	19.550261709	12.330105769	4.348476624
F	17.937462344	10.831577267	5.117515262
F	–0.555167297	4.778422842	9.960913606
F	11.536473138	8.843999058	6.983946874
F	5.816132018	2.765557521	8.119697971
F	9.986525508	9.835365672	8.401002570
F	7.345045250	3.778596021	6.695691543
F	10.159271763	10.540108506	6.188304864
F	7.173979638	4.480877903	8.908948502
F	9.266539114	8.439227892	6.682543829
F	8.093599855	2.392609301	8.410042540
F	17.839268667	11.096449090	11.968474129
F	–0.478433509	5.070077290	3.100604511
F	0.953206773	6.864462824	3.473128892
F	16.411224893	12.897249279	11.616280421
F	15.950239824	10.858677041	10.608921911
F	1.400887772	4.817757378	4.469422068
F	17.772731540	12.110181960	9.890364541
F	–0.421542603	6.071568912	5.186053441
H	13.881116195	4.481002892	7.176061793
H	3.433602668	10.515089807	8.016517611
H	11.511475256	5.563459717	8.138890961
H	5.783850402	11.591905927	7.000100035
H	9.562979910	4.074878932	6.882315967

H	7.758524972	10.115945436	8.231183781
H	8.647197696	2.363076204	5.781243830
H	8.699316888	8.431795974	9.357511710
H	9.561282910	–0.639342742	2.751388301
H	7.817352249	5.412279892	12.378895087
H	11.265799579	–1.521153848	1.592481585
H	6.108242044	4.513481818	13.541827215
H	13.865436179	–2.366223929	1.188967657
H	3.509485826	3.648701684	13.925989449
H	15.363703061	–0.684788345	2.787572955
H	2.010920244	5.326105226	12.327081684
H	7.504627182	–0.888406841	2.314215202
H	9.873726008	5.156426828	12.799622405
H	12.338994689	–0.951237677	6.425690058
H	5.002778370	5.066606360	8.600971252
H	13.958816677	–2.304720380	8.194792607
H	3.343288272	3.717842918	6.860425440
H	16.307190385	–0.868417286	8.190224572
H	1.014112976	5.180070554	6.887136065
H	17.731166771	0.758837659	7.713784855
H	–0.389570401	6.812046714	7.374804873
H	18.507041532	3.884094777	4.772112414
H	–1.123417469	9.940401527	10.325308889
H	17.601145062	4.762250798	2.879176220
H	–0.215265716	10.799218069	12.207150787
H	15.663615987	5.466418060	1.036426019
H	1.718755152	11.488425212	14.056937892
H	13.444294043	4.021450866	1.827286574
H	3.942807362	10.059474076	13.250601955
H	–1.935519039	7.560431302	6.212319674
H	19.290293025	1.484235706	8.892437953
H	12.384030131	7.478147064	14.561990177
H	4.990295796	1.420122609	0.552427688
H	7.402595884	0.368723356	–0.356074893
H	9.975173663	6.425514513	15.479176051
H	8.074532732	8.011896328	14.272600712
H	9.298332009	1.959707109	0.851781797
H	7.205996270	9.758452906	13.178103577
H	10.163753614	3.699745434	1.954248697
H	9.140909038	6.671855531	4.978161666
H	8.217181152	12.711239854	10.131291368
H	7.404439690	7.547364406	6.078320226
H	9.953986593	13.592154852	9.032288602
H	4.770722513	8.169288036	6.646887284
H	12.588894360	14.202104670	8.449874402
H	3.323338332	6.393958638	5.107743654
H	14.035596281	12.421172419	9.979906358
H	11.165817411	6.984299371	5.437815674
H	6.187939761	13.019687571	9.679548600
H	11.657738428	8.450357285	2.771665461
H	5.723431985	14.504385529	12.339813437
H	11.144522869	9.205269322	4.311864775
H	6.223049263	15.251004597	10.790599426
H	10.036663950	8.125030584	3.421132653
H	7.337179561	14.173628252	11.676917192
H	8.625017042	–2.094740866	4.298199627

