Supplementary Material (ESI) for Chemical Communications

Supplementary materials for article

Unexpected ligand substitutions in the cluster core $\{Re_6Se_8\}$: synthesis and structure of the novel cluster compound $Cs_{11}(H_3O)[Re_6Se_4O_4Cl_6]_3 \cdot 4H_2O$

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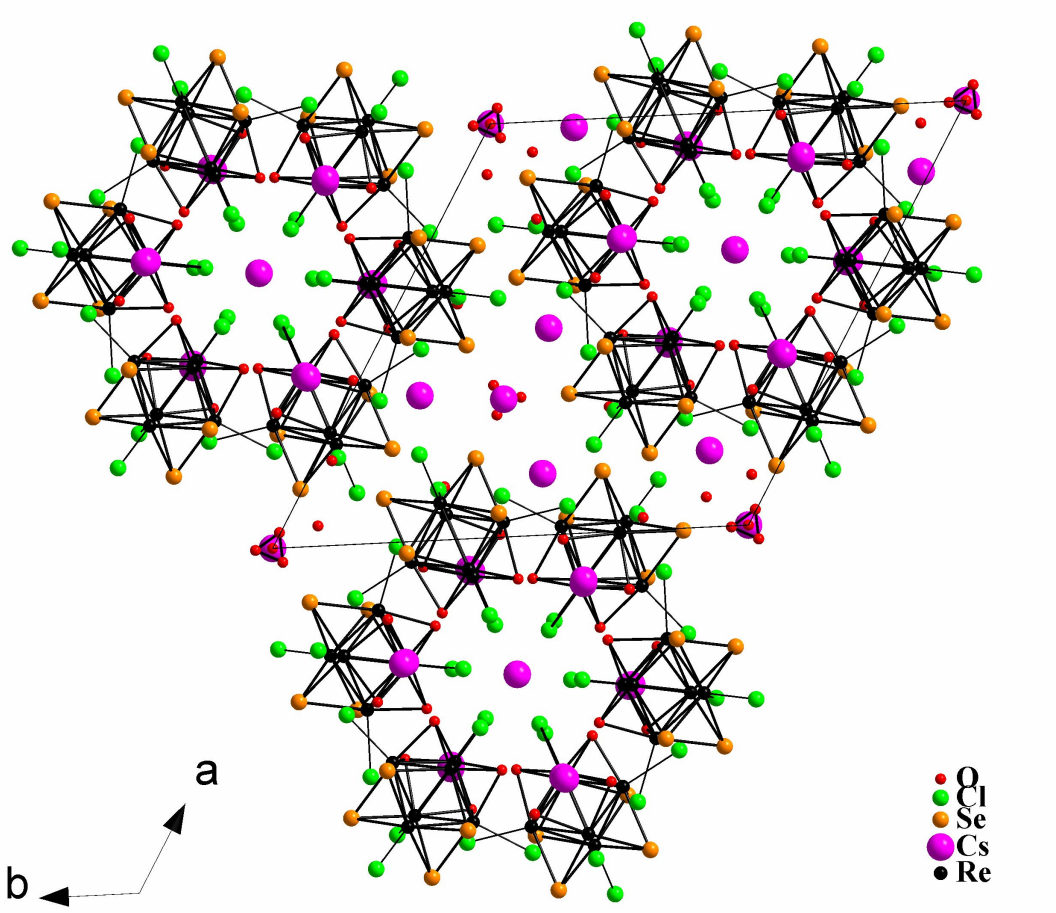

Figure S1. A fragment of a honeycomb-like double layer of $Cs_{11}(H_3O)[Re_6Se_4O_4Cl_6]_3 \cdot 4H_2O$.

