Electronic Supplementary Material (ESI) for Dalton Transactions.

Supramolecular assembly and structural transformation of d^{10}-metal complexes containing (aza-15-crown-5)dithiocarbamate

Biing-Chiau Tzeng,*[,a] Chung-Lun Wu,[a] Jun-Wei Hung,[a] Su-Ying Chien[b] and Gene-Hsiang Lee[b]

[a]Department of Chemistry and Biochemistry, National Chung Cheng University, 168 University Road, Min-Hsiung, Chiayi 62102, Taiwan

[b]Department of Chemistry, National Taiwan University, 1, Sec. 4, Roosevelt Road, Taipei 10617, Taiwan

Table S1 Crystallographic Data of **1-6**.

	1	**2**	**2'**	**3**	**4**	**5**	**6**
Empirical formula	$C_{11}H_{20}AgNO_4S_2$	$C_{52}H_{92}Cu_4N_8O_{16}S_8$	$C_{88}H_{160}Cu_8N_8O_{32}S_{16}$	$C_{22}H_{42}AgLiN_2O_9S_4$	$C_{22}H_{40}AgN_2NaO_8S_4$	$C_{22}H_{40}AgKN_2O_8S_4$	$C_{22}H_{40}AgN_2O_8RbS_4$
Formula weight	402.27	1595.97	2863.51	721.62	719.66	735.77	782.14
Crystal system	Orthorhombic	Tetragonal	Triclinic	Triclinic	Monoclinic	Hexagonal	Hexagonal
Space group	Pccn	I-4	P-1	P-1	C2/c	$P6_522$	$P6_522$
a (Å)	16.7239(16)	19.5073(4)	13.0623(9)	10.0460(19)	31.430(6)	9.656(2)	9.70500(7)
b (Å)	21.489(3)	19.5073(4)	13.8962(10)	10.0552(19)	20.015(5)	9.656(2)	9.70500(7)
c (Å)	8.2014(9)	8.9948(2)	17.5548(12)	16.237(3)	18.982(4)	57.87(2)	58.1123(7)
α(°)	90	90	75.058(2)	93.574(2)	90	90	90
β(°)	90	90	79.229(2)	104.499(3)	95.95(2)	90	90
γ(°)	90	90	74.115(2)	96.368(2)	90	120	120
V ($Å^3$), Z	2947.5(6), 8	3422.83(16), 2	2937.9(4), 1	1571.2(5), 2	11877(5), 16	4672(3), 6	4740.12(9), 6
F(000) (e)	1632	1664	1488	748	5952	2280	2388
μ(Mo-Kα) (mm^{-1})	1.659	1.537	1.779	0.955	1.021	1.093	2.477
T (K)	100(2)	150(2)	150(2)	173(2)	173(2)	173(2)	150(2)
Reflections collected	13261	38501	53694	5583	44976	36217	43051
Independent reflections (Fo≥2σ(Fo))	2592 (R_{int}=0.056)	5003 (R_{int}=0.045)	13392 (R_{int}=0.083)	5583 (R_{int}=0.050)	13527 (R_{int}=0.177	3589 (R_{int}=0.047)	4631 (R_{int}=0.045)
Refined parameters	172	200	698	381	693	186	174
Goodness-of-fit on F^2	1.047	1.046	1.009	1.105	0.929	1.336	1.125
R^a, $R_w{}^b$ (I≥2σ(I))	0.0350, 0.0812	0.0178, 0.0414	0.0526, 0.1150	0.0925, 0.2254	0.0728, 0.1627	0.0648, 0.1479	0.0274, 0.0672
R^a, $R_w{}^b$ (all data)	0.0457, 0.0882	0.0190, 0.0417	0.0934, 0.1371	0.1015, 0.2316	0.1918, 0.2123	0.0666, 0.1488	0.0287, 0.0677

$^aR=\Sigma\,||F_o|-|F_c||\,/\,\Sigma\,|F_o|$. $^bwR_2=\{[\Sigma w(F_o^2-F_c^2)^2/\Sigma[w(F_o^2)^2]\}^{1/2}$.

