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# CROSS SECTIONS FOR ION PRODUCTION IN REACTIONS OF $H^+$ WITH $D_2$. EFFECTS OF VIBRATIONAL AND ROTATIONAL EXCITED STATES OF $D_2$.

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# Cross Sections for Ion Production in Reactions of $H^+$ with $D_2$. Effects of Vibrational and Rotational Excited States of $D_2$.

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Cross sections for production of $D_2^+$, $D^+$, and $HD^+$ ions in the reaction of $H^+$ with $D_2$ were calculated in the center-of-mass collision energy range of 2.5 eV$\leqq E_{cm} \leqq$ 8.0 eV by using a trajectory surface hopping (TSH) method with ab initio three-dimensional potential energy surfaces(3D-PES's). The calculations were carried out with $D_2$ reactants in the vibrational and rotational states with quantum numbers (v=0 to 3, j=1,5,10), and (v, j) dependence of each ion production was evaluated. It was found that the $D_2^+$ production is enhanced remarkably as the vibrational and rotational (v, j) state becomes high, where the vibrational excited state has the primary effect and the rotational excited state has the secondary effect. Compared with the $D_2^+$ production, the effect of vibrational excited state v on the $D^+$ and $HD^+$ production is small. The production of latter two ions is almost independent of the rotational excited state j.

Keywords : Ion Production Cross Section, State Selected Cross Section, Trajectory-surface-hopping, Ab Initio Potential Surfaces, $H_3^+$, $H^+$, $D_2$, $D_2^+$, $HD^+$, $D^+$

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+Department of Materials Science

# $H^+ + D_2$反応におけるイオン生成の断面積.
# $D_2$の振動回転励起状態がイオン生成に与える効果

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（1998年9月2日受理）

$H^+$と$D_2$の反応で生じる$D_2^+$、$D^+$、および$HD^+$イオン生成の断面積を、重心衝突エネルギー$E_{cm}$= 2.5－8.0 eVの範囲内で、非経験的分子軌道計算で得られた$H_3^+$の3次元ポテンシャル面上でのトラジェクトリーサーフェスホッピング(TSH)法を用いることにより、評価した。反応物$D_2$の初期状態が各イオン生成に与える影響を調べるために、$D_2$の振動および回転の量子数をv= 0－3、j= 1, 5 , 10に設定して計算を行った。 その結果、$D_2^+$イオンの生成は、$D_2$の振動回転状態(v, j)が高くなるに従って著しく増大することが分かった。$D_2^+$生成の飛躍的な増大には、$D_2$の振動励起が主要な役割を果たし、回転励起は補助的な効果を与えた。$D_2^+$生成と比較して、$D_2$の振動状態が$D^+$および$HD^+$イオンの生成に与える効果は一桁小さく、$D_2$の回転状態に対する効果は殆ど無視しうる大きさであった。

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# 1. Introduction

Ion-molecule reactions occurring in the $H_3^+$ system and its isotopic variants have been studied theoretically as well as experimentally[1]. The absolute cross sections for ion production in the reactions $H^+ + D_2(v=0)$, $D^+ + H_2(v=0)$, and $D^+ + D_2(v=0)$ were measured by Ochs and Teloy[2] and by Schlier et al.[3] with an estimated error of $\pm 10$ to 20% using a guided beam method, where v represents the vibrational quantum number. These cross sections were calculated theoretically by using a trajectory surface hopping (TSH) method with diatomics-in-molecules potential energy surfaces (DIM-PES's)[3-7]. The TSH calculations with DIM-PES's reproduce the $D^+$ and $HD^+$ production cross sections for the $H^+ + D_2$ reaction within the experimental uncertainty, but show systematic deviations from the experiments for other reactions[3]. Except for the region near the threshold energy, the disagreement with the experiment is attributed to the faulty repulsive wall of the ground state DIM-PES's[3,8].

In a recent paper[9] we also reported similar TSH calculations with ab initio three-dimensional (3D)-PES's, instead of DIM-PES's, which were calculated by the full configuration interaction method with a [8s6p2d1f] Gaussian-type basis set[10]. Compared with the TSH calculation with DIM-PES's, the energy dependence of experimental cross sections is reproduced better for the $D^+ + H_2$ and $D^+ + D_2$ systems by the use of the ab initio PES's. Although the TSH calculations with the ab initio PES's are systematically larger than the experiments for the $H^+ + D_2$ system, they almost coincide with each other within the corresponding uncertainties[2,9].

In this paper we present the cross sections for ion production from the reaction of $H^+$ with $D_2$ in vibrational and rotational excited states with quantum numbers (v=0 to 3, j=1,5,10). Three kinds of ions $D_2^+$, $D^+$, and $HD^+$ can be observed in the reaction of $H^+$ with $D_2$. These processes involving vibrationally and rotationally excited molecular species are of great importance for a plasma modeling of fusion reactor divertor[11], but there are no available data. So we undertook the TSH calculation with the ab initio 3D-PES's, and estimated how the vibrational and rotational excited states of $D_2$ affect each ion production in the collision energy range $2.5\ \mathrm{eV} \leq E_{cm} \leq 8.0\ \mathrm{eV}$.

# 2. Computational Method

The TSH calculation was carried out as before[9], except that the probability of surface hopping (nonadiabatic electronic transition) was evaluated by using the formula

established by Zhu and Nakamura (ZN)[12] instead of the Landau-Zener (LZ) formula[13-16]. All parameters in the ZN formula can be estimated directly from the ab initio PES's[12]. The hopping probability was calculated with the ZN formula when a surface hop was possible under the conventional TSH model[5].

## 3. Results and Discussion

Figures 1 to 3 show the cross sections for $D_2^+$ production by the electron transfer $H^+ + D_2 \rightarrow D_2^+ + H$. As the vibrational state v becomes high, the $D_2^+$ production is enhanced remarkably with the increase of energy $E_{cm.}$ Fig.4 illustrates the section of ab initio PES's at R = 5.29 Å (10 bohr) in the $C_{2v}$ geometry, where R is the distance between $H^+$ and $D_2$. In our TSH calculation, the surface hopping takes place on the avoided crossing point of two PES's. The avoided crossing between the $H^+ + D_2$ and $H + D_2^+$ electronic states arises in the region where the internuclear distance of $D_2$ (r) is about 1.32 Å (2.5 bohr) and R is larger than 2.65 Å (5 bohr)[10]. Thus the $D_2^+$ production is induced by such a $H^+ + D_2$ collision as $D_2$ is excited into the vibrational state with quantum number $v > 6$, because the vibration amplitude of $D_2$ in the $v > 6$ state is sufficient to reach the internuclear distance of r = 1.32 Å. If $D_2$ is in the vibrational excited state in advance, further vibrational excitation into the $v > 6$ state is brought about more easily by the collision with $H^+$, and that should cause the remarkable enhancement of the $D_2^+$ production.

The $D_2^+$ production cross section for $v \geqq 1$ also increases appreciably as the rotational state j becomes high. If $D_2$ is in the rotational excited state, the centrifugal force of the $D_2$ rotator contributes to the enlargement of D-D bond length, which should promote the $D_2^+$ production. From Figs.1 to 3, however, it is concluded that the vibrational excited state v has the primary effect on the $D_2^+$ production, and the rotational excited state j has the secondary effect.

Figs.5 to 7 show the cross sections for $D^+$ production. As v becomes larger, the $D^+$ production is reduced at $E_{cm}$ below 4 eV, while it is enhanced above 5 eV. The $D^+$ ions are produced from reactions $H^+ + D_2 \rightarrow D^+ + HD$ (nuclear rearrangement) and $H^+ + D_2 \rightarrow D^+ + H + D$ (dissociation). Threshold energy of dissociation is 4.52 eV for the $H^+ + D_2(v=0, j=1)$ system and 3.11 eV for $H^+ + D_2(v=3, j=10)$. Thus, most of $D^+$ ions are produced by the nuclear rearrangement at $E_{cm}$ below 4 eV. (The v dependence of $D^+$ production by the nuclear rearrangement is discussed later with the $HD^+$ production.) With the increase

of $E_{cm}$, the nuclear rearrangement decreases monotonically, while the dissociation increases[9]. Above 6 eV, the $D^+$ production from dissociation becomes more dominant than that from nuclear rearrangement. Figs.8 to 10 show contribution of the dissociation $H^+ + D_2 \rightarrow D^+ + H + D$ to the $D^+$ production. The dissociation is enhanced as the vibrational state v becomes high. From Figs.5 and 10 it is clearly demonstrated that the increase of $D^+$ production cross section with increasing v above 5 eV is due to the contribution of dissociation.

Figs.11 to 13 show the $HD^+$ production cross sections from the reaction $H^+ + D_2 \rightarrow HD^+ + D$. As v becomes largr, the $HD^+$ production is enhanced at $E_{cm}$ below about 5 eV. At low collision energies both the $HD^+$ and $D^+$ ions are produced via the H-D pair formation[6]. The $HD^+$ ion can be formed if the internal energy of the H-D pair is sufficient to reach the internuclear distance of 1.32 Å, where the avoided crossing of two PES's arises[17]. On the other hand, the $D^+$ ion (neutral HD molecule) is formed if the H-D pair is not in the vibrational excited state sufficient to reach the internuclear distance of 1.32 Å. In the present calculation the sum of cross sections for above two reactions $H^+ + D_2 \rightarrow D^+ + HD$ and $H^+ + D_2 \rightarrow HD^+ + D$ is almost independent of v. Figs.14 to 16 show the summed cross sections for the $H^+ + D_2$ system. It can be seen from Figs.5 to 7 and Figs.11 to 16 that the vibrational excited state v promotes the $HD^+$ production and reduces the $D^+$ production at the same time at $E_{cm}$ below about 5 eV.

