Spectroscopic properties of $K_5Li_2UF_{10}$.

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Streszczenie

A new uranium (III) fluoro-complex of the formula $K_5Li_2UF_{10}$ has been synthesised and characterised by X-ray powder diffraction and electronic absorption spectra measurements. The compound crystallises in the orthorhombic system, space group *Pnma*, with $a = 20.723$, $b = 7.809$, $c = 6.932$ Å, $V = 1121.89$ Å^3, $Z = 4$ and is isostructural with its $K_5Li_2NdF_{10}$ and $K_5Li_2LaF_{10}$ analogous. The absorption spectrum of a polycrystalline sample of $K_5Li_2UF_{10}$ was recorded at 4.2 K in the 3500–45,000 cm^{-1} range and is discussed. The observed crystal-field levels were assigned and fitted to parameters of the simplified angular overlap model (AOM) and next to those of a semi-empirical Hamiltonian, which was representing the combined atomic and one-electron crystal-field interactions. The starting values of the AOM parameters were obtained from ab initio calculations. The analysis of the spectra enabled the assignment of 71 crystal-field levels of U^{3+} with a relatively small r.m.s. deviation of 37 cm^{-1}. The total splitting of 714 cm^{-1} was calculated for the $^4I_{9/2}$ ground multiplet.

Adres publiczny

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