The effect of molecular geometry on He*-H_2 autoionization reaction

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A new technology developed by Ed Narevicius [1,2] enables chemical reactions to proceed at very low temperatures, close to absolute zero. For example, a Penning ionization reaction was observed on the collision of an excited helium atom and a hydrogen molecule. The investigation of such reactions is enabled by generating a complex potential energy surface (CPES). In our research, using CPESs obtained by Bhattacharya and coworkers [3], we study the Penning ionization reaction rate during the collision of He^* (^{3}P,1s2p) and H_2 as related to their geometry. Our results demonstrate that due to the large anisotropy of the CPESs, the molecular geometry during the ionization reaction observed in the experiment, was almost exclusively the B_1 T-shape geometry, although the ionization could theoretically occur also in the other geometries. Figure 1 shows an excellent agreement between the reaction rate coefficient calculated assuming the B_1 symmetry of the T-shape geometry (without any fitting or scaling parameter) and the measured coefficient. The reaction rate coefficients for each geometry were calculated using a simple closed-form expression [4], which yielded a good agreement with the experimental results of the collision between He^* (^{3}S,1s2s) and H_2 [5].

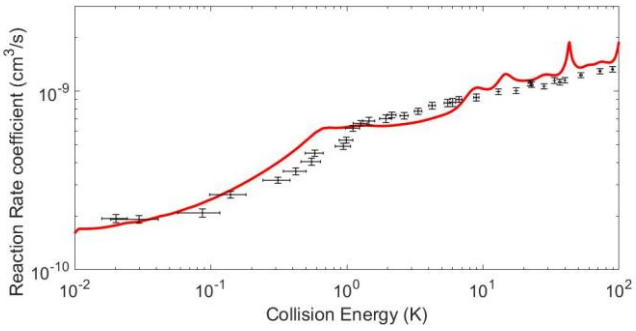

Figure 1: Comparison of the measured reaction rate coefficient with the coefficient calculated assuming the B_1 T-shape geometry (in red).

References

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