From Figs.5 to 7 and 11 to 13 it is known that both the $HD^+$ and $D^+$ production is almost independent of the rotational state j.

Compared with the $HD^+$ and $D^+$ production cross sections, the $D_2^+$ production cross section shows remarkable (v, j) dependence. The $D_2^+$ production cross section, which is less than 1.0 $Å^2$ for (v=0,j=1) at $E_{cm}$=8.0 eV, becomes more than 7.0 $Å^2$ for (v=3,j=10). In the $D^+$ and $DH^+$ production, the difference of cross sections between different rovibrational states is less than 0.5 $Å^2$ in the calculated energy range.

The (v, j) dependence is also observed in the maximum of impact parameter ($b_{max}$) selected to determine the $D_2^+$ production cross section. The value of $b_{max}$ for the $D_2^+$ production, which is less than 1.5 Å for (v=0, j=1), increases as the rovibrational state (v, j) becomes high and exceeds 2.7 Å for (v=3, j=10) in the calculated energy range. The values of $b_{max}$ for the $HD^+$ and $D^+$ production, which are not so sensitive to the rovibrational state (v, j), are less than 1.5 Å and 1.25 Å, respectively, for all (v, j) at $E_{cm} \geqq 3$ eV. When $D_2$ is in the vibrational excited state in advance, the $D_2^+$ production

takes place with less energy capture in the $H^+ + D_2$ collision with larger impact parameter. In the $HD^+$ and $D^+$ production, $H^+$ need to approach $D_2$ closely to create the H-D pair or to cut the D-D pair, so that the molecular size of $D_2$ and $HD_2^+$ should restrict $b_{max}$ more rigidly.

Finally, we discuss the accuracy of the present calculation. In the previous study[9], ion production cross sections were calculated for the reaction of $H^+$ with $D_2$(v=0,j=1) in the range of 2.5 eV$\leqq E_{cm} \leqq$ 8.0 eV, where the classical treatment for the nuclear motion was considered to be appropriate because the quantum effect such as tunneling is not significant[8,9]. In the present study, ion production cross sections were calculated for the reaction of $H^+$ with $D_2$ in the rovibrational excited states. The rovibrational energy level of $D_2$ (v=3,j=10) is 1.41 eV higher than that of $D_2$(v=0,j=1). It is thought that the bundle of trajectories calculated for the $H^+ + D_2$ (v=3,j=10) system at $E_{cm}$ = 6.59 eV covers the same area of PES's as the bundle for the $H^+ + D_2$(v=0,j=1) system at $E_{cm}$ = 8.0 eV with different density distribution. Since the ion production cross sections for $H^+ + D_2$(v=0, j=1) are in agreement with the experiments within the uncertainty of about $\pm$30 %[9] and the cross sections for other rovibrational states (v, j) are given by smooth curves in the calculated energy range, serious problem may not happen on our PES's.

In the present calculation the hopping probability was evaluated by the ZN formula[12], instead of the LZ formula[9]. The use of LZ formula is not appropriate when a trajectory crosses an avoided crossing point with energy near the threshold. The ZN formula used is applicable to the whole range of energies above threshold and more accurate than the LZ formula. Therefore, the present TSH calculation with the ZN formula is more reliable than the previous calculation with the LZ formula.

In order to evaluate the applicability of TSH calculation[18], experiments with excited $D_2$ molecule are strongly requested.

## 4. Summary and Concluding Remarks

The cross sections for the production of $HD^+$, $D^+$, and $D_2^+$ ions in the reaction of $H^+$ with $D_2$(v=0 to 3, j=1,5,10) were calculated in the energy range 2.5 eV$\leqq E_{cm} \leqq$ 8.0 eV by using the TSH method with ab initio 3D-PES's. As the rovibrational (v, j) state becomes high, the $D_2^+$ production is enhanced remarkably with the increase of $E_{cm}$. The vibrational excited state v has the primary effect on the $D_2^+$ production and the rotational

excited state j has the secondary effect. Although the $HD^+$ and $D^+$ production shows the v dependence, its effect is small compared with the case for $D_2^+$ production, and the production of these two ions is almost independent of the rotational state j. The $D_2^+$ ion production is induced when $D_2$ is excited into high rovibrational state by the collision with $H^+$ and the amplitude of this oscillation is sufficient to reach the avoided crossing point. On the other hand, the $HD^+$ and $D^+$ ion production is brought about via the particle rearrangement (H-D pair formation) or dissociation.

These cross sections are fundamental to accurate modeling of the plasma power exhaust by the neutral hydrogen gas in the fusion reactor divertor. It has been shown that the $D_2^+$ production, which is endothermic for the $H^+ + D_2(v \leqq 3)$ system, is the dominant reaction for $E_{cm} \leqq 8.0$eV. It is expected that the (v, j) dependence of each ion production obtained for the $H^+ + D_2$ system applies to the ion production occurring in other isotopic variants.

## Acknowledgements

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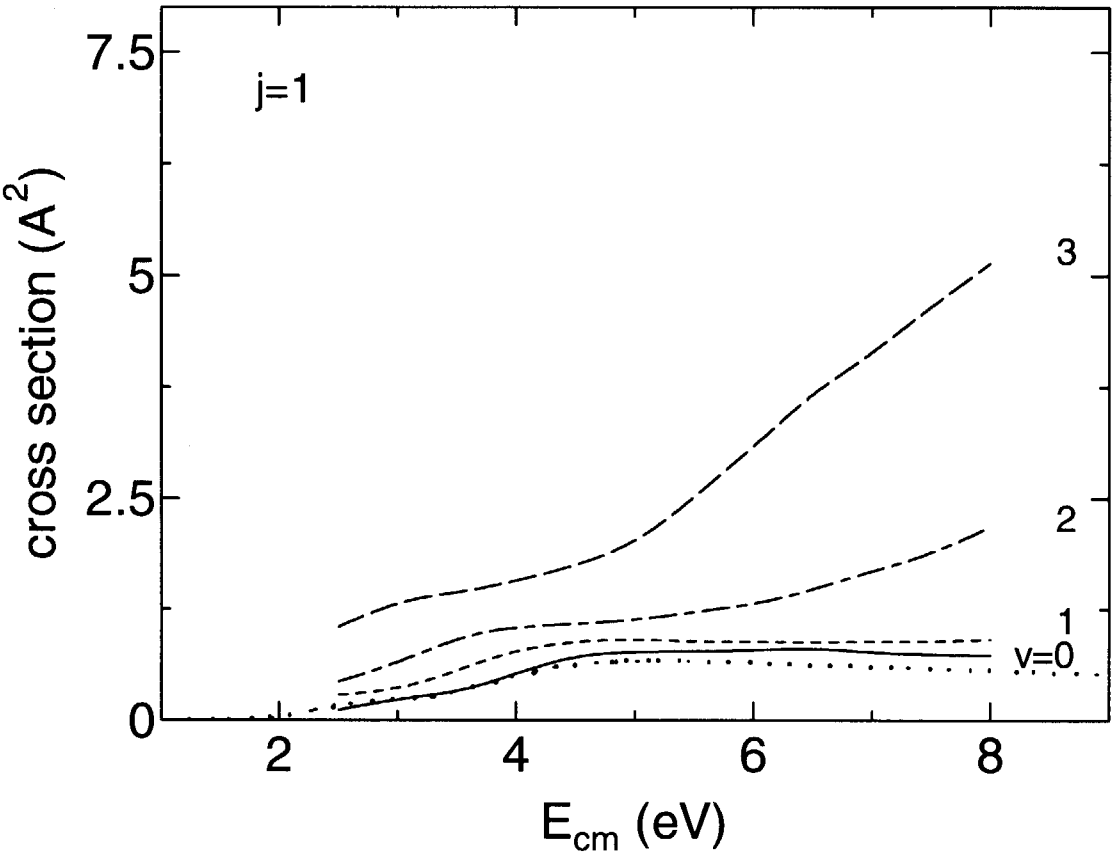


Fig.1 Absolute cross sections for the reactions $H^+ + D_2(v=0 \text{ to } 3, j=1) \rightarrow D_2^+ + H$. The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

