

Charge transfer process contribution to the zero-field splitting of the S-state transition ions

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Abstract

The zero-field splitting of the S state due to the virtual electron transfer processes from the ligands into an unfilled shell ($4f$) of a paramagnetic ion has been calculated. A simple analytical formula has been deduced for the spin-Hamiltonian parameters. The paramagnetic centres: $\text{LiCaAlF}_6:\text{Fe}^{3+}$, $\text{LiSrAlF}_6:\text{Fe}^{3+}$, $\text{Al}_2\text{O}_3:\text{Fe}^{3+}$, $\text{LiCaAlF}_6:\text{Gd}^{3+}$, $\text{LiSrAlF}_6:\text{Gd}^{3+}$, $\text{Al}_2\text{O}_3:\text{Gd}^{3+}$ and $\text{YBa}_2\text{Cu}_3\text{O}_{6+y}:\text{Gd}^{3+}$ with $y = 0.91, 0.95$ have been considered as an example. In all cases the calculated values of the D-parameter are in agreement with the electron paramagnetic resonance data within an order of magnitude and in the sign as well.

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