

Two pairs of 1:2 nickel(II) and copper(II) metal-complex dyes showing the same *trans* configuration and azo-hydrazone transformation but different thermal properties

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Electronic Supporting Information

Table SI1 Hydrogen bonding parameters (Å, °) in complexes 1-4.

D-H...A	D-H	H...A	D...A	∠DHA	Symmetry code
1					
C10-H10...O3	0.93	2.53	3.372(6)	151	$x, 1+y, z$
2					
C18-H18C...O4	0.98	2.52	3.504(4)	179	$1/2-x, 1/2+y, -1/2-z$
C11-H11...N3	0.95	2.59	3.294(5)	131	$1-x, -y, -z$
C8-H8...O6	0.95	2.41	3.234(4)	145	$1/2-x, 1/2-y, -z$
C3-H3...O5	0.95	2.50	3.411(8)	162	$1/2+x, 1/2-y, 1/2+z$
3					
C3-H3...O5	0.93	2.45	3.241(2)	143	$1-x, -y, 1-z$
C18-H18C...O2	0.96	2.43	3.150(3)	131	$-1+x, y, 1+z$
C19-H19A...O4	0.96	2.38	3.340(3)	173	$2-x, -y, 1-z$
C19-H19C...O1	0.96	2.48	3.365(3)	154	$x, y, 1+z$
4					
C19-H19A...O3	0.96	2.49	3.440(7)	173	$1+x, y, z$
C19-H19C...O1	0.96	2.45	3.305(7)	148	$2-x, 1-y, 1-z$

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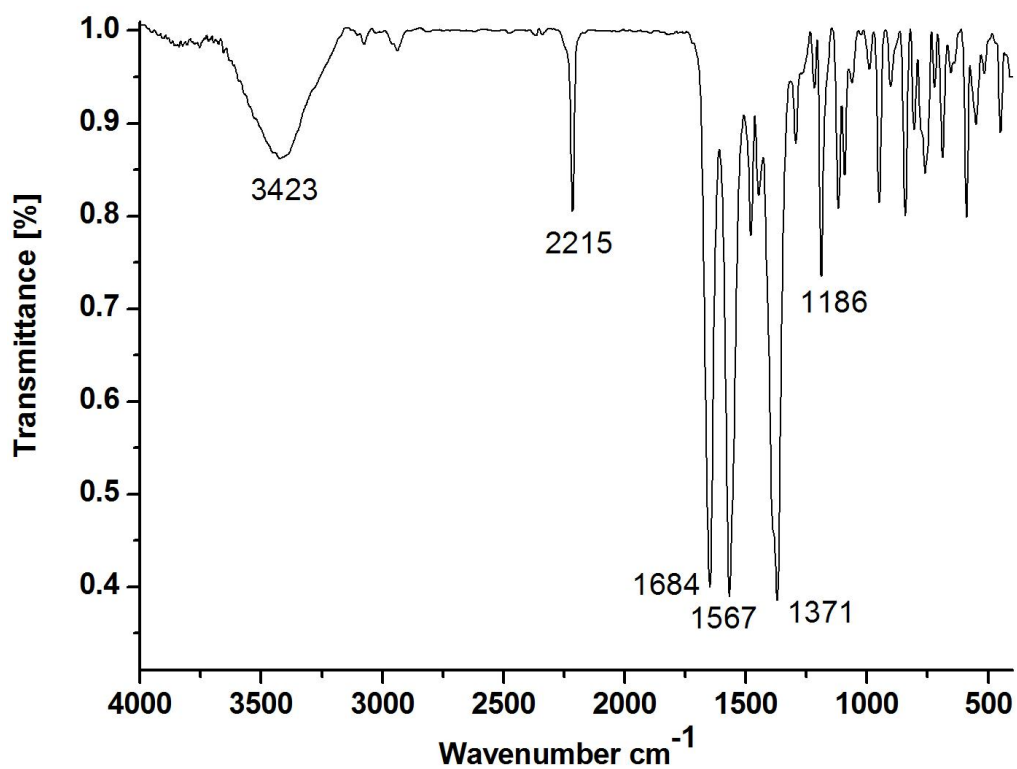


