SUPPORTING INFORMATION

THE EFFECT OF THE ORGANOMETALLIC FRAGMENT R= -$CCHCo_2(CO)_6$ ON THE PROPERTIES OF THE $M_2\{OOCR\}_4$ CLUSTERS, (M = Mo and Cu)

Víctor Calvo-Pérez[1]*, Andrés Vega[1,2], Evgenia Spodine[1]

Figure 1S. Crystal packing of compound **1b**. Carbon monoxide has been deleted to show the molybdenum cluster and the 1,4-xylene stacking that forms the chain.

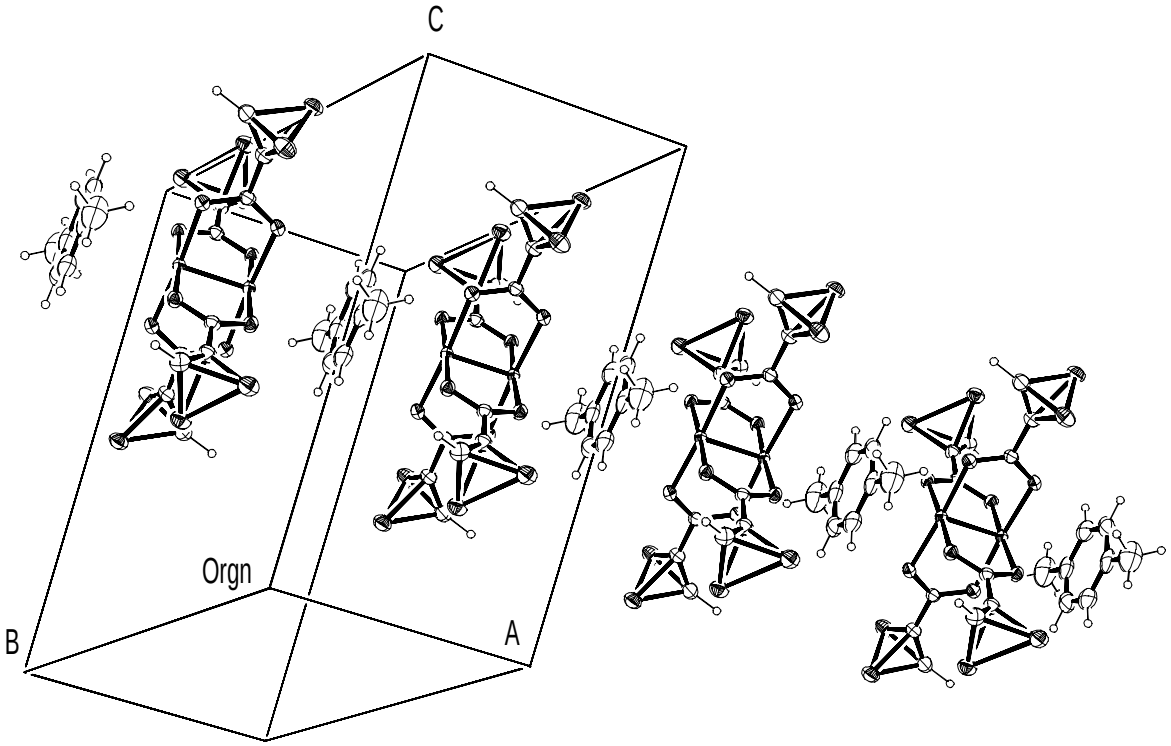


Figure 2S Packing of compound **1b**. Carbon monoxide has been deleted to show the metallic core and the numbering scheme of the 1,4-xylene.

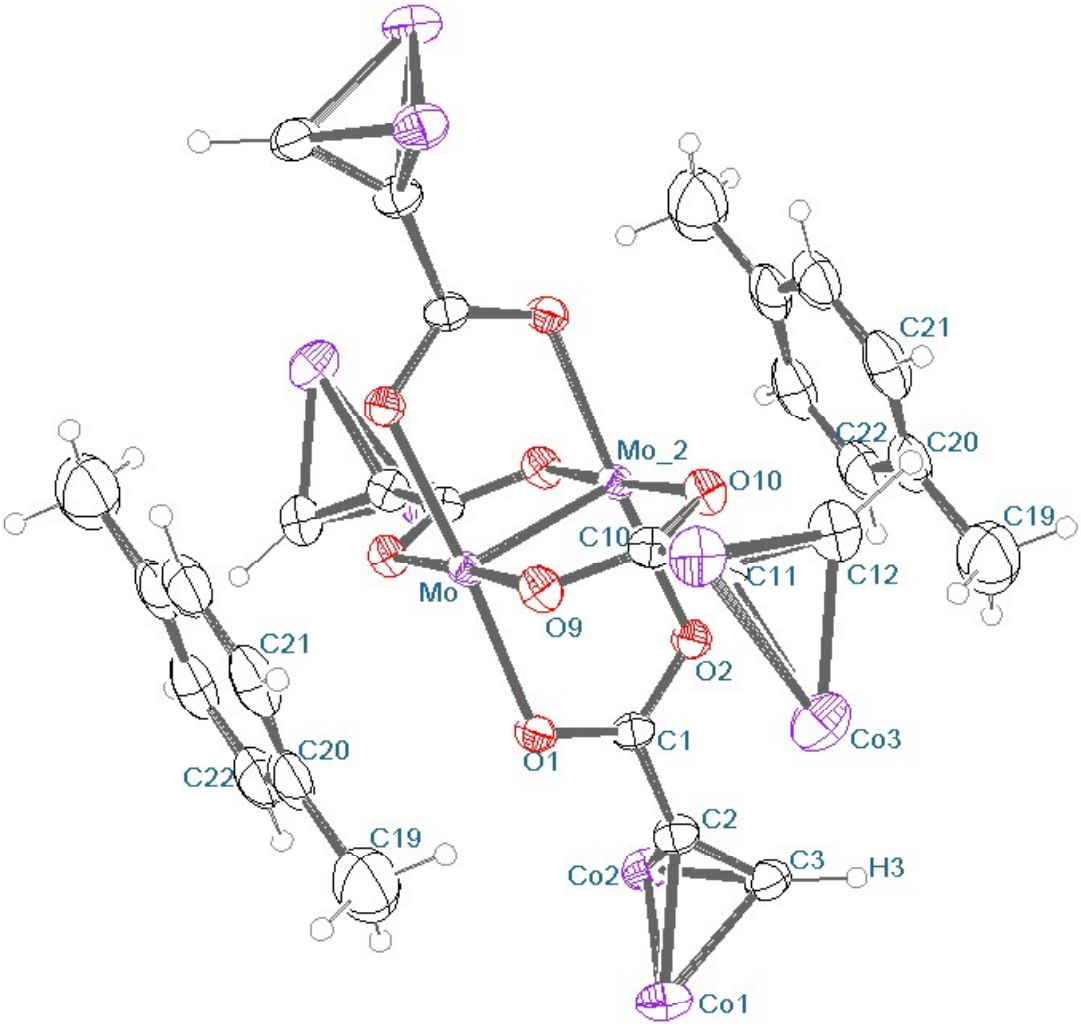


Figure 3S Molecular connectivity of compound **1c**. Carbon monoxide included to show the cluster ligand and the location of the toluene along the Mo-Mo axis. The methyl groups on the toluene (C111) are disordered over four positions. The hydrogen atoms were not found.