Supporting Information

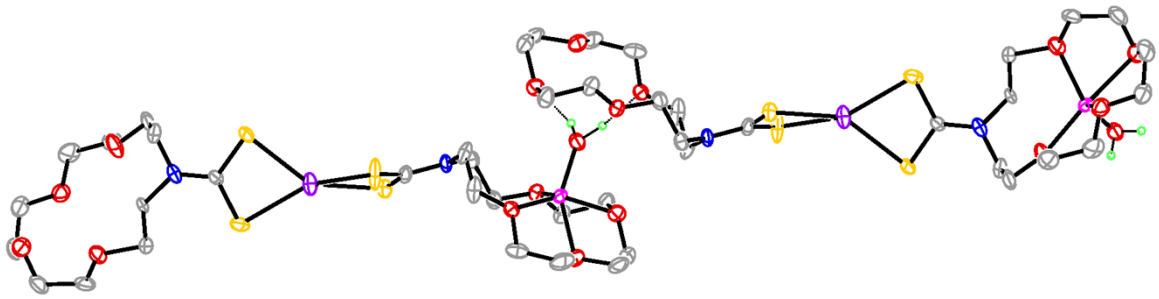

Figure S1. The packing diagram of complex **3** with each Li^+ ion of 50 % disorder.

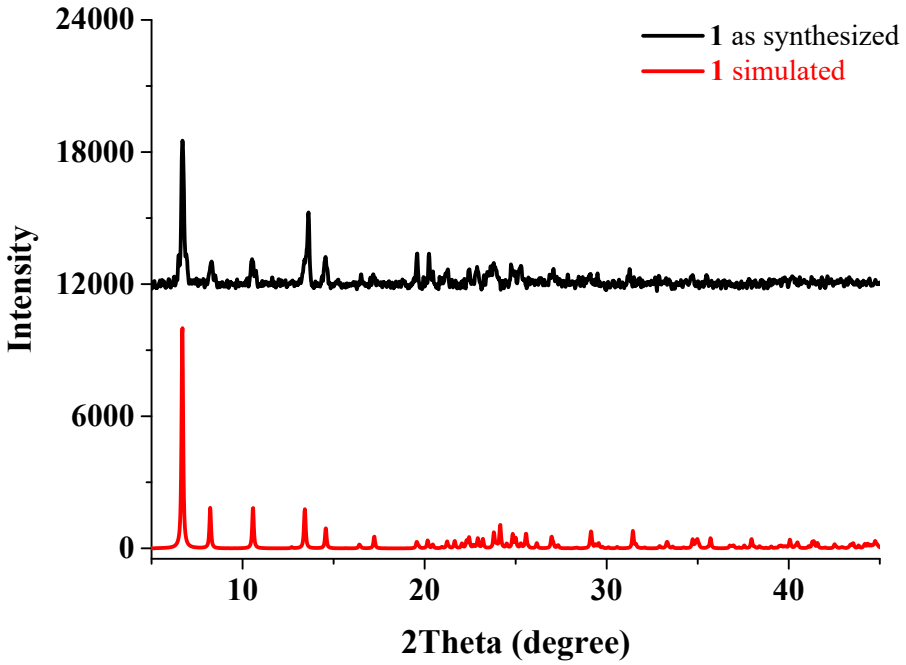

Figure S2. The experimental and simulated powder X-ray diffraction patterns of complex **1**.