Fig. SI1. FT-IR spectrum of complex 1

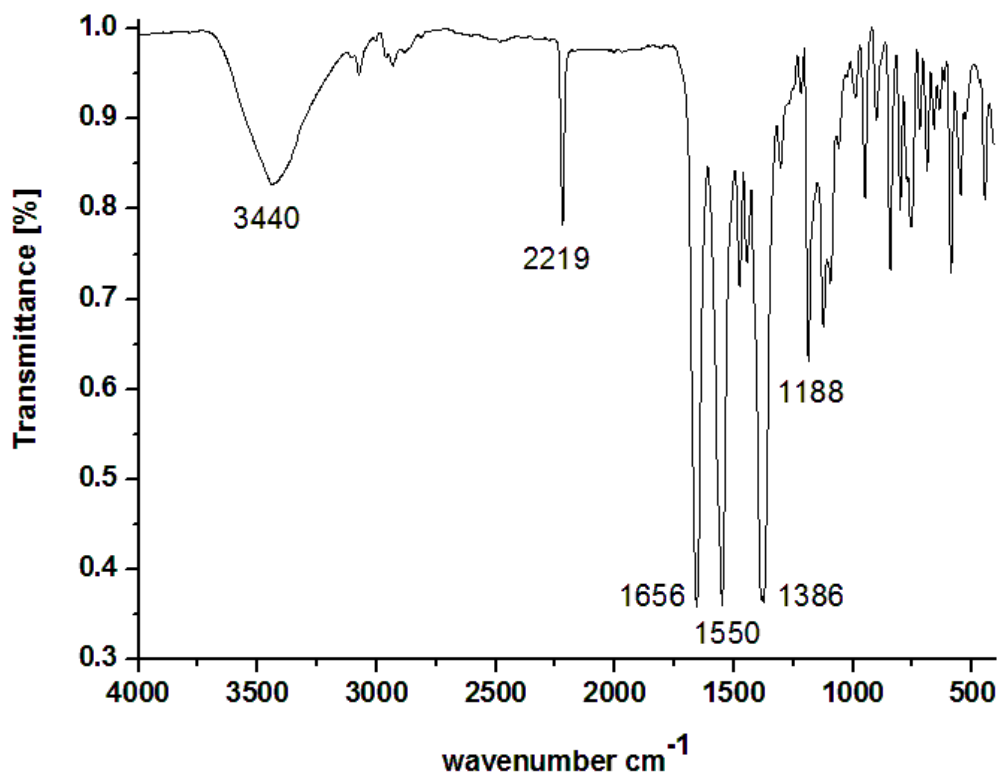


Fig. SI2. FT-IR spectrum of complex 2

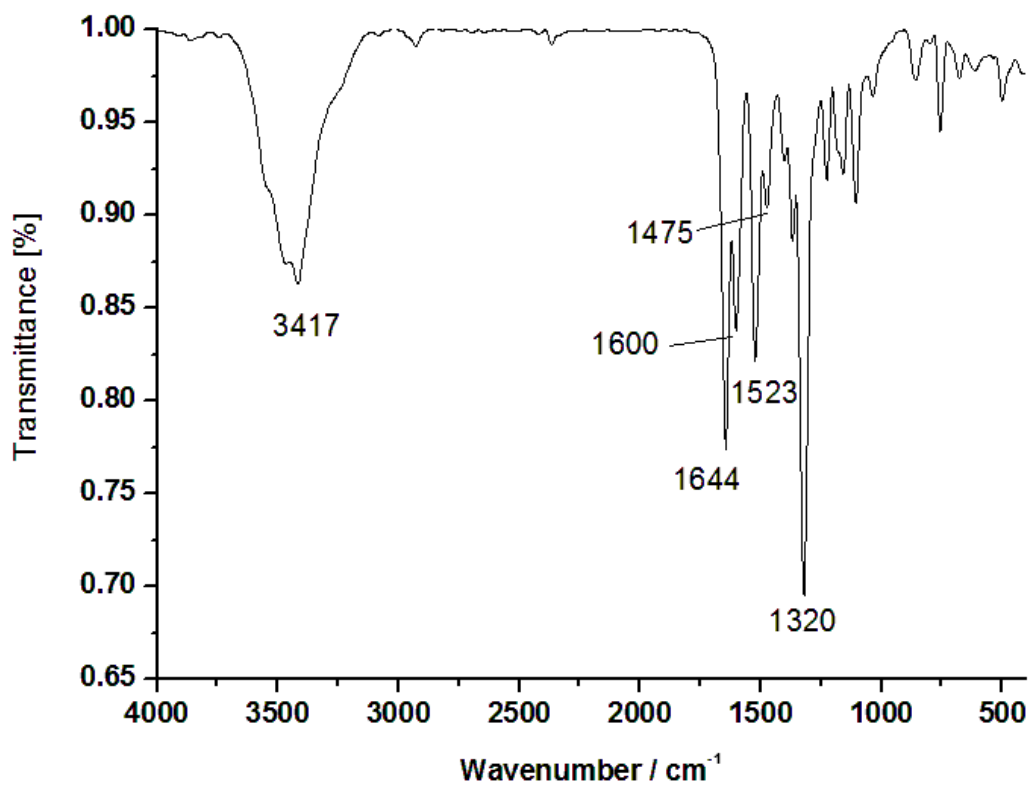


