# Total, Partial, and Differential Ionization Cross Sections in Proton-Hydrogen Atom Collisions in the Energy Region of 0.1–10 keV/u

#### Lukáš Pichla)

Foundation of Computer Science Laboratory, University of Aizu, Tsuruga, Ikki, Aizu-Wakamatsu, Fukushima 965-8580, Japan

## Shiyang Zoub)

Department of Fusion Science, School of Mathematical and Physical Science, Graduate University for Advanced Studies, Oroshi-cho 322-6, Toki, Gifu 509-5292, Japan

#### Mineo Kimura<sup>c)</sup>

Graduate School of Sciences, Kyushu University, Fukuoka 812-8581, Japan

### Izumi Murakami<sup>d)</sup> and Takako Kato<sup>e)</sup>

National Institute for Fusion Science, Oroshi-cho 322-6, Toki, Gifu 509-5292, Japan

(Received 26 June 2003; revised manuscript received 15 December 2003; accepted 29 December 2003; published online 2 December 2004)

Single-differential, partial, and total ionization cross sections for the proton-hydrogen atom collision system in the energy region of 0.1–10 keV/u are determined by using the molecular-orbital close-coupling method within a semiclassical formalism. The present cross sections are in an excellent agreement with the recent experiments of Shah *et al.* [J. Phys. B. **31**, L757 (1998)], but decrease more rapidly than the cross sections measured by Pieksma *et al.* [Phys. Rev. Lett. **73**, 46 (1994)] with decreasing energy. The numerical data for all calculated cross sections are included in this paper. A critical evaluation of the existing data for the ionization process in the keV energy range is performed both for the experiment and theory. The recommended data are obtained from a converged close-coupling expansion, which in total includes 362 bound and continuum channels with their wave functions augmented by the electron translation factor in order to insure the correct scattering boundary condition. © *2004 American Institute of Physics*.

[DOI: 10.1063/1.1710897]

Key words: charge transfer; hydrogen atom; ionization; semiclassical molecular orbital close coupling two center Coulomb functions.

#### 3.4. Differential Ionization Cross Sections **Contents** 3.5. Charge Transfer and Target Excitation...... 1038 2.1. Molecular Orbital Coupled Equations. . . . . . 1034 2.2. Two Coulomb Center Functions...... 1034 Appendix A: One-Electron Diatomic-Molecule 3.2. Total Ionization Cross Sections (TICS)..... 1035 Appendix B: Separation of Angular Couplings... 1048 List of Tables <sup>a)</sup>Author to whom correspondence should be addressed; electronic mail: 1. Molecular basis sets for the close-coupling basis lukas@u-aizu.ac.jp b)Present address: Institute for Molecular Science, Myodaiji, Okazaki 444-8585, Japan; electronic mail: zou@ims.ac.jp Total ionization cross sections.............................. 1036 c)Electronic mail: mineoscc@mbox.nc.kyushu-u.ac.jp Partial ionization cross sections................. 1037 3. d)Electronic mail: mizumi@nifs.ac.jp Single differential cross sections e)Electronic mail: takako@nifs.ac.jp © 2004 American Institute of Physics.

5.	Single differential cross sections	
	at $E = 0.42 \text{ keV/amu}$	1041
6.	Single differential cross sections	
	at $E = 0.74 \text{ keV/amu}$	1042
7.	Single differential cross sections	
	at $E = 1.06 \mathrm{keV/amu}$	1043
8.	Single differential cross sections	
0	at $E = 1.38 \text{ keV/amu}$ .	1043
9.	Single differential cross sections	1044
10	at $E = 1.70 \text{keV/amu}$ .	1044
10.	Single differential cross sections at $E = 2.02 \text{ keV/amu}$	1044
11	Single differential cross sections	1044
11.	at $E = 2.34 \text{ keV/amu}$	1045
12.	Single differential cross sections	1015
	at $E = 2.65 \text{ keV/amu}$	1045
13.	Single differential cross sections	
	at $E = 2.97 \text{ keV/amu}$	1046
14.	Single differential cross sections	
	at $E = 3.29 \text{ keV/amu}$	1046
15.	Single differential cross sections	
	at $E = 3.61 \text{ keV/amu}$	1047
16.	Single differential cross sections	
	at $E=3.93 \text{ keV/amu}$	1047
17.	Single differential cross sections	1040
10	at $E = 4.25 \text{ keV/amu}$ .	1048
10.	Single differential cross sections at $E = 4.57 \text{ keV/amu}$ .	1048
10	Single differential cross sections	1046
17.	at $E = 4.89 \text{ keV/amu}$ .	1049
20.	Single differential cross sections	1017
-0.	at $E = 5.21 \text{ keV/amu}$ .	1049
21.	Single differential cross sections	
	at $E = 5.53 \text{ keV/amu}$	1050
22.	Single differential cross sections	
	at $E = 5.85 \text{ keV/amu}$	1050
23.	Single differential cross sections	
	at $E = 6.17 \text{ keV/amu}$	1051
24.	Single differential cross sections	
25	at $E = 6.49 \text{ keV/amu}$ .	1051
25.	Single differential cross sections	1052
26	at E = 6.81 keV/amu	1052
20.	Single differential cross sections at $E = 7.13 \text{ keV/amu}$ .	1052
27	Single differential cross sections	1032
27.	at $E=7.45 \text{ keV/amu}$ .	1053
28.	Single differential cross sections	1000
	at $E = 7.76 \mathrm{keV/amu}$	1053
29.	Single differential cross sections	
	at $E = 8.08 \text{ keV/amu}$	1054
30.	Single differential cross sections	
	at $E = 8.40 \text{ keV/amu}$	1054
31.	Single differential cross sections	
22		1055
32.	Single differential cross sections	1055
	at $E = 9.04 \text{ keV/amu}$	1000

33.	Single differential cross sections	
	at $E = 9.36 \text{ keV/amu}$	1056
34.	Single differential cross sections	
	at $E = 9.68 \text{ keV/amu}$	1056
35.	Single differential cross sections	
	at $E = 10.0 \mathrm{keV/amu}$	1057
	List of Figures	
1.	Total ionization cross sections of proton—	
	hydrogen system: (a) and (b) are for low and high	
	energy regions, respectively	1033
2.	Partial ionization cross sections (integrated over	
	the ejected electron energy) as a function of the	
	collision energy $E$ for the 11 partial waves	1036
3.	Same as Fig. 2 except for the ejected electron	
	energy is fixed at $\epsilon$ =0.01 Ry	1038
4.	Single differential ionization cross sections for	
	proton-hydrogen system as a function of	
	ejected electron energy $\epsilon$ and collision	
	energy $E$	1038
5.	Ejected electron distribution for proton-	
	hydrogen system as a function of electron	
	velocity, $v_e$ , and impact parameter, $b$ , at the	
	collision energy $E = 10 \text{ keV/u.} \dots$	1039
6.	Cross section comparison (hydrogen-proton	
	system) for: (a) excitation to $2s$ and $2p$	
	levels and (b) capture into $2s$ and $2p$	

### 1. Introduction

levels of atomic hydrogen in collisions

Proton impact ionization from various atoms and molecules has attracted many researchers over many years since it serves as an important and challenging problem in atomic physics. It is one of the most fundamental processes in various applications such as fusion reactors (plasma edge processes, cooling rate estimates), radiation damage in biological matters (including cancer treatment), energy loss of heavy ions in solid targets, and ion-beam technologies (etching, thin-film manufacturing).

There has been a vast amount of effect directed at the full understanding of the emissions during ion-atom collisions both from the experimental and theoretical perspectives. Several publications have provided a partial overview of these studies. 1-5 Yet, our understanding of even the basic prototype ion-atom collision system, proton on hydrogen atom, is not completely satisfactory, especially at low energies below a few keV. At keV energies, the total ionization cross sections measured in the experiment of Pieksma et al.<sup>6</sup> were found substantially larger than the recent measurements of Shah et al. below 10 keV/u, and decreasing more slowly with the decreasing energy. At 1 keV/u, the cross sections of Pieksma et al.<sup>6</sup> exceed the values by Shah et al.<sup>7</sup> by as much as ~4 times. Numbers from the highly accurate experiments<sup>8,9</sup> and elaborate calculations<sup>10–12</sup> disagree by 20% at the peak of ionization cross section of 50 keV/u. The above experimental and theoretical results are summarized in

Fig. 1 together with other rigorous theoretical contributions over the years. Detailed discussions on these studies are provided in the following paragraphs.

Describing the ionization process correctly with high precision, probabilities of other concurrent processes, in particular elastic scattering, target excitation, and electron capture to the projectile should be considered simultaneously in low-to-intermediate collision energies. It is not possible to describe one process accurately without treating all on equal footing since the ionization is strongly intertwined with other inelastic and elastic processes. Because proton—hydrogen atom interactions are known to be relatively weak, and also many channels couple closely, computing high accuracy cross sections for ionization of this collision system requires us to include a huge number of channels carefully, and remains one of the difficult and challenging problems in collision physics.

There is a series of theoretical and experimental works to obtain accurate ionization cross sections, based on a variety of approaches. In theory, the methods commonly used include the molecular orbital close coupling method (MOCC), or atomic orbital close coupling (AOCC), the perturbative method, and the classical trajectory Monte Carlo method (CTMC), and some of the most recent ones are cited below. Even among extensive and reliable theoretical investigations particularly based on the close coupling scheme, discrepancies of ambiguous origin arise in the energy dependence and magnitude below the intermediate energy. A study based on the MOCC includes SethuRaman et al., 13 and Thorson and his co-workers, 14,15 and those by using the various types of the AOCC are Winter and Lin,16 McLaughlin et al.,17 Fritsch and Lin,<sup>18</sup> and other authors.<sup>11,12</sup> Most recently, a study based on the two-center AOCC approach was carried out by Toshima, 10 who calculated ionization cross sections for collision energy 1-800 keV/u, obtaining results 20% higher than the experiments of Shah et al. 8,9 at the ionization cross section peak. Two recent calculations by Kolakowska and Sidky<sup>11,12</sup> agree well with Toshima<sup>10</sup> and Shah's et al. experiment<sup>7</sup> at energies 4–10 keV/u, but decrease more rapidly than those by Shah et al.7 below 4 keV/u. Two different types of the hidden crossing calculation, i.e., the inclusion or neglect of radial decoupling mechanism were performed, and corresponding two results based on the approach of Ovchinnikov and Macek<sup>19</sup> were found to be largely different.<sup>6,20</sup> The result obtained by the neglect of the decoupling mechanism is found to provide good agreement with Shah et al.7 The present formalism builds on evaluating measurable quantities in the real coordinate space. We therefore directly compute bound- and continuum-state wave functions, radial and angular couplings among all states involved, and solve the dynamics in the molecular-state basis. 21-25

In the experiment, the proton-hydrogen atom system is the simplest ion-atom system but yet one of the most difficult ones to be studied for a number of reasons including the difficulty of producing pure hydrogen atoms. A few experimental references are: Pieksma *et al.*,<sup>6</sup> Shah *et al.*,<sup>7</sup> Fite

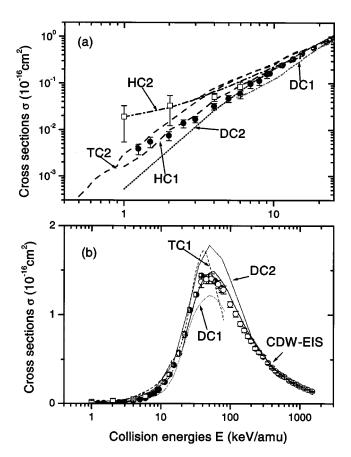


Fig. 1. Total ionization cross sections of proton—hydrogen system: (a) and (b) are for low and high energy regions, respectively. Circles with error bars, measured cross sections of Shah *et al.* (Refs. 7–9). Squares with error bars, measured cross sections of Pieksma *et al.* (Ref. 6); HC2, hidden crossing theory with *S* and *T* and radial decoupling promotion mechanisms (Ref. 20); HC1, hidden crossing theory with only *S* and *T* promotion mechanisms (Ref. 6); TC2, close-coupling triple-center calculations of Shah *et al.* (Ref. 7); TC1, close-coupling triple-center calculations of McLaughlin *et al.* (Ref. 17); DC2, two-center close-coupling calculations of Toshima (Ref. 10); DC1, two-center close-coupling calculations of Fritsch and Lin (Ref. 18); CDW-EIS, continuum distorted wave eikonal initial state approximation of Crothers and McCann (Ref. 35); (solid line) present results.

et al., 26 but as described above, a serious discrepancy exists between the most recent measurements.

It can be seen in Fig. 1 that the experimental results are only in a very rough general accord. Therefore reliable theoretical values must play an important role for recommending the set of cross sections that is to be used in applications and also the method that describes the dynamics of ionizing collisions best. Nevertheless, for such purpose the previous theoretical calculations differ even to a higher extent than the experimental data. This can be seen in Fig. 1(a) at low keV energy, whether it is the difference between the hiddencrossing calculations with and without the radial decoupling promotion mechanism<sup>6,20</sup> or the difference between the close-coupling calculations based on the two-center<sup>10</sup> versus the three-center expansion. In addition, it is important to note that the hidden-crossing method relies on the complex coordinate and analytical continuation, and therefore the evaluation of measurable quantities such as differential ion-

ization cross sections or spatial probability distributions of the electron during the collision is not straightforward. The present method, in contrast, provides for all of these quantities before the total ionization cross sections are calculated.

Because of the uncertainty on the ionization cross section values below a few keV/u, both in theory and experiments as summarized above, we have undertaken the project to calculate the differential ionization cross sections (DICSs) and the total ionization cross sections (TICSs) for ionization of atomic hydrogen by proton impact at the low collision energy range 0.1–10 keV/u. In addition, charge transfer and excitation channels were also considered. Electron transfer factor (ETF) has been included to ensure correct scattering boundary conditions. All results obtained are given both in tabular and graphical forms.

## 2. Theoretical Method

### 2.1. Molecular Orbital Coupled Equations

Let us assume the internuclear distance between proton and hydrogen to be described classically by a vector  $\mathbf{R}(t)$ , and solve the resulting time-dependent Schorödinger equation for the electron system with Hamiltonian  $H_{\rm el}$ ,

$$i(h/2\pi)\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = H_{el}(\mathbf{r},\mathbf{R}(t))\Psi(\mathbf{r},t).$$
 (1)

We expand the state vector  $\Psi$  in an ETF-modified molecular basis set, and integrate over electron coordinates  $\mathbf{r}$ . Then for the expansion coefficients  $a_n(t)$  in the MOCC method one obtains the coupled equations (up to the first order in velocity  $\mathbf{v}$ )

$$i(h/2\pi)\frac{da_k(t)}{dt} = \sum_{n \neq k} \left[ \dot{R}(P^R + A^R) + R\dot{\theta}(P^\theta + A^\theta) \right]_{kn}$$

$$\times a_n(t) \exp\left[ -\frac{i}{(h/2\pi)} \int_{-\epsilon_k(t')}^{t} (\epsilon_n(t')) dt' \right], \tag{2}$$

with  $\Theta = \angle(\mathbf{v}, \mathbf{R})$ , where the usual coupling terms  $P^{27}$ 

$$P_{kn}^{R} = -i(h/2\pi)(\epsilon_{k} - \epsilon_{n})^{-1} \left\langle \phi_{k} \left[ \left[ \frac{\partial H_{el}}{\partial R} \right]_{r} \right] \phi_{n} \right\rangle, \quad (3)$$

$$P_{kn}^{\theta} = -R^{-1} \langle \phi_k | \hat{L}_v | \phi_n \rangle \tag{4}$$

are corrected by the radial and angular ETF terms

$$A_{kn}^{R} = \operatorname{im}/(h/2\pi)(\epsilon_{k} - \epsilon_{n}) \langle \phi_{k} | z f_{n}(\mathbf{r}; \mathbf{R}) | \phi_{n} \rangle, \quad (5)$$

$$A_{kn}^{\theta} = \operatorname{im}/(h/2\pi)(\epsilon_k - \epsilon_n) \langle \phi_k | x f_n(\mathbf{r}; \mathbf{R}) | \phi_n \rangle.$$
 (6)

Here, m is the reduced electron mass, L is the electronic orbital angular momentum, and  $\mathbf{r} = (x, y, z)$ , with z being parallel to  $\mathbf{R}$ . The switching functions  $f_n(\mathbf{r}; \mathbf{R})$  which describe the correlation of electron motion on nuclei, in general, depend on the molecular-state wave function  $\phi_n(\mathbf{r}; \mathbf{R})$ . We have employed the switching function derived by Thorson

et al.<sup>22</sup> for the  $\rm H_2^+$  system, based on the analytical twocenter decomposition of exact wave functions. All these coupling matrix elements are evaluated using Gauss–Legendre and Gauss–Laguerre quadratures with relative errors  $\leq 1 \times 10^{-8}$ .

Before moving on to solve the close-coupled Eqs. (2), a few important comments associated with the ETF's modified molecular orbital expansion approach need to be discussed. This is the non-Hermitian Hamiltonian matrix (P+A) in Eq. (2). In any calculation, we need to replace the full Hilbert space spanned by the true discrete and continuum states with a truncated subspace. As a result, certain operators in the equations of motion cannot be fully represented, and unless great care is taken they may not even be accurately represented within the truncated subspace. This is true in particular for the propagator itself. Thus, a theory should consider the flux loss from the truncated subspace, and then, in contrast with the exact close-coupled equations, the closecoupled equations for the wave function in the truncated subspace are necessarily nonunitary, i.e., they should not conserve probabilities. Our locally non-Hermitian Hamiltonian matrix (P+A) allows us to consider the escape of electrons from the subspace spanned by the truncated basis. Importantly, the flux loss effects decrease with the basis size increase, and the probability conservation is satisfied approximately on a sufficiently large basis set. By implementing the ETFs, the basis sets of relatively small size can be considered as complete with sufficient accuracy. In the present study, we find the probability conservation is better than  $1 \times 10^{-3}$  with a basis set including ten bound states and 11 continuum partial waves.

#### 2.2. Two Coulomb Center Functions

Next, we briefly summarize the computation of matrix elements in Eqs. (3)–(6).  ${\rm H_2}^+$  is a prototype one-electron two-nuclei system, which is separable in the conventional prolate spheroidal coordinates,  ${\bf r}=(\xi,\eta,\phi)$ , and the corresponding eigenvalues  $\epsilon_k$  and wave functions  $\phi_k({\bf r};R)$  can be calculated with great numerical accuracy. <sup>28–34</sup> The wave function is factored out

$$\phi_k(\xi, \eta, \varphi; R) = C_k(R) \Lambda_k(\xi, R) M_k(\eta, R) e^{i\mu\varphi}, \quad (7)$$

where  $C_k(R)$  is a normalization constant, and functions  $\Lambda_k(\xi,R)$  and  $M_k(\eta,R)$  describe the quasiradial and quasiangular motions of electron, respectively. The index  $\mu$  labels the component of electronic angular momentum on the  $\mathbf{R}$  axis. The letter k stands for the three quantum numbers  $E, \mu$ , and A (A is equivalent to the orbital angular momentum for R=0). The one dimensional wave functions in Eq. (7) are found in semianalytical forms, and the coupling terms in Eqs. (3)–(6) are then readily computed. Details of the method can be found in Refs. 28–34 and have been summarized in Appendices A and B.

The state vector  $\Psi$  in Eq. (1) is composed of noninteracting g (gerade) and u (ungerade) components, and thus there are corresponding sets of g and u close-coupled Eqs. (2). If index "1" designates the initial states in each set  $(1s\sigma_g)$  or

 $2p\sigma_u$ , respectively), then the initial conditions for Eqs. (2) (corresponding to "proton A plus atom B") is

$$a_k(t=-\infty) = 1/\sqrt{2}\,\delta_{1k}\,,\tag{8}$$

and (for given energy E and each impact parameter b) the final-state amplitude  $a_k(E,b)$  is computed. Once the final-state amplitude  $a_k(t=+\infty)$  is obtained, we can define the probability of excitation/or ionization to the molecular state k as

$$P_k(E,b) = |a_k(t=\infty)|^2,$$
 (9)

and the corresponding individual cross section reads

$$Q_k(E) = 2\pi \int P_k(E,b)b \, db. \tag{10}$$

In ionization problems,  $Q_k(E)$  is the partial ionization cross section, labeled by  $\epsilon$ ,  $\lambda$ , and  $\mu$ . Hence the differential ionization cross section is determined by summing  $Q(\epsilon, \lambda, \mu; E)$  over quantum numbers  $\lambda$ ,  $\mu$ 

$$\frac{d\sigma}{d\epsilon} = \sum_{\lambda,\mu} Q(\epsilon,\lambda,\mu;E)$$
 (11)

and the total ionization cross section

$$\sigma = \int \frac{d\sigma}{d\epsilon} d\epsilon \tag{12}$$

is obtained by integrating the energy distribution of ejected electrons.

#### 3. Results and Discussion

#### 3.1. Basis Sets and Convergence

To compute the ionization cross sections, we have carried out systematic calculations with basis sets A, B, and C, as listed in Table 1. Comparing the numerical results with different basis sets allows us to study the convergence of ionization cross sections with the basis size. In addition, some selected calculation have been done on the ungerade component of basis set C without  $2p \pi_u$  (set D) to understand the role of upper levels in the ionization dynamics. The continuum component is common in the basis sets A (direct ionization), B, C (indirect ionization), and D (reference basis set), which contains 32 energies below 1.0 Ry for each partial wave; then the total continuum states are accounted for up to 352. Within the straight-line approximation, we have solved the coupled differential equations, Eq. (2), for 100 impact parameters arranged in (0.0-6.0) a.u. at 32 collision energies from 0.1 to 10 keV/u. The results shown below were obtained by using the basis set C.

The energy of ejected electrons is explicitly included in the equations of motion via the coupling terms in Eq. (2), while the total ionization cross section requires a formal integration over the whole continuum. Therefore, we need to revert to a discrete sampling scheme as described further. Our study and also previous works in the literature 15,34 find the couplings with continuum states to be generally weak,

TABLE 1. Molecular basis sets for the close-coupling basis sets

Sets	Gerade basis states	Ungerade basis states	Number of all states
Continuum	$ \epsilon s \sigma_g\rangle \  \epsilon d\sigma_g\rangle,  \epsilon d\pi_g\rangle \  \epsilon g \sigma_e\rangle,  \epsilon g \pi_e\rangle$	$  \epsilon p \sigma_u\rangle,  \epsilon p \pi_u\rangle   \epsilon f \sigma_u\rangle,  \epsilon f \pi_u\rangle   \epsilon h \sigma_u\rangle,  \epsilon h \pi_u\rangle $	
	5 partial waves, for 32 energies	6 partial waves, for 32 energies	$11 \times 32 = 352$
Bound	all above, plus	all above, plus	
A	$ 1s\sigma_g\rangle$	$ 2p\sigma_u\rangle$	354
В	all above, plus $ 3d\pi_g\rangle$ $ 3d\sigma_g\rangle$	all above, plus $ 2p\pi_u\rangle$ $ 3p\sigma_u\rangle$	
	$ 2s\sigma_g\rangle$	$ 3p\pi_u\rangle$	360
C	all above, plus	all above, plus	
	$ 4d\pi_g angle$	$ 4f\sigma_u\rangle$	362
D	_	all above, minus $ 2p\pi_u\rangle$	196ª

<sup>a</sup>Set D contains 4 discrete states  $(2p\sigma_u, 3p\sigma_u, 3p\pi_u, 4f\sigma_u)$  and 192 continuum states (32 energies for the 6 *u*-partial waves above).

and the full close-coupled Eqs. (2) can be partitioned into separate groups. Each group contains the strongly coupled symmetry allowed discrete states (cf. Table 1) and several partial waves for continuum electron with the same energy; these are coupled by weak radial or angular interactions. Truncation in the partial wave expansion of the continuum electron is based on a rapid decrease of the couplings with the increasing angular momentum number ( $\sim$ 3 orders of magnitude for ejected electron with l=5). Next, we calculate the differential ionization cross sections at a certain set of separate energy points, interpolate these with B splines, and finally integrate the spline function over the whole continuum analytically. Thus the convergence in the number of continuum states can be controlled through the convergence of B-spline interpolation. Ionization cross sections decrease rapidly with the ejected electron energy increase, and the necessary number of interpolation points derives from the number of B-spline terms which can accurately represent this function shape. Logarithm equally spaced mesh points of ejected electron energy were conveniently used in our calculation. The differential cross sections already vary smoothly with free electron energies on the 32 point grid.

#### 3.2. Total Ionization Cross Sections (TICS)

Figure 1 shows the present TICSs along with some earlier theoretical and experimental results. The present MOCC results are found to agree better with Shah *et al.*<sup>7</sup> below 10 keV/u. The present results are smaller than those of the triple-center AOCC calculations, although they exhibit closer agreement at collision energies lower than 1.5 keV/u. The hidden-crossing calculation including *S* and *T* promotions and the radial decoupling mechanism is about 30% larger than the present results at 10 keV/u. Their cross section decreases more slowly with the decreasing energy, and thus at 1 keV/u the difference from our calculations is as high as a factor of 6. Yet, the present values are in better agreement

with the hidden-crossing method including S and T promotions, with the discrepancies better than 30% in all energies. Below 2 keV/u, however, the hidden-crossing results decrease faster, and correspondingly, those cross sections are by a factor of 2 smaller than the present results at 1 keV/u. The present results agree well with the two-center AOCC result of Toshima. 10 In the energy range from 4–10 keV/u, however, the cross sections by Toshima become smaller than the present results and sharply decrease below 4 keV/u. The present results are also compared with the measurements of Pieksma et al.,6 and Shah et al.7 Our results are found to be 25% below the measured results of Pieksma et al.6 at 6 keV/u, and decrease more rapidly with the decreasing energy, the discrepancies being up to a factor of 6 at the lowest collision energy of 1 keV/u considered. However, our results are in excellent agreement with the recent experimental data of Shah et al., since they lie within the experimental error bars in the entire energy range considered.

The numerical results for total ionization cross sections are given in Table 2.

