

# Photodetachment cross sections for molecular anions of astrophysical interest

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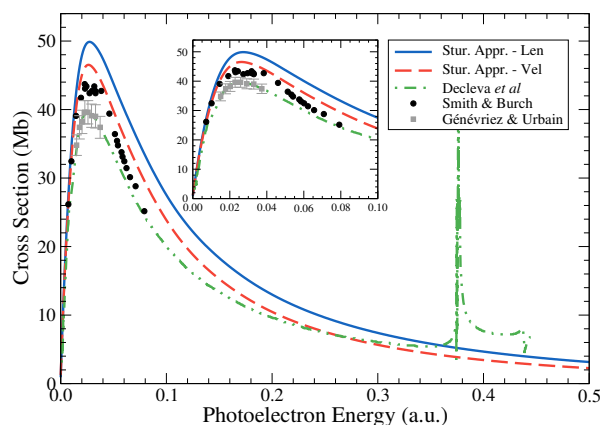
**Synopsis** We calculate photodetachment cross sections for small molecular anions of astrophysical interest, such as  $\text{CN}^-$ . The initial states are obtained using the complete active space self-consistent field, while the ejected electron is described through an expansion in Generalized Sturmian Functions with appropriate boundary conditions.

More than 30 years ago, Herbst suggested that negative molecular ions could be formed in the interstellar medium (ISM) through radiative attachment of a low-energy electron to a neutral radical [1]. The existence of anions in the ISM was recently confirmed with the discovery of several carbon chain negative molecular ions in space [2]. The formation of these anions is assumed to happen through radiative electronic attachment. The corresponding cross sections can be obtained from the photodetachment cross sections using detailed balance.

In this contribution, photodetachment cross sections are obtained using a Sturmian approach with generalized Sturmian functions (GSFs) [3, 4]. The approach has been used to study, among others, single photoionization of atoms and small molecules [5, 6]. In that case the ejected electron asymptotically feels a positive unit charge. For the photodetachment of atomic or molecular anions, the scattering wave function describing the ejected electron is expanded in a set of GSFs with zero asymptotic charge. The scattering amplitude is directly extracted from the expansion coefficients, without the need of calculating a transition matrix element.

We first considered  $\text{H}^-$  to test our methodology. The ground state of the anion was calculated using a B-spline basis, in the one-electron approximation. Even with a modest description of the target, we obtain a cross section (see Fig. 1) that is in agreement with other theoretical [7] and experimental [8, 9] data.

We will present calculations for small molecules, in particular for  $\text{CN}^-$ . The electronic wave functions are computed using the complete active space self consistent field (CASSCF) method and using the augmented double zeta (aug-cc-pVDZ) basis set. The full valence space was chosen as active space every time.



**Figure 1.** Cross section for the photodetachment of  $\text{H}^-$ . We compare our results using the Sturmian approach in the length and velocity gauges with theoretical calculations reported in Ref. [7] and with experimental data reported in Refs. [8, 9].

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## References

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