Supporting Information

Effect of Intermolecular Anionic Interactions on Spin Crossover of Two Triple-Stranded Dinuclear Fe(II) Complexes Showing Above Room Temperature Spin Transition

S. Athira‡, Dibya Jyoti Mondal‡, Shraoshee Shome, Bijoy Dey, and Sanjit Konar *[a]

[a]Department of Chemistry
Indian Institute of Science Education and Research Bhopal
Bhopal By-pass Road, Bhauri, Madhya Pradesh, India-462066
E-mail: skonar@iiserb.ac.in

‡ These authors contributed equally to this work.

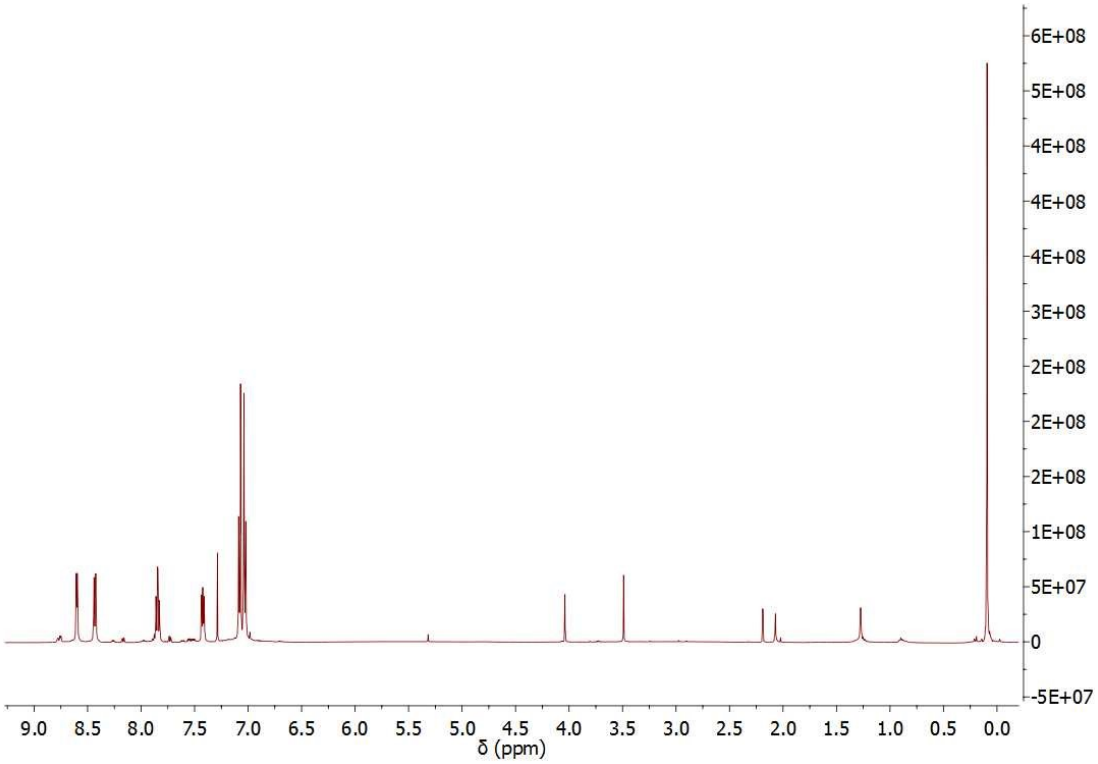

Figure S1.[1]H-NMR spectrum of Ligand (L).