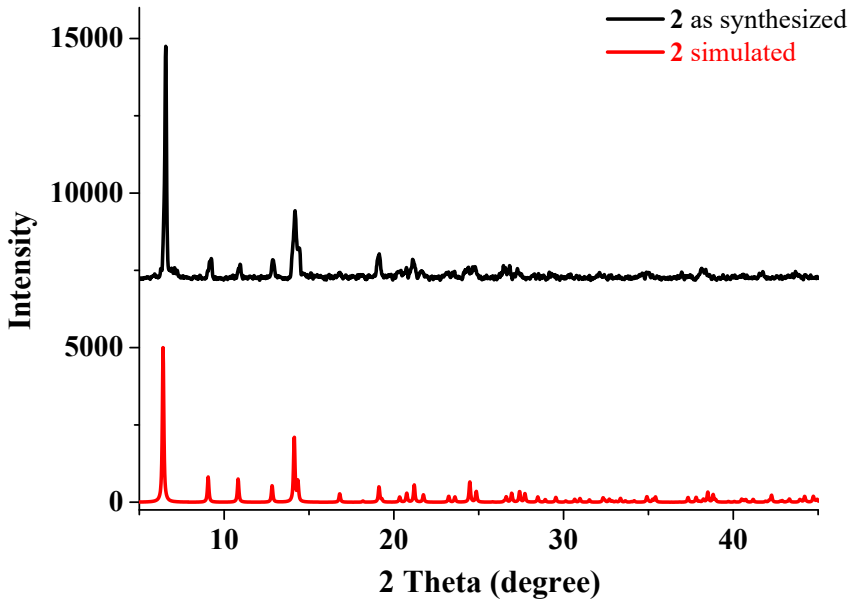

Figure S3. The experimental and simulated powder X-ray diffraction patterns of complex **2**.

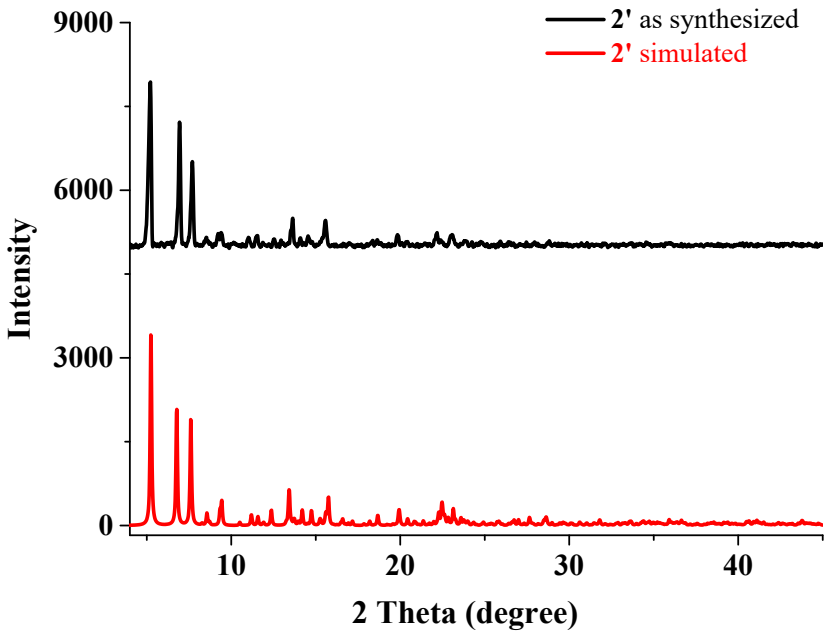

Figure S4. The experimental and simulated powder X-ray diffraction patterns of complex **2'**.

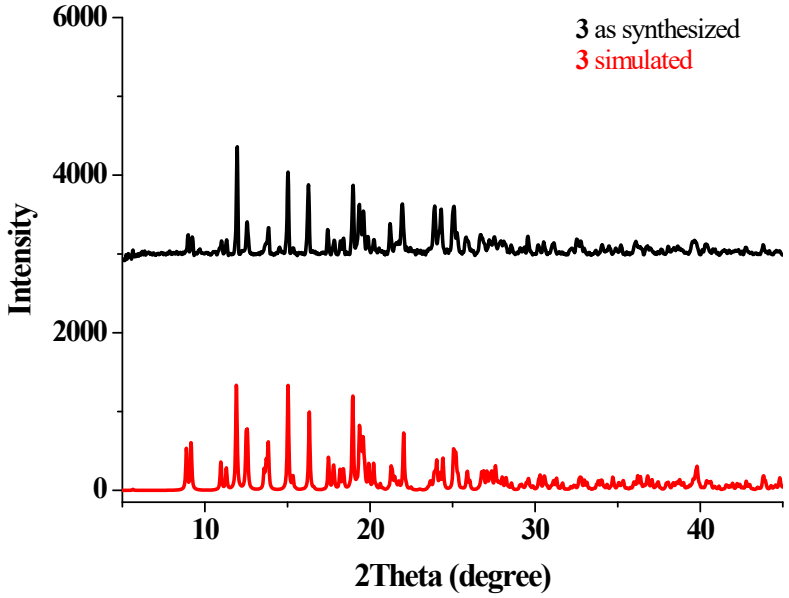

Figure S5. The experimental and simulated powder X-ray diffraction patterns of complex **3**.

