

PAPER • OPEN ACCESS

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

To cite this article: B ywicka and P Moejko 2020 *J. Phys.: Conf. Ser.* **1412** 152076

View the [article online](#) for updates and enhancements.



**IOP | ebooks™**

Bringing together innovative digital publishing with leading authors from the global scientific community.

Start exploring the collection—download the first chapter of every title for free.

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

B Żywicka<sup>1\*</sup> and P Możejko<sup>2†</sup>

<sup>1</sup>Nicolaus Copernicus High School No. I, ul. Waly Piastowskie 6, 80-855 Gdańsk, Poland

<sup>2</sup>Department of Atomic, Molecular and Optical Physics, Faculty of Applied Physics and Mathematics, Gdańsk University of Technology, Gabriela Narutowicza 11/12, 80-233 Gdańsk, Poland

**Synopsis** The total cross sections for the single electron-impact ionization of 5-chloropyridine (5-C<sub>5</sub>H<sub>4</sub>ClN) and 5-bromopyridine (5-C<sub>5</sub>H<sub>4</sub>BrN) 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<sub>5</sub>H<sub>4</sub>ClN) and 5-bromopyridine (5-C<sub>5</sub>H<sub>4</sub>BrN) 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 binding 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.

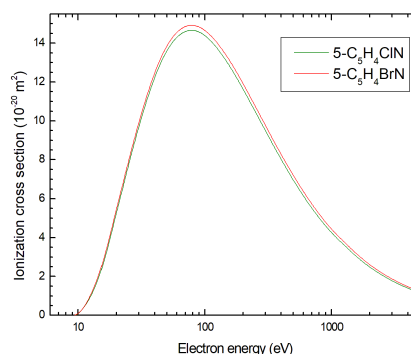
The ionization thresholds for studied targets calculated in the present work are listed in table 1 together with respective values obtained recently for pyridine, 2-chloropyridine and 2-bromopyridine molecules [4].

\*E-mail: [boshena@mif.pg.gda.pl](mailto:boshena@mif.pg.gda.pl)

†E-mail: [paw@pg.edu.pl](mailto:paw@pg.edu.pl)

**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.

This work has been supported by the Polish Ministry of Science and Higher Education. Numerical computations have been performed at the Academic Computer Center in Gdańsk.

### References

- [1] Hwang W *et al* 1996 *J. Chem. Phys.* **104** 2956
- [2] Zakrzewski V G *et al* 1993 *J. Comp. Chem.* **14** 13
- [3] Karwasz G P *et al* 2014 *Int. J. Mass Spectrom.* **365-366** 232
- [4] Szmytkowski Cz *et al* 2018 *Mol. Phys.* **117** 395