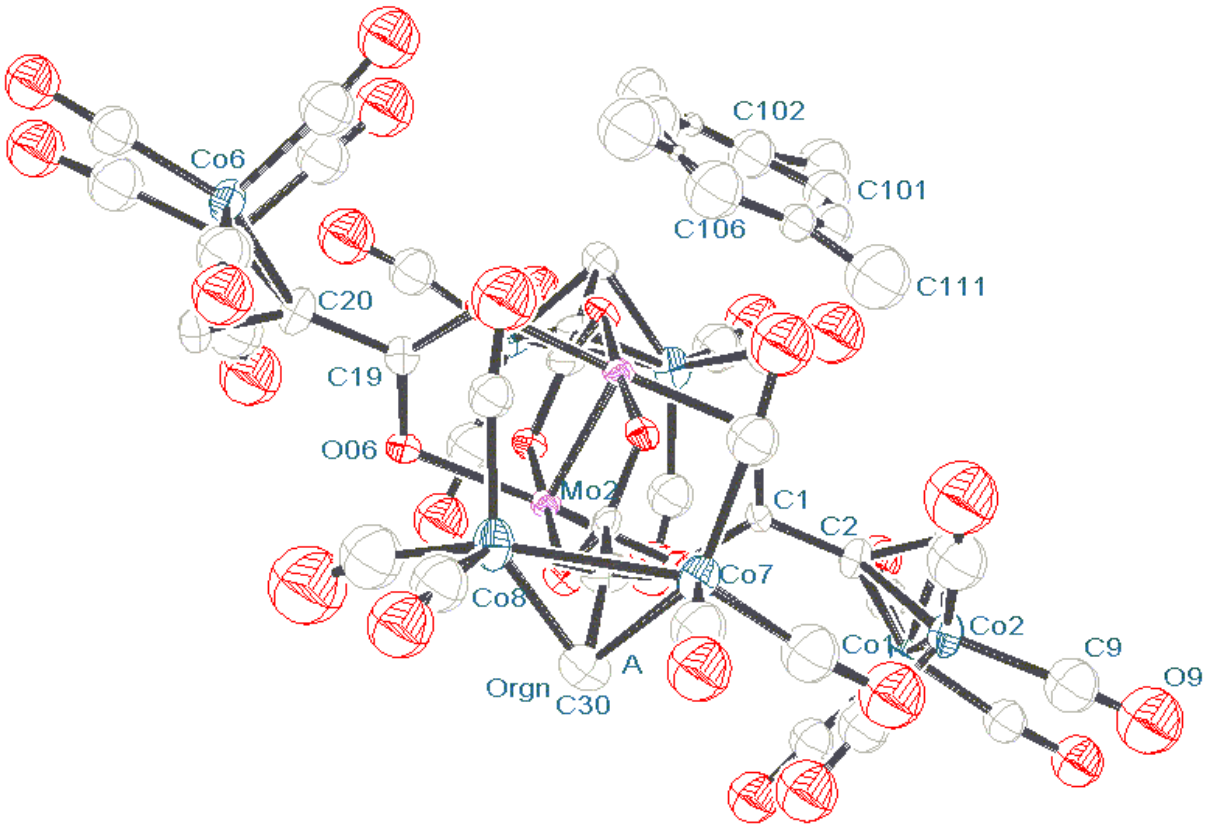


Figure 4S Fragment analysis of compound **1b** supermolecule. Only the benzene π-manifold shown for clarity. There are no great significant overlaps with the molybdenum manifold, except for the Mo π* orbitals. The basis set was LANL2DZ.