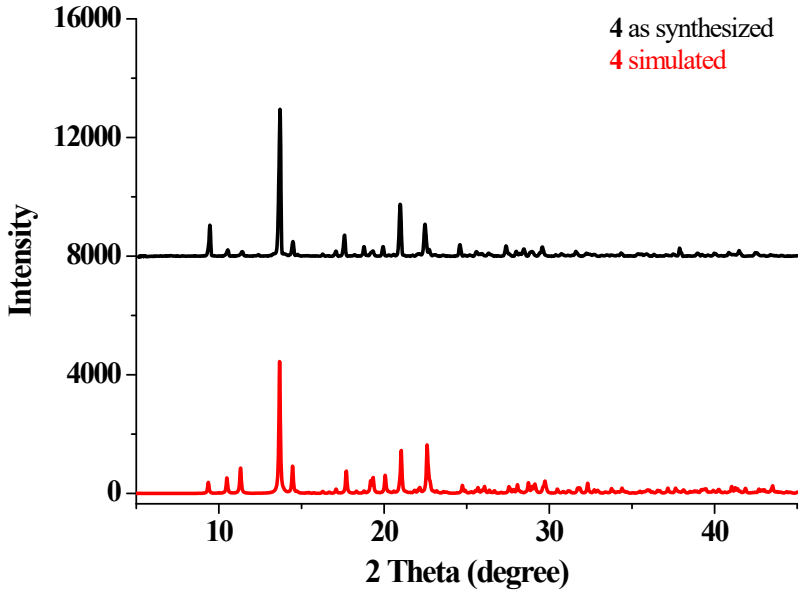

Figure S6. The experimental and simulated powder X-ray diffraction patterns of complex **4**.

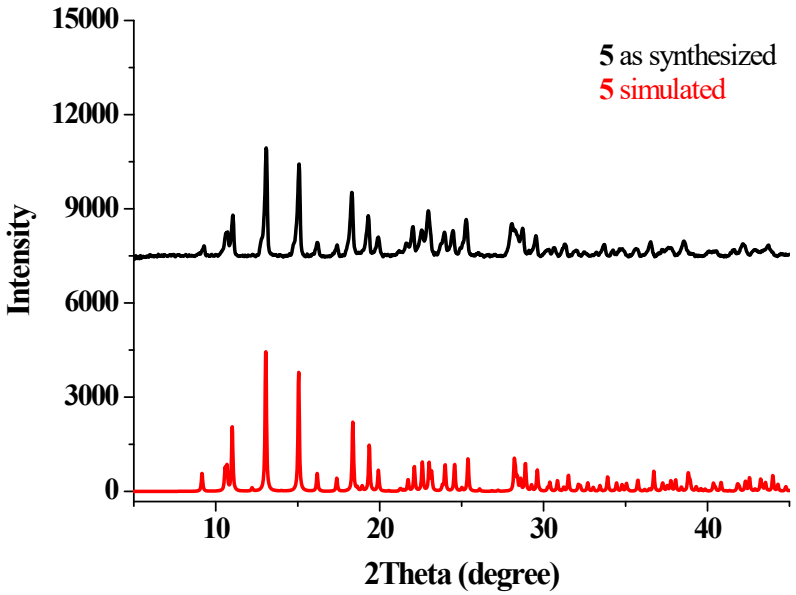

Figure S7. The experimental and simulated powder X-ray diffraction patterns of complex **5**.

