

**Supporting Information for:
 Homo- And Heterometallic Luminescent 2-D Stilbene Metal-Organic Frameworks**

Christina A. Bauer,^{a,b,*} Simon C. Jones,^c Tiffany L. Kinnibrugh,^d Paul Tongwa,^d
 Richard A. Farrell,^a Avinash Vakil,^b Tatiana V. Timofeeva,^d
 Victor N. Khrustalev^{d,e} and Mark D. Allendorf^f

^a Dept. of Chemistry and Biochemistry, University of California Los Angeles, Los Angeles, CA 90095, USA

^b Dept. of Chemistry, Whittier College, Whittier, CA 90608, USA. Fax: (1) 562 698 4067; Tel: (1) 562 907 4200, ext. 4420; E-mail: cbauer@whittier.edu

^c Dept. of Chemistry and Biochemistry, Georgia Institute of Technology, Atlanta, GA 30032, USA

^d Dept. of Natural Sciences, New Mexico Highlands University, Las Vegas, NM 87701, USA

^e Institute of Organoelement Compounds, Moscow, 119991, Russia

^f Sandia National Laboratories, Livermore, CA 94550, USA

Table S1 Crystallographic data for **2**, **3** and **5–8** (e.s.d.s in parentheses).

Compound	Cd ₃ L ₃ (DMF) ₂ 2	Mn ₃ L ₃ (DMF) ₂ 3	Zn ₂ CdL ₃ (DMF) ₂ 5	Zn ₂ MnL ₃ (DMF) ₂ 6	Zn ₂ CoL ₃ (DMF) ₂ 7	Co ₂ MnL ₃ (DMF) ₂ 8
Empirical formula	C ₅₄ H ₄₄ N ₂ O ₁₄ Cd ₃	C ₅₄ H ₄₄ N ₂ O ₁₄ Mn ₃	C ₅₄ H ₄₄ CdN ₂ O ₁₄ Zn ₂	C ₅₄ H ₄₄ MnN ₂ O ₁₄ Zn ₂	C ₅₄ H ₄₄ CoN ₂ O ₁₄ Zn ₂	C ₅₄ H ₄₄ Co ₂ MnN ₂ O ₁₄
Formula mass	1282.11	1109.73	1188.05	1130.59	1134.58	1117.71
Temp. (K)	100.0(2)	100.0(2)	100.0(2)	100.0(2)	100.0(2)	100.0(2)
Crystal system	Trigonal	Trigonal	Trigonal	Trigonal	Trigonal	Trigonal
Space group	<i>R</i> $\bar{3}$	<i>R</i> $\bar{3}$	<i>R</i> $\bar{3}$	<i>R</i> $\bar{3}$	<i>R</i> $\bar{3}$	<i>R</i> $\bar{3}$
<i>a</i> (Å)	16.488(3)	16.3456(19)	16.1672(10)	16.1173(16)	16.1476(19)	16.147(2)
<i>c</i> (Å)	16.704(7)	16.590(4)	16.6171(10)	16.617(3)	16.476(4)	16.617(4)
γ (deg.)	120.0	120.0	120.0	120.0	120.0	120.0
<i>V</i> (Å ³)	3933(3)	3838.7(15)	3761.4(4)	3738.3(12)	3720.5(15)	3752.0(15)
<i>Z</i>	3	3	3	3	3	3
<i>d</i> _{calc} (g/cm ³)	1.624	1.440	1.573	1.507	1.519	1.484
<i>F</i> (000)	1914	1707	1806	1737	1743	1719
μ (mm ⁻¹)	1.273	0.797	1.439	1.275	1.361	0.974
2 θ _{max} (deg.)	60	60	56	60	60	60
Reflections collected	14415	14674	16570	19140	18962	19174
Independent reflections	2503	2480	1973	2406	2396	2419
Reflections observed	1585	1998	1639	1714	1980	1812
Data/restraints/parameters	2503/26/123	2480/16/123	1973/20/81	2406/8/117	2396/8/117	2419/10/123
<i>R</i> ₁ /w <i>R</i> ₂ [<i>I</i> ≥ 2σ(<i>I</i>)]	0.0335/0.0525	0.0584/0.1574	0.0661/0.1618	0.0382/0.0899	0.0375/0.1077	0.0372/0.0941
<i>R</i> ₁ /w <i>R</i> ₂ (all data)	0.0547/0.0543	0.0715/0.1661	0.0789/0.1708	0.0609/0.0965	0.0455/0.1120	0.0543/0.0991
GOF on F ²	0.924	1.033	1.001	0.937	1.062	0.946
Largest difference peak/hole (e/Å ³)	0.907/-0.867	1.171/-0.640	1.193/-1.195	0.751/-0.459	0.916/-0.435	0.580/-0.383

