Electronic supplementary information (ESI)

Iron(III) complexes of 2-methyl-6-(pyrimidin-2-yl-hydrazonomethyl)-phenol as spin-crossover molecular materials

Juan Yuan,[a,b] Mei-Jiao Liu,[a] Cai-Ming Liu,[c] and Hui-Zhong Kou*,[a]

[a] Department of Chemistry, Tsinghua University, Beijing 100084, P. R. China
[b] School of Pharmacy, Henan University of Traditional Chinese Medicine, Zhengzhou 450046, P. R. China
[c] Beijing National Laboratory for Molecular Sciences, Center for Molecular Science, Institute of Chemistry, Chinese Academy of Sciences, Beijing 100190, P. R. China

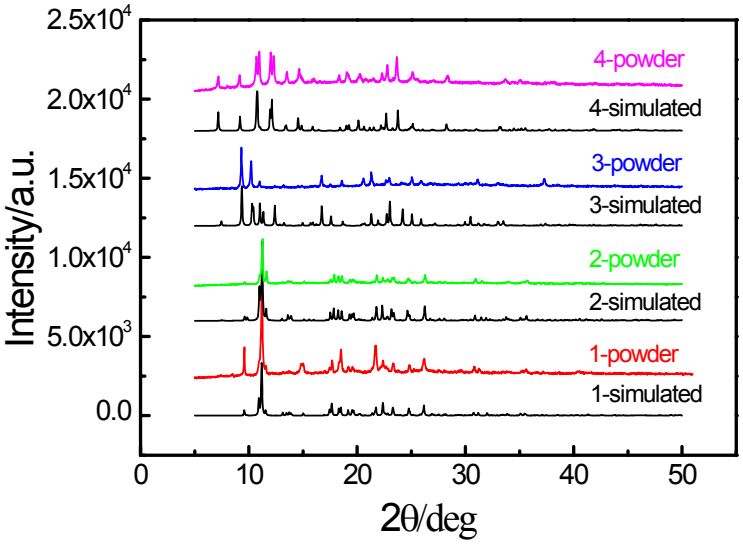

Fig. S1. Simulated and experimental XRD patterns for complexes **1-4**.

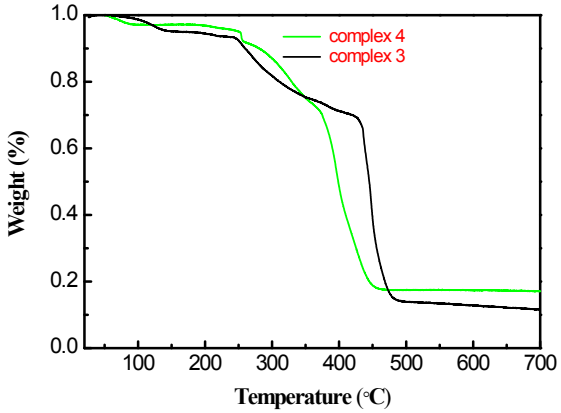

Fig. S2. TGA curves of desolvated complexes **3** and **4**.