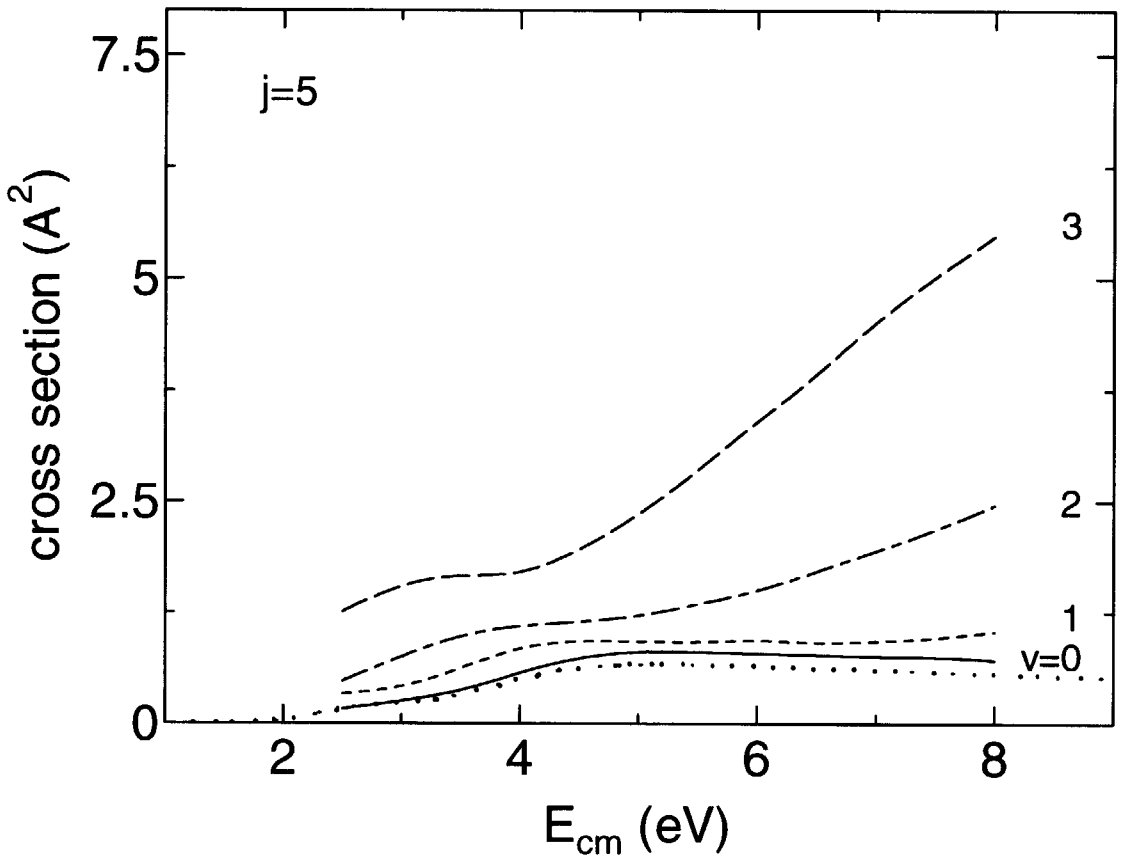


Fig.2 Absolute cross sections for the reactions $H^+ + D_2(v=0 \text{ to } 3, j=5) \rightarrow D_2^+ + H$. The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

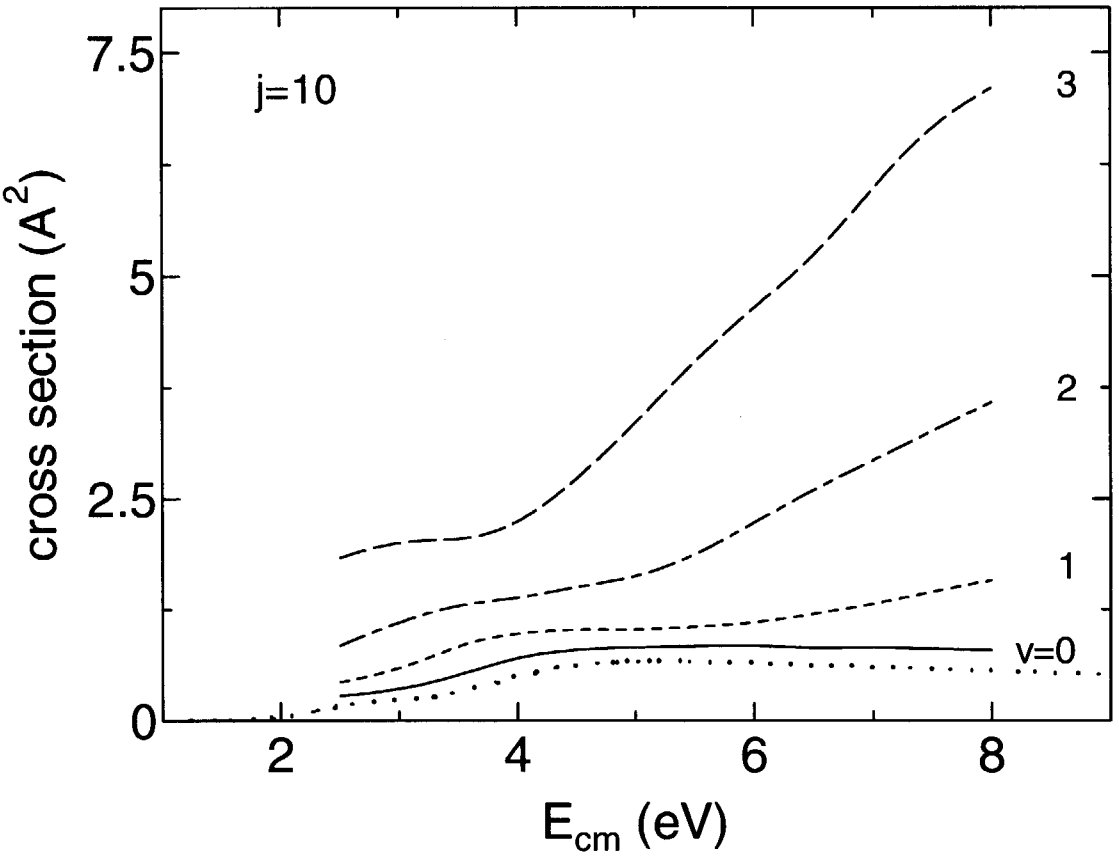


Fig.3 Absolute cross sections for the reactions $H^+ + D_2$(v=0 to 3, j=10) → $D_2^+ + H$. The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

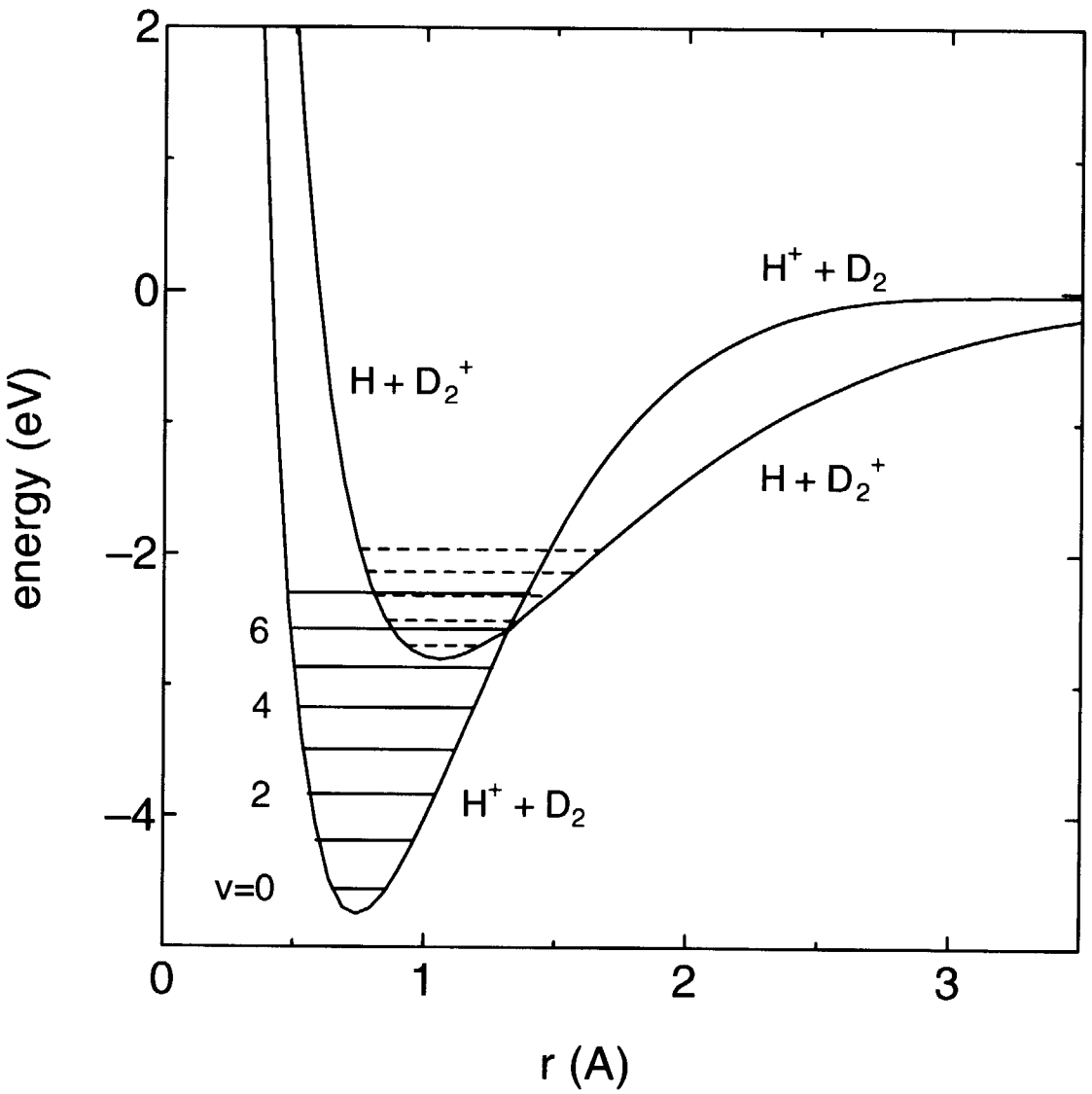


Fig.4 Section of potential energy surfaces for R=5.29 Å in the $C_{2v}$ geometry. r is the distance between two deuterons. The vibrational energy levels of $D_2$ and $D_2^+$ are shown by solid and dotted lines, respectively.