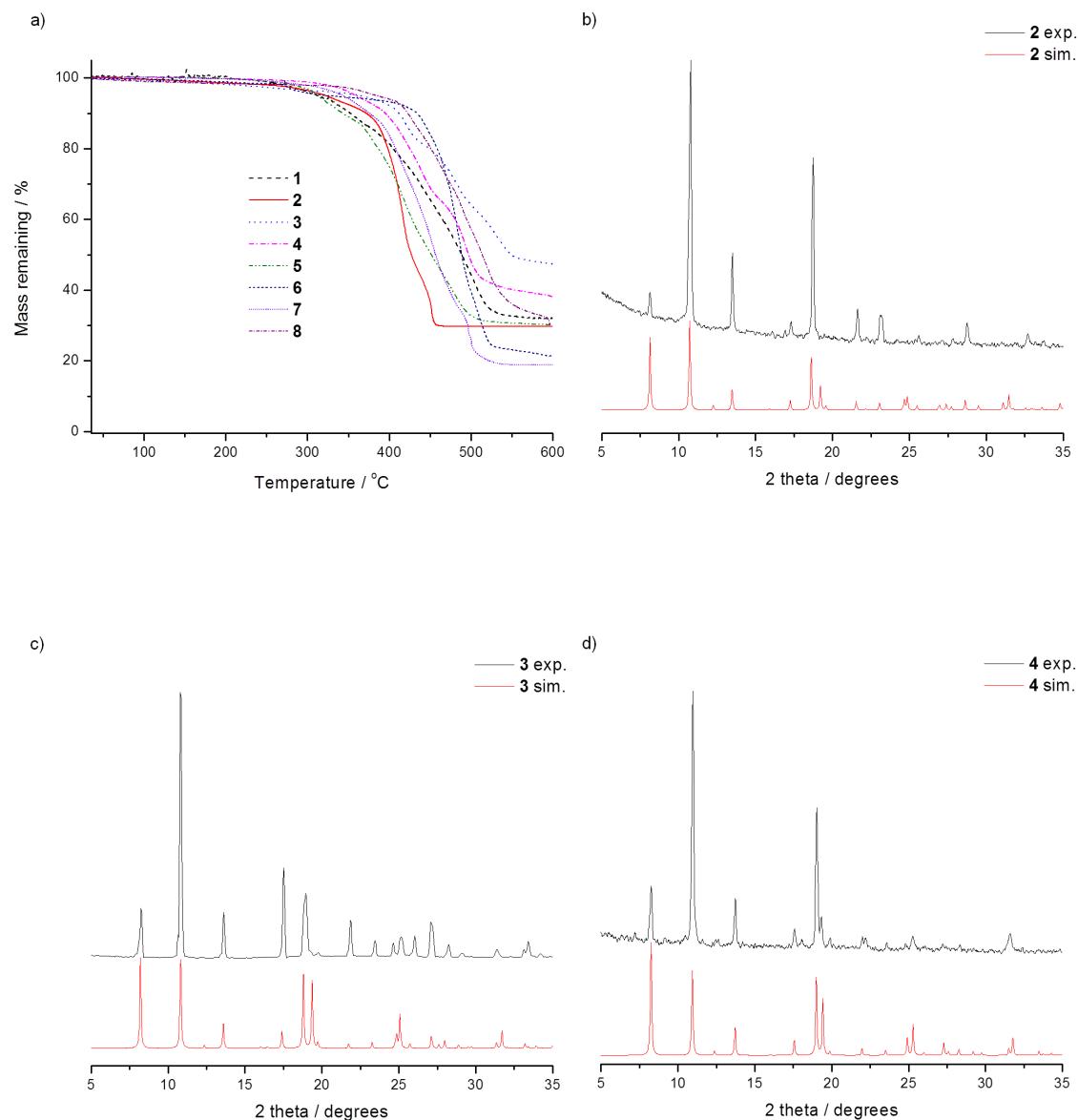


Fig. S1 (a) TGA data for compounds **1-8**; comparison of measured (black) and simulated (red) powder XRD patterns for **2** (b), **3** (c) and **4** (d). Powder XRD data for **1** are shown in Bauer *et al.*, *J. Am. Chem. Soc.*, 2007, **129**, 7136.

