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Competition between Jahn-Teller instability and uniaxial magnetism in Ca_3CoMO_6 (M = Mn, Co, Rh) YUEMEI ZHANG, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, HONGJUN XIANG, National Renewable Energy Laboratory, 1617 Cole Blvd., Golden, CO 80401, ERJUN KAN, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204, A. VILLESUZANNE, Institut de Chimie de la Matiere Condensee de Bordeaux (ICMCB-CNRS), Universite Bordeaux I, 87 Avenue du Dr. A. Schweitzer, 33608 Pessac Cedex, France, M.-H. WHANGBO, Department of Chemistry, North Carolina State University, Raleigh, NC 27695-8204 — Ca_3CoMO_6 (M = Mn, Co, Rh) exhibits a uniaxial magnetism, because the Co^{n+} ions of their CoO_6 trigonal prisms (n = 2 or 3) possess an electron configuration with unevenly filled degenerate d-states, so the Co^{n+} ions have a nonzero magnetic moment only along the axis of the rotational symmetry causing the degeneracy (i.e., the 3-fold rotational axis along the $CoMO_6$ chain). Such ions lead to Jahn-Teller (JT) instability, and the associated distortion removes the rotational symmetry responsible for the uniaxial magnetism. We investigated how these opposing factors compete in Ca_3CoMO_6 (M = Mn, Co, Rh) on the basis of first principles DFT calculations.

Yuemei Zhang
Dept of Chemistry, North Carolina State University, Raleigh, NC 27695-8204

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