STRUCTURE OF $ScBr_3$ AND Sc_2Br_6 MOLECULES DETERMINED BY THE SYNCHRONOUS GAS-PHASE ELECTRON DIFFRACTION AND MASS SPECTROMETRIC EXPERIMENT AND QUANTUM CHEMICAL CALCULATIONS

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The structure of monomeric and dimeric molecules of scandium tribromide is studied by the synchronous electron diffraction and mass spectrometric experiment at T = 888(10) K and also by the quantum chemical calculations. The experimental data on the structural parameters of $ScBr_3$ molecule were obtained for the first time; also for the first time the molecular structure of Sc_2Br_6 dimeric molecule was studied. It is found that the $ScBr_3$ molecule has the C_{3v} effective configuration with the distance r_g(Sc–Br) = 2.430(3) Å and the valence angle $\angle_g$(Br–Sc–Br) = 117.6(5)°. The equilibrium structure of the given molecule is planar with D_{3h} symmetry. According to a theoretical study by DFT and MP2 methods, Sc_2Br_6 molecule has the equilibrium structure of D_{2h} symmetry with four Sc–Br bridge bonds. It was confirmed by the results of the electron diffraction analysis.

Keywords: gas-phase electron diffraction, quantum chemistry, mass spectrometry, scandium tribromide, scandium tribromide dimer, molecular structure, frequencies of vibrations.