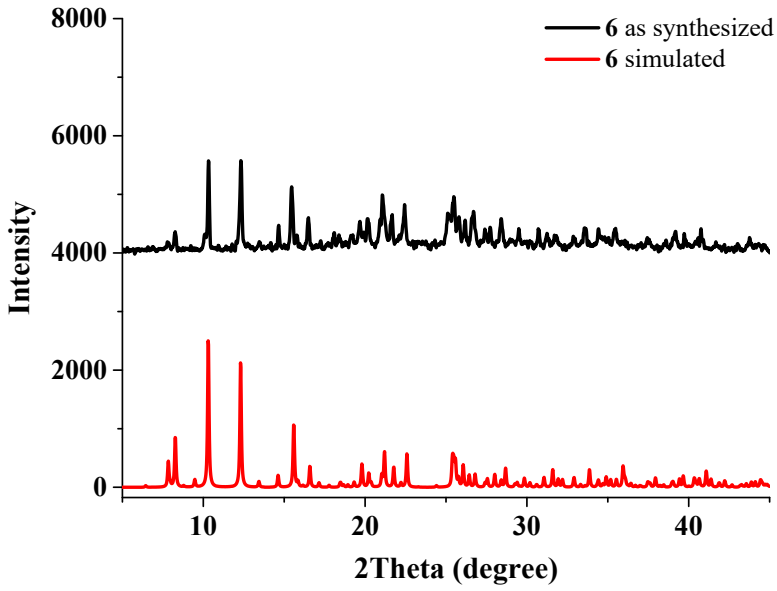

Figure S8. The experimental and simulated powder X-ray diffraction patterns of complex **6**.

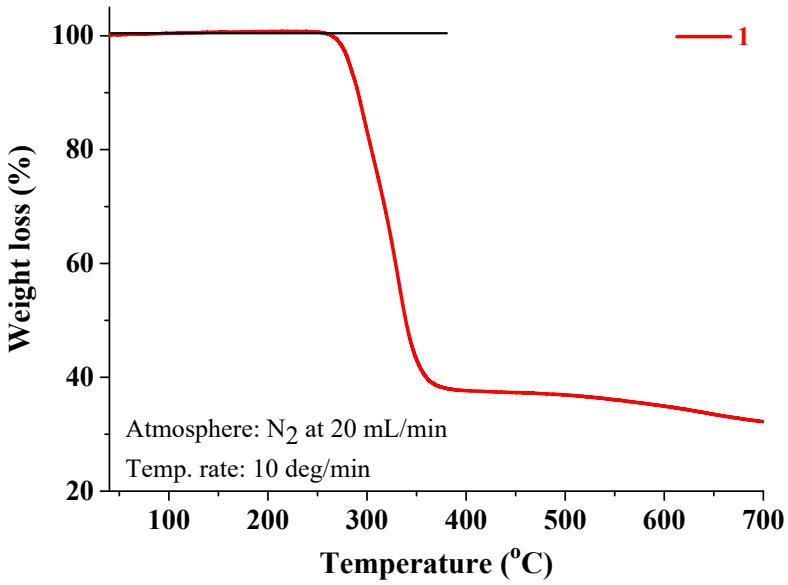

Figure S9. The TGA trace of complex **1**.

