Supporting material

State-to-State Differential Cross Sections for the Reactive Scattering of $H^*(n)$ with o-D_2

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Theoretical method and Figures S1, S2, S3

Theoretical Method

The potential energy surface (PES) employed in the present study was newly constructed in terms of the internal coordinates (r_1, r_2, θ) shown in **Fig.S3**, where r_1 is the distance between the two D atoms, r_2 is the distance between H^+ and one of the D atoms, and θ is the enclosed bond angle. All the *ab* initio calculations were carried out at the CCSD/aug-cc-pvqz level of theory by using MOLPRO[1] and Gaussian[2] package. We use 50 points for r_1 from 0.7 to 20.0 a_0 with the restriction of $r_2 \geq r_1$, and the angle θ runs from 60^0 to 180^0 in increments of 10^0 by utilizing the symmetry of the system. This set of grids gives a total of ~12000 symmetry-unique points. In addition, ~1300 points on the perpendicular bisector line as shown in Fig.S1 are added to calculate energies and first order derivatives on the dividing line. Based on these ~13000 *ab* initio points the PES was constructed by the three-dimensional spline scheme[3,4]. The new PES is quite close to the existing PES[5], but with some small differences mainly due to different *ab initio* methods employed. The original data for the PES and the spline program are available at

http://www.QMD.dicp.ac.cn/research/PES/HD2+

The reactant-coordinate-based(RCB) [6,7] time-dependent wave packet method is used here to study the $H^+ + D_2$ reaction at the state to state level by propagating initial state selected wave packets only in reactant coordinates. The RCB method has particular advantages over the other approaches to reactions with deep wells as has been demonstrated[8,9]. The numerical parameters used in the time-dependent wave packet calculation are as follows: A total of 191 sine functions (among them, 127 for the interaction region) are employed for the translational coordinate in the range of [0.0, 22.0]α_0. A total of 47 vibrational functions are employed in the range of [0.6, 22.0]α_0 for the reagent D_2 in the interaction region. We use total of 90 rotational basis. The permutation symmetry of the diatomic reagent is used, which saves half of the angular grid points. Calculations are carried out for all the total angular momentum J up to 59 to converge differential cross sections of the title reaction for collision energies up to 0.6 eV. The full K (the projection of the total angular momentum onto the scattering velocity vector) blocks are used in the calculation for each J. The total propagation time is 400,000 au to accomplish the wave packet propagation from the reagent channel to the product channel. For higher J partial waves, the wave packet is propagated for a shorter time because the reaction probability in the low energy range is negligible. We put the dividing surface at 16.0α_0. in the product coordinates to extract the state-to-state information. For each reactant K block, we use only 3 potential optimized discrete variable representation (PODVR) points for product HD and 12 Gaussian-Legendre quadrature points for the rotational motion of the diatomic product. **Fig.S1** shows the total differential cross section calculated at 0.526 eV collision energy for the $H^+ + D_2(\nu=0, j=0) \rightarrow HD + D^+$ reaction.

Fig.S2 shows angular distributions for the D products from phtotodissociation of CD_4 at 121.6 nm in the lab frame with or without LN_2-cooled copper block. The strong attenuation in the forward scattering direction (θ_{Lab}=-50~-70^o) by the HI beam has been observed. The strong elastic/inelastic scattering between D atoms with HI molecule is possibly responsible for this attenuation.

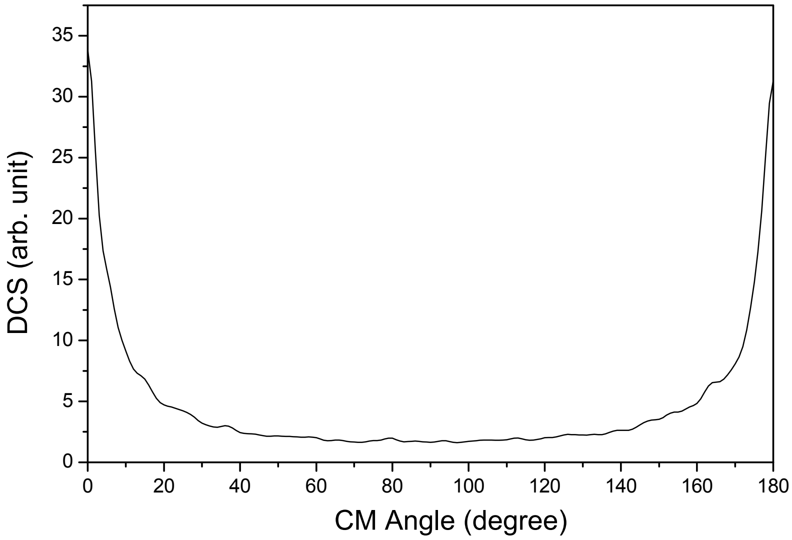

Fig S1 Total differential cross section calculated at 0.526 eV collision energy for the $H^+ + D_2(v=0, j=0) \rightarrow HD + D^+$ reaction.

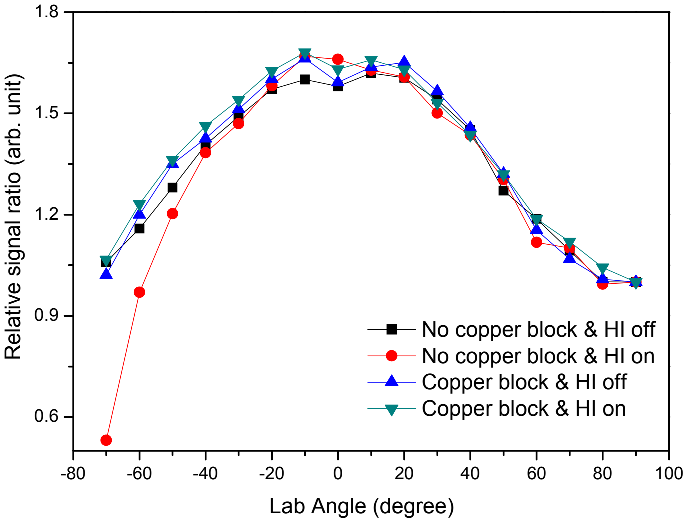

Fig S2 Angular distributions for the D products from phtotodissociation of CD_4 at 121.6 nm in the lab frame with or without LN_2-cooled copper block. The strong attenuation in the forward scattering direction (θ_{Lab}=-50~-70^{o}) by the HI beam has been observed.

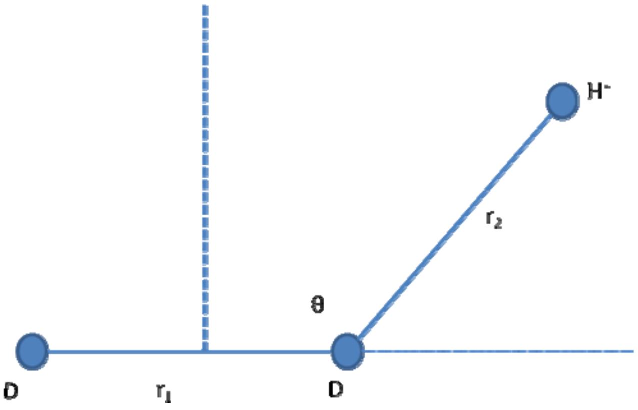

Fig S3 The internal coordinates used for three-dimensional spline for H_3^+ system

Reference:

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