

# Supplementary Materials: The First Homoleptic Complex of Seven-Coordinated Osmium: Synthesis and Crystallographical Evidence of Pentagonal Bipyramidal Polyhedron of Heptacyanoosmate(IV)

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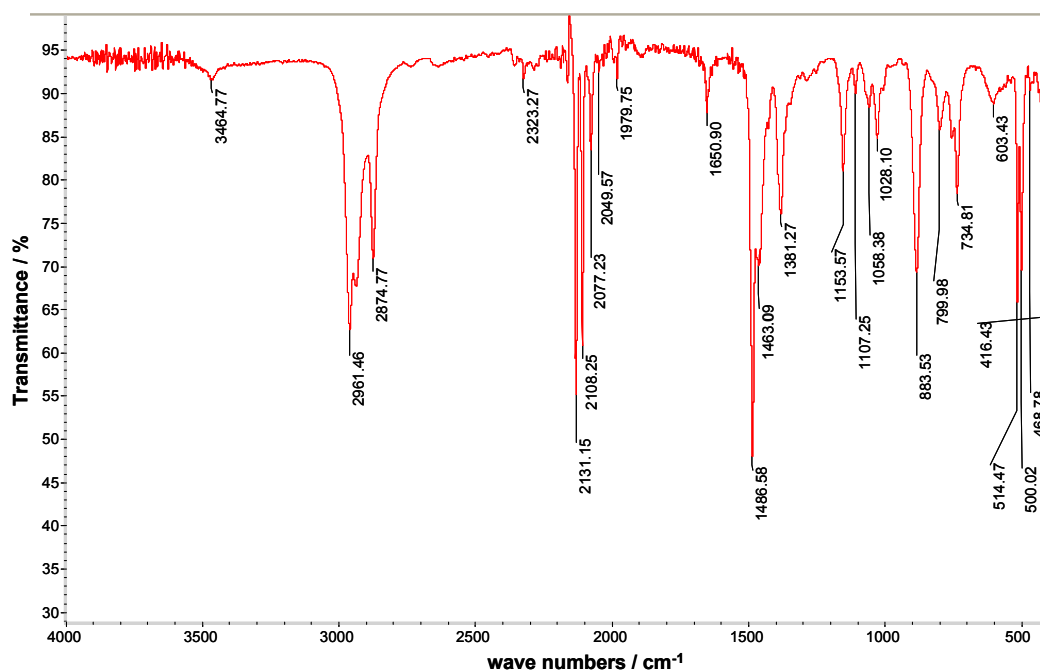


Figure S1. IR spectrum of  $(n\text{-Bu}_4\text{N})_3[\text{Os}(\text{CN})_7] \cdot 0.5\text{H}_2\text{O}$  (1) (reflectance).