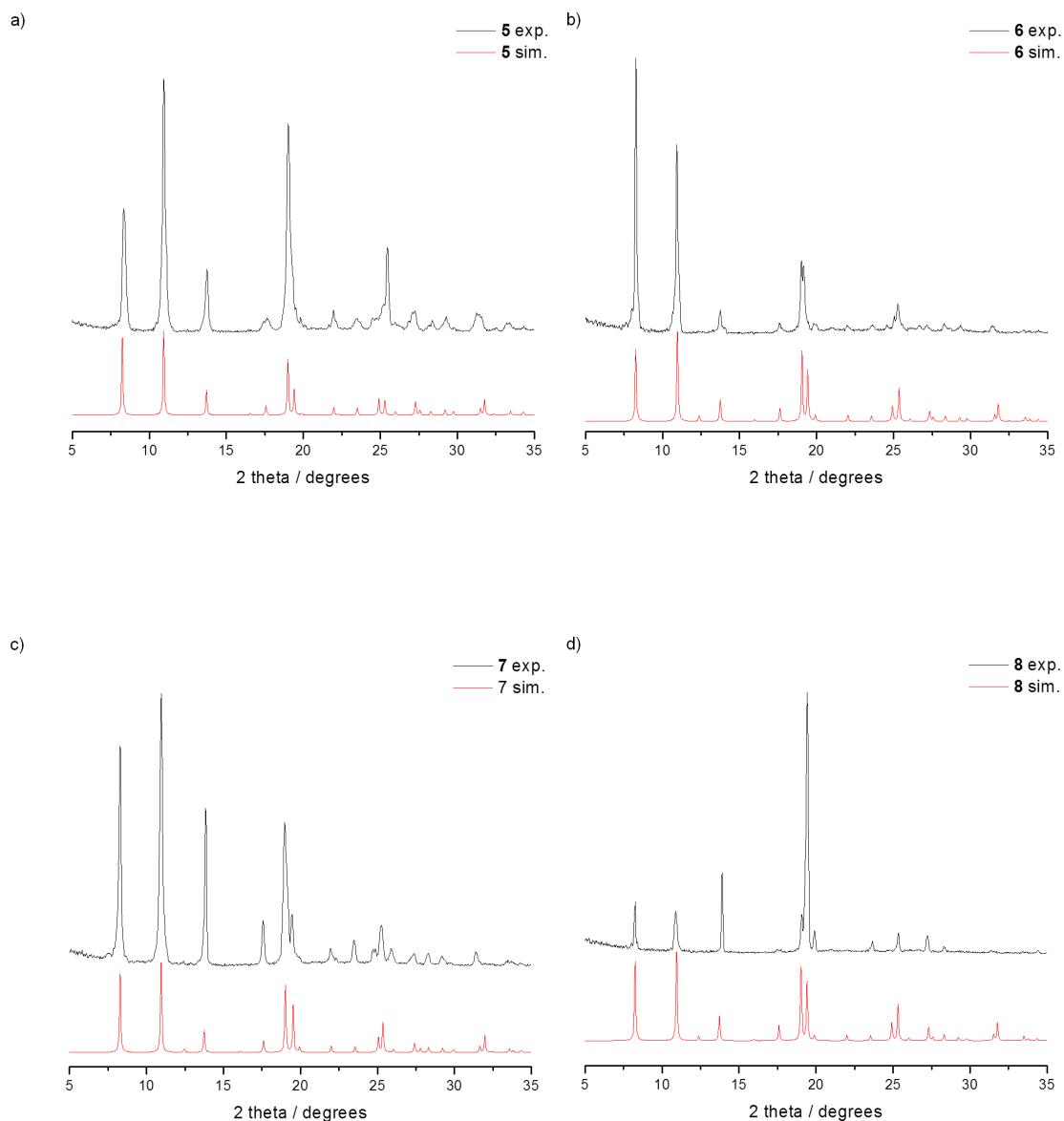


Fig. S2 Comparison of measured (black) and simulated (red) powder XRD patterns for **5** (a), **6** (b), **7** (c) and **8** (d).

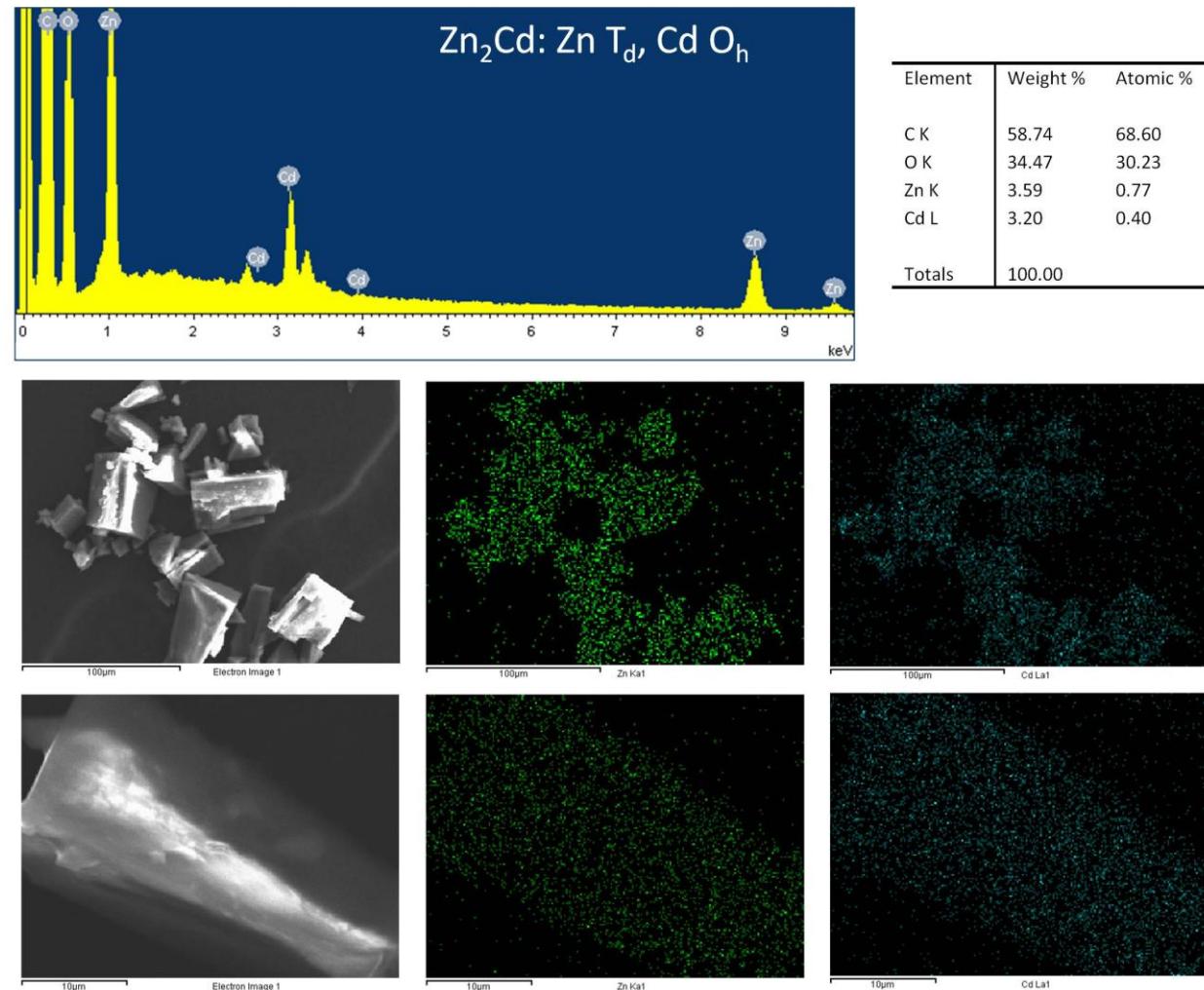


Fig. S3 EDS data for **5** showing observed ~2:1 ratio between Zn and Cd, and uniform distribution of Zn and Cd in the crystals within the resolution limit of the experiment.