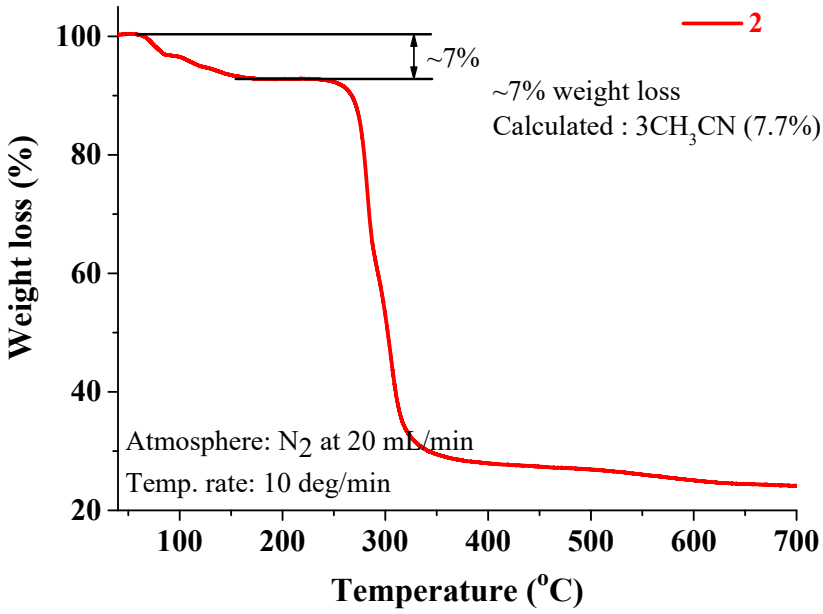

Figure S10. The TGA trace of complex **2**.

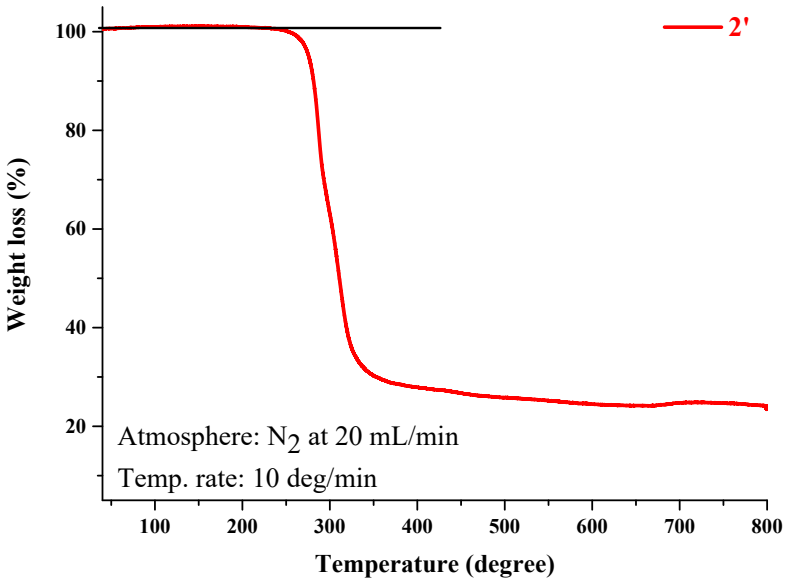

Figure S11. The TGA trace of complex **2'**.

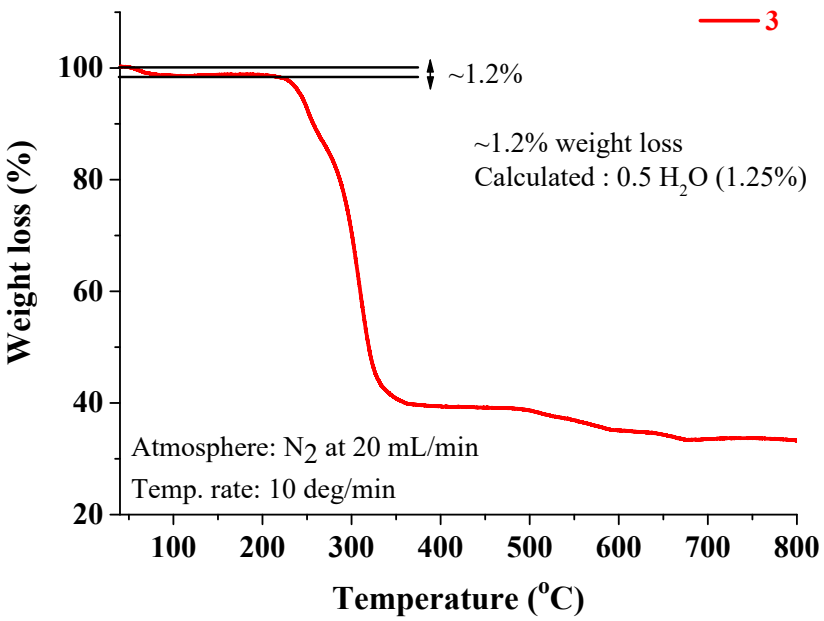

Figure S12. The TGA trace of complex **3**.

