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Dissociative Ionization of BF_3 and its fragments[1] MILKA NIKOLIC, MARIJA RASKOVIC, SVETOZAR POPOVIC, LEPOSAVA VUSKOVIC, Old Dominion University — Dominant contribution of particular molecular orbitals to the individual fragment production exists, in some cases, in the dissociative ionization by electron impact [1]. We have calculated the electron-impact ionization rates of BF_3 and its fragments. In our calculation electronic structures of BF_3 and its fragments were described with several empirical basic sets. After geometry optimization using density functional method B3LYP, MO parameters were calculated with UHF, CCSD(T) and OVGF methods [2]. Electron-impact ionization cross-sections were calculated employing the Binary-Encounter-Bethe approximation and results were compared with available experimental data. In the absence of clear-cut assignment, the fractional MO-fragment correlation was made using geometry considerations. As the final test of the method, we compared the ionization rates for electron energy distribution present in sheath mode of the repetitively pulsed d.c. diode system with those obtained experimentally.

[1] S. Popovic, S. Williams, and L.Vuskovic, Phys. Rev. A 73, 022711, (2006).
[2] Y-K Kim, K. K. Irikura, AIP conferences proceedings 543, 220 (2000).

[1]Spported by DOE.

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