MOLECULAR STRUCTURE OF $ErCl_3$ AND $YbCl_3$ ACCORDING TO THE DATA OF THE SIMULTANEOUS ELECTRON DIFFRACTION AND MASS SPECTROMETRIC EXPERIMENT

N. I. Giricheva,[1] S. A. Shlykov,[2] G. V. Girichev,[2] E. V. Chernova,[1] and E. A. Lapykina[1]

UDC 539.27: 544.18: 621.384.8: 544.666: 544.668

The saturated vapors of $ErCl_3$ and $YbCl_3$ were studied in a simultaneous electron diffraction and mass spectrometric experiment at 1165 K and 1170 K, respectively. In the vapors of these compounds, we found up to 3 mol.% dimers along with the monomers. The parameters of the r_g effective configuration of the monomer molecules were determined. For $ErCl_3$ and $YbCl_3$, the internuclear distances r_g(Ln–Cl) were 2.436(5) Å and 2.416(5) Å, and the bond angles $\angle_g$(Cl–Ln–Cl) were 117.0(10)° and 117.2(10)°, respectively. The equilibrium configurations and vibration frequencies of the monomer and dimer molecules were calculated by the HF, B3LYP, and MP2 methods using the combination of the ECP_D energy-consistent quasirelativistic core potential, including 4*f* electrons [Kr4d^{10}4f^n], and the contracted [5*s*4*p*3*d*] valence basis set for Er and Yb atoms and the MIDIX [4*s*3*p*1*d*] basis set for Cl atoms. The parameters of the effective r_g configuration of the monomer molecules corresponding to the temperature of the experiment were calculated. The difference between the calculated equilibrium r_e(Ln–Cl) and temperature-averaged r_g(Ln–Cl) distances was found to be 0.001-0.002 Å and did not exceed the error of the r_g(Ln–Cl) parameter determined in the electron diffraction experiment. The experimental parameters of the r_g structure were shown to be consistent with the idea about the planar equilibrium geometrical configuration of $ErCl_3$ and $YbCl_3$ molecules.

Keywords: gas-phase electron diffractometry, mass spectrometry, erbium trichloride, ytterbium trichloride, vapor composition, molecular structure, vibration frequencies, quantum-chemical calculations, anharmonicity of vibrations.