Fig. SI3. FT-IR spectrum of complex 3

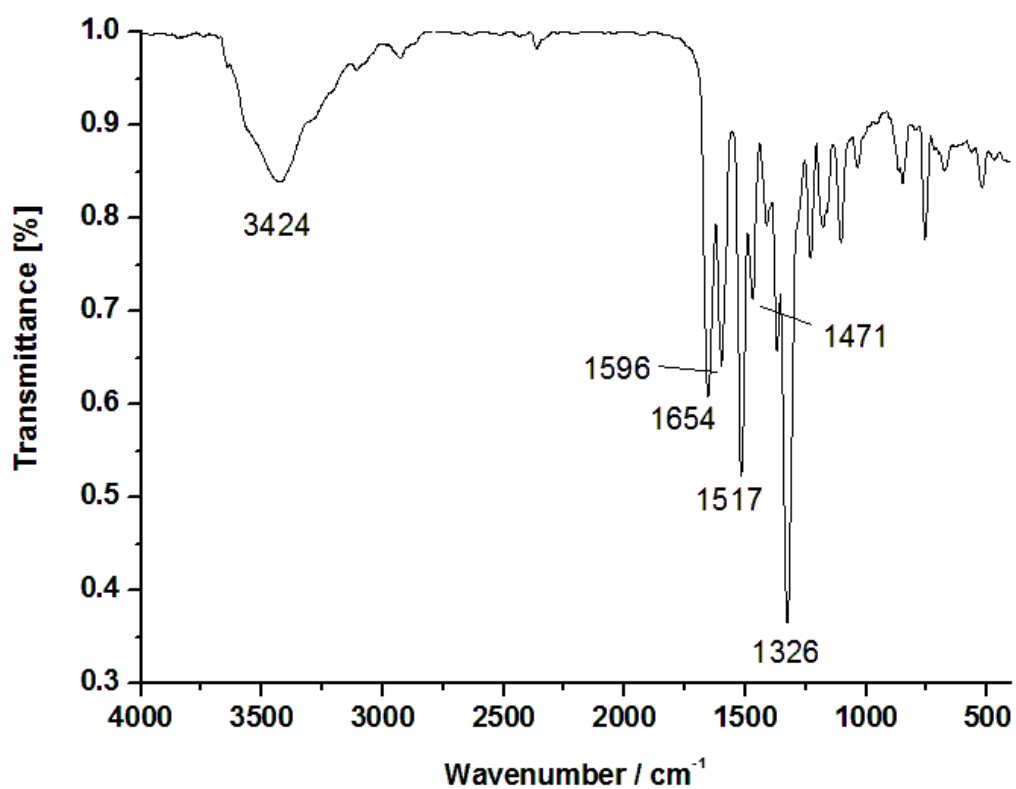


Fig. SI4. FT-IR spectrum of complex 4

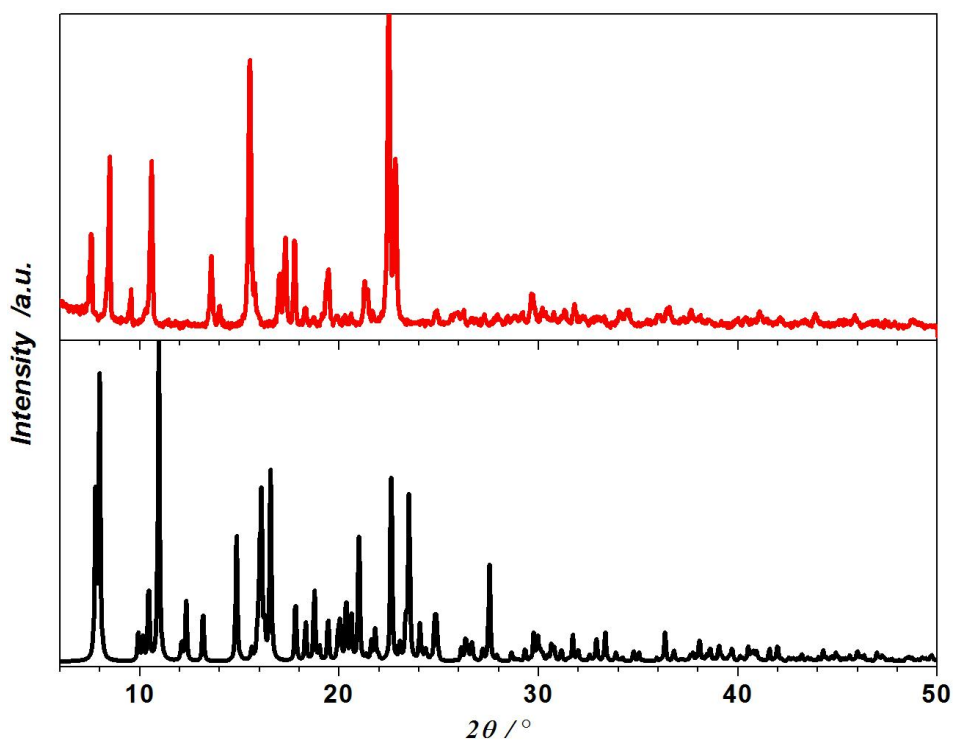


