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 diagram of **3** and **5:**

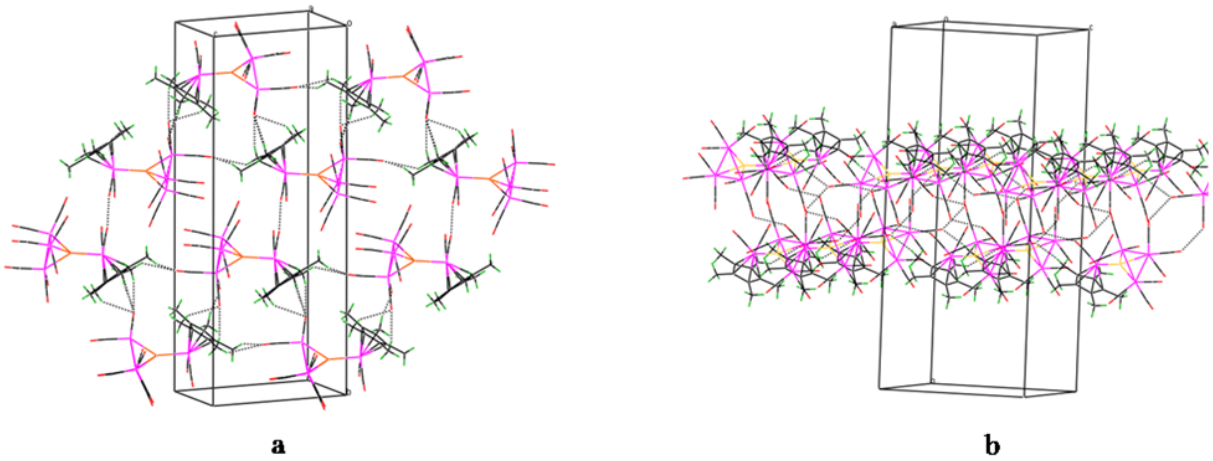

Fig. S1. (a) Crystal packing diagram of **3** linked through C-H•••O interactions. (b) Crystal packing diagram of **5** linked through C-H•••O interactions.

Spectroscopic data of **4:**MS (MALDI): m/z 808 $[M+H-11CO]^+$. isotope envelope $C_{10}H_{16}Os_3Ru$: requires 808, m/z. ^1H NMR (22 °C, 400 MHz, $[D_6]$-benzene): δ = 1.99 (s, 15H, 1Cp*), -18.34 (s, 1H, Os-H-Os). ^{13}C NMR (22 °C, 100 MHz, $[D_6]$-benzene): δ = 196.1, 191.3 (*C*O), 101.8 (C_5Me_5), 11.3 (C_5Me_5). IR νbar/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**.