M. H. F. Bettega[†], C. Winstead^{*}, M. A. P. Lima[‡], V. McKoy^{*}

[†]Departamento de Física, Universidade Federal do Paraná, Caixa Postal 19044, 81531-990, Curitiba, Paraná, Brazil

*A. A. Noyes Laboratory of Chemical Physics, California Institute of Technology, Pasadena, California, 91125

[‡]Instituto de Física "Gleb Wataghin", Universidade Estadual de Campinas, Caixa Postal 6165, 13083-970, Campinas, São Paulo, Brazil

There have been several recent theoretical [1, 2, 3, 4, 5] and experimental [6, 7, 8] studies of elastic electron collisions with N₂O. One focus of interest has been the well-known Π shape resonance located near 2.2 eV, whose position has been correctly described by some calculations [1, 3, 5]. In particular, Winstead and McKoy presented a procedure to avoid target overcorrelation in resonant problems, which located the Π shape resonance at its experimental position. In general, the various calculated cross sections agree well with one another, and they also agree with experiment at energies above $\sim 10 \text{ eV}$, but at lower energies agreement with experiment is poorer. As Kitajima et al. pointed out, the calculated differential cross sections differ most from the experiment at angles below $\sim 60^{\circ}$, as shown in the figure. Similar behavior was noted in C_2H_4 and several other molecules that display low-energy resonances [9].



Fig. 1. Elastic differential cross sections for N_2O . Solid line, our recent calculation with a larger number of configurations; dashed line, results of Ref. [3]; squares, results of Ref. [7]; circles, results of Ref. [8].

Here we revisit the scattering of low-energy

electrons by N₂O and C₂H₄ in order to understand the origin of the discrepancies seen between theory and experiment in the elastic differential cross section. Our calculations employ the Schwinger multichannel method at different levels of approximation: static–exchange, static– exchange plus polarization, and polarization with multichannel coupling. Our previous calculations at the static–exchange level indicated that the inclusion of nuclear motion (stretching and bending vibrations) does not significantly affect the behavior of the differential cross sections at angles below ~ 60°. This behavior is also unchanged by the inclusion of a few open channels in the calculation.

References

- B. K. Sarpal, K. Pfingst, B. M. Nestmann, and S. Peyerinhoff, J. Phys. B 29, 857 (1996).
- [2] S. E. Michelin, T. Kroin, and M.-T. Lee, J. Phys. B 29, 4319 (1996).
- [3] L. A. Morgan, C. J. Gillian, J. Tenyson, and X. Chen, J. Phys. B **30**, 4087 (1997).
- [4] S. M. S. da Costa and M. H. F. Bettega, Eur. Phys. J. D 3, 67 (1998).
- [5] C. Winstead and V. McKoy, Phys. Rev. A 57, 3589 (1998).
- [6] C. Szmytkowski, G. Karwasz, and K. Maciag, Chem. Phys. Lett. 107, 481 (1984).
- [7] W. M. Johnstone and W. R. Newell, J. Phys. B 26, 129 (1993).
- [8] M. Kitajima, Y. Sakamoto, R. J. Gulley, M. Hoshino, J. C. Gibson, H. Tanaka, and S. J. Buckman, J. Phys. B 33, 1687 (2000).
- [9] S. J. Buckman and L. T. Chadderton, 52nd Gaseous Electronics Conference, Norfolk, Virginia, October 5–8, 1999.