#### 3.3. Partial Cross Sections

Figure 2 illustrates the partial cross sections for different partial waves of ejected electron, and the related numerical data are summarized in Table 3.

In particular, Fig. 2 shows the distribution of partial ionization cross sections which are integrated over the ejected electron energy in the interval (0,1) Ry. The partial ionization cross sections as a function of collision energy represent our statement that the ionization is significant only in two or three (l,m) channels either for g components or for u components. In case of g components,  $s\sigma$ ,  $d\sigma$  and  $d\pi$  are the important channels below 4 keV/amu, but the partial ionization cross section of s $\sigma$  increases much more rapidly than the other two, and exceeds them by order of magnitude at E = 10 keV/u. The channels  $p\sigma$ ,  $p\pi$ , and  $f\pi$  are important in the case of u components, and the partial ionization cross section of  $p\sigma$  is much greater than those of other channels except E < 2 keV/u, where the cross section of  $p\pi$  is the largest one. However, the distribution of ejected electrons over partial waves depends on the energy of free electron significantly, which is illustrated in Fig. 3 by the partial ionization cross sections for one fixed energy of the ejected electron,  $\epsilon$ =0.01 Ry. In this particular case, the ionization in u components is dominated by  $p\pi$  and  $p\sigma$  channels and their contributions are almost the same at the highest energy considered, 10 keV/u.

#### 3.4. Differential Ionization Cross Sections (DICS)

In addition to the accurate integral ionization cross sections (cf. Fig. 1) obtained presently, in Fig. 4 we give the single DICSs as a function of ejected electron energy  $\epsilon$  and collision energy E. Cross sections of g and u components are shown in the upper (a) and lower (b) parts, respectively. Ionization cross section decreases rapidly with the final electron energy increasing and collision energy decreasing. Ionization

TABLE 2. Total ionization cross sections (units  $10^{-16} \, \text{cm}^2$ )<sup>a</sup>

$E_{\rm c.m.}^{\ \ b}$	σ	$E_{\rm c.m.}$	σ	$E_{\mathrm{c.m.}}$	σ	$E_{\mathrm{c.m.}}$	σ
0.10	$6.16^{-5}$	2.65	$1.49^{-2}$	5.21	$5.19^{-2}$	7.76	$1.07^{-1}$
0.42	$6.92^{-4}$	2.97	$1.85^{-2}$	5.53	$5.78^{-2}$	8.08	$1.15^{-1}$
0.74	$1.78^{-3}$	3.29	$2.24^{-2}$	5.85	$6.38^{-2}$	8.40	$1.24^{-1}$
1.06	$3.11^{-3}$	3.61	$2.66^{-2}$	6.17	$7.01^{-2}$	8.72	$1.33^{-1}$
1.38	$4.83^{-3}$	3.93	$3.11^{-2}$	6.49	$7.68^{-2}$	9.04	$1.43^{-1}$
1.70	$6.83^{-3}$	4.25	$3.59^{-2}$	6.81	$8.37^{-2}$	9.36	$1.53^{-1}$
2.02	$9.03^{-3}$	4.57	$4.09^{-2}$	7.13	$9.09^{-2}$	9.68	$1.63^{-1}$
2.34	$1.17^{-2}$	4.89	$4.63^{-2}$	7.45	$9.86^{-2}$	10.0	$1.74^{-1}$

<sup>a</sup>Superscript *i* denotes the order of magnitude, i.e.,  $\times 10^{i}$ .

<sup>b</sup>Collision energy E<sub>c.m.</sub> is measured in keV/amu.

is significant only when the collision energy E is above 3 keV/u for g components and 1 keV/u for u components. At the collision energy  $E=10\,\mathrm{keV/u}$ , the differential cross sections of  $\epsilon=0.01\,\mathrm{Ry}$  is about 2 orders of magnitude greater than that of  $\epsilon=1.0\,\mathrm{Ry}$ . Differential cross section  $d\sigma/d\epsilon$  of u components is about 1 order of magnitude greater than that of g components at their maxima. We have projected the differential cross sections  $d\sigma/d\epsilon$  on the bottom plane in this figure. There is a region in the two projections in which for a constant  $d\sigma/d\epsilon$  the ratio of  $\epsilon/E$  is a constant. It shows that a small group of electrons gains energies from incident protons

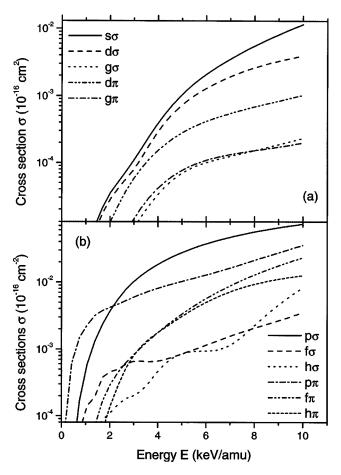


Fig. 2. Partial ionization cross sections (integrated over the ejected electron energy) as a function of the collision energy E for the 11 partial waves: (a) g components and (b) u components.

TABLE 3. Partial ionization cross sections (units  $10^{-16} \, \text{cm}^2$ )

E (keV/u)	0.10	0.42	0.74	1.06	1.38	1.70	2.02	2.34
sσ	$4.48^{-8}$	$3.43^{-7}$	$1.62^{-6}$	$4.47^{-6}$	$1.12^{-5}$	$2.14^{-5}$	$3.55^{-5}$	5.11 <sup>-5</sup>
$p\sigma$	$4.98^{-8}$	$2.21^{-7}$	$4.92^{-7}$	$3.40^{-6}$	$9.35^{-6}$	$1.77^{-5}$	$2.84^{-5}$	$4.12^{-5}$
$d\sigma$	$3.82^{-8}$	$1.60^{-7}$	$2.91^{-7}$	$5.64^{-7}$	$7.14^{-7}$	$6.77^{-7}$	$9.72^{-7}$	$2.94^{-6}$
$f\sigma$	$2.80^{-10}$	$6.18^{-9}$	$2.36^{-8}$	$1.31^{-7}$	$5.83^{-7}$	$1.38^{-6}$	$2.70^{-6}$	$4.95^{-6}$
$g\sigma$	$1.41^{-11}$	$8.29^{-10}$	$2.06^{-8}$	$6.77^{-7}$	$2.87^{-6}$	$6.75^{-6}$	$1.30^{-5}$	$2.28^{-5}$
$\overset{\smile}{h}\sigma$	$5.10^{-6}$	$1.76^{-5}$	$1.68^{-4}$	$5.85^{-4}$	$1.30^{-3}$	$2.34^{-3}$	$3.75^{-3}$	$5.54^{-3}$
$p\pi$	$4.84^{-6}$	$2.03^{-5}$	$5.64^{-5}$	$1.40^{-4}$	$1.91^{-4}$	$3.78^{-4}$	$4.56^{-4}$	$4.97^{-4}$
$d\pi$	$4.42^{-6}$	$3.11^{-5}$	$4.02^{-5}$	$5.06^{-5}$	$6.08^{-5}$	$8.62^{-5}$	$1.12^{-4}$	$1.47^{-4}$
$f\pi$	$4.62^{-5}$	$6.15^{-4}$	$1.47^{-3}$	$2.26^{-3}$	$3.16^{-3}$	$3.75^{-3}$	$4.19^{-3}$	$4.67^{-3}$
$g\pi$	$7.83^{-7}$	$7.07^{-6}$	$1.66^{-5}$	$2.85^{-5}$	$6.96^{-5}$	$1.67^{-4}$	$2.96^{-4}$	$4.45^{-4}$
$\stackrel{\smile}{h}\pi$	$1.43^{-7}$	$9.09^{-7}$	$2.20^{-5}$	$3.45^{-5}$	$3.12^{-5}$	$6.01^{-5}$	$1.41^{-4}$	$2.82^{-4}$
$\sigma_{ m total}$	$6.16^{-5}$	$6.92^{-4}$	$1.78^{-3}$	$3.11^{-3}$	$4.83^{-3}$	$6.83^{-3}$	$9.03^{-3}$	$1.17^{-2}$
E (keV/u)	2.65	2.97	3.29	3.61	3.93	4.25	4.57	4.89
sσ	$7.26^{-5}$	1.07-4	$1.60^{-4}$	$2.40^{-4}$	$3.55^{-4}$	5.11-4	$7.09^{-4}$	9.48 <sup>-4</sup>
$p\sigma$	$5.62^{-5}$	$7.77^{-5}$	$1.15^{-4}$	$1.77^{-4}$	$2.68^{-4}$	$3.84^{-4}$	$5.21^{-4}$	$6.73^{-4}$
$d\sigma$	$6.06^{-6}$	$1.00^{-5}$	$1.53^{-5}$	$2.23^{-5}$	$3.13^{-5}$	$4.20^{-5}$	$5.37^{-5}$	$6.57^{-5}$
$f\sigma$	$8.53^{-6}$	$1.38^{-5}$	$2.07^{-5}$	$2.93^{-5}$	$3.93^{-5}$	$5.02^{-5}$	$6.15^{-5}$	$7.30^{-5}$
$g\sigma$	$3.70^{-5}$	$5.65^{-5}$	$8.12^{-5}$	$1.11^{-4}$	$1.45^{-4}$	$1.82^{-4}$	$2.22^{-4}$	$2.64^{-4}$
$h\sigma$	$7.64^{-3}$	$9.96^{-3}$	$1.24^{-2}$	$1.51^{-2}$	$1.78^{-2}$	$2.07^{-2}$	$2.36^{-2}$	$2.66^{-2}$
$p\pi$	$5.86^{-4}$	$6.52^{-4}$	$6.59^{-4}$	$6.46^{-4}$	$6.54^{-4}$	$6.91^{-4}$	$7.50^{-4}$	$8.20^{-4}$
$d\pi$	$1.80^{-4}$	$1.99^{-4}$	$2.33^{-4}$	$3.07^{-4}$	$4.32^{-4}$	$5.81^{-4}$	$7.19^{-4}$	$8.25^{-4}$
$f\pi$	$5.24^{-3}$	$5.89^{-3}$	$6.57^{-3}$	$7.26^{-3}$	$7.94^{-3}$	$8.62^{-3}$	$9.29^{-3}$	$9.98^{-3}$
$g\pi$	$6.12^{-4}$	$8.08^{-4}$	$1.04^{-3}$	$1.33^{-3}$	$1.68^{-3}$	$2.09^{-3}$	$2.57^{-3}$	$3.13^{-3}$
$h\pi$	$5.00^{-4}$	$7.77^{-4}$	$1.08^{-3}$	$1.38^{-3}$	$1.69^{-3}$	$2.04^{-3}$	$2.43^{-3}$	$2.90^{-3}$
$\sigma_{ m total}$	$1.49^{-2}$	$1.85^{-2}$	$2.24^{-2}$	$2.66^{-2}$	$3.11^{-2}$	$3.59^{-2}$	$4.09^{-2}$	$4.63^{-2}$
E (keV/u)	5.21	5.53	5.85	6.17	6.49	6.81	7.13	7.45
sσ	1.23-3	1.54-3	$1.90^{-3}$	$2.29^{-3}$	$2.72^{-3}$	$3.20^{-3}$	$3.74^{-3}$	$4.32^{-3}$
$p\sigma$	$8.38^{-4}$	$1.01^{-3}$	$1.20^{-3}$	$1.39^{-3}$	$1.59^{-3}$	$1.79^{-3}$	$2.01^{-3}$	$2.22^{-3}$
$d\sigma$	$7.71^{-5}$	$8.74^{-5}$	$9.66^{-5}$	$1.05^{-4}$	$1.13^{-4}$	$1.20^{-4}$	$1.28^{-4}$	$1.36^{-4}$
$f\sigma$	$8.41^{-5}$	$9.45^{-5}$	$1.04^{-4}$	$1.13^{-4}$	$1.21^{-4}$	$1.28^{-4}$	$1.35^{-4}$	$1.41^{-4}$
$g\sigma$	$3.07^{-4}$	$3.50^{-4}$	$3.93^{-4}$	$4.35^{-4}$	$4.78^{-4}$	$5.19^{-4}$	$5.61^{-4}$	$6.04^{-4}$
$\overset{\circ}{h}\sigma$	$2.97^{-2}$	$3.27^{-2}$	$3.58^{-2}$	$3.89^{-2}$	$4.19^{-2}$	$4.50^{-2}$	$4.80^{-2}$	$5.10^{-2}$
$p\pi$	$8.99^{-4}$	$9.87^{-4}$	$1.09^{-3}$	$1.20^{-3}$	$1.33^{-3}$	$1.47^{-3}$	$1.62^{-3}$	$1.77^{-3}$
$d\pi$	$8.93^{-4}$	$9.24^{-4}$	$9.33^{-4}$	$9.40^{-4}$	$9.73^{-4}$	$1.06^{-3}$	$1.22^{-3}$	$1.48^{-3}$
$f\pi$	$1.07^{-2}$	$1.15^{-2}$	$1.23^{-2}$	$1.33^{-2}$	$1.43^{-2}$	$1.55^{-2}$	$1.68^{-2}$	$1.83^{-2}$
$g\pi$	$3.76^{-3}$	$4.48^{-3}$	$5.27^{-3}$	$6.15^{-3}$	$7.11^{-3}$	$8.15^{-3}$	$9.27^{-3}$	$1.05^{-2}$
$h\pi$	$3.43^{-3}$	$4.03^{-3}$	$4.67^{-3}$	$5.35^{-3}$	$6.05^{-3}$	$6.76^{-3}$	$7.45^{-3}$	$8.14^{-3}$
$\sigma_{ m total}$	$5.19^{-2}$	$5.78^{-2}$	$6.38^{-2}$	$7.01^{-2}$	$7.68^{-2}$	$8.37^{-2}$	$9.09^{-2}$	$9.86^{-2}$
E (keV/u)	7.76	8.08	8.40	8.72	9.04	9.36	9.68	10.00
sσ	$4.98^{-3}$	$5.69^{-3}$	$6.48^{-3}$	$7.34^{-3}$	$8.28^{-3}$	$9.30^{-3}$	$1.04^{-2}$	$1.16^{-2}$
$p\sigma$	$2.44^{-3}$	$2.66^{-3}$	$2.88^{-3}$	$3.10^{-3}$	$3.31^{-3}$	$3.53^{-3}$	$3.73^{-3}$	$3.93^{-3}$
$d\sigma$	$1.45^{-4}$	$1.54^{-4}$	$1.65^{-4}$	$1.76^{-4}$	$1.89^{-4}$	$2.02^{-4}$	$2.16^{-4}$	$2.31^{-4}$
$f\sigma$	$1.47^{-4}$	$1.53^{-4}$	$1.59^{-4}$	$1.66^{-4}$	$1.73^{-4}$	$1.80^{-4}$	$1.89^{-4}$	$1.98^{-4}$
$g\sigma$	$6.48^{-4}$	$6.93^{-4}$	$7.41^{-4}$	$7.91^{-4}$	$8.43^{-4}$	$8.99^{-4}$	$9.58^{-4}$	$1.02^{-3}$
$h\sigma$	$5.40^{-2}$	$5.69^{-2}$	$5.98^{-2}$	$6.27^{-2}$	$6.55^{-2}$	$6.83^{-2}$	$7.11^{-2}$	$7.38^{-2}$
$p\pi$	$1.93^{-3}$	$2.10^{-3}$	$2.28^{-3}$	$2.47^{-3}$	$2.68^{-3}$	$2.92^{-3}$	$3.20^{-3}$	$3.52^{-3}$
1_	$1.86^{-3}$	$2.36^{-3}$	$3.00^{-3}$	$3.78^{-3}$	$4.69^{-3}$	$5.74^{-3}$	$6.91^{-3}$	$8.21^{-3}$
$d\pi$	1.00-2	$2.16^{-2}$	$2.35^{-2}$	$2.56^{-2}$	$2.79^{-2}$	$3.03^{-2}$	$3.29^{-2}$	$3.56^{-2}$
$f\pi$	$1.99^{-2}$	2.10	2.00					
	$1.18^{-2}$	$1.32^{-2}$	$1.46^{-2}$	$1.62^{-2}$	$1.78^{-2}$	$1.95^{-2}$	$2.13^{-2}$	$2.32^{-2}$
$f\pi$	$   \begin{array}{c}     1.99 \\     1.18^{-2} \\     8.80^{-3} \\     1.07^{-1}   \end{array} $	$1.32^{-2}$ $9.43^{-3}$ $1.15^{-1}$	$   \begin{array}{c}     1.46^{-2} \\     1.00^{-2} \\     1.24^{-1}   \end{array} $	$1.62^{-2}  1.06^{-2}  1.33^{-1}$	$   \begin{array}{c}     1.78^{-2} \\     1.11^{-2} \\     1.43^{-1}   \end{array} $	$1.95^{-2}  1.16^{-2}  1.53^{-1}$	$2.13^{-2}$ $1.21^{-2}$ $1.63^{-1}$	$ \begin{array}{c} 2.32^{-2} \\ 1.26^{-2} \\ 1.74^{-1} \end{array} $

in a single impulse, and comes out with a large excess energy. Such a process is analogous to electron capture to continuum in which the projectile transfers a part of its kinetic energy to the target in a constant rate and results free electron with  $\nu_e{\sim}V_p$ .

The ejected electron distributions of the g and u components are shown in Fig. 5, as a function of ejected electron velocity,  $\nu_e$ , and impact parameter, b, at the fixed collision

energy of 10 keV/u. The g and u components are shown in the upper (a) and lower (b) parts, respectively. We can see that the electron distributions tend to peak near  $\nu_e \sim V_p/2$ , i.e., the saddle point electron, but there is no linear relationship to  $V_p$  for electron velocity  $\nu_e$  at the peak. Therefore, the maxima of ionization probabilities cannot be regarded as a saddle-point electron emission.

Tables 4-35 show the differential cross section data as a

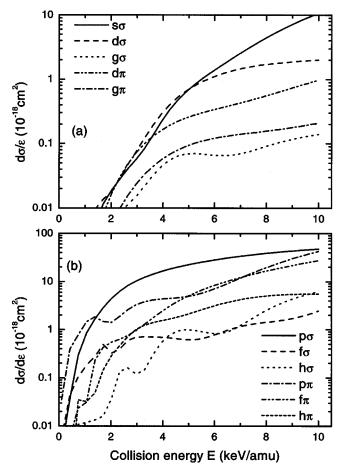


Fig. 3. Same as Fig. 2 except for the ejected electron energy is fixed at  $\epsilon$ =0.01 Ry: (a) g components and (b) u components.

function of partial wave numbers and 32 ejected electron energies (0.01–1 Ry), one table per each of the 32 projectile energies in the range (0.1–10) keV/au.

#### 3.5. Charge Transfer and Target Excitation

Figure 6 shows the cross sections of charge transfer and target excitation along with some earlier theoretical and experimental results. Our results are in good agreement with the experimental results and other rigorous calculations below 6 keV/u. The agreement became less satisfactory as the energy increases above 10 keV/u. Above 10 keV/u, the higher-order corrections of the ETF's become important, and additional discrete states need to be included in the MOCC calculations since there is a uniform increase in the number of weakly coupled channels.

#### 4. Data Evaluation

In the following, we will briefly discuss the differences between the experimental data, especially those that arise in measurements by Shah *et al.*<sup>7</sup> and Pieksma *et al.*,<sup>6</sup> and also the major disagreements of theoretical calculations. An absolute agreement of the present calculations with the measurements of Shah *et al.*<sup>7</sup> is stated here.

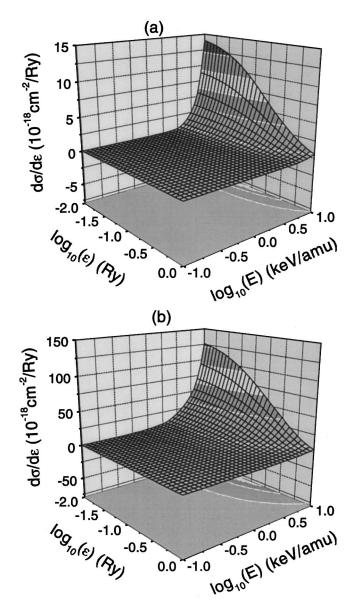


Fig. 4. Single differential ionization cross sections for proton—hydrogen system as a function of ejected electron energy  $\epsilon$  and collision energy E: (a) g components and (b) u components. Numerical values are obtained by present ETF-modified molecular close-coupling calculations with basis

#### 4.1. Experimental Data

The disagreement between the experimental measurements by Pieksma *et al.*<sup>6</sup> and Shah *et al.*<sup>7</sup> is likely to be due to the very different schemes employed by these authors. A crossed-beam method incorporating time-of-flight analysis and coincidence counting of the collision products were used by Shah *et al.*<sup>7</sup> Their cross sections obtained in the energy range 1.25–1500 keV/u were declared with very small experimental uncertainties. In these experiments, a momentum-analyzed beam of protons from an accelerator adjustable in energy (1.25–1500) keV/u was arranged to intersect (at right angles) in a high vacuum region a thermal energy beam of highly dissociated hydrogen. Slow ions and electrons formed

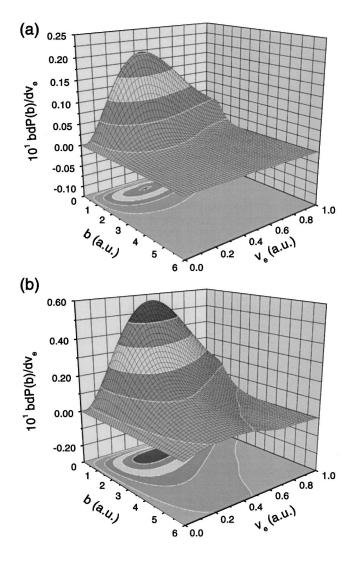


Fig. 5. Ejected electron distribution for proton—hydrogen system as a function of electron velocity,  $v_e$ , and impact parameter, b, at the collision energy  $E\!=\!10~{\rm keV/u:}~(a)~g$  components and (b) u components. Numerical values are obtained by present ETF-modified molecular close-coupling calculations with basis set C.

as collision products in the crossed beam region were extracted by transverse electric field and separately counted by particle multipliers. Product  $H^+$  ions arising from collisions with  $H_2$  or other background gas species were recognized by their characteristic times of flight to multiplier. The required  $H^+$  ions from the ionization process could be distinguished from those arising from the charge transfer process by counting the  $H^+$  ions with the electrons from the same ionizing events.

Experimental studies by Pieksma *et al.*,<sup>6</sup> on the other hand, focused especially on the identification of saddle-point electrons which are to have a half of the collision velocity in the asymptotic space region. They also produced total ionization cross sections at (1–6) keV/u, which were found to follow such characteristic dependence on the collision velocity near the very threshold. In the experiments by Pieksma *et al.*,<sup>6</sup> a pulsed stabilized proton beam was crossed with a

partially dissociated thermal hydrogen beam produced by a rf discharge source. Electrons were detected by means of a magnetic time-of-flight (TOF) spectrometer, which could collect the electrons ejected in the forward hemisphere as long as the approximate transmission condition  $k \sin \vartheta$  $\leq$ 0.42 a.u. was satisfied. Here k is the electron velocity and  $\vartheta$  is the ejection angle with respect to the symmetry axis of the spectrometer. The rf source Pieksma et al.6 used was causing a severe background of slow electrons appearing as a constant term in the recorded TOF distributions, a problem which was dealt with by subtracting the TOF measured with the rf source switched off. However, a complete suppression was considered to be impossible by Pieksma et al.<sup>6</sup> Further, the difference spectrum was also to be corrected for the constant background of uncorrelated rf source electrons. In addition, the electron spectrum of ionizing H<sup>+</sup>-H<sub>2</sub> collisions also had to be corrected for. The total ionization cross sections were then obtained by integration over the ejected electron velocity. This resulted in cross sections two times higher than that of Shah et al. 7 at 6 keV/amu, which also decrease much more rapidly with energy decreasing. The discrepancy between the values of Pieksma et al.<sup>6</sup> and Shah et al.<sup>7</sup> are as large as the factor of  $\sim$ 6 at the lowest energy considered (1 keV/amu).

In summary, the measured data from Shah *et al.*<sup>7</sup> should be recommended for the *total* ionization cross section because in their experiments all electrons and ions were extracted by very reliable methods. Pieksma *et al.*,<sup>6</sup> on the other hand, accurately measured especially the electron velocity distributions. Therefore their low-energy total ionization cross sections are very small—subtracting the background rf electrons from the total signal in this region causes a big problem due to the minor number of electrons produced by the proton-impact ionization.

