Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

An Eleven-Vertex Metallaborane with Tetracapped Pentagonal Bipyramidal Geometry

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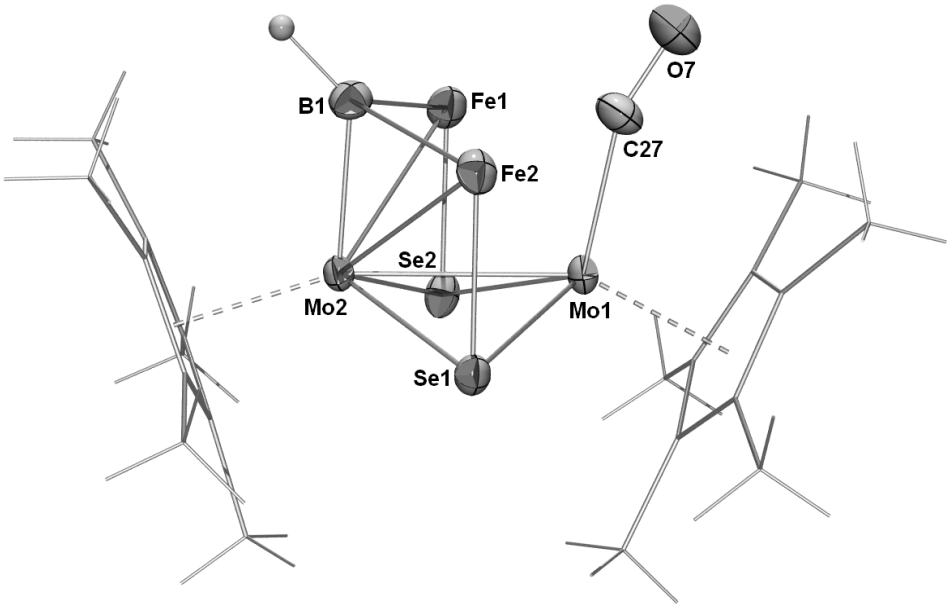

Figure S1: Molecular structure of **I** (30% probability ellipsoids). Carbonyl ligands are excluded for clarity. Selected bond lengths (Å) and angles (°): Mo1–Mo2 2.9053(4), Mo2–B1 2.077(5), B1–Fe1 2.277(5), Mo1–Se1 2.4743(5), Mo1–Se2 2.4674(5); Mo2–B1–Fe1 80.64(18), Fe1–B1–Fe2 105.4(2), Se2–Mo1–Se1 96.200(18).

X-ray Structure Determination. The crystal data for **2** and **I** were collected and integrated using Bruker Axs kappa apex2 CCD diffractometer, with graphite monochromated Mo–Kα (λ = 0.71073 Å) radiation at 273 and 298 K respectively. The structures were solved by heavy atom methods using SHELXS-97 or SIR92[1] and refined using SHELXL-97.[2,3] CCDC-854064 (**2**) and CCDC-854874 (**I**)

contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac. uk/data_request/cif.

References

(1) A. Altomare, G. Cascarano, C. Giacovazzo and A. Guagliardi, *J. Appl. Cryst.*, 1993, **26**, 343.

(2) G. M. Sheldrick, SHELXS-97; University of Göttingen: Germany, 1997**.**

(3) G. M. Sheldrick, SHELXS-97; University of Göttingen: Germany, 1997.