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ABSTRACT

The reaction of ground state carbon, $C(^3P_j)$, with the propargyl radical, $C_3H_3(X^2B_2)$, is investigated at an average collision energy of 42.0 $kJmol^{-1}$ employing the crossed molecular beams technique and a universal mass spectrometric detector. The laboratory angular distribution and time-of-flight spectra of the C_4H_2 product are recorded at m/e = 50. Forward-convolution fitting of our data reveals the formation of diacetylene, HCCCCH, in its $X^1\Sigma_g^+$ electronic ground state. The reaction dynamics are governed by an initial attack of $C(^3P_j)$ to the π-electron density at the acetylenic carbon atom of the propargyl radical, followed by a [1,4]-hydrogen migration to the n-C_4H_3 isomer. A final carbon-hydrogen bond rupture yields atomic hydrogen and diacetylene thru a tight exit transition state located 30 - 60 $kJmol^{-1}$ above the products. This first successful crossed molecular beams study of a reaction between an atom and a free radical marks the beginning of the next generation of crossed beams experiments elucidating the formation of molecular species in combustion processes, chemical vapor deposition, in the interstellar medium, outflows of carbon stars, and hydrocarbon-rich planetary atmospheres via radical - radical reactions.

I. INTRODUCTION

The chemical reaction dynamics of atomic carbon in its $C(^3P_j)$ electronic ground state with unsaturated hydrocarbon molecules are of major importance in interstellar chemistry [1,2], combustion processes [3,4,5], and chemical vapor deposition [6,7,8]. Recently, we initiated these studies in our lab elucidating the chemical dynamics and reaction products of exothermic atom-molecule reactions (1)-(4) employing the crossed beams technique with electron impact ionizer coupled to a quadrupole mass spectrometer. These investigations provided collision energy dependent (8.8 - 45.0 $kJmol^{-1}$), doubly differential cross sections to both interstellar tricarbon hydride radicals [9], l/c-C_3H, and to hitherto unobserved interstellar propargyl [10] [C_3H_3 (X^2B_2)], n-C_4H_3 (X^2A') [11], and methylpropargyl [12] [C_4H_5 (X^2B_2/X^2A'')] radicals:

(1a) $C(^3P_j) + C_2H_2(X^1\Sigma^+_g) \rightarrow$ l-$C_3H(X^2\Pi_j) + H(^2S_{1/2})$,

(1b) $\rightarrow$ c-$C_3H(X^2B_2) + H(^2S_{1/2})$,

(2) $C(^3P_j) + C_2H_4(X^1A_g) \rightarrow C_3H_3(X^2B_2) + H(^2S_{1/2})$,

(3) $C(^3P_j) + CH_3CCH(X^1A_1) \rightarrow$ n-$C_4H_3(X^2A') + H(^2S_{1/2})$,

(4) $C(^3P_j) + C_3H_6(X^1A') \rightarrow C_4H_5(X^2B_2/X^2A'') + H(^2S_{1/2})$.

The explicit identification of this carbon-hydrogen exchange under single collision conditions elucidated the importance of a one-step pathway to free hydrocarbon radicals. This mechanism can be employed further to predict large scale concentrations of unobserved interstellar radicals C_3H_3, C_4H_3, and C_4H_5 in extraterrestrial environments [2].

The work described above is just the beginning towards a better understanding of the importance of neutral-neutral reactions in contrast to ion - molecule reactions in the formation of molecules and radicals in extraterrestrial environments. The chemical dynamics of atom-radical as well as radical-radical reactions in the hydrogen deficient C-H-system are completely unknown. Both reaction classes, however, are expected to have a profound impact on chemistry in interstellar and hydrocarbon-rich planetary environments at very low

temperatures down to 10 K: reactive encounters between carbon atoms with open shell hydrocarbons such as CH, C_2H, C_2H_3, and C_3H_3 radicals are thought to resemble prototype reactions proceeding without any barrier in the entrance channel. Therefore, these reactions are strongly expected to form complex species even in the coldest known interstellar clouds where the average kinetic energy of reactant molecules are about 0.08 $kJmol^{-1}$. In this communication, we present the chemical dynamics of atomic carbon reacting with the propargyl radical to form C_4H_2 isomers diacetylene [reaction (5)], butatrienylidene [reaction (6)], and/or the cyclic isomer cyclopropenylidenecarbene [reaction (7)] [13, 14, 15]:

(5) $C\,(^3P_j) + C_3H_3\,(X^2B_2) \rightarrow C_4H_3 \rightarrow C_4H_2\,(X^1\Sigma_g^+) + H(^2S_{1/2})$ $\Delta_R H^0 = -385 \pm 30\ kJmol^{-1}$

(6) $\rightarrow CCCCH_2\,(X^1A_1) + H(^2S_{1/2})$ $\Delta_R H^0 = -203 \pm 30\ kJmol^{-1}$.