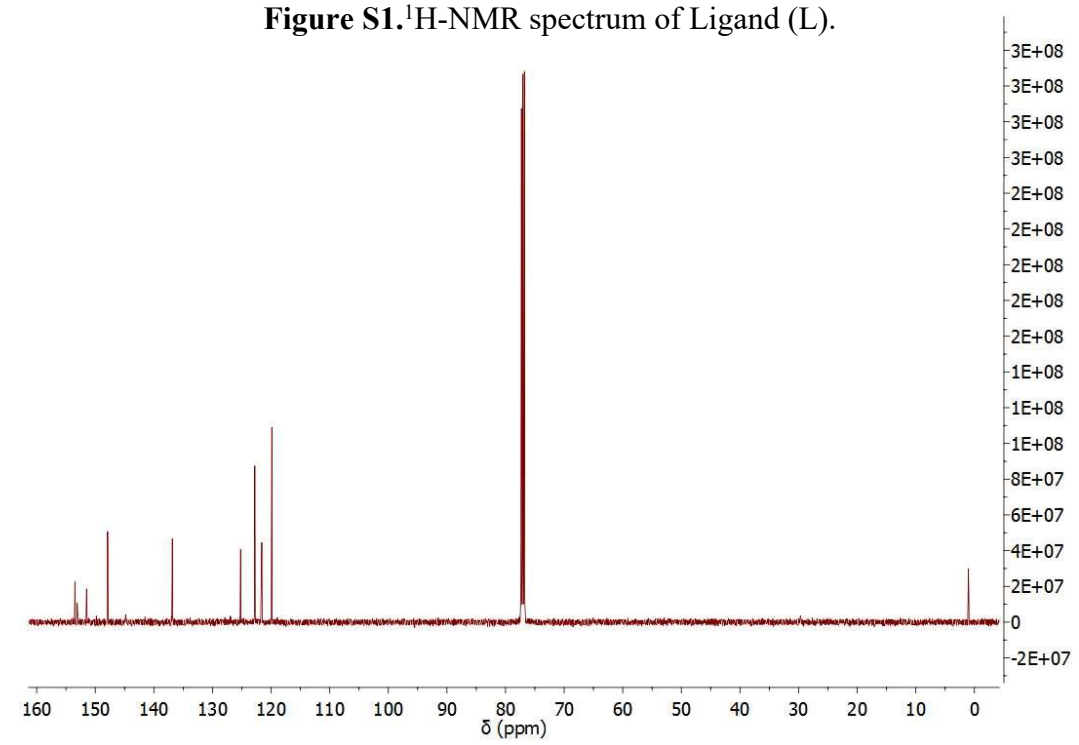

Figure S2. [13]C NMR spectrum of Ligand (L).

Table S1. Crystallographic data for complex **1** and **2.**

	Complex **1 (LS-LS) (CCDC No. 2182188)**	Complex **1** (HS-LS) **(CCDC No. 2205321)**	Complex **2** **(CCDC No. 2182187)**
Empirical formula	C77H77Fe2N18O22.5F12S4	C77H77Fe2N18O22.5F12S4	C73.35H79.4Fe2N18O27.35Cl4
Formula weight	2082.32	1891.29	1904.21
Temperature/K	120.0	294.00	100.0
Crystal system	monoclinic	monoclinic	monoclinic
Space group	*C2/c*	*C2/c*	$P2_1/c$
a/Å	33.680(3)	34.197(2)	15.2707(4)
b/Å	14.0309(12)	14.3395(9)	22.8316(6)
c/Å	39.333(4)	39.517(3)	23.0331(6)
α/°	90	90	90
β/°	109.649(2)	109.422(2)	95.936(2)
γ/°	90	90	90
Volume/Å^3	17505(3)	18275(2)	7963.4(5)
Z	4	8	4
ρ_{calc}g/cm^3	1.534	1.375	1.554
μ/mm^{-1}	0.533	0.477	0.592
F(000)	8240.0	7728.0	3816.0
Crystal size/mm^3	0.45 × 0.36 × 0.3	0.45 × 0.36 × 0.3	0.45 × 0.38 × 0.33
Radiation	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.398 to 49.602	3.85 to 49.566	4.596 to 52.84
Index ranges	-39 ≤ h ≤ 39, -16 ≤ k ≤ 16, -44 ≤ l ≤ 46	-36 ≤ h ≤ 40, -16 ≤ k ≤ 16, -46 ≤ l ≤ 46	-19 ≤ h ≤ 18, -28 ≤ k ≤ 28, -28 ≤ l ≤ 28
Reflections collected	135555	88841	88182
Independent reflections	15061 [R_{int} = 0.1227, R_{sigma} = 0.0787]	15552 [R_{int} = 0.0909, R_{sigma} = 0.0682]	16295 [R_{int} = 0.1172, R_{sigma} = 0.0940]
Data/restraints/parameters	15061/0/1192	15552/751/1350	16295/0/1145
Goodness-of-fit on F^2	1.034	1.239	1.011
Final R indexes [I>=2σ (I)]	R_1 = 0.1249, wR_2 = 0.3418	R_1 = 0.1025, wR_2 = 0.2996	R_1 = 0.1230, wR_2 = 0.3124
Final R indexes [all data]	R_1 = 0.1886, wR_2 = 0.3866	R_1 = 0.1522, wR_2 = 0.3457	R_1 = 0.1880, wR_2 = 0.3607
Largest diff. peak/hole / e Å^{-3}	2.52/-1.51	1.84/-0.52	5.33/-2.17

