Electron-impact ionization cross section calculations for 5-chloropyridine and 5-bromopyridine molecules

Electron-impact ionization cross section calculations for 5-chloropyridine and 5-bromopyridine molecules

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Synopsis The total cross sections for the single electron-impact ionization of 5-chloropyridine (5-C_5H_4ClN) and 5-bromopyridine (5-C_5H_4BrN) molecules have been calculated using binary-encounter-Bethe method for electron energies ranging from the ionization threshold up to 5 keV.

In the present work we have studied positive ionization of 5-chloropyridine (5-C_5H_4ClN) and 5-bromopyridine (5-C_5H_4BrN) molecules by electron impact. The total cross sections (ICSs) for the single electron-impact ionization have been calculated using the binary-encounter-Bethe (BEB) model [1] for electron energies ranging from the ionization threshold up to 5 keV. All quantities necessary in the BEB calculations, like the electron binging energy and the orbital kinetic energy, have well defined physical meaning and have been evaluated with the Hartree-Fock method using the GAUSSIAN code and the Gaussian 6-311G++(2d,2p) basis set. Since obtained that way ionization energies usually differ from experimental ones, we have performed also outer valence Green function calculations of correlated electron affinities and ionization potentials [2]. ICS obtained with the BEB method usually are in good agreement (within ±15%) with experimental data [3].

In figure 1 the calculated ICSs are shown. The ionization threshold behavior of the obtained ionization cross sections is very similar. Both ICS functions almost merge for electron-impact energies up to 50 eV. For electron energies higher than 50 eV the ionization cross section for 5-bromopyridine molecule is slightly higher than that for 5-chloropyridine molecule.

The ionization thresholds for studied targets calculated in the present work are listed in table 1 together with respective values obtained recently for pyridine, 2-chloropyridine and 2-bromopyridine molecules [4].

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Table 1. The ionization thresholds for pyridine molecule and its halogenated derivatives.

Molecule	Ionization Potential (eV)
Pyridine	9.638 [4]
2-chloropyridine	9.520 [4]
2-bromopyridine	9.372 [4]
5-chloropyridine	9.509
5-bromopyridine	9.372

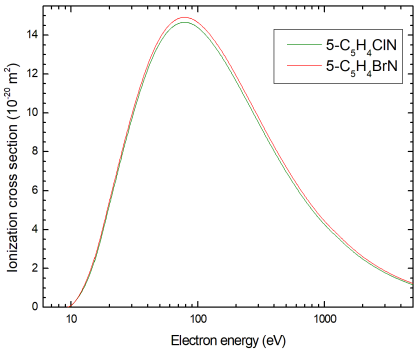

Figure 1. Comparison of the cross sections for electron-impact ionization of 5-chloropyridine and 5-bromopyridine molecules.

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References

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