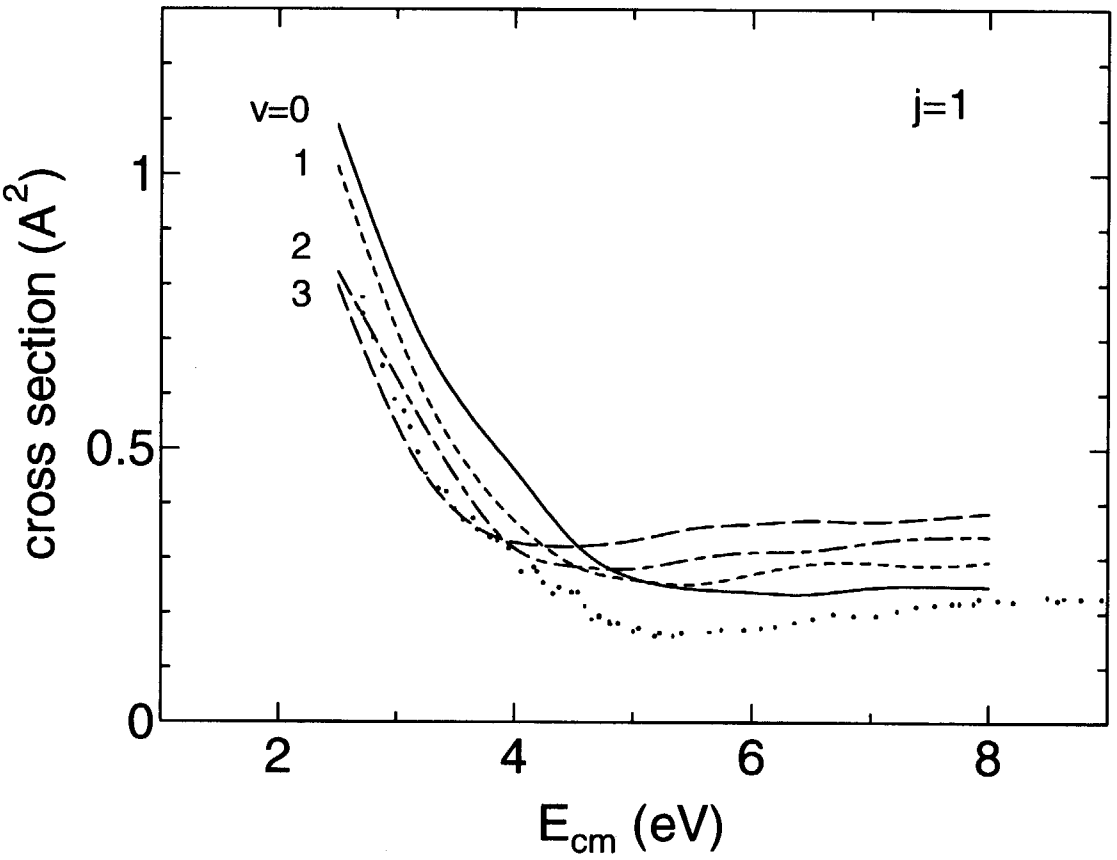


Fig.5 Absolute cross sections for the $D^+$ production from the reactions $H^+ + D_2$(v=0 to 3, j=1). The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

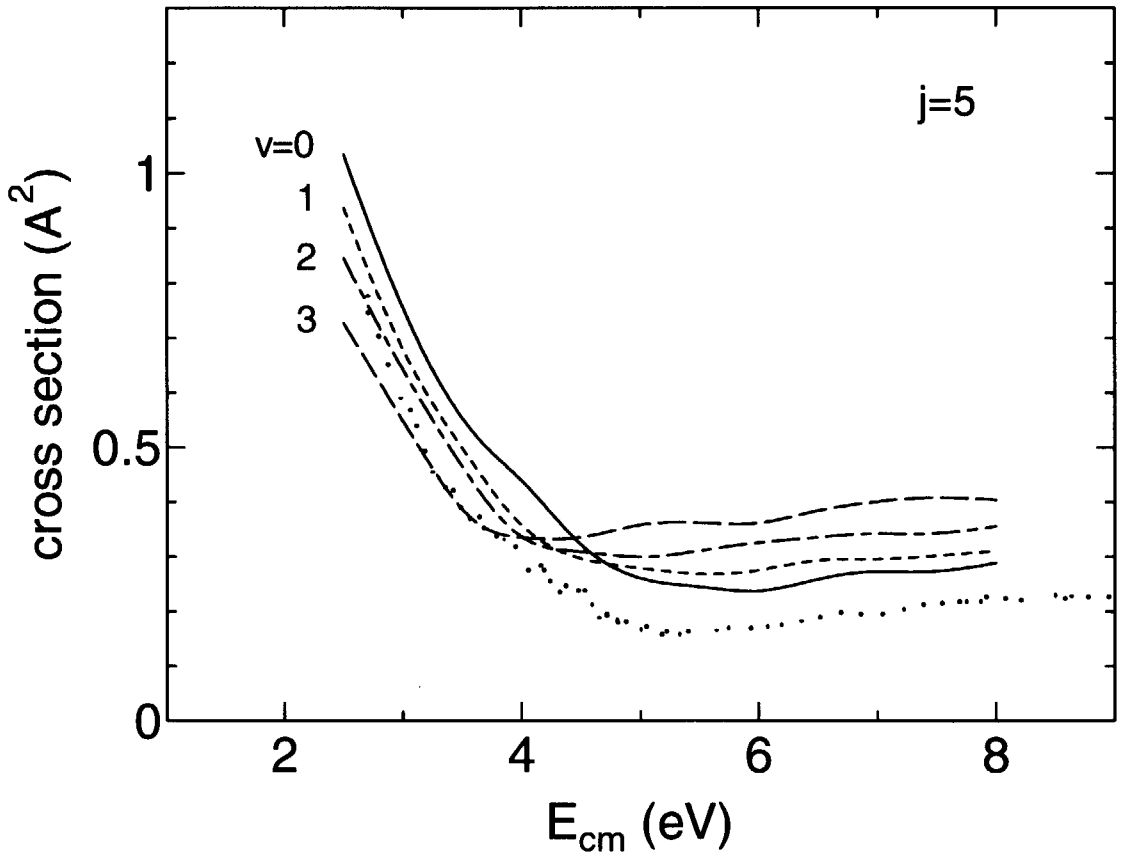


Fig.6 Absolute cross sections for the $D^+$ production from the reactions $H^+ + D_2$(v=0 to 3, j=5). The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

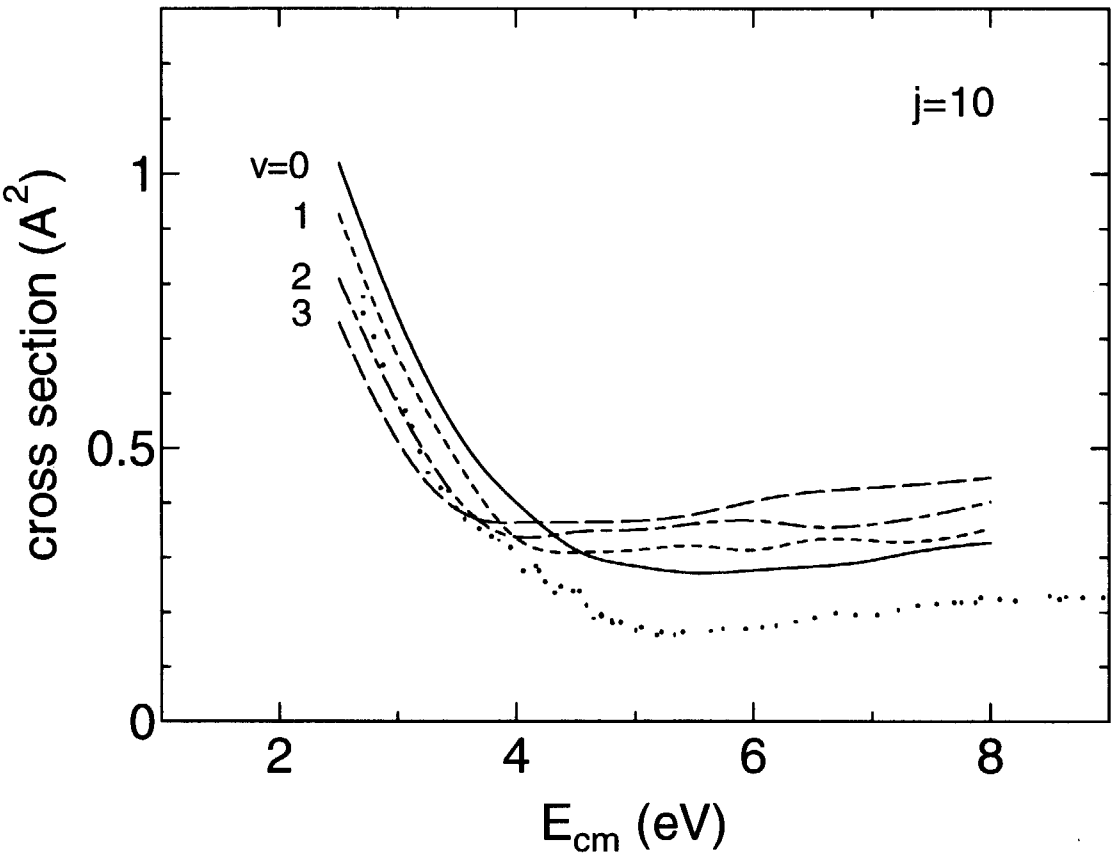


Fig.7 Absolute cross sections for the $D^+$ production from the reactions $H^+ + D_2$(v=0 to 3, j=10). The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

