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***N*-Heterocyclic Carbene Adducts of Molybdenum tetra-Carboxylate Complexes.**

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Table 1S: X-ray Crystallographic Data for Compounds **1a**, **2a**, **3a** and **1b**.

	(1a)	(2a)	(3a)	(1b)
Empirical Formula	C ₂₉ H ₂₄ F ₁₂ Mo ₂ N ₂ O ₈	C ₂₉ H ₃₆ Mo ₂ N ₂ O ₈	C _{44.50} H ₆₄ Mo ₂ N ₂ O ₈	C ₇₀ H ₈₂ F ₁₂ Mo ₂ N ₄ O ₈
FW (g.mol ⁻¹)	948.38	732.48	946.85	1527.27
Crystal System	Monoclinic	Triclinic	Monoclinic	Orthorhombic
Space Group	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	<i>P</i> 2 ₁ / <i>a</i>	<i>P</i> 2 ₁ 2 ₁ 2 ₁
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073
<i>a</i> (Å)	8.5050(2)	8.4000(2)	11.2778(2)	16.61270(10)
<i>b</i> (Å)	17.1100(3)	17.3732(4)	27.5134(6)	19.3204(2)
<i>c</i> (Å)	24.4660(3)	21.3704(4)	15.7145(4)	45.9155(5)
α (°)	90	84.852(2)	90	90
β (°)	95.5790(10)	87.660(2)	97.019(2)	90
γ (°)	90	76.240(2)	90	90
Volume (Å ³)	3543.44(11)	3016.35(12)	4839.52(18)	14737.2(2)
Crystal Size (mm ³)	0.200 x 0.150 x 0.150	0.250 x 0.250 x 0.200	0.770 x 0.230 x 0.120	0.300 x 0.250 x 0.250
Density (Mgm ⁻³)	1.778	1.613	1.300	1.377
<i>Z</i>	4	4	4	8
μ (Mo K α) (mm ⁻¹)	0.820	0.883	0.566	0.424
Theta range (°)	7.876 to 27.494	3.021 to 29.440	2.791 to 27.500	3.550 to 25.009
Reflections Collected	55010	22264	52926	163154
Independent Reflections	7882	13796	11088	25323
<i>R</i> _{int}	0.0675	0.0311	0.0264	0.1260
<i>R</i> ₁ , w <i>R</i> ₂ [<i>I</i> > 2 σ (<i>I</i>)]	0.0347, 0.0684	0.0421, 0.0711	0.0323, 0.0812	0.0706, wR2 = 0.1079
<i>R</i> indices (all data)	0.0561, 0.0754	0.0746, 0.0823	0.0392, 0.0855	0.1138, wR2 = 0.1177
Flack Parameter	-	-	-	0.126(14)
Largest diff. peak and hole (e.Å ⁻³)	0.739, -0.505	0.867, -0.555	1.132, -0.565	0.590, -0.500
CCDC Reference	1477588	1477587	1477589	1477590

Table 2S: X-ray Crystallographic Data for Compounds **1c**, **1d**, **2d**, **4** and **5**.