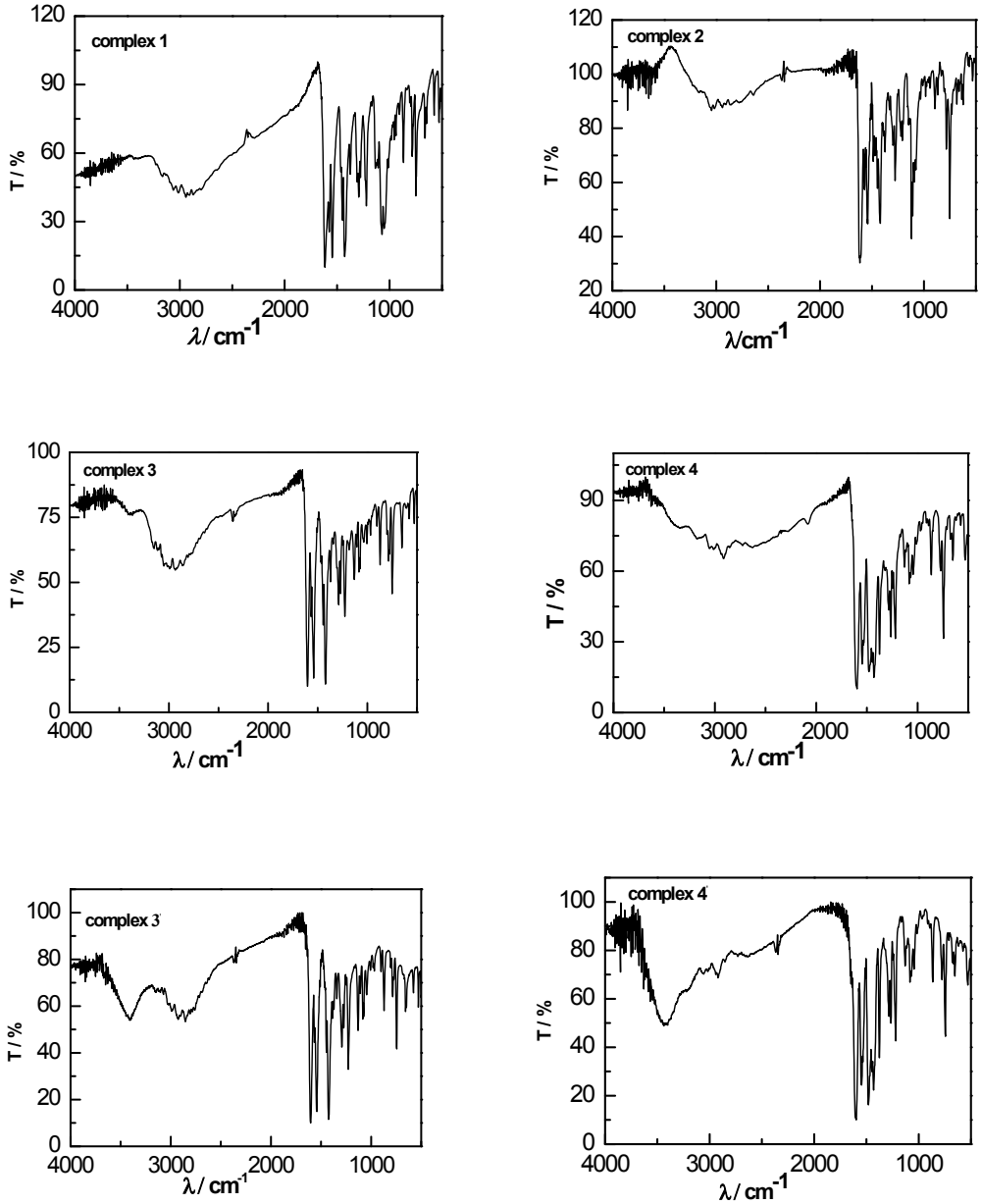

Fig. S3. IR spectra of complexes **1-4, 3' and 4'**.

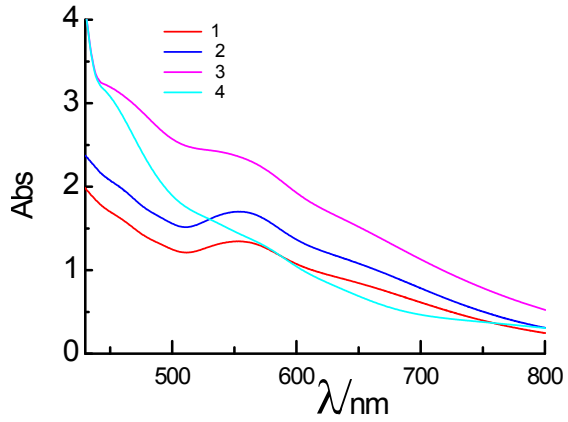

Fig. S4. The visible spectra for complexes **1-4** in a 5×10^{-5} mol/L DMF solution.

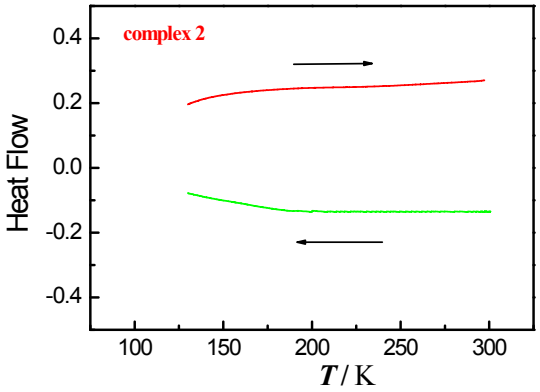

Fig. S5. DSC curves for complex **2** in the heating and cooling modes.