### 4.2. Theoretical Data

In order to compare theoretical results for the total ionization cross sections of the proton-hydrogen system, refer again to Fig. 1(b), in which various calculations are compared for a broader energy range (0.1-1000) keV/amu. Here, the TICS values from Toshima<sup>10</sup> are 20% higher than the experimental values of Shah et al. 8,9 around E= 100 keV/amu, yet they are in a good agreement in the high energy region. Triple-center close-coupling calculations<sup>7,17</sup> predicted the cross sections at low to intermediate energies to be larger than the high-accuracy measurement data<sup>7,8</sup> up to a factor of 2, and they decrease much faster at collision energies above 50 keV/amu. They are also found to oscillate with collision energies. The continuum distorted wave eikonal initial state (CDW-EIS) approximation, is a high energy theory by Crothers and McCann. 35 The CDW-EIS calculated cross sections are in a good agreement with the measurements by Shah et al. 8,9 for energies above 25 keV/amu. All the above theories predicted TICSs decreasing much more rapidly than our results and the experimental data below 1.5 keV/amu. Within the entire energy region dealt with in the present

TABLE 4. Single differential cross sections (in  $10^{-16} \, \text{cm}^2$ ) at  $E = 0.10 \, \text{keV/amu}$ 

				,				
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$7.80^{-7}$	$7.65^{-7}$	$7.49^{-7}$	$7.30^{-7}$	$7.11^{-7}$	$6.90^{-7}$	$6.70^{-7}$	$6.50^{-7}$
$p\sigma$	$3.32^{-5}$	$3.31^{-5}$	$3.29^{-5}$	$3.27^{-5}$	$3.25^{-5}$	$3.22^{-5}$	$3.20^{-5}$	$3.17^{-5}$
$d\sigma$	$2.31^{-7}$	$2.31^{-7}$	$2.32^{-7}$	$2.33^{-7}$	$2.35^{-7}$	$2.38^{-7}$	$2.43^{-7}$	$2.49^{-7}$
$f\sigma$	$5.73^{-5}$	$5.80^{-5}$	$5.87^{-5}$	$5.94^{-5}$	$5.98^{-5}$	$5.97^{-5}$	$5.85^{-5}$	$5.57^{-5}$
$g\sigma$	$7.38^{-7}$	$7.24^{-7}$	$7.08^{-7}$	$6.91^{-7}$	$6.73^{-7}$	$6.54^{-7}$	$6.36^{-7}$	$6.18^{-7}$
$h\sigma$	$3.29^{-6}$	$3.31^{-6}$	$3.63^{-6}$	$4.35^{-6}$	$5.54^{-6}$	$7.16^{-6}$	$8.94^{-6}$	$1.03^{-5}$
$p\pi$	$3.51^{-4}$	$3.47^{-4}$	$3.43^{-4}$	$3.41^{-4}$	$3.40^{-4}$	$3.42^{-4}$	$3.48^{-4}$	$3.57^{-4}$
$d\pi$	$1.65^{-9}$	$1.65^{-9}$	$1.65^{-9}$	$1.65^{-9}$	$1.64^{-9}$	$1.67^{-9}$	$1.59^{-9}$	$1.54^{-9}$
$f\pi$	$9.95^{-6}$	$1.01^{-5}$	$1.02^{-5}$	$1.03^{-5}$	$1.02^{-5}$	$1.00^{-5}$	$9.58^{-6}$	$8.87^{-6}$
$g\pi$	$1.09^{-10}$	$1.10^{-10}$	$1.10^{-10}$	$1.11^{-10}$	$1.12^{-10}$	$1.12^{-10}$	$1.10^{-10}$	$1.04^{-10}$
$\stackrel{\scriptstyle \circ}{h}\pi$	$3.86^{-7}$	$4.04^{-7}$	$4.25^{-7}$	$4.48^{-7}$	$4.75^{-7}$	$5.03^{-7}$	$5.29^{-7}$	$5.51^{-7}$
<b>ε</b> (Ry)	0.010	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	$6.30^{-7}$	$6.05^{-7}$	$5.72^{-7}$	5.27 <sup>-7</sup>	$4.75^{-7}$	$4.31^{-7}$	$4.04^{-7}$	$3.69^{-7}$
$p\sigma$	$3.14^{-5}$	$3.11^{-5}$	$3.08^{-5}$	$3.03^{-5}$	$2.98^{-5}$	$2.90^{-5}$	$2.81^{-5}$	$2.71^{-5}$
$d\sigma$	$2.57^{-7}$	$2.64^{-7}$	$2.67^{-7}$	$2.65^{-7}$	$2.62^{-7}$	$2.64^{-7}$	$2.74^{-7}$	$2.77^{-7}$
$f\sigma$	$5.14^{-5}$	$4.67^{-5}$	$4.38^{-5}$	$4.50^{-5}$	$4.84^{-5}$	$4.62^{-5}$	$3.60^{-5}$	$3.27^{-5}$
$g\sigma$	$6.01^{-7}$	$5.82^{-7}$	$5.55^{-7}$	$5.17^{-7}$	$4.67^{-7}$	$4.21^{-7}$	$3.89^{-7}$	$3.54^{-7}$
$h\sigma$	$1.03^{-5}$	$8.08^{-6}$	$4.19^{-6}$	$1.34^{-6}$	$2.99^{-6}$	$7.33^{-6}$	$5.76^{-6}$	$6.94^{-7}$
$p\pi$	$3.69^{-4}$	$3.82^{-4}$	$3.91^{-4}$	$3.90^{-4}$	$3.72^{-4}$	$3.35^{-4}$	$2.86^{-4}$	$2.48^{-4}$
$d\pi$	$1.48^{-9}$	$1.41^{-9}$	$1.35^{-9}$	$1.33^{-9}$	$1.34^{-9}$	$1.31^{-9}$	$1.20^{-9}$	$1.10^{-9}$
	$7.85^{-6}$	$6.54^{-6}$	$5.11^{-6}$	$3.88^{-6}$	$3.35^{-6}$	$3.91^{-6}$	$5.43^{-6}$	$6.80^{-6}$
$f\pi$	$9.33^{-11}$	$7.76^{-11}$	$5.11$ $5.99^{-11}$	$4.63^{-11}$	$4.32^{-11}$	$4.96^{-11}$	$5.43$ $5.37^{-11}$	$4.61^{-11}$
$g\pi$	$5.62^{-7}$	$5.55^{-7}$	$5.26^{-7}$	$4.81^{-7}$	$4.32$ $4.39^{-7}$	$4.23^{-7}$	$4.44^{-7}$	$4.84^{-7}$
$h\pi$	3.02	3.33	3.20	4.01	4.39	4.23	4.44	4.04
$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$3.08^{-7}$	$2.62^{-7}$	$2.19^{-7}$	$1.79^{-7}$	$1.43^{-7}$	$1.09^{-7}$	8.33-8	$5.70^{-8}$
$p\sigma$	$2.59^{-5}$	$2.44^{-5}$	$2.28^{-5}$	$2.14^{-5}$	$1.97^{-5}$	$1.72^{-5}$	$1.58^{-5}$	$1.30^{-5}$
$d\sigma$	$2.62^{-7}$	$2.61^{-7}$	$2.53^{-7}$	$2.37^{-7}$	$2.21^{-7}$	$2.05^{-7}$	$1.77^{-7}$	$1.48^{-7}$
$f\sigma$	$3.62^{-5}$	$2.58^{-5}$	$2.91^{-5}$	$1.95^{-5}$	$2.16^{-5}$	$1.61^{-5}$	$1.09^{-5}$	$8.82^{-6}$
$g\sigma$	$2.95^{-7}$	$2.53^{-7}$	$2.12^{-7}$	$1.63^{-7}$	$1.26^{-7}$	$9.33^{-8}$	$6.08^{-8}$	$3.69^{-8}$
$h\sigma$	$6.53^{-6}$	$5.14^{-6}$	$5.47^{-6}$	$6.89^{-6}$	$1.14^{-5}$	$9.68^{-6}$	$1.11^{-5}$	$1.33^{-5}$
$p\pi$	$2.40^{-4}$	$2.50^{-4}$	$2.34^{-4}$	$1.85^{-4}$	$1.67^{-4}$	$1.58^{-4}$	$1.22^{-4}$	$1.12^{-4}$
$d\pi$	$1.10^{-9}$	$1.01^{-9}$	$9.23^{-10}$	$8.79^{-10}$	$7.91^{-10}$	$7.10^{-10}$	$6.61^{-10}$	$6.06^{-10}$
	$6.28^{-6}$	$3.70^{-6}$	$2.35^{-6}$	$4.07^{-6}$	$3.70^{-6}$	$1.60^{-6}$	$2.95^{-6}$	$1.15^{-6}$
$f\pi$	$3.83^{-11}$	$3.70$ $3.37^{-11}$	$2.35^{-11}$	$2.82^{-11}$	$1.98^{-11}$	$1.66^{-11}$	$1.88^{-11}$	$1.62^{-11}$
$g\pi h\pi$	$5.26^{-7}$	$5.45^{-7}$	$4.92^{-7}$	$4.82^{-7}$	$5.10^{-7}$	$4.80^{-7}$	$4.59^{-7}$	$4.29^{-7}$
ε (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ	4.33-8	$3.02^{-8}$	$2.02^{-8}$	1.47-8	1.08-8	8.41 <sup>-9</sup>	6.60-9	5.26 <sup>-9</sup>
$p\sigma$	$1.16^{-5}$	$9.14^{-6}$	$7.15^{-6}$	$5.54^{-6}$	$4.13^{-6}$	$3.06^{-6}$	$2.22^{-6}$	$1.50^{-6}$
$d\sigma$	$1.10^{-7}$	$9.14^{-8}$	$7.13^{-8}$	$5.12^{-8}$	$3.27^{-8}$	$2.02^{-8}$	$1.09^{-8}$	5.43 <sup>-9</sup>
$f\sigma$	$7.10^{-6}$	5.39 <sup>-6</sup>	$3.55^{-6}$	$2.05^{-6}$	$1.32^{-6}$	$8.52^{-7}$	$4.10^{-7}$	$1.57^{-7}$
	$2.03^{-8}$	$9.22^{-9}$	$2.97^{-9}$	$4.25^{-10}$	8.25 <sup>-11</sup>	$6.50^{-10}$	$1.15^{-9}$	$1.37$ $1.29^{-9}$
$g\sigma$	$1.59^{-5}$	$1.60^{-5}$	$1.43^{-5}$	$1.04^{-5}$	8.35 <sup>-6</sup>	$7.37^{-6}$	$5.22^{-6}$	$3.48^{-6}$
$h\sigma$	$8.52^{-5}$	$7.00^{-5}$	$5.57^{-5}$	$4.19^{-5}$	$3.06^{-5}$	$2.15^{-5}$	$1.48^{-5}$	$9.83^{-6}$
$p\pi$	$5.44^{-10}$	$4.86^{-10}$	$4.48^{-10}$	$4.19^{-10}$	$3.06^{-10}$	$3.45^{-10}$	$3.19^{-10}$	$9.83$ $2.92^{-10}$
$d\pi$	1.06=6	$1.09^{-6}$	$5.94^{-7}$	4.07	$3.75^{-10}$ $3.40^{-7}$	$3.45^{-7}$ $3.09^{-7}$	$2.25^{-7}$	$1.51^{-7}$
$f\pi$	$1.86^{-6}$		5.94 '	$4.60^{-7}$	3.40 ' 3.40-11		2.23	1.31
$g\pi$	$1.63^{-11}$	$1.61^{-11}$	$1.81^{-11}$	$2.08^{-11}$	$2.40^{-11}$	$2.77^{-11}$	$3.33^{-11}$	$3.94^{-11}$
$h\pi$	$3.96^{-7}$	$3.40^{-7}$	$2.94^{-7}$	$2.41^{-7}$	$1.89^{-7}$	$1.44^{-7}$	$1.03^{-7}$	$6.89^{-8}$

work, the only consistent agreement between experiment and theory within the measurement error bars is that of the data by Shah  $et\ al.^7$  and the present results.

#### 5. Conclusion

We have computed single-differential, partial, and total ionization cross sections for the proton-hydrogen atom collision system in the energy region of 0.1–10 keV/u. All data are included in numerical and graphical form with this paper.

In a series of tables, we present single differential ionization cross sections resolved with respect to electron angular momentum, energy of the ejected electron, and collision energy of the nuclei. It is found that the upper electronic levels promote ionization for g components, while in the case of u components the upper levels behave as trap for the ionization flux to continuum, especially the excitation to  $2p\pi_u$  state. The present cross sections are in excellent agreement with the recent experiments of Shah  $et\ al.^7$  but decrease more rapidly than the cross sections measured by Pieksma  $et\ al.^6$  with decreasing energy. The numerical data for all cross section-

TABLE 5. Single differential cross sections (in  $10^{-16} \, \text{cm}^2$ ) at  $E = 0.42 \, \text{keV/amu}$ 

			Treferitiar ero.		110 cm )			
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
$s\sigma$	$4.16^{-6}$	$4.11^{-6}$	$4.05^{-6}$	$3.99^{-6}$	$3.91^{-6}$	$3.83^{-6}$	$3.75^{-6}$	$3.65^{-6}$
$p\sigma$	$3.71^{-4}$	$3.64^{-4}$	$3.57^{-4}$	$3.48^{-4}$	$3.38^{-4}$	$3.26^{-4}$	$3.13^{-4}$	$2.98^{-4}$
$d\sigma$	$1.00^{-6}$	$1.02^{-6}$	$1.05^{-6}$	$1.08^{-6}$	$1.11^{-6}$	$1.15^{-6}$	$1.20^{-6}$	$1.26^{-6}$
$f\sigma$	$4.41^{-4}$	$4.33^{-4}$	$4.23^{-4}$	$4.11^{-4}$	$3.96^{-4}$	$3.77^{-4}$	$3.54^{-4}$	$3.26^{-4}$
$g\sigma$	$2.97^{-6}$	$2.91^{-6}$	$2.86^{-6}$	$2.79^{-6}$	$2.73^{-6}$	$2.66^{-6}$	$2.58^{-6}$	$2.51^{-6}$
$h\sigma$	$4.69^{-5}$	$4.61^{-5}$	$4.55^{-5}$	$4.52^{-5}$	$4.57^{-5}$	$4.70^{-5}$	$4.97^{-5}$	$5.42^{-5}$
$p\pi$	$3.93^{-3}$	$3.96^{-3}$	$3.98^{-3}$	$4.02^{-3}$	$4.06^{-3}$	$4.10^{-3}$	$4.16^{-3}$	$4.22^{-3}$
$d\pi$	$2.16^{-8}$	$2.15^{-8}$	$2.14^{-8}$	$2.12^{-8}$	$2.11^{-8}$	$2.07^{-8}$	$2.05^{-8}$	$2.02^{-8}$
$f\pi$	$5.76^{-5}$	$5.79^{-5}$	$5.80^{-5}$	$5.81^{-5}$	$5.79^{-5}$	$5.75^{-5}$	$5.66^{-5}$	$5.51^{-5}$
$g \pi$	$1.31^{-8}$	$1.34^{-8}$	$1.37^{-8}$	$1.41^{-8}$	$1.45^{-8}$	$1.49^{-8}$	$1.53^{-8}$	$1.56^{-8}$
$\stackrel{\circ}{h}\pi$	$2.41^{-6}$	$2.16^{-6}$	$1.89^{-6}$	$1.61^{-6}$	$1.33^{-6}$	$1.06^{-6}$	$8.12^{-7}$	$6.23^{-7}$
ε (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	$3.54^{-6}$	$3.41^{-6}$	$3.26^{-6}$	$3.08^{-6}$	$2.85^{-6}$	$2.57^{-6}$	$2.24^{-6}$	1.91 <sup>-6</sup>
$p\sigma$	$2.81^{-4}$	$2.61^{-4}$	$2.40^{-4}$	$2.16^{-4}$	$1.90^{-4}$	$1.63^{-4}$	$1.36^{-4}$	$1.11^{-4}$
$d\sigma$	$1.32^{-6}$	$1.39^{-6}$	$1.46^{-6}$	$1.51^{-6}$	$1.53^{-6}$	$1.51^{-6}$	$1.42^{-6}$	$1.29^{-6}$
$f\sigma$	$2.94^{-4}$	$2.58^{-4}$	$2.19^{-4}$	$1.82^{-4}$	$1.52^{-4}$	$1.32^{-4}$	$1.24^{-4}$	$1.20^{-4}$
$g\sigma$	$2.43^{-6}$	$2.35^{-6}$	$2.27^{-6}$	$2.18^{-6}$	$2.06^{-6}$	$1.90^{-6}$	$1.69^{-6}$	$1.44^{-6}$
$h\sigma$	$6.08^{-5}$	$6.97^{-5}$	$8.05^{-5}$	$9.17^{-5}$	$1.00^{-4}$	$1.03^{-4}$	$9.57^{-5}$	$8.16^{-5}$
$p\pi$	$4.28^{-3}$	$4.34^{-3}$	$4.38^{-3}$	$4.40^{-3}$	$4.37^{-3}$	$4.26^{-3}$	$4.06^{-3}$	$3.74^{-3}$
$d\pi$	$1.97^{-8}$	$1.91^{-8}$	$1.85^{-8}$	$1.78^{-8}$	$1.71^{-8}$	$1.66^{-8}$	$1.63^{-8}$	$1.62^{-8}$
$f\pi$	$5.29^{-5}$	$4.97^{-5}$	$4.55^{-5}$	$4.04^{-5}$	$3.47^{-5}$	$2.93^{-5}$	$2.55^{-5}$	$2.49^{-5}$
$g\pi$	$1.58^{-8}$	$1.57^{-8}$	$1.54^{-8}$	$1.47^{-8}$	$1.36^{-8}$	$1.21^{-8}$	$1.05^{-8}$	$8.70^{-9}$
$h\pi$	$5.28^{-7}$	$5.72^{-7}$	$8.06^{-7}$	$1.28^{-6}$	$2.01^{-6}$	$2.96^{-6}$	$4.01^{-6}$	$4.93^{-6}$
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$1.65^{-6}$	$1.51^{-6}$	$1.47^{-6}$	$1.38^{-6}$	$1.17^{-6}$	$9.38^{-7}$	$7.20^{-7}$	5.95 <sup>-7</sup>
$p\sigma$	$8.82^{-5}$	$6.97^{-5}$	$5.51^{-5}$	$4.32^{-5}$	$3.27^{-5}$	$2.42^{-5}$	$2.02^{-5}$	$1.91^{-5}$
$d\sigma$	$1.14^{-6}$	$1.05^{-6}$	$1.02^{-6}$	$9.66^{-7}$	$8.84^{-7}$	$8.81^{-7}$	$8.06^{-7}$	$5.98^{-7}$
$f\sigma$	$1.10^{-4}$	$9.10^{-5}$	$8.04^{-5}$	$8.75^{-5}$	$7.92^{-5}$	$5.65^{-5}$	$6.10^{-5}$	$3.41^{-5}$
$g\sigma$	$1.19^{-6}$	$1.02^{-6}$	$8.98^{-7}$	$7.36^{-7}$	$5.11^{-7}$	$3.72^{-7}$	$2.72^{-7}$	$1.49^{-7}$
$h\sigma$	$7.24^{-5}$	$8.48^{-5}$	$1.15^{-4}$	$1.22^{-4}$	$8.50^{-5}$	$9.32^{-5}$	$1.29^{-4}$	$8.03^{-5}$
$p\pi$	$3.34^{-3}$	$2.90^{-3}$	$2.53^{-3}$	$2.32^{-3}$	$2.25^{-3}$	$2.15^{-3}$	$1.87^{-3}$	$1.48^{-3}$
$d\pi$	$1.61^{-8}$	$1.58^{-8}$	$1.52^{-8}$	$1.49^{-8}$	$1.48^{-8}$	$1.43^{-8}$	$1.37^{-8}$	$1.35^{-8}$
$f\pi$	$2.88^{-5}$	$3.66^{-5}$	$4.43^{-5}$	$4.49^{-5}$	$3.33^{-5}$	$1.58^{-5}$	$1.06^{-5}$	$2.16^{-5}$
$g\pi$	$6.82^{-9}$	$4.66^{-9}$	$2.39^{-9}$	$7.10^{-10}$	$1.85^{-10}$	$4.05^{-10}$	$8.12^{-10}$	$7.95^{-10}$
$h\pi$	$5.45^{-6}$	$5.39^{-6}$	$4.78^{-6}$	$3.72^{-6}$	$2.52^{-6}$	$2.03^{-6}$	$2.48^{-6}$	$2.74^{-6}$
<b>ε</b> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ	5.74 <sup>-7</sup>	$4.30^{-7}$	3.48 <sup>-7</sup>	$3.10^{-7}$	$2.38^{-7}$	1.98 <sup>-7</sup>	1.61 <sup>-7</sup>	1.23 <sup>-7</sup>
$p\sigma$	$1.86^{-5}$	$1.77^{-5}$	$1.54^{-5}$	$1.31^{-5}$	$1.03^{-5}$	$8.13^{-6}$	$6.84^{-6}$	$6.07^{-6}$
$d\sigma$	$5.31^{-7}$	$3.97^{-7}$	$2.95^{-7}$	$2.17^{-7}$	$1.45^{-7}$	$8.56^{-8}$	$4.43^{-8}$	$2.34^{-8}$
$f\sigma$	$2.95^{-5}$	$2.18^{-5}$	$1.37^{-5}$	$1.03^{-5}$	$5.80^{-6}$	$3.56^{-6}$	$1.59^{-6}$	$6.47^{-7}$
$g\sigma$	$9.16^{-8}$	$3.77^{-8}$	$1.28^{-8}$	$2.36^{-9}$	$7.95^{-10}$	$2.92^{-9}$	$4.87^{-9}$	$5.76^{-9}$
$h\sigma$	$1.09^{-4}$	$7.49^{-5}$	$6.61^{-5}$	$6.23^{-5}$	$4.73^{-5}$	$3.30^{-5}$	$2.46^{-5}$	$1.42^{-5}$
$p\pi$	$1.24^{-3}$	$1.07^{-3}$	$8.01^{-4}$	$6.27^{-4}$	$4.58^{-4}$	$3.33^{-4}$	$2.26^{-4}$	$1.51^{-4}$
$d\pi$	$1.29^{-8}$	$1.26^{-8}$	$1.22^{-8}$	$1.16^{-8}$	$1.11^{-8}$	$1.05^{-8}$	$9.92^{-9}$	$9.23^{-9}$
$f\pi$	$2.15^{-5}$	$7.11^{-6}$	$1.09^{-5}$	$7.37^{-6}$	$5.57^{-6}$	$3.19^{-6}$	$3.37^{-6}$	$2.15^{-6}$
$g \pi$	$3.03^{-10}$	$1.16^{-10}$	$2.24^{-10}$	$1.37^{-10}$	$1.85^{-10}$	$1.83^{-10}$	$2.38^{-10}$	$2.97^{-10}$
$\stackrel{\circ}{h}\pi$	$2.51^{-6}$	$2.09^{-6}$	$1.83^{-6}$	$1.55^{-6}$	$1.25^{-6}$	$9.44^{-7}$	$6.86^{-7}$	$4.62^{-7}$
7. 11	2.51	2.07	1.05	1.55	1.23	7.77	0.00	7.02

spresented here were obtained with a semiclassical molecular-orbital close-coupling method using the electron translation factor. This method provides all measurable quantities in the real coordinate space before the total ionization cross sections can be finally calculated.

Previous experimental and theoretical methods were critically evaluated throughout the manuscript, especially in Sec. 4. For the total ionization cross sections, the data by Shah *et al.*<sup>7</sup> are recommended. Experimental data reported by Pieksma *et al.*<sup>6</sup> provide valuable insight, especially into the

velocity distributions of ionized electrons. Hidden-crossing calculations yield different results based on the promotion mechanisms considered. Also the previous close-coupling calculations differed based on the number of expansion centers and did not exhibit a fully satisfactory agreement with the experiments. Within the energy region of 100-10 keV/u considered here, the only consistent agreement between experiment and theory until present is that of the data by Shah *et al.*<sup>7</sup> and our results. The state-resolved differential cross sections are reported for the first time, in this detail.

