



Optical spectrum and crystal-field analysis of uranium trifluoride.

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Streszczenie

The first low temperature absorption spectrum and crystal-field analysis of uranium trifluoride are presented. The measurements have been performed on a polycrystalline sample in the 4000–30,000 cm^{-1} range at 4.2 K. One may notice the largest crystal-field splitting of SLJ multiplets among all so far reported data for uranium(III) as well as in polycrystalline samples and U^{3+} doped single crystals. In the presented analysis 94 experimental crystal-field levels, observed in 0–24,116 cm^{-1} energy range, have been identified and fitted to a semiempirical Hamiltonian representing the combined atomic and crystal-field interactions at the C_2 site symmetry. In order to exclude a possible influence of inaccuracy in the description of the free-ion multiplets on crystal-field parameters a number of additional freely varied parameters associated with the centroids of the free-ion multiplets were introduced. In the final step of the fitting procedure eight free-ion and 14 CF parameters were freely varied giving. The performed calculation procedure enabled the determination of good starting values, reliable crystal-field parameters and a small r.m.s. deviation.

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