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Cr^{III}–Cr^{III} interactions in two alkoxo-bridged heterometallic Zn_2Cr_2 complexes self-assembled from zinc oxide, Reinecke's salt and diethanolamine.

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Two new tetranuclear complexes, $[Zn_2Cr_2(NCS)_4(Dea)_2(HDea)_2]\cdot 4DMSO$ (**1**; DMSO = dimethyl sulfoxide) and $[Zn_2Cr_2(NCS)_4(Dea)_2(HDea)_2]\cdot 2CH_3CN$ (**2**), were prepared from zinc oxide, Reinecke's salt, $NH_4[Cr(NCS)_4(NH_3)_2]\cdot H_2O$, ammonium thiocyanate, and a nonaqueous solution of diethanolamine (H_2Dea) in a reaction carried out under open air. Both compounds have similar centrosymmetric crystal structures based on a tetranuclear $\{Zn_2Cr_2(\mu_3\text{-}O)_2(\mu\text{-}O)_4\}$ core. Variable-temperature magnetic susceptibility measurements of **1** and **2** show weak antiferromagnetic coupling between chromium centers. The magnetic data and high-field, high-frequency electron paramagnetic resonance spectra were analyzed in terms of the spin Hamiltonianwith J = 13.7 cm^{-1}, j = 1.1 cm^{-1}, D_{Cr} = 0.3864 cm^{-1}, E_{Cr} = −0.1104 cm^{-1}, D_{12} = −0.1873 cm^{-1}, and E_{12} = −0.0155 cm^{-1} for **1** and J = 9.4 cm^{-1}, j = 0.8 cm^{-1}, D_{Cr} = 0.3564 cm^{-1}, E_{Cr} = −0.0647 cm^{-1}, D_{12} = −0.1850 cm^{-1}, and E_{12} = −0.0112 cm^{-1} for **2**. Density functional theory (DFT) calculations were employed to calculate the zero-field splitting on Cr^{3+} ions. Calculations of the exchange integrals J were attempted by using the "broken-symmetry" DFT method.

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