TABLE 6. Single differential cross sections (in  $10^{-16} \, \text{cm}^2$ ) at  $E = 0.74 \, \text{keV/amu}$ 

					•	<u> </u>		
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$1.15^{-5}$	$1.14^{-5}$	$1.12^{-5}$	$1.11^{-5}$	$1.09^{-5}$	$1.07^{-5}$	$1.05^{-5}$	$1.02^{-5}$
$p\sigma$	$2.93^{-3}$	$2.89^{-3}$	$2.84^{-3}$	$2.79^{-3}$	$2.73^{-3}$	$2.66^{-3}$	$2.58^{-3}$	$2.48^{-3}$
$d\sigma$	$3.76^{-6}$	$3.67^{-6}$	$3.58^{-6}$	$3.47^{-6}$	$3.34^{-6}$	$3.21^{-6}$	$3.06^{-6}$	$2.90^{-6}$
$f\sigma$	$1.06^{-3}$	$1.04^{-3}$	$1.02^{-3}$	$9.94^{-4}$	$9.66^{-4}$	$9.33^{-4}$	$8.95^{-4}$	$8.50^{-4}$
$g\sigma$	$5.98^{-6}$	$5.87^{-6}$	$5.74^{-6}$	$5.59^{-6}$	$5.42^{-6}$	$5.22^{-6}$	$4.99^{-6}$	$4.72^{-6}$
$\overset{\circ}{h}\sigma$	$1.08^{-4}$	$1.07^{-4}$	$1.06^{-4}$	$1.05^{-4}$	$1.03^{-4}$	$1.01^{-4}$	$9.84^{-5}$	$9.52^{-5}$
$p\pi$	$7.76^{-3}$	$7.80^{-3}$	$7.84^{-3}$	$7.89^{-3}$	$7.95^{-3}$	$8.02^{-3}$	$8.10^{-3}$	$8.18^{-3}$
$d\pi$	$1.15^{-7}$	$1.13^{-7}$	$1.10^{-7}$	$1.08^{-7}$	$1.05^{-7}$	$1.02^{-7}$	$9.92^{-8}$	$9.59^{-8}$
$f\pi$	$2.36^{-4}$	$2.38^{-4}$	$2.39^{-4}$	$2.41^{-4}$	$2.41^{-4}$	$2.42^{-4}$	$2.41^{-4}$	$2.39^{-4}$
	$6.13^{-7}$	$5.99^{-7}$	$5.84^{-7}$	$5.66^{-7}$	$5.46^{-7}$	$5.23^{-7}$	$4.97^{-7}$	$4.68^{-7}$
$g\pi h\pi$	$3.49^{-4}$	$3.47^{-4}$	$3.45^{-4}$	$3.42^{-4}$	$3.38^{-4}$	$3.23$ $3.34^{-4}$	$3.29^{-4}$	$3.23^{-4}$
	3.49	3.47	3.43	3.42	3.36	3.34	3.29	3.23
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	$9.98^{-6}$	$9.73^{-6}$	$9.49^{-6}$	$9.28^{-6}$	$9.09^{-6}$	8.93 <sup>-6</sup>	$8.77^{-6}$	$8.54^{-6}$
$p\sigma$	$2.38^{-3}$	$2.27^{-3}$	$2.14^{-3}$	$2.01^{-3}$	$1.86^{-3}$	$1.71^{-3}$	$1.56^{-3}$	$1.40^{-3}$
$d\sigma$	$2.73^{-6}$	$2.57^{-6}$	$2.42^{-6}$	$2.31^{-6}$	$2.26^{-6}$	$2.30^{-6}$	$2.44^{-6}$	$2.68^{-6}$
$f\sigma$	$8.00^{-4}$	$7.43^{-4}$	$6.82^{-4}$	$6.18^{-4}$	$5.55^{-4}$	$4.97^{-4}$	$4.48^{-4}$	$4.10^{-4}$
$g\sigma$	$4.43^{-6}$	$4.12^{-6}$	$3.80^{-6}$	$3.48^{-6}$	$3.20^{-6}$	$2.96^{-6}$	$2.79^{-6}$	$2.65^{-6}$
$h\sigma$	$9.15^{-5}$	$8.74^{-5}$	$8.33^{-5}$	$7.98^{-5}$	$7.76^{-5}$	$7.75^{-5}$	$7.91^{-5}$	$8.02^{-5}$
$p\pi$	$8.28^{-3}$	$8.37^{-3}$	$8.45^{-3}$	$8.51^{-3}$	$8.52^{-3}$	$8.46^{-3}$	$8.29^{-3}$	$7.97^{-3}$
$d\pi$	$9.25^{-8}$	$8.90^{-8}$	$8.55^{-8}$	$8.20^{-8}$	$7.85^{-8}$	$7.50^{-8}$	$7.15^{-8}$	$6.81^{-8}$
$f\pi$	$2.35^{-4}$	$2.28^{-4}$	$2.18^{-4}$	$2.03^{-4}$	$1.83^{-4}$	$1.57^{-4}$	$1.27^{-4}$	$9.52^{-5}$
$g\pi$	$4.35^{-7}$	$3.99^{-7}$	$3.60^{-7}$	$3.18^{-7}$	$2.74^{-7}$	$2.30^{-7}$	$1.88^{-7}$	$1.50^{-7}$
$\stackrel{\circ}{h}\pi$	$3.15^{-4}$	$3.05^{-4}$	$2.93^{-4}$	$2.78^{-4}$	$2.59^{-4}$	$2.36^{-4}$	$2.09^{-4}$	$1.79^{-4}$
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$8.14^{-6}$	$7.47^{-6}$	$6.57^{-6}$	$5.62^{-6}$	$4.86^{-6}$	$4.37^{-6}$	$4.03^{-6}$	$3.75^{-6}$
$p\sigma$	$1.24^{-3}$	$1.08^{-3}$	$9.24^{-4}$	$7.63^{-4}$	$5.96^{-4}$	$4.32^{-4}$	$2.87^{-4}$	$1.83^{-4}$
$d\sigma$	$2.97^{-6}$	$3.22^{-6}$	$3.30^{-6}$	$3.15^{-6}$	$2.81^{-6}$	$2.25^{-6}$	$1.45^{-6}$	$9.31^{-7}$
$f\sigma$	$3.80^{-4}$	$3.49^{-4}$	$3.12^{-4}$	$2.69^{-4}$	$2.20^{-4}$	$1.60^{-4}$	$9.33^{-5}$	$5.80^{-5}$
$g\sigma$	$2.46^{-6}$	$2.14^{-6}$	$1.67^{-6}$	$1.19^{-6}$	$9.03^{-7}$	$7.67^{-7}$	$5.26^{-7}$	$2.69^{-7}$
$h\sigma$	$7.75^{-5}$	$7.05^{-5}$	$7.03^{-5}$	$9.57^{-5}$	$1.38^{-4}$	$1.34^{-4}$	$8.54^{-5}$	$1.03^{-4}$
$p\pi$	$7.49^{-3}$	$6.87^{-3}$	$6.17^{-3}$	$5.51^{-3}$	$5.00^{-3}$	$4.70^{-3}$	$4.45^{-3}$	$4.03^{-3}$
$d\pi$	$6.47^{-8}$	$6.16^{-8}$	$5.88^{-8}$	$5.63^{-8}$	$5.36^{-8}$	$5.11^{-8}$	$5.02^{-8}$	$5.03^{-8}$
$f\pi$	$6.48^{-5}$	$4.16^{-5}$	$3.03^{-5}$	$3.16^{-5}$	$3.90^{-5}$	$4.07^{-5}$	$3.01^{-5}$	$1.77^{-5}$
$g \pi$	$1.17^{-7}$	$9.23^{-8}$	$7.44^{-8}$	$6.21^{-8}$	$5.22^{-8}$	$4.13^{-8}$	$2.77^{-8}$	$1.36^{-8}$
$\overset{\circ}{h}\pi$	$1.46^{-4}$	$1.13^{-4}$	$8.22^{-5}$	$5.78^{-5}$	$4.23^{-5}$	$3.68^{-5}$	$3.82^{-5}$	$3.83^{-5}$
<b>ε</b> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ	3.38-6	$2.75^{-6}$	$2.36^{-6}$	2.11-6	$1.70^{-6}$	$1.42^{-6}$	1.13 <sup>-6</sup>	8.96 <sup>-7</sup>
$p\sigma$	$1.21^{-4}$	$7.93^{-5}$	$4.84^{-5}$	$3.42^{-5}$	$2.89^{-5}$	$2.36^{-5}$	$1.63^{-5}$	$1.02^{-5}$
$d\sigma$	$1.01^{-6}$	$8.65^{-7}$	$6.16^{-7}$	$3.26^{-7}$	$2.64^{-7}$	$1.55^{-7}$	$8.55^{-8}$	$4.24^{-8}$
$f\sigma$	$5.38^{-5}$	$4.11^{-5}$	$2.84^{-5}$	$1.97^{-5}$	$1.04^{-5}$	$9.01^{-6}$	$2.90^{-6}$	$1.88^{-6}$
$g\sigma$	$1.77^{-7}$	$7.47^{-8}$	$3.09^{-8}$	$6.95^{-9}$	$3.31^{-9}$	$6.51^{-9}$	$1.00^{-8}$	$1.07^{-8}$
$h\sigma$	$1.14^{-4}$	$1.09^{-4}$	$9.58^{-5}$	$9.53^{-5}$	$7.89^{-5}$	$6.22^{-5}$	$4.47^{-5}$	$3.53^{-5}$
$p\pi$	$3.36^{-3}$	$2.73^{-3}$	$2.29^{-3}$	$1.83^{-3}$	$1.36^{-3}$	$1.02^{-3}$	$7.06^{-4}$	$4.81^{-4}$
$d\pi$	$4.87^{-8}$	$4.64^{-8}$	$4.44^{-8}$	$4.33^{-8}$	$4.09^{-8}$	$3.89^{-8}$	$3.65^{-8}$	$3.40^{-8}$
$f\pi$	$2.10^{-5}$	$3.07^{-5}$	$2.08^{-5}$	$1.03^{-5}$	$1.58^{-5}$	$7.57^{-6}$	$7.83^{-6}$	$3.92^{-6}$
	$4.24^{-9}$	$1.14^{-9}$	$1.71^{-9}$	$1.66^{-9}$	$3.97^{-10}$	$4.42^{-10}$	$3.58^{-10}$	$4.80^{-10}$
$g\pi$	$3.21^{-5}$	$2.21^{-5}$	$1.71$ $1.41^{-5}$	$1.00^{-5}$	$8.29^{-6}$	$5.22^{-6}$	$3.45^{-6}$	$2.09^{-6}$
$h \pi$	3.41	2.21	1.41	1.10	0.29	3.22	5.43	2.09

## 6. Acknowledgments

Support by a Grant-in-Aid of the Japan Society for the Promotion of Science (JSPS) for young scientists is hereby gratefully acknowledged (L.P.). One of us (S.Z.) would like to thank the Japanese Government for the award of a scholarship to support his study in Japan. This work was supported in part by the Ministry of Education, Science, Sport, Culture and Technology, JSPS, and the National Institute for Fusion Science (L.P. and M.K.).

## 7. Appendix A: One-Electron Diatomic-Molecule Orbitals

The Hamiltonian of one electron moving in the field of two fixed charges  $Z_A$  and  $Z_B$  is given as

$$h_{\rm el} = -\frac{1}{2m} \nabla_r^2 - \frac{Z_A}{r_A} - \frac{Z_B}{r_B}.$$
 (A1)

Table 7. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=1.06\,\mathrm{keV/amu}$ 

Table 8. Single differential cross sections (in  $10^{-16} \,\mathrm{cm}^2$ ) at  $E = 1.38 \,\mathrm{keV/amu}$ 

										1.501	xc v/airia							
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\overline{\epsilon}$ (	(Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ				$2.62^{-5}$			$2.50^{-5}$	$2.45^{-5}$	S	$s\sigma$	$5.41^{-5}$	$5.40^{-5}$	$5.38^{-5}$	5.37-5	$5.36^{-5}$	$5.35^{-5}$	5.34-5	5.33 <sup>-5</sup>
$p\sigma$	$8.44^{-3}$	$8.36^{-3}$	$8.26^{-3}$	$8.16^{-3}$	$8.04^{-3}$	$7.90^{-3}$	$7.73^{-3}$	$7.54^{-3}$	Į.	$p\sigma$	$1.66^{-2}$	$1.65^{-2}$	$1.63^{-2}$	$1.61^{-2}$	$1.58^{-2}$	$1.55^{-2}$	$1.52^{-2}$	$1.49^{-2}$
$d\sigma$						$3.07^{-5}$			a	$d\sigma$	$9.55^{-5}$						$9.07^{-5}$	
$f\sigma$	$1.81^{-3}$	$1.80^{-3}$	$1.79^{-3}$	$1.77^{-3}$	$1.76^{-3}$	$1.75^{-3}$	$1.73^{-3}$	$1.71^{-3}$	f	$f\sigma$	$2.77^{-3}$	$2.70^{-3}$	$2.63^{-3}$	$2.55^{-3}$	$2.45^{-3}$	$2.35^{-3}$	$2.23^{-3}$	$2.11^{-3}$
$g\sigma$						$1.11^{-5}$			9	$g\sigma$							$1.06^{-5}$	
$h\sigma$	$1.19^{-4}$	$1.23^{-4}$	$1.27^{-4}$	$1.32^{-4}$	$1.38^{-4}$	$1.45^{-4}$	$1.53^{-4}$	$1.62^{-4}$		$h\sigma$	$1.33^{-4}$	$1.33^{-4}$	$1.34^{-4}$	$1.34^{-4}$	$1.34^{-4}$	$1.34^{-4}$	$1.34^{-4}$	$1.34^{-4}$
$p\pi$	$1.46^{-2}$	$1.44^{-2}$	$1.42^{-2}$	$1.39^{-2}$	$1.36^{-2}$	$1.33^{-2}$	$1.29^{-2}$	$1.24^{-2}$		υπ	$1.85^{-2}$	$1.85^{-2}$	$1.85^{-2}$	$1.84^{-2}$	$1.84^{-2}$	$1.83^{-2}$	$1.82^{-2}$	$1.81^{-2}$
$d\pi$						$2.33^{-6}$			a	$d\pi$	$1.28^{-5}$	$1.25^{-5}$	$1.22^{-5}$	$1.18^{-5}$	$1.14^{-5}$	$1.10^{-5}$	$1.05^{-5}$	$9.93^{-6}$
$f\pi$	$3.14^{-4}$	$2.92^{-4}$	$2.68^{-4}$	$2.43^{-4}$	$2.16^{-4}$	$1.89^{-4}$	$1.62^{-4}$	$1.36^{-4}$	f	$f\pi$	$2.29^{-3}$	$2.23^{-3}$	$2.15^{-3}$	$2.07^{-3}$	$1.97^{-3}$	$1.86^{-3}$	$1.74^{-3}$	$1.60^{-3}$
$g\pi$						$1.12^{-5}$			,	$g\pi$	$3.41^{-5}$	$3.39^{-5}$	$3.36^{-5}$	$3.33^{-5}$	$3.30^{-5}$	$3.27^{-5}$	$3.23^{-5}$	$3.19^{-5}$
$\stackrel{\circ}{h}\pi$						$3.18^{-4}$				$h\pi$	$4.82^{-4}$	$4.69^{-4}$	$4.53^{-4}$	$4.37^{-4}$	$4.19^{-4}$	$4.00^{-4}$	$3.79^{-4}$	$3.58^{-4}$
$\epsilon$ (Ry)		0.038	0.044		0.059	0.069	0.080	0.093	$\epsilon$ (	(Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$	$2.40^{-5}$			$2.20^{-5}$					S	$s\sigma$	$5.33^{-5}$			$5.35^{-5}$				
$p\sigma$						$5.71^{-3}$			Į.	$p\sigma$							$1.10^{-2}$	
$d\sigma$	$3.08^{-5}$	$3.09^{-5}$	$3.10^{-5}$	$3.12^{-5}$	$3.13^{-5}$	$3.14^{-5}$	$3.12^{-5}$	$3.05^{-5}$	a	$d\sigma$	$8.75^{-5}$	$8.53^{-5}$	$8.27^{-5}$	$7.95^{-5}$	$7.58^{-5}$	$7.15^{-5}$	$6.66^{-5}$	$6.13^{-5}$
$f\sigma$						$1.49^{-3}$			f	$f\sigma$							$1.18^{-3}$	
$g\sigma$						$6.77^{-6}$			8	$g\sigma$							$7.48^{-6}$	
$h\sigma$						$1.94^{-4}$			h	$h\sigma$							$1.14^{-4}$	
$p\pi$						$9.33^{-3}$			P	$p\pi$							$1.49^{-2}$	
$d\pi$	$1.96^{-6}$	$1.82^{-6}$	$1.67^{-6}$	$1.51^{-6}$	$1.34^{-6}$	$1.17^{-6}$	$1.01^{-6}$	$8.41^{-7}$	a	$d\pi$	$9.34^{-6}$	$8.71^{-6}$	$8.05^{-6}$	$7.35^{-6}$	$6.62^{-6}$	$5.88^{-6}$	$5.14^{-6}$	$4.41^{-6}$
$f\pi$						$1.10^{-4}$			f	$f\pi$	$1.45^{-3}$	$1.28^{-3}$	$1.11^{-3}$	$9.19^{-4}$	$7.27^{-4}$	$5.41^{-4}$	$3.70^{-4}$	$2.27^{-4}$
$g \pi$						$8.70^{-6}$			8	$g \pi$							$2.78^{-5}$	
$h\pi$	$3.21^{-4}$	$3.24^{-4}$	$3.28^{-4}$	$3.33^{-4}$	$3.37^{-4}$	$3.40^{-4}$	$3.39^{-4}$	$3.33^{-4}$	h	$h\pi$	$3.37^{-4}$	$3.15^{-4}$	$2.95^{-4}$	$2.76^{-4}$	$2.60^{-4}$	$2.46^{-4}$	$2.36^{-4}$	$2.28^{-4}$
									_									
$\epsilon$ (Ry)		0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (	(Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$	$1.83^{-5}$	$1.76^{-5}$	$1.68^{-5}$	$1.59^{-5}$	$1.47^{-5}$	$1.31^{-5}$	$1.14^{-5}$	$1.01^{-5}$	S	$s\sigma$	$5.15^{-5}$	$4.91^{-5}$	$4.56^{-5}$	$4.12^{-5}$	$3.64^{-5}$	$3.21^{-5}$	$2.86^{-5}$	$2.60^{-5}$
$p\sigma$	$4.26^{-3}$	$3.74^{-3}$	$3.22^{-3}$	$2.71^{-3}$	$2.23^{-3}$	$1.78^{-3}$	$1.34^{-3}$	$9.42^{-4}$	Ľ	$p\sigma$	$9.26^{-3}$	$8.29^{-3}$	$7.25^{-3}$	$6.17^{-3}$	$5.10^{-3}$	$4.08^{-3}$	$3.19^{-3}$	$2.45^{-3}$
$d\sigma$	$2.91^{-5}$	$2.68^{-5}$	$2.33^{-5}$	$1.89^{-5}$	$1.41^{-5}$	$9.59^{-6}$	$6.37^{-6}$	$5.19^{-6}$	a	$d\sigma$	$5.59^{-5}$	$5.08^{-5}$	$4.66^{-5}$	$4.37^{-5}$	$4.18^{-5}$	$3.98^{-5}$	$3.54^{-5}$	$2.72^{-5}$
$f\sigma$	$1.12^{-3}$	$9.28^{-4}$	$7.52^{-4}$	$6.32^{-4}$	$5.70^{-4}$	$4.90^{-4}$	$3.20^{-4}$	$1.52^{-4}$	f	$f\sigma$	$1.08^{-3}$	$1.06^{-3}$	$1.05^{-3}$	$1.03^{-3}$	$9.73^{-4}$	$8.66^{-4}$	$6.86^{-4}$	$4.53^{-4}$
$g\sigma$	$3.59^{-6}$	$2.79^{-6}$	$2.27^{-6}$	$1.95^{-6}$	$1.64^{-6}$	$1.26^{-6}$	$9.08^{-7}$	$6.27^{-7}$	و	gσ	$7.02^{-6}$	$6.39^{-6}$	$5.25^{-6}$	$3.65^{-6}$	$2.06^{-6}$	$1.05^{-6}$	$7.45^{-7}$	$5.96^{-7}$
$h\sigma$						$1.35^{-4}$			ĥ	$h\sigma$	$1.26^{-4}$	$1.41^{-4}$	$1.51^{-4}$	$1.47^{-4}$	$1.37^{-4}$	$1.54^{-4}$	$2.03^{-4}$	$2.00^{-4}$
$p\pi$	$8.47^{-3}$	$8.47^{-3}$	$8.58^{-3}$	$8.66^{-3}$	$8.52^{-3}$	$8.02^{-3}$	$7.13^{-3}$	$6.09^{-3}$	Į	$p\pi$	$1.28^{-2}$	$1.17^{-2}$	$1.06^{-2}$	$9.78^{-3}$	$9.23^{-3}$	$8.97^{-3}$	$8.81^{-3}$	$8.45^{-3}$
$d\pi$	$6.87^{-7}$	$5.47^{-7}$	$4.26^{-7}$	$3.29^{-7}$	$2.57^{-7}$	$2.07^{-7}$	$1.73^{-7}$	$1.46^{-7}$	a	$d\pi$	$3.69^{-6}$	$3.01^{-6}$	$2.37^{-6}$	$1.81^{-6}$	$1.34^{-6}$	$9.70^{-7}$	$7.16^{-7}$	$5.51^{-7}$
$f\pi$	$2.21^{-4}$	$2.49^{-4}$	$2.52^{-4}$	$2.23^{-4}$	$1.65^{-4}$	$9.51^{-5}$	$4.50^{-5}$	$3.29^{-5}$	f	$f\pi$							$2.02^{-4}$	
$g\pi$	$6.03^{-6}$	$4.91^{-6}$	$3.75^{-6}$	$2.67^{-6}$	$1.76^{-6}$	$1.10^{-6}$	$7.06^{-7}$	$4.86^{-7}$	و	$g\pi$	$2.52^{-5}$	$2.33^{-5}$	$2.07^{-5}$	$1.74^{-5}$	$1.36^{-5}$	$9.60^{-6}$	$5.98^{-6}$	$3.30^{-6}$
$\stackrel{\circ}{h}\pi$	$3.19^{-4}$	$2.95^{-4}$	$2.59^{-4}$	$2.11^{-4}$	$1.57^{-4}$	$1.02^{-4}$	$5.60^{-5}$	$2.75^{-5}$		$h\pi$	$2.22^{-4}$	$2.15^{-4}$	$2.05^{-4}$	$1.89^{-4}$	$1.65^{-4}$	$1.32^{-4}$	$9.43^{-5}$	$5.65^{-5}$
$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (	(Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ	9.42-6	8.77-6	$7.62^{-6}$	$6.35^{-6}$	$5.50^{-6}$	$4.61^{-6}$	$3.66^{-6}$	2.93-6		sσ	$2.41^{-5}$	$2.22^{-5}$	1.92-5	$1.59^{-5}$	$1.35^{-5}$	$1.14^{-5}$	$9.05^{-6}$	$7.19^{-6}$
$p\sigma$	$6.28^{-4}$	$4.10^{-4}$	$2.52^{-4}$	$1.28^{-4}$	$6.69^{-5}$	$4.63^{-5}$	$3.38^{-5}$			$p\sigma$	$1.81^{-3}$	$1.24^{-3}$	$7.50^{-4}$	$4.11^{-4}$	$2.28^{-4}$	$1.16^{-4}$	$5.65^{-5}$	$3.86^{-5}$
$d\sigma$	5.30-6	$4.30^{-6}$	$2.06^{-6}$	7.67-7	$6.01^{-7}$	$3.38^{-7}$	$1.17^{-7}$			$d\sigma$	$1.70^{-5}$	$9.19^{-6}$	5.71 <sup>-6</sup>	$4.62^{-6}$	$2.56^{-6}$	$6.82^{-7}$	$3.59^{-7}$	$1.45^{-7}$
fσ	$1.02^{-4}$	8 43-5	$6.91^{-5}$	$3.07^{-5}$	$1.53^{-5}$	$9.09^{-6}$	$7.62^{-6}$	$2.73^{-6}$		fσ	$2.66^{-4}$	$1.92^{-4}$	$1.33^{-4}$	$6.01^{-5}$	$3.46^{-5}$	$1.87^{-5}$	$5.73^{-6}$	$3.09^{-6}$
$g\sigma$						$7.98^{-9}$			J	gσ	$3.26^{-7}$	$2.40^{-7}$					$2.19^{-8}$	
$h\sigma$						$6.89^{-5}$				$h\sigma$	$1.43^{-4}$	$2.04^{-4}$					$6.10^{-5}$	
$p\pi$	$5.24^{-3}$	$4.65^{-3}$	$4.04^{-3}$	$3.23^{-3}$	$2.50^{-3}$	$1.93^{-3}$	$1.38^{-3}$	$9.65^{-4}$		$p\pi$	$7.65^{-3}$	$6.51^{-3}$	$5.43^{-3}$	$4.61^{-3}$	$3.80^{-3}$	$2.90^{-3}$	$2.17^{-3}$	$1.55^{-3}$
$d\pi$	$1.22^{-7}$	$1.04^{-7}$	$9.50^{-8}$	$9.06^{-8}$	$8.49^{-8}$	$7.88^{-8}$	$7.47^{-8}$	$6.83^{-8}$		$d\pi$	$4.34^{-7}$	$3.40^{-7}$	$2.73^{-7}$	$2.42^{-7}$	$2.20^{-7}$	$1.91^{-7}$	$1.70^{-7}$	$1.53^{-7}$
$f\pi$						$1.16^{-5}$				a f π							$1.84^{-5}$	
gπ						$1.03^{-8}$			,	, gπ							$2.18^{-8}$	
$\overset{\circ}{h}\pi$						$4.91^{-6}$				$h\pi$							$1.78^{-6}$	
	00							2.00	,,	•••								

In the prolate spheroidal coordinates, the corresponding Schrödinger equation is separable, and we obtain for the wave function components

$$\[ \frac{d^2}{d\phi^2} - \mu^2 \] \Omega(\phi) = 0, \tag{A2}$$

$$\[ \frac{d^2}{d\xi} (\xi^2 - 1) \frac{d}{d\xi} - \frac{\mu^2}{\xi^2 - 1} + RZ_+ \xi - c^2 (\xi^2 - 1) + A \] X(\xi, R)$$

$$= 0, \tag{A3}$$

$$\[ \frac{d^2}{d\eta} (1 - \eta^2) \frac{d}{d\eta} - \frac{\mu^2}{1 - \eta^2} + RZ_+ \eta - c^2 (1 - \eta^2) - A \] \times Y(\eta, R) = 0, \tag{A4}$$

where c is the energy parameter, i.e.,  $\epsilon=-2c^2/R^2$  (discrete state) or  $\epsilon=2c^2/R^2$  (continuum state),  $Z_+$  and  $Z_-$  are charge parameters given by  $Z_+=Z_B+Z_A$  and  $Z_-=Z_B-Z_A$ . Here  $\mu$ 

Table 9. Single differential cross sections (in  $10^{-16} \, \text{cm}^2$ ) at  $E = 1.70 \, \text{keV/amu}$ 

Table 10. Single differential cross sections (in  $10^{-16} \,\mathrm{cm}^2$ ) at  $E = 2.02 \,\mathrm{keV/amu}$ 

