CONTRIBUTION OF THE CLOSED d-ELECTRON SHELL OF THE TI⁺ ION TO CHEMICAL BOND

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Summary

A method that takes into account the influence of the crystal lattice field on the radial wave functions of an activator ion has been developed, with the electron density of lattice ions being approximated by a Gaussian distribution. The radial wave functions of a Tl⁺ ion embedded into KCl, KBr, and KI crystal lattices have been calculated. The results of calculations confirm the assumption made earlier about the existence of a new type of chemical bonds. These bonds are caused by a change of the self-energy of *d*-electrons, which belong to the activator ion's electron shell.