Supplementary materials

Mononuclear pyrazole-pyrazolate complexes of Co(II), Cu(II) and Zn

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Table S1.
Crystal data and structure refinement parameters for complexes **1**–**4**

Parameters	**1**	**2**	**3**	**4**
CCDC	2430824	2430825	2430826	2430827
Empirical formula	$C_{20}H_{18}F_{12}N_8Zn$	$C_{20}H_{18}F_{12}N_8Co$	$C_{20}H_{18}N_8F_{12}Cu$	$C_{31}H_{38}N_8O_4F_{12}Cl_2Cu_2$
Formula weight	663.79	657.35	661.96	1012.67
Temperature/K	296(2)	296(2)	120(2)	150(2)
Crystal system	triclinic	triclinic	orthorhombic	monoclinic
Space group	P-1	P-1	Aba2	C2/c
a/Å	8.7719(14)	9.466(14)	17.982(3)	20.9937(13)
b/Å	11.2287(18)	11.005(16)	17.969(3)	10.3294(6)
c/Å	15.981(3)	14.72(2)	15.915(3)	20.7409(13)
α/°	70.082(3)	109.39(2)	90	90
β/°	89.231(3)	101.21(2)	90	107.4360(10)
γ/°	72.118(3)	91.60(2)	90	90
Volume/Å^3	1401.1(4)	1412(4)	5142.2(14)	4291.1(5)
Z	2	2	8	4
ρ_{calc}g/cm^3	1.573	1.546	1.710	1.568
μ/mm^{-1}	0.982	0.712	0.964	1.212
F(000)	664	658	2648	2048
Crystal size/mm^3	0.38 × 0.22 × 0.1	0.32 × 0.14 × 0.08	0.32 × 0.14 × 0.04	0.36 × 0.18 × 0.1
2Θ range for data collection/°	2.7 to 52.0	4.4 to 52.0	4.5 to 58.0	5.1 to 58.0
Index ranges	-10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -19 ≤ l ≤ 19	-11 ≤ h ≤ 7, -10 ≤ k ≤ 13, -18 ≤ l ≤ 18	0 ≤ h ≤ 24, 0 ≤ k ≤ 23, -21 ≤ l ≤ 21	-28 ≤ h ≤ 28, -14 ≤ k ≤ 14, -27 ≤ l ≤ 28
Reflections collected	12505	6797	6763	23063
Independent reflections	5499 [R_{int} = 0.0234, R_{sigma} = 0.0306]	5320 [R_{int} = 0.0200, R_{sigma} = 0.0516]	6763 [R_{int} = 0.0, R_{sigma} = 0.0548]	5679 [R_{int} = 0.0221, R_{sigma} = 0.0191]
Data/restraints/parameters	5499/24/422	5320/18/412	6763/1/383	5679/6/289
Goodness-of-fit on F^2	1.033	1.016	1.032	1.025
Final R indexes [I>=2σ (I)]	R_1 = 0.0540, wR_2 = 0.1507	R_1 = 0.0524, wR_2 = 0.1314	R_1 = 0.0376, wR_2 = 0.0925	R_1 = 0.0417, wR_2 = 0.1097
Final R indexes [all data]	R_1 = 0.0803, wR_2 = 0.1727	R_1 = 0.0885, wR_2 = 0.1517	R_1 = 0.0440, wR_2 = 0.0966	R_1 = 0.0490, wR_2 = 0.1146