(7) $\rightarrow c\text{-}C_4H_2\,(X^1A_1) + H(^2S_{1/2})$ $\Delta_R H^0 = -45 \pm 30\ kJmol^{-1}$.

II. EXPERIMENT AND DATA ACQUISITION

Investigating the chemical dynamics of radical-radical reactions using the crossed molecular beams technique is quite challaging. Compared to $C(^3P_j)$ reactions (1)-(4), the secondary neat hydrocarbon beam must be replaced by a ca. 10 % beam of the radical precursor seeded in helium. Even assuming an excellent conversion of 10 % into radicals, the reactive scattering signal drops by two orders of magnitude to gain a comparable signal to noise ratio to reactions (1)-(4) if the reactive scattering cross sections are comparable. The experiment is performed with a universal crossed molecular beam apparatus described in ref. [16] in detail. Briefly, a pulsed supersonic carbon beam is generated via laser ablation of graphite in the primary source chamber [17]. The 65 mJ, 30 Hz, 266 nm output of a Spectra Physics GCR-270-30 Nd:YAG laser is focused to a 0.1 - 0.2 mm spot onto a rotating graphite rod, and ablated carbon atoms are seeded into helium gas held at 4 atm backing pressure. A four slot chopper wheel located between skimmer of the primary source and the interaction region, slices a 9 μs segment of the pulsed carbon beam to select a velocity $v_0 = 2765 \pm 14\ ms^{-1}$ and

a speed ratio S = 3.0 ± 0.3. The pulsed propargyl radical beam is produced in the secondary source region via photodissociation of 10 % propargyl bromide precursor seeded in helium carrier gas at 1 atm stagnation pressure. The 80 mJ, 193 nm output of a Lamda Physik Compex 110 excimer laser is focussed 5 mm downstream of the pulsed valve nozzle to a rectangle of 1 × 4 mm. These operation parameters yield a propargyl beam with a velocity v_0 = 1220 ± 20 ms^{-1} and a speed ratio S = 14.0 ± 0.5. Time-of-flight spectra of reactively scattered species were monitored using a triply differentially pumped quadrupole mass spectrometer with an electron-impact ionizer [18, 19] in 5.0° steps with respect to the carbon beam at m/e = 51 and m/e = 50. To gain information on the reaction dynamics, the time-of-flight (TOF) spectra and the laboratory angular distribution (LAB) are fit using a forward-convolution technique [20] yielding the translational energy flux distribution $P(E_T)$ and angular distribution $T(\theta)$ in the center-of-mass reference frame.

Since both the carbon and propargyl beams are pulsed, extreme care has to be taken to select the correct time delay between the primary and secondary pulsed valve prior to the crossing at 90° in the interaction region. An improper timing would have resulted in reaction of $C(^3P_j)$ with the slow part of the secondary beam containing predominantly propargyl bromide precursor to form C_4H_3 detectable at m/e = 51 and m/e = 50 as well as Br atoms. Here, we optimize this delay by monitoring the excimer laser correlated integrated intensity of the time-of-flight (TOF) spectra at m/e = 50 versus the delay time of the second pulsed valve. Signal at m/e = 50 recorded with the excimer laser ''off'' originates only from reaction of atomic carbon with the propargyl bromide precursor and the fragmentation of the C_4H_3 product in the electron impact ionizer. However, signal with the excimer laser ''on'' can arise from reaction of carbon atoms with propargyl bromide as well as propargyl radicals. Therefore, a correct time delay should show no signal at m/e = 50 with the excimer laser ''off'', but only with the excimer laser ''on''. Further, the laser ''on'' TOFs at the correct delay time should show no intensity at m/e = 51. This optimization procedure results in triggering the second pulsed valve between 7 and 15 μs prior to the primary pulsed valve.

III. RESULTS

Reactive scattering signal was only observed at m/e = 50, i.e. C_4H_2, c.f. Figs. 1-2; no signal was detected at m/e = 51, unconditionally supporting the absence of propargyl bromide reacting with atomic carbon in our experimental conditions. The LAB distribution of the C_4H_2 product (Fig. 1) peaks at 55° near the center-of-mass angle of 55±1°, but shows a slight forward shape with respect to the carbon beam if we compare intensities at 45^0 and 50^0 with those at 55^0 and 60^0, respectively. Due to the limiting signal to noise ratio, no data could be obtained at angles smaller than 45^0 and larger than 65^0. Best fits of our data yield translational energy distributions $P(E_T)$s extending to 300 - 420 $kJmol^{-1}$, whereas the total available energy gives 427 ± 30 $kJmol^{-1}$ to form the diacetylene isomer, c.f. reaction (5). Finally, the $P(E_T)$s depict a maximum about 30 - 60 $kJmol^{-1}$, demonstrating a repulsive carbon-hydrogen bond rupture to result in a tight exit transition state.

