Calculations of cross sections for vibrational EELS of cyclopropane

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Hydrocarbon species are known as sources of carbon atoms during chemical vapour decomposition reactions [1]. Among them cyclopropane, C_3H_6, is found to be present in cooler edges of fusion plasmas [2]. Therefore qualitative and quantitative understanding of different events during the electron-cyclopropane collisions is important for initiating a great variety of processes.

In this work we apply Discrete Momentum Representation (DMR) method for calculation of elastic and vibrationally inelastic cross sections for electrons scattered by the cyclopropane molecules. Static-exchange approximation is employed for the collision energy range of 2-20 eV. We have analyzed all the 21 normal modes and the quantitative results have been compared with previous calculations of *Čurík and Gianturco* [3] where only 3 full-symmetric modes were computed. We also carried out a qualitative comparison with experimental data of Allan and Andric [4]. We have confirmed the presence of shape resonances of different symmetries in different vibrational modes and our cross sections compare well with those of *Čurík and Gianturco* for the excitations of modes where comparison is available, as can be seen on Fig.1.

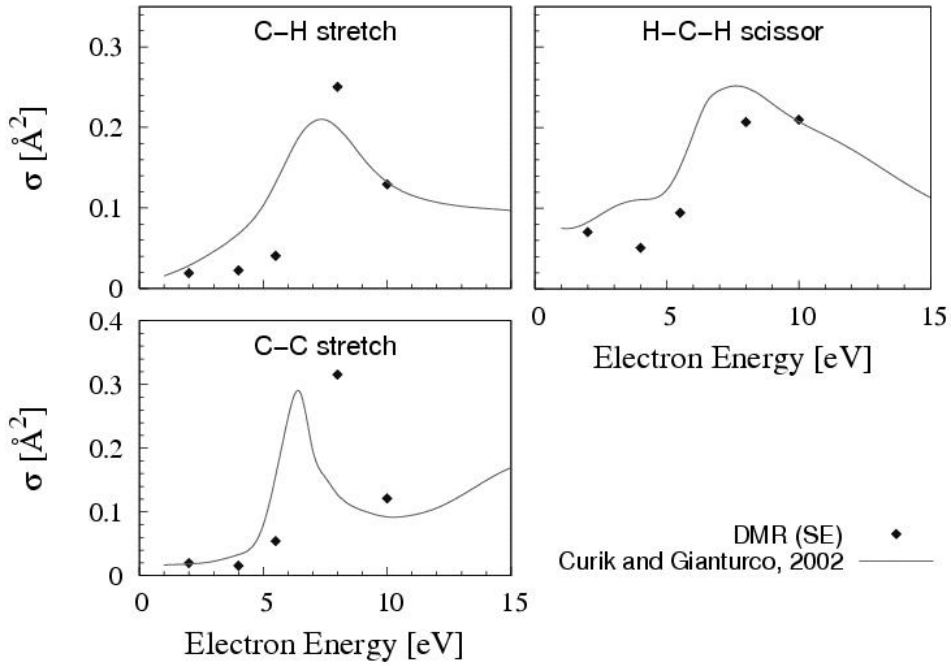

Fig. 1: Comparison of integral cross sections for the excitation of 3 vibrational modes. Diamonds represent DMR results and full curve are calculations of Curik and Gianturco [3].

References:

[1] Matus L G, Powell J A and Salupo C, 1991, *Appl. Phys. Lett.* **59** 1170
[2] Tawara H, Itikawa Y, Nishimura H, Tanaka H and Nakamura Y, 1990, *Report NIFS-DATQA-6*
[3] Čurík R and Gianturco F A, 2002, *J. Phys. B.* **35** 1235
[4] Allan M and Andric L, 1996, *J. Chem. Phys.* **105** 3559