$R_1 = \Sigma||F_o| - |F_c||/ \Sigma F_o$, $R_2 = [\Sigma\{w(F_o^2 - Fc^2)^2\}/\Sigma\{w(F_o^2)^2\}]^{1/2}$

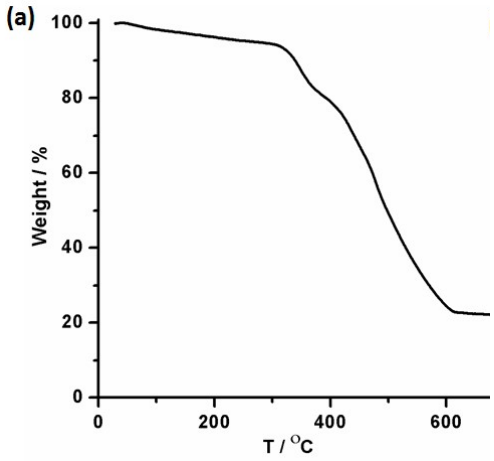

Figure S3. TGA diagram for complex **1.**

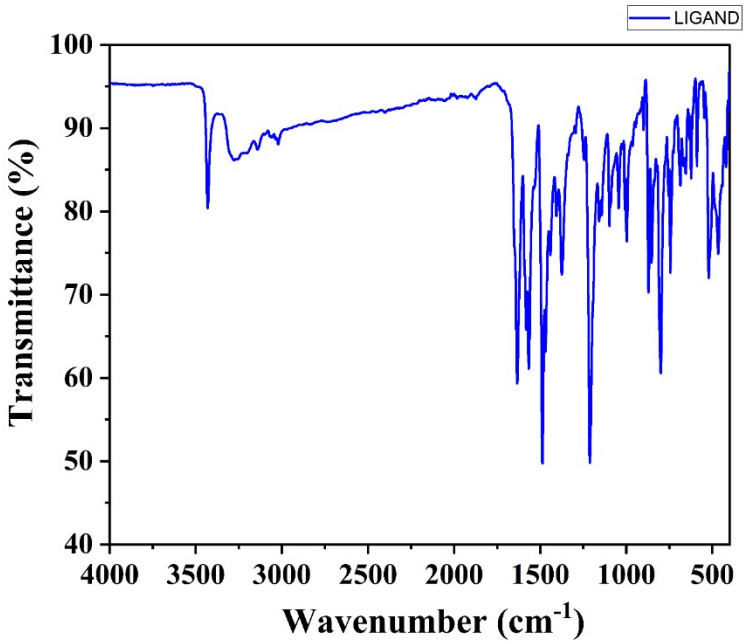

Figure S4. FT-IR spectrum of Ligand.