The center-of-mass angular flux distribution $T(\theta)$ is slightly forward scattered with respect to the carbon beam yielding an intensity ratio of $I(0^0)/I(180^0) = 1.7 \pm 0.3$ within the error limits. This finding implies a) one microchannel to C_4H_2 thru an osculating complex or b) two microchannels giving an isotropic as well as a forward scattered contribution. Finally, the weak $T(\theta)$ polarization results from a poor coupling between the initial **L** and final orbital angular momentum **L'** with L' < 0.15-0.2 L indicating that most of the total angular momentum channels into rotational excitation of the C_4H_2 product.

IV. DISCUSSION

Figure 4 displays a schematic energy level diagram of the title reaction. Five reaction pathways on the ground state doublet surface are theoretically feasible. Defining the acetylenic carbon atom of the propargyl radical as C1, the central C atom as C2, the olefinic as C3, and the attacking one as C4, these are addition to C3, C2, or C1 forming the C_4H_3 isomers {1}, {2}, and {3}, as well as $C(^3P_j)$ insertion into the acetylenic C-H

bond yielding n-C_4H_3 (X^2A') {4} or insertion into an olefinic C-H-bond to form the iso C_4H_3 (X^2A') isomer {5}. Hereafter, [1,4]-H migration in {3} to {4}, a [3,4]-H migration in {1} to {5}, ring closure of {2} to {6} followed by a [1,4]-H-migration to {7} are theoretically possible. A final C-H bond rupture in {4} or {5} could form diacetylene {8}, and a C4-H cleavage in {4} could yield butatrienylidene {9} as well. Comparing the scattering range with limit circles of the C_4H_2 isomers and analyzing the high energy cut-off of the $P(E_T)$ strongly suggests that c-C_4H_2 {10} is not the major contribution. Therefore, we restrict the discussion on C_4H_2 isomers to diacetylene {8} and butatrienylidene {9}.

The crucial question to be answered is the nature of the decomposing C_4H_3 complex, i.e {4} and/or {5}. The forward peaked center of mass angular distribution requires that the attacking $C(^3P_j)$ and the leaving H atom must be located on opposite sites of the rotation axis of the fragmenting C_4H_3 complex. A detailed analyses of the principal rotational axes of {4} and {5} employing ab initio geometries from refs. [21, 22] alone clearly shows that {5} must rotate around its A axis to account for this $T(\theta)$ shape. The final C-H bond cleavage, however, would yield a linear diacetylene molecule, rotating about its internuclear axis. Due to the vanishing moment of inertia around the A axis, this rotation is energetically not accessible, and {5} can be excluded as the fragmenting C_4H_3 complex. The same argument strictly eliminates a decomposing {4} excited to A-like rotations, but rotations around the B/C axes contribute to the observed $T(\theta)$, leading to diacetylene {8} in the final C-H bond rupture excited to B-like rotations. The preferred olefinic bond cleavage in {4} as compared to the acetylenic one goes hand in hand with olefinic C-H bonds about 60 - 80 $kJmol^{-1}$ weaker than acetylenic ones.

Based on our crossed beam data alone, we cannot distinguish between the reaction path to {4}, i.e. a single insertion process into the acetylenic C1-H bond, or an initial addition to C1 followed by a hydrogen migration to {4}. Keeping in mind that $C(^3P_j)$ insertions are symmetry-forbidden and are expected to hold an entrance barrier, and comparing our findings with the chemical dynamics of reaction (1) and (3) studied

earlier, we find that $C(^3P_j)$ does not insert into C-H bonds, but rather attacks preferentially the carbon atom with the highest π-electron density, in our title reaction the acetylenic C1. Likewise, acceptable impact parameters leading to reaction supports the elucidated chemical dynamics. Here, attack to the olefinic C3 atom is expected to proceed almost perpendicular to the C_3H_3 molecular plane. The acetylenic C1-C2 bond, however, shows almost cylindrical symmetry, and in plane as well as out of plane approach geometries can lead to a C_4H_3 intermediate. Therefore, we conclude that the reaction between atomic carbon and propargyl radical is initiated by an attack to the C1 atom yielding {3}, followed by a hydrogen migration to {4} and a final bond rupture to form atomic hydrogen and diacetylene {8}.