=1.70	ke V/amu								= 2.02	keV/amu	l						
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ				$1.14^{-4}$					$s\sigma$		$1.88^{-4}$						$1.74^{-4}$
$p\sigma$				$2.76^{-2}$					$p\sigma$		$4.39^{-2}$						
$d\sigma$				$1.38^{-4}$					$d\sigma$		$1.76^{-4}$						
$f\sigma$	$4.91^{-3}$	$4.90^{-3}$	$4.88^{-3}$	$4.86^{-3}$	$4.84^{-3}$	$4.81^{-3}$	$4.77^{-3}$	$4.72^{-3}$	$f\sigma$	$3.22^{-3}$	$3.20^{-3}$	$3.19^{-3}$	$3.18^{-3}$	$3.16^{-3}$	$3.14^{-3}$	$3.12^{-3}$	$3.11^{-3}$
$g\sigma$				$7.93^{-6}$					$g\sigma$		$2.85^{-5}$						
$h\sigma$	$1.60^{-4}$	$1.59^{-4}$	$1.59^{-4}$	$1.60^{-4}$	$1.62^{-4}$	$1.64^{-4}$	$1.69^{-4}$	$1.75^{-4}$	$h\sigma$	$3.71^{-4}$	$3.57^{-4}$	$3.41^{-4}$	$3.25^{-4}$	$3.08^{-4}$	$2.91^{-4}$	$2.73^{-4}$	$2.57^{-4}$
$p\pi$				$1.49^{-2}$					$p\pi$		$1.41^{-2}$						
$d\pi$				$2.83^{-5}$					$d\pi$		$5.65^{-5}$						
$f\pi$	4.26	4.21	4.14	$4.07^{-3}$ $7.74^{-5}$	3.98	3.88	3.76	3.62	$f\pi$	5.44	$5.42^{-3}$ $1.66^{-4}$	5.38	5.34	5.29	5.23	5.15	5.06
$g\pi$				$1.34^{-3}$					$g\pi$		$2.80^{-3}$						
$-h\pi$	1.40	1.43	1.39	1.34	1.29	1.24	1.18	1.12	$-h\pi$	2.85	2.80	2.75	2.08	2.01	2.55	2.45	2.33
<b>ε</b> (Ry)			0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)		0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$				$9.50^{-5}$			$8.36^{-5}$		$s\sigma$		$1.67^{-4}$						$1.38^{-4}$
$p\sigma$				$2.20^{-2}$					$p\sigma$		$3.70^{-2}$						
$d\sigma$				$1.39^{-4}$					$d\sigma$		$1.73^{-4}$						
$f\sigma$				$4.34^{-3}$					$f\sigma$		$3.07^{-3}$						
$g\sigma$				$9.57^{-6}$					$g\sigma$		$1.39^{-5}$						
$h\sigma$	1.84-4	1.98-4	$2.15^{-4}$	$2.38^{-4}$	$2.66^{-4}$	2.98-4	$3.30^{-4}$	$3.56^{-4}$	$h\sigma$	$2.42^{-4}$	$2.30^{-4}$	$2.22^{-4}$	$2.19^{-4}$	2.23-4	$2.37^{-4}$	$2.63^{-4}$	$3.04^{-4}$
$p\pi$				$1.64^{-2}$					$p\pi$		$1.42^{-2}$						
$d\pi$				$1.79^{-5}$					$d\pi$		$4.10^{-5}$						
$f\pi$	3.46	3.26	3.04	$2.78^{-3}$ $6.03^{-5}$	2.49	2.16	1.80	1.43	$f\pi$	4.95	$4.81^{-3}$ $1.30^{-4}$	4.64	4.43	4.17	3.86	3.49	3.07
$g\pi$	6.78	0.54	6.29	$8.26^{-4}$	5.77	5.52	5.28	5.05	$g\pi$		$1.30^{-3}$ $2.13^{-3}$						
$-h\pi$	1.05	9.80	9.04	8.26	7.46	6.65	5.85	5.06	$-h\pi$	2.25	2.13	2.02	1.89	1./5	1.61	1.47	1.31
$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)			0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$				$7.11^{-5}$			$6.40^{-5}$	$5.77^{-5}$	$s\sigma$	$1.32^{-4}$	$1.27^{-4}$		$1.15^{-4}$			$9.84^{-5}$	$9.17^{-5}$
$p\sigma$				$1.11^{-2}$					$p\sigma$		$2.20^{-2}$						
$d\sigma$				$8.56^{-5}$					$d\sigma$		$1.73^{-4}$						
$f\sigma$				$1.46^{-3}$					$f\sigma$		$2.99^{-3}$						
$g\sigma$				$2.13^{-6}$					$g\sigma$		$6.15^{-6}$						
$h\sigma$				$2.44^{-4}$					$h\sigma$		$4.36^{-4}$						
$p\pi$				$1.33^{-2}$					$p\pi$		$1.59^{-2}$						
$d\pi$	9.24	7.61	6.08	$4.68^{-6}$ $2.03^{-4}$	3.46	2.45	1.69	1.19	$d\pi$	1.89	$1.58^{-5}$ $2.06^{-3}$	1.29	1.02	7.68	5.52	3.74	2.43
$f\pi$				$3.97^{-5}$					$f\pi$	2.59	$7.49^{-5}$	1.52	1.01	5.82	2.80	1.29	1.09
$g\pi$	4.82	4.59 °	4.32	$3.97^{-3}$ $2.18^{-4}$	3.51	2.91	2.19	1.44	$g\pi$	8.08	$9.85^{-4}$	0.97	6.49	5.97	2.05-4	4.50	5.45
$h\pi$	4.30	3.30	2.85	2.18	1.57	1.06	0.81	4.42	$h\pi$	1.15	9.85	8.10	0.30	4.51	2.85	1.48	5.70
<b>ϵ</b> (Ry)				0.552			0.862	1.000	$\epsilon$ (Ry)	0.353	0.410		0.552		0.743	0.862	1.000
$s\sigma$				$3.25^{-5}$					$s\sigma$	$8.34^{-5}$	$7.37^{-5}$	$6.39^{-5}$	$5.47^{-5}$	$4.62^{-5}$	$3.83^{-5}$	$3.08^{-5}$	$2.40^{-5}$
$p\sigma$	$3.49^{-3}$	$2.44^{-3}$	$1.64^{-3}$	$1.04^{-3}$	$5.79^{-4}$	$2.77^{-4}$	$1.32^{-4}$	$6.45^{-5}$	$p\sigma$	$6.18^{-3}$	$4.47^{-3}$	$3.01^{-3}$	$1.89^{-3}$	$1.13^{-3}$	$6.35^{-4}$	$2.94^{-4}$	$1.24^{-4}$
$d\sigma$	$3.81^{-5}$	$3.08^{-5}$	$1.95^{-5}$	$9.41^{-6}$	$4.95^{-6}$	$3.24^{-6}$	$1.21^{-6}$	$2.97^{-7}$	$d\sigma$	$5.44^{-5}$	$4.25^{-5}$	$3.43^{-5}$	$2.45^{-5}$	$1.29^{-5}$	$5.57^{-6}$	$2.99^{-6}$	$1.21^{-6}$
$f\sigma$				$1.25^{-4}$					$f\sigma$		$4.63^{-4}$						
$g\sigma$				$1.23^{-7}$					$g\sigma$		$4.35^{-7}$						
$h\sigma$				$1.72^{-4}$					$h\sigma$		$1.77^{-4}$						
$p\pi$				$5.85^{-3}$					$p\pi$		$8.92^{-3}$						
$d\pi$				$4.03^{-7}$ $2.92^{-5}$					$d\pi$		$1.13^{-6}$						
$f\pi$	1.63	$9.40^{-3}$	3.64	$2.92^{-3}$ $1.11^{-6}$	$3.15^{-3}$	1.65	1.91	1.78	$f\pi$		$1.53^{-4}$ $1.26^{-5}$						
$g\pi$	7.95	3.81	1.90	8.13 <sup>-6</sup>	5.45	1.55	5.01	5.08	$g\pi$	2.29	$1.26^{-5}$ $2.04^{-5}$	2.42-5	2.65	1.46	0.0/	1.6/	5.65
$h\pi$	3.20	2.55	1./9	8.15	2.51	5.15	3.91 °	1.89	$h\pi$	1.88	2.04	3.42	5.54	1.96	5.51 °	4.11	5.11

and A are the separation constants. The solution of Eq. (A2) gives  $\Omega(\phi) = \exp(i\mu\pi)/\sqrt{2\pi}$ . Finally, the electronic boundand continuum-state wave function

$$\varphi_k(\mathbf{r};R) = \varphi_k(\xi,\eta,\varphi;R)$$

can be factorized and written as

$$\varphi_k(\xi, \eta, \phi; R) = C_k(R) X_k(\xi; R) Y_k(\eta; R) \exp(i\mu\phi) / \sqrt{2\pi},$$
(A5)

where  $C_k(R)$  is the normalization constant, and functions  $X_k(\xi,R)$  and  $Y_k(\eta,R)$  describe the quasiradial and quasiangular motions of electron, respectively. The index  $\mu$  labels the component of electronic angular momentum on the R axis. Several methods have been developed through the years which can treat these kinds of differential equations (A2), (A3), and (A4) in which the separation constant A and energy constant c are R dependent.

The bound state wave functions both  $X(\xi,R)$  and  $Y(\eta,R)$  can be expanded in a suitable power series (there are several

Table 11. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=2.34\,\mathrm{keV/amu}$ 

TABLE 12. Single differential cross sections (in  $10^{-16} \,\mathrm{cm}^2$ ) at  $E = 2.65 \,\mathrm{keV/amu}$ 

- 2.34	ke v/aiiiu	l							- 2.03	Ke v/aiiiu	1						
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$2.81^{-4}$	$2.79^{-4}$	2.77-4	$2.74^{-4}$	$2.72^{-4}$	$2.68^{-4}$	$2.64^{-4}$	$2.60^{-4}$	sσ	$4.09^{-4}$	$4.08^{-4}$	$4.06^{-4}$	$4.04^{-4}$	$4.01^{-4}$	$3.98^{-4}$	$3.94^{-4}$	$3.89^{-4}$
$p\sigma$	$6.28^{-2}$	$6.22^{-2}$	$6.15^{-2}$	$6.07^{-2}$	$5.98^{-2}$	$5.87^{-2}$	$5.76^{-2}$	$5.62^{-2}$	$p\sigma$	$8.25^{-2}$	$8.18^{-2}$	$8.09^{-2}$	$7.99^{-2}$	$7.88^{-2}$	$7.75^{-2}$	$7.60^{-2}$	$7.44^{-2}$
$d\sigma$	$2.92^{-4}$	$2.89^{-4}$	$2.86^{-4}$	$2.82^{-4}$	$2.78^{-4}$	$2.73^{-4}$	$2.68^{-4}$	$2.62^{-4}$	$d\sigma$			$4.64^{-4}$	$4.57^{-4}$	$4.49^{-4}$	$4.40^{-4}$	$4.30^{-4}$	$4.18^{-4}$
$f\sigma$	$3.95^{-3}$	$3.90^{-3}$	$3.85^{-3}$	$3.79^{-3}$	$3.72^{-3}$	$3.64^{-3}$	$3.56^{-3}$	$3.45^{-3}$	fσ	$5.92^{-3}$	$5.86^{-3}$	$5.78^{-3}$	$5.70^{-3}$	$5.61^{-3}$	$5.50^{-3}$	$5.37^{-3}$	$5.23^{-3}$
$g\sigma$				$7.59^{-5}$				$6.62^{-5}$	$g\sigma$	$1.14^{-4}$	$1.13^{-4}$					$1.07^{-4}$	
$h\sigma$	$1.36^{-3}$	$1.32^{-3}$	$1.27^{-3}$	$1.22^{-3}$	$1.16^{-3}$	$1.10^{-3}$	$1.04^{-3}$	$9.65^{-4}$	$h\sigma$	$1.60^{-3}$	$1.57^{-3}$	$1.53^{-3}$	$1.49^{-3}$	$1.44^{-3}$	$1.39^{-3}$	$1.33^{-3}$	$1.27^{-3}$
$p\pi$	$1.90^{-2}$	$1.88^{-2}$	$1.86^{-2}$	$1.84^{-2}$	$1.81^{-2}$	$1.78^{-2}$	$1.75^{-2}$	$1.72^{-2}$	$p\pi$	$2.61^{-2}$	$2.58^{-2}$	$2.55^{-2}$	$2.52^{-2}$	$2.48^{-2}$	$2.43^{-2}$	$2.38^{-2}$	$2.33^{-2}$
$d\pi$	$9.89^{-5}$			$9.28^{-5}$			$8.41^{-5}$	$8.05^{-5}$	$d\pi$	$1.58^{-4}$	$1.56^{-4}$	$1.53^{-4}$	$1.49^{-4}$	$1.46^{-4}$	$1.41^{-4}$	$1.36^{-4}$	$1.31^{-4}$
$f\pi$	$6.29^{-3}$	$6.27^{-3}$	$6.24^{-3}$	$6.21^{-3}$	$6.17^{-3}$	$6.13^{-3}$	$6.08^{-3}$	$6.01^{-3}$	$f\pi$	$7.49^{-3}$	$7.45^{-3}$	$7.39^{-3}$	$7.33^{-3}$	$7.27^{-3}$	$7.19^{-3}$	$7.11^{-3}$	$7.02^{-3}$
$g\pi$	$3.03^{-4}$	$2.99^{-4}$	$2.94^{-4}$	$2.88^{-4}$	$2.82^{-4}$	$2.75^{-4}$	$2.67^{-4}$	$2.58^{-4}$	$g\pi$	$4.90^{-4}$	$4.84^{-4}$	$4.76^{-4}$	$4.68^{-4}$	$4.59^{-4}$	$4.48^{-4}$	$4.36^{-4}$	$4.22^{-4}$
$\stackrel{\stackrel{\circ}{h}\pi}{=}$	$4.64^{-3}$	$4.58^{-3}$	$4.50^{-3}$	$4.41^{-3}$	$4.31^{-3}$	$4.21^{-3}$	$4.09^{-3}$	$3.96^{-3}$	$\stackrel{\stackrel{\scriptstyle \circ}{h}\pi}{=}$	$7.19^{-3}$	$7.08^{-3}$	$6.97^{-3}$	$6.84^{-3}$	$6.69^{-3}$	$6.54^{-3}$	$6.36^{-3}$	$6.18^{-3}$
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	$2.54^{-4}$	$2.48^{-4}$	$2.41^{-4}$	$2.33^{-4}$	$2.25^{-4}$	$2.15^{-4}$	$2.05^{-4}$	1.94-4	sσ	$3.84^{-4}$	3.77-4	$3.69^{-4}$	$3.60^{-4}$	$3.49^{-4}$	$3.36^{-4}$	$3.21^{-4}$	$3.04^{-4}$
$p\sigma$				$4.89^{-2}$					$p\sigma$							$5.55^{-2}$	
$d\sigma$				$2.36^{-4}$					$d\sigma$							$3.00^{-4}$	
$f\sigma$				$2.92^{-3}$					$f\sigma$							$3.47^{-3}$	
$g\sigma$	$6.26^{-5}$	$5.85^{-5}$	$5.37^{-5}$	$4.82^{-5}$	$4.21^{-5}$	$3.56^{-5}$	$2.89^{-5}$	$2.23^{-5}$	$g\sigma$	$1.02^{-4}$	$9.93^{-5}$	$9.55^{-5}$	$9.09^{-5}$	$8.53^{-5}$	$7.85^{-5}$	$7.03^{-5}$	$6.09^{-5}$
$h\sigma$	$8.92^{-4}$	$8.16^{-4}$	$7.40^{-4}$	$6.66^{-4}$	$5.95^{-4}$	$5.30^{-4}$	$4.71^{-4}$	$4.22^{-4}$	$h\sigma$							$8.20^{-4}$	
$p\pi$				$1.59^{-2}$					$p\pi$							$1.80^{-2}$	
$d\pi$	$7.65^{-5}$	$7.22^{-5}$	$6.75^{-5}$	$6.25^{-5}$	$5.72^{-5}$	$5.17^{-5}$	$4.61^{-5}$	$4.05^{-5}$	$d\pi$		$1.18^{-4}$				$8.66^{-5}$	$7.77^{-5}$	$6.87^{-5}$
$f\pi$	$5.94^{-3}$	$5.84^{-3}$	$5.73^{-3}$	$5.58^{-3}$	$5.40^{-3}$	$5.17^{-3}$	$4.88^{-3}$	$4.51^{-3}$	$f\pi$	$6.92^{-3}$	$6.81^{-3}$	$6.69^{-3}$	$6.55^{-3}$	$6.38^{-3}$	$6.19^{-3}$	$5.94^{-3}$	$5.65^{-3}$
$g\pi$	$2.47^{-4}$	$2.36^{-4}$	$2.24^{-4}$	$2.10^{-4}$	$1.96^{-4}$	$1.81^{-4}$	$1.66^{-4}$	$1.50^{-4}$	$g \pi$	$4.06^{-4}$	$3.89^{-4}$	$3.70^{-4}$	$3.49^{-4}$	$3.26^{-4}$	$3.01^{-4}$	$2.76^{-4}$	$2.49^{-4}$
$h\pi$	$3.82^{-3}$	$3.67^{-3}$	$3.51^{-3}$	$3.34^{-3}$	$3.17^{-3}$	$2.98^{-3}$	$2.78^{-3}$	$2.56^{-3}$	$h\pi$	$5.98^{-3}$	$5.77^{-3}$	$5.54^{-3}$	$5.31^{-3}$	$5.07^{-3}$	$4.82^{-3}$	$4.56^{-3}$	$4.28^{-3}$
$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ				$1.57^{-4}$					sσ	$2.85^{-4}$						$1.82^{-4}$	
$p\sigma$				$2.52^{-2}$					$p\sigma$	$4.77^{-2}$						$2.13^{-2}$	
$d\sigma$				$1.91^{-4}$					$d\sigma$							$1.84^{-4}$	
$f\sigma$				$2.05^{-3}$					$f\sigma$							$1.57^{-3}$	
$g\sigma$				$6.86^{-6}$					$g\sigma$							$6.86^{-6}$	
$h\sigma$				$4.03^{-4}$					$h\sigma$							$4.55^{-4}$	
$p\pi$				$1.55^{-2}$					$p\pi$							$1.47^{-2}$	
$d\pi$				$2.00^{-5}$					$d\pi$							$1.66^{-5}$	
$f\pi$				$2.26^{-3}$					$f\pi$							$1.28^{-3}$	
$g \pi$	$1.35^{-4}$	$1.22^{-4}$	$1.09^{-4}$	$9.90^{-5}$	$9.00^{-5}$	$8.17^{-5}$	$7.24^{-5}$	$6.06^{-5}$	$g \pi$	$2.22^{-4}$	$1.96^{-4}$	$1.72^{-4}$	$1.51^{-4}$	$1.33^{-4}$	$1.18^{-4}$	$1.05^{-4}$	$9.15^{-5}$
$h\pi$	$2.33^{-3}$	$2.08^{-3}$	$1.79^{-3}$	$1.48^{-3}$	$1.15^{-3}$	$8.17^{-4}$	$5.02^{-4}$	$2.43^{-4}$	$h\pi$	$3.98^{-3}$	$3.64^{-3}$	$3.25^{-3}$	$2.80^{-3}$	$2.30^{-3}$	$1.75^{-3}$	$1.20^{-3}$	$6.98^{-4}$
$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ				$7.88^{-5}$		$5.71^{-5}$	$4.60^{-5}$		sσ	$1.63^{-4}$				$9.20^{-5}$			
$p\sigma$				$3.28^{-3}$					$p\sigma$							$9.41^{-4}$	
$d\sigma$	$1.05^{-4}$	$7.29^{-5}$	$4.98^{-5}$	$3.60^{-5}$	$2.53^{-5}$	$1.38^{-5}$	$5.52^{-6}$	$2.46^{-6}$	$d\sigma$	$1.54^{-4}$	$1.23^{-4}$	$8.60^{-5}$	$5.49^{-5}$	$3.61^{-5}$	$2.40^{-5}$	$1.28^{-5}$	$4.77^{-6}$
$f\sigma$				$3.19^{-4}$					$f\sigma$	$1.71^{-3}$	$1.52^{-3}$	$1.03^{-3}$	$5.19^{-4}$	$2.85^{-4}$	$2.13^{-4}$	$1.45^{-4}$	$5.27^{-5}$
$g\sigma$				$3.67^{-7}$					$g\sigma$							$2.98^{-7}$	
$h\sigma$				$1.93^{-4}$					$h\sigma$							$1.25^{-4}$	
$p\pi$	$1.11^{-2}$	$9.88^{-3}$	$8.95^{-3}$	$8.07^{-3}$	$6.94^{-3}$	$5.64^{-3}$	$4.47^{-3}$	$3.43^{-3}$	$p\pi$							$5.18^{-3}$	
$d\pi$	$3.39^{-6}$	$2.08^{-6}$	$1.37^{-6}$	$9.66^{-7}$	$6.78^{-7}$	$5.17^{-7}$	$4.44^{-7}$	$3.86^{-7}$	$d\pi$	$7.42^{-6}$	$4.42^{-6}$	$2.59^{-6}$	$1.65^{-6}$	$1.12^{-6}$	$7.61^{-7}$	$5.66^{-7}$	$4.79^{-7}$
$f\pi$				$8.86^{-5}$					$f\pi$							$1.90^{-5}$	
$g \pi$				$6.77^{-6}$					$g \pi$	$7.48^{-5}$	$5.45^{-5}$	$3.33^{-5}$	$1.62^{-5}$	$6.63^{-6}$	$3.04^{-6}$	$1.47^{-6}$	$4.35^{-7}$
$h\pi$	$7.50^{-5}$	$1.14^{-5}$	$2.50^{-5}$	$5.51^{-5}$	$5.48^{-5}$	$2.67^{-5}$	$6.78^{-6}$	$6.19^{-6}$	$h\pi$	$3.10^{-4}$	$8.00^{-5}$	$1.15^{-5}$	$4.52^{-5}$	$8.19^{-5}$	$6.58^{-5}$	$2.41^{-5}$	$6.50^{-6}$

possibilities,<sup>31,32</sup> e.g., obtaining recursion relations for the coefficients and solving them by matrix or infinite continued fraction methods). In the present study, the radial wave function  $X(\xi,R)$  is expanded in

$$X(\xi;R) = (\xi^2 - 1)^{\mu/2} (\xi + 1)^{\sigma} \exp(-c\xi) \sum_{t=0}^{\infty} g_t \left(\frac{\xi - 1}{\xi + 1}\right)^t$$
(A6)

with

$$\sigma = R(1 + Z_R/Z_A)/2c - \mu - 1$$
,

and the angular wave function  $Y(\eta,R)$  is expanded in

$$Y(\eta;R) = \exp(-c \eta) \sum_{l=\mu} d_l P_l^{\mu}(\eta).$$
 (A7)

Here  $P_l^{\mu}(\eta)$  denotes the associated Legendre polynomials. The obtained three term recursion relations for  $g_t$  and  $d_l$  are then solved by the infinite continued fraction method. Using this method it was possible to obtain the potential curves with accuracy better than ten significant digits. To compute the electronic wave functions and couplings simply, the function  $Y(\eta,R)$  is written as

Table 13. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=2.97\,\mathrm{keV/amu}$ 

TABLE 14. Single differential cross sections (in  $10^{-16} \text{ cm}^2$ ) at E = 3.29 keV/amu