H	8.740117039	3.979666657	10.801654875
H	7.477325158	–3.124864125	3.397982632
H	9.881473797	2.935192131	11.693229281
H	7.003680880	–2.389873619	4.960871320
H	10.359610181	3.680095052	10.136243976
H	13.595970127	6.486849971	5.321721624
H	3.757296448	12.531082599	9.819707015
H	13.300513682	8.246443921	5.340271568
H	4.058885350	14.289308883	9.781165604
H	13.744932291	7.442586758	3.813152212
H	3.623116713	13.501775995	11.319657313
H	4.938862153	–1.294505216	3.978501807
H	12.428582471	4.768297158	11.115685264
H	5.335982171	–2.083737225	2.427571805
H	12.038263534	3.956284249	12.656594390
H	5.081923783	–0.317787901	2.485786920
H	12.295298483	5.722501958	12.623927884
H	11.987417257	8.293505775	9.095250090
H	5.367104099	2.238285350	5.995964151
H	13.994853775	6.512590186	8.458011394
H	3.362664558	0.444565711	6.609785485
H	15.849316706	6.845938155	10.472209326
H	1.512870502	0.793472001	4.594611815
H	16.864786506	7.750292241	12.289096298
H	0.502818768	1.708492813	2.777603099
H	1.188809594	4.647446137	–0.369855031
H	16.196525951	10.681323482	15.447235790
H	2.539549468	6.366227474	–0.900814652
H	14.853437744	12.404492817	15.983212701
H	4.686941856	8.088108016	–0.770080912
H	12.712657298	14.133699898	15.860509116
H	6.283764356	7.015340850	1.199196316
H	11.101249474	13.064401069	13.900908206
H	–0.329992243	3.766162356	–1.547462094
H	17.711723074	9.777076908	16.614054489
H	–2.271073107	2.254571727	–2.013319372
H	19.656579615	8.266566175	17.063430307
H	–2.648565563	3.935407643	–2.485302057
H	20.028901219	9.942248531	17.555855004
H	–3.318855251	3.270033787	–0.977598291
H	20.702410989	9.297598035	16.040730177
H	–4.935039811	8.023191728	6.729261472
H	22.292360465	1.940208894	8.380026903
H	–4.251538470	7.275277211	5.269264960
H	21.603900105	1.187167161	9.835143053
H	–3.891558212	8.981127878	5.642036508
H	21.253054211	2.897263756	9.472406578
H	–2.384948724	5.288887357	0.171237289
H	19.765618732	11.330132550	14.921226341
H	–1.550594360	5.908822916	–1.272256463
H	18.924432887	11.926793161	16.370957409
H	–0.646319677	5.625859311	0.237441060
H	18.026209233	11.662031128	14.854066560
H	19.513361171	–0.261186899	7.024786069
H	–2.166924671	5.797902418	8.069344492
H	20.397272136	–0.689258277	8.514975757