	(1c)	(1d)	(2d)	(4)	(5)
Empirical Formula	C ₂₆ H ₃₂ F ₁₂ Mo ₂ N ₄ O ₈	C ₃₀ H ₄₀ F ₁₂ Mo ₂ N ₄ O ₈	C ₅₈ H ₈₄ Mo ₂ N ₄ O ₈	C ₃₆ H ₆₆ Mo ₂ N ₂ O ₁₀	C ₄₀ H ₆₂ Cl ₂ Mo ₂ N ₄ O ₄
FW (g.mol ⁻¹)	948.43	1004.54	1157.17	878.78	925.71
Crystal System	Triclinic	Monoclinic	Triclinic	Monoclinic	Triclinic
Space Group	<i>P</i> -1	<i>P</i> 2 ₁ / <i>n</i>	<i>P</i> -1	Cc	<i>P</i> -1
Wavelength (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
<i>a</i> (Å)	11.3739(6)	9.8400(2)	8.5480(2)	12.21900(10)	9.8940(2)
<i>b</i> (Å)	12.0093(7)	12.2550(3)	11.9010(3)	21.1750(2)	11.8630(2)
<i>c</i> (Å)	13.5043(8)	16.1040(2)	15.0010(4)	17.9860(2)	12.7570(3)
α (°)	90.405(5)	90	100.6310(10)	90	102.557(1)
β (°)	106.754(5)	91.3730(10)	102.629(2)	103.5920(10)	106.210(1)
γ (°)	91.534(4)	90	102.0870(10)	90	93.427(1)
Volume (Å ³)	1765.44(18)	1941.41(7)	1413.08(6)	4523.32(8)	1391.76(5)
Crystal Size (mm ³)	0.200 x 0.100 x 0.100	0.500 x 0.380 x 0.380	0.300 x 0.130 x 0.080	0.200 x 0.100 x 0.050	0.200 x 0.130 x 0.100
Density (Mgm ⁻³)	1.784	1.718	1.360	1.290	1.214
Z	2	2	1	4	1
μ (Mo K α) (mm ⁻¹)	0.824	0.755	0.499	0.603	0.585
Theta range (°)	3.167 to 28.279	7.929 to 31.017	8.516 to 27.421	4.142 to 32.004	3.544 to 30.687
Reflections Collected	15978	30529	26722	50052	8488 ^a
Independent Reflections	8722	6069	6165	14898	8488
R_{int}	0.0314	0.0298	0.0688	0.0692	0.0373 ^b
R_1 . wR_2 [$I > 2\sigma(I)$]	0.0492, 0.1138	0.0321, 0.0810	0.0300, 0.0690	0.0351, 0.0853	0.0355, 0.1174
<i>R</i> indices (all data)	0.0674, 0.1269	0.0363, 0.0838	0.0386, 0.0728	0.0440, 0.0929	0.0412, 0.1212
Flack Parameter	-	-	-	0.17(3)	-
Largest diff. peak and hole	1.892, -1.069	1.213, -1.259	0.602, -0.654	0.702, -0.642	1.83, -0.75
CCDC Reference	1477591	1477593	1477592	1477594	1477595

^a after SQUEEZE; ^b before SQUEEZE

S1: Molecular structure of complex 2d

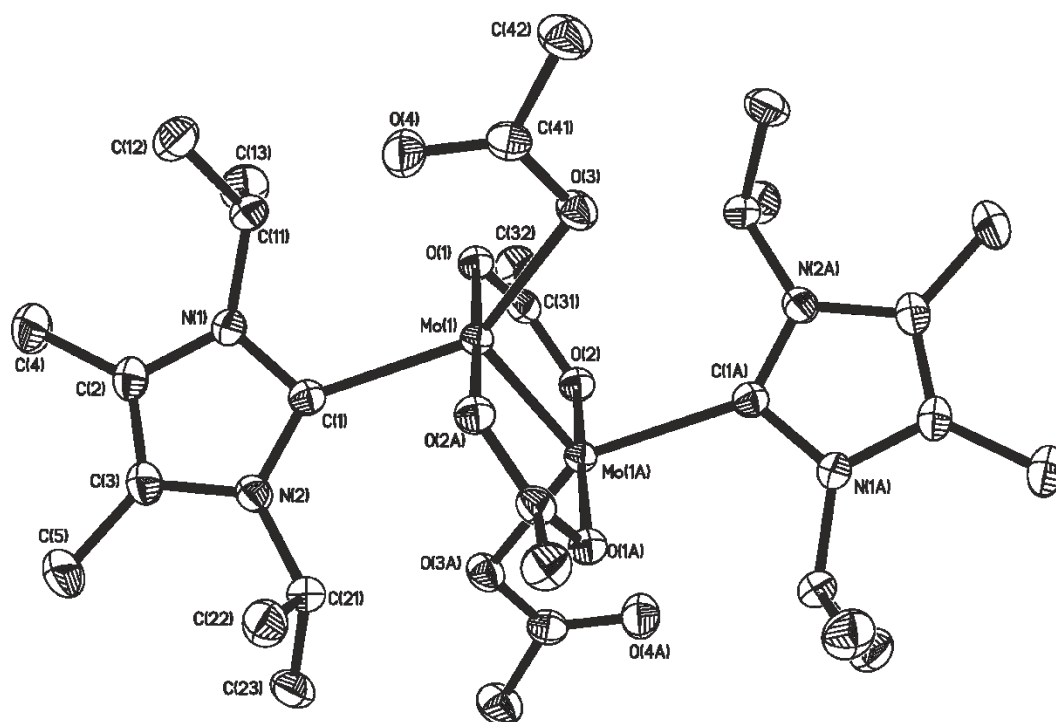


Figure S1: Molecular structure of the molecular structure $[\text{Mo}_2(\mu\text{-OAc})_2(\text{OAc})_2(\text{L}^{\text{d}})_2]$ (**2d**). The solvent of crystallisation and hydrogen atoms have been removed for clarity, and thermal ellipsoids are shown at 50 % probability. Symmetry transformations used to generate equivalent atoms: $1 -x, -y, -z+1$.