Magnetic interactions in hexanuclear cluster compounds of niobium and tantalum

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Octahedral hexanuclear clusters of Mo, W, Nb and Ta draw attention in the solid state research due to interesting phenomena they exert such as superconductivity at high critical fields and specific thermoelectric properties. Nb and Ta halide clusters, with the $[M_6L_{12}]^{n+}$ structural unit exist in three different oxidation states (n = 2, 3 or 4). Magnetic interactions between paramagnetic clusters (n = 3) have been noticed experimentally some time ago, whereas the role of bridging atoms (L) has been revealed using ^{19}F ssNMR spectroscopy only 5 years ago [1]. More recently, a model of Heisenberg antiferromagnet ($\mathcal{H} = -J\sum_{i,j} \boldsymbol{S}_i \cdot \boldsymbol{S}_j$) has been proposed for several Ta_6 halide cluster compounds [2]. Symmetry of the lattice determines the onset of an unusual long-range ordering. Usefulness of broad-band ssNMR and NQR spectroscopies in the investigation of these phase transitions will be discussed.

[1] R. Knoll, J. Sokolovski, Y. BenHaim, A. I. Shames, S. D. Goren, H. Shaked, J.-Y. Thépot, C. Perrin and S. Cordier, Physica B **381** (2006) 47

[2] B. Perić, S. Cordier, J. Cuny, R. Gautier, T. Guizouarn and P. Planinić, Chem. Eur. J. (2011) (DOI: 10.1002/chem.201002332)