Supporting Information

Mixed-Metal Chalcogenide Tetrahedral Clusters with an Exo-polyhedral Metal Fragment

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I. Supplementary Data

I.1 Fig. S1 Crystal packing diagrams for 3 and 5.
I.2 Fig. S2 Proposed molecular structure of 4

I.1 Fig. S1: Crystal packing diagram of 3 and 5:

![Crystal packing diagram of 3 and 5](image)

**Fig. S1.** (a) Crystal packing diagram of 3 linked through C-H···O interactions. (b) Crystal packing diagram of 5 linked through C-H···O interactions.
Spectroscopic data of 4: MS (MALDI): m/z 808 [M+H-11CO]+. Isotope envelope C_{10}H_{16}Os_{3}Ru: requires 808, m/z. \(^1\)H NMR (22 °C, 400 MHz, [D\(_6\)]-benzene): \(\delta = 1.99\) (s, 15H, 1Cp*), -18.34 (s, 1H, Os-H-Os). \(^{13}\)C NMR (22 °C, 100 MHz, [D\(_6\)]-benzene): \(\delta = 196.1, 191.3\) (CO), 101.8 (C\(_5\)Me\(_5\)), 11.3 (C\(_5\)Me\(_3\)). IR \(\nu\)bar/cm\(^{-1}\): 2080, 2051, 1929 (CO). Elemental analysis (%) calcd for C\(_{21}\)H\(_{16}\)O\(_{11}\)RuOs\(_3\): C, 22.60; H, 1.44. Found: C, 21.96; H, 1.49.

Note that all our attempts to get a suitable X-ray data from the tiny crystals of 4 failed and thus, compound 4 has been characterized based on the spectroscopic data and combustion analysis. Based on the spectroscopic data, combustion analysis and a poor X-ray data a plausible structure has been proposed in Fig. S2.

I.2  Fig. S2: Proposed molecular structure of 4.