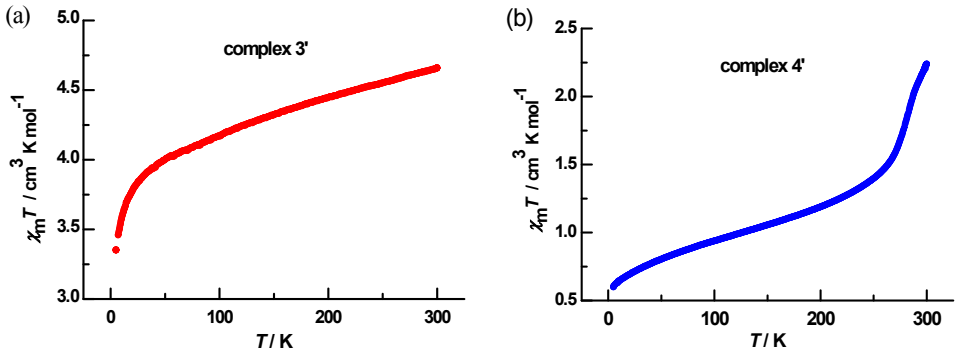

Fig. S6. Temperature dependence of $\chi_{\mathrm{m}}T$ for complexes **3′** (a) and **4′** (b).

Table S1 Electrochemical data of complexes **1-4**

Complex	E_{pc} /v	E_{pa} /v	$E_{1/2}$ /v	ΔE_p /mv
1	–0.97	–0.74	–0.86	230
2	–0.94	–0.73	–0.84	210
3	–0.92	–0.70	–0.81	220
4	–0.91	–0.72	–0.82	190

vs. SCE $E_{1/2}$=1/2 (E_{pa}+ E_{pc}) ΔE_p= E_{pa}–E_{pc}

Table S2 Magnetic and structural data for $[Fe^{III}(L')_2]^+$ analogous complexes

