ELECTRONIC SUPPLEMENTARY INFORMATION

Unprecedented coordination of dithiocarbimate in homodimetallic, trinuclear heterometallic and heteroleptic complexes: synthesis, crystal and molecular structures and properties†

Bandana Singh[a] , Michael G. B. Drew§[b], Gabriele Kociok-Kohn[c] , Kieran C. Molloy§[c] and Nanhai Singh,*‡[a]

[a] Department of Chemistry, Faculty of Science, Banaras Hindu University, Varanasi 221005, India

*E-mail: nsingh@bhu.ac.in, Fax: 91 542 2368127 Tel: 91 542 2307321*108*

[b] Department of Chemistry, University of Reading, Whiteknights, Reading, RG6 6AD. U.K.
[c] Department of Chemistry, University of Bath, Bath, UK BA2 7AY

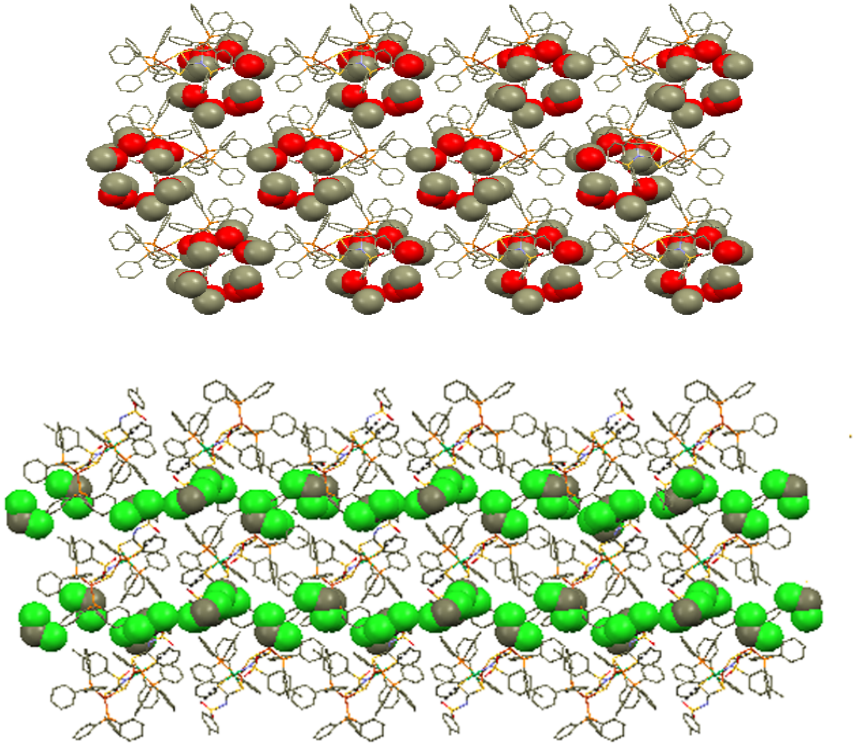

Figure S1. Molecular packing diagram of **1** (top) and **2** (bottom), showing the solvent molecules, methanol in **1** and dichloromethane in **2** as spheres, grey carbon, green chlorine, red oxygen. The solvent packing shows cavity like motif along the *a* axis in **1** and channel like motif along the *b* axis in **2**. Hydrogen atoms are omitted for clarity.

Table S1. Hydrogen bond geometry (Å, °) show inter- and intra- molecular interaction

Complex	D-H···A	D-H	H···A	D···A	D-H···A
1	O-H0···O2[a]	0.82	2.32	2.813	119
	O3-H3A···O4	0.82	1.94	2.753	170
	O4-H4A···O7	0.82	1.92	2.702	158
	O6-H6A···O3	0.82	2.21	2.890	140
	O7-H7A···O1[b]	0.82	2.26	2.840	128
	C4-H4···O1	0.93	2.53	2.907	105
	O7-H7A···S1[a]	0.82	2.92	3.664	148
2	C90-H90B···O2[c]	0.97	2.70	3.281	144
	C89-H89A···O3[d]	0.97	2.66	3.159	111
	C91-H91A···O4[d]	0.96	2.70	3.647	164
	C34-H34···N1[d]	0.92	2.44	3.323	157
	C81-H81···S4[e]	0.92	2.96	3.847	160
	C89-H89B···S2[f]	0.97	2.86	3.641	137
	C43-H43···Cl6[d]	0.93	2.90	3.694	143
3	C(20)–H(20)…S(2)[a]	0.95	2.93	3.682	136
	C(30)–H(30)…O(2)[a]	0.95	2.64	3.415	138
	C(42)–H(42)…O(2)[g]	0.95	2.41	3.329	162
4	C(20)–H(20)…S(2)[a]	0.95	2.90	3.661	138
	C(30)–H(30)…O(2)[a]	0.95	2.66	3.435	130
	C(42)–H(42)…O(2)[g]	0.95	2.41	3.332	163

Symmetry code: [a] = x, -1+y, z; [b] = x, 3/2-y, -1/2+ z; [c] = x, 1+y, z; [d] = 1+x, y; [e] = 1-x, -y; [f] = -x, -y, 2-z ; [g] = 1+x, -1+y, z.

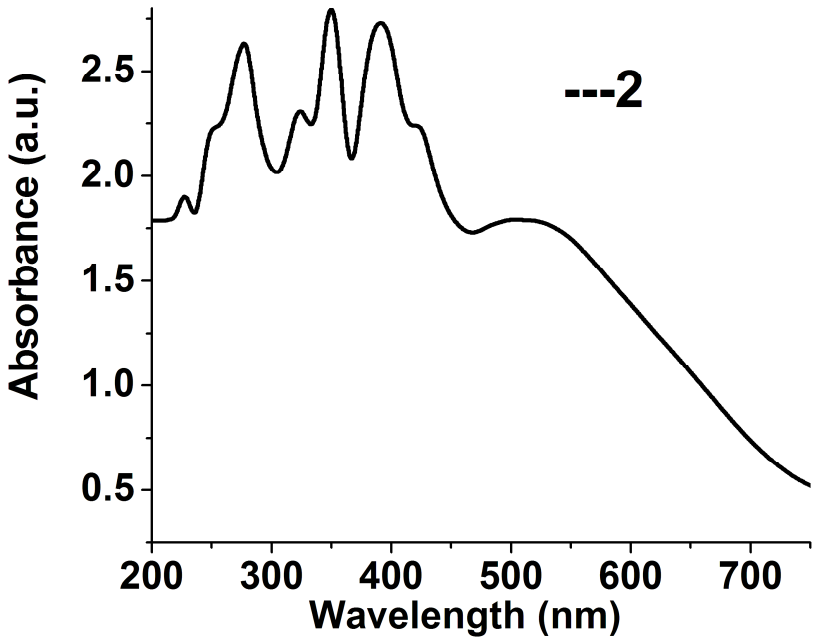

Figure S2. Electronic absorption spectra (as solid) in nujol mull of complex **2.**