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Kolekcja

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Streszczenie

The absorption spectrum of tris[hydrotris(1-pyrazolyl)borato]uranium(III) (UTp_3) was run at room and low temperatures. From the spectra obtained, a truncated crystal field (CF) splitting pattern could be derived, and simulated by fitting the free parameters of a phenomenological Hamiltonian achieving an r.m.s. deviation of 37.7 cm^{-1} for 29 assignments. The parameters used allow the insertion of the Tp ligand into empirical spectrochemical, nephelauxetic and relativistic nephelauxetic series of U^{III} compounds, and the set-up of experimentally based nonrelativistic and relativistic molecular orbital schemes of UTp_3 in the f range. Using the wavefunctions and eigenvalues of the fit, the experimentally determined temperature dependence (in the range 1.34–294.4 K) of μ^2_{eff} could be reproduced adopting an orbital reduction factor k = 0.99.

Słowa kluczowe

uranium, N ligands, Optical properties, crystal field analysis, paramagnetic susceptibility, electronic structures

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