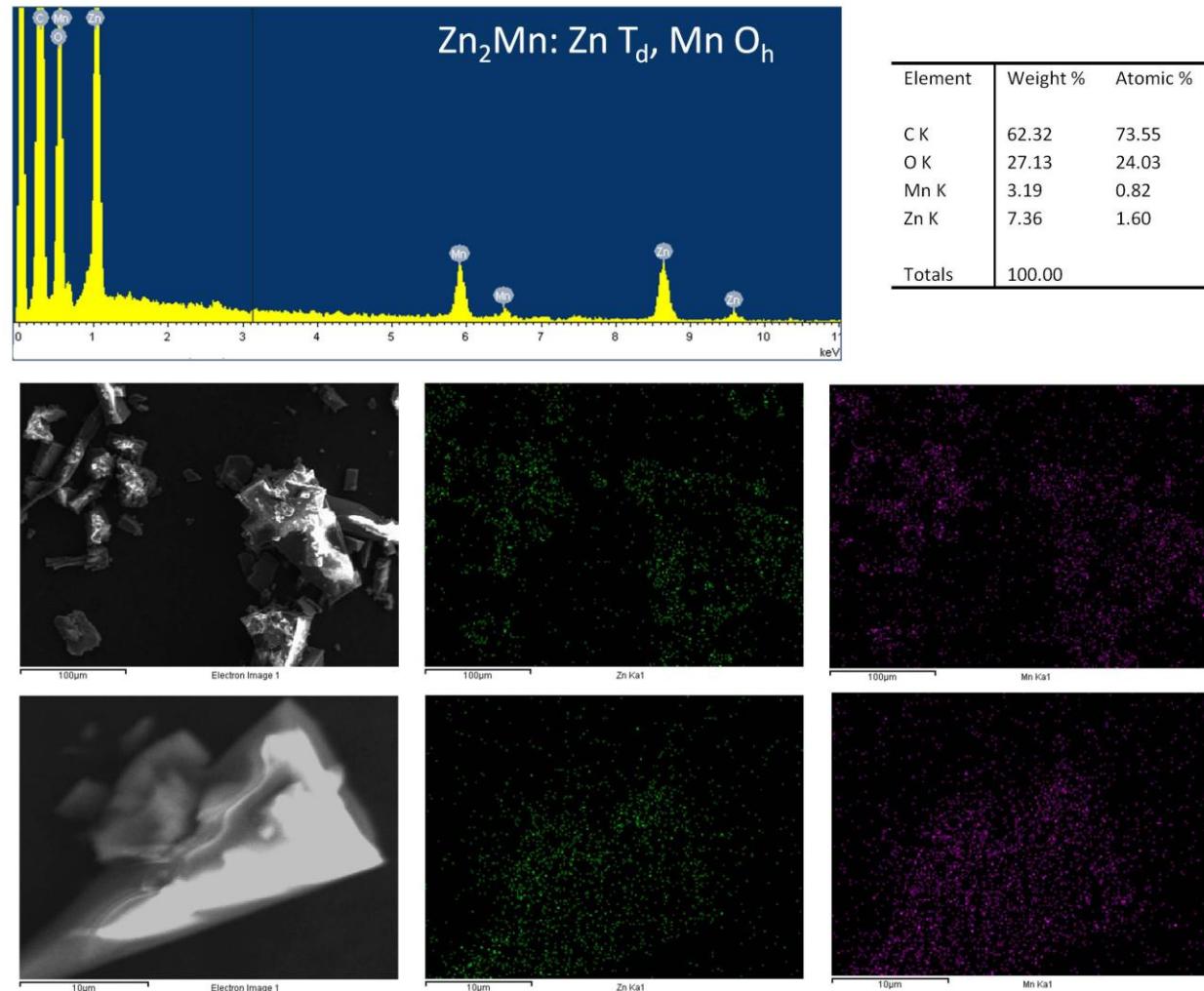


Fig. S4 EDS data for **6** showing observed ~2:1 ratio between Zn and Mn, and uniform distribution of Zn and Mn in the crystals within the resolution limit of the experiment.