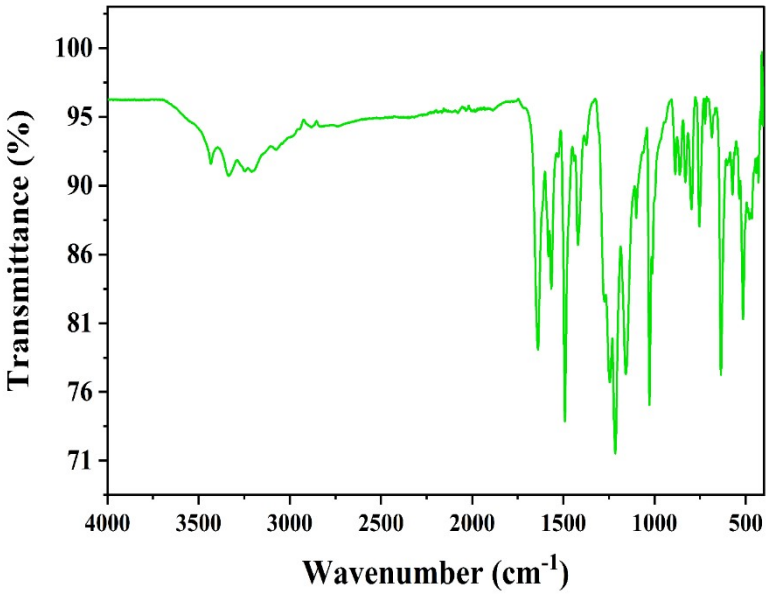

Figure S5. FT-IR spectrum of Complex **1.**

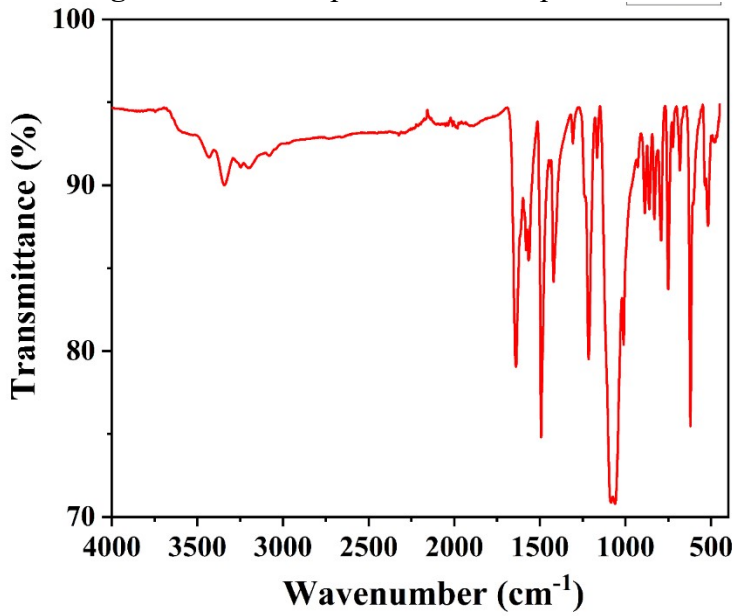

Figure S6. FT-IR spectrum of Complex **2.**

