Supplementary Information

Structural characterization and magnetic properties studies of a mixed-valence $\{Co^{III}Co^{II}4\}$ complex with a μ_4-oxo tetrahedral $\{Co^{II}_4\}$ motif

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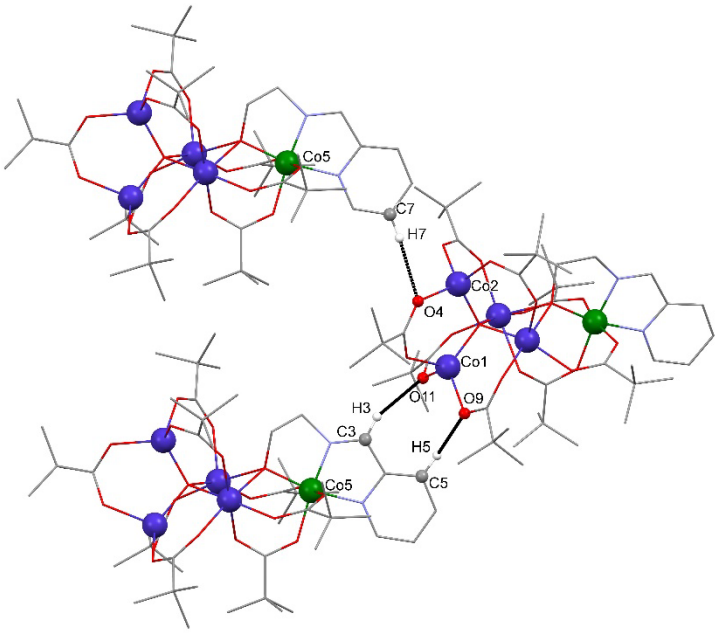

Figure SI1. Capped sticks molecular representation of complex **1** showing the C-H···O inter-molecular interactions pattern. H atoms have been removed for sake of clarity, except for the H atoms involved in the interactions. Colour code: Green: Co(III); Blue: Co(II); Red: O; Light Blue: N; Grey: C; White: H.

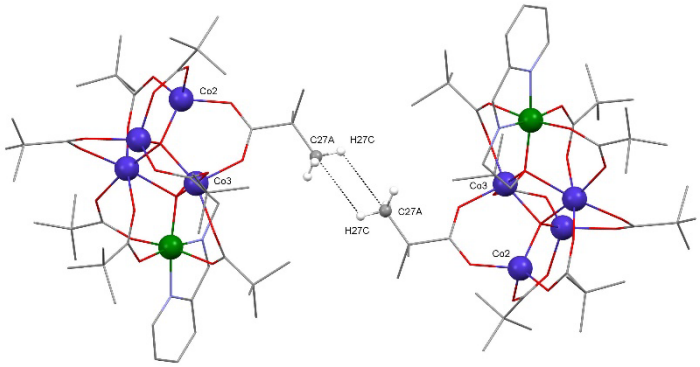

Figure SI2. Capped sticks molecular representation of complex **1** showing the C-H···C-H pivalates inter-molecular interactions pattern. H atoms have been removed for sake of clarity, except for the H atoms involved in the interactions. Colour code: Green: Co(III); Blue: Co(II); Red: O; Light Blue: N; Grey: C; White: H.

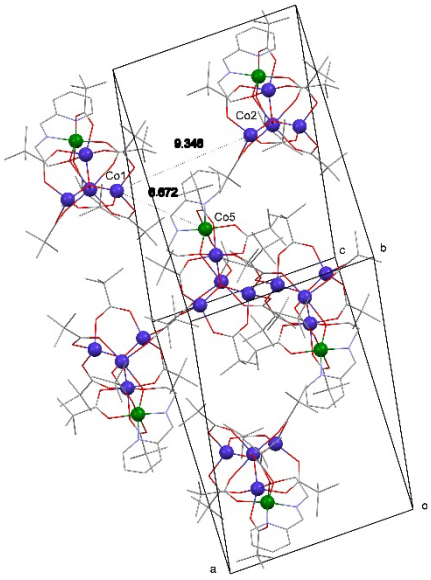

Figure SI3. Capped sticks molecular representation of complex **1** crystal packing showing the closest Co···Co inter-molecular distances (Å). H atoms have been removed for sake of clarity. Colour code: Green: Co(III); Blue: Co(II); Red: O; Light Blue: N; Grey: C.

