

Electronic Supplementary Information

Mixed-metal clusters with {Re₃Mo₃Se₈} core: from polymeric solid to soluble species with multiple redox transitions

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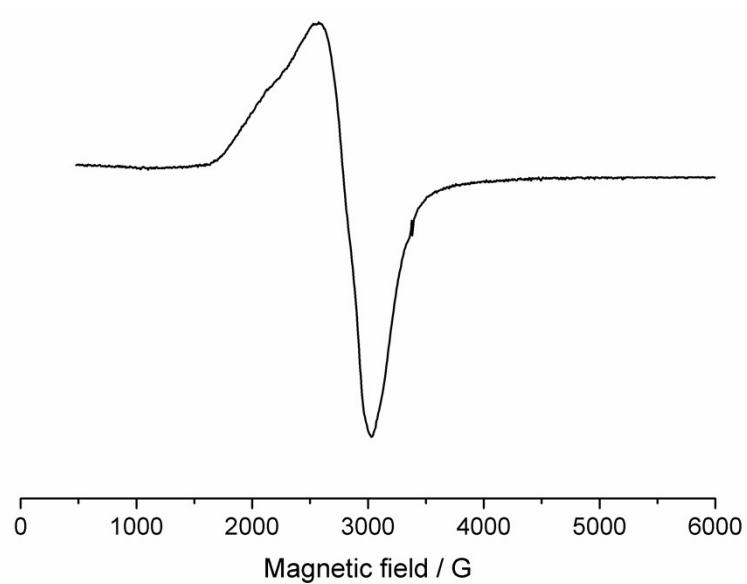


Figure S1. EPR spectra of polycrystalline sample of compound **4** at 77K ($g = 2.430$).

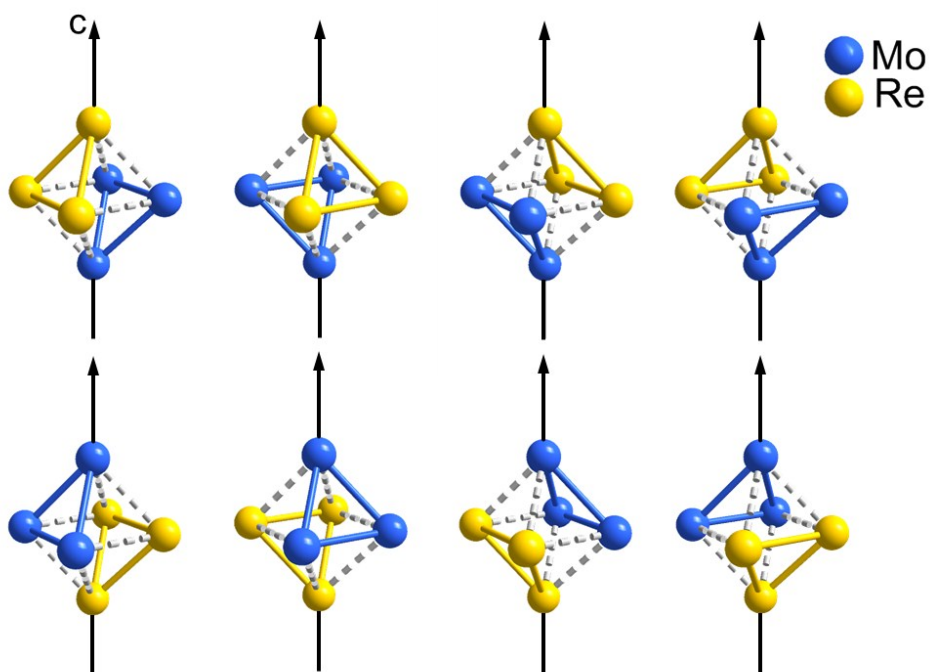


Figure S2. The possible orientations of *fac*-{Re₃Mo₃} isomer toward the fourfold axis in the crystal structure of compound **1**.