- 2.97	ke v/amu	<u>l</u>							- 3.29	ke v/aiiii	1						
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$5.72^{-4}$	$5.71^{-4}$	$5.70^{-4}$	$5.68^{-4}$	$5.66^{-4}$	$5.63^{-4}$	$5.60^{-4}$	5.57-4	$s\sigma$	$8.41^{-4}$	$8.38^{-4}$	$8.35^{-4}$	8.31-4	$8.27^{-4}$	$8.22^{-4}$	$8.16^{-4}$	$8.10^{-4}$
$p\sigma$				$9.94^{-2}$	$9.81^{-2}$	$9.66^{-2}$			$p\sigma$	$1.22^{-1}$	$1.21^{-1}$					$1.14^{-1}$	
$d\sigma$			$7.36^{-4}$	$7.25^{-4}$	$7.13^{-4}$	$6.99^{-4}$	$6.84^{-4}$	$6.66^{-4}$	$d\sigma$	$1.21^{-3}$	$1.20^{-3}$	$1.18^{-3}$	$1.17^{-3}$	$1.15^{-3}$	$1.13^{-3}$	$1.11^{-3}$	$1.08^{-3}$
$f\sigma$				$6.67^{-3}$		$6.44^{-3}$	$6.30^{-3}$	$6.14^{-3}$	$f\sigma$							$6.38^{-3}$	
$g\sigma$	$1.52^{-4}$	$1.50^{-4}$	$1.49^{-4}$	$1.48^{-4}$	$1.46^{-4}$	$1.44^{-4}$	$1.42^{-4}$	$1.40^{-4}$	$g\sigma$							$1.98^{-4}$	
$h\sigma$				$1.12^{-3}$					$h\sigma$							$1.21^{-3}$	
$p\pi$				$3.19^{-2}$					$p\pi$							$3.62^{-2}$	
$d\pi$	$2.37^{-4}$	$2.33^{-4}$	$2.29^{-4}$	$2.25^{-4}$	$2.19^{-4}$	$2.13^{-4}$	$2.07^{-4}$	$1.99^{-4}$	$d\pi$	$3.33^{-4}$	$3.28^{-4}$	$3.23^{-4}$	$3.16^{-4}$	$3.10^{-4}$	$3.02^{-4}$	$2.93^{-4}$	$2.83^{-4}$
$f\pi$	$9.59^{-3}$	$9.49^{-3}$	$9.37^{-3}$	$9.25^{-3}$	$9.11^{-3}$	$8.96^{-3}$	$8.79^{-3}$	$8.61^{-3}$	$f\pi$	$1.29^{-2}$	$1.27^{-2}$	$1.25^{-2}$	$1.23^{-2}$	$1.20^{-2}$	$1.17^{-2}$	$1.14^{-2}$	$1.11^{-2}$
$g \pi$	$7.25^{-4}$	$7.16^{-4}$	$7.06^{-4}$	$6.95^{-4}$	$6.83^{-4}$	$6.68^{-4}$	$6.52^{-4}$	$6.33^{-4}$	$g \pi$	$9.96^{-4}$	$9.86^{-4}$	$9.74^{-4}$	$9.60^{-4}$	$9.44^{-4}$	$9.26^{-4}$	$9.05^{-4}$	$8.82^{-4}$
$h\pi$	9.98-3	9.83	9.67 <sup>-3</sup>	$9.49^{-3}$	9.29-3	9.07 <sup>-3</sup>	8.83	8.58-3	$h\pi$	1.23-2	1.21-2	1.19-2	1.17-2	1.14-2	1.12-2	$1.09^{-2}$	1.06 <sup>-2</sup>
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	5.53-4	5.47-4	5.41-4	5.33-4	5.23-4	$5.11^{-4}$	$4.96^{-4}$	$4.77^{-4}$	$s\sigma$	$8.03^{-4}$	$7.95^{-4}$	$7.85^{-4}$	$7.75^{-4}$	$7.63^{-4}$	$7.49^{-4}$	$7.32^{-4}$	$7.13^{-4}$
$p\sigma$				$8.22^{-2}$					$p\sigma$							$8.60^{-2}$	
$d\sigma$				$5.72^{-4}$					$d\sigma$							$7.86^{-4}$	
$f\sigma$				$5.29^{-3}$					$f\sigma$							$4.45^{-3}$	
$g\sigma$	$1.37^{-4}$	$1.34^{-4}$	$1.30^{-4}$	$1.26^{-4}$	$1.21^{-4}$	$1.16^{-4}$	$1.09^{-4}$	$1.00^{-4}$	$g\sigma$	$1.88^{-4}$	$1.82^{-4}$	$1.76^{-4}$	$1.70^{-4}$	$1.62^{-4}$	$1.55^{-4}$	$1.47^{-4}$	$1.37^{-4}$
$h\sigma$	$9.49^{-4}$	$9.11^{-4}$	$8.75^{-4}$	$8.44^{-4}$	$8.20^{-4}$	$8.08^{-4}$	$8.10^{-4}$	$8.26^{-4}$	$h\sigma$							$8.04^{-4}$	
$p\pi$	$2.92^{-2}$	$2.83^{-2}$	$2.74^{-2}$	$2.63^{-2}$	$2.52^{-2}$	$2.39^{-2}$	$2.26^{-2}$	$2.12^{-2}$	$p \pi$	$3.50^{-2}$	$3.42^{-2}$	$3.33^{-2}$	$3.22^{-2}$	$3.09^{-2}$	$2.95^{-2}$	$2.79^{-2}$	$2.62^{-2}$
$d\pi$				$1.60^{-4}$					$d\pi$							$1.79^{-4}$	
$f\pi$				$7.76^{-3}$					$f\pi$							$8.29^{-3}$	
$g \pi$	$6.12^{-4}$	$5.88^{-4}$	$5.61^{-4}$	$5.32^{-4}$	$4.99^{-4}$	$4.64^{-4}$	$4.27^{-4}$	$3.87^{-4}$	$g \pi$	$8.55^{-4}$	$8.25^{-4}$	$7.91^{-4}$	$7.53^{-4}$	$7.11^{-4}$	$6.65^{-4}$	$6.15^{-4}$	$5.61^{-4}$
$h\pi$	8.31	8.03	7.73	$7.44^{-3}$	7.13	6.83	6.52	6.20	$h\pi$	1.02 -	9.90	9.56	9.21	8.88	8.56	$8.25^{-3}$	7.94
ε (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195		0.263	0.305
$s\sigma$	$4.55^{-4}$	$4.30^{-4}$	$4.01^{-4}$	$3.69^{-4}$	$3.35^{-4}$	$3.02^{-4}$	$2.72^{-4}$	$2.46^{-4}$	$s\sigma$	$6.90^{-4}$	$6.62^{-4}$	$6.28^{-4}$	$5.89^{-4}$	$5.44^{-4}$	$4.94^{-4}$	$4.42^{-4}$	$3.90^{-4}$
$p\sigma$	$6.09^{-2}$	$5.57^{-2}$		$4.47^{-2}$					$p\sigma$							$3.55^{-2}$	
$d\sigma$				$2.75^{-4}$					$d\sigma$	$6.61^{-4}$	$5.92^{-4}$	$5.21^{-4}$	$4.48^{-4}$	$3.78^{-4}$	$3.15^{-4}$	$2.62^{-4}$	$2.23^{-4}$
$f\sigma$				$2.11^{-3}$					$f\sigma$							$1.21^{-3}$	
$g\sigma$				$4.82^{-5}$					$g\sigma$							$2.97^{-5}$	
$h\sigma$				$8.12^{-4}$					$h\sigma$							$6.75^{-4}$	
$p\pi$				$1.67^{-2}$					$p \pi$							$1.59^{-2}$	
$d\pi$				$5.81^{-5}$					$d\pi$							$4.62^{-5}$	
$f\pi$				$4.71^{-3}$					$f\pi$							$3.22^{-3}$	
$g \pi$				$2.28^{-4}$					$g \pi$	$5.05^{-4}$	$4.47^{-4}$	$3.89^{-4}$	$3.34^{-4}$	$2.83^{-4}$	$2.39^{-4}$	$2.03^{-4}$	$1.73^{-4}$
$h\pi$	5.86 <sup>-3</sup>	5.48	5.03	$4.48^{-3}$	3.83	3.08	2.27	1.46	$h\pi$	7.62	7.27	6.83	6.28	5.57	4.69	$3.65^{-3}$	2.55
ε (Ry)	0.353		0.476	0.552	0.640	0.743	0.862	1.000	<b>ε</b> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ	$2.24^{-4}$	$2.05^{-4}$	$1.84^{-4}$	$1.58^{-4}$	$1.31^{-4}$	$1.07^{-4}$	$8.88^{-5}$	$7.16^{-5}$	sσ	$3.41^{-4}$	$2.99^{-4}$	$2.62^{-4}$	$2.27^{-4}$	$1.90^{-4}$	$1.54^{-4}$	$1.23^{-4}$	$9.89^{-5}$
$p\sigma$	$1.80^{-2}$	$1.34^{-2}$	$9.65^{-3}$	$6.71^{-3}$	$4.50^{-3}$	$2.77^{-3}$	$1.48^{-3}$	$7.27^{-4}$	$p\sigma$	$2.34^{-2}$	$1.78^{-2}$	$1.29^{-2}$	$8.93^{-3}$	$5.96^{-3}$	$3.81^{-3}$	$2.19^{-3}$	$1.10^{-3}$
$d\sigma$	$1.74^{-4}$	$1.57^{-4}$	$1.27^{-4}$	$8.88^{-5}$	$5.45^{-5}$	$3.38^{-5}$	$2.12^{-5}$	$1.05^{-5}$	$d\sigma$	$1.96^{-4}$	$1.77^{-4}$	$1.56^{-4}$	$1.24^{-4}$	$8.38^{-5}$	$4.94^{-5}$	$2.95^{-5}$	$1.73^{-5}$
$f\sigma$	$1.26^{-3}$	$1.33^{-3}$	$1.25^{-3}$	$8.86^{-4}$	$4.50^{-4}$	$2.45^{-4}$	$1.86^{-4}$	$1.09^{-4}$	$f\sigma$		$9.83^{-4}$			$6.73^{-4}$	$3.46^{-4}$	$2.07^{-4}$	
$g\sigma$				$5.71^{-7}$					$g\sigma$							$5.80^{-7}$	
$h\sigma$				$3.60^{-4}$					$h\sigma$							$1.69^{-4}$	
$p\pi$				$9.53^{-3}$					$p \pi$							$6.50^{-3}$	
$d\pi$				$3.05^{-6}$					$d\pi$							$1.49^{-6}$	
$f\pi$				$1.33^{-4}$					$f\pi$							$2.78^{-5}$	
$g \pi$				$3.24^{-5}$					$g \pi$							$4.57^{-6}$	
$h\pi$	7.76-4	2.94 <sup>-4</sup>	5.52-3	$2.25^{-5}$	8.03	1.02-4	5.90 <sup>-3</sup>	1.47 <sup>-3</sup>	$h\pi$	1.51-3	6.91 <sup>-4</sup>	1.98-4	2.54 <sup>-5</sup>	5.63 <sup>-5</sup>	1.18-4	$9.98^{-5}$	3.67 <sup>-3</sup>

$$Y(\eta;R) = \sum_{l=\mu} d_l P_l^{\mu}(\eta).$$
 (A8)

The same procedure can be used to calculate the separation constant and the angular wave function for the continuum states. However, the radial part must be calculated numerically. Integration starts from  $\xi=1$  with  $|\Lambda(\xi=1,R)|<+\infty$  to a sufficient larger value of  $\xi_{\rm max}$ , where  $X(\xi,R)$  accurately matches the asymptotic boundary condition

$$X(\xi \to \infty; R) \to \frac{1}{c\,\xi} \sin\left(c\,\xi' - \frac{RZ_+}{2c} \ln(2c\,\xi) - \frac{\lambda\,\pi}{2} + \delta_{\lambda\,\mu}\right), \tag{A9}$$

and  $\delta_{\lambda\mu}$  is the phase shift for the radial function. Let us note that A represents the eigenvalue of the constant of separation, which comes from the additional symmetry in the two-center Coulomb system. The system with this degree of symmetry is described by the invariant operator  $\hat{A}$ 

Table 15. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at  $E=3.61\,\mathrm{keV/amu}$ 

Table 16. Single differential cross sections (in  $10^{-16} \,\mathrm{cm}^2$ ) at  $E = 3.93 \,\mathrm{keV/amu}$ 

	RC 17 dillio	•															
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$1.34^{-3}$			$1.32^{-3}$			$1.28^{-3}$	$1.26^{-3}$	$s\sigma$		$2.15^{-3}$				$2.06^{-3}$		$2.00^{-3}$
$p\sigma$	$1.42^{-1}$	$1.41^{-1}$	$1.39^{-1}$	$1.38^{-1}$	$1.36^{-1}$	$1.35^{-1}$	$1.33^{-1}$	$1.30^{-1}$	$p\sigma$	$1.61^{-1}$	$1.60^{-1}$	$1.59^{-1}$	$1.57^{-1}$	$1.55^{-1}$	$1.54^{-1}$	$1.51^{-1}$	$1.49^{-1}$
$d\sigma$	$1.91^{-3}$	$1.89^{-3}$	$1.87^{-3}$		$1.82^{-3}$	$1.79^{-3}$	$1.75^{-3}$		$d\sigma$		$2.83^{-3}$			$2.72^{-3}$	$2.67^{-3}$	$2.61^{-3}$	
$f\sigma$	$6.99^{-3}$	$6.91^{-3}$	$6.81^{-3}$	$6.70^{-3}$	$6.58^{-3}$	$6.44^{-3}$	$6.28^{-3}$	$6.11^{-3}$	$f\sigma$	$6.89^{-3}$	$6.81^{-3}$	$6.72^{-3}$	$6.61^{-3}$	$6.50^{-3}$	$6.37^{-3}$	$6.23^{-3}$	$6.06^{-3}$
$g\sigma$	$3.19^{-4}$	$3.15^{-4}$	$3.10^{-4}$	$3.05^{-4}$	$3.00^{-4}$	$2.93^{-4}$	$2.86^{-4}$	$2.78^{-4}$	$g\sigma$	$4.38^{-4}$	$4.33^{-4}$	$4.28^{-4}$	$4.21^{-4}$	$4.14^{-4}$	$4.06^{-4}$	$3.97^{-4}$	$3.86^{-4}$
$h\sigma$						$2.57^{-3}$			$h\sigma$	$5.24^{-3}$	$5.17^{-3}$	$5.09^{-3}$	$4.99^{-3}$	$4.87^{-3}$	$4.74^{-3}$	$4.59^{-3}$	$4.42^{-3}$
$p\pi$	$4.14^{-2}$	$4.13^{-2}$				$4.06^{-2}$			$p\pi$	$4.33^{-2}$	$4.33^{-2}$	$4.33^{-2}$	$4.33^{-2}$	$4.33^{-2}$	$4.32^{-2}$	$4.31^{-2}$	$4.29^{-2}$
$d\pi$						$4.03^{-4}$			$d\pi$		$5.51^{-4}$						
$f\pi$	$1.74^{-2}$	$1.72^{-2}$	$1.68^{-2}$	$1.65^{-2}$	$1.61^{-2}$	$1.57^{-2}$	$1.52^{-2}$	$1.47^{-2}$	$f\pi$	$2.33^{-2}$	$2.29^{-2}$	$2.25^{-2}$	$2.20^{-2}$	$2.14^{-2}$	$2.08^{-2}$	$2.02^{-2}$	$1.94^{-2}$
$g\pi$						$1.21^{-3}$			$g\pi$		$1.59^{-3}$						
$h\pi$	$1.40^{-2}$	$1.38^{-2}$	$1.35^{-2}$	$1.32^{-2}$	$1.30^{-2}$	$1.26^{-2}$	$1.23^{-2}$	$1.20^{-2}$	$h\pi$	$1.52^{-2}$	$1.50^{-2}$	$1.47^{-2}$	$1.44^{-2}$	$1.41^{-2}$	$1.38^{-2}$	$1.34^{-2}$	$1.30^{-2}$
<b>ε</b> (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	$1.24^{-3}$	1 22-3	1 20-3	1 17-3	1 15-3	$1.12^{-3}$	1 09-3	$1.06^{-3}$	sσ	1 96-3	1.92-3	1 87-3	1.82-3	1 77-3	1 71-3	1 65-3	$1.58^{-3}$
$p\sigma$						$1.08^{-1}$			pσ		$1.43^{-1}$						$1.11^{-1}$
$d\sigma$						$1.35^{-3}$			$d\sigma$		$2.41^{-3}$						
$f\sigma$						$4.73^{-3}$			$f\sigma$		$5.70^{-3}$						
$g\sigma$						$2.11^{-4}$			$g\sigma$		$3.60^{-4}$						
$h\sigma$	$2.24^{-3}$	$2.10^{-3}$	$1.95^{-3}$	$1.79^{-3}$	$1.62^{-3}$	$1.46^{-3}$	$1.31^{-3}$	$1.19^{-3}$	$h\sigma$	$4.22^{-3}$	$3.99^{-3}$	$3.73^{-3}$	$3.45^{-3}$	$3.14^{-3}$	$2.80^{-3}$	$2.46^{-3}$	$2.12^{-3}$
$p\pi$	$3.95^{-2}$	$3.89^{-2}$	$3.81^{-2}$	$3.72^{-2}$	$3.61^{-2}$	$3.47^{-2}$	$3.31^{-2}$	$3.13^{-2}$	$p\pi$	$4.27^{-2}$	$4.23^{-2}$	$4.18^{-2}$	$4.12^{-2}$	$4.03^{-2}$	$3.92^{-2}$	$3.77^{-2}$	$3.60^{-2}$
$d\pi$	$3.65^{-4}$	$3.50^{-4}$	$3.33^{-4}$	$3.14^{-4}$	$2.93^{-4}$	$2.71^{-4}$	$2.47^{-4}$	$2.23^{-4}$	$d\pi$	$4.67^{-4}$	$4.48^{-4}$	$4.28^{-4}$	$4.05^{-4}$	$3.79^{-4}$	$3.52^{-4}$	$3.23^{-4}$	$2.93^{-4}$
$f\pi$						$1.08^{-2}$			$f\pi$	$1.86^{-2}$	$1.77^{-2}$	$1.68^{-2}$	$1.58^{-2}$	$1.48^{-2}$	$1.37^{-2}$	$1.26^{-2}$	$1.16^{-2}$
$g\pi$	$1.13^{-3}$	$1.09^{-3}$	$1.05^{-3}$	$1.00^{-3}$	$9.52^{-4}$	$8.95^{-4}$	$8.33^{-4}$	$7.66^{-4}$	$g\pi$	$1.41^{-3}$	$1.37^{-3}$	$1.32^{-3}$	$1.27^{-3}$	$1.21^{-3}$	$1.15^{-3}$	$1.07^{-3}$	$9.93^{-4}$
$\stackrel{\circ}{h}\pi$	$1.16^{-2}$	$1.12^{-2}$	$1.09^{-2}$	$1.05^{-2}$	$1.02^{-2}$	$9.87^{-3}$	$9.59^{-3}$	$9.34^{-3}$	$\stackrel{\circ}{h}\pi$	$1.26^{-2}$	$1.22^{-2}$	$1.19^{-2}$	$1.15^{-2}$	$1.12^{-2}$	$1.09^{-2}$	$1.07^{-2}$	$1.05^{-2}$
(D.)	0.100	0.125	0.145	0.160	0.105	0.226	0.262	0.205	(D.)	0.100	0.125	0.145	0.160	0.105	0.226	0.262	0.205
	0.108		0.145		0.195	0.226	0.263	0.305		0.108		0.145		0.195		0.263	0.305
$s\sigma$			$9.36^{-4}$		$8.29^{-4}$		$6.93^{-4}$	$6.15^{-4}$	$s\sigma$		$1.44^{-3}$						$9.13^{-4}$
$p\sigma$						$5.07^{-2}$			$p\sigma$		$9.60^{-2}$						
$d\sigma$						$5.31^{-4}$ $1.48^{-3}$			$d\sigma$		$1.51^{-3}$ $3.63^{-3}$						
$f\sigma$						$\frac{1.48}{7.82^{-5}}$			$f\sigma$		$\frac{3.63}{2.03^{-4}}$						
$g\sigma$						$1.29^{-3}$			$g\sigma$		$1.56^{-3}$						
$h\sigma$						1.29 <sup>3</sup> 1.83 <sup>-2</sup>			$h\sigma$		$3.15^{-2}$						
$p\pi$						1.83 <sup>2</sup> 8.47 <sup>-5</sup>			$p\pi$		$2.30^{-4}$						
$d\pi$						$5.07^{-3}$			$d\pi$		$9.56^{-3}$						
$f\pi$						$3.07^{-4}$			$f\pi$				$6.23^{-4}$				
$g \pi h \pi$	0.94	0.19	3.42											1.7.0			
	$0.10^{-3}$	0 02-3	0.40-3	0.01-3	7 22-3	6.41-3	5 24-3	2.29	$g\pi$								
	$9.10^{-3}$	8.83 <sup>-3</sup>	$8.49^{-3}$	8.01 <sup>-3</sup>	7.33 <sup>-3</sup>	6.41 <sup>-3</sup>	5.24 <sup>-3</sup>	3.89 <sup>-3</sup>	$h\pi$		$1.02^{-2}$						
ε (Ry)	0.353	0.410	0.476	$8.01^{-3}$ $0.552$	$7.33^{-3}$ $0.640$	$6.41^{-3}$ $0.743$	$5.24^{-3}$ $0.862$	3.89 <sup>-3</sup>	$\frac{\stackrel{\circ}{h}\pi}{-}$	$1.04^{-2}$ $0.353$	$1.02^{-2}$ $0.410$	$1.00^{-2}$ $0.476$	$9.67^{-3}$ $0.552$	$9.07^{-3}$ $0.640$	$8.18^{-3}$ $0.743$	$6.94^{-3}$ $0.862$	5.41 <sup>-3</sup> 1.000
	0.353 5.35 <sup>-4</sup>	0.410 4.57 <sup>-4</sup>	0.476 3.87 <sup>-4</sup>	$8.01^{-3}$ $0.552$ $3.27^{-4}$	$7.33^{-3}$ $0.640$ $2.73^{-4}$	$6.41^{-3}$ $0.743$ $2.23^{-4}$	$5.24^{-3}$ $0.862$ $1.76^{-4}$	$ \begin{array}{c} 3.89^{-3} \\ \hline 1.000 \\ 1.37^{-4} \end{array} $	$\frac{\stackrel{\circ}{h}\pi}{-}$	$   \begin{array}{r}     1.04^{-2} \\     0.353 \\     \hline     8.01^{-4}   \end{array} $	$   \begin{array}{r}     1.02^{-2} \\     \hline     0.410 \\     \hline     6.85^{-4}   \end{array} $	$   \begin{array}{r}     1.00^{-2} \\     \hline     0.476 \\     \hline     5.73^{-4}   \end{array} $	$9.67^{-3}$ $0.552$ $4.73^{-4}$	$9.07^{-3}$ $0.640$ $3.88^{-4}$	$8.18^{-3}$ $0.743$ $3.15^{-4}$	$6.94^{-3}$ $0.862$ $2.49^{-4}$	$ \begin{array}{c} 5.41^{-3} \\ 1.000 \\ \hline 1.91^{-4} \end{array} $
<u>ε (Ry)</u>	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup>	0.476 3.87 <sup>-4</sup> 1.67 <sup>-2</sup>	$8.01^{-3}$ $0.552$ $3.27^{-4}$ $1.17^{-2}$	$7.33^{-3}$ $0.640$ $2.73^{-4}$ $7.74^{-3}$	$ \begin{array}{c} 6.41^{-3} \\ 0.743 \\ 2.23^{-4} \\ 4.95^{-3} \end{array} $	$ \begin{array}{r} 5.24^{-3} \\ 0.862 \\ \hline 1.76^{-4} \\ 2.98^{-3} \end{array} $	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup>	$\frac{h\pi}{\epsilon \text{ (Ry)}}$	$   \begin{array}{r}     1.04^{-2} \\     0.353 \\     \hline     8.01^{-4} \\     3.45^{-2}   \end{array} $	$   \begin{array}{r}     1.02^{-2} \\     \hline     0.410 \\     \hline     6.85^{-4} \\     2.72^{-2}   \end{array} $	$   \begin{array}{r}     1.00^{-2} \\     \hline     0.476 \\     \hline     5.73^{-4} \\     2.06^{-2}   \end{array} $	$9.67^{-3}$ $0.552$ $4.73^{-4}$ $1.47^{-2}$	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup>	$8.18^{-3}$ $0.743$ $3.15^{-4}$ $6.30^{-3}$	$ \begin{array}{r} 6.94^{-3} \\ 0.862 \\ \hline 2.49^{-4} \\ 3.84^{-3} \end{array} $	$ \begin{array}{r} 5.41^{-3} \\ 1.000 \\ \hline 1.91^{-4} \\ 2.15^{-3} \end{array} $
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup>	0.476 3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup>	$ \begin{array}{c} 8.01^{-3} \\ 0.552 \\ 3.27^{-4} \\ 1.17^{-2} \\ 1.55^{-4} \end{array} $	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup>	$ \begin{array}{c} 6.41^{-3} \\ 0.743 \\ 2.23^{-4} \\ 4.95^{-3} \\ 7.38^{-5} \end{array} $	5.24 <sup>-3</sup> 0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup>	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup>	$\frac{h\pi}{\epsilon \text{ (Ry)}}$ $\frac{\epsilon \text{ (Ry)}}{s\sigma}$	$ \begin{array}{c} 1.04^{-2} \\ 0.353 \\ 8.01^{-4} \\ 3.45^{-2} \\ 4.19^{-4} \end{array} $	$ \begin{array}{c} 1.02^{-2} \\ 0.410 \\ \hline 6.85^{-4} \\ 2.72^{-2} \\ 3.17^{-4} \end{array} $	$ \begin{array}{r} 1.00^{-2} \\ 0.476 \\ \hline 5.73^{-4} \\ 2.06^{-2} \\ 2.45^{-4} \end{array} $	$9.67^{-3}$ $0.552$ $4.73^{-4}$ $1.47^{-2}$ $1.94^{-4}$	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup>	$ \begin{array}{c} 8.18^{-3} \\ 0.743 \\ 3.15^{-4} \\ 6.30^{-3} \\ 1.04^{-4} \end{array} $	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup>
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup>	0.476 3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup>	$7.33^{-3}$ $0.640$ $2.73^{-4}$ $7.74^{-3}$ $1.17^{-4}$ $7.26^{-4}$	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup>	5.24 <sup>-3</sup> 0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup>	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$	$ \begin{array}{c} 1.04^{-2} \\ 0.353 \\ 8.01^{-4} \\ 3.45^{-2} \\ 4.19^{-4} \\ 7.19^{-4} \end{array} $	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup>	1.00 <sup>-2</sup> 0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup>
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup>	$0.410$ $4.57^{-4}$ $2.25^{-2}$ $2.20^{-4}$ $8.00^{-4}$ $1.02^{-5}$	0.476  3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup>	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup>	5.24 <sup>-3</sup> 0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup>	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup> 5.17 <sup>-7</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{\sigma}{\rho\sigma}$ $d\sigma$	$ \begin{array}{r} 1.04^{-2} \\ 0.353 \\ \hline 8.01^{-4} \\ 3.45^{-2} \\ 4.19^{-4} \\ 7.19^{-4} \\ 3.45^{-5} \end{array} $	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup>	0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup>
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup> 5.04 <sup>-4</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup> 1.02 <sup>-5</sup> 3.39 <sup>-4</sup>	0.476 3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup> 3.32 <sup>-4</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup> 3.16 <sup>-4</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup> 3.63 <sup>-4</sup>	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup> 3.54 <sup>-4</sup>	0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup> 1.63 <sup>-4</sup>	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup> 5.17 <sup>-7</sup> 1.38 <sup>-4</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$	1.04 <sup>-2</sup> 0.353 8.01 <sup>-4</sup> 3.45 <sup>-2</sup> 4.19 <sup>-4</sup> 7.19 <sup>-4</sup> 3.45 <sup>-5</sup> 9.05 <sup>-4</sup>	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup> 5.46 <sup>-4</sup>	0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup> 3.51 <sup>-4</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup> 2.80 <sup>-4</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup> 2.67 <sup>-4</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup> 3.72 <sup>-4</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup> 2.57 <sup>-4</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup> 1.38 <sup>-4</sup>
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$ $f\sigma$ $g\sigma$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup> 5.04 <sup>-4</sup> 1.50 <sup>-2</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup> 1.02 <sup>-5</sup> 3.39 <sup>-4</sup> 1.40 <sup>-2</sup>	0.476  3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup> 3.32 <sup>-4</sup> 1.27 <sup>-2</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup> 3.16 <sup>-4</sup> 1.12 <sup>-2</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup> 3.63 <sup>-4</sup> 9.66 <sup>-3</sup>	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup> 3.54 <sup>-4</sup> 8.32 <sup>-3</sup>	0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup> 1.63 <sup>-4</sup> 7.02 <sup>-3</sup>	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup> 5.17 <sup>-7</sup> 1.38 <sup>-4</sup> 5.65 <sup>-3</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{\sigma}{s\sigma}$ $f\sigma$ $g\sigma$ $h\sigma$ $p\pi$	0.353 8.01 <sup>-4</sup> 3.45 <sup>-2</sup> 4.19 <sup>-4</sup> 7.19 <sup>-4</sup> 3.45 <sup>-5</sup> 9.05 <sup>-4</sup> 1.57 <sup>-2</sup>	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup> 5.46 <sup>-4</sup> 1.46 <sup>-2</sup>	0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup> 3.51 <sup>-4</sup> 1.34 <sup>-2</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup> 2.80 <sup>-4</sup> 1.19 <sup>-2</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup> 2.67 <sup>-4</sup> 1.03 <sup>-2</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup> 3.72 <sup>-4</sup> 8.83 <sup>-3</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup> 2.57 <sup>-4</sup> 7.48 <sup>-3</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup> 1.38 <sup>-4</sup> 6.11 <sup>-3</sup>
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup> 5.04 <sup>-4</sup> 1.50 <sup>-2</sup> 3.87 <sup>-5</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup> 1.02 <sup>-5</sup> 3.39 <sup>-4</sup> 1.40 <sup>-2</sup> 2.67 <sup>-5</sup>	0.476  3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup> 3.32 <sup>-4</sup> 1.27 <sup>-2</sup> 1.69 <sup>-5</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup> 3.16 <sup>-4</sup> 1.12 <sup>-2</sup> 9.86 <sup>-6</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup> 3.63 <sup>-4</sup> 9.66 <sup>-3</sup> 5.81 <sup>-6</sup>	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup> 3.54 <sup>-4</sup> 8.32 <sup>-3</sup> 3.75 <sup>-6</sup>	0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup> 1.63 <sup>-4</sup> 7.02 <sup>-3</sup> 2.51 <sup>-6</sup>	1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup> 5.17 <sup>-7</sup> 1.38 <sup>-4</sup> 5.65 <sup>-3</sup> 1.65 <sup>-6</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$	0.353 8.01 <sup>-4</sup> 3.45 <sup>-2</sup> 4.19 <sup>-4</sup> 7.19 <sup>-4</sup> 3.45 <sup>-5</sup> 9.05 <sup>-4</sup> 1.57 <sup>-2</sup> 5.51 <sup>-5</sup>	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup> 5.46 <sup>-4</sup> 1.46 <sup>-2</sup> 3.94 <sup>-5</sup>	0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup> 3.51 <sup>-4</sup> 1.34 <sup>-2</sup> 2.60 <sup>-5</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup> 2.80 <sup>-4</sup> 1.19 <sup>-2</sup> 1.58 <sup>-5</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup> 2.67 <sup>-4</sup> 1.03 <sup>-2</sup> 9.29 <sup>-6</sup>	0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup> 3.72 <sup>-4</sup> 8.83 <sup>-3</sup> 5.87 <sup>-6</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup> 2.57 <sup>-4</sup> 7.48 <sup>-3</sup> 3.98 <sup>-6</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup> 1.38 <sup>-4</sup> 6.11 <sup>-3</sup> 2.64 <sup>-6</sup>
ε (Ry)  sσ  pσ  dσ  fσ  gσ  hσ  pπ	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup> 5.04 <sup>-4</sup> 1.50 <sup>-2</sup> 3.87 <sup>-5</sup> 2.14 <sup>-3</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup> 1.02 <sup>-5</sup> 3.39 <sup>-4</sup> 1.40 <sup>-2</sup> 2.67 <sup>-5</sup> 1.27 <sup>-3</sup>	0.476 3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup> 3.32 <sup>-4</sup> 1.27 <sup>-2</sup> 1.69 <sup>-5</sup> 6.38 <sup>-4</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup> 3.16 <sup>-4</sup> 1.12 <sup>-2</sup> 9.86 <sup>-6</sup> 2.91 <sup>-4</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup> 3.63 <sup>-4</sup> 9.66 <sup>-3</sup> 5.81 <sup>-6</sup> 1.51 <sup>-4</sup>	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup> 3.54 <sup>-4</sup> 8.32 <sup>-3</sup> 3.75 <sup>-6</sup> 9.15 <sup>-5</sup>	0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup> 1.63 <sup>-4</sup> 7.02 <sup>-3</sup> 2.51 <sup>-6</sup> 4.34 <sup>-5</sup>	3.89 <sup>-3</sup> 1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 5.17 <sup>-7</sup> 1.38 <sup>-4</sup> 5.65 <sup>-3</sup> 1.65 <sup>-6</sup> 1.79 <sup>-5</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{\sigma}{s\sigma}$ $f\sigma$ $g\sigma$ $h\sigma$ $p\pi$	0.353 8.01 <sup>-4</sup> 3.45 <sup>-2</sup> 4.19 <sup>-4</sup> 7.19 <sup>-4</sup> 3.45 <sup>-5</sup> 9.05 <sup>-4</sup> 1.57 <sup>-2</sup> 5.51 <sup>-5</sup> 2.88 <sup>-3</sup>	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup> 5.46 <sup>-4</sup> 1.46 <sup>-2</sup> 3.94 <sup>-5</sup> 1.87 <sup>-3</sup>	0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup> 3.51 <sup>-4</sup> 1.34 <sup>-2</sup> 2.60 <sup>-5</sup> 1.04 <sup>-3</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup> 2.80 <sup>-4</sup> 1.19 <sup>-2</sup> 1.58 <sup>-5</sup> 4.97 <sup>-4</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup> 2.67 <sup>-4</sup> 1.03 <sup>-2</sup> 9.29 <sup>-6</sup> 2.25 <sup>-4</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup> 3.72 <sup>-4</sup> 8.83 <sup>-3</sup> 5.87 <sup>-6</sup> 1.17 <sup>-4</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup> 7.48 <sup>-3</sup> 3.98 <sup>-6</sup> 6.09 <sup>-5</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup> 1.38 <sup>-4</sup> 6.11 <sup>-3</sup> 2.64 <sup>-6</sup> 2.47 <sup>-5</sup>
$ \frac{\epsilon \text{ (Ry)}}{s\sigma} $ $ \frac{s\sigma}{p\sigma} $ $ d\sigma $ $ f\sigma $ $ g\sigma $ $ h\sigma $ $ p\pi $ $ d\pi $	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup> 5.04 <sup>-4</sup> 1.50 <sup>-2</sup> 3.87 <sup>-5</sup> 2.14 <sup>-3</sup> 1.93 <sup>-4</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup> 1.02 <sup>-5</sup> 3.39 <sup>-4</sup> 1.40 <sup>-2</sup> 2.67 <sup>-5</sup> 1.27 <sup>-3</sup> 1.59 <sup>-4</sup>	0.476  3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup> 3.32 <sup>-4</sup> 1.27 <sup>-2</sup> 1.69 <sup>-5</sup> 6.38 <sup>-4</sup> 1.23 <sup>-4</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup> 3.16 <sup>-4</sup> 1.12 <sup>-2</sup> 9.86 <sup>-6</sup> 2.91 <sup>-4</sup> 8.36 <sup>-5</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup> 3.63 <sup>-4</sup> 9.66 <sup>-3</sup> 5.81 <sup>-6</sup> 1.51 <sup>-4</sup> 4.60 <sup>-5</sup>	0.743 0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup> 3.54 <sup>-4</sup> 8.32 <sup>-3</sup> 3.75 <sup>-6</sup> 9.15 <sup>-5</sup> 1.98 <sup>-5</sup>	0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup> 1.63 <sup>-4</sup> 7.02 <sup>-3</sup> 4.34 <sup>-5</sup> 7.65 <sup>-6</sup>	3.89 <sup>-3</sup> 1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup> 5.17 <sup>-7</sup> 1.38 <sup>-4</sup> 5.65 <sup>-6</sup> 1.79 <sup>-5</sup> 3.35 <sup>-6</sup>	$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{\sigma}{s\sigma}$	1.04 <sup>-2</sup> 0.353 8.01 <sup>-4</sup> 3.45 <sup>-2</sup> 4.19 <sup>-4</sup> 7.19 <sup>-4</sup> 3.45 <sup>-5</sup> 9.05 <sup>-4</sup> 1.57 <sup>-2</sup> 5.51 <sup>-5</sup> 2.88 <sup>-3</sup> 2.45 <sup>-4</sup>	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup> 5.46 <sup>-4</sup> 1.46 <sup>-2</sup> 3.94 <sup>-5</sup> 1.87 <sup>-3</sup> 2.02 <sup>-4</sup>	1.00 <sup>-2</sup> 0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup> 3.51 <sup>-4</sup> 1.34 <sup>-2</sup> 2.60 <sup>-5</sup> 1.04 <sup>-3</sup> 1.61 <sup>-4</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup> 2.80 <sup>-4</sup> 1.158 <sup>-5</sup> 4.97 <sup>-4</sup> 1.16 <sup>-4</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup> 2.67 <sup>-4</sup> 1.03 <sup>-2</sup> 9.29 <sup>-6</sup> 6.99 <sup>-5</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup> 3.72 <sup>-4</sup> 8.83 <sup>-3</sup> 5.87 <sup>-6</sup> 1.117 <sup>-4</sup> 3.30 <sup>-5</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup> 2.57 <sup>-4</sup> 7.48 <sup>-3</sup> 3.98 <sup>-6</sup> 6.09 <sup>-5</sup> 1.27 <sup>-5</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup> 1.38 <sup>-4</sup> 6.11 <sup>-3</sup> 2.64 <sup>-6</sup> 2.47 <sup>-5</sup> 5.16 <sup>-6</sup>
$\frac{\epsilon \text{ (Ry)}}{s\sigma}$ $\frac{s\sigma}{p\sigma}$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$	0.353 5.35 <sup>-4</sup> 2.89 <sup>-2</sup> 2.68 <sup>-4</sup> 8.43 <sup>-4</sup> 1.92 <sup>-5</sup> 5.04 <sup>-4</sup> 1.50 <sup>-2</sup> 3.87 <sup>-5</sup> 2.14 <sup>-3</sup> 1.93 <sup>-4</sup>	0.410 4.57 <sup>-4</sup> 2.25 <sup>-2</sup> 2.20 <sup>-4</sup> 8.00 <sup>-4</sup> 1.02 <sup>-5</sup> 3.39 <sup>-4</sup> 1.40 <sup>-2</sup> 2.67 <sup>-5</sup> 1.27 <sup>-3</sup> 1.59 <sup>-4</sup>	0.476  3.87 <sup>-4</sup> 1.67 <sup>-2</sup> 1.86 <sup>-4</sup> 7.90 <sup>-4</sup> 5.25 <sup>-6</sup> 3.32 <sup>-4</sup> 1.27 <sup>-2</sup> 1.69 <sup>-5</sup> 6.38 <sup>-4</sup> 1.23 <sup>-4</sup>	8.01 <sup>-3</sup> 0.552 3.27 <sup>-4</sup> 1.17 <sup>-2</sup> 1.55 <sup>-4</sup> 8.06 <sup>-4</sup> 2.34 <sup>-6</sup> 3.16 <sup>-4</sup> 1.12 <sup>-2</sup> 9.86 <sup>-6</sup> 2.91 <sup>-4</sup> 8.36 <sup>-5</sup>	7.33 <sup>-3</sup> 0.640 2.73 <sup>-4</sup> 7.74 <sup>-3</sup> 1.17 <sup>-4</sup> 7.26 <sup>-4</sup> 8.23 <sup>-7</sup> 3.63 <sup>-4</sup> 9.66 <sup>-3</sup> 5.81 <sup>-6</sup> 1.51 <sup>-4</sup> 4.60 <sup>-5</sup>	0.743 2.23 <sup>-4</sup> 4.95 <sup>-3</sup> 7.38 <sup>-5</sup> 4.77 <sup>-4</sup> 5.64 <sup>-7</sup> 3.54 <sup>-4</sup> 8.32 <sup>-3</sup> 3.75 <sup>-6</sup> 9.15 <sup>-5</sup>	0.862 1.76 <sup>-4</sup> 2.98 <sup>-3</sup> 4.16 <sup>-5</sup> 2.58 <sup>-4</sup> 7.92 <sup>-7</sup> 1.63 <sup>-4</sup> 7.02 <sup>-3</sup> 4.34 <sup>-5</sup> 7.65 <sup>-6</sup>	3.89 <sup>-3</sup> 1.000 1.37 <sup>-4</sup> 1.59 <sup>-3</sup> 2.40 <sup>-5</sup> 1.73 <sup>-4</sup> 5.17 <sup>-7</sup> 1.38 <sup>-4</sup> 5.65 <sup>-6</sup> 1.79 <sup>-5</sup> 3.35 <sup>-6</sup>	ε (Ry)  sσ  pσ  dσ  fσ  gσ  hσ  hσ  pπ  dπ  fπ	1.04 <sup>-2</sup> 0.353 8.01 <sup>-4</sup> 3.45 <sup>-2</sup> 4.19 <sup>-4</sup> 7.19 <sup>-4</sup> 3.45 <sup>-5</sup> 9.05 <sup>-4</sup> 1.57 <sup>-2</sup> 5.51 <sup>-5</sup> 2.88 <sup>-3</sup> 2.45 <sup>-4</sup>	0.410 6.85 <sup>-4</sup> 2.72 <sup>-2</sup> 3.17 <sup>-4</sup> 6.81 <sup>-4</sup> 1.80 <sup>-5</sup> 5.46 <sup>-4</sup> 1.46 <sup>-2</sup> 3.94 <sup>-5</sup> 1.87 <sup>-3</sup>	1.00 <sup>-2</sup> 0.476 5.73 <sup>-4</sup> 2.06 <sup>-2</sup> 2.45 <sup>-4</sup> 6.62 <sup>-4</sup> 8.68 <sup>-6</sup> 3.51 <sup>-4</sup> 1.34 <sup>-2</sup> 2.60 <sup>-5</sup> 1.04 <sup>-3</sup> 1.61 <sup>-4</sup>	9.67 <sup>-3</sup> 0.552 4.73 <sup>-4</sup> 1.47 <sup>-2</sup> 1.94 <sup>-4</sup> 6.44 <sup>-4</sup> 4.01 <sup>-6</sup> 2.80 <sup>-4</sup> 1.158 <sup>-5</sup> 4.97 <sup>-4</sup> 1.16 <sup>-4</sup>	9.07 <sup>-3</sup> 0.640 3.88 <sup>-4</sup> 9.89 <sup>-3</sup> 1.50 <sup>-4</sup> 6.32 <sup>-4</sup> 1.70 <sup>-6</sup> 2.67 <sup>-4</sup> 1.03 <sup>-2</sup> 9.29 <sup>-6</sup> 6.99 <sup>-5</sup>	8.18 <sup>-3</sup> 0.743 3.15 <sup>-4</sup> 6.30 <sup>-3</sup> 1.04 <sup>-4</sup> 5.27 <sup>-4</sup> 7.82 <sup>-7</sup> 3.72 <sup>-4</sup> 8.83 <sup>-3</sup> 5.87 <sup>-6</sup> 1.117 <sup>-4</sup> 3.30 <sup>-5</sup>	0.862 2.49 <sup>-4</sup> 3.84 <sup>-3</sup> 6.04 <sup>-5</sup> 3.30 <sup>-4</sup> 8.95 <sup>-7</sup> 2.57 <sup>-4</sup> 7.48 <sup>-3</sup> 3.98 <sup>-6</sup> 6.09 <sup>-5</sup> 1.27 <sup>-5</sup>	1.000 1.91 <sup>-4</sup> 2.15 <sup>-3</sup> 3.27 <sup>-5</sup> 1.97 <sup>-4</sup> 7.89 <sup>-7</sup> 1.38 <sup>-4</sup> 6.11 <sup>-3</sup> 2.64 <sup>-6</sup> 2.47 <sup>-5</sup> 5.16 <sup>-6</sup>