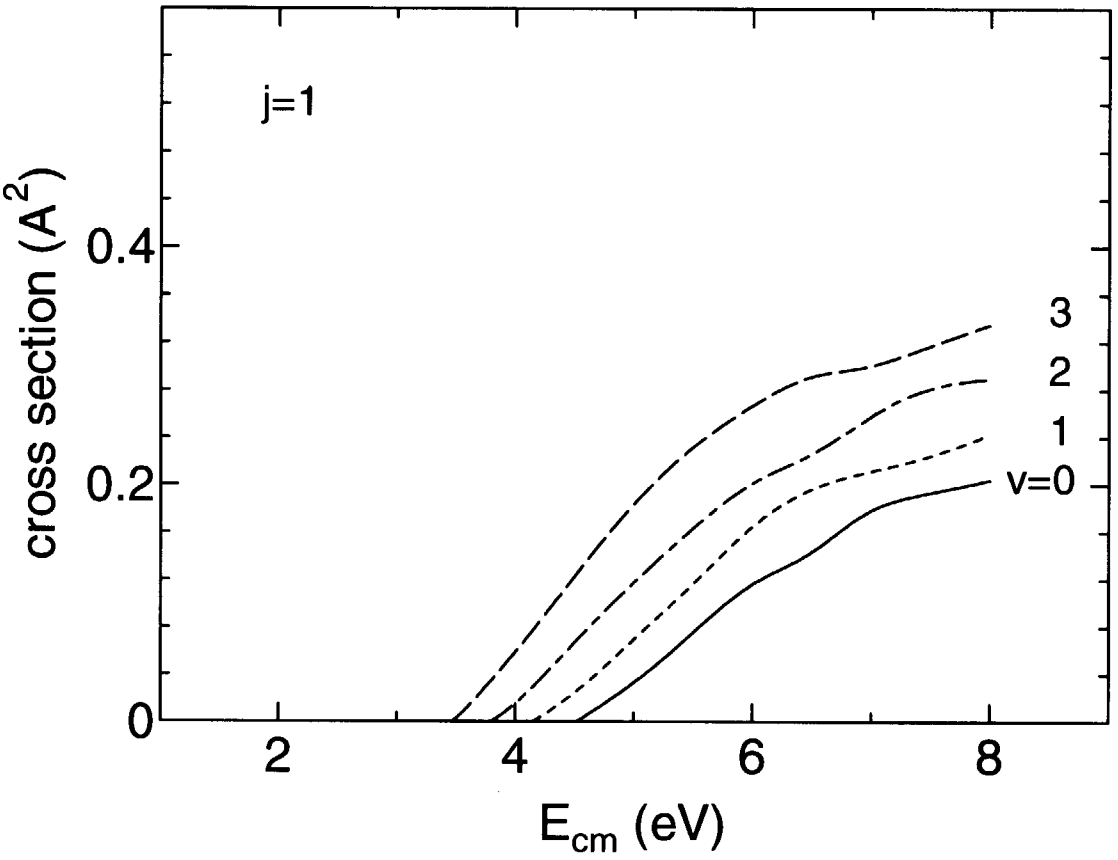


Fig.8 Contribution of the dissociation $H^+ + D_2(v, j=1) \rightarrow D^+ + H + D$ to the $D^+$ production.

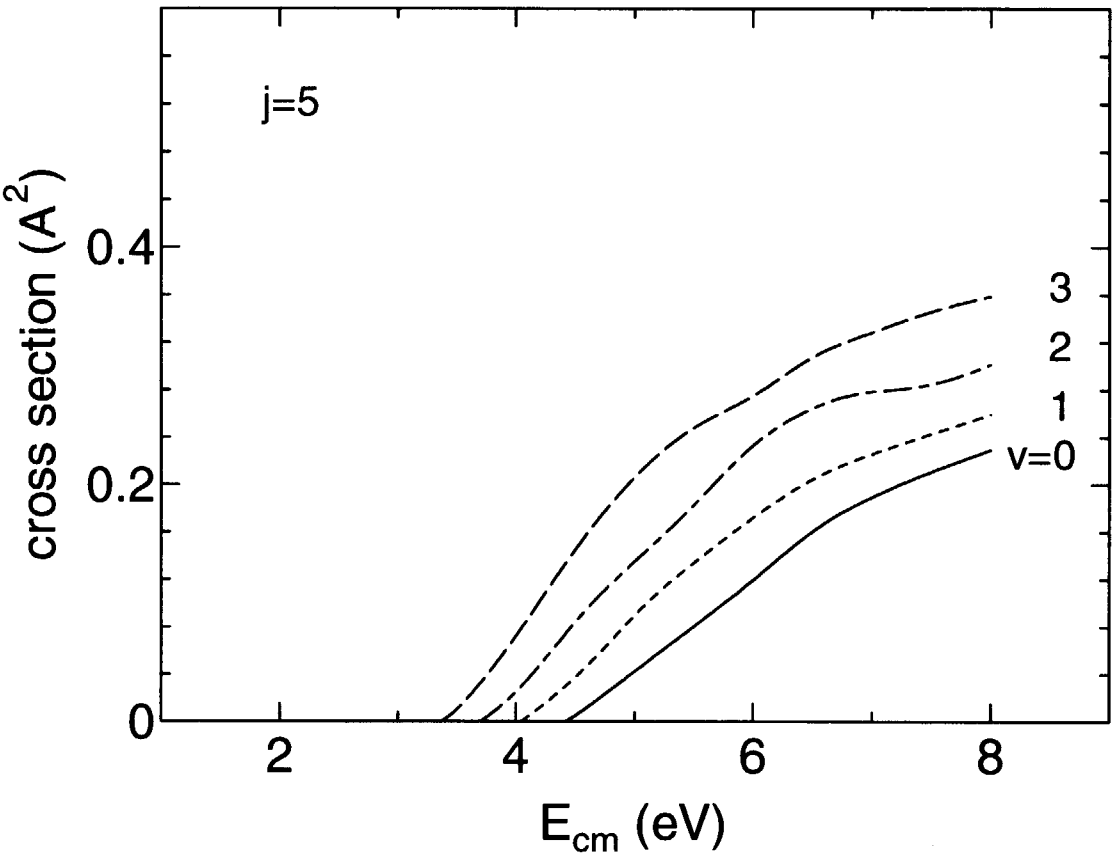


Fig.9 Contribution of the dissociation $H^+ + D_2(v, j=5) \rightarrow D^+ + H + D$ to the $D^+$ production.

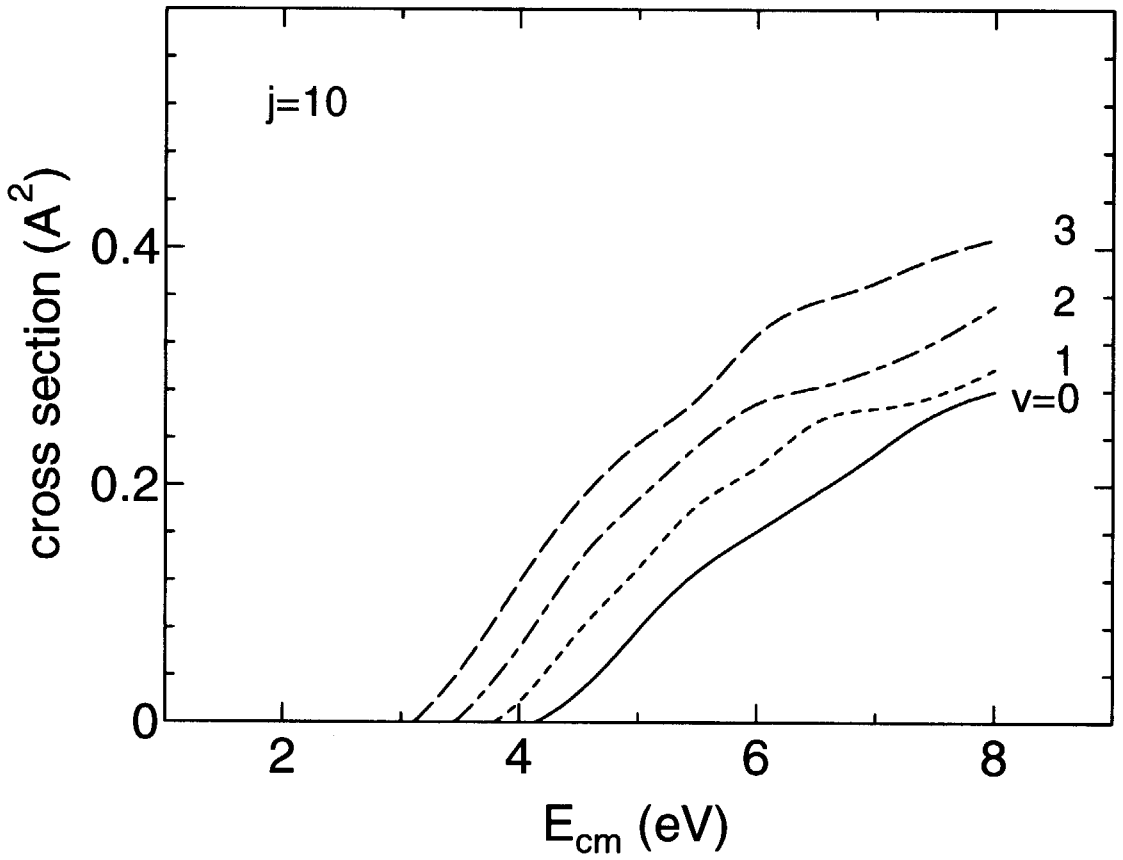


Fig.10 Contribution of the dissociation $H^+ + D_2(v, j=10) \rightarrow D^+ + H + D$ to the $D^+$ production.