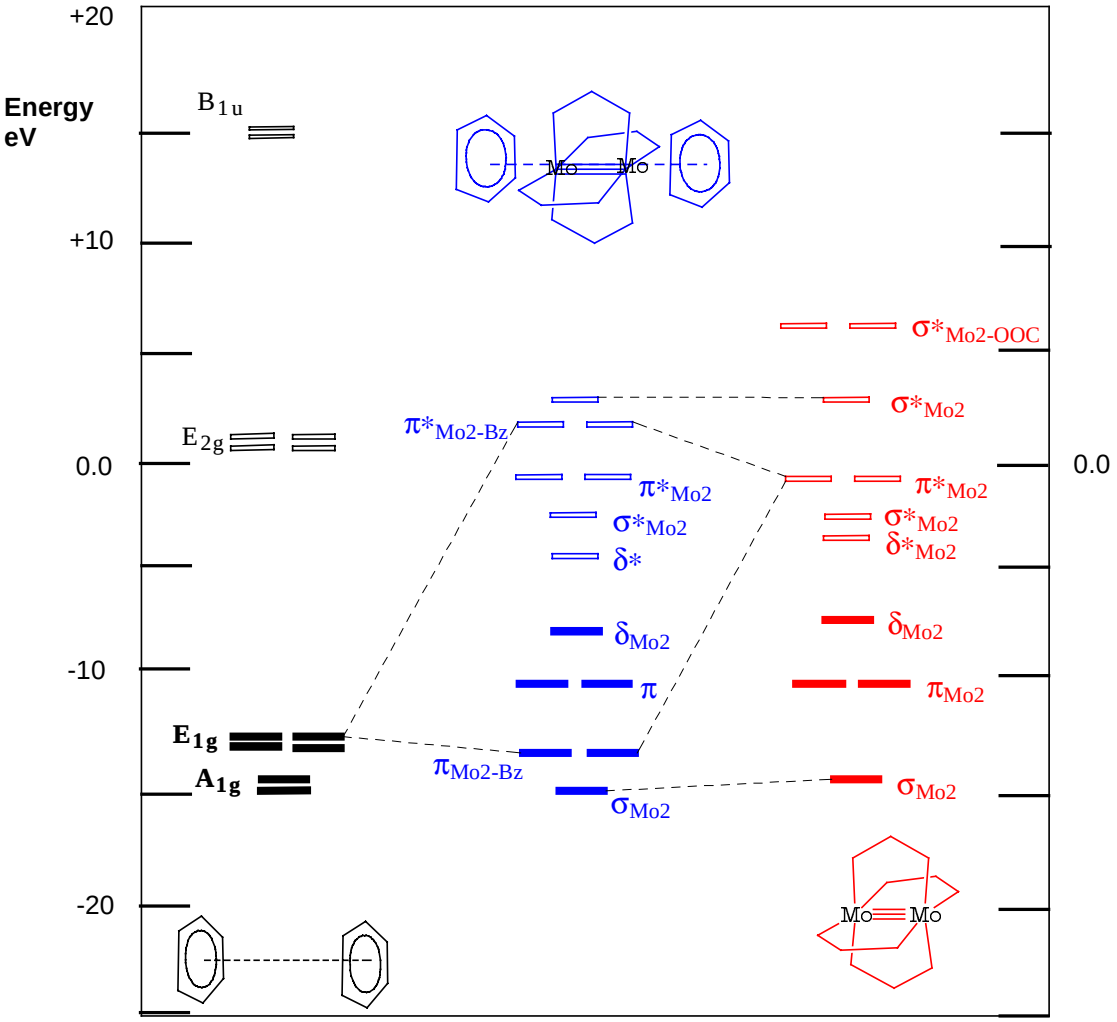


Figure 5S Cyclic voltammetry compound **1b** in acetone 0.1M Bu_4N ClO_4 at 100 mV/s. The quasi reversible couple correspond to the dimolybdenum core.

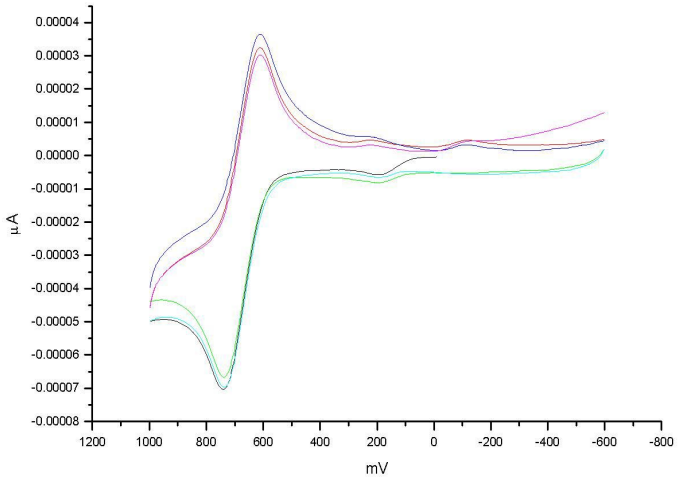


Figure 5S Cyclic voltammetry compound **1b** in acetone 0.1M Bu_4N ClO_4 at 100 mV/s. The irreversible reduction occurring at –1100 mV produces a series cobalt fragments that did not occur during narrower potential scans (c.a. 0 to +1200 mV).

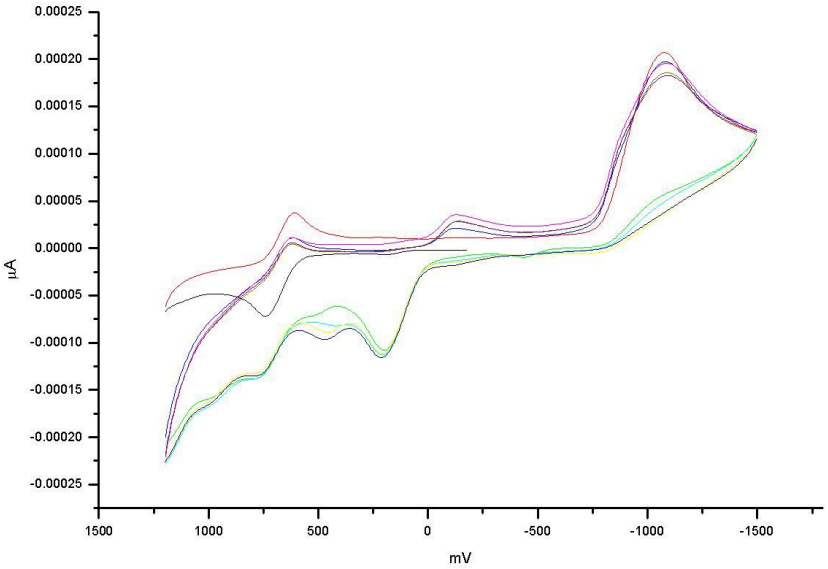
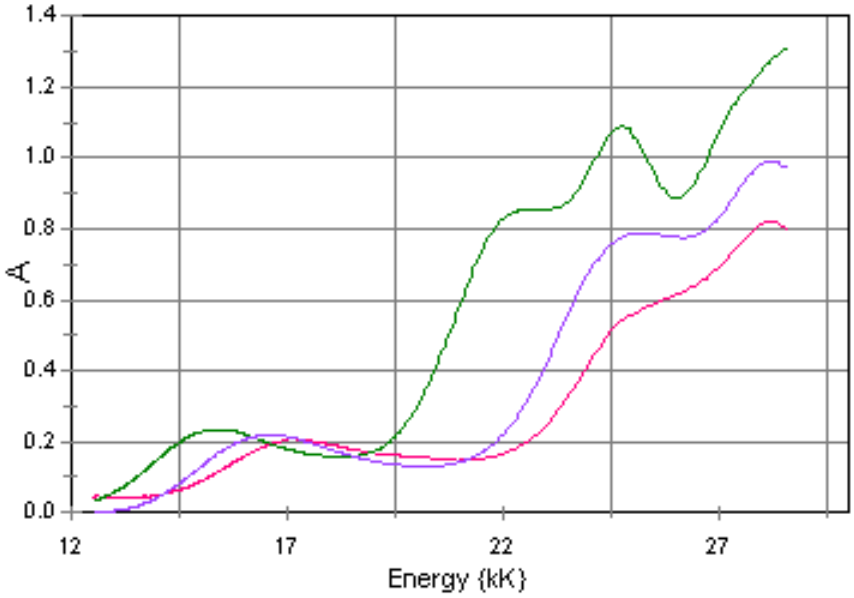


Figure 6S Electronic spectra of compound **1b** in three different solvents. tetrahydrofurane (green), toluene (blue), CH_2Cl_2 (red).



Computational results. Comparison of experimental and optimized distances and angles for $Mo_2\{OOCCCHCo_2(CO)_6\}_4$ using toluene as a polarizable continuum media (PCM).

