Crystal lattice effect on the quenching of the intracluster magnetic interaction in [V12B18O60H6] 10- polyoxometalate

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In the present work, the synthesis and structural characterization of four new polyoxovanadoborate (BVO) frameworks based on the [V12B 18O60H6]10- polyanion are reported: (NH4)8(1,3-diapH2)[V12B 18O60H6]·5H2O (1), K 8(NH4)2[V12B18O 60H6]·18H2O (2), K10[V 12B18O60H6]·10H2O (3) and K8Cs2[V12B18O 60H6]·10H2O (4). A global antiferromagnetic behaviour is observed for these 10VIV/2V V mixed valence clusters. The magnetic data of 1, 2 and 3, which present different countercation environments, show that 1 is more coupled than 2 and 3. DFT calculations show that the positive charges strongly influence the polarization mechanism of the spin density of the vanadyl groups and the extent of the magnetic orbitals, therefore corroborating the experimental observation of the quenching effect of the magnetic coupling between vanadium centres of 2 and 3.