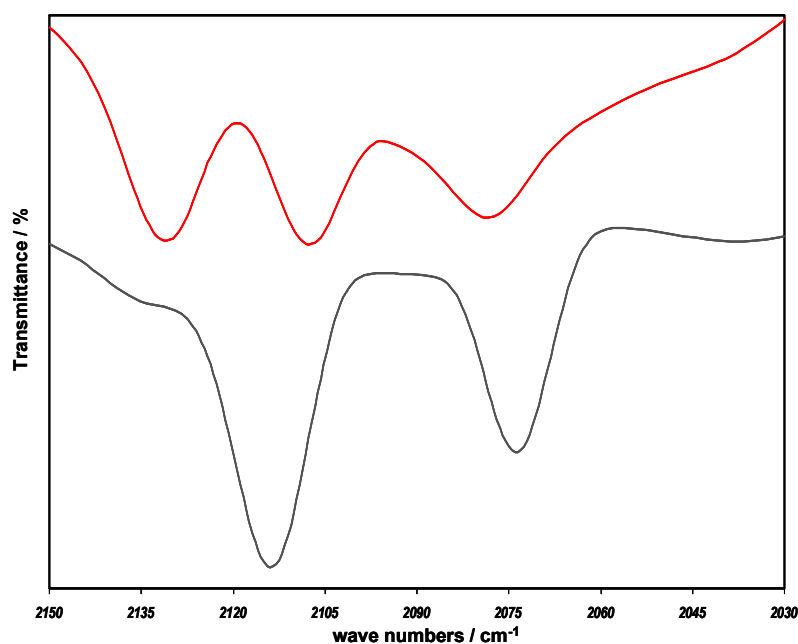
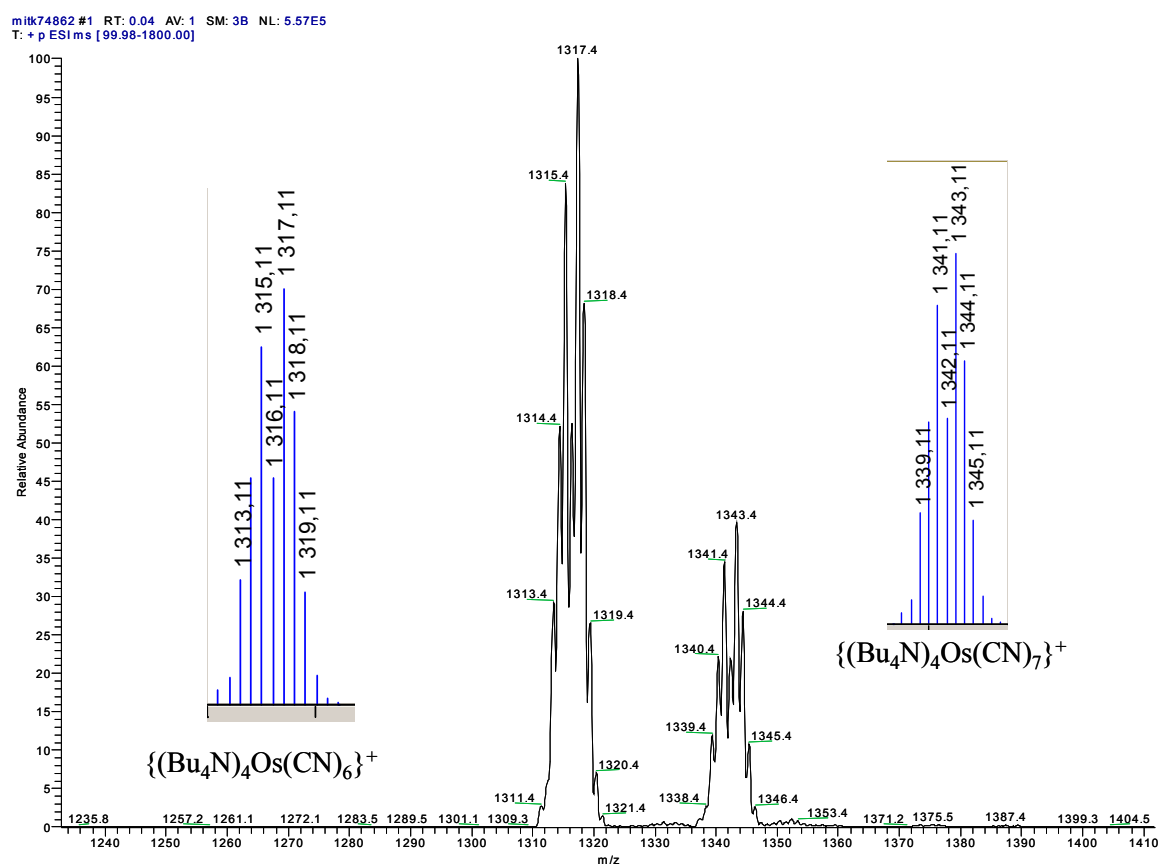