$$\hat{A} = L^2 - \frac{R^2}{4} \left( \Delta - \frac{\partial^2}{\partial z^2} \right) - R(\cos \theta_A - \cos \theta_B) - c^2,$$

where L is the orbital angular momentum of the electron. At the united-atom limit R=0,  $\hat{A}$  reduces to  $-L^2$ , and the corresponding eigenvalue is therefore  $A=-\lambda(\lambda+1)$ .

Summarizing, the one electron diatomic orbitals are labeled by two more quantum numbers  $\lambda$ ,  $\mu$ , in addition to energy. Bound states are denoted  $\phi(n\lambda\mu;\mathbf{r},\mathbf{R})$ , with energy eigenvalues  $\epsilon(n\lambda\mu;R) < 0$ , and continuum states

 $\phi(\epsilon \lambda \mu; \mathbf{r}, \mathbf{R})$  with continuous eigenvalues  $\epsilon > 0$ . At each value of R, these wave functions must satisfy the conventional orthogonality relations

$$\langle \phi(n'\lambda'\mu';\mathbf{R}) \big| \phi(n\lambda\mu;\mathbf{R}) \rangle = \delta_{nn'} \delta_{\lambda\lambda'} \delta_{\mu\mu'},$$

$$\langle \phi(\epsilon' \lambda' \mu'; \mathbf{R}) | \phi(n \lambda \mu; \mathbf{R}) \rangle = 0,$$
 (A10)

Table 17. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=4.25\,\mathrm{keV/amu}$ 

TABLE 18. Single differential cross sections (in  $10^{-16} \text{ cm}^2$ ) at E = 4.57 keV/amu

-4.23	ke v/aiiit	1							-4.57	ke v/ami							
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
$s\sigma$	$3.31^{-3}$	$3.28^{-3}$	$3.25^{-3}$	$3.22^{-3}$	$3.19^{-3}$	$3.14^{-3}$	$3.10^{-3}$	$3.04^{-3}$	sσ	$4.72^{-3}$	$4.69^{-3}$	$4.65^{-3}$	$4.61^{-3}$	$4.56^{-3}$	$4.50^{-3}$	$4.43^{-3}$	$4.36^{-3}$
$p\sigma$				$1.76^{-1}$					$p\sigma$							$1.88^{-1}$	
$d\sigma$				$3.85^{-3}$					$d\sigma$							$4.82^{-3}$	
$f\sigma$				$6.48^{-3}$					$f\sigma$							$6.02^{-3}$	
$g\sigma$				$5.37^{-4}$					$g\sigma$	$6.42^{-4}$	$6.38^{-4}$	$6.34^{-4}$	$6.29^{-4}$	$6.23^{-4}$	$6.16^{-4}$	$6.07^{-4}$	$5.97^{-4}$
$h\sigma$				$7.33^{-3}$					$h\sigma$							$8.70^{-3}$	
$p\pi$				$4.48^{-2}$					$p\pi$							$4.68^{-2}$	
$d\pi$				$6.50^{-4}$					$d\pi$							$7.18^{-4}$	
$f\pi$				$2.87^{-2}$					$f\pi$							$3.33^{-2}$	
$g \pi$				$1.86^{-3}$					$g \pi$							$2.07^{-3}$	
$-h\pi$	1.65-2	1.63-2	1.60-2	$1.56^{-2}$	1.53-2	1.49-2	1.45-2	1.41 <sup>-2</sup>	$h\pi$	1.82-2	1.79-2	1.76-2	1.72-2	1.68-2	1.64-2	$1.60^{-2}$	1.55 <sup>-2</sup>
<b>ε</b> (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$				$2.76^{-3}$					$s\sigma$		$4.18^{-3}$		$3.96^{-3}$			$3.52^{-3}$	
$p\sigma$				$1.52^{-1}$					$p\sigma$							$1.51^{-1}$	
$d\sigma$				$3.14^{-3}$					$d\sigma$							$3.56^{-3}$	
$f\sigma$				$5.34^{-3}$					$f\sigma$							$4.92^{-3}$	
$g\sigma$				$4.34^{-4}$					$g\sigma$							$4.57^{-4}$	
$h\sigma$				$5.48^{-3}$					$h\sigma$							$5.72^{-3}$	
$p\pi$				$4.42^{-2}$					$p\pi$							$4.49^{-2}$	
$d\pi$				$4.99^{-4}$					$d\pi$							$4.84^{-4}$	
$f\pi$				$2.03^{-2}$					$f\pi$							$1.99^{-2}$	
$g \pi$				$1.55^{-3}$					$g \pi$	$1.99^{-3}$	$1.94^{-3}$	$1.88^{-3}$	$1.82^{-3}$	$1.75^{-3}$	$1.67^{-3}$	$1.58^{-3}$	$1.48^{-3}$
$-h\pi$	1.37-2	1.33-2	1.29-2	$1.26^{-2}$	1.23-2	1.20-2	1.19-2	1.18 <sup>-2</sup>	$-h\pi$	1.51-2	1.47-2	1.43-2	1.39-2	1.36-2	1.34-2	$1.32^{-2}$	1.32-2
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$	$2.23^{-3}$	$2.10^{-3}$	$1.97^{-3}$	$1.84^{-3}$	$1.71^{-3}$	$1.57^{-3}$	$1.43^{-3}$	$1.29^{-3}$	$s\sigma$	$3.17^{-3}$	$2.98^{-3}$	$2.78^{-3}$	$2.57^{-3}$	$2.37^{-3}$	$2.16^{-3}$	$1.95^{-3}$	$1.75^{-3}$
$p\sigma$	$1.19^{-1}$	$1.10^{-1}$	$1.01^{-1}$	$9.08^{-2}$	$8.04^{-2}$	$6.99^{-2}$	$5.95^{-2}$		$p\sigma$	$1.34^{-1}$	$1.25^{-1}$	$1.14^{-1}$	$1.04^{-1}$	$9.21^{-2}$	$8.03^{-2}$	$6.86^{-2}$	
$d\sigma$	$2.33^{-3}$	$2.14^{-3}$	$1.94^{-3}$	$1.73^{-3}$	$1.51^{-3}$	$1.29^{-3}$	$1.07^{-3}$	$8.54^{-4}$	$d\sigma$							$1.49^{-3}$	
$f\sigma$				$3.31^{-3}$					$f\sigma$							$2.25^{-3}$	
$g\sigma$				$2.06^{-4}$					$g\sigma$							$1.51^{-4}$	
$h\sigma$	$2.93^{-3}$	$2.41^{-3}$	$1.96^{-3}$	$1.64^{-3}$	$1.47^{-3}$	$1.45^{-3}$	$1.48^{-3}$	$1.45^{-3}$	$h\sigma$							$1.43^{-3}$	
$p\pi$				$3.00^{-2}$					$p\pi$							$2.33^{-2}$	
$d\pi$				$2.15^{-4}$					$d\pi$							$1.50^{-4}$	
$f\pi$				$9.00^{-3}$					$f\pi$							$6.58^{-3}$	
$g \pi$				$7.99^{-4}$					$g\pi$							$5.87^{-4}$	
$h\pi$	$1.17^{-2}$	$1.17^{-2}$	$1.16^{-2}$	$1.14^{-2}$	$1.09^{-2}$	$1.00^{-2}$	$8.74^{-3}$	$7.07^{-3}$	$h\pi$	$1.33^{-2}$	$1.33^{-2}$	$1.33^{-2}$	$1.32^{-2}$	$1.28^{-2}$	$1.20^{-2}$	$1.07^{-2}$	$8.88^{-3}$
$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ				6.73 <sup>-4</sup>					sσ							$4.58^{-4}$	
$p\sigma$				$1.79^{-2}$					$p\sigma$							$5.96^{-3}$	
$d\sigma$				$2.58^{-4}$					$d\sigma$							$1.15^{-4}$	
$f\sigma$				$5.56^{-4}$					$f\sigma$							$3.65^{-4}$	
$g\sigma$				$6.44^{-6}$					$g\sigma$							$1.57^{-6}$	
$h\sigma$				$3.22^{-4}$					$h\sigma$							$3.11^{-4}$	
$p\pi$	1.00	1.02	11.0	$1.25^{-2}$	1.07	7.00	, . , .	0.00	$p\pi$							$8.32^{-3}$	
$d\pi$				$2.34^{-5}$					$d\pi$							$8.28^{-6}$	
$f\pi$				$7.87^{-4}$					$f\pi$							$1.04^{-4}$	
$g \pi$				$1.51^{-4}$					$g \pi$							$3.15^{-5}$	
$h\pi$	$5.14^{-3}$	$3.19^{-3}$	$1.55^{-3}$	$4.87^{-4}$	$5.63^{-5}$	$5.09^{-5}$	$1.49^{-4}$	$1.42^{-4}$	$h\pi$	$6.71^{-3}$	$4.42^{-3}$	$2.36^{-3}$	$8.86^{-4}$	$1.56^{-4}$	$2.50^{-5}$	$1.30^{-4}$	$1.68^{-4}$

$$\langle \phi(\epsilon' \lambda' \mu'; \mathbf{R}) | \phi(\epsilon \lambda \mu; \mathbf{R}) \rangle = \delta(\epsilon' - \epsilon) \delta_{\lambda \lambda'} \delta_{\mu \mu'}.$$

The prolate spheroidal quantum numbers  $\lambda$ ,  $\mu$  are analogous to spherical polar quantum number l, m. Numerical calculations show that the orthogonality relations are satisfied better than eight significant digits for  $R \leq 40$  for the wave functions used in our calculation.