View along the c axes

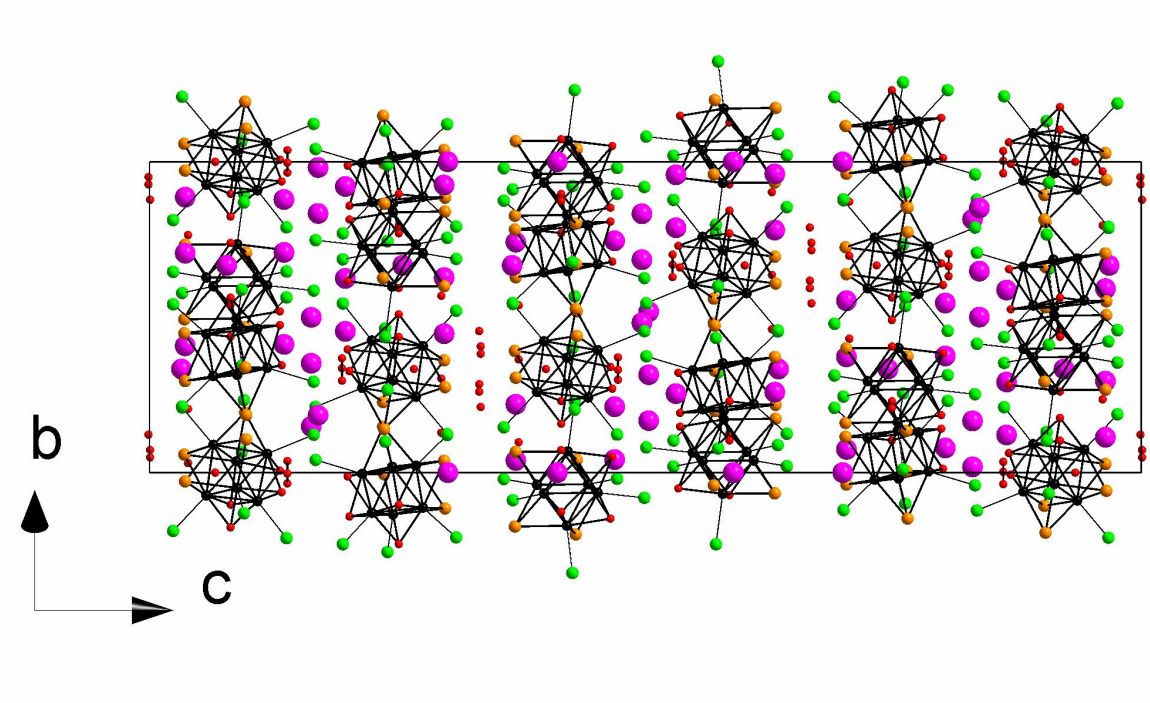

Figure S2. Unit cell of $Cs_{11}(H_3O)[Re_6Se_4O_4Cl_6]_3 \cdot 4H_2O$. View along the a axes

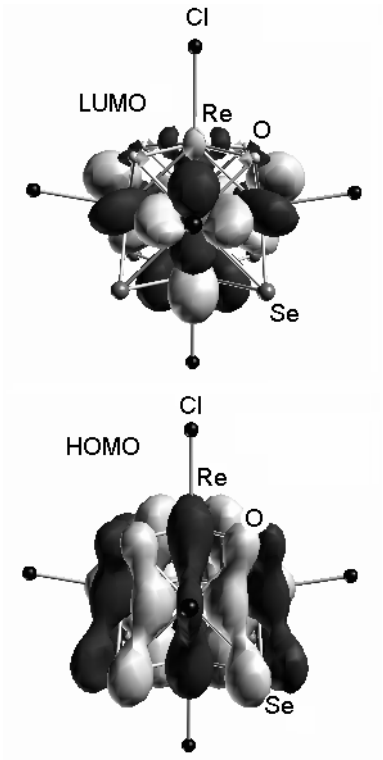

Figure S3. The schematic figures of HOMO and LUMO for C_{4v} $Re_6O_4Se_4Cl_6$. The non degenerated HOMO, $44b_1$ is antibonding character and is formed from the valent 5d-orbitals of Re atoms (~ 65 %), with the O and Se valent *p*-orbitals contributions (~12% and ~17 %). The non degenerated LUMO, $45b_1$ is largely centered on the rhenium atoms (~98 % of the valent 5d-orbitals). The calculated HOMO-LUMO energy gap is 2.56 eV.