Isotope effect in reactive collisions of O^- with H_2, D_2 and HD

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Synopsis We have calculated cross sections for the reaction of oxygen anion with the hydrogen molecule and its isotopic analogs producing the neutral H_2O molecule by electron detachment or OH^- (OD^-) through proton (deuteron) transfer. We found strong isotopic effect in agreement with recent measurements of colleagues from our faculty [1]. We also predict strong asymetry in OH^-/OD^- production when oxygen anion reacts with HD molecule.

Water is almost omnipresent in both laboratory and space environment. Its creation in the interstellar clouds in gas phase can proceed through the associative detachment reaction

$$O^- + H_2 \rightarrow H_2O + e^-.$$

The reaction is exotermic with large cross section at very low energies exceeding the Langevin cross section [2]. It is competing with OH^- production, which is also exoenergetic but much less efficient at subtermal energies.

In our previous work [2, 3] we have studied the global shape of all three potential energy surfaces connected to groung state O^- + H_2 asymptote. We have also localized the crossing of the anion state and the neutral state, determining thus the electron autodetachment region. To characterize the electron detachment process we studied the electron collisions with water molecule at relevant geometries in [3] with the R-matrix method. Based on this information we constructed preliminary model of the reaction dynamics and performed quantum scattering calculation with limited dimensionality to asses the capture cross section at very low energies [2].

In this work we will present more detailed classical trajectory Monte-Carlo calculations of the reaction cross sections for different isotopic variants of the collision O^- + H_2, D_2 and HD. We will show that while the associative detachment cross section is quite insensitive to isotope effect, the production of the hydroxyl anion is very sensitive to the mass of hydrogen atoms. The reactions can thus lead to strong asymetry in isotopic composition of interstellar molecular clouds.

References

[1] R. Plašil, Š. Roučka, J. Glosík, *private communication.*

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