H	–3.038832854	5.383981598	6.568063878
H	21.276012233	–0.035296989	7.094361691
H	–3.928550754	6.022862323	7.988091689
H	–0.487366841	0.835944420	11.258547275
H	17.838146734	6.898943151	3.862588671
H	–0.606455936	2.624294773	11.036374897
H	17.958254460	8.689062245	4.063101066
H	–1.648345813	1.755143800	12.261941754
H	19.007468342	7.804749275	2.855179368
H	17.285408468	2.266667324	9.952637230
H	0.082994200	8.325207155	5.168413070
H	17.070932118	3.795877528	10.926481093
H	0.313284105	9.809637697	4.132749579
H	17.543481580	3.895957448	9.207062844
H	–0.155611276	9.987586256	5.846293746
N	12.627513823	3.225989107	6.060528388
N	4.710736315	9.264116721	9.110165384
N	11.264223039	3.115382707	5.998011586
N	6.073772112	9.154373435	9.146789649
N	11.605715801	1.517354904	4.373164009
N	5.748824948	7.551938942	10.763941680
N	12.234937906	–0.102438253	2.876442247
N	5.139197860	5.924486614	12.254292717
N	13.522386200	0.185576477	3.260887277
N	3.854294995	6.205340990	11.866031383
N	13.992601997	0.328156474	6.198562765
N	3.366056635	6.362124818	8.844167131
N	15.239939192	0.324389642	6.764618040
N	2.109376144	6.366223519	8.295683653
N	15.711198663	2.060226727	5.351681398
N	1.658931731	8.109723528	9.712034577
N	15.985901823	3.628605114	3.708696390
N	1.404217563	9.673865534	11.367978198
N	14.675913458	3.369682184	3.396785441
N	2.717824479	9.415835661	11.675190779
N	15.546955413	3.370444433	9.532065853
N	1.833971556	9.426808154	5.542932126
N	11.163043667	8.795717783	13.483606158
N	6.206644903	2.741119641	1.632624401
N	9.804962583	8.952255572	13.425388462
N	7.564449468	2.898868615	1.694570656
N	10.204849353	10.561960524	11.829189105
N	7.158420755	4.516358422	3.281876182
N	10.878127100	12.133648600	10.303691160
N	6.481070703	6.093827499	4.800295214
N	12.158671443	11.742304604	10.613942732
N	5.200598989	5.707593057	4.483148190
N	13.176519244	8.725300627	10.770898623
N	4.182216307	2.681877770	4.320561750
N	14.398934332	8.252460062	11.180072935
N	2.961821022	2.209825849	3.903375895
N	14.194616846	9.739142117	12.905871138
N	3.174907879	3.701115287	2.182409583
N	13.788667767	11.420128737	14.408938362
N	3.593035597	5.380397486	0.680329756
N	12.604995114	11.602739176	13.737072468

N	4.774266924	5.559332672	1.357337979
N	0.393394217	1.980385421	12.771011029
N	16.969246609	8.025256397	2.330073337
O	15.121010641	2.475772152	8.790377187
O	2.252498830	8.554446904	6.315578627
O	14.866220297	4.334810173	9.916526257
O	2.522627655	10.370852045	5.125193372
O	0.160057394	1.594580216	13.928478311
O	17.218913920	7.650850385	1.172073659
O	1.468701798	2.470977290	12.402358137
O	15.882844451	8.495524081	2.692625345
S	7.204666298	0.515451715	4.245089773
S	10.165374339	6.585574411	10.886222919
S	–2.552380474	8.739502727	8.205685593
S	19.912461867	2.681987770	6.911651191
S	5.818243932	11.614918361	11.595605790
S	11.545445804	5.562849605	3.535365962
S	–0.887068706	2.656235604	0.502391150
S	18.272182265	8.697780823	14.550083324

1[BF_4]$_2$·$MeNO_2$ (phase 1), high-spin			
Fe	4.171764868	7.428967422	6.565213644
Fe	2.740346713	10.856130130	14.041530665
Fe	12.559561450	4.761503052	8.577330535
Fe	13.991202909	1.334344600	1.100879633
B	–0.565362969	9.054365095	7.654913467
B	0.866620601	9.230414893	0.176740651
B	17.296681387	3.135977091	7.487979853
B	15.864399907	2.962198138	14.966069790
B	7.741330975	–0.381446745	4.297379632
B	6.309305544	6.477036665	11.773566127
B	10.421939244	5.712995389	3.368779314
B	8.990320992	12.571299208	10.845189660
C	4.743610253	9.743356937	4.556775226
C	3.310968891	8.540578969	12.033996590
C	11.987503938	2.447084708	10.585576464
C	13.420452175	3.649529889	3.108766274
C	3.980092698	10.365232385	3.546322160
C	2.546620115	7.918060522	11.024557988
C	12.750958715	1.825169465	11.596046808
C	14.184632180	4.271959256	4.118379584
C	2.779996096	9.686390229	3.499138193
C	1.346820974	8.597424586	10.977346976
C	13.951000139	2.504096125	11.643434392
C	15.384541996	3.592782674	4.165520594
C	1.905196548	7.782148006	4.913524996
C	0.473568588	10.503284742	12.390383401
C	14.825870109	4.408434486	10.229199629
C	16.258192040	1.687356915	2.752101333
C	0.652231647	7.546331291	4.374484379
C	–0.779293992	10.739545559	11.851362717
C	16.078799757	4.644265697	10.768281362
C	17.511146969	1.451265445	3.291044161
C	–0.125169710	6.529361957	4.964653864
C	–1.556010625	11.757328095	12.440990632