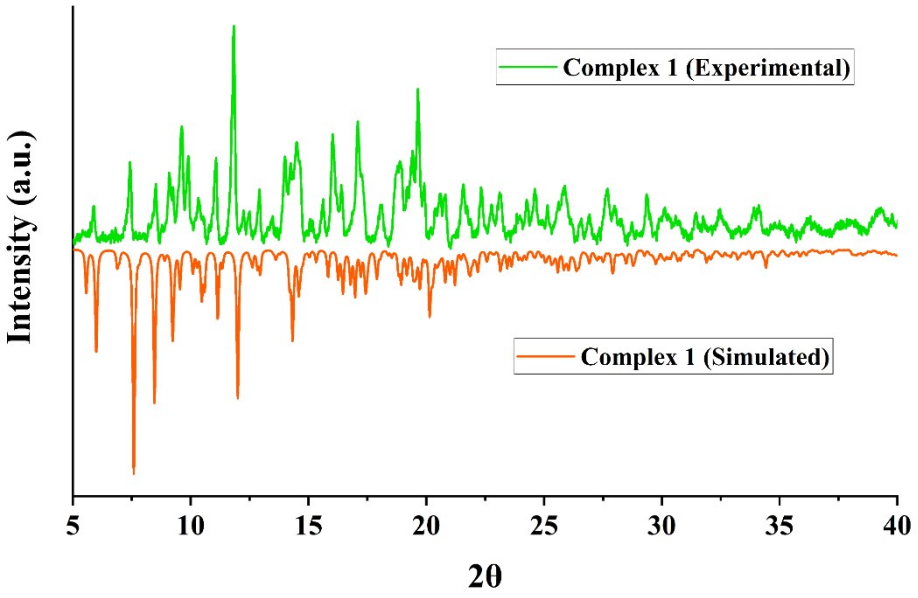

Figure S7. P-XRD plot of complex **1.**

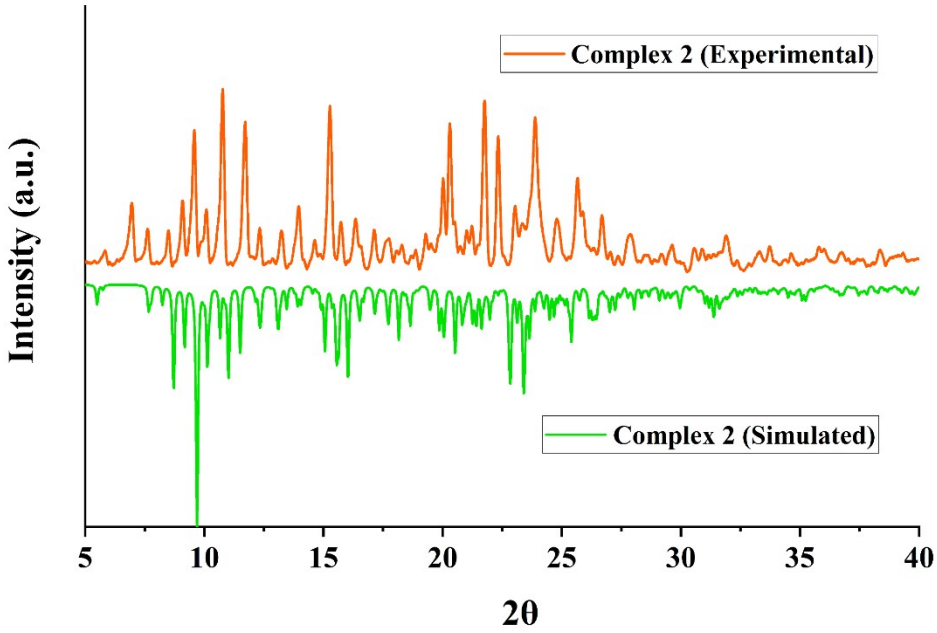

Figure S8. P-XRD plot of complex **2**.

