EVAPORATION THERMODYNAMICS OF YTTRIUM TRIFLUORIDE IN THE FORM OF MOLECULES YF_3 AND Y_2F_6

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Due to the ongoing work on obtaining reliable thermodynamic data of yttrium halides, new calculations of functions for YF3 and Y2F6 in gas phase were performed using quantum-chemical calculations by MP2 and CCSD(T) methods. Enthalpy of sublimation of yttrium trifluoride in the form of monomer was updated whereas enthalpy of YF3(g) formation was calculated on the basis of existing data on vapor pressure of yttrium trifluoride using new thermodynamic functions of YF3 molecules. Ab initio calculations of dissociation energy of dimer molecules Y2F6 on monomer two YF3 was carried out. Using this data sublimation enthalpy of yttrium trifluoride in dimer form was found and formation enthalpy of Y2F6(g) was calculated. The composition of yttrium trifluoride vapor was calculated as follows: the ratio of Y2F6 pressure to that of YF3 in the range between 1400 and 3000 K increased from 10-4 to 10-2. The thermodynamic and thermochemical values obtained were introduced into IVTANTERMO database.