C	16.856232505	5.661236493	10.178153307
C	18.288173138	0.433912344	2.701066192
C	17.782775073	–0.284282485	1.593557224
C	0.379895852	5.811167077	6.072295996
C	16.351220005	6.379428862	9.070479747
C	–1.050514651	12.475682285	13.548347365
C	1.635165599	6.155089024	6.535403451
C	0.204533016	12.131191108	14.011601799
C	15.095991707	6.035489365	8.607287715
C	16.527571773	0.059960995	1.130499053
C	16.259321486	–1.374042714	–0.930905080
C	1.902932693	4.720946986	8.596759288
C	14.828219828	7.469552707	6.545839446
C	0.472822433	13.565154528	16.073008951
C	15.206356618	–1.493421999	–1.817789121
C	2.955781828	4.601343252	9.483746203
C	13.775403098	7.589001962	5.658786572
C	1.525576130	13.684059414	16.960204635
C	14.186583243	–0.647380141	–1.326721933
C	3.975753816	5.447262065	8.992851927
C	12.755474769	6.743037713	6.149684944
C	2.545209991	12.837732840	16.469317440
C	–2.020462130	7.123810644	2.942631885
C	–3.452040912	11.162363856	10.419791197
C	18.750994809	5.067142484	12.200670980
C	20.183459921	1.027808074	4.723213580
C	–3.160949501	6.471776803	2.161790261
C	–4.592383384	11.814150665	9.638499038
C	19.891134851	5.719384353	12.981847185
C	21.323527415	0.375433804	5.504405929
C	–2.369870537	8.549026651	3.360285912
C	–3.802123344	9.737858517	10.839338474
C	19.100573545	3.641849521	11.783434294
C	20.533458147	2.452830676	4.305417444
C	15.049550551	3.646625901	–0.760978386
C	3.113137157	9.740101258	8.428329123
C	13.618175551	2.450189468	6.714414714
C	1.681976105	8.543962212	15.903340025
C	14.418352533	4.580786728	–1.614934268
C	3.744250908	10.673948485	9.282690259
C	12.987086138	1.516247521	5.860139730
C	2.313081531	7.609643708	16.757187191
C	13.071407231	4.282384532	–1.572529520
C	5.091340030	10.376281063	9.239451954
C	11.640010916	1.813983302	5.903238746
C	3.660057337	7.907921692	16.714828481
C	11.797341828	2.603708631	–0.183099303
C	6.365577909	8.698519248	7.849020218
C	10.365714114	3.491921042	7.293378748
C	4.934278327	9.586569938	15.325478014
C	10.477223578	2.968061623	–0.410231056
C	7.685665373	9.063055821	8.076012617
C	9.045637313	3.127339317	7.066308992
C	6.254361044	9.222032320	15.552550924
C	8.677111284	8.371062774	7.349104129
C	7.245823382	9.913912867	14.825561369

C	8.054110976	3.819382096	7.793068216
C	9.485800615	2.276048244	0.316691323
C	8.306368181	7.348118514	6.445570601
C	6.875132230	10.936805282	13.921955090
C	8.424802103	4.842412747	8.696541108
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1[BF_4]$_2$·MeCN, high-spin			
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1[BF_4]$_2$·MeCN, low-spin