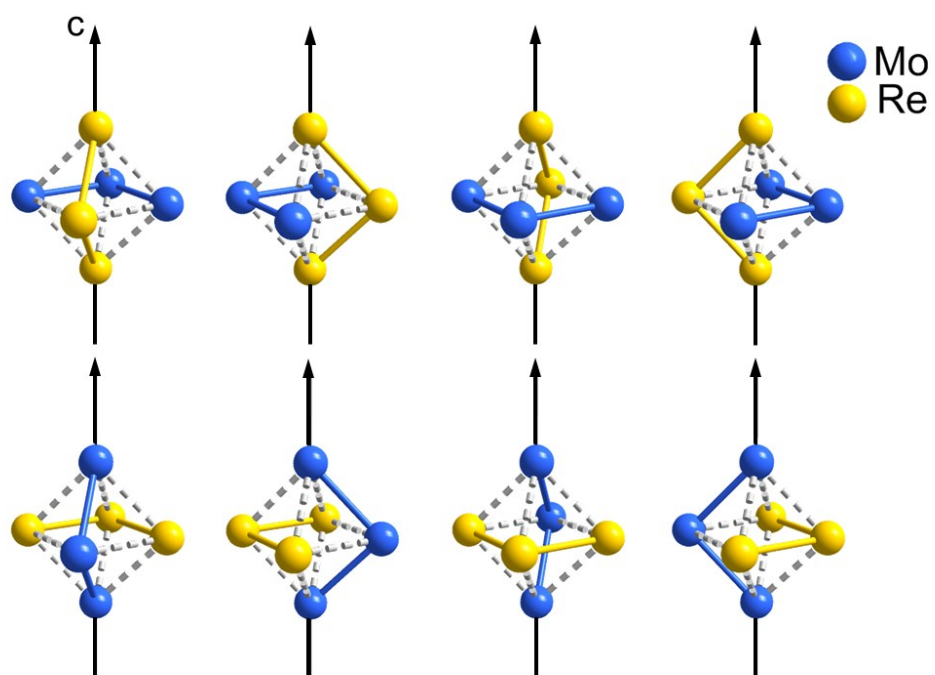


Figure S3. The possible orientations of $mer\text{-}\{\text{Re}_3\text{Mo}_3\}$ isomer toward the fourfold axis in the crystal structure of compound **1**.

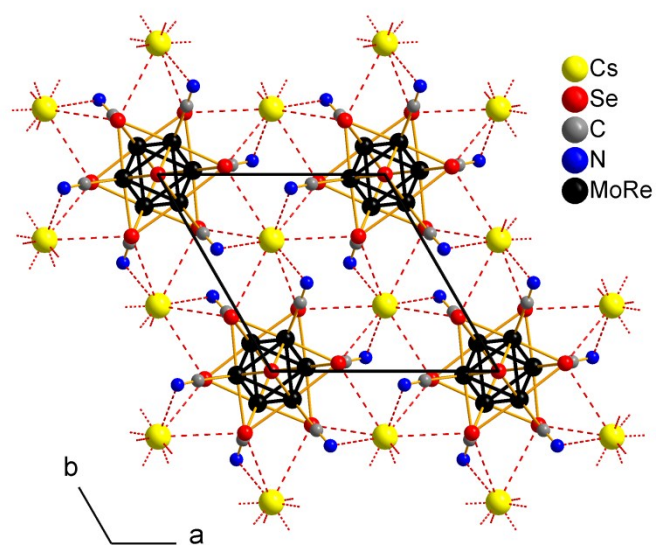


Figure S4. Fragment of crystal packing in **3**. Extra framework cations and solvate H_2O molecules are omitted for clarity.