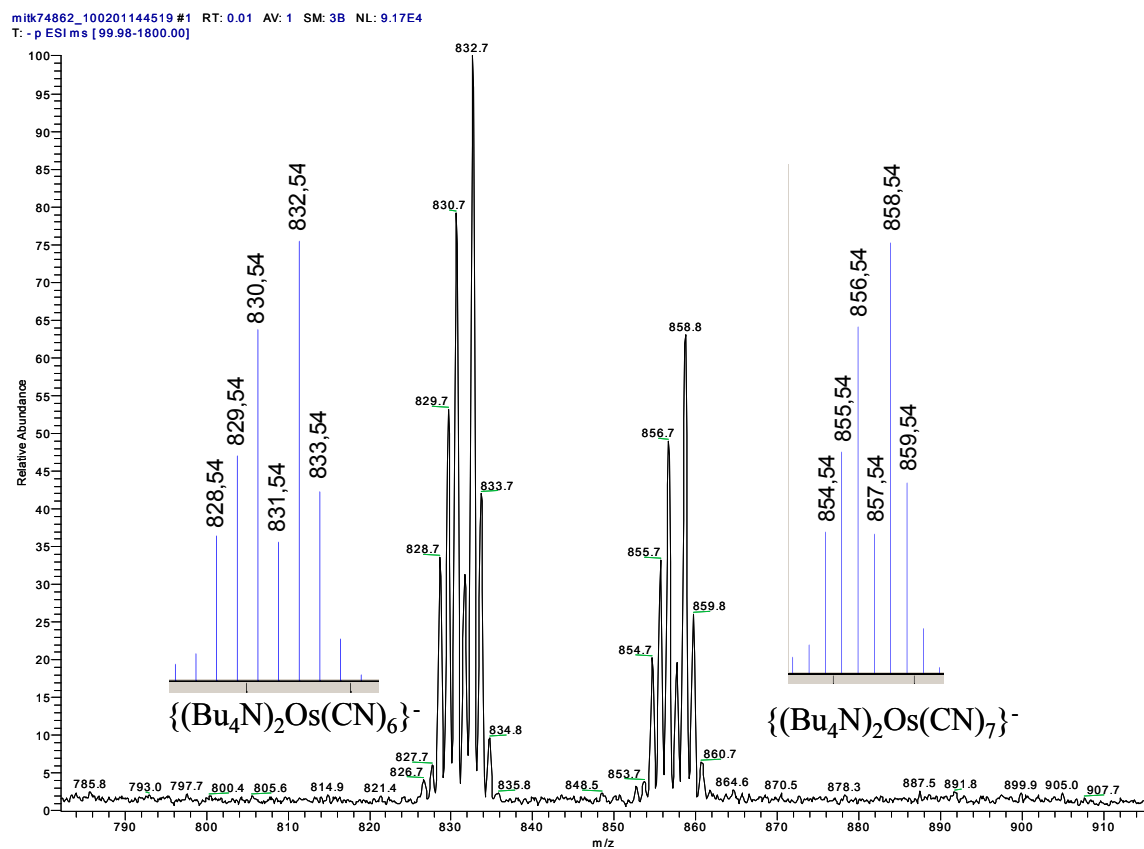