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C	32.352767598	36.141006413	41.688714045
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C	45.271682019	25.857624511	39.916565851
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C	3.322037431	–4.440416383	–2.933146816
C	–3.383856089	–1.100754838	–8.428579710
C	4.995402058	–7.117666619	1.267235113
C	–4.995402058	7.117666619	–1.267235113
C	3.383856089	1.100754838	8.428579710
C	–2.285587779	–1.937740622	–8.713167775
C	3.896822801	–7.954329967	1.551480847
C	–3.896822801	7.954329967	–1.551480847
C	2.285587779	1.937740622	8.713167775
C	–1.325445406	–1.621211008	–7.769986924
C	2.937234957	–7.637860532	0.607724748
C	–2.937234957	7.637860532	–0.607724748

C	1.325445406	1.621211008	7.769986924
C	–4.443152332	3.706900129	–3.946701948
C	–6.056749905	2.309140879	3.213418156
C	4.443152332	–3.706900129	3.946701948
C	6.056749905	–2.309140879	–3.213418156
C	–3.621918168	4.341446819	–2.991761664
C	–5.235890899	1.674335323	4.168517954
C	3.621918168	–4.341446819	2.991761664
C	5.235890899	–1.674335323	–4.168517954
C	–2.484100053	3.565178381	–2.908901748
C	–4.097938631	2.450356652	4.251783786
C	2.484100053	–3.565178381	2.908901748
C	4.097938631	–2.450356652	–4.251783786
C	2.281265278	1.066590029	–2.193463004
C	0.666602117	4.946960512	4.969058565
C	–2.281265278	–1.066590029	2.193463004
C	–0.666602117	–4.946960512	–4.969058565
C	2.638822908	2.506375794	–2.547126446
C	1.024034947	3.507351146	4.614548707
C	–2.638822908	–2.506375794	2.547126446
C	–1.024034947	–3.507351146	–4.614548707
C	3.408482244	0.363616764	–1.435136934
C	1.793069166	5.649363687	5.728969303
C	–3.408482244	–0.363616764	1.435136934
C	–1.793069166	–5.649363687	–5.728969303
Cl	–0.837300085	2.484883272	0.240266502
Cl	0.776804703	3.528146786	–6.920920288
Cl	0.837300085	–2.484883272	–0.240266502
Cl	–0.776804703	–3.528146786	6.920920288
Cl	–7.681737489	5.699929079	–4.098058637
Cl	–9.293740029	0.313876887	3.063037028
Cl	7.681737489	–5.699929079	4.098058637
Cl	9.293740029	–0.313876887	–3.063037028
H	–8.179263676	3.526591639	–8.244576557
H	–9.792444436	2.489386164	–1.082372157
H	9.792444436	–2.489386164	1.082372157
H	8.179263676	–3.526591639	8.244576557
H	–9.174652274	0.460704426	–5.317921890
H	–10.787056857	5.555576473	1.844256533
H	9.174652274	–0.460704426	5.317921890
H	10.787056857	–5.555576473	–1.844256533
H	–2.361096240	3.656914757	–7.957884989
H	–3.974140800	2.359042898	–0.796715123
H	3.974140800	–2.359042898	0.796715123
H	2.361096240	–3.656914757	7.957884989
H	–3.834557323	5.444886870	–9.471357841
H	–5.447998934	0.570043828	–2.308660644
H	5.447998934	–0.570043828	2.308660644
H	3.834557323	–5.444886870	9.471357841
H	–6.437232997	4.610259144	–9.127747820
H	–8.050582293	1.404765491	–1.964772862
H	8.050582293	–1.404765491	1.964772862
H	6.437232997	–4.610259144	9.127747820
H	5.568053291	–7.479315336	–3.563669058
H	–3.955974123	–1.463087974	–3.597491270
H	3.955974123	1.463087974	3.597491270