Besides the chemical reaction dynamics, these results are of fundamental importance to interstellar as well as solar system chemistry as in Titan's stratosphere[23,24], the Jovian atmosphere [25] as well as Neptune, Uranus, Saturn and Triton [26,27]. Since C_3H_3 can be formed thru reaction (2) and photodissociation of C_3H_4 isomers [28], the title reaction is strongly suggested to be included in chemical reaction networks modeling these extraterrestrial environments. Further, reaction of $C(^3P_j)$ with C_3H_3 provides an alternative pathway to diacetylene hitherto thought to be solely synthesized via reaction (8) [29,30,31,32]:

(8) $$C_2H + C_2H_2 \rightarrow C_4H_3 \rightarrow C_4H_2 + H.$$

Future investigations of the title reaction will be performed at lower collision energies to elucidate a potential transition from a forward to isotropic center of mass angular distribution as the collision energy drops. If this is verified experimentally, {4} is a long-lived complex at lower, but an osculating one at higher collision energies. Likewise, the existence of a second isomer as detected around the circumstellar envelope of IRC +10216 and toward TMC-1 [33,34,35,36], $CCCCH_2$, will be investigated by replacing $HCCCH_2$ by $HCCCD_2$. Despite this open question, the present work clearly demonstrates that the investigation of the chemical reaction dynamics of radical - radical as well as atom - radical reactions employing the crossed molecular beam technique is technologically feasible and extendible to other systems. For example, preliminary reactive

scattering experiments of $C(^3P_j)$ with the vinyl radical, C_2H_3, [37] show laser correlated signal at interstellar C_3H_2 radicals at m/e = 38 - boldly to go where no one has gone before...

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Fig. 1. Lower: Newton diagram for the reaction $C(^3P_j) + C_3H_3$ at a collision energy of 42.0 $kJmol^{-1}$. The circle stands for the maximum center-of-mass recoil velocity in the center-of-mass reference frame of C_4H_2 isomers. From outer to inner: diacetylene, butatrienylidene, and cyclopropenylidenecarbene. Upper: Laboratory angular distribution of C_3H_3 at m/e = 50. Circles and 1σ error bars indicate experimental data, the solid line the calculated distribution. C.M. designates the center-of-mass angle of 55.0°.

Fig. 2. Time-of-flight data at the center-of-mass angle of 55.0°. The dashed line indicates the experimental data, the solid line the fit.

Fig. 3. Lower: Center-of-mass angular flux distribution for the reaction $C(^3P_j) + C_3H_3$. Upper: Center-of-mass translational energy flux distribution for the reaction $C(^3P_j) + C_3H_3$. Solid lines represent the best fit, dashed lines limit the range of acceptable fits within 1σ error bars.

Fig. 4. Schematic energy level diagram for the reaction $C(^3P_j) + C_3H_3$. Solid dashed lines: no ab-initio calculations have been performed on these structures. E_{av} indicates the total available energy.