(1)	Observed	Calculated	Error
Mo-O1	2.105(3)	2.136	-0.031
Mo-O2a	2.094(3)	2.136	-0.042
Mo-O10	2.113(2)	2.136	-0.023
Mo-O11a	2.106(3)	2.136	-0.030
Mo-Moa	2.099(1)	2.130	+0.031
C1-O1	1.260(4)	1.282	+0.022
C1-O2	1.281(4)	1.282	+0.001
C10-O10	1.272(4)	1.282	+0.010
C10-O11	1.271(4)	1.282	+0.011
C1-C2	1.458(5)	1.487	+0.029
C2-C3	1.337(6)	1.326	-0.011
C8-O8	1.123(7)	1.128	+0.005
C4-O4	1.121(7)	1.125	+0.004
Co1-Co2	2.473(1)	2.467	-0.006
Co3-Co4	2.466(2)	2.467	-0.001
Co2-C9	1.811(5)	1.802	+0.009
C12-H12	1.047	1. 080	+0.033
O1-Mo-O10	89.5(1)	90.0	+0.5
O1-Mo-O11a	90.3(1)	90.0	-0.3
O10-Mo2-O2a	90.6(1)	90.0	-0.6
O2a-Mo-O11a	89.4(1)	90.0	+0.6
O1-Mo2-O2a	176.4(1)	180.0	+3.6
O10-Mo-O11a	176.3(1)	180.0	+3.7
O1-C1-O2	122.8(3)	122.6	-0.2
C1-C2-C3	143.8(4)	140.8	-3.0
O10-C10-O11	122.9(3)	122.6	-0.3
C10-C11-C12	140.9(4)	140.8	-0.1

Table 1S. Atomic Coordinates (Å x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **1b**

atom	x	y	z	U(eq)
Mo	3761(1)	51(1)	5017(1)	29(1)
O1	4585(3)	1597(2)	6165(2)	37(1)
C1	6142(5)	1971(3)	6491(2)	36(1)
O2	7214(3)	1482(2)	6119(2)	36(1)
C2	6773(5)	2959(3)	7363(3)	42(1)
C3	8175(6)	3733(3)	7909(3)	49(1)
Co1	6186(1)	4256(1)	8125(1)	53(1)
Co2	7018(1)	2975(1)	8585(1)	49(1)
C4	6380(10)	4894(5)	7373(4)	92(2)
O4	6570(10)	5281(6)	6891(4)	161(3)
C5	3898(8)	3763(5)	8007(4)	74(2)
O5	2486(6)	3437(4)	7918(4)	114(2)
C6	6827(8)	5451(4)	9234(4)	75(2)
O6	7261(8)	6187(3)	9930(3)	124(2)
C7	8243(7)	2044(5)	8363(4)	67(1)
O7	9003(7)	1467(4)	8199(4)	112(2)
C8	4922(8)	2104(5)	8505(4)	68(1)
O8	3619(6)	1547(4)	8408(4)	112(2)
C9	7809(8)	3847(5)	9809(4)	76(2)
O9	8319(8)	4394(4)	10567(3)	120(2)
O10	4005(3)	798(2)	4121(2)	37(1)
C10	5438(5)	981(3)	3864(2)	35(1)
O11	6639(3)	683(2)	4084(2)	38(1)
C11	5779(5)	1579(3)	3306(3)	42(1)
C12	6935(6)	1856(4)	2834(3)	52(1)
Co3	6408(1)	3147(1)	3692(1)	59(1)
Co4	4665(1)	1626(1)	2248(1)	50(1)
C13	7330(10)	4129(5)	3268(5)	88(2)
O13	7928(8)	4704(4)	2978(4)	145(3)
C14	7940(10)	3642(5)	4704(5)	105(2)
O14	8890(10)	3945(5)	5338(5)	179(3)
C15	4710(10)	3583(5)	4270(4)	81(2)
O15	3604(8)	3811(4)	4596(4)	128(2)
C16	4874(7)	2354(4)	1548(4)	68(1)
O16	5037(7)	2809(4)	1114(3)	105(2)
C17	4322(7)	300(5)	1320(4)	67(1)
O17	4159(7)	-540(3)	729(3)	98(1)
C18	2540(8)	1534(5)	2537(4)	74(2)
O18	1264(6)	1503(5)	2743(4)	115(2)
C19	1170(10)	2266(6)	5437(6)	120(3)
C20	561(6)	1094(5)	5210(5)	72(2)
C21	48(6)	303(6)	4298(5)	73(2)
C22	497(6)	773(5)	5903(4)	73(2)
C23	9530(10)	2130(6)	935(5)	108(2)
C24	9774(7)	1030(5)	455(4)	73(2)
C25	10894(8)	837(5)	-160(4)	78(2)
C26	8871(8)	162(6)	588(4)	84(2)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE 2S. Bond lengths (Å) for **1b**

Mo-O2#2	2.094(3)	Mo-Mo#2	2.099(1)
Mo-O1	2.105(3)	Mo-O11#2	2.106(3)
Mo-O10	2.113(2)	Mo-C22	3.301(5)
Mo-C20	3.326(5)	Mo-C21	3.411(5)
Mo-Mo#2	6.202(2)	O1-C1	1.260(4)
C1-O2	1.281(4)	C1-C2	1.458(5)
O2-Mo#2	2.094(3)	C2-C3	1.337(6)
C2-Co1	1.937(4)	C2-Co2	1.962(4)
C3-Co2	1.951(5)	C3-Co1	1.964(5)
Co1-C4	1.785(6)	Co1-C6	1.808(6)
Co1-C5	1.818(7)	Co1-Co2	2.473(1)
Co2-C7	1.800(6)	Co2-C9	1.811(5)
Co2-C8	1.820(6)	C4-O4	1.121(7)
C5-O5	1.122(7)	C6-O6	1.127(6)
C7-O7	1.113(6)	C8-O8	1.123(7)
C9-O9	1.125(6)	O10-C10	1.272(4)
C10-O11	1.271(4)	C10-C11	1.468(5)
O11-Mo#2	2.106(3)	C11-C12	1.328(6)
C11-Co4	1.944(4)	C11-Co3	1.963(4)
C12-Co3	1.949(5)	C12-Co4	1.960(4)
Co3-C14	1.784(7)	Co3-C13	1.816(6)
Co3-C15	1.817(7)	Co3-Co4	2.466(2)
Co4-C17	1.787(6)	Co4-C16	1.814(5)
Co4-C18	1.825(6)	C13-O13	1.125(7)
C14-O14	1.118(8)	C15-O15	1.124(8)
C16-O16	1.125(6)	C17-O17	1.141(6)
C18-O18	1.116(7)	C19-C20	1.487(8)
C20-C22	1.372(8)	C20-C21	1.384(9)
C21-C22#2	1.368(8)	C23-C24	1.498(9)
C24-C25	1.373(8)	C24-C26	1.376(8)
C25-C26#2	1.365(9)	C3-H3	1.047
C12-H12	1.047	C19-H19b	0.959
C19-H19a	0.960	C19-H19c	0.960
C21-H21a	0.960	C22-H22a	0.960
C23-H23b	0.960	C23-H23a	0.961
C23-H23c	0.961	C25-H25a	0.960
C26-H26a	0.960		