H	–5.568053291	7.479315336	3.563669058
H	7.959941202	–8.705383231	–4.309274686
H	–6.348018964	–2.689100119	–2.852220416
H	6.348018964	2.689100119	2.852220416
H	–7.959941202	8.705383231	4.309274686
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H	–8.267114252	–1.215519594	–4.166326576
H	8.267114252	1.215519594	4.166326576
H	–9.879295641	7.231826860	2.995538216
H	–10.245695192	3.718690507	–8.808850398
H	–11.859594664	2.297884574	–1.646534435
H	11.859594664	–2.297884574	1.646534435
H	10.245695192	–3.718690507	8.808850398
H	0.976795460	–6.947421978	–1.251516554
H	0.636181196	–0.930273726	–5.912093382
H	–0.636181196	0.930273726	5.912093382
H	–0.976795460	6.947421978	1.251516554
H	–0.163888905	1.984022751	–2.776443896
H	–1.777270108	4.030262398	4.384441708
H	0.163888905	–1.984022751	2.776443896
H	1.777270108	–4.030262398	–4.384441708
H	–4.325511831	–0.998498272	–8.958478990
H	5.936826439	–7.015475271	1.797587459
H	–5.936826439	7.015475271	–1.797587459
H	4.325511831	0.998498272	8.958478990
H	–2.191264730	–2.687800835	–9.489076264
H	3.801905768	–8.704242881	2.327450709
H	–3.801905768	8.704242881	–2.327450709
H	2.191264730	2.687800835	9.489076264
H	–0.324733980	–2.010881329	–7.600648597
H	1.936590273	–8.027458230	0.437874914
H	–1.936590273	8.027458230	–0.437874914
H	0.324733980	2.010881329	7.600648597
H	–5.431782155	3.985750191	–4.302165641
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H	–3.838443815	5.243547766	–2.433935402
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H	3.838443815	–5.243547766	2.433935402
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H	–1.586424104	3.659203449	–2.308128077
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H	1.586424104	–3.659203449	2.308128077
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H	1.356000975	1.015370589	–1.598654508
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H	–1.356000975	–1.015370589	1.598654508
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H	–10.426759638	5.930032155	–7.651883672
H	–12.039749527	0.086368073	–0.490278142
H	12.039749527	–0.086368073	0.490278142
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H	–9.226912688	4.930328852	–6.792926108
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H	9.226912688	–4.930328852	6.792926108

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H	–10.862978878	5.106847331	–6.126527664
H	–12.475850273	0.908793495	1.035527005
H	10.862978878	–5.106847331	6.126527664
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H	–12.870538602	4.048608832	–7.231803505
H	–14.483540933	1.967243785	–0.068149039
H	14.483540933	–1.967243785	0.068149039
H	12.870538602	–4.048608832	7.231803505
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H	–14.283523595	2.934775299	–1.558792522
H	14.283523595	–2.934775299	1.558792522
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H	–12.433489157	4.850066987	–8.763314024
H	–14.047330214	1.166718091	–1.600367636
H	14.047330214	–1.166718091	1.600367636
H	12.433489157	–4.850066987	8.763314024
H	2.815915400	3.066628254	–1.617627721
H	1.199846122	2.946161275	5.543713030
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H	1.845941816	3.009952207	–3.115977595
H	0.231559596	3.004554100	4.044424697
H	–1.845941816	–3.009952207	3.115977595
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H	3.560436311	2.532430011	–3.149087855
H	1.946266926	3.481426955	4.013535969
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H	–1.946266926	–3.481426955	–4.013535969
H	4.332632917	0.346635353	–2.032671265
H	2.717596031	5.667499363	5.132054787
H	–4.332632917	–0.346635353	2.032671265
H	–2.717596031	–5.667499363	–5.132054787
H	–1.520001781	–6.680041637	–5.991903542
H	3.136156063	–0.667495255	–1.173170053
H	–3.136156063	0.667495255	1.173170053
H	1.520001781	6.680041637	5.991903542
H	3.604837284	0.918387318	–0.504892085
H	1.989038352	5.093649354	6.658726942
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H	1.462559483	1.538519439	1.840889246
H	3.075362611	4.474654939	–5.320700155
H	–1.462559483	–1.538519439	–1.840889246
H	–3.075362611	–4.474654939	5.320700155
H	2.125730016	0.209891844	1.466074038
H	3.736485430	5.804245063	–5.695966687
H	–2.125730016	–0.209891844	–1.466074038
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N	–6.159538376	1.475848637	–6.464000229
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N	7.772280187	–4.540210866	–0.697644280
N	–5.497908066	3.123952778	–7.904646746
N	–7.110952916	2.891912184	–0.742902708
N	7.110952916	–2.891912184	0.742902708