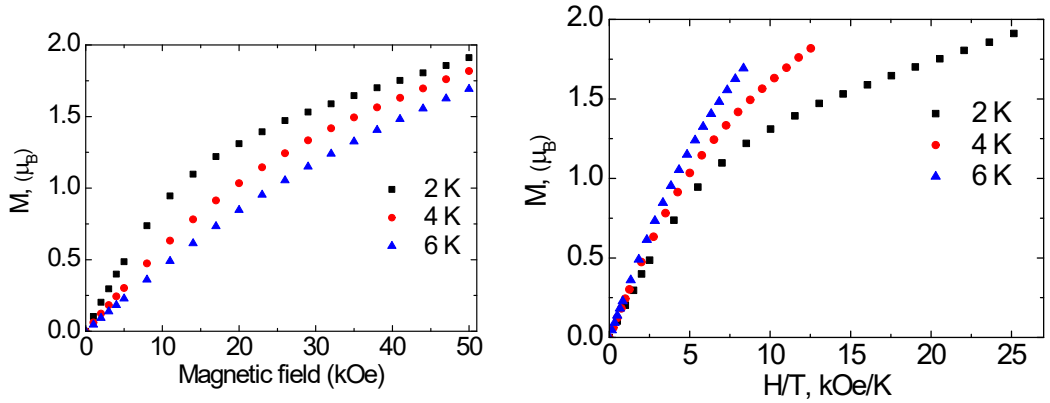

Figure S1. The M(H) and M(H/T) dependences at different temperatures for complex **2**.

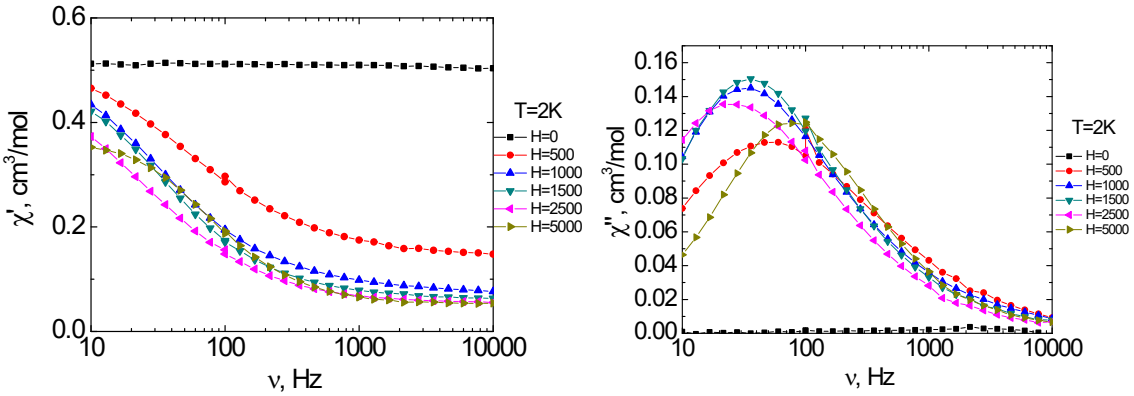

Figure. S2. Frequency dependencies of real, χ' (left) and imaginary, χ'' (right) components of dynamic magnetic susceptibility for complex **2** at T = 2 K under various dc magnetic fields. Solid lines are visual guides.