Complexes	spin state	Fe-N_{imine}/ Å	Fe-$N_{pyridyl}$ (N_{amine})/ Å	Fe-$O_{phenolate}$/ Å	Ref
$[Fe(qsal)_2]NCSe$	LS	1.936, 1.945	1.969, 1.986	1.867, 1.874	[39]
$[Fe(SalEen)_2]ClO_4 \cdot 0.5H_2O$	LS	1.939, 1.934	2.046, 2.071	1.888, 1.885	[50]
$[Fe(SalEen)_2]ClO_4$	LS	1.935, 1.935	2.045, 2.049	1.884, 1.877	[50]
$[Fe(4\text{-}Br\text{-}sal_2trien)][MnCr(ox)_3]_{0.67}Cl_{0.33}$	LS	1.931, 1.933	1.999, 2.003	1.887, 1.888	[51]
$Fe(5\text{-}Br\text{-}qsal)_2Ni(dmit)_2$	LS	1.961, 1.956	1.986, 1.972	1.898, 1.903	[52]
$[Fe(qnal)_2][Pd(dmit)_2]_5$	LS	1.945, 1.935	1.950, 1.969	1.885, 1.888	[41]
$[Fe(qsal)_2]_2[Fe(CN)_5(NO)]$	LS (Fe1)	2.06	2.06	1.90	[59]
$[Fe(acpa)_2]ClO_4$	LS	1.92	1.97	1.89	[60]
$[Fe(qnal\text{-}OMe)_2]PF_6 \cdot acetone$	LS	1.989	2.025	1.843	[61]
$Fe(4\text{-}MeO–SalEen)_2PF_6$	LS (Fe1)	1.925, 1.925	2.047, 2.058	1.881, 1.879	[55]
	LS (Fe2)	1.928, 1.935	2.039, 2.042	1.883, 1.884	[55]
$Fe(4\text{-}MeO–SalEen)_2NO_3$	LS	1.934, 1.934	2.040, 2.040	1.889, 1.889	[55]
$[Fe^{III}(3\text{-}MeO\text{-}SalEen)_2]PF_6$	LS	1.925, 1.920	2.045, 2.057	1.872, 1.872	[56]
$[Fe(3\text{-}OMe\text{-}salEen)_2]ClO_4$	LS	1.920, 1.919	2.056, 2.062	1.886, 1.884	[57]
$[Fe(3\text{-}OMe\text{-}salBen)_2]ClO_4$	LS	1.928, 1.936	2.057, 2.041	1.882, 1.870	[57]
$[Fe(salEen)_2]_2[Fe(CN)_5(NO)]$	LS	1.944, 1.945	2.050, 2.068	1.879, 1.882	[58]
$[Fe(acpa)_2]PF_6$	LS (96.1%)	1.942, 1.942	1.989, 1.989	1.889, 1.889	[53]
$[Fe(acpa)_2]BPh_4$	LS (96.7%)	1.933, 1.933	1.973, 1.980	1.884, 1.898	[53]
$[Fe(mph)_2]_2(ClO_4)_2$	HS (35%)	2.136, 2.143	2.147, 2.153	1.886, 1.937	[3]
	HS (35%)	2.167, 2.131	2.120, 2.152	1.882, 1.925	[3]
4	HS (70%)	2.016, 2.009	2.041, 2.032	1.881, 1.882	This work
$[Fe(qsal)_2][Ni(dmit)_2]_3$	HS (84%)	1.935, 1.982	2.035, 2.015	1.871, 1.861	[49]
$[Fe(qsal)_2][Ni(dmit)_2]_3$	HS (84%)	1.991, 1.968	1.956, 2.019	1.894, 1.866	[49]
$[Fe^{III}(3\text{-}MeO\text{-}SalEen)_2]PF_6$	HS (96%)	2.117, 2.139	2.223, 2.239	1.936, 1.904	[56]
$[Fe(acpa)_2]PF_6$	HS (97.7%)	2.082, 2.082	2.155, 2.155,	1.939, 1.941	[54]
1	HS	2.147, 2.141	2.166, 2.177	1.890, 1.886	This work
2	HS	2.139, 2.142	2.172, 2.177	1.885, 1.886	This work
3	HS	2.161, 2.119	2.140, 2.154	1.877, 1.877	This work
$[Fe(qsal)_2]_2[Fe(CN)_5(NO)]$	HS (Fe1)	2.14	2.14	1.92	[59]
	HS (Fe2)	2.15	2.15	1.92	[59]
$[Fe(acpa)_2]ClO_4$	HS	2.05	2.11	1.92	[60]
$[Fe(qnal\text{-}OMe)_2]PF_6 \cdot acetone$	HS	2.101	2.151	1.922	[61]
$[Fe(qnal\text{-}OMe)_2]BPh_4 \cdot 2MeOH$	HS	2.096, 2.097	2.146, 2.144	1.909, 1.918	[61]
$[Fe(pap)_2]ClO_4 \cdot H_2O$	HS	2.112, 2.135	2.216, 2.146	1.929, 1.926	[40]
$[Fe(salpm)_2]ClO_4$	HS (Fe1)	2.092, 2.093	2.156, 2.181	1.911, 1.917	[23]
	HS (Fe2)	2.105, 2.103	2.166, 2.156	1.917, 1.896	[23]
$[Fe(SalEen)_2]ClO_4$	HS	2.089, 2.079	2.191, 2.220	1.908, 1.932	[50]
	HS	2.061, 2.056	2.183, 2.192	1.910, 1.904	[50]
$[Fe(3\text{-}Br\text{-}sal_2\text{-}trien)][Mn^{II}Cr(ox)_3]$	HS	2.129, 2.133	2.171, 2.174	1.915, 1.921	[51]
$Fe(5\text{-}Br\text{-}qsal)_2Ni(dmit)_2$	HS	2.104, 2.110	2.144, 2.114	1.923, 1.922	[52]
$[Fe(qnal)_2][Pd(dmit)_2]_5$	HS	2.102, 2.102	2.129, 2.133	1.921, 1.908	[41]
$Fe(4\text{-}MeO–SalEen)_2PF_6$	HS (Fe1)	2.068, 2.055	2.194, 2.229	1.917, 1.923	[55]

	HS (Fe2)	2.057, 2.071	2.165, 2.179	1.916, 1.921	[55]
$Fe(4\text{-}MeO\text{–}SalEen)_2NO_3$	HS	2.090, 2.090	2.221, 2.221	1.925, 1.925	[55]
$[Fe(3\text{-}OMe\text{-}salEen)_2]ClO_4$	HS	2.091, 2.070	2.192, 2.226	1.915, 1.911	[57]
$[Fe(3\text{-}OMe\text{-}salBen)_2]ClO_4$	HS	2.070, 2.082	2.195, 2.223	1.901, 1.915	[57]
$[Fe(salEen)_2]_2[Fe(CN)_5(NO)]$	HS	2.070, 2.064	2.161, 2.187	1.902, 1.908	[58]
$[Fe(3\text{-}OEt\text{-}SalAPA)_2](ClO_4)\cdot C_6H_5Br$	HS	2.106, 2.077	2.158, 2.200	1.915, 1.919	[46]
$[Fe(3\text{-}OEt\text{-}SalAPA)_2](ClO_4)\cdot C_6H_5Cl$	HS	2.094, 2.096	2.172, 2.196	1.910, 1.916	[46]