Quantemol Electron Collisions

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UCL

Easy Set Up for Molecular Targets

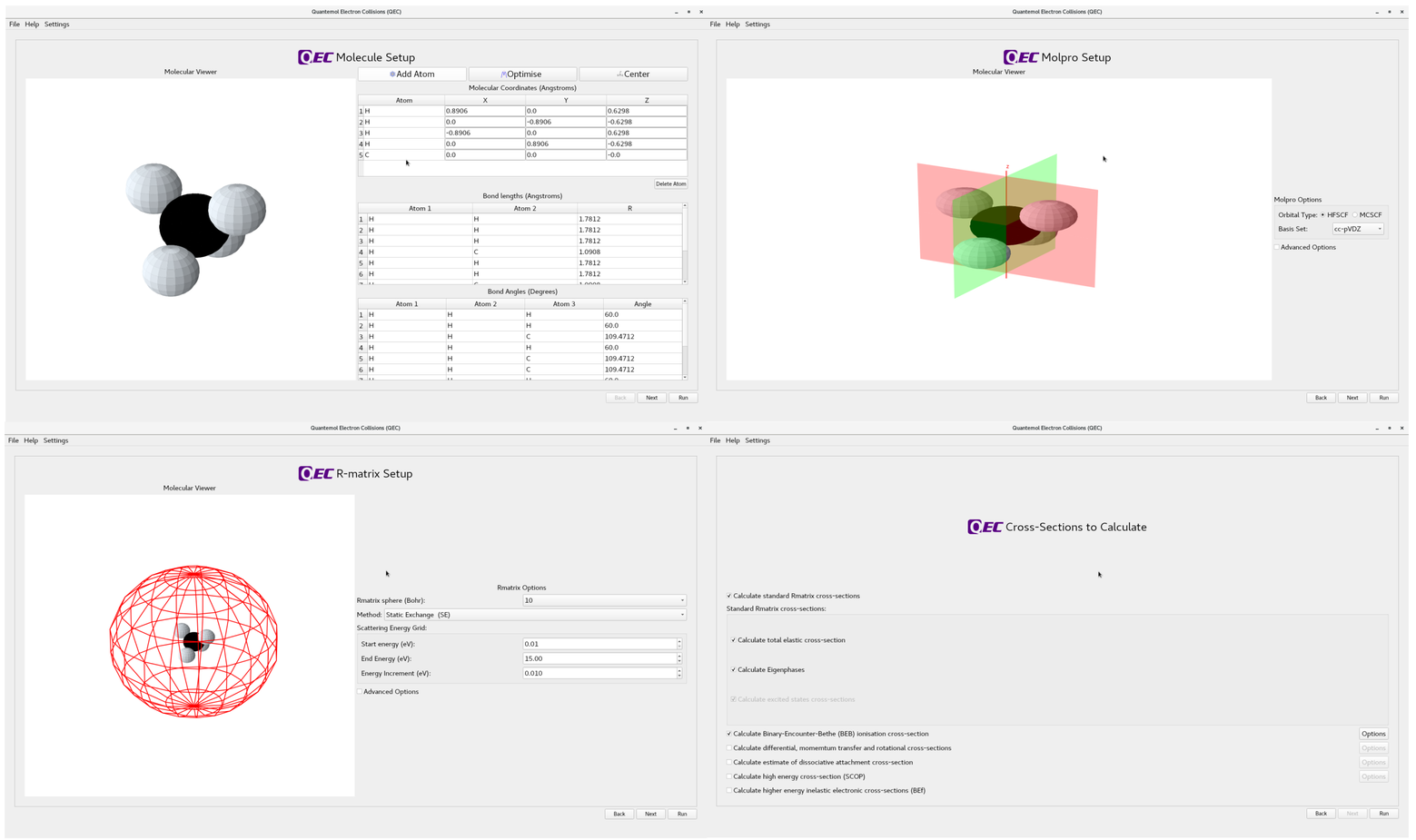
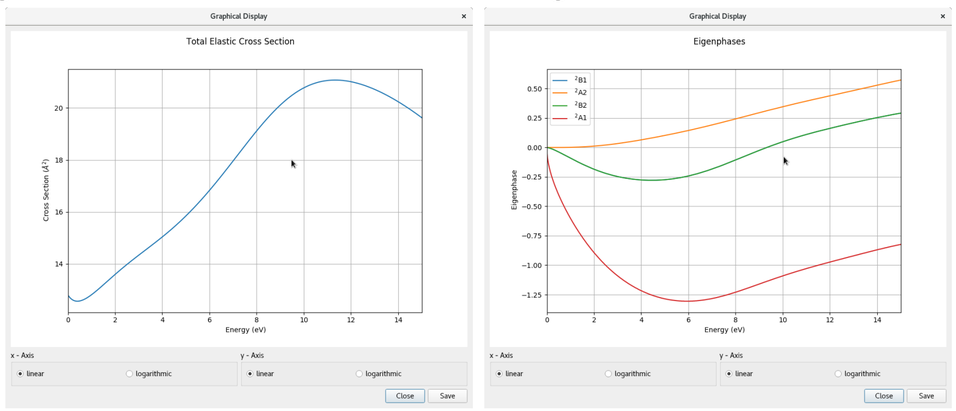