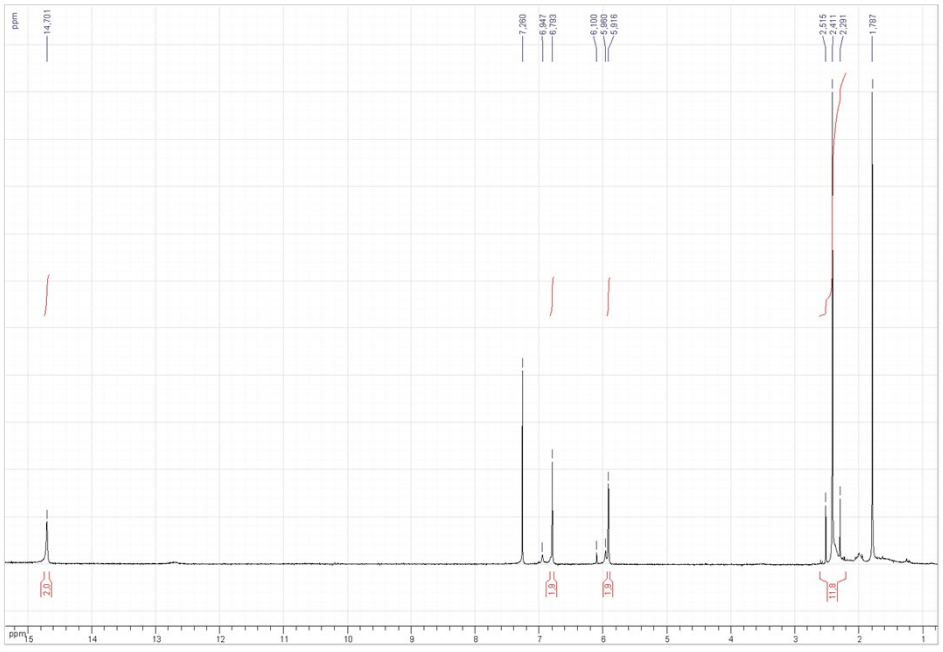

Figure S3. ^{1}H NMR ($CDCl_3$, 400 MHz) of 1.

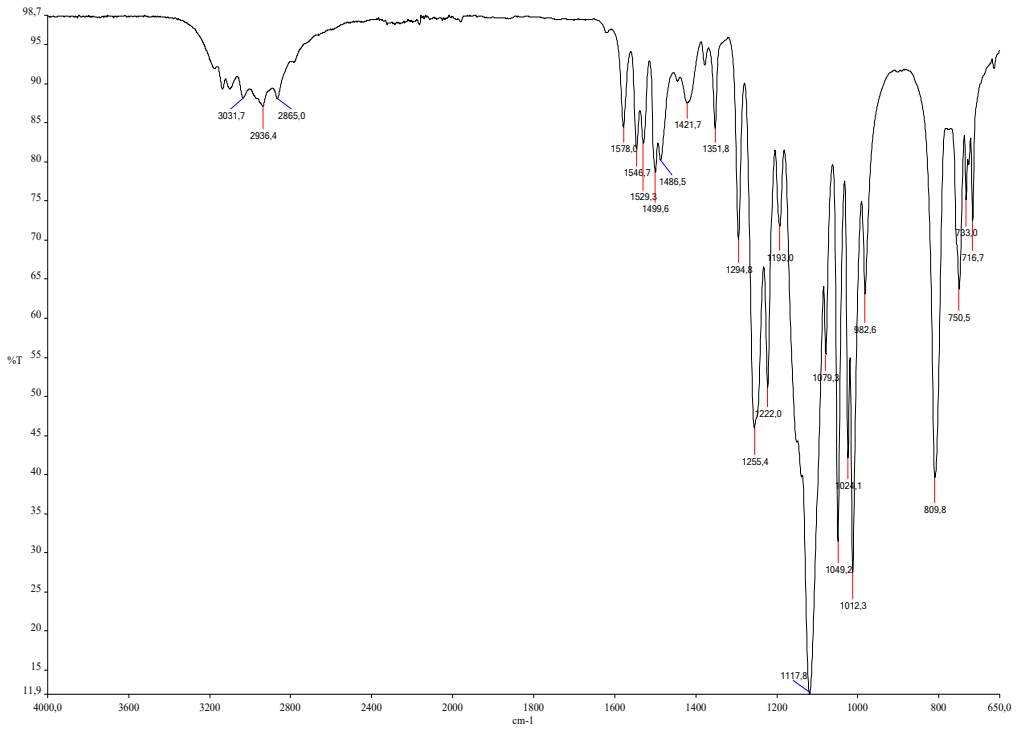

Figure S4. IR spectrum of 1.

