THERMODYNAMIC FUNCTIONS AND ENERGY STABILITY OF YTTRIUM TRICHLORIDE AND ITS DIMER

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Experimental and theoretical data on the structure and vibrational frequencies of yttrium trichloride and its dimer was critically analyzed. The analysis enabled to choose the values of molecular constants and to perform thermodynamic functions calculations. Enthalpy of sublimation of yttrium trichloride in the form of monomer was updated whereas enthalpy of YCl3(g) formation was calculated on the basis of existing data on vapor pressure of yttrium trichloride using new thermodynamic functions of YCl3 molecules. Enthalpy of sublimation of yttrium trichloride in the form of a dimer was found and the enthalpy of Y2Cl6(g) formation was calculated using literature data on the composition of vapor at the temperature of 1312 K. The composition of yttrium trichloride vapor in the temperature range between 1317 and 1646 K was calculated: the ratio of Y2Cl6 pressure to that of YCl3 increased from 0.15 to 0.21. The obtained values are added to IVTANTERMO software.