TABLE 2S. Angles (deg) for **1b continued**

O2-Mo#2-Mo#2	91.89(8)	O2-Mo#2-O1	176.4(1)
Mo-Mo#2-O1	91.71(8)	O2-Mo#2-O11#2	89.4(1)
Mo-Mo#2-O11#2	91.38(7)	O1-Mo-O11#2	90.3(1)
O2-Mo#2-O10	90.6(1)	Mo-Mo#2-O10	92.30(7)
O1-Mo-O10	89.5(1)	O11-Mo#2-O10	176.3(1)
O2-Mo#2-C22	106.9(1)	Mo-Mo#2-C22	158.3(1)
O1-Mo-C22	69.6(1)	O11-Mo#2-C22	78.4(1)
O10-Mo-C22	98.1(1)	O2-Mo#2-C20	103.1(1)
Mo-Mo#2-C20	159.9(1)	O1-Mo-C20	73.4(1)
O11-Mo#2-C20	101.9(1)	O10-Mo-C20	74.5(1)
C22-Mo-C20	23.9(1)	O2-Mo#2-C21	80.8(1)
Mo-Mo#2-C21	157.5(1)	O1-Mo-C21	95.9(1)
O11-Mo#2-C21	109.7(1)	O10-Mo-C21	66.7(1)
C22-Mo-C21	41.3(1)	C20-Mo-C21	23.7(2)
O2-Mo#2-Mo#2	84.05(7)	Mo-Mo#2-Mo#2	175.37(2)
O1-Mo-Mo#2	92.35(8)	O11-Mo#2-Mo#2	86.38(7)
O10-Mo-Mo#2	89.97(7)	C22-Mo-Mo#2	24.4(1)
C20-Mo-Mo#2	24.6(1)	C21-Mo-Mo#2	23.6(1)
C1-O1-Mo	116.8(2)	O1-C1-O2	122.8(3)
O1-C1-C2	120.0(3)	O2-C1-C2	117.1(3)
C1-O2-Mo#2	116.7(2)	C3-C2-C1	143.8(4)
C3-C2-Co1	71.1(3)	C1-C2-Co1	140.3(3)
C3-C2-Co2	69.6(3)	C1-C2-Co2	123.9(3)
Co1-C2-Co2	78.8(2)	C2-C3-Co2	70.5(3)
C2-C3-Co1	68.9(3)	Co2-C3-Co1	78.4(2)
C4-Co1-C6	99.4(3)	C4-Co1-C5	100.8(3)
C6-Co1-C5	104.5(3)	C4-Co1-C2	99.9(2)
C6-Co1-C2	142.3(2)	C5-Co1-C2	103.2(2)
C4-Co1-C3	98.5(3)	C6-Co1-C3	105.1(2)
C5-Co1-C3	141.2(2)	C2-Co1-C3	40.1(2)
C4-Co1-Co2	147.4(2)	C6-Co1-Co2	98.8(2)
C5-Co1-Co2	100.4(2)	C2-Co1-Co2	51.1(1)
C3-Co1-Co2	50.6(1)	C7-Co2-C9	99.8(3)
C7-Co2-C8	100.9(3)	C9-Co2-C8	106.7(3)
C7-Co2-C3	96.8(2)	C9-Co2-C3	107.1(2)
C8-Co2-C3	138.2(2)	C7-Co2-C2	99.3(2)
C9-Co2-C2	143.7(2)	C8-Co2-C2	99.6(2)
C3-Co2-C2	40.0(2)	C7-Co2-Co1	146.1(2)
C9-Co2-Co1	100.3(2)	C8-Co2-Co1	99.1(2)
C3-Co2-Co1	51.1(1)	C2-Co2-Co1	50.2(1)
O4-C4-Co1	177.1(7)	O5-C5-Co1	178.4(6)
O6-C6-Co1	178.1(6)	O7-C7-Co2	177.8(5)
O8-C8-Co2	176.5(5)	O9-C9-Co2	179.1(7)
C10-O10-Mo	116.0(2)	O11-C10-O10	122.9(3)
O11-C10-C11	117.0(3)	O10-C10-C11	120.1(3)
C10-O11-Mo#2	117.2(2)	C12-C11-C10	140.9(4)
C12-C11-Co4	70.8(3)	C10-C11-Co4	139.0(3)
C12-C11-Co3	69.6(3)	C10-C11-Co3	129.9(3)
Co4-C11-Co3	78.3(2)	C11-C12-Co3	70.7(3)
C11-C12-Co4	69.5(3)	Co3-C12-Co4	78.3(2)
C14-Co3-C13	99.4(3)	C14-Co3-C15	97.8(4)
C13-Co3-C15	105.6(3)	C14-Co3-C12	102.6(3)
C13-Co3-C12	102.4(3)	C15-Co3-C12	141.9(2)
C14-Co3-C11	100.6(2)	C13-Co3-C11	140.3(3)
C15-Co3-C11	105.2(2)	C12-Co3-C11	39.7(2)
C14-Co3-Co4	149.9(2)	C13-Co3-Co4	100.5(2)
C15-Co3-Co4	98.2(2)	C12-Co3-Co4	51.1(1)
C11-Co3-Co4	50.5(1)	C17-Co4-C16	97.3(2)
C17-Co4-C18	100.9(3)	C16-Co4-C18	104.4(3)
C17-Co4-C11	104.2(2)	C16-Co4-C11	143.4(2)
C18-Co4-C11	100.2(2)	C17-Co4-C12	99.1(2)

C16-Co4-C12	108.2(2)	C18-Co4-C12	138.9(2)
C11-Co4-C12	39.8(2)	C17-Co4-Co3	149.4(2)
C16-Co4-Co3	97.1(2)	C18-Co4-Co3	101.4(2)
C11-Co4-Co3	51.2(1)	C12-Co4-Co3	50.7(2)
O13-C13-Co3	177.0(7)	O14-C14-Co3	179.4(8)
O15-C15-Co3	176.8(7)	O16-C16-Co4	178.6(6)
O17-C17-Co4	177.7(6)	O18-C18-Co4	177.7(6)
C22-C20-C21	118.5(5)	C22-C20-C19	120.4(7)
C21-C20-C19	121.0(7)	C22-C20-Mo	77.1(3)
C21-C20-Mo	81.6(3)	C19-C20-Mo	111.1(4)
C22-C21#2-C20	120.5(5)	C22-C21#2-Mo	81.2(3)
C20-C21-Mo	74.7(3)	C21-C22#2-C20	120.9(6)
C21-C22#2-Mo	80.9(3)	C20-C22-Mo	79.1(3)
C25-C24-C26	116.7(6)	C25-C24-C23	121.0(6)
C26-C24-C23	122.2(6)	C26-C25#2-C24	121.0(6)
C25-C26#2-C24	122.2(6)	H3-C3-C2	143.46
H3-C3-Co2	136.27	H3-C3-Co1	130.99
H12-C12-C11	141.07	H12-C12-Co3	136.79
H12-C12-Co4	132.34	H19b-C19-H19a	109.49
H19b-C19-H19c	109.59	H19b-C19-C20	109.61
H19a-C19-H19c	109.42	H19a-C19-C20	108.57
H19c-C19-C20	110.13	H21a-C21-C22#2	120.01
H21a-C21-C20	119.48	H22a-C22-C21#2	119.89
H22a-C22-C20	119.11	H23b-C23-H23a	109.42
H23b-C23-H23c	109.43	H23b-C23-C24	109.64
H23a-C23-H23c	109.49	H23a-C23-C24	109.65
H23c-C23-C24	109.19	H25a-C25-C26#2	119.42
H25a-C25-C24	119.59	H26a-C26-C25#2	119.20
H26a-C26-C24	118.55		

