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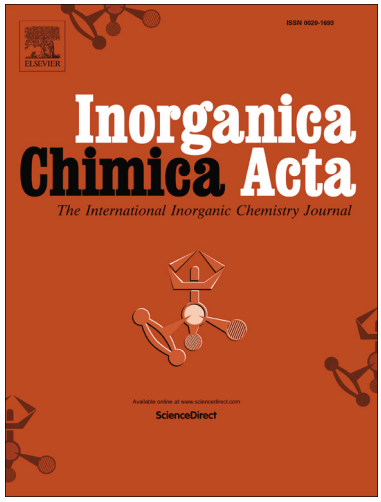

Theoretical insight into the superexchange mechanism of coupling in $f^1 - f^1$ system. The case of study $Ce_2(COT)_3$ compound

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Theoretical insight into the superexchange mechanism of coupling in $f^1 - f^1$ system. The case of study $Ce_2(COT)_3$ compound.

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Abstract

This work present a detailed theoretical determination of the spin-Hamiltonian parameters for $Ce_2(COT)_3$ molecule. A qualitative model to explain the origin of the small value of the Zero Field Splitting (ZFS) is developed concluding that, because of the symmetry reasons the spin orbit coupling (SOC) contribution to ZFS value is minimal and the value is the result only of dipole-dipole interaction. Magnetic susceptibility and g-factors are determined from the analysis of the magnetization matrices using different active spaces and the properties could be rationalized throughout the relationship between the monomer $[Ce(COT)_2]^-$ and bimetallic molecule. Finally a possible mechanism to explain the antiferromagnetic coupling of the magnetic moments of both centers is proposed using the states generated when $4f_{z^3}$ and $5d_{z^2}$ metal orbitals are included in the calculations. The active space employed in this point produce the best results at all levels of theory used in this work (CASSCF, MRCI+CIS and DDCIn n = 2, 3).