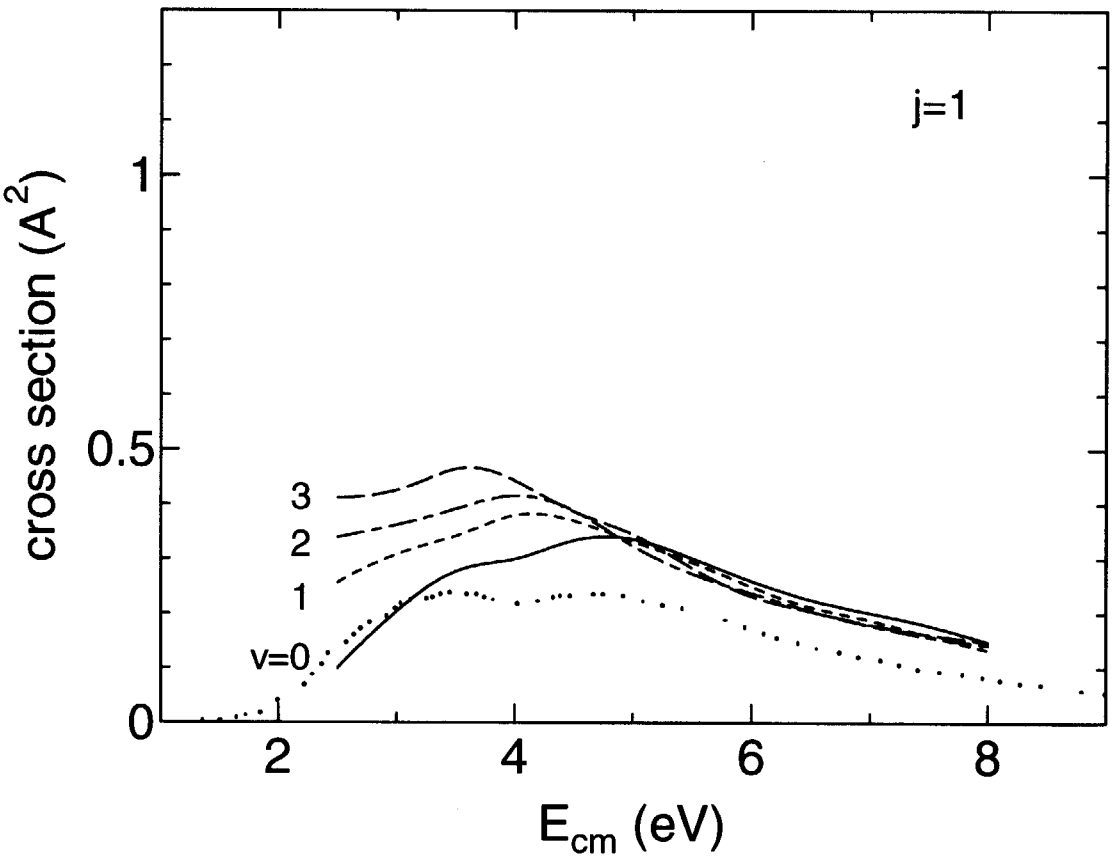


Fig.11 Absolute cross sections for the reactions $H^+ + D_2(v=0 \text{ to } 3, j=1) \rightarrow HD^+ + D$. The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

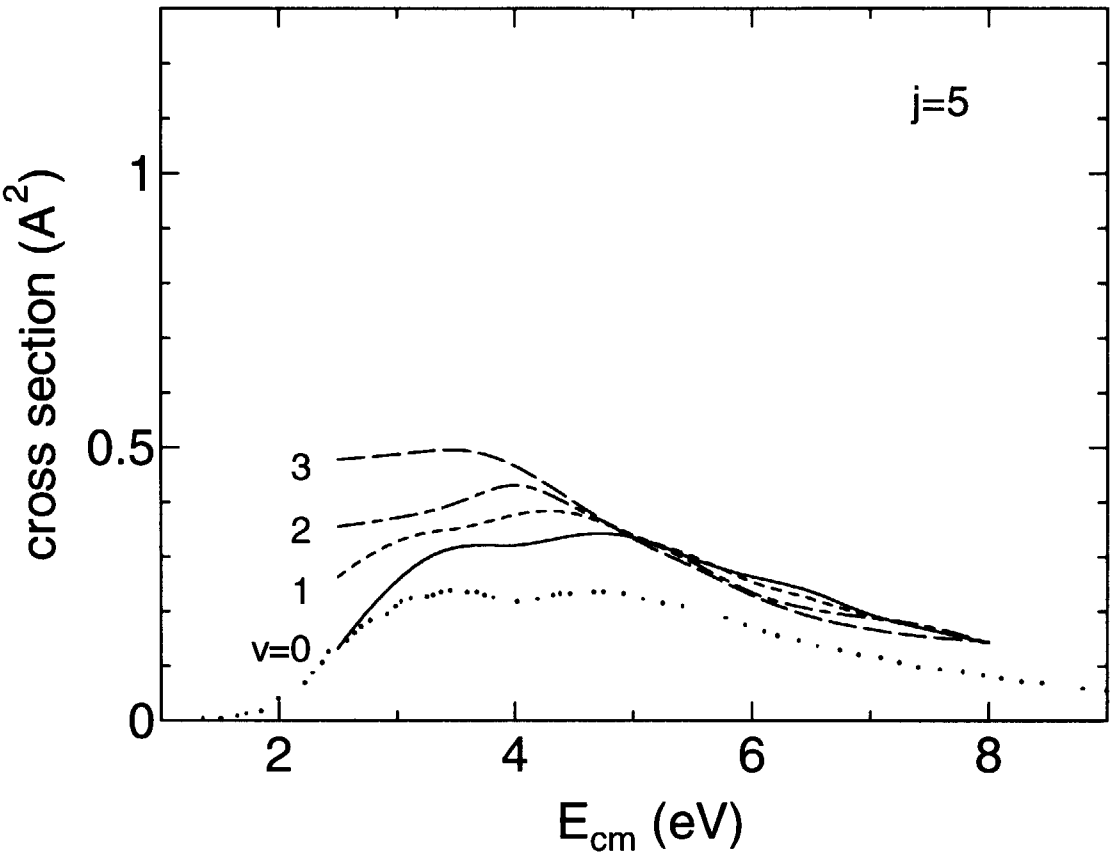


Fig.12 Absolute cross sections for the reactions $H^+ + D_2(v=0 \text{ to } 3, j=5) \rightarrow HD^+ + D$. The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

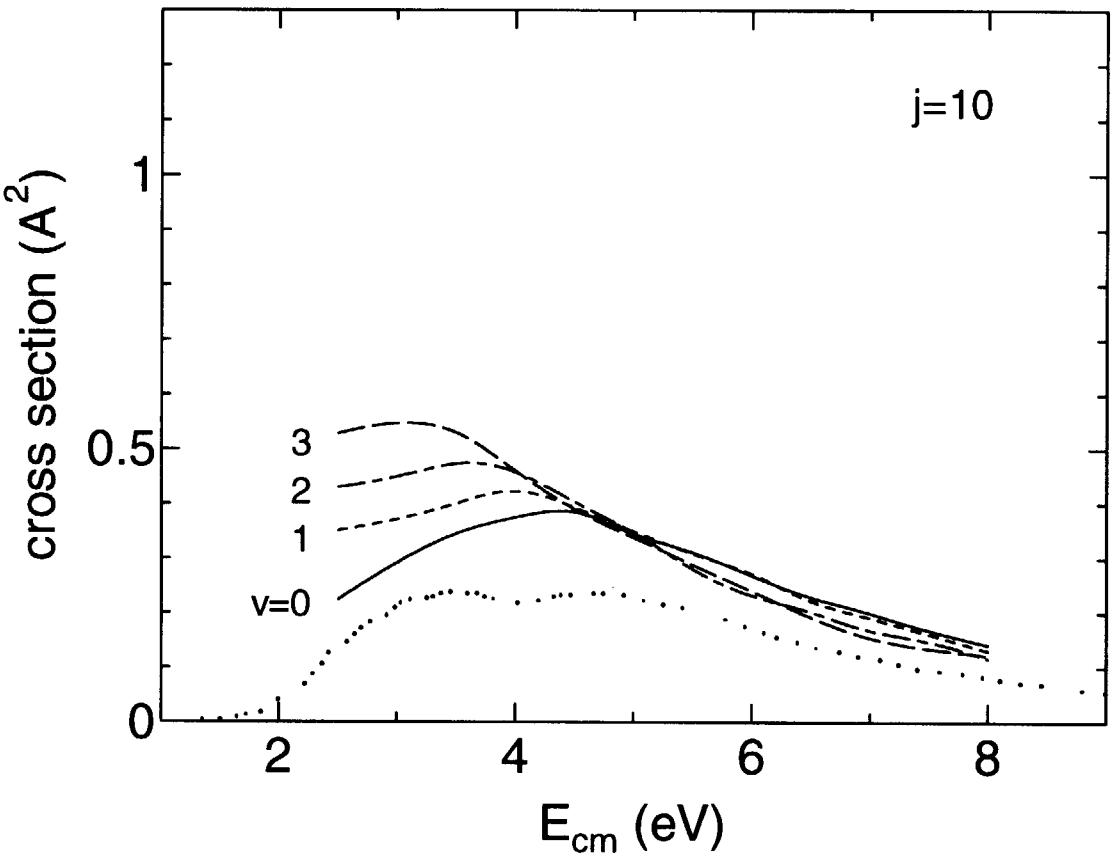


Fig.13 Absolute cross sections for the reactions $H^+ + D_2$(v=0 to 3, j=10) → $HD^+ + D$. The cross section is given as a function of center-of-mass collision energy $E_{cm}$. The experimental data for v=0 (Ref.2) are plotted by dots in the figure.