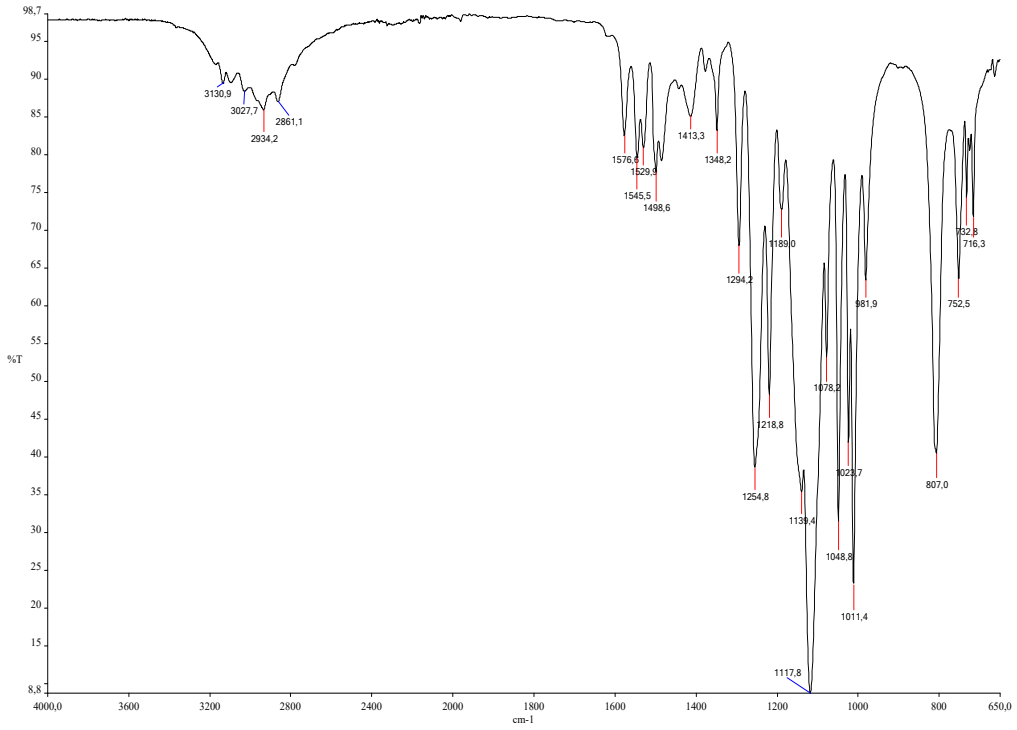

Figure S5. IR spectrum of 2.

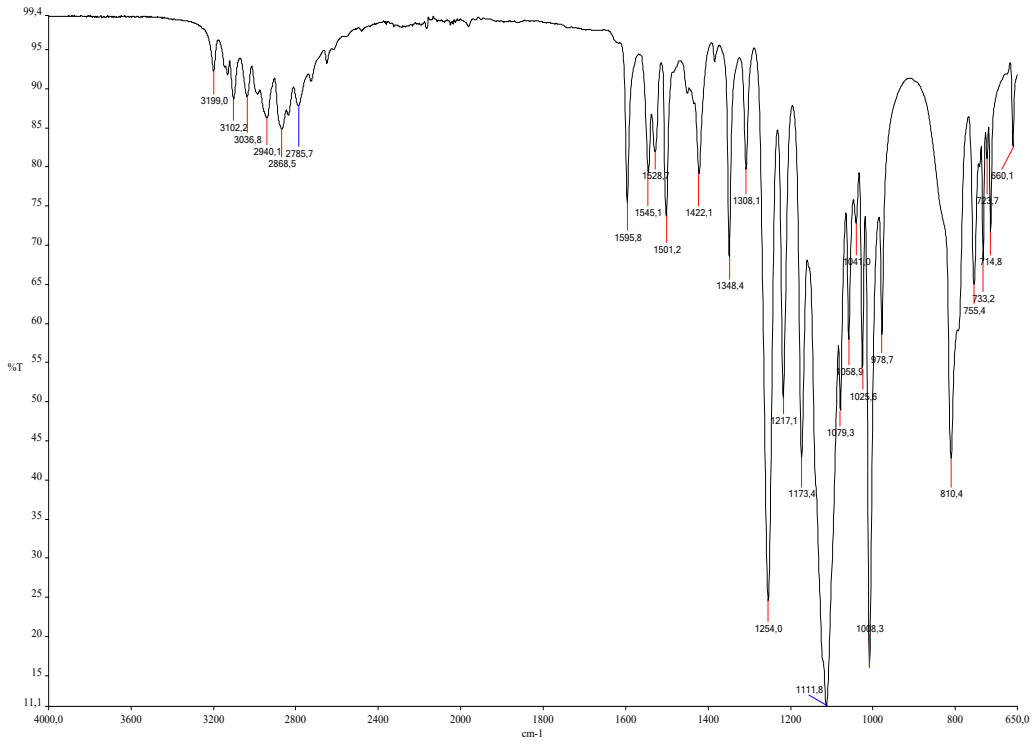

Figure S6. IR spectrum of 3.

