Moment direction and off-octahedral distortions in K_2CoF_4 and CoO

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We have analyzed two cobalt compounds, K_2CoF_4 and CoO, with an aim to explain their magnetocrystalline anisotropy i.e. the origin of the given direction of the Co magnetic moment. In both these compounds Co ions are divalent. They are both antiferromagnetic below 107 and 291 K, respectively. In our atomic-like approach QUASST the d electrons in these compounds form the highly-correlated atomic-like system $3d^7$ realizing the high-spin state resulting from the octahedral subterm $^4T_{1g}$ (^4F). We have derived the low-energy electronic structure taking additionally into account the tetragonal distortion and the relativistic spin-orbit interaction. We have found that the tetragonal distortion determines the direction of the Co moment. The moment direction along the tetragonal axis is realized in case of the tetragonal compression explaining experimental results. We have calculated the orbital moment. These theoretical findings we treat as a large superiority of our atomistic approach over presently-in-fashion *ab initio* methods which are unable to provide e. g. low-energy (say, in the 5 meV scale) electronic structure, anisotropy and the orbital moment.