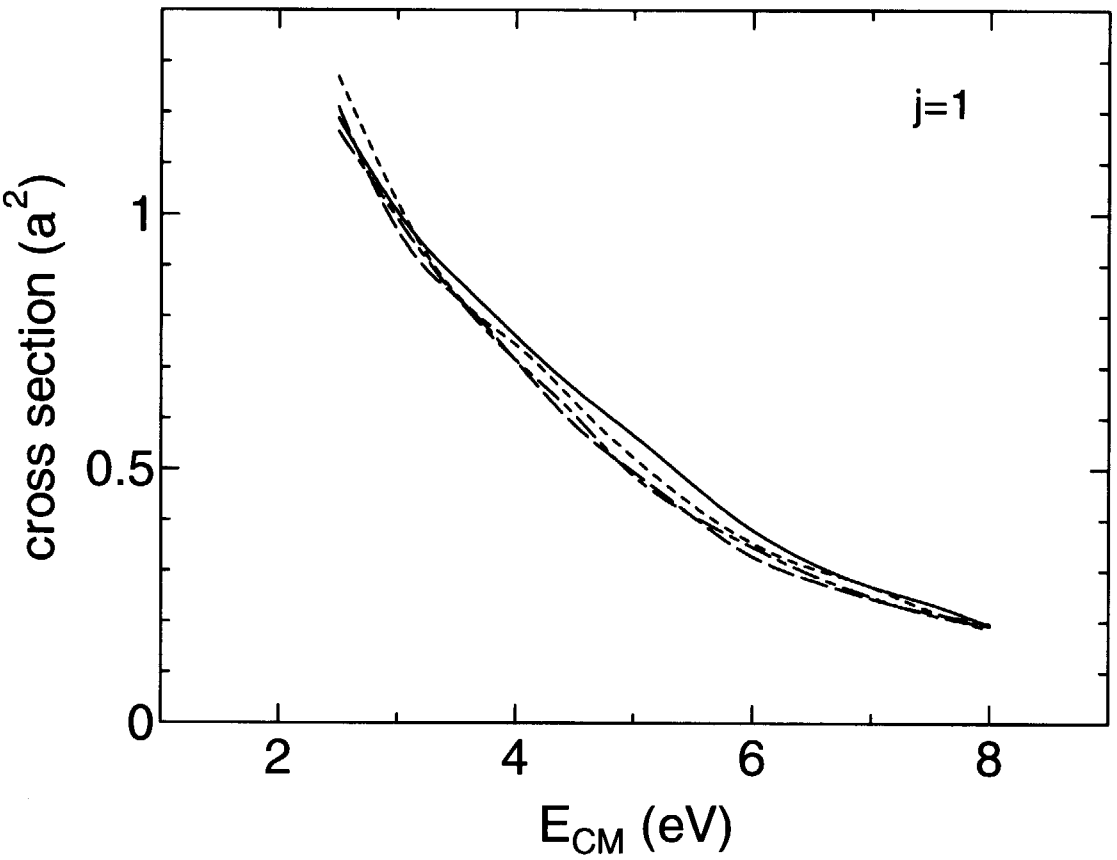


Fig.14 The sum of cross sections for the reactions $H^+ + D_2(v,j=1) \rightarrow D^+ + HD$ and $H^+ + D_2(v, j=1) \rightarrow HD^+ + D$.

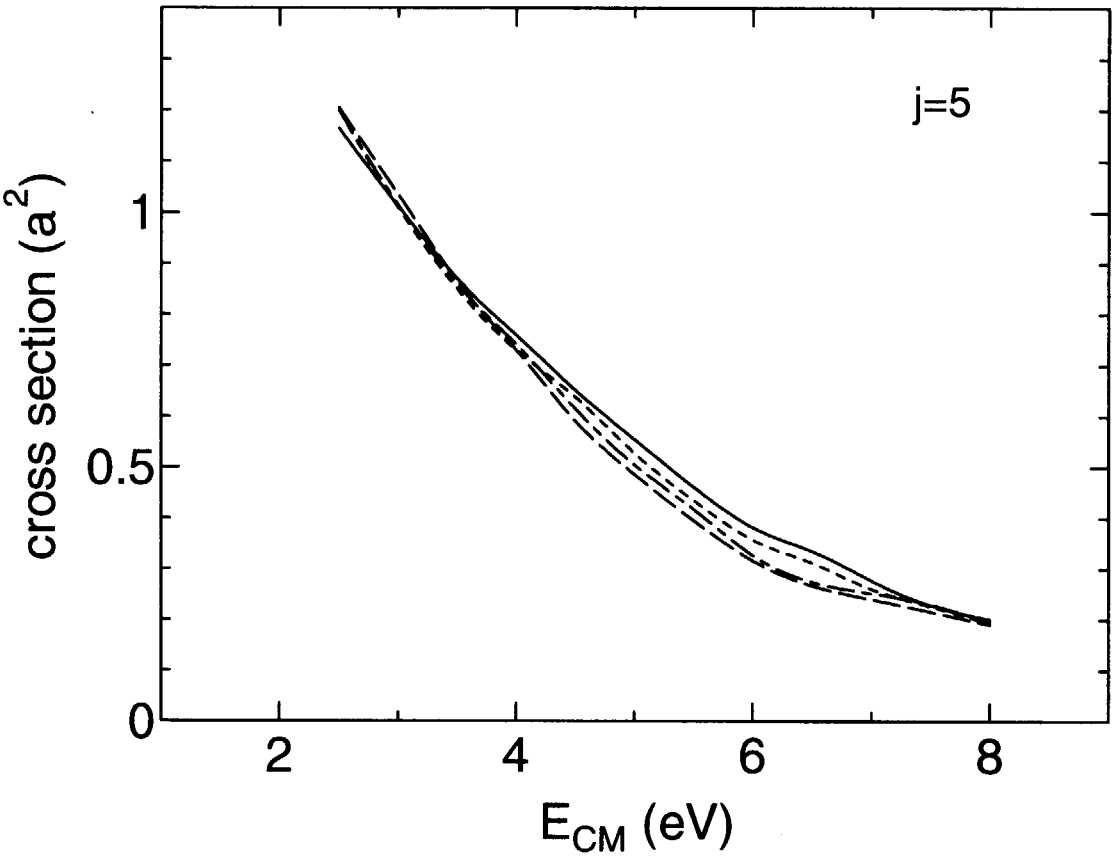


Fig.15 The sum of cross sections for the reactions $H^+ + D_2(v,j=5) \rightarrow D^+ + HD$ and $H^+ + D_2(v, j=5) \rightarrow HD^+ + D$.

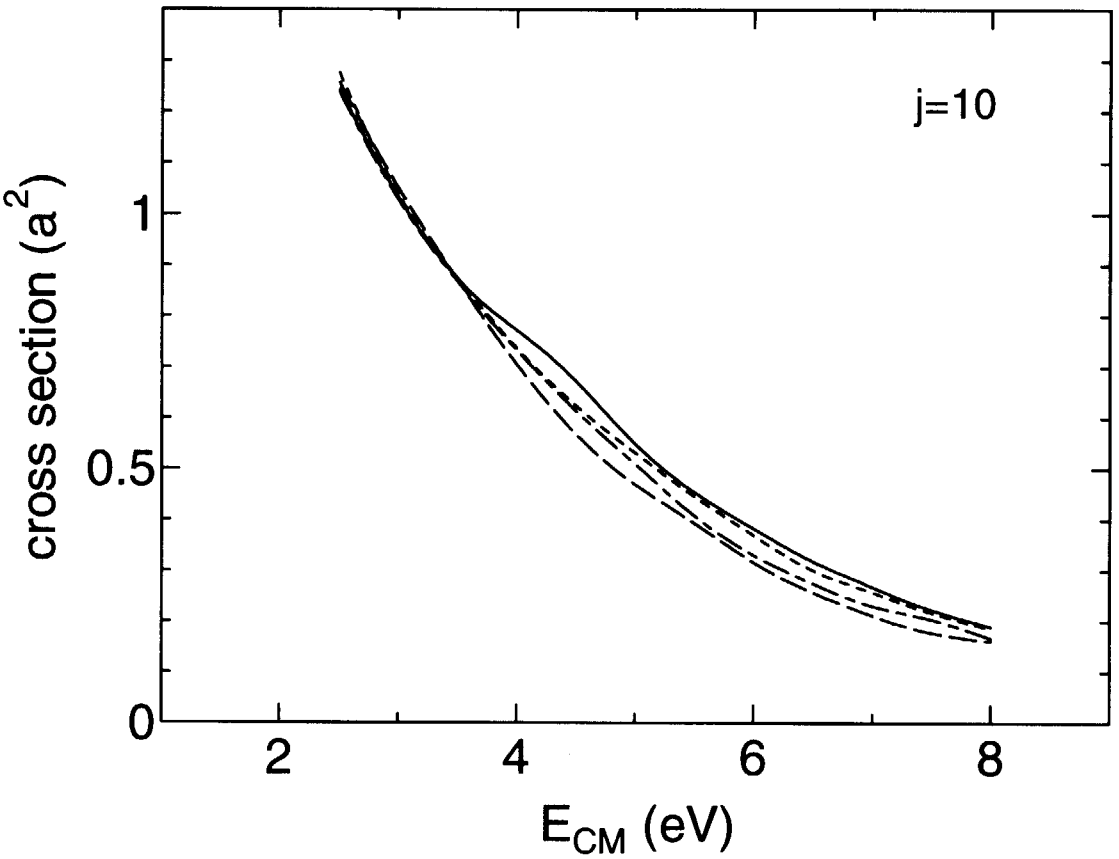


Fig.16 The sum of cross sections for the reactions $H^+ + D_2(v,j=10) \rightarrow D^+ + HD$ and $H^+ + D_2(v, j=10) \rightarrow HD^+ + D$.

