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

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A.L.Johnson@bath.ac.uk
<table>
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<tr>
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<th>(1a)</th>
<th>(2a)</th>
<th>(3a)</th>
<th>(1b)</th>
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<td>C_{29}H_{24}F_{12}Mo_{2}N_{2}O_{8}</td>
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<td>FW (g mol⁻¹)</td>
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<td>Monoclinic</td>
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<tr>
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<td>P2₁/a</td>
<td>P2₁2₁2₁</td>
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<td>Wavelength (Å)</td>
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<td>0.71073</td>
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<td>a (Å)</td>
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<td>b (Å)</td>
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<td>Crystal Size (mm³)</td>
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<td>0.0421, 0.0711</td>
<td>0.0323, 0.0812</td>
<td>0.0706, wR₂ = 0.1079</td>
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Table 2S: X-ray Crystallographic Data for Compounds 1c, 1d, 2d, 4 and 5.

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<td><strong>Empirical Formula</strong></td>
<td>C₃₀H₃₂F₁₂Mo₂N₄O₈</td>
<td>C₃₀H₃₂F₁₂Mo₂N₄O₈</td>
<td>C₃₀H₃₂Mo₂N₄O₈</td>
<td>C₃₀H₃₂Mo₂N₂O₁₀</td>
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<td><strong>FW (g.mol⁻¹)</strong></td>
<td>948.43</td>
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<td>P₂₁/n</td>
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<td><strong>Wavelength (Å)</strong></td>
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<td><strong>a (Å)</strong></td>
<td>11.3739(6)</td>
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<td><strong>b (Å)</strong></td>
<td>12.0093(7)</td>
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<td><strong>α (°)</strong></td>
<td>90.405(5)</td>
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<tr>
<td><strong>β (°)</strong></td>
<td>106.754(5)</td>
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<td><strong>γ (°)</strong></td>
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<td><strong>Crystal Size (mm³)</strong></td>
<td>0.200 x 0.100 x 0.100</td>
<td>0.500 x 0.380 x 0.380</td>
<td>0.300 x 0.130 x 0.080</td>
<td>0.200 x 0.100 x 0.050</td>
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<td><strong>Density (Mgm⁻³)</strong></td>
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<td><strong>Z</strong></td>
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<td><strong>μ (Mo Kα) (mm⁻¹)</strong></td>
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<td><strong>Theta range (°)</strong></td>
<td>3.167 to 28.279</td>
<td>7.929 to 31.017</td>
<td>8.516 to 27.421</td>
<td>4.142 to 32.004</td>
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<td><strong>Reflections Collected</strong></td>
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<td>30529</td>
<td>26722</td>
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<td><strong>Independent Reflections</strong></td>
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<td><strong>Rint</strong></td>
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<td>0.0373⁷⁻¹⁷⁻¹</td>
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<td><strong>R₁, wR₂ [I&gt;2σ(I)]</strong></td>
<td>0.0492, 0.1138</td>
<td>0.0321, 0.0810</td>
<td>0.0300, 0.0690</td>
<td>0.0351, 0.0853</td>
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<td><strong>R indices (all data)</strong></td>
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<td>0.0440, 0.0929</td>
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<td><strong>Flack Parameter</strong></td>
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<td>0.17(3)</td>
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<tr>
<td><strong>Largest diff. peak and hole</strong></td>
<td>1.892, -1.069</td>
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⁷ after SQUEEZE; ⁸ before SQUEEZE
**Figure S1:** Molecular structure of the molecular structure [Mo₂(μ-OAc)₂(OAc)₂(L²)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.