Figure S2.  $\text{CN}^-$  valance stretch region in the IR spectra of:  $(n\text{-Bu}_4\text{N})_3[\text{Os}(\text{CN})_7](\text{H}_2\text{O})_{0.5}$  (red) and  $(n\text{-Bu}_4\text{N})_3[\text{Re}(\text{CN})_7]$  (black) (reflectance).

Figure S3a. MS-ESI spectrum of the reaction mixture of **1** (cationic part).Figure S3b. MS-ESI spectrum of the reaction mixture of **1** (anionic part 1).

44901 #1 RT: 0.00 AV: 1 SM: 3B NL: 4.00E4  
0-359.98]

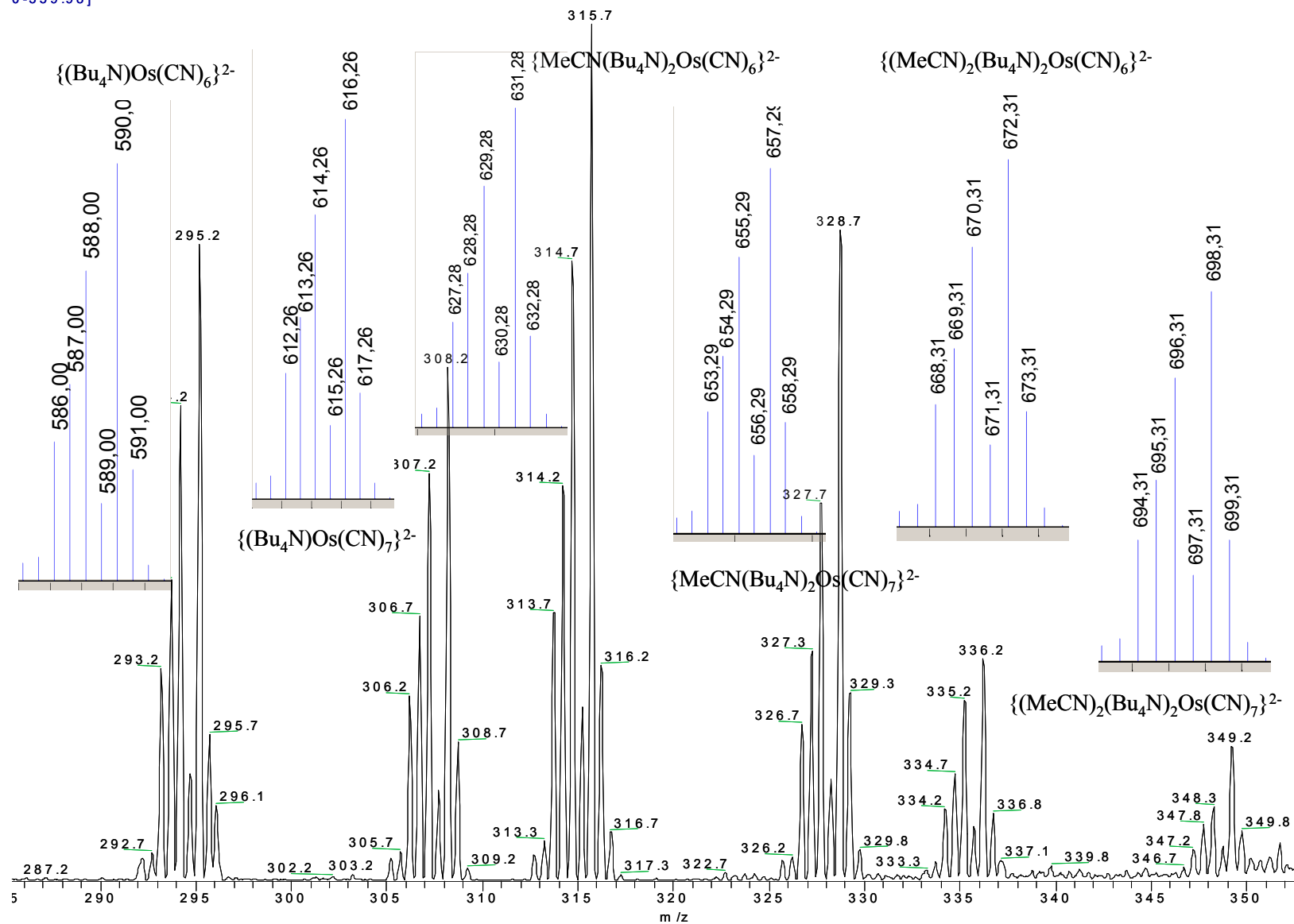


Figure S3c. MS-ESI spectrum of the reaction mixture of 1 (anionic part 2).