N	5.497908066	–3.123952778	7.904646746
N	–4.219823253	2.801492283	–7.527778572
N	–5.832753892	3.214725394	–0.366656886
N	5.832753892	–3.214725394	0.366656886
N	4.219823253	–2.801492283	7.527778572
N	8.163671668	–6.184906177	–2.256965646
N	–6.551324814	–0.168656134	–4.904629087
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N	–8.163671668	6.184906177	2.256965646
N	6.808039649	–6.256541306	–2.395911972
N	–5.195728371	–0.240310732	–4.765441403
N	5.195728371	0.240310732	4.765441403
N	–6.808039649	6.256541306	2.395911972
N	–2.149524347	0.870585512	–5.278083666
N	–3.762476592	5.145724136	1.883450574
N	2.149524347	–0.870585512	5.278083666
N	3.762476592	–5.145724136	–1.883450574
N	3.470873285	–6.662866769	–0.184040243
N	–1.858502391	–0.645905801	–6.978198649
N	1.858502391	0.645905801	6.978198649
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N	–3.128196468	–0.316067059	–7.374962250
N	4.740428559	–6.333172596	0.213289568
N	–4.740428559	6.333172596	–0.213289568
N	3.128196468	0.316067059	7.374962250
N	–2.644370210	2.531542270	–3.785632934
N	–4.257777913	3.484093872	3.375053062
N	2.644370210	–2.531542270	3.785632934
N	4.257777913	–3.484093872	–3.375053062
N	–3.851506703	2.612777426	–4.430342769
N	–5.464742323	3.403175783	2.730040443
N	3.851506703	–2.612777426	4.430342769
N	5.464742323	–3.403175783	–2.730040443
O	6.415212992	–6.431939409	3.982060707
O	–8.027012744	–0.418125512	3.176780849
O	8.027012744	0.418125512	–3.176780849
O	–6.415212992	6.431939409	–3.982060707
O	8.737798231	–6.618718158	4.553427491
O	–10.350345837	–0.604540968	2.608171594
O	10.350345837	0.604540968	–2.608171594
O	–8.737798231	6.618718158	–4.553427491
O	–8.056549142	5.151781441	–2.781536833
O	–9.666867057	0.860787439	4.380560771
O	8.056549142	–5.151781441	2.781536833
O	9.666867057	–0.860787439	–4.380560771
O	–7.526999092	4.597458687	–5.052658467
O	–9.140338458	1.417255431	2.109244388
O	7.526999092	–4.597458687	5.052658467
O	9.140338458	–1.417255431	–2.109244388
O	2.309260512	1.045398437	1.941524200
O	3.921375757	4.969070389	–5.220487321
O	–2.309260512	–1.045398437	–1.941524200
O	–3.921375757	–4.969070389	5.220487321
O	–0.158751653	2.462436700	1.543245442
O	1.456186807	3.547861395	–5.618284291
O	0.158751653	–2.462436700	–1.543245442

O	–1.456186807	–3.547861395	5.618284291
O	1.600086232	2.754405356	–7.877272100
O	–0.011309229	3.256695088	–0.715319562
O	0.011309229	–3.256695088	0.715319562
O	–1.600086232	–2.754405356	7.877272100
O	–2.145653912	3.123210244	0.382645822
O	–0.533320385	2.893577369	–6.778146281
O	2.145653912	–3.123210244	–0.382645822
O	0.533320385	–2.893577369	6.778146281
O	0.621095961	4.891368204	–7.434079700
O	–0.996728709	1.122388042	–0.273723724
O	0.996728709	–1.122388042	0.273723724
O	–0.621095961	–4.891368204	7.434079700
S	–10.585027410	2.258867256	–6.923835972
S	–12.197893229	3.757378566	0.238878636
S	10.585027410	–2.258867256	6.923835972
S	12.197893229	–3.757378566	–0.238878636
S	1.995986779	0.065253415	–3.702695180
S	0.382786933	5.949458362	3.460281827
S	–1.995986779	–0.065253415	3.702695180
S	–0.382786933	–5.949458362	–3.460281827