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::
1: x, y, z 2: -x, -y, -z

TABLE 3S. Anisotropic displacement parameters ($Å^2$ x 10^3) for **1b**

atom	U11	U22	U33	U23	U13	U12
Mo	27(1)	34(1)	28(1)	13(1)	5(1)	14(1)
O1	36(1)	37(1)	34(1)	10(1)	5(1)	16(1)
C1	43(2)	33(2)	29(2)	12(2)	3(2)	13(2)
O2	31(1)	37(1)	34(1)	11(1)	1(1)	11(1)
C2	48(2)	39(2)	37(2)	14(2)	1(2)	15(2)
C3	55(3)	39(2)	44(2)	12(2)	6(2)	11(2)
Co1	74(1)	40(1)	41(1)	12(1)	7(1)	24(1)
Co2	61(1)	46(1)	37(1)	16(1)	3(1)	16(1)
C4	151(7)	86(4)	66(4)	37(3)	21(4)	68(4)
O4	261(8)	194(6)	141(5)	134(5)	83(5)	140(6)
C5	75(4)	75(4)	67(3)	16(3)	9(3)	41(3)
O5	75(3)	126(4)	124(4)	35(3)	15(3)	41(3)
C6	110(5)	48(3)	61(3)	18(3)	9(3)	29(3)
O6	214(6)	59(3)	62(3)	-4(2)	3(3)	37(3)
C7	79(4)	71(3)	63(3)	36(3)	9(3)	31(3)
O7	140(4)	131(4)	120(4)	75(3)	39(3)	93(4)
C8	73(4)	73(4)	69(3)	41(3)	22(3)	20(3)
O8	81(3)	119(4)	152(5)	85(4)	34(3)	12(3)
C9	109(5)	64(3)	48(3)	22(3)	2(3)	23(3)
O9	177(5)	100(3)	45(2)	12(2)	-20(3)	24(3)
O10	36(1)	46(2)	39(1)	24(1)	5(1)	18(1)
C10	41(2)	37(2)	30(2)	15(2)	5(2)	14(2)
O11	36(1)	46(2)	39(1)	23(1)	8(1)	15(1)
C11	47(2)	48(2)	38(2)	23(2)	6(2)	17(2)
C12	46(2)	66(3)	54(3)	36(2)	8(2)	17(2)
Co3	69(1)	50(1)	58(1)	30(1)	-1(1)	11(1)
Co4	57(1)	59(1)	44(1)	32(1)	6(1)	18(1)
C13	96(5)	67(4)	91(4)	46(3)	-10(4)	-5(3)
O13	175(6)	106(4)	146(5)	92(4)	-2(4)	-29(4)
C14	124(6)	76(4)	95(5)	29(4)	-36(5)	20(4)
O14	202(7)	136(5)	138(5)	24(4)	-98(5)	36(5)
C15	110(5)	58(3)	76(4)	29(3)	23(4)	27(3)
O15	155(5)	91(4)	143(5)	43(3)	83(4)	52(4)
C16	89(4)	67(3)	55(3)	36(3)	6(3)	22(3)
O16	146(4)	107(3)	94(3)	79(3)	12(3)	31(3)
C17	84(4)	67(3)	55(3)	37(3)	2(3)	17(3)
O17	136(4)	65(3)	78(3)	20(2)	-1(3)	27(3)
C18	63(3)	112(5)	63(3)	51(3)	7(3)	32(3)
O18	70(3)	194(6)	105(4)	83(4)	25(3)	51(3)
C19	91(5)	112(6)	178(9)	78(6)	37(5)	41(5)
C20	40(3)	79(4)	123(5)	59(4)	32(3)	33(3)
C21	44(3)	113(5)	98(5)	71(4)	27(3)	39(3)
C22	43(3)	95(4)	84(4)	39(3)	18(3)	27(3)
C23	121(6)	117(6)	94(5)	51(5)	33(4)	40(5)
C24	73(4)	94(4)	55(3)	39(3)	10(3)	22(3)
C25	74(4)	92(4)	75(4)	50(4)	16(3)	12(3)
C26	71(4)	115(5)	75(4)	51(4)	27(3)	24(4)

The anisotropic displacement factor exponent takes the form
$2\ pi^2\ [h^2a^2U(11) + ... + 2hka^*b^*U(12)]$

TABLE 4S. Hydrogen Coordinates (Å x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **1b**

atom	x	y	z	U(eq)
H3	9430(20)	4130(30)	7910(30)	50
H12	8000(40)	1670(40)	2560(30)	80(20)
H19A	1463	2682	6099	80
H19B	2151	2402	5157	80
H19C	299	2472	5212	80
H21A	82	515	3805	80
H22A	854	1315	6537	80
H23A	8713	2117	1339	80
H23B	10590	2656	1293	80
H23C	9143	2323	478	80
H25A	11515	1411	-295	80
H26A	8043	265	993	80