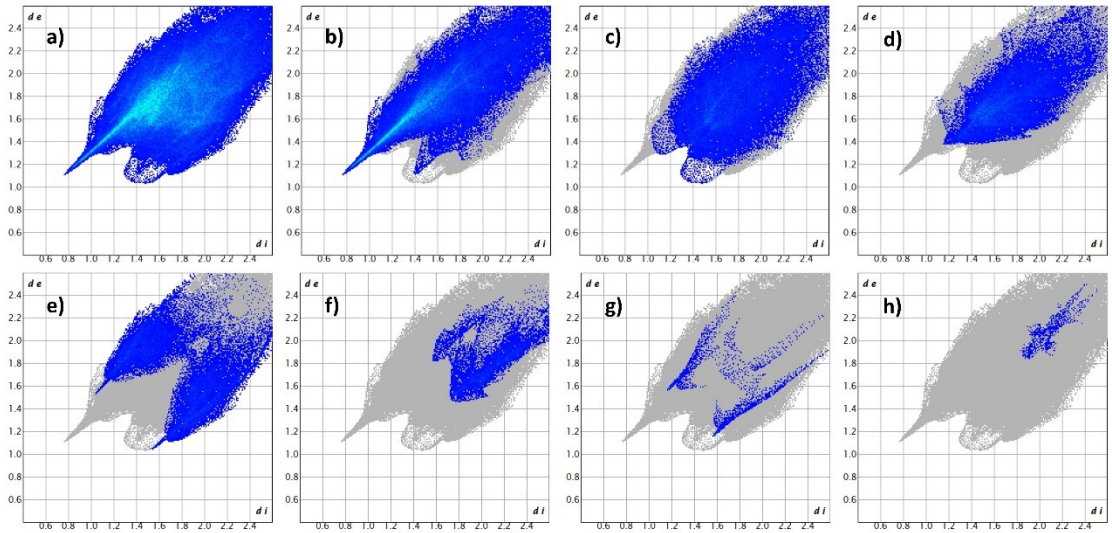

Figure S9. Fingerprint plots for a) All major types of interactions b) O-H c) H-H d) H-F e) C-H f) O-C g) N-H h) C-C interactions present in complex **1** at 120 K**.**

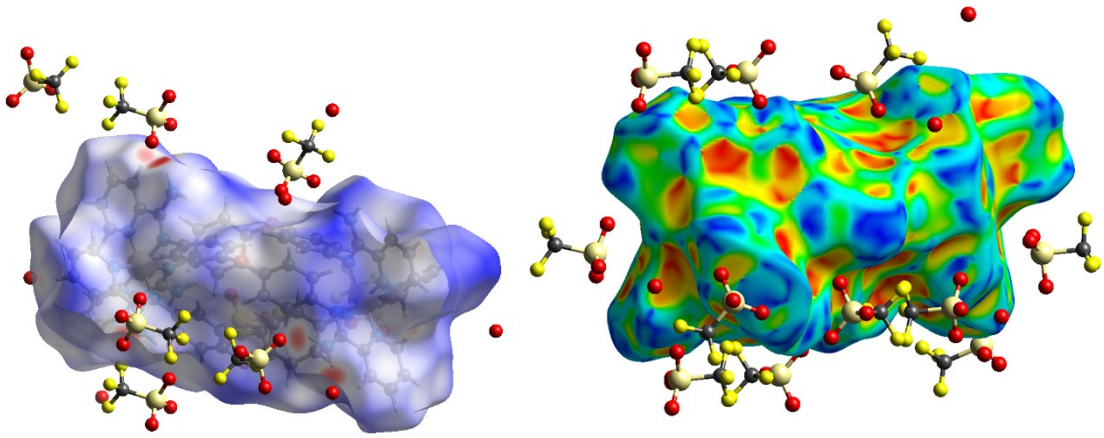

Figure S10. Intermolecular interactions in complex **1** through Hirshfeld surface mapping by d_{norm} function (left) and shape-index (right) at 120 K.

