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Calculations of cross sections data for scattering of electrons on BF3 MARIJA VRANIC, MARIJA RADMILOVIC-RADJENOVIC, ZORAN LJ. PETROVIC, Institute of Physics, POB 68, 11080 Zemun, Serbia, HEMAL N. VARAMBHIA, JONATHAN TENNYSON, Department of Physics and Astronomy, University College London, Gower Street, WC1E, 6BT, UK — In recent years there has been a need to establish extensive databases of atomic and molecular collisional cross sections. Boron trifluoride is used as a dopant in ion implantation, for initiating polymerisation of unsaturate compounds, as a catalyst in isomerization, alkylation, esterification, condensation, and is used in sensitive neutron detectors. This work dealing with BF3 is focused on computing the total (integrated) and excitation electron scattering cross-sections by using the R-matrix method. This data will enable a more accurate calculation of the transport coefficients. The R-Matrix code Quantemol-N has been used for the calculations. The basis set used in this calculation was 6- 311G, and the method was CI (Configuration Interaction). The computed total and BEB ionization cross sections were compared to known experimental studies. The results indicate the presence of a shape resonance of symmetry B1 (A2" in D3h) at around 4.5 eV.

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