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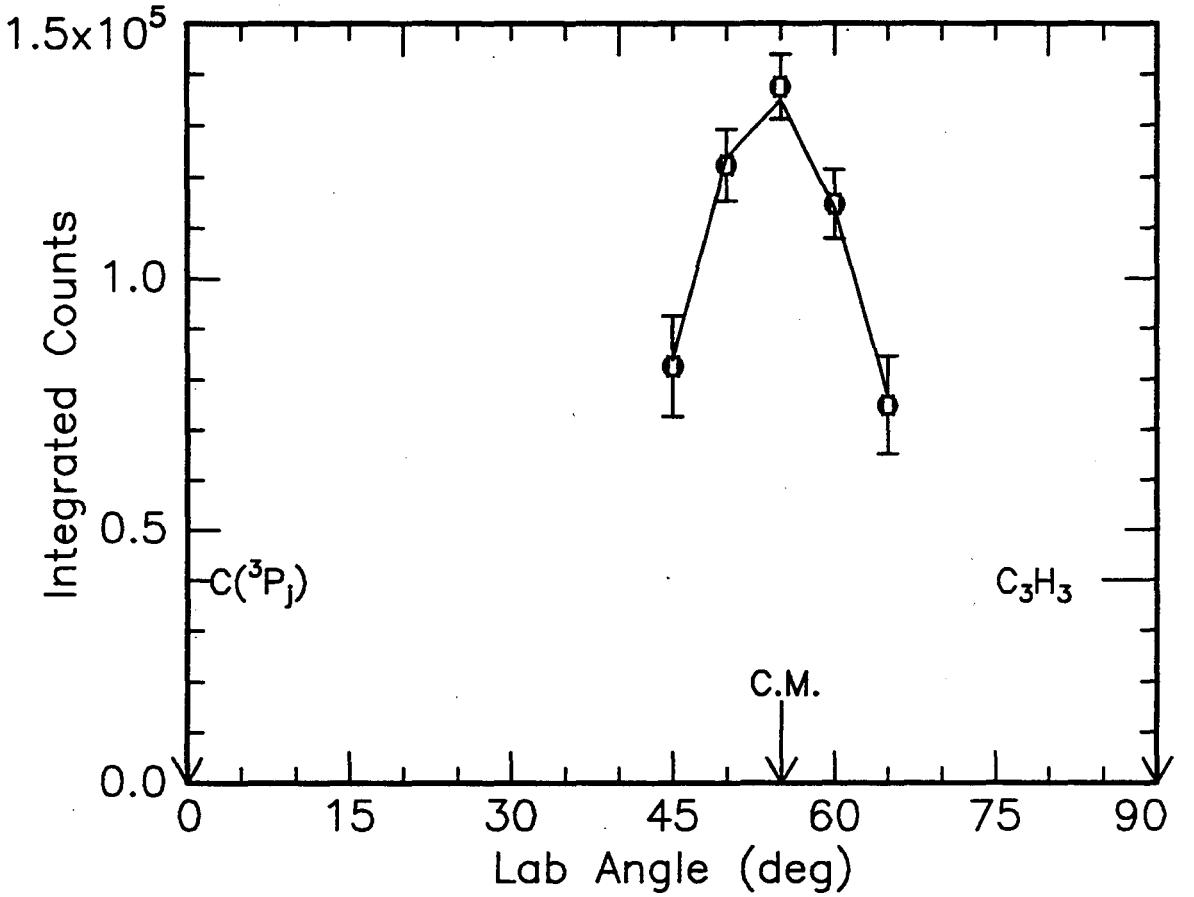
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