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Magnetic ordering, frustration and possible spin liquid state from 1D Cr₃-triangles in the TiCrIr_{2-x}Os_xB₂ series

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A new series of compounds TiCrIr_{2-x}Os_xB₂ (x=0-2) was successfully synthesized and characterized using X-ray diffraction as well as energy-dispersive X-ray analysis. All members of the series crystallize in the hexagonal non-centrosymmetric Ti_{1+x}Os_{2-x}RuB₂ structure type (space group P62m, no. 189, Pearson symbol hP18). The structure contains trigonal planar B₄ units strongly interacting with triangles of magnetically active Cr atoms, which are stacked on each other to form isolated Cr₃-chains along the c-axis. Magnetization measurements of TiCrIr₂B₂ (34 valence electrons, VE) reveal ferrimagnetic behavior below T_c=275 K with a large, negative Weiss constant of -750 K. Density functional theory calculations demonstrate magnetic frustration due to indirect antiferromagnetic interactions within the Cr₃ triangles competing with direct ferromagnetic interactions. Tuning the valence electron count by replacing Ir with Os changes the magnetic behavior in the series. Magnetization measurements of TiCrIrOsB₂ (33 VE) and TiCrOs₂B₂ (32 VE) exhibit paramagnetic behavior with features reminiscent of the spin liquid state. Interestingly, the crystal orbital Hamilton population (COHP) of TiCrIr₂B₂ indicates Cr-Cr antibonding interactions above 32.9 VE, but part of the Cr-Cr antibonding region is already occupied in TiCrOs₂B₂ even though it has 32 valence electrons. Therefore, the TiCrIr_{2-x}Os_xB₂ (x=0-2) series do not follow rigid band approximation.

Biography

Boniface P T Fokwa completed his PhD in 2003 from the Dresden University of Technology (Germany) and Post-doctoral studies from the RWTH Aachen University (Germany). He is an Associate Editor for Encyclopedia of Inorganic and Bioinorganic Chemistry (Wiley). He has published more than 70 papers in reputed journals and has won several awards including the prestigious Heisenberg Fellowship from the German Research Foundation and was Visiting Scientist at University of Auckland (New Zealand) and Cornell University as well as Visiting Professor at UCLA.

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