Fig. SI5. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for complex 1.

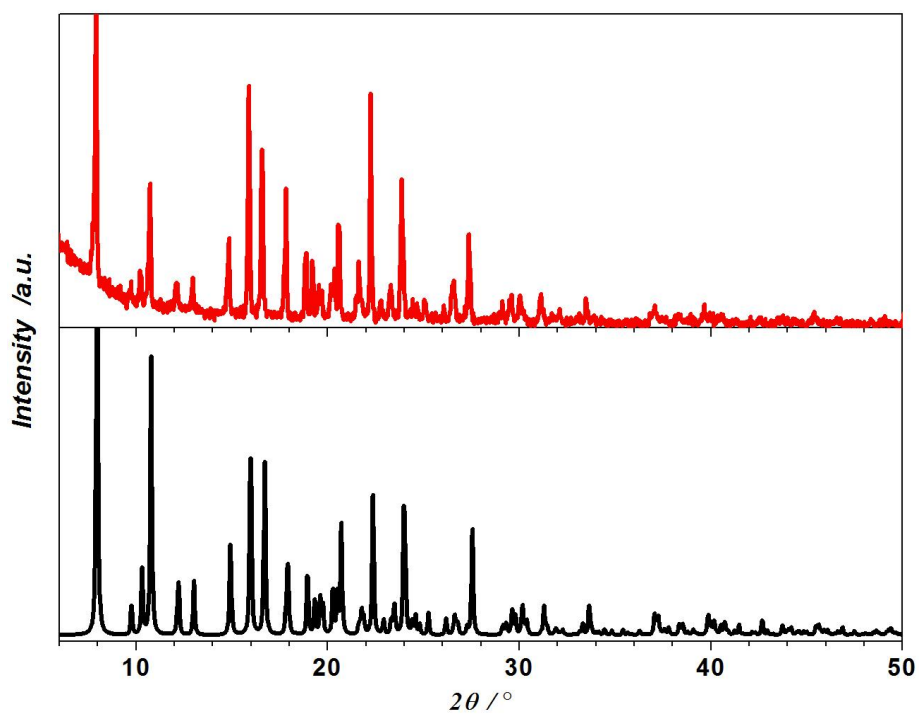


Fig. SI6. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for complex 2.