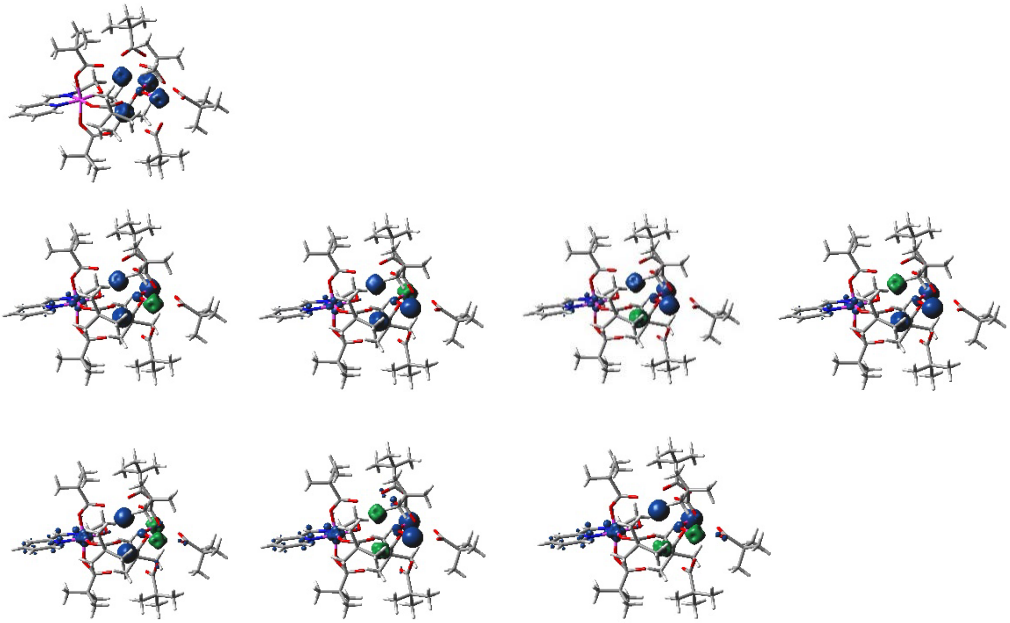

Figure SI4. Spin density iso-surfaces (0.02 a.u.), as arising from BS calculations of complex **1** (see details in text). Top: HS state; Middle: BS states converged after sequentially flipping each Co(II) site spin density; Bottom: BS states converged after sequentially flipping three Co(II)-Co(II) sites pair spin density.

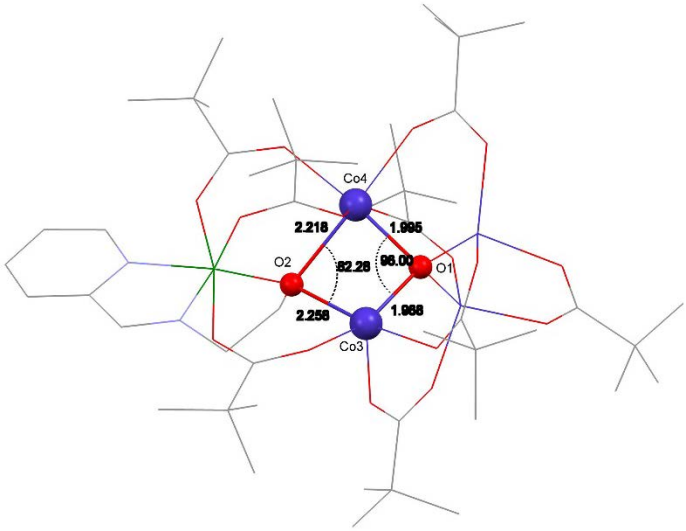

Figure SI5. Main metrics describing the Co(3)-Co(4) exchange interaction pathway in complex **1**. Angles in degrees, distances in Å.

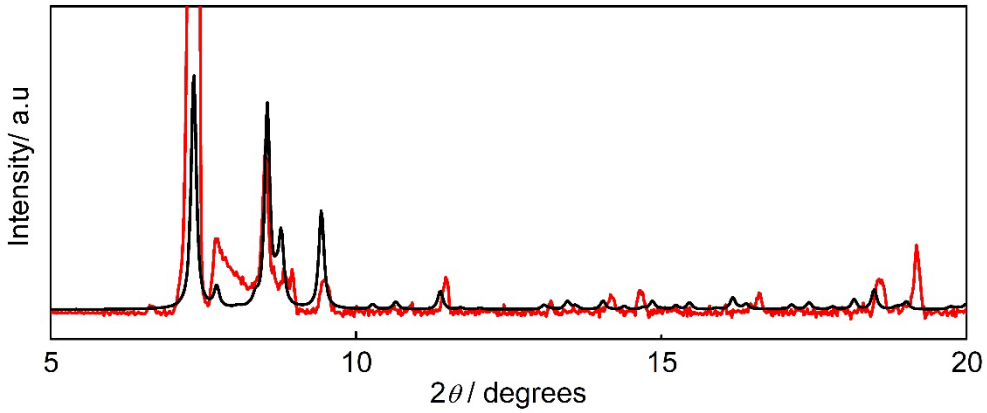

Figure SI6. Powder X-ray diffractogram collected at room temperature of polycrystalline sample of complex **1**. Red line: experimental; Black line: simulated from single crystal structural information.