TABLE 5S. Atomic Coordinates (Å x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **2**

atom	x	y	z	U(eq)
Cu	1440(3)	5338(2)	103(2)	39(1)
O1	2770(20)	4290(10)	-540(10)	42(4)
C1	1990(30)	3770(20)	-930(20)	37(6)
O2	230(20)	3760(10)	-690(10)	45(4)
C2	3120(30)	3060(20)	-1530(20)	57(7)
C3	4640(30)	2490(20)	-1590(20)	38(6)
Co1	2646(5)	1985(3)	-1950(3)	64(1)
Co2	3942(5)	3652(3)	-2932(3)	69(1)
C4	460(50)	2360(30)	-2270(30)	130(10)
O4	-1040(30)	2690(20)	-2350(20)	160(10)
C5	2360(50)	950(20)	-860(20)	100(10)
O5	2340(30)	220(20)	-50(20)	128(9)
C6	3600(30)	1200(20)	-2820(20)	80(10)
O6	4320(30)	760(20)	-3370(20)	140(10)
C7	5230(40)	3350(20)	-3990(20)	80(10)
O7	6090(30)	3010(20)	-4630(20)	140(10)
C8A	4700(60)	4970(20)	-3080(60)	170(30)
C8B	5860(30)	4390(30)	-3010(60)	140(30)
O8	5980(30)	5200(20)	-2930(20)	190(10)
C9	1970(40)	4510(30)	-3470(30)	140(20)
O9	800(40)	4990(30)	-3770(30)	230(20)
O10	1530(20)	4160(10)	1410(10)	49(4)
C10	330(30)	3580(20)	1690(20)	33(6)
O11	-960(20)	3680(10)	1250(10)	60(5)
C11	630(30)	2580(20)	2590(20)	35(6)
C12	-350(30)	1920(20)	3380(20)	42(6)
Co3	2210(4)	1838(3)	3639(3)	54(1)
Co4	1119(4)	1144(3)	2469(3)	59(1)
C13	4340(40)	2240(20)	3000(20)	69(8)
O13	5650(20)	2440(20)	2510(20)	140(9)
C14	1740(40)	2610(30)	4520(30)	110(10)
O14	1450(40)	3120(20)	5040(20)	160(10)
C15	2770(30)	580(20)	4600(20)	56(8)
O15	3000(20)	-280(10)	5200(20)	87(7)
C16	1170(30)	-260(20)	3250(20)	75(9)
O16	930(30)	-1110(10)	3720(20)	130(10)
C17	-500(40)	1330(20)	1580(20)	80(10)
O17	-1580(30)	1400(20)	1120(20)	114(8)
C18	3090(30)	1240(20)	1550(20)	75(9)
O18	4400(30)	1300(20)	1020(20)	124(9)
O1W	3640(20)	6150(10)	90(10)	56(5)

U(eq) is defined as 1/3 the trace of the Uij tensor.

TABLE 6S. Bond lengths (Å) for **2**

Cu-O1	1.98(1)	Cu-O2#2	1.90(1)
Cu-O10	1.96(1)	Cu-O11#2	1.95(2)
Cu-O1W	2.16(1)	Cu-Cu#2	2.631(5)
C1-O1	1.29(2)	C1-O2	1.34(2)
C1-C2	1.55(1)	C2-C3	1.29(3)
Co1-C2	1.85(2)	Co2-C2	1.88(2)
Co1-C3	1.99(2)	Co2-C3	2.06(2)
Co1-Co2	2.471(5)	Co1-C5	1.69(3)
Co1-C4	1.76(4)	Co1-C6	1.87(3)
C4-O4	1.17(4)	C5-O5	1.21(3)
C6-O6	1.14(3)	Co2-C7	1.77(3)
Co2-C8A	1.89(1)	Co2-C8B	1.89(1)
Co2-C9	1.83(3)	C7-O7	1.19(3)
C8A-O8	1.15(1)	C8B-O8	1.15(1)
C9-O9	1.07(3)	C10-O10	1.25(2)
C10-O11	1.21(2)	C10-C11	1.51(3)
C11-C12	1.36(2)	Co3-C11	1.93(2)
Co4-C11	1.96(2)	Co3-C12	2.04(2)
Co4-C12	2.01(2)	Co3-Co4	2.452(5)
Co3-C13	1.82(3)	Co3-C14	1.82(3)
Co3-C15	1.79(3)	C13-O13	1.14(3)
C14-O14	1.14(3)	C15-O15	1.17(3)
Co4-C16	1.82(3)	Co4-C17	1.83(3)
Co4-C18	1.81(3)	C16-O16	1.13(3)
C17-O17	1.11(3)	C18-O18	1.15(3)

TABLE 6S. Angles (deg) for **2 continued**

O2-Cu#2-O11#2	89.0(6)	O2-Cu#2-O10	92.6(6)
O11-Cu#2-O10	166.9(5)	O2-Cu#2-O1	168.9(5)
O11-Cu#2-O1	89.2(6)	O10-Cu-O1	86.6(6)
O2-Cu#2-O1W	93.3(5)	O11-Cu#2-O1W	90.7(5)
O10-Cu-O1W	102.2(5)	O1-Cu-O1W	97.7(5)
C1-O1-Cu	122(1)	O1-C1-O2	119(2)
O1-C1-C2	119(2)	O2-C1-C2	122(2)
C1-O2-Cu#2	129(1)	C3-C2-C1	142(2)
C3-C2-Co1	76(1)	C1-C2-Co1	133(2)
C3-C2-Co2	79(2)	C1-C2-Co2	121(2)
Co1-C2-Co2	83.0(8)	C2-C3-Co1	65(1)
C2-C3-Co2	64(1)	Co1-C3-Co2	75.3(7)
C5-Co1-C4	100(2)	C5-Co1-C2	105(1)
C4-Co1-C2	105(1)	C5-Co1-C6	98(1)
C4-Co1-C6	101(1)	C2-Co1-C6	141(1)
C5-Co1-C3	98(1)	C4-Co1-C3	144(1)
C2-Co1-C3	39.1(7)	C6-Co1-C3	108(1)
C5-Co1-Co2	150(1)	C4-Co1-Co2	101(1)
C2-Co1-Co2	49.1(7)	C6-Co1-Co2	98(1)
C3-Co1-Co2	53.7(6)	C7-Co2-C9	104(2)
C7-Co2-C2	144(1)	C9-Co2-C2	103(2)
C7-Co2-C8B	83(2)	C9-Co2-C8B	115(2)
C2-Co2-C8B	107(2)	C7-Co2-C8A	101(3)
C9-Co2-C8A	83(2)	C2-Co2-C8A	106(3)
C7-Co2-C3	109(1)	C9-Co2-C3	140(2)
C2-Co2-C3	37.8(7)	C8B-Co2-C3	92(2)
C8A-Co2-C3	111(2)	C7-Co2-Co1	103(1)
C9-Co2-Co1	100(1)	C2-Co2-Co1	47.8(6)
C8B-Co2-Co1	142(2)	C8A-Co2-Co1	154(3)
C3-Co2-Co1	51.0(5)	O4-C4-Co1	168(3)
O5-C5-Co1	173(4)	O6-C6-Co1	174(3)
O7-C7-Co2	172(3)	O8-C8A-Co2	133(3)
O8-C8B-Co2	135(3)	O9-C9-Co2	178(6)
C10-O10-Cu	118(1)	O11-C10-O10	127(2)
O11-C10-C11	117(2)	O10-C10-C11	116(2)
C10-O11-Cu#2	127(1)	C12-C11-C10	138(2)
C12-C11-Co3	74(1)	C10-C11-Co3	143(2)
C12-C11-Co4	72(1)	C10-C11-Co4	123(1)
Co3-C11-Co4	78.1(8)	C11-C12-Co4	68(1)
C11-C12-Co3	66(1)	Co4-C12-Co3	74.5(8)
C15-Co3-C14	95(2)	C15-Co3-C13	104(1)
C14-Co3-C13	100(1)	C15-Co3-C11	143(1)
C14-Co3-C11	104(1)	C13-Co3-C11	103(1)
C15-Co3-C12	108(1)	C14-Co3-C12	97(1)
C13-Co3-C12	142(1)	C11-Co3-C12	39.9(7)
C15-Co3-Co4	97.4(8)	C14-Co3-Co4	149(1)
C13-Co3-Co4	104.6(8)	C11-Co3-Co4	51.5(5)
C12-Co3-Co4	52.1(6)	C18-Co4-C16	107(1)
C18-Co4-C17	98(1)	C16-Co4-C17	103(1)
C18-Co4-C11	102(1)	C16-Co4-C11	141(1)
C17-Co4-C11	98(1)	C18-Co4-C12	141(1)
C16-Co4-C12	104(1)	C17-Co4-C12	99(1)
C11-Co4-C12	40.1(7)	C18-Co4-Co3	97(1)
C16-Co4-Co3	100.2(8)	C17-Co4-Co3	147(1)
C11-Co4-Co3	50.4(6)	C12-Co4-Co3	53.4(6)
O13-C13-Co3	171(3)	O14-C14-Co3	178(4)
O15-C15-Co3	173(2)	O16-C16-Co4	169(3)
O17-C17-Co4	173(3)	O18-C18-Co4	176(3)