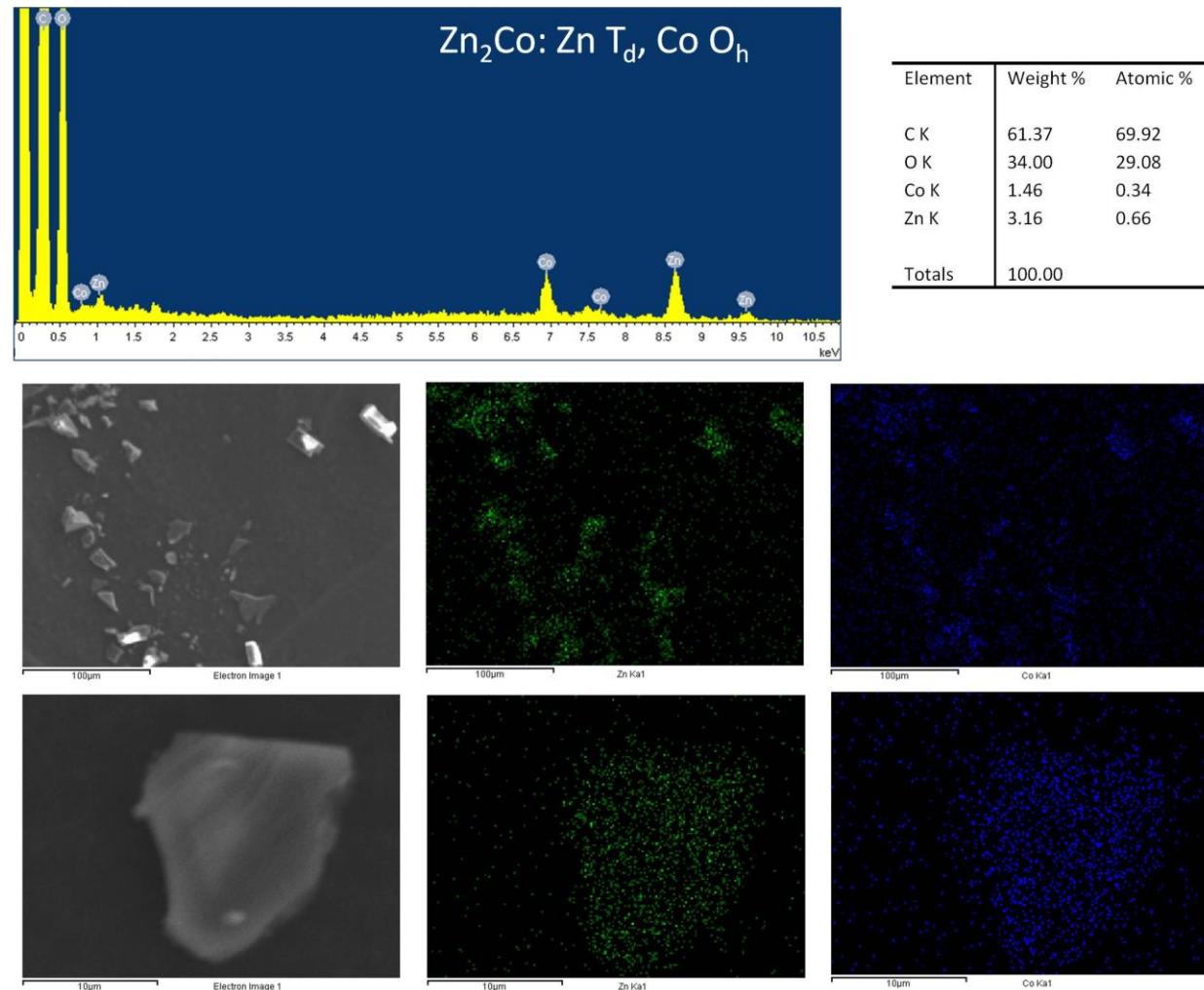


Fig. S5 EDS data for **7** showing observed ~2:1 ratio between Zn and Co, and uniform distribution of Zn and Co in the crystals within the resolution limit of the experiment.