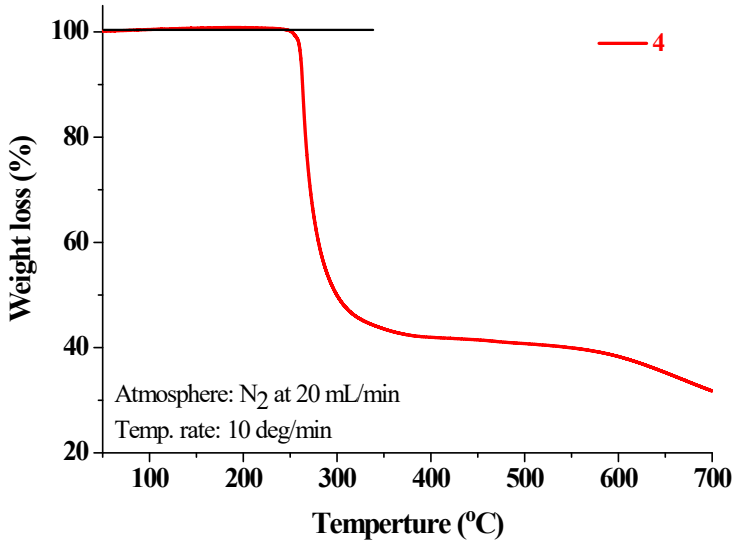

Figure S13. The TGA trace of complex **4**.

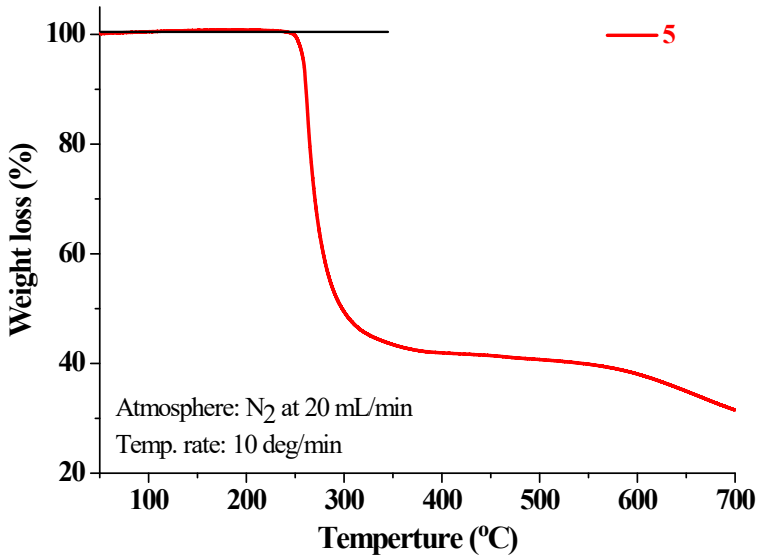

Figure S14. The TGA trace of complex **5**.

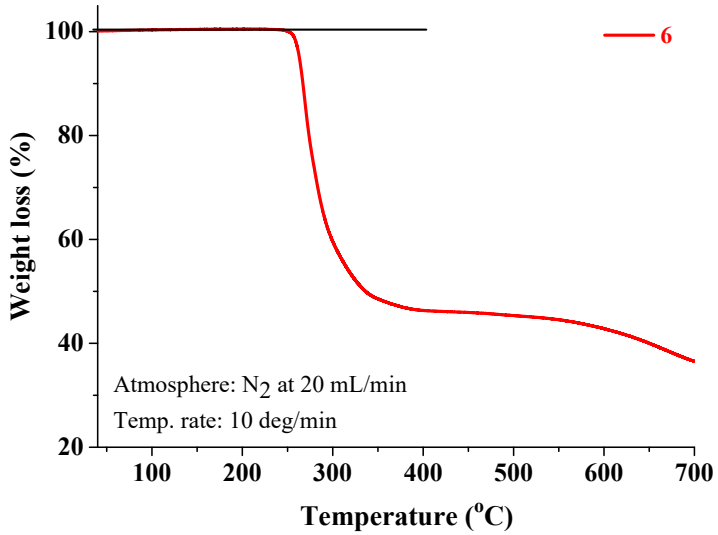

Figure S15. The TGA trace of complex **6**.