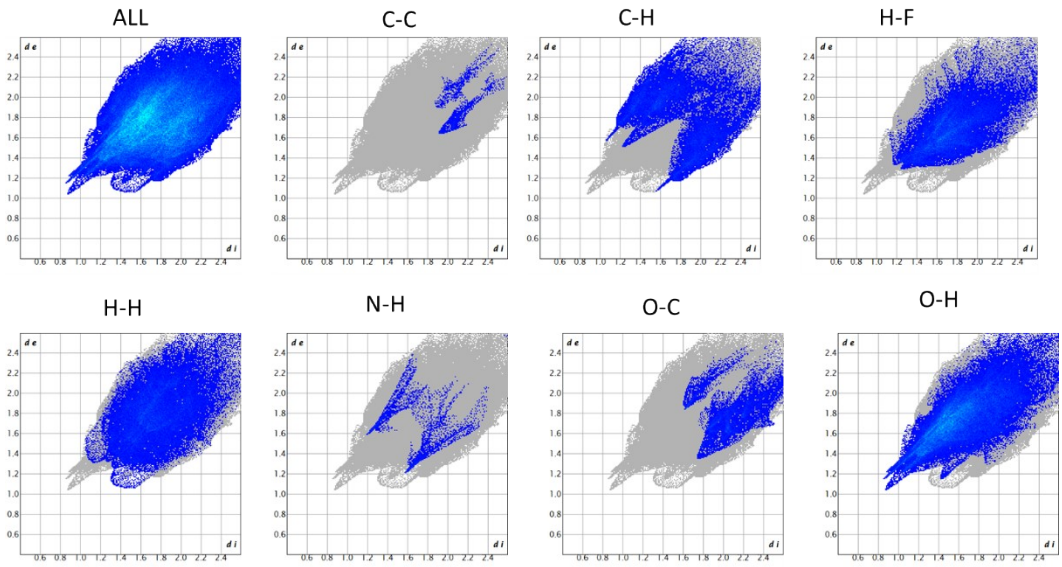

Figure S11. Fingerprint plots for a) All major types of interactions b) O-H c) H-H d) H-F e) C-H f) O-C g) N-H h) C-C interactions present in complex 1 at 294 K.

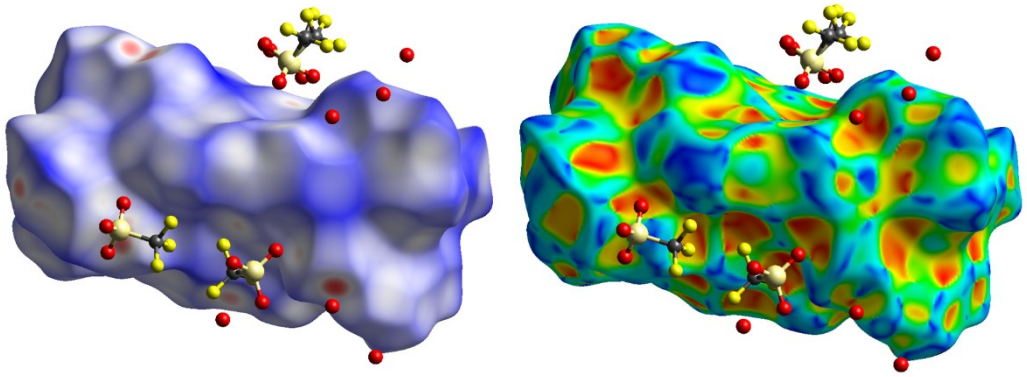

Figure S12. Intermolecular interactions in complex **1** through Hirshfeld surface mapping by d_{norm} function (left) and shape-index (right) at 294 K.