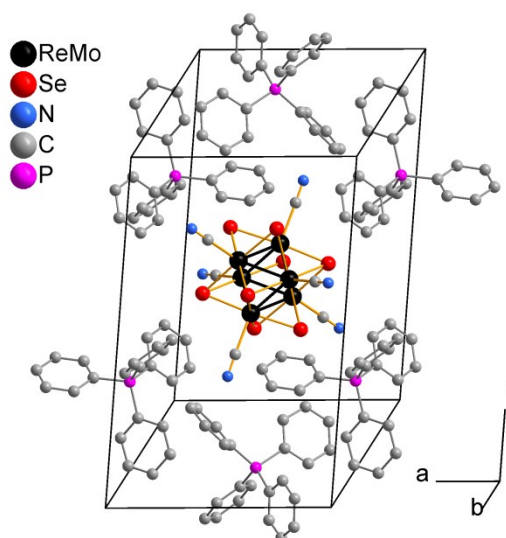


Figure S5. Fragment of crystal packing in **4**. Hydrogen atoms and solvate CH_3CN molecules are omitted for clarity.

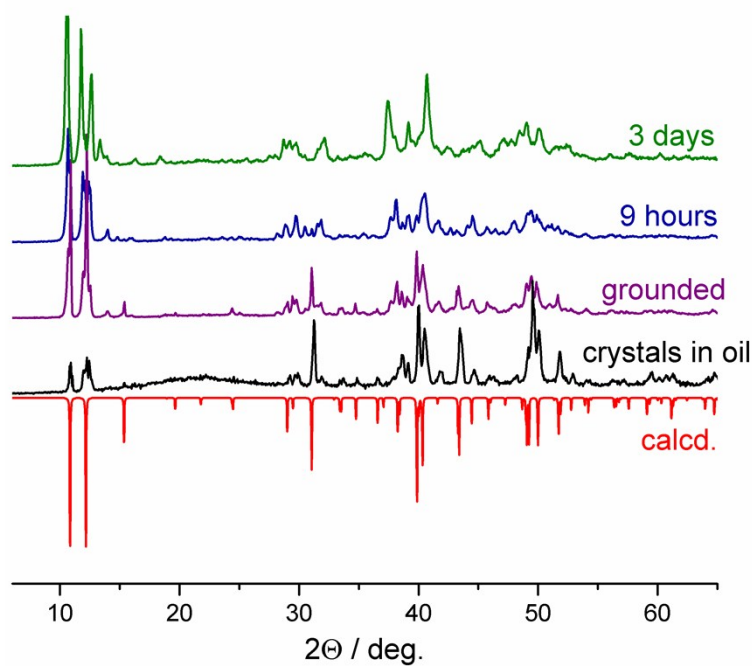


Figure S6. Powder XRD patterns for compound **1**. Down up: calculated pattern (red line); freshly prepared sample of **1** grounded in mineral oil (black line); freshly prepared sample of **1** grounded in CCl_4 (purple line); the sample **1** grounded in CCl_4 and exposed in air for 9 hours (blue line); the sample **1** grounded in CCl_4 and exposed in air for 3 days (green line).