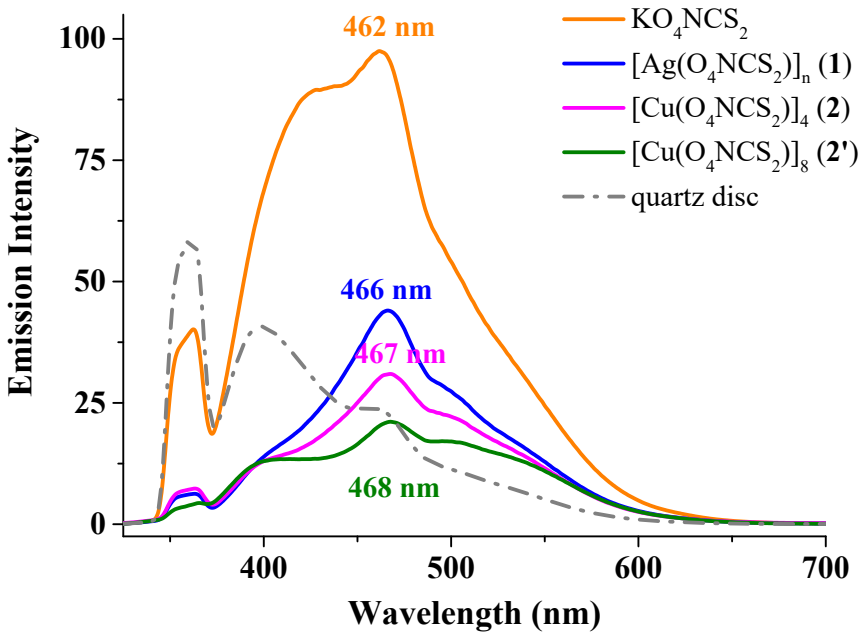

Figure S16. Luminescence spectra for solid samples of KO_4NCS_2 (orange line), complexes **1** (blue line), **2** (pink line), and **2'** (green line) and quartz disc (background : gray dash dotted line) at room temperature. The excitation wavelength is 350 nm.

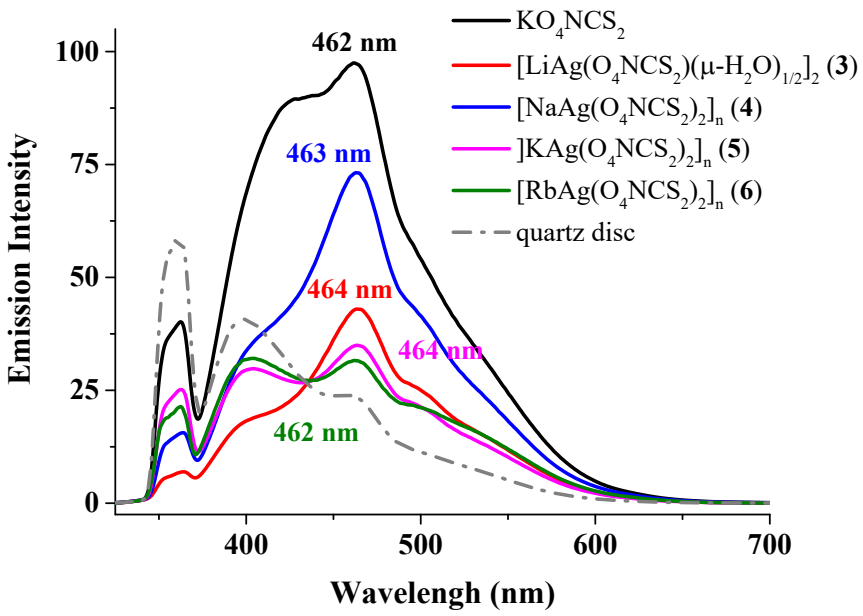

Figure S17. Luminescence spectra for solid samples of KO_4NCS_2 (purple line), complexes **3** (red line), **4** (blue line), **5** (pink line), and **6** (green line) and quartz disc (background : gray dash dotted line) at room temperature. The excitation wavelength is 350 nm.