Electron scattering by the pyrazine molecule: elastic and inelastic cross sections considering up to 139 open channels

Murilo O. Silva[1], Giseli M. Moreira[2], Márcio H. F. Bettega[1]
and Romarly F. da Costa[3]

[1]Departamento de Física, Universidade Federal do Paraná,
81531-980 Curitiba, Paraná, Brazil
[2] Departamento de Física, Universidade Estadual do Centro-Oeste,
85040-167 Guarapuava, Paraná, Brazil
[3]Centro de Ciências Naturais e Humanas, Universidade Federal do ABC,
09210-580 Santo André, São Paulo, Brazil

In this work we present integral and differential cross sections, as well as excitation functions, for the elastic scattering of low energy electrons by the pyrazine molecule. Electronically inelastic integral cross sections involving the transitions from the ground state to the first three singlet excited states and the first three triplet excited states of the pyrazine molecule by electron impact are also reported. The calculations were performed by using the Schwinger multichannel method implemented with pseudopotentials (SMCPP) [1] according to the minimum orbital basis for single configuration interactions (MOB-SCI) [2] strategy at a close-coupling level of up to 139 open channels. Our results are compared with the theoretical and experimental data available in the literature. Present elastic cross sections are in good agreement with previous calculated [3,4,5] and measured [6] results. On the other hand, only a marginal level of agreement between present and previous [4] calculed cross sections and the lack of measuremets for the electronic excitation cross sections highlight the need of further investigations.

[1] M. H. F. Bettega *et al.* , Phys. Rev. A **47**, 1111 (1993).

[2] R. F. da Costa *et al.* , J. Phys. B **38**, 4363 (2005).

[3] C. Winstead and V. McKoy, Phys. Rev. A **76**, 012712 (2007).

[4] Z. Mašín and J. D. Gorfinkiel, J. Chem. Phys. **135**, 144308 (2011).

[5] A. G. Sanz *et al.* , J. Chem. Phys. **139**, 184310 (2013).

[6] P. Palihawadana *et al.* , J. Chem. Phys. **137**, 204307 (2012).