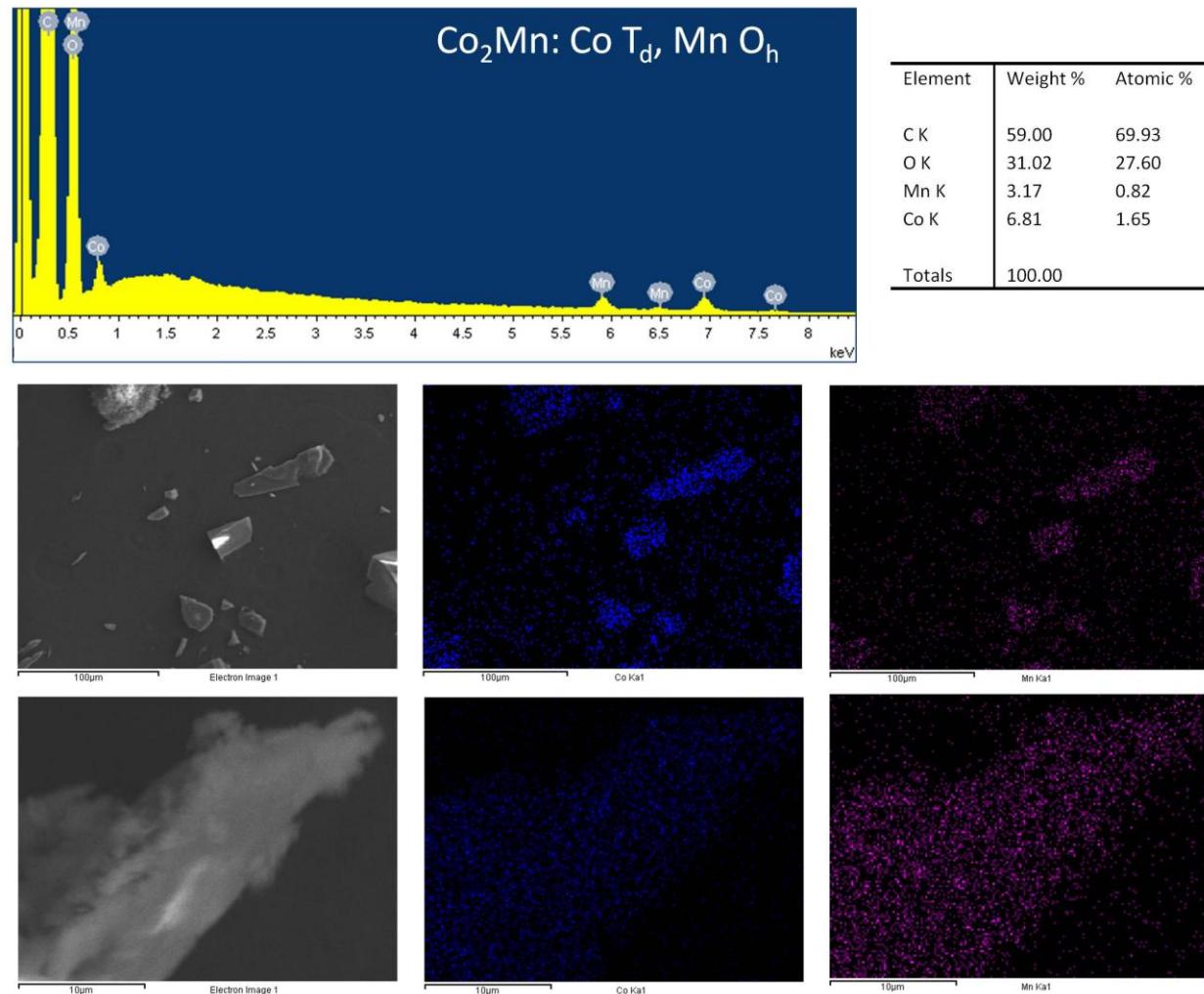


Fig. S6 EDS data for **8** showing observed ~2:1 ratio between Co and Mn, and uniform distribution of Co and Mn in the crystals within the resolution limit of the experiment.