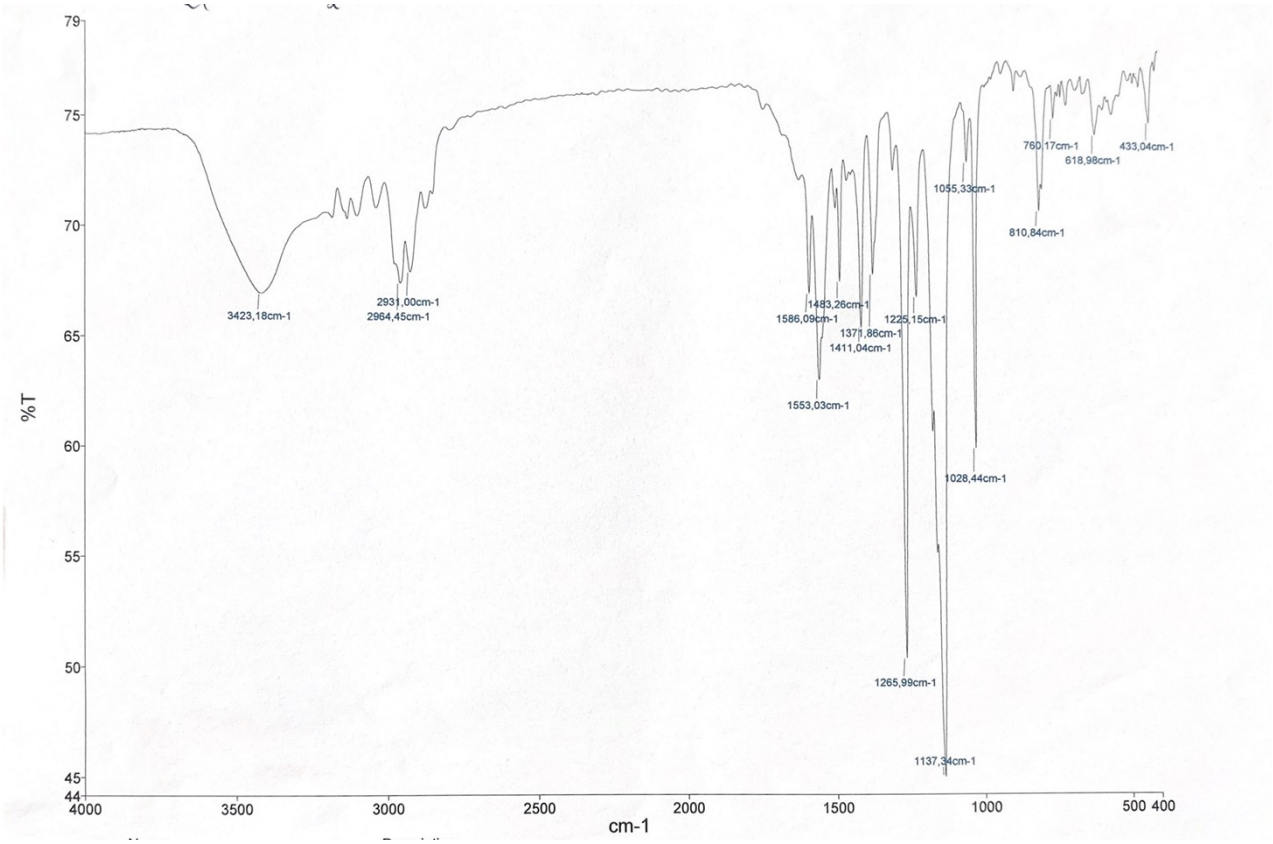

Figure S7. IR spectrum of 4.