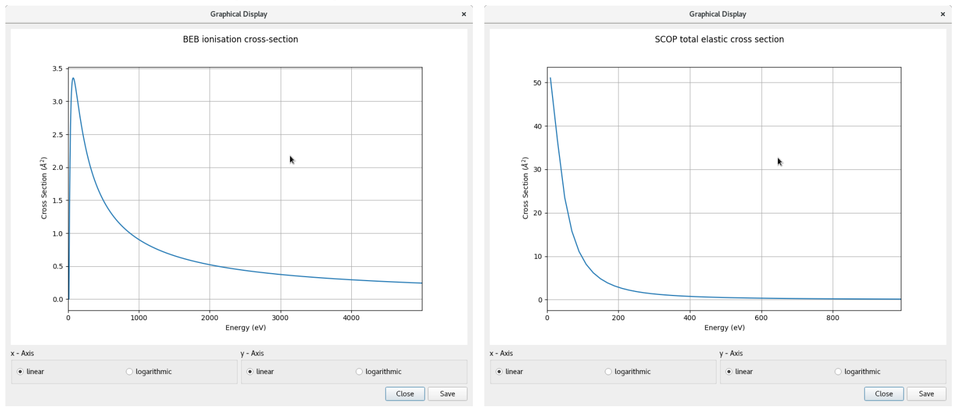
Fig 1: a) Easy set up of molecular targets. Optimize geometry using Molpro. Load an xyz file. b) Symmetry determination using Molpro. Select between HF or MCSCF orbitals. Default valence active space. c) Simplified r-matrix setup. Select r-matrix sphere size, select correlation method, and scattering energy grid. d) Select cross sections.

Results

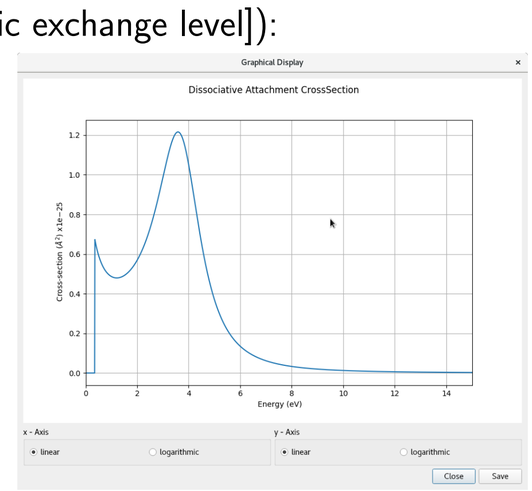
- Methane in cc-pVDZ at the Static Exchange level, with rmatrix sphere of 10 Bohr.
- Fig 2: Total elastic cross section and eigenphases:



- Fig 3: Binary-Encounter-Bethe ionisation cross section and high energy cross section(SCOP):

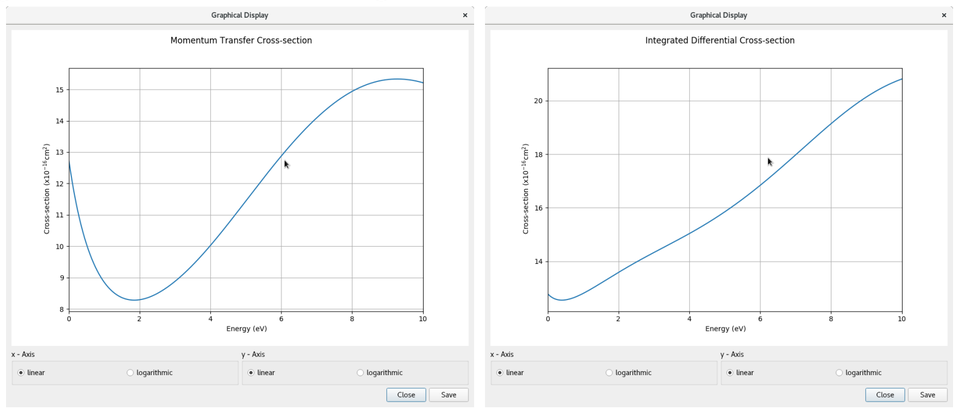


- Fig 4: Dissociative Electron Attachment cross-section (DEA [CO cc-pvdz at the static exchange level]):

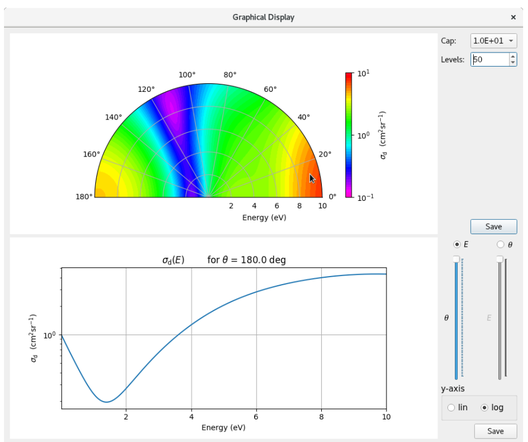


More Results

- Methane in cc-pVDZ at the Static Exchange level, with rmatrix sphere of 10 Bohr.
- Additional cross sections from POLYDCS code.
- Fig 5: Momentum and Integrated differential cross sections:



- Fig 6: Differential cross-section:



Read all about it

1. J. Tennyson et al, *J. Phys.: Conf. Ser.* **86** (2007), 012001.
2. H. -J. Werner et al, *WIREs Comput. Mol. Sci.*, **2**, (2012), 242.
3. J. Benda et al, *Comput. Phys. Comms* (to be submitted).
4. B. Cooper et al, *Preprints* (2019) 2019070126. (Later in Atoms.)