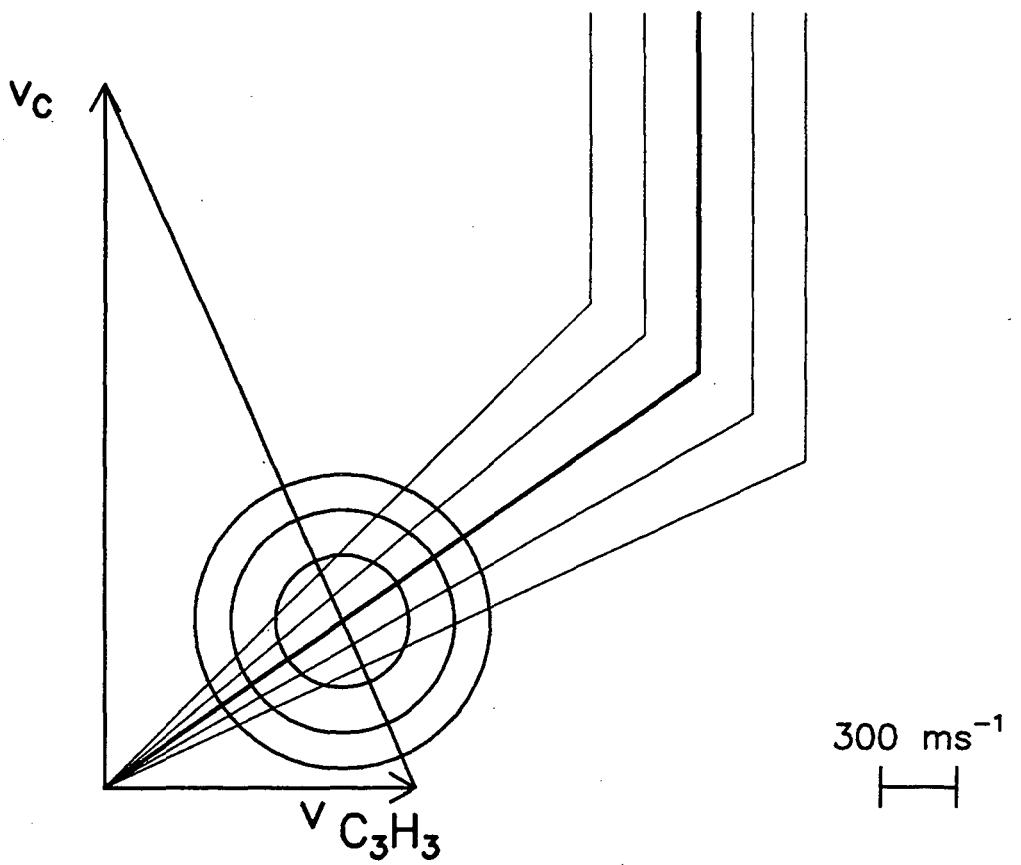
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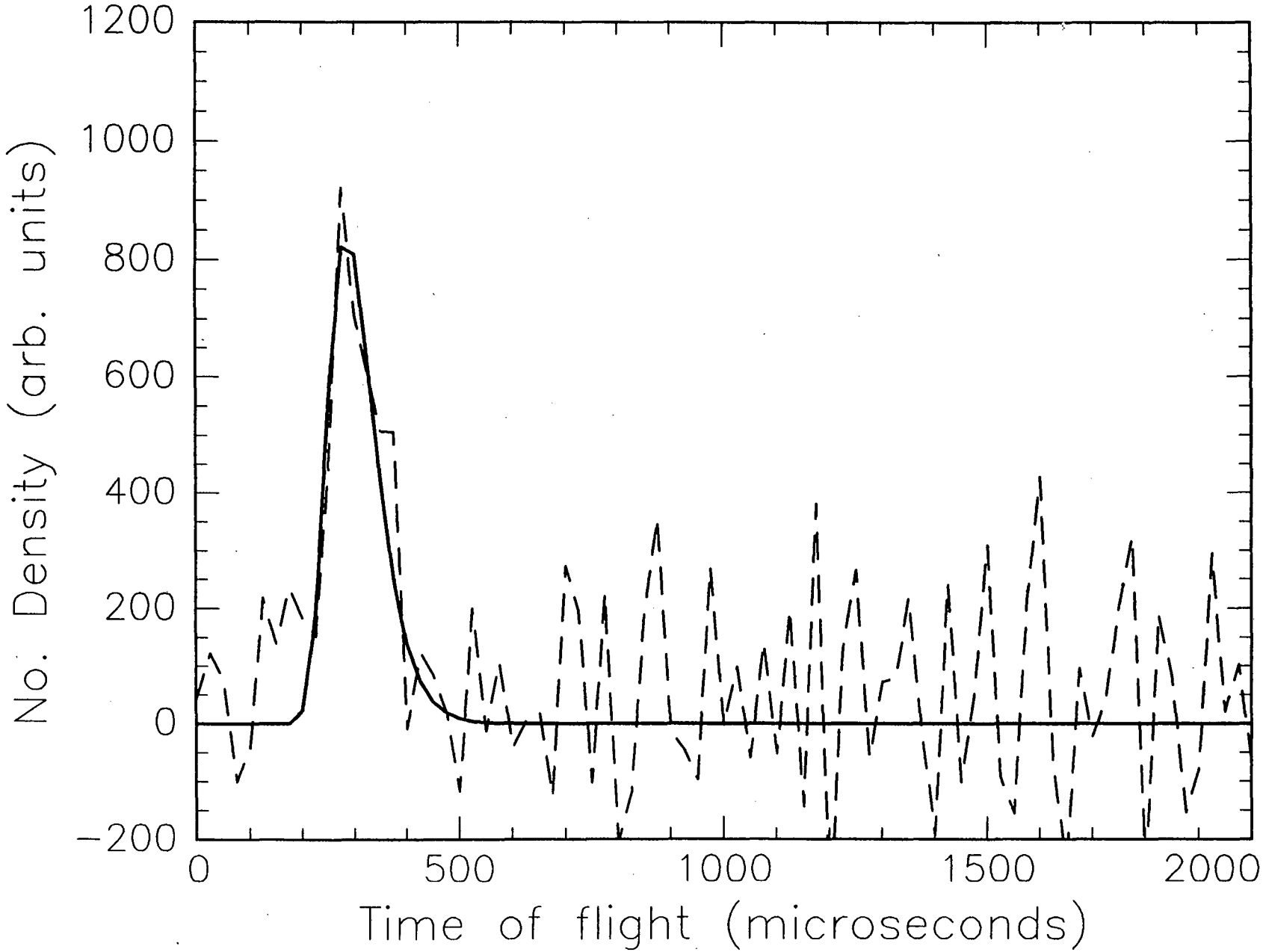