# 国際単位系 (SI) と換算表

**表 1　SI基本単位および補助単位**

| 量 | 名称 | 記号 |
|---|---|---|
| 長さ | メートル | m |
| 質量 | キログラム | kg |
| 時間 | 秒 | s |
| 電流 | アンペア | A |
| 熱力学温度 | ケルビン | K |
| 物質量 | モル | mol |
| 光度 | カンデラ | cd |
| 平面角 | ラジアン | rad |
| 立体角 | ステラジアン | sr |

**表 2　SIと併用される単位**

| 名称 | 記号 |
|---|---|
| 分，時，日 | min，h，d |
| 度，分，秒 | °，′，″ |
| リットル | l，L |
| トン | t |
| 電子ボルト | eV |
| 原子質量単位 | u |

1 eV = 1.60218 × $10^{-19}$ J

1 u = 1.66054 × $10^{-27}$ kg

**表 5　SI接頭語**

| 倍数 | 接頭語 | 記号 |
|---|---|---|
| $10^{18}$ | エクサ | E |
| $10^{15}$ | ペタ | P |
| $10^{12}$ | テラ | T |
| $10^{9}$ | ギガ | G |
| $10^{6}$ | メガ | M |
| $10^{3}$ | キロ | k |
| $10^{2}$ | ヘクト | h |
| $10^{1}$ | デカ | da |
| $10^{-1}$ | デシ | d |
| $10^{-2}$ | センチ | c |
| $10^{-3}$ | ミリ | m |
| $10^{-6}$ | マイクロ | μ |
| $10^{-9}$ | ナノ | n |
| $10^{-12}$ | ピコ | p |
| $10^{-15}$ | フェムト | f |
| $10^{-18}$ | アト | a |

**表 3　固有の名称をもつSI組立単位**

| 量 | 名称 | 記号 | 他のSI単位による表現 |
|---|---|---|---|
| 周波数 | ヘルツ | Hz | $s^{-1}$ |
| 力 | ニュートン | N | m·kg/$s^2$ |
| 圧力，応力 | パスカル | Pa | N/$m^2$ |
| エネルギー，仕事，熱量 | ジュール | J | N·m |
| 工率，放射束 | ワット | W | J/s |
| 電気量，電荷 | クーロン | C | A·s |
| 電位，電圧，起電力 | ボルト | V | W/A |
| 静電容量 | ファラド | F | C/V |
| 電気抵抗 | オーム | Ω | V/A |
| コンダクタンス | ジーメンス | S | A/V |
| 磁束 | ウェーバ | Wb | V·s |
| 磁束密度 | テスラ | T | Wb/$m^2$ |
| インダクタンス | ヘンリー | H | Wb/A |
| セルシウス温度 | セルシウス度 | ℃ | |
| 光束 | ルーメン | lm | cd·sr |
| 照度 | ルクス | lx | lm/$m^2$ |
| 放射能 | ベクレル | Bq | $s^{-1}$ |
| 吸収線量 | グレイ | Gy | J/kg |
| 線量当量 | シーベルト | Sv | J/kg |

**表 4　SIと共に暫定的に維持される単位**

| 名称 | 記号 |
|---|---|
| オングストローム | Å |
| バーン | b |
| バール | bar |
| ガル | Gal |
| キュリー | Ci |
| レントゲン | R |
| ラド | rad |
| レム | rem |

1 Å = 0.1 nm = $10^{-10}$ m

1 b = 100 $fm^2$ = $10^{-28}$ $m^2$

1 bar = 0.1 MPa = $10^5$ Pa

1 Gal = 1 cm/$s^2$ = $10^{-2}$ m/$s^2$

1 Ci = 3.7 × $10^{10}$ Bq

1 R = 2.58 × $10^{-4}$ C/kg

1 rad = 1 cGy = $10^{-2}$ Gy

1 rem = 1 cSv = $10^{-2}$ Sv

（注）

1. 表1－5は「国際単位系」第5版，国際度量衡局 1985年刊行による。ただし，1 eVおよび1 uの値はCODATAの1986年推奨値によった。
2. 表4には海里，ノット，アール，ヘクタールも含まれているが日常の単位なのでここでは省略した。
3. barは，JISでは流体の圧力を表わす場合に限り表2のカテゴリーに分類されている。
4. EC閣僚理事会指令ではbar，barnおよび「血圧の単位」mmHgを表2のカテゴリーに入れている。

## 換　算　表

| 力 | N(=$10^5$ dyn) | kgf | lbf |
|---|---|---|---|
| | 1 | 0.101972 | 0.224809 |
| | 9.80665 | 1 | 2.20462 |
| | 4.44822 | 0.453592 | 1 |

粘度　1 Pa·s(N·s/$m^2$) = 10 P(ポアズ)(g/(cm·s))

動粘度　1 $m^2$/s = $10^4$ St(ストークス)($cm^2$/s)

| 圧力 | MPa(=10 bar) | kgf/$cm^2$ | atm | mmHg(Torr) | lbf/$in^2$(psi) |
|---|---|---|---|---|---|
| | 1 | 10.1972 | 9.86923 | 7.50062 × $10^3$ | 145.038 |
| | 0.0980665 | 1 | 0.967841 | 735.559 | 14.2233 |
| | 0.101325 | 1.03323 | 1 | 760 | 14.6959 |
| | 1.33322 × $10^{-4}$ | 1.35951 × $10^{-3}$ | 1.31579 × $10^{-3}$ | 1 | 1.93368 × $10^{-2}$ |
| | 6.89476 × $10^{-3}$ | 7.03070 × $10^{-2}$ | 6.80460 × $10^{-2}$ | 51.7149 | 1 |

| エネルギー・仕事・熱量 | J(=$10^7$ erg) | kgf·m | kW·h | cal(計量法) | Btu | ft·lbf | eV |
|---|---|---|---|---|---|---|---|
| | 1 | 0.101972 | 2.77778 × $10^{-7}$ | 0.238889 | 9.47813 × $10^{-4}$ | 0.737562 | 6.24150 × $10^{18}$ |
| | 9.80665 | 1 | 2.72407 × $10^{-6}$ | 2.34270 | 9.29487 × $10^{-3}$ | 7.23301 | 6.12082 × $10^{19}$ |
| | 3.6 × $10^6$ | 3.67098 × $10^5$ | 1 | 8.59999 × $10^5$ | 3412.13 | 2.65522 × $10^6$ | 2.24694 × $10^{25}$ |
| | 4.18605 | 0.426858 | 1.16279 × $10^{-6}$ | 1 | 3.96759 × $10^{-3}$ | 3.08747 | 2.61272 × $10^{19}$ |
| | 1055.06 | 107.586 | 2.93072 × $10^{-4}$ | 252.042 | 1 | 778.172 | 6.58515 × $10^{21}$ |
| | 1.35582 | 0.138255 | 3.76616 × $10^{-7}$ | 0.323890 | 1.28506 × $10^{-3}$ | 1 | 8.46233 × $10^{18}$ |
| | 1.60218 × $10^{-19}$ | 1.63377 × $10^{-20}$ | 4.45050 × $10^{-26}$ | 3.82743 × $10^{-20}$ | 1.51857 × $10^{-22}$ | 1.18171 × $10^{-19}$ | 1 |

1 cal = 4.18605 J (計量法)

= 4.184 J (熱化学)

= 4.1855 J (15 °C)

= 4.1868 J (国際蒸気表)

仕事率　1 PS (仏馬力)

= 75 kgf·m/s

= 735.499 W

| 放射能 | Bq | Ci |
|---|---|---|
| | 1 | 2.70270 × $10^{-11}$ |
| | 3.7 × $10^{10}$ | 1 |

| 吸収線量 | Gy | rad |
|---|---|---|
| | 1 | 100 |
| | 0.01 | 1 |

| 照射線量 | C/kg | R |
|---|---|---|
| | 1 | 3876 |
| | 2.58 × $10^{-4}$ | 1 |

| 線量当量 | Sv | rem |
|---|---|---|
| | 1 | 100 |
| | 0.01 | 1 |

（86年12月26日現在）

CROSS SECTIONS FOR ION PRODUCTION IN REACTIONS OF $H^+$ WITH $D_2$. EFFECTS OF VIBRATIONAL AND ROTATIONAL EXCITED STATES OF $D_2$.