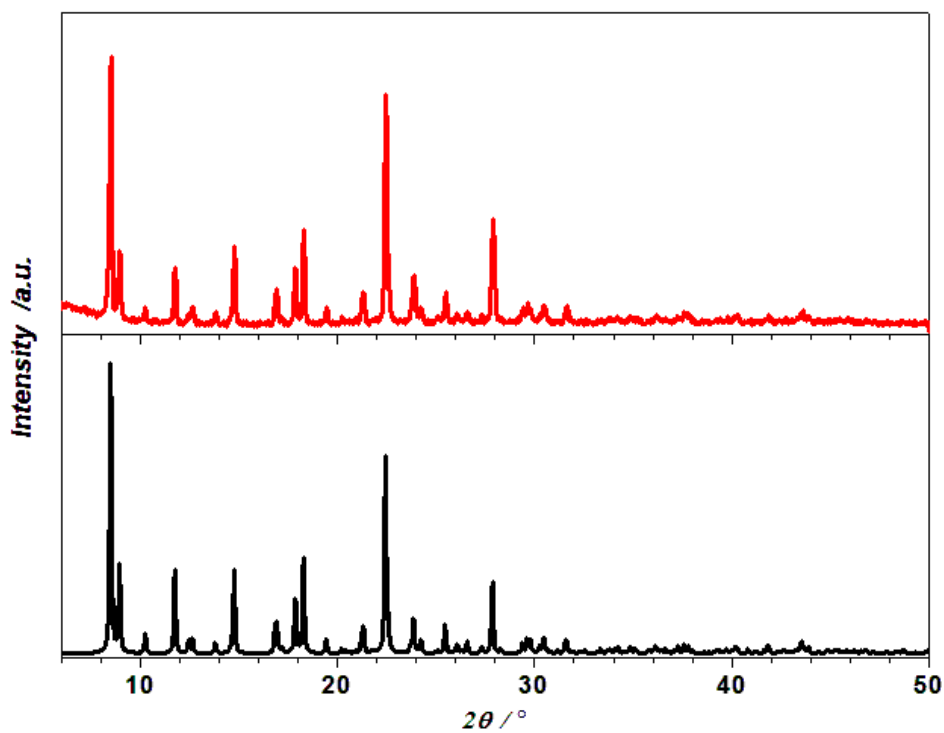


Fig. SI7. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for complex **3**.

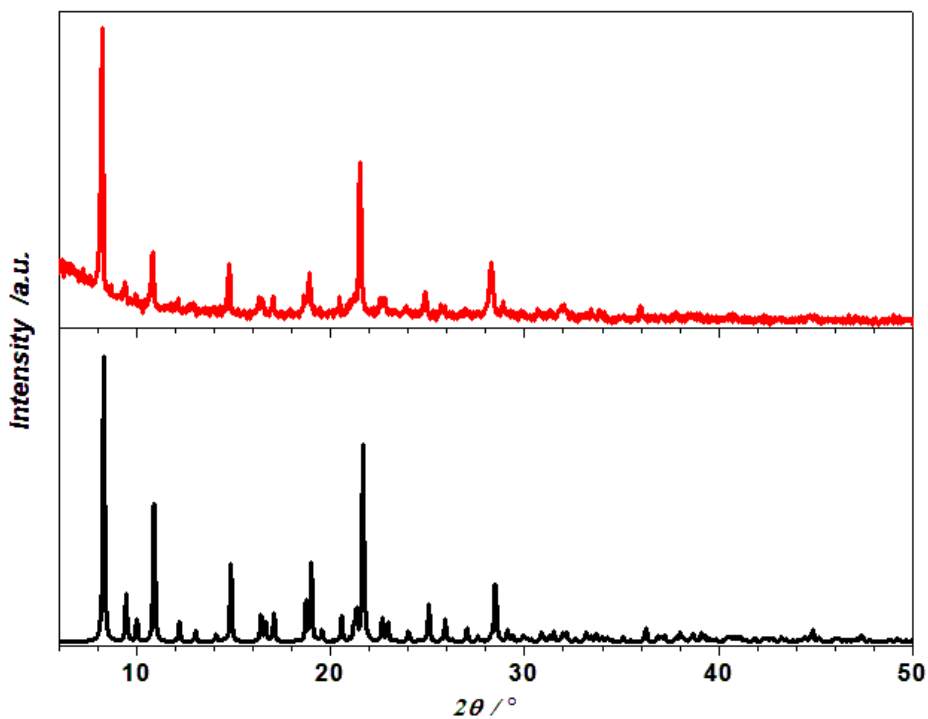


Fig. SI8. The simulative (black line) and experimental (red line) powder X-ray diffraction patterns for complex **4**.

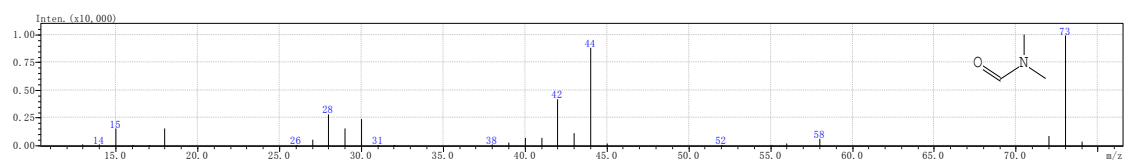


Fig. SI9. Standard mass spectrum of DMF from the GC-MS database.