

Convergent close-coupling calculations of electrons scattering on HeH^+

L. H. Scarlett^a, M. C. Zammit^b, I. Bray^a, B. I. Schneider^c, D. V. Fursa^a

^a*Department of Physics and Astronomy, Curtin University, Perth, Western Australia 6102, Australia*

^b*Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico 87545, USA*

^c*National Institute of Standards and Technology, Gaithersburg, Maryland 20899-8422, USA*

We have applied the molecular convergent close-coupling (MCCC) method to study electron scattering on HeH^+ . Along with the hydrogen molecule, HeH^+ is expected to form in the cooler edge and divertor regions of fusion reactors, where it is well-known that electron collisions with molecular species play an important role in governing the plasma dynamics. Previous calculations for this collision system have been almost exclusively limited to low-energy rovibrational excitation, and the only available measurements are for helium ion production following electron-impact dissociation of HeH^+ .

Figure 1 presents MCCC cross sections for dissociative excitation and ionisation of HeH^+ leading to He^+ fragments. Comparison is made with measurements from Lecointre *et. al.* [2] and Strömholm *et. al.* [3], and the complex Kohn calculations of Orel & Rescigno [1]. The MCCC DE calculations agree with the measurements of Strömholm *et. al.* [3] at low energies, and are in reasonable agreement with Lecointre *et. al.* [2] for ionisation. However, the MCCC total He^+ production cross section is 30% larger than measurements at the cross section peak. With only one set of measurements and no other calculations in this energy region the source of the discrepancy is not clear, and further experimental and theoretical work would be desirable to clarify the situation.

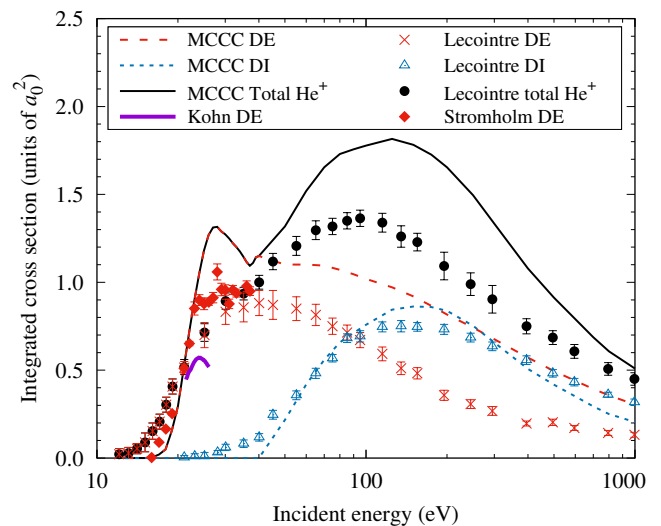


Figure 1: *Cross sections for production of He^+ from electron-impact dissociative excitation (DE) and ionisation (DI) of HeH^+ . Comparison is made between the MCCC calculations, the Kohn calculations of Orel & Rescigno [1], and the measurements of Lecointre *et. al.* [2] and Strömholm *et. al.* [3].*

[1] A. E. Orel, T. N. Rescigno, *Phys. Rev. A* **44**, 4328 (1991)

[2] J. Lecointre, J. J. Jureta, X. Urbain, P. Defrance *J. Phys. B At. Mol. Opt. Phys.* **47**, 015203 (2014)

[3] C. Strömholm, J. Semaniak, S. Rosén, H. Danared, S. Datz, W. van der Zande, M. Larsson, L. J. Dube, *Phys. Rev. A* **54**, 3086 (1996)