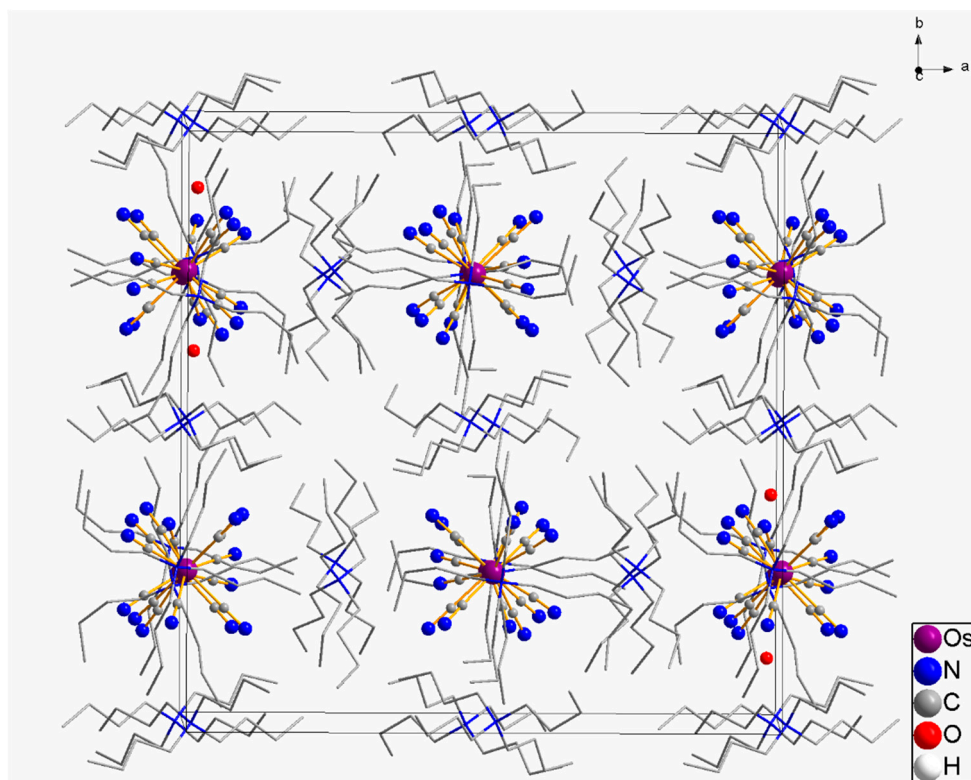


Figure S4. The crystal packing in **1**.

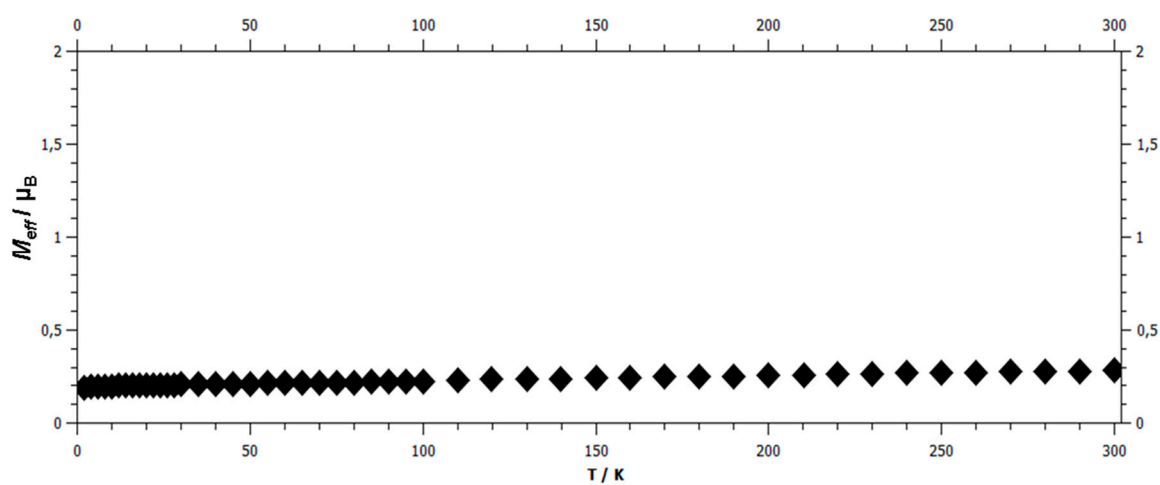


Figure S5. The temperature dependence for the effective magnetic moment of the polycrystalline sample of **1**. Non-zero value of  $M_{eff}$  can be explained by a large measurement error caused by the considerable diamagnetic contribution of  $n\text{-Bu}_4\text{N}^+$  cations and cyanide ligands because their contribution in molecular weight is almost 85%.



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