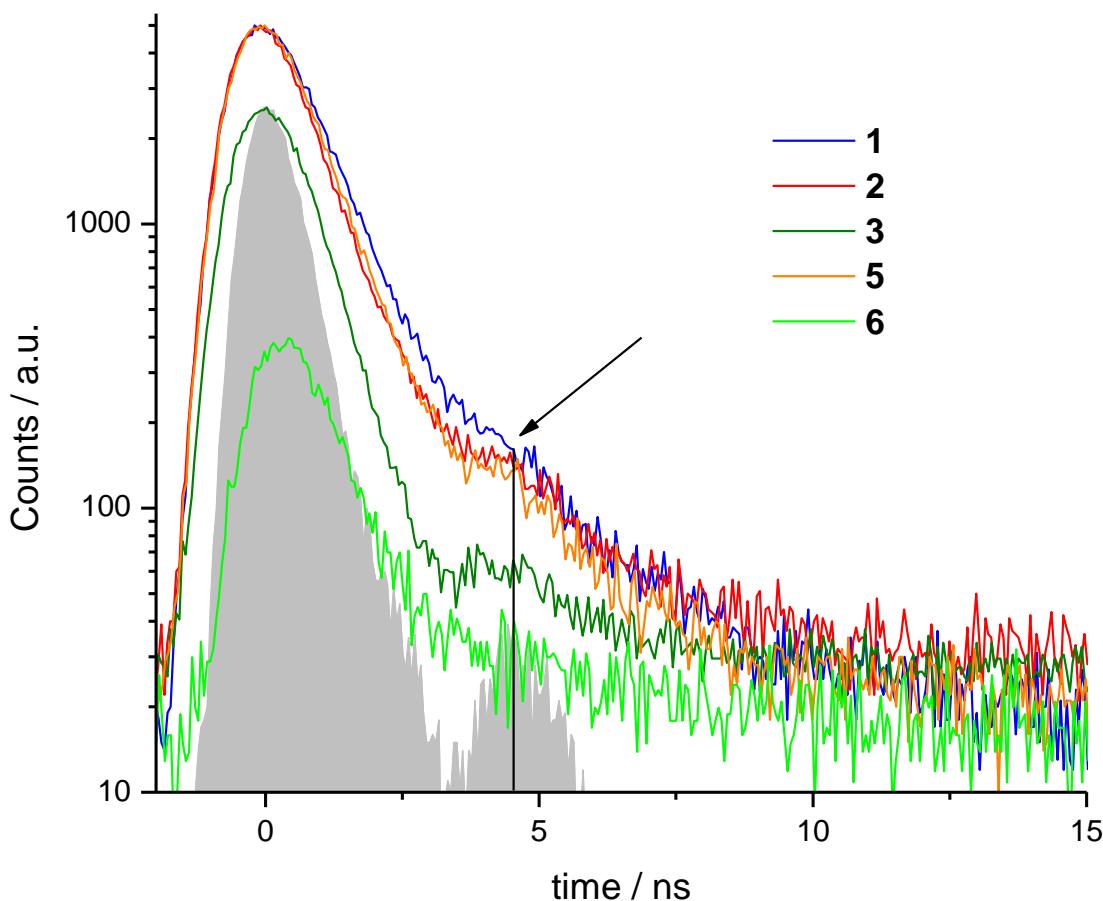


Fig. S7 TCSPC emission decay data measured for the emission of **1-3**, **5** and **6** after excitation at 330 nm, detected at 440 nm (the third vibronic peak). The grey shaded curve represents the instrument response function measured by scattering of LUDOX® HS-40 colloidal silica (40% suspension in water) under these conditions; the shoulder at ~4.5 ns indicated arises from the instrument response and is not a feature of the species investigated.