1[ClO$_4$]$_2$·H$_2$O, low-spin			
Fe	–3.835899714	1.354980199	–6.003198644
Fe	–5.658512794	4.664228060	1.354643987
Fe	3.835899714	–1.354980199	6.003198644
Fe	5.658512794	–4.664228060	–1.354643987
C	–5.981065322	2.590776930	–7.401770742
C	–7.805663173	3.430379850	–0.042491862
C	7.805663173	–3.430379850	0.042491862
C	5.981065322	–2.590776930	7.401770742
C	–7.295180956	2.908693794	–7.721506734
C	–9.120146092	3.113860089	–0.361857394
C	9.120146092	–3.113860089	0.361857394
C	7.295180956	–2.908693794	7.721506734
C	–8.307009176	2.179336922	–7.064765338
C	–10.130980443	3.843617344	0.295830847
C	8.307009176	–2.179336922	7.064765338
C	10.130980443	–3.843617344	–0.295830847
C	–7.966128901	1.170033044	–6.135785941
C	–9.788761466	4.852756376	1.224543486
C	7.966128901	–1.170033044	6.135785941
C	9.788761466	–4.852756376	–1.224543486
C	–6.626759558	0.946312807	–5.901069110
C	–8.449010092	5.075303489	1.458601859
C	6.626759558	–0.946312807	5.901069110
C	8.449010092	–5.075303489	–1.458601859
C	–2.702869011	3.605122252	–7.876665244
C	–4.528902421	2.414372060	–0.522760811
C	4.528902421	–2.414372060	0.522760811
C	2.702869011	–3.605122252	7.876665244
C	–3.291423298	4.536720909	–8.760308657
C	–5.119235303	1.485681434	–1.408291307
C	5.119235303	–1.485681434	1.408291307
C	3.291423298	–4.536720909	8.760308657

C	–4.644755860	4.264422511	–8.749300662
C	–6.472301921	1.758861049	–1.394866150
C	6.472301921	–1.758861049	1.394866150
C	4.644755860	–4.264422511	8.749300662
C	6.285170888	–6.916717064	–3.448664670
C	–4.466332416	–0.895001624	–3.907108599
C	4.466332416	0.895001624	3.907108599
C	–6.285170888	6.916717064	3.448664670
C	7.485712260	–7.508933929	–3.907018414
C	–5.667962284	–1.484602022	–3.448200449
C	5.667962284	1.484602022	3.448200449
C	–7.485712260	7.508933929	3.907018414
C	8.505190347	–6.896591149	–3.204171992
C	–6.686241299	–0.872031378	–4.152616672
C	6.686241299	0.872031378	4.152616672
C	–8.505190347	6.896591149	3.204171992
C	–10.198681023	3.946319422	–8.262694129
C	–12.022548210	2.076990062	–0.901980924
C	12.022548210	–2.076990062	0.901980924
C	10.198681023	–3.946319422	8.262694129
C	–9.827714628	5.157268073	–7.416466333
C	–11.649034371	0.865815949	–0.057225008
C	11.649034371	–0.865815949	0.057225008
C	9.827714628	–5.157268073	7.416466333
C	–11.659478872	3.992791386	–8.708395219
C	–13.483970035	2.029227965	–1.345335606
C	13.483970035	–2.029227965	1.345335606
C	11.659478872	–3.992791386	8.708395219
C	–1.305802348	0.085432626	–5.921548247
C	–3.129599640	5.936100567	1.431901242
C	1.305802348	–0.085432626	5.921548247
C	3.129599640	–5.936100567	–1.431901242
C	1.886421696	–6.283393859	–1.910029888
C	–0.062055906	–0.258801886	–5.442586194
C	0.062055906	0.258801886	5.442586194
C	–1.886421696	6.283393859	1.910029888
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