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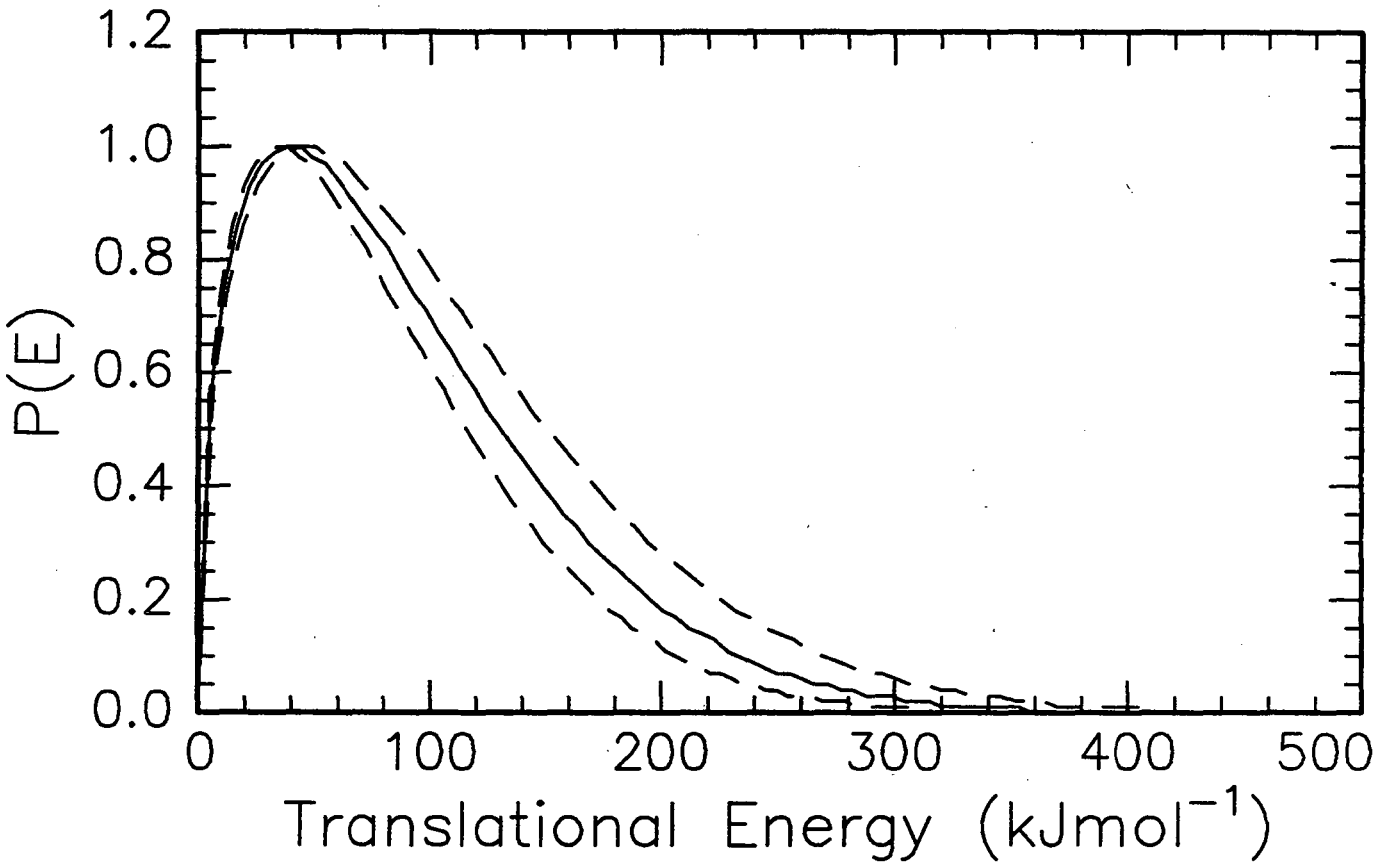
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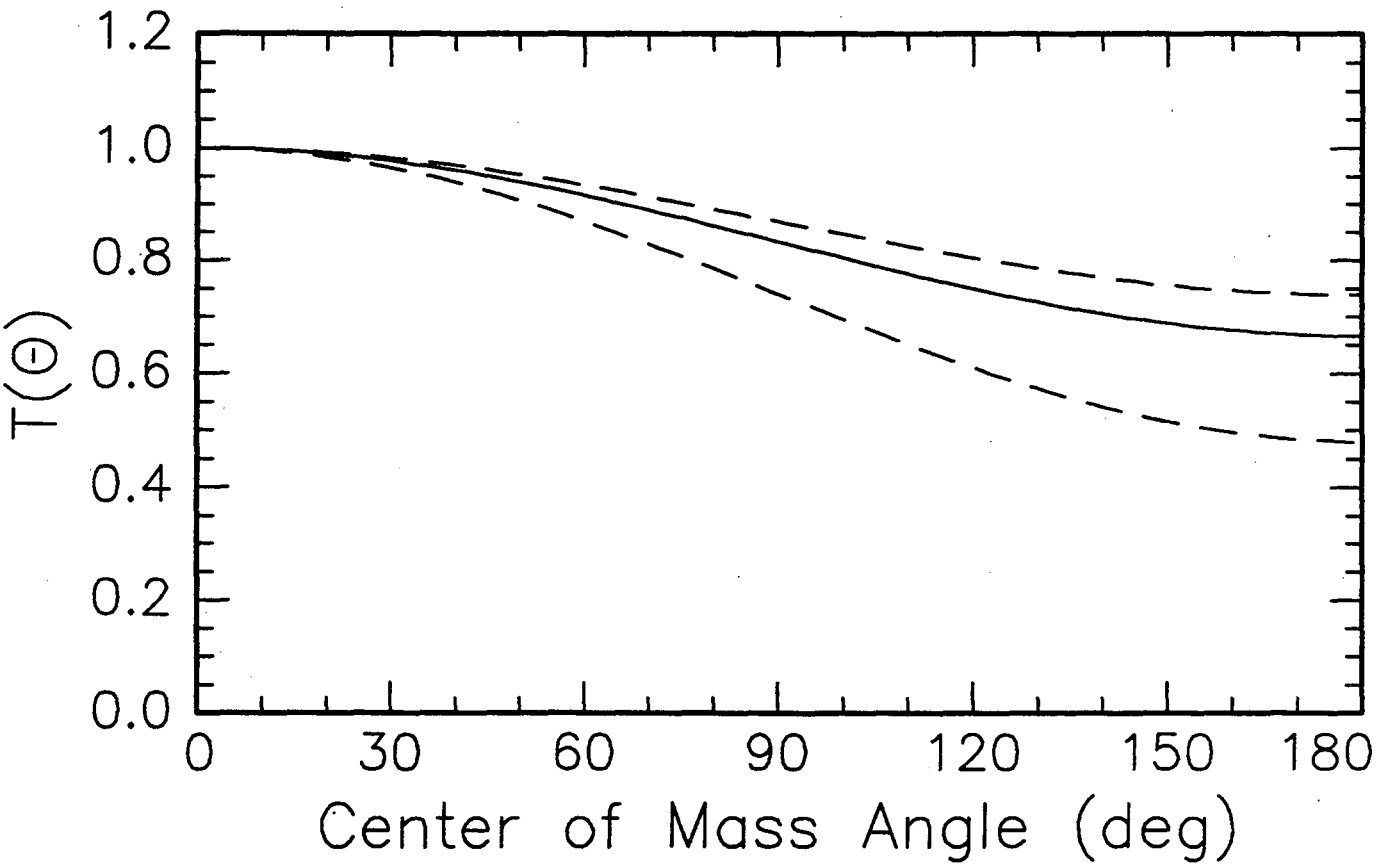