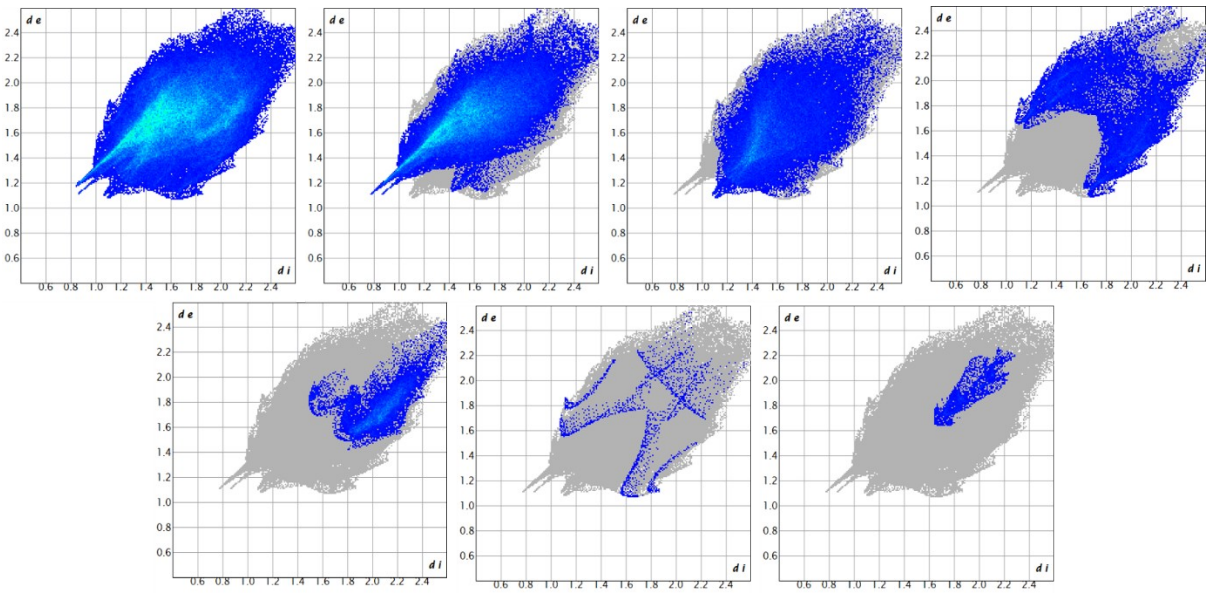

Figure S13. Fingerprint plots for a) All major types of interactions b) O-H c) H-H d) C-H e) O-C f) N-H g) C-C interactions present in complex **2**.

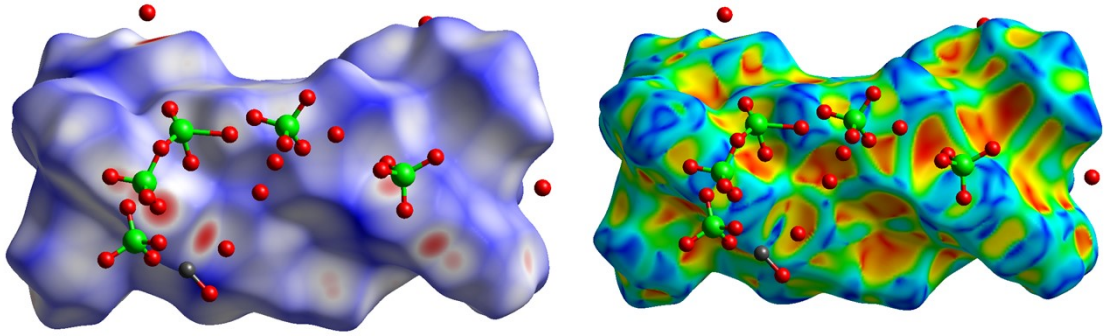

Figure S14. Intermolecular interactions in complex **2** through Hirshfeld surface mapping by d_{norm} function (left) and shape-index (right).

Table S2. Selected bond lengths (Å) and bite angles (˚) for complex **1** at 120 K

	Fe-N_{amine} (Å)		Fe-$N_{pyridine}$ (Å)		Bite Angles (˚)
	N1	1.994(8)	N2	1.984(8)	81.302(3)
Fe1	N3	1.984(9)	N4	1.951(8)	81.140(3)
	N5	2.013(6)	N6	1.954(8)	79.998(3)
	N10	1.985(9)	N11	1.976(9)	80.750(4)
Fe2	N12	2.000(6)	N13	1.976(9)	80.672(3)
	N14	2.000(7)	N15	1.960(9)	79.997(3)

Table S3. Selected bond lengths (Å) and bite angles (˚) for complex **2** at 120 K.

	Fe-N_{amine} (Å)		Fe-$N_{pyridine}$ (Å)		Bite Angles (˚)
	N2	2.005(7)	N1	1.956(7)	81.2(3)
Fe1	N4	1.995(7)	N3	1.967(7)	80.5(3)
	N6	1.998(7)	N5	1.962(7)	80.6(3)
	N11	2.014(7)	N10	1.963(7)	79.68(6)
Fe2	N13	2.013(7)	N12	1.978(8)	80.60(3)
	N15	1.976(7)	N14	1.973(7)	80.30(3)

Table S4. Selected atom distances (Å) for complex **1** at 120 and 294 K.

HS-LS (294 K)	**Distance (A)**	**LS-LS (120 K)**	**Distance (A)**
O22-H18a	2.648	O12-H9a	2.383
O16-H7a	2.477	O14-H16b	2.239
O20-H4a	2.319	O9-H7a	2.085

Table S5. Percentage Hirshfeld surface interaction calculated from crystal explorer for compound **1** at two different temperatures.

Complex 1	**HS-LS (294 K)**	**LS-LS (100 K)**
O-H	35.9	39.6
H-H	19.6	23.9
C-H	15.3	11.9
O-C	5.3	4.2
N-H	1.5	0.9
C-C	0.8	0.4
H-F	17	15.5
Others	4.6	3.6