# INVESTIGATION OF STATIC AND DYNAMIC MAGNETISM IN NICKEL(II) COMPLEXES

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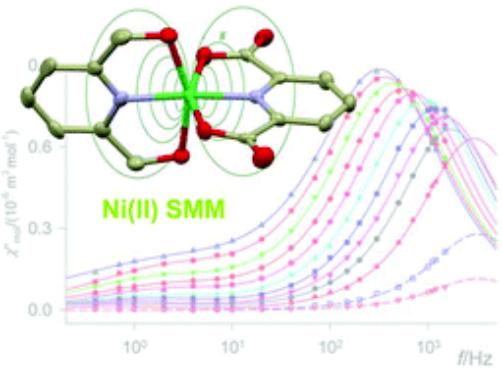


Single ion magnetism (SIM) represents very attractive phenomena that accelerated a development of the coordination chemistry. One of the principal problems in this area is the understanding the relaxation phenomena that cause a degradation of the magnetic ordering and define the lifetime of the SIM. The Orbach process climbing over the barrier to spin reversal represents only one of the numerous relaxation processes. In its theory, the axial zero-field splitting parameter *D*, in combination with the rhombic zero-field splitting *E*, plays a key role. A number of hexacoordinate, pentacoordinate, and tetracoordinate Ni(II) complexes has been investigated by applying the Generalized Crystal Field Theory and *ab initio* calculations. The geometry of the coordination polyhedron covers $D_{4h}$, $D_{3h}$, $D_{2h}$, $D_{2d}$, $C_{4v}$, $C_{3v}$, $C_{2v}$, and $D_{5d}$ symmetry. The calculated spin-Hamiltonian parameters, as well as the relaxation parameters were compared with the experimental data [1, 2].

[1] Rajnák, C., Titiš, J., Boča, R., *Magnetochemistry* **2021**, 7 (6), art. no. 76.

[2] Titiš, J. et al., *Dalton Transactions* **2019**, 48 (31), pp. 11647.