INFLUENCE OF THE Tl^+-ION ELECTRONIC STATE ON THE ISOTROPIC d-BOND WITH LIGANDS

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S u m m a r y

The radial wave functions of an activator Tl^+ ion in the excited electronic state $5d^{10}6s6p$ have been calculated making use of the Hartree-Torrance method. The energy eigenvalues for d-, s-, and p-electrons of the Tl^+ ion introduced into KCl, KBr, and KI crystals have been determined. The energy of the isotropic d-bond with ligands has been shown to grow, if the electronic state of the Tl^+ ion becomes excited. This growth is responsible for a substantial reconstruction of thallium complexes within the lifetime of the Tl^+ excited electronic state.