

## Cold inelastic collisions of $\text{He}(^1\text{S})$ with the smallest astrophysical anion observed, $\text{CN}^-(^1\Sigma^+)$ : an accurate quantum dynamical study.

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**Synopsis** Accurate state-to-state rovibrational inelastic collisional cross sections involving the smallest molecular anion astronomically detected with  $\text{He}(^1\text{S})$  based on two recently computed energy surfaces will be presented. A detailed comparison between the collisional findings provided either using a high-level of accuracy in the potential energy surface or taking advantage of the full-dimensional approach will be discussed.

In dense and dark regions of the interstellar medium, two-body inelastic collisions involving p-/o- $\text{H}_2(^1\Sigma_g^+)$  and  $\text{He}(^1\text{S})$  as projectiles are known to be crucial. They affect in fact the populations of the internal rovibrational levels involved in the radiative transitions by which a given species can be observed and its abundance inferred. If collisions with  $\text{He}(^1\text{S})$  are not as important as those involving p-/o- $\text{H}_2(^1\Sigma_g^+)$  on the basis of their column densities ratio, the former however provide an interesting choice for testing theory and supporting experimental measurements [1, 2].

$\text{CN}^-(^1\Sigma^+)$  is the smallest detected interstellar anion and to support the observations as well as to help to predict its abundance in interstellar regions other than the molecular envelope IRC+10216 where it has been observed, accurate inelastic collisional rate coefficients with the  $\text{He}(^1\text{S})$  and p-/o- $\text{H}_2(^1\Sigma_g^+)$  are essential [3].

Two potential energy surfaces for the ground electronic state of the  $\text{CN}^-$ -He anionic van der Waals complex have been recently constructed [4]. The first describes the complex in the rigid-rotor approxima-

tion at the CCSD(T)/aug-cc-pV{5,6}Z (cp corrected) +  $\Delta\text{CCSDT/cc-pV}\{\text{T,Q}\}\text{Z} + \Delta\text{CCSDT(Q)/cc-pVTZ}$  + rel. CCSD(T)/aug-cc-pV{5,6}Z-DK + core-valence CCSD(T)/aug-cc-pwCV{5,6}Z level and shows a general accuracy of about 0.2/0.4  $\text{cm}^{-1}$ . The second one is full-dimensional at the CCSD(T)/aug-cc-pV{5,6}Z (cp corrected) level and is averaged on the lowest anionic diatom vibrational wave functions. Assuming the system  $\text{CN}^-$ -He as a prototype for polar negatively charged van der Waals complexes, a detailed comparison between the inelastic collisional findings obtained using either the full-dimensional approach or very high level of accuracy will be presented and discussed.

### References

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