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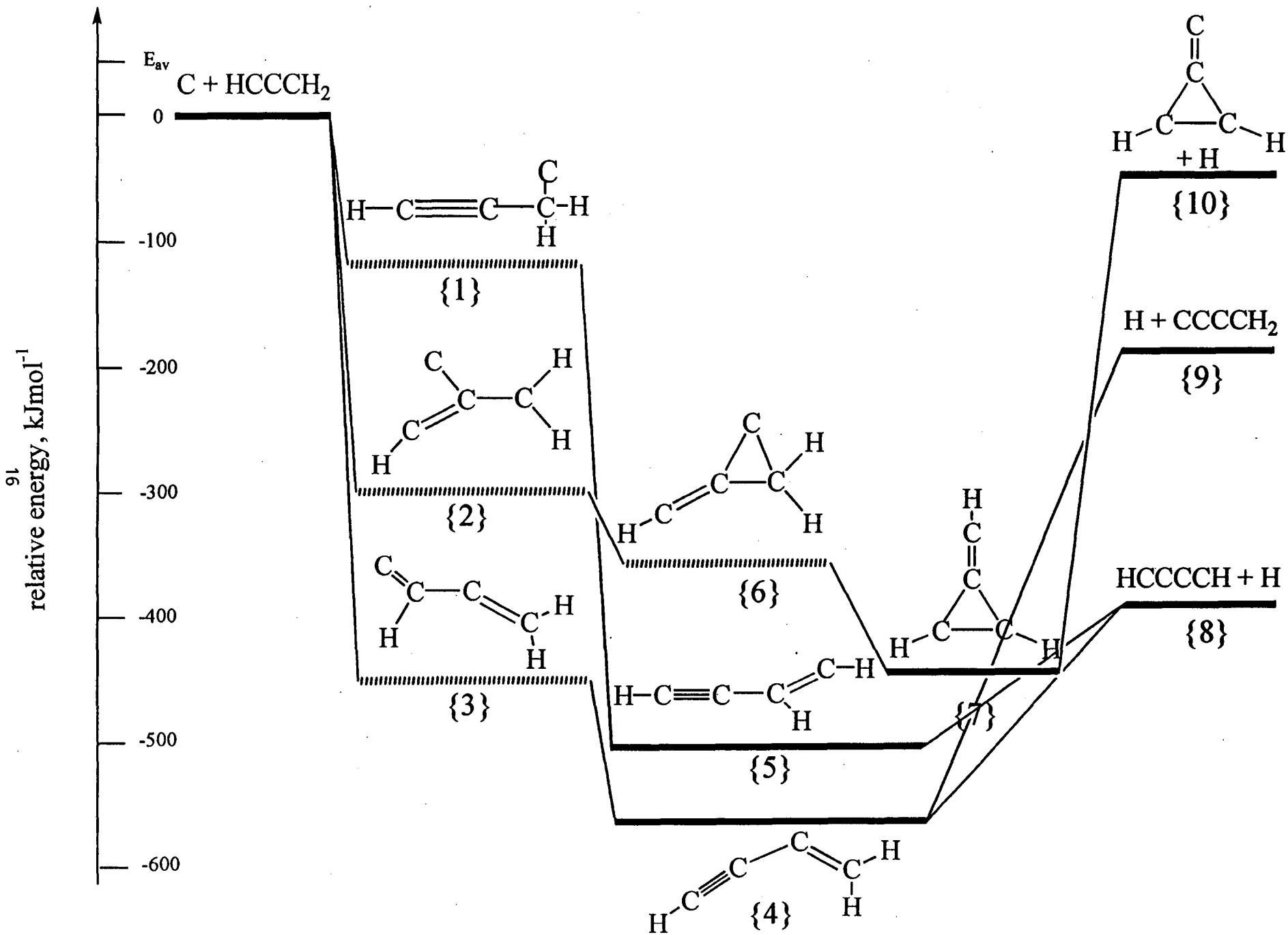
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