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Molecular Analogue of the Perovskete Repeating Unit[1] XIANGGUO LI, YUN-PENG WANG, ANNALIESE E. THUIJS, KHALIL A. ABBOUD, GEORGE CHRISTOU, X.-G. ZHANG, HAI-PING CHENG, Univ of Florida - Gainesville — The perovskite manganites $AMnO_3$ and their doped analogues $A_{1-x}B_xMnO_3$ are a fascinating family of magnetic oxides exhibiting a rich variety of properties. They are thus under intense investigation along multiple fronts, one of which is how their structural and physical properties are modified at the nanoscale when needed at this size regime. We investigate the electronic and magnetic properties of the molecular compound $[Ce_3Mn_8O_8(O_2CPh)_{18}(HO_2CPh)_2]$ (Ce_3Mn_8) that bears a striking structural resemblance to the repeating unit seen in the perovskite manganites, using first-principles method. We show that Ce_3Mn_8 exhibits both the combination of pairwise Mn_2^{III} ferro- and antiferromagnetic exchange interactions and the resultant spin vector alignments that are found within the C-type antiferromagnetic perovskites. The first-principles calculations reveal not only the expected nearest-neighbor Mn_2^{III} exchange parameters but also an unusual, direct metal-to-metal channel through the central Ce^{IV} for magnetic couplings, originating from a virtual exchange involving the Ce^{IV} f-orbitals.

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