Estimated standard deviations are given in the parenthesis.
Symmetry operators ::
1: x, y, z 2: -x, -y, -z

TABLE 7S. Anisotropic displacement parameters (Å^2 x 10^3) for **2**

atom	U11	U22	U33	U23	U13	U12
Cu	39(2)	33(2)	47(2)	-14(2)	-7(2)	-5(2)
O(1)	26(9)	50(10)	50(10)	-23(9)	2(8)	-2(8)
O(2)	50(10)	40(10)	50(10)	-28(9)	-1(9)	-9(8)
Co(1)	48(3)	75(3)	96(3)	-64(3)	5(2)	-9(2)
Co(2)	72(3)	73(3)	67(3)	-40(3)	0(2)	-1(2)
C(5)	190(40)	90(30)	20(20)	-10(20)	40(20)	-50(30)
O(5)	190(20)	100(20)	110(20)	-70(20)	30(20)	-50(20)
C(6)	50(20)	110(30)	120(30)	-70(20)	0(20)	-10(20)
O(6)	170(30)	110(20)	160(20)	-100(20)	-20(20)	0(20)
C(7)	100(30)	80(30)	80(30)	-30(20)	-40(20)	-10(20)
O(7)	180(30)	130(20)	110(20)	-70(20)	30(20)	0(20)
C(9)	60(30)	190(40)	170(40)	-70(40)	-80(30)	40(30)
O(9)	160(30)	340(40)	190(30)	-110(30)	-120(30)	100(30)
O(10)	40(10)	60(10)	40(10)	-1(9)	-23(9)	-4(9)
O(11)	9(8)	70(10)	100(10)	-20(10)	-14(9)	0(8)
Co(3)	53(3)	49(3)	52(3)	-7(2)	-11(2)	-6(2)
Co(4)	52(3)	52(3)	75(3)	-21(2)	-14(2)	-4(2)
O(13)	50(10)	210(20)	170(20)	-90(20)	40(20)	-40(20)
C(14)	30(20)	190(40)	150(40)	-90(30)	10(20)	-20(20)
O(14)	180(30)	170(30)	130(20)	-80(20)	-50(20)	20(20)
C(15)	50(20)	70(20)	60(20)	-20(20)	0(20)	-20(20)
O(15)	90(20)	50(10)	90(20)	20(10)	-20(10)	-10(10)
C(16)	80(20)	40(20)	110(30)	-40(20)	-20(20)	0(20)
O(16)	140(20)	20(10)	240(30)	-20(20)	-60(20)	0(10)
O(17)	110(20)	100(20)	170(20)	-70(20)	-40(20)	-20(10)
C(18)	50(20)	70(20)	110(30)	-50(20)	10(20)	10(20)
O(18)	110(20)	150(20)	90(20)	-30(20)	20(20)	0(20)
O(1W)	40(10)	50(10)	70(10)	0(10)	-12(9)	-15(8)

TABLE 8S. Hydrogen Coordinates (Å x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for **2**

atom	x	y	z	U(eq)
H(2W)	4379	5992	805	80

Table 9s. Summary of crystal data and refinement details for $Mo_2[OOCCCHCo_2(CO)_6]_4$(Toluene) **1c**

Empirical Formula	C52 Co8 Mo2 O32
Formula Weight (AMU)	1799.98
Crystal Color and Habit	black, needle
Crystal Size (mm)	0.20 x 0.30 x 0.20
Crystal System and Space Group	Monoclinic, P21/n
Cell Dimensions :: (Å and deg.)	
a : 8.345(5)	
b : 27.06(2) beta : 95.90(5)	
c : 26.28(1)	
Cell Volume ($Å^3$)	5903(6)
Z (formula units/cell)	4.
Density (calculated) (g/ml)	2.021
Absorption Coefficient (μ, mm^{-1})	2.691
F(000)	3504.
Diffractometer	Siemens R3m Diffractometer
Radiation Source and Wavelength (A)	MoKa lambda 0.7107
Data Collection Temperature (degK)	293(2)
Two-theta range (deg)	3.02 to 40.02
Scan Type and Speed (deg/min)	? : ?
Scan width (deg)	?
Background Measurements	stationary crystal&counter method
Standard Reflections	0 every 0 reflections
Index ranges	0<h< 8 ; 0<k< 26 ; -25<l< 25
Reflection Collected	5470
Observed Reflections	2965
Observation criterion	>2sigma(I)
Absorption Correction Method	?
Structure Solution Program	SHELXS-86 (Sheldrick, 1990)
Structure Refinement Program	SHELXL-93 (Sheldrick, 1993)
Number of l.s. Parameters	508
Residuals (observed data)	R(F)=0.0869 : wR(F^2)= .0000
Residuals (all data)	R(F)=0.1696 : wR(F^2)= .2609
Goodness-of-fit (all data)	S(F^2)=0.0000
Largest and Mean l.s. shifts (delta/sig)	0.000 : 0.000
Largest e- Density Peak and Hole (e/A^3)	0.720 : -0.684

- Notes ----------

$w=1/[\backslash s^2(Fo^2)+(0.0810P)^2+125.6564P]$ where $P=(Fo^2+2Fc^2)/3$