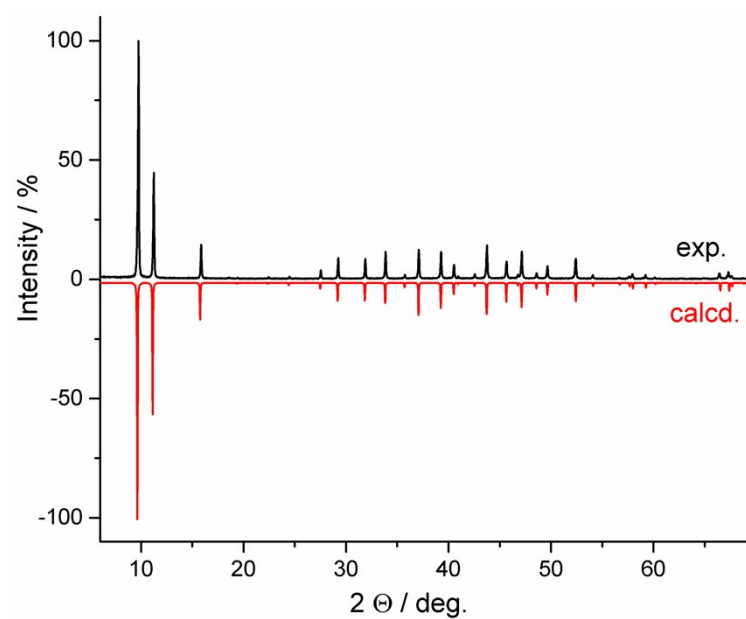


Figure S7. Powder XRD patterns (recorded, black vs calculated, red) for compound **2**.

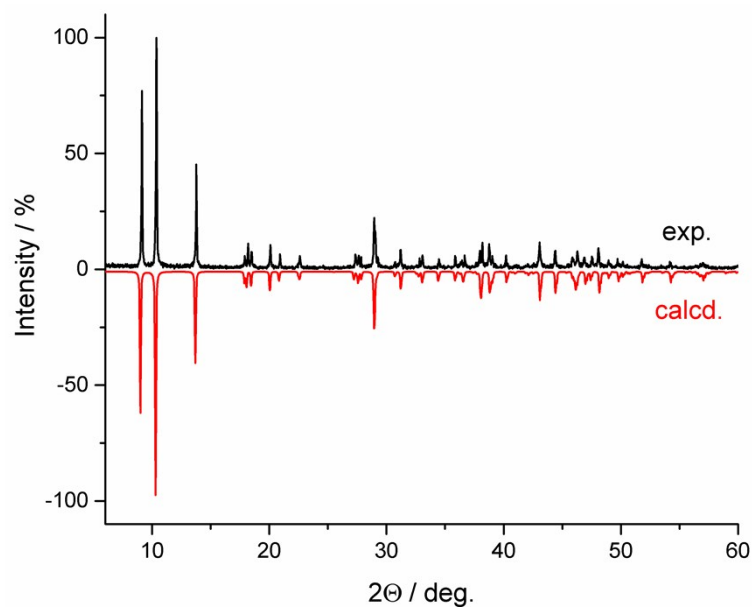


Figure S8. Powder XRD patterns (recorded, black vs calculated, red) for compound **3**.

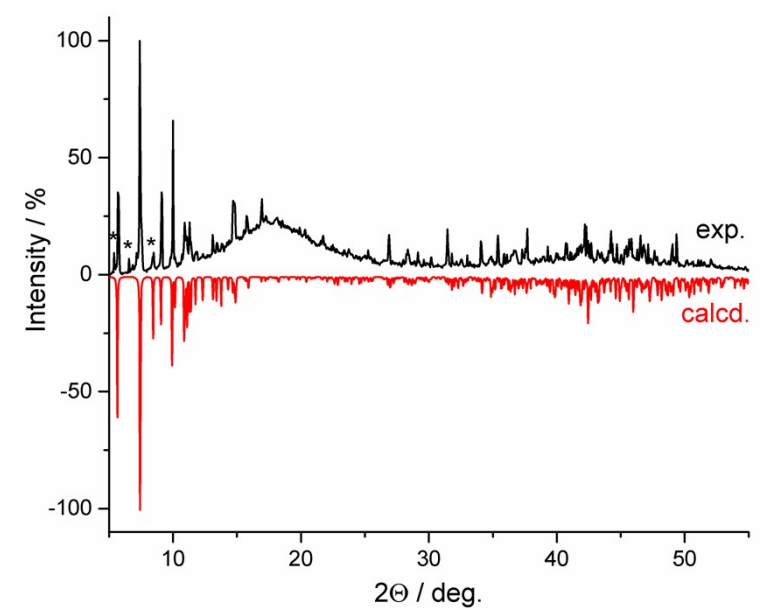


Figure S9. Powder XRD patterns (recorded, black vs calculated, red) for compound **4** in mineral oil. The asterisks mark the crystalline products of desolvation.