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Magnetic order on a frustrated lattice due to orbital degrees of freedom in RO_2 hyperoxides ANDRZEJ M. OLEŚ, Jagellonian University, Cracow, Poland, KRZYSZTOF WOHLFELD, MARIA DAGHOFER, IFW Dresden, Germany — The alkali RO_2 hyperoxides (R=Rb,Cs,K) crystallize in a frustrated bct lattice. Nevertheless, all of the members of the family of alkali RO_2 hyperoxides have long range layered C-type antiferromagnetic (C-AF) order at low temperature. We show that including the almost degenerate p-orbital degrees of freedom in a realistic spin-orbital model can resolve this contradiction [1]. Although a priori the orbital degrees of freedom do not remove frustration in spin system, we show that the anomalously large interorbital hopping together with the orbital order induced by the lattice stabilize the C-AF order in this class of compounds, in agreement with generalized Goodenough-Kanamori rules formulated here.

[1] K. Wohlfeld, M. Daghofer, and A.M. Oleś, EPL 96, 27001 (2011).

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