Cold inelastic collisions of He(^{1}S) with the smallest astrophysical anion observed, $CN^-(^1\Sigma^+)$: 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 He(^{1}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-$H_2(^1\Sigma_g^+)$ and He(^{1}S) as projectiles are known to be crucial. They affect in fact the populations of the internal rovitational levels involved in the radiative transitions by which a given species can be observed and its abundance inferred. If collisions with He(^{1}S) are not as important as those involving p-/o-$H_2(^1\Sigma_g^+)$ on the basis of their column densities ratio, the former however provide an interesting choice for testing theory and supporting experimental measurements [1, 2].

$CN^-(^1\Sigma^+)$ 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 He(^{1}S) and p-/o-$H_2(^1\Sigma_g^+)$ are essential [3].

Two potential energy surfaces for the ground electronic state of the CN^--He anionic van der Waals complex have been recently constructed [4]. The first describes the complex in the rigid-rotor approximation at the CCSD(T)/aug-cc-pV{5,6}Z (cp corrected) + $\triangle$CCSDT/cc-pV{T,Q}Z + $\triangle$CCSDT(Q)/cc-pVTZ + rel. CCSD(T)/aug-cc-pV{T,Q}Z-DK + core-valence CCSD(T)/aug-cc-pwCV{T,Q}Z level and shows a general accuracy of about 0.2/0.4 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 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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