## 8. Appendix B: Separation of Angular Couplings

Let us show the separation of angular couplings in molecular orbital (MO) expansion, by transforming the coordinate system from a space-fixed coordinate system to a molecular-rotating coordinate system. Let  $\mathbf{r} = (x, y, z)$  be the coordinate of electron in the space-fixed frame, while

Table 19. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at  $E=4.89\,\mathrm{keV/amu}$ 

Table 20. Single differential cross sections (in  $10^{-16} \,\mathrm{cm^2}$ ) at  $E = 5.21 \,\mathrm{keV/amu}$ 

=4.89	keV/amu	l							= 5.21	keV/amu	1						
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
$s\sigma$	$6.35^{-3}$			$6.21^{-3}$												$7.73^{-3}$	
$p\sigma$				$2.13^{-1}$												$2.24^{-1}$	
$d\sigma$	$6.56^{-3}$	$6.50^{-3}$		$6.36^{-3}$												$7.35^{-3}$	
$f\sigma$	$6.17^{-3}$	$6.14^{-3}$	$6.10^{-3}$	$6.05^{-3}$	$6.00^{-3}$	$5.95^{-3}$	$5.89^{-3}$	$5.82^{-3}$	5	$6.14^{-3}$	$6.11^{-3}$	$6.07^{-3}$	$6.03^{-3}$	$5.99^{-3}$	$5.94^{-3}$	$5.89^{-3}$	$5.83^{-3}$
$g\sigma$				$6.84^{-4}$												$6.96^{-4}$	
$h\sigma$				$9.84^{-3}$												$9.66^{-3}$	
$p\pi$	$4.83^{-2}$	$4.84^{-2}$	$4.85^{-2}$	$4.86^{-2}$	$4.87^{-2}$	$4.88^{-2}$	$4.89^{-2}$	$4.91^{-2}$	$p\pi$	$5.21^{-2}$	$5.21^{-2}$	$5.21^{-2}$	$5.21^{-2}$	$5.21^{-2}$	$5.22^{-2}$	$5.22^{-2}$	$5.22^{-2}$
$d\pi$	9.06	8.97	8.85	$8.72^{-4}$	8.58	8.41	8.22	8.00								$9.17^{-4}$	
$f\pi$	4.74	4.67	4.59 2	$4.49^{-2}$ $2.44^{-3}$	4.39 -	4.27	4.13	3.98 -	3	5.71 2	5.63	5.53 2	5.43	5.30 2	5.16	$5.01^{-2}$ $2.61^{-3}$	4.83
$g\pi$				$1.93^{-2}$						2.77	2.75	2.73	2.71	2.68	2.65	$2.61^{\circ}$ $2.03^{-2}$	2.57
$-h\pi$	2.04	2.00 -	1.97	1.93	1.88	1.84	1.79 -	1.74	$-h\pi$	2.31	2.21 -	2.23	2.18	2.14 -	2.08 -	2.03	1.97
<i>ϵ</i> (Ry)	0.033		0.044	0.051	0.059	0.069	0.080	0.093		0.033		0.044	0.051	0.059		0.080	0.093
$s\sigma$				$5.37^{-3}$		$5.01^{-3}$			$s\sigma$		$7.33^{-3}$		$6.96^{-3}$	$6.75^{-3}$			
$p\sigma$	$2.00^{-1}$	$1.96^{-1}$	$1.92^{-1}$	$1.86^{-1}$	$1.81^{-1}$	$1.74^{-1}$	$1.67^{-1}$	$1.58^{-1}$	$p\sigma$	$2.18^{-1}$	$2.13^{-1}$	$2.09^{-1}$	$2.03^{-1}$	$1.97^{-1}$	$1.90^{-1}$	$1.82^{-1}$	$1.73^{-1}$
$d\sigma$				$5.25^{-3}$												$5.54^{-3}$	
$f\sigma$				$5.46^{-3}$												$5.32^{-3}$	
$g\sigma$				$6.16^{-4}$												$6.13^{-4}$	
$h\sigma$	$9.35^{-3}$	$9.15^{-3}$	$8.90^{-3}$	$8.58^{-3}$	$8.18^{-3}$	$7.68^{-3}$	$7.08^{-3}$	$6.37^{-3}$								$7.87^{-3}$	
$p\pi$				$4.92^{-2}$												$5.08^{-2}$	
$d\pi$				$6.84^{-4}$							$8.37^{-4}$						
$f\pi$	$3.81^{-2}$	$3.63^{-2}$	$3.43^{-2}$	$3.21^{-2}$	$2.98^{-2}$	$2.73^{-2}$	$2.48^{-2}$	$2.22^{-2}$	3	$4.64^{-2}$	$4.42^{-2}$	$4.18^{-2}$	$3.92^{-2}$	$3.64^{-2}$	$3.35^{-2}$	$3.04^{-2}$	$2.72^{-2}$
$g\pi$	$2.26^{-3}$	2.21	2.15	$2.08^{-3}$ $1.56^{-2}$	$2.01^{-3}$	1.92	1.83	$1.72^{-3}$	0	$2.52^{-3}$	$2.46^{-3}$	$2.40^{-3}$	2.33	$2.25^{-3}$	$2.16^{-3}$	$2.06^{-3}$ $1.70^{-2}$	1.95
$h\pi$	1.69 -	1.64	1.60 -2	1.56	1.53	1.51	1.50 -2	1.50	$h\pi$	1.92 -	1.86 -2	1.81 -	1.77	1.73	1.71 -2	1.70 2	1.70 -2
<i>ε</i> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$				$3.49^{-3}$												$3.39^{-3}$	
$p\sigma$				$1.16^{-1}$												$8.77^{-2}$	
$d\sigma$				$2.95^{-3}$												$2.41^{-3}$	
$f\sigma$				$4.24^{-3}$												$3.41^{-3}$	
$g\sigma$				$3.34^{-4}$												$2.35^{-4}$	
$h\sigma$				$2.86^{-3}$												$1.47^{-3}$	
$p\pi$	$4.54^{-2}$	$4.34^{-2}$	$4.09^{-2}$	$3.77^{-2}$	$3.41^{-2}$	$3.02^{-2}$	$2.62^{-2}$	$2.25^{-2}$	$p\pi$	$4.86^{-2}$	$4.68^{-2}$	$4.44^{-2}$	$4.14^{-2}$	$3.77^{-2}$	$3.36^{-2}$	$2.92^{-2}$	$2.50^{-2}$
$d\pi$	$4.65^{-4}$	$4.15^{-4}$	3.63-4	$3.13^{-4}$	$2.65^{-4}$	$2.20^{-4}$	$1.80^{-4}$	$1.45^{-4}$								$2.10^{-4}$	
$f\pi$				$1.26^{-2}$					$f\pi$							$8.55^{-3}$	
$g\pi$				$1.19^{-3}$ $1.53^{-2}$					0							$8.63^{-4}$ $1.51^{-2}$	
$-h\pi$	1.51	1.52	1.53	1.53	1.49 -	1.41 -	1.28	1.08 -	$h\pi$	1.72 -	1.74	1.76	1.76	1.73	1.65	1.51	1.30 -2
<i>ε</i> (Ry)	0.353					0.743	0.862	1.000	<i>ε</i> (Ry)	0.353	0.410		0.552	0.640	0.743	0.862	1.000
$s\sigma$	$2.03^{-3}$	$1.75^{-3}$	$1.48^{-3}$	$1.22^{-3}$	$9.82^{-4}$	$7.73^{-4}$	$5.98^{-4}$				$2.24^{-3}$		$1.56^{-3}$			$7.64^{-4}$	
$p\sigma$	$5.34^{-2}$	$4.24^{-2}$	$3.28^{-2}$	$2.45^{-2}$	$1.75^{-2}$	$1.17^{-2}$	$7.27^{-3}$	$4.22^{-3}$	$p\sigma$							$8.70^{-3}$	
$d\sigma$	$1.29^{-3}$	$9.86^{-4}$	$7.15^{-4}$	$4.95^{-4}$	$3.35^{-4}$	$2.26^{-4}$	$1.48^{-4}$	$8.73^{-5}$	$d\sigma$							$1.87^{-4}$	
$f\sigma$	$1.41^{-3}$	$8.15^{-4}$	$5.23^{-4}$	$4.59^{-4}$	$4.30^{-4}$	$3.71^{-4}$	$3.28^{-4}$	$2.65^{-4}$	$f\sigma$							$2.89^{-4}$	
$g\sigma$	$1.05^{-4}$	$6.63^{-5}$	$3.54^{-5}$	$1.59^{-5}$	$6.69^{-6}$	$3.49^{-6}$	$2.34^{-6}$	$1.81^{-6}$	$g\sigma$	$1.33^{-4}$	$8.80^{-5}$	$4.99^{-5}$	$2.36^{-5}$	$9.80^{-6}$	$4.73^{-6}$	$3.23^{-6}$	$2.39^{-6}$
$h\sigma$	$1.30^{-3}$	$1.15^{-3}$	$8.72^{-4}$	$5.65^{-4}$	$3.21^{-4}$	$1.92^{-4}$	$2.39^{-4}$	$2.66^{-4}$	$h\sigma$							$1.91^{-4}$	
$p\pi$	$1.94^{-2}$	$1.70^{-2}$	$1.52^{-2}$	$1.36^{-2}$	$1.21^{-2}$	$1.04^{-2}$	$8.74^{-3}$	$7.25^{-3}$	$p\pi$							$9.14^{-3}$	
$d\pi$				$4.23^{-5}$												$1.43^{-5}$	
$f\pi$				$1.54^{-3}$					<i>j</i>							$1.92^{-4}$	
$g\pi$				$2.24^{-4}$												$6.25^{-5}$	
$h\pi$	8.44	5.81	3.34 <sup>-3</sup>	$1.43^{-3}$	3.43	2.23	1.01	1.81	$h\pi$	1.03	7.36	4.47	2.11	6.29	5.99	$6.72^{-5}$	1.81

 $\mathbf{r}' = (x', y', z')$  denotes the same vector in the rotating molecular frame. The relation between these two is then given by

$$x' = x \cos \Theta \cos \Phi + y \cos \Theta \sin \Phi - z \sin \Theta$$
, (B1)

$$y' = -x \sin \Phi + y \cos \Phi, \tag{B2}$$

$$z' = x \sin \Theta \cos \Phi + y \sin \Theta \sin \Phi + z \cos \Theta$$
. (B3)

Here  $(\Theta,\Phi)$  are the usual spherical polar angles of the vector **R** in the space-fixed frame. In the spherical polar coordinates, the gradient  $-i\nabla^R$  (while keeping **r** fixed) can be written as

$$-i\nabla_{R} = \mathbf{e}_{R}(-i\partial/\partial R)_{xyz} + \mathbf{e}_{\Theta}R^{-1}(-i\partial/\partial \Theta)_{xyz} + \mathbf{e}_{\Phi}(R\sin\Theta)^{-1}(-i\partial/\partial \Theta)_{xyz},$$
(B4)

where  $\mathbf{e}_R$ ,  $\mathbf{e}_\Theta$ , and  $\mathbf{e}_\Phi$  are the unit vectors of the spherical

Table 21. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=5.53\,\mathrm{keV/amu}$ 

Table 22. Single differential cross sections (in  $10^{-16} \text{ cm}^2$ ) at E = 5.85 keV/amu

- 5.55	KC V/aiiiu	1							- 3.63	Ke v/aiii	u						
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018		0.024	0.028	$\epsilon$ (Ry)		0.012	0.013	0.016	0.018		0.024	0.028
$s\sigma$	$1.03^{-2}$			$1.00^{-2}$			$9.68^{-3}$	$9.53^{-3}$	$s\sigma$	$1.27^{-2}$	$1.26^{-2}$		$1.24^{-2}$				$1.17^{-2}$
$p\sigma$	$2.55^{-1}$	$2.53^{-1}$	$2.51^{-1}$	$2.50^{-1}$	$2.47^{-1}$	$2.45^{-1}$	$2.42^{-1}$	$2.39^{-1}$	$p\sigma$	$2.72^{-1}$	$2.71^{-1}$	$2.69^{-1}$	$2.67^{-1}$	$2.65^{-1}$	$2.62^{-1}$	$2.59^{-1}$	$2.56^{-1}$
$d\sigma$	$9.24^{-3}$	$9.17^{-3}$	$9.09^{-3}$	$9.00^{-3}$	$8.90^{-3}$	$8.78^{-3}$	$8.64^{-3}$	$8.48^{-3}$	$d\sigma$		$1.05^{-2}$			$1.02^{-2}$			
$f\sigma$	$6.49^{-3}$	$6.45^{-3}$	$6.40^{-3}$	$6.35^{-3}$	$6.29^{-3}$	$6.22^{-3}$	$6.16^{-3}$		$f\sigma$		$7.19^{-3}$			$6.96^{-3}$		$6.77^{-3}$	$6.67^{-3}$
$g\sigma$	$6.91^{-4}$	$6.91^{-4}$	$6.91^{-4}$	$6.92^{-4}$					$g\sigma$	6.69-4	$6.69^{-4}$	$6.70^{-4}$	$6.71^{-4}$	$6.72^{-4}$	$6.73^{-4}$	$6.74^{-4}$	$6.75^{-4}$
$h\sigma$				$9.10^{-3}$ $5.75^{-2}$					$h\sigma$	8.38	$8.41^{-3}$ $6.57^{-2}$	8.43	8.46	$8.49^{-3}$	8.52	$8.55^{-3}$ $6.36^{-2}$	$8.57^{-3}$ $6.31^{-2}$
$p\pi$				$1.06^{-3}$					$p\pi$		$6.57^{-2}$ $1.17^{-3}$					0.36	$1.05^{-3}$
$d\pi$ $f\pi$	$6.74^{-2}$	6.65-2	6.54-2	$6.42^{-2}$	6.29-2	6.12-2	5.05-2	9.77 5.75 <sup>-2</sup>	$d\pi$ $f\pi$	7.02-2	$7.72^{-2}$	7.13	7.47-2	7.22-2	$7.15^{-2}$	6.05-2	6.72-2
$g\pi$				$2.96^{-3}$					$g\pi$	3.28 <sup>-3</sup>	$3.26^{-3}$	$3.24^{-3}$	$3.21^{-3}$	$\frac{7.32}{3.17^{-3}}$	$\frac{7.13}{3.14^{-3}}$	$3.10^{-3}$	$3.05^{-3}$
$\overset{g}{h}\pi$				$2.48^{-2}$					$h\pi$	$2.97^{-2}$	$2.92^{-2}$	$2.87^{-2}$	$2.81^{-2}$	$2.74^{-2}$	$2.67^{-2}$	$2.60^{-2}$	$2.52^{-2}$
	2.00	2.00	2.00			2.07						2.07	2.01		2.07	2.00	
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)		0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$	$9.37^{-3}$			$8.72^{-3}$					$s\sigma$		$1.13^{-2}$						
$p\sigma$				$2.20^{-1}$					$p\sigma$		$2.47^{-1}$						
$d\sigma$				$7.60^{-3}$					$d\sigma$		$9.33^{-3}$						
$f\sigma$				$5.81^{-3}$ $6.83^{-4}$					$f\sigma$		$6.46^{-3}$ $6.77^{-4}$						
$g\sigma$				$6.83^{-3}$ $8.89^{-3}$				0.00	$g\sigma$		$8.57^{-3}$					$6.67^{-4}$ $7.88^{-3}$	
$h\sigma$				$5.57^{-2}$					$h\sigma$	6.25-2	$6.19^{-2}$	8.54 5 6.12 <sup>-2</sup>	6.05-2	8.35 5 5.07 <sup>-2</sup>	5.20 <sup>-2</sup>	7.88 5 5.70 <sup>-2</sup>	7.49 5 5.67 <sup>-2</sup>
$p\pi$ $d\pi$				$8.42^{-4}$					$d\pi$		$9.87^{-4}$						
$f\pi$				$4.71^{-2}$					$f\pi$		$6.20^{-2}$						
$g\pi$				$2.56^{-3}$					$g\pi$		$2.93^{-3}$						
$\overset{s}{h}\pi$				$2.00^{-2}$					$\overset{s}{h}\pi$	$2.45^{-2}$	$2.37^{-2}$	$2.30^{-2}$	$2.24^{-2}$	$2.20^{-2}$	$2.16^{-2}$	$2.15^{-2}$	$2.16^{-2}$
$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$7.12^{-3}$	$6.71^{-3}$	$6.27^{-3}$	$5.81^{-3}$	5.32-3	$4.82^{-3}$	$4.30^{-3}$	$3.79^{-3}$	sσ	$8.72^{-3}$	8.23-3	$7.70^{-3}$	$7.15^{-3}$	$6.57^{-3}$	$5.96^{-3}$	5.33-3	$4.70^{-3}$
$p\sigma$				$1.41^{-1}$					ρσ		$1.80^{-1}$						
$d\sigma$	$5.78^{-3}$	$5.33^{-3}$	$4.85^{-3}$	$4.36^{-3}$	$3.86^{-3}$	$3.37^{-3}$	$2.90^{-3}$	$2.44^{-3}$	$d\sigma$	$6.79^{-3}$	$6.26^{-3}$	$5.71^{-3}$	$5.14^{-3}$	$4.55^{-3}$	$3.97^{-3}$	$3.41^{-3}$	$2.88^{-3}$
$f\sigma$				$4.97^{-3}$					$f\sigma$		$5.75^{-3}$						
$g\sigma$				$4.76^{-4}$					$g\sigma$		$6.15^{-4}$						
$h\sigma$				$4.18^{-3}$					$h\sigma$	$6.95^{-3}$	$6.27^{-3}$	$5.44^{-3}$	$4.51^{-3}$	$3.55^{-3}$	$2.65^{-3}$	$1.93^{-3}$	$1.45^{-3}$
$p\pi$				$4.48^{-2}$					$p\pi$		$5.34^{-2}$						
$d\pi$				$4.03^{-4}$					$d\pi$		$5.74^{-4}$						
$f\pi$				$1.80^{-2}$					$f\pi$		$3.01^{-2}$						
$g\pi$				$1.58^{-3} \\ 2.01^{-2}$					$g\pi$		$2.10^{-3}$ $2.22^{-2}$						
$-h\pi$	1.95	1.97	2.00	2.01	1.99	1.91	1./6	1.53	$h\pi$	2.18	2.22	2.25	2.21	2.26	2.18	2.02	1./8
$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
sσ	$3.29^{-3}$	$2.80^{-3}$	$2.35^{-3}$	$1.94^{-3}$					sσ		$3.46^{-3}$					$1.17^{-3}$	$8.80^{-4}$
$p\sigma$	$6.78^{-2}$	$5.42^{-2}$	$4.20^{-2}$	$3.15^{-2}$			$1.02^{-2}$	$6.09^{-3}$	$p\sigma$	$7.53^{-2}$			$3.53^{-2}$		$1.79^{-2}$	$1.18^{-2}$	$7.15^{-3}$
$d\sigma$				$8.61^{-4}$					$d\sigma$		$1.91^{-3}$						
$f\sigma$	$2.41^{-3}$	$1.59^{-3}$	$9.04^{-4}$	$5.12^{-4}$	$3.90^{-4}$	$3.37^{-4}$	$2.65^{-4}$	$2.24^{-4}$	$f\sigma$		$1.97^{-3}$						
$g\sigma$				$3.32^{-5}$					$g\sigma$	$2.01^{-4}$	$1.39^{-4}$	$8.60^{-5}$	$4.49^{-5}$	$1.96^{-5}$	$8.33^{-6}$	$4.99^{-6}$	$3.81^{-6}$
$h\sigma$		$1.02^{-3}$		$6.46^{-4}$					$h\sigma$		$9.96^{-4}$						
$p\pi$				$1.48^{-2}$					$p\pi$		$2.13^{-2}$						
$d\pi$				$6.37^{-5}$					$d\pi$		$1.35^{-4}$						
$f\pi$				$2.38^{-3}$ $3.03^{-4}$					$f\pi$		$5.47^{-3}$ $5.89^{-4}$						
$g\pi$				$3.03^{-4}$ $2.92^{-3}$					$g\pi$		$1.09^{-2}$						
$h\pi$	1.24 -	9.08	3.75	2.92	1.02	1.51	3.98	1.08	$h\pi$	1.46	1.09 2	/.1/	3.8/	1.51	3.06	2.86	1.40

polar system at **R** (they coincide with the z', x', and y', respectively). Using Eqs. (B1)–(B3) the components of this operator can be rewritten

$$-i(\partial/\partial R)_{xyz} = -i(\partial/\partial R)_{x'y'z'}, \tag{B5}$$

$$-i(\partial/\partial\Theta)_{xyz} = -i(\partial/\partial\Theta)_{x'y'z'} - \hat{L}_{y'}, \qquad (B6)$$

$$-i(\partial/\partial\Phi)_{xyz} = -i(\partial/\partial\Phi)_{x'y'z'} + [\sin\Theta\hat{L}_{x'} - \cos\Theta\hat{L}_{z'}],$$
(B7)

where  $L_{x',y',z'}$  are the components of the electronic orbital angular momentum operator. The vector **P** is therefore expressed as <sup>14</sup>

$$\mathbf{P}_{k'k} = P_{k'k}^R \mathbf{e}_R + P_{k'k}^{\Theta} \mathbf{e}_{\Theta} + P_{k'k}^{\Phi} \mathbf{e}_{\Phi} , \qquad (B8)$$

where

$$P_{k'k}^{R} = \langle \phi_{k'} | (-i\partial/\partial R) | \phi_{k} \rangle,$$

$$P_{k'k}^{\Theta} = -R^{-1} \langle \phi_{k'} | \hat{L}_{y'} | \phi_{k} \rangle,$$
(B9)

Table 23. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=6.17\,\mathrm{keV/amu}$ 

Table 24. Single differential cross sections (in  $10^{-16}$  cm<sup>2</sup>) at E = 6.49 keV/amu

- 0.17	KC v/aiiiu	l.							- 0.49	Ke v/aiii							
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)		0.012	0.013	0.016	0.018	0.021	0.024	0.028
$s\sigma$				$1.51^{-2}$					$s\sigma$	$1.88^{-2}$	$1.86^{-2}$		$1.83^{-2}$				$1.72^{-2}$
$p\sigma$	$2.90^{-1}$	$2.89^{-1}$	$2.87^{-1}$	$2.85^{-1}$	$2.82^{-1}$	$2.79^{-1}$	$2.76^{-1}$	$2.72^{-1}$	$p\sigma$	$3.07^{-1}$	$3.06^{-1}$	$3.04^{-1}$	$3.02^{-1}$	$2.99^{-1}$	$2.96^{-1}$	$2.93^{-1}$	$2.89^{-1}$
$d\sigma$				$1.15^{-2}$					$d\sigma$	$1.29^{-2}$	$1.29^{-2}$	$1.28^{-2}$	$1.27^{-2}$	$1.26^{-2}$	$1.24^{-2}$	$1.23^{-2}$	$1.21^{-2}$
$f\sigma$				$8.06^{-3}$					$f\sigma$							$8.81^{-3}$	
$g\sigma$				$6.53^{-4}$					$g\sigma$							$6.48^{-4}$	
$h\sigma$				$8.29^{-3}$					$h\sigma$							$8.90^{-3}$	
$p\pi$				$7.50^{-2}$					$p\pi$							$8.36^{-2}$	
$d\pi$	$1.25^{-3}$	$1.24^{-3}$	$1.22^{-3}$	$1.21^{-3}$	$1.19^{-3}$	$1.17^{-3}$	$1.14^{-3}$	$1.11^{-3}$	$d\pi$	$1.31^{-3}$	$1.30^{-3}$	$1.28^{-3}$	$1.27^{-3}$	$1.25^{-3}$	$1.23^{-3}$	$1.20^{-3}$	$1.17^{-3}$
$f\pi$				$8.58^{-2}$					$f\pi$							$9.12^{-2}$	
$g\pi$				$3.45^{-3}$ $3.14^{-2}$					$g\pi$							$3.58^{-3}$ $3.20^{-2}$	
$-h\pi$	3.33	3.28	3.21	3.14	3.07	2.99	2.90	2.82	$-h\pi$	3.09	3.03	3.30	3.48	3.39	3.30	3.20	3.10
<b>ε</b> (Ry)		0.038	0.044		0.059	0.069	0.080	0.093	$\epsilon$ (Ry)		0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$				$1.29^{-2}$					$s\sigma$							$1.37^{-2}$	
$p\sigma$				$2.51^{-1}$					$p\sigma$							$2.41^{-1}$	
$d\sigma$				$9.98^{-3}$					$d\sigma$							$9.94^{-3}$	
$f\sigma$				$6.94^{-3}$					$f\sigma$							$7.25^{-3}$	
$g\sigma$				$6.63^{-4}$					$g\sigma$							$6.54^{-4}$	
$h\sigma$	8.35	8.34	8.31	$8.24^{-3}$ $6.68^{-2}$	8.12	$7.95^{-3}$	$7.69^{-3}$	7.33	$h\sigma$	8.85	8.79	8.71	8.60	8.43	8.20	$7.88^{-3}$ $6.84^{-2}$	$7.46^{-3}$
$p\pi$				6.68 <sup>2</sup> 9.67 <sup>-4</sup>					$p\pi$							6.84 <sup>2</sup> 8.54 <sup>-4</sup>	
$d\pi$				$6.47^{-2}$					$d\pi$	1.14	1.10	7.05-2	7.42-2	9.68	9.14	$5.95^{-2}$	7.91
$f\pi$				$3.00^{-3}$					$f\pi$							$2.88^{-3}$	
$g \pi h \pi$				$2.49^{-2}$					$g \pi$ $h \pi$	3.45	2.00-2	2.30	3.21	3.11	$3.00^{\circ}$	$2.88$ $2.59^{-2}$	2.75
	2.13	2.04	2.30	2.49	2.43	2.39	2.30	2.36		3.00	2.90	2.01	2.12	2.03	2.01	2.39	
<i>ϵ</i> (Ry)		0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)			0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$			$9.25^{-3}$		$7.92^{-3}$			$5.70^{-3}$	$s\sigma$		$1.17^{-2}$			$9.36^{-3}$			$6.80^{-3}$
$p\sigma$				$1.65^{-1}$					$p\sigma$							$1.26^{-1}$	
$d\sigma$				$5.97^{-3}$					$d\sigma$							$4.56^{-3}$	
$f\sigma$				$5.86^{-3}$					$f\sigma$							$4.95^{-3}$	
$g\sigma$				$5.76^{-4}$					$g\sigma$							$4.38^{-4}$	
$h\sigma$				$4.59^{-3}$					$h\sigma$							$2.22^{-3}$	
$p\pi$				$5.16^{-2}$					$p\pi$							$4.17^{-2}$	
$d\pi$				$4.78^{-4}$ $2.54^{-2}$					$d\pi$							$3.08^{-4}$ $1.53^{-2}$	
$f\pi$				$1.93^{-3}$					$f\pi$							$1.53^{-2}$ $1.45^{-3}$	
$g\pi$				$1.93^{-2}$ $2.54^{-2}$					$g\pi$							$2.58^{-2}$	
$-h\pi$	2.41	2.40	2.31	2.34	2.33	2.40	2.30	2.03	$h\pi$	2.03	2.09	2.73	2.80	2.80	2.74	2.36	2.32
<b>ε</b> (Ry)			0.476	0.552	0.640	0.743	0.862	1.000	<b>ϵ</b> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
$s\sigma$				$2.86^{-3}$				$1.06^{-3}$	$s\sigma$		$5.01^{-3}$						$1.25^{-3}$
$p\sigma$	$8.28^{-2}$	$6.68^{-2}$	$5.22^{-2}$	$3.93^{-2}$	$2.86^{-2}$	$2.01^{-2}$	$1.34^{-2}$	$8.28^{-3}$	$p\sigma$		$7.32^{-2}$					$1.50^{-2}$	
$d\sigma$				$1.30^{-3}$					$d\sigma$							$4.31^{-4}$	
$f\sigma$	$3.07^{-3}$	$2.26^{-3}$	$1.47^{-3}$	$8.21^{-4}$	$4.47^{-4}$	$3.20^{-4}$	$2.50^{-4}$	$1.83^{-4}$	$f\sigma$	$3.34^{-3}$	$2.50^{-3}$	$1.70^{-3}$	$1.00^{-3}$	$5.30^{-4}$	$3.24^{-4}$	$2.47^{-4}$	$1.75^{-4}$
$g\sigma$	$2.39^{-4}$	$1.69^{-4}$	$1.08^{-4}$	$5.88^{-5}$	$2.67^{-5}$	$1.11^{-5}$	$5.95^{-6}$	$4.51^{-6}$	$g\sigma$							$7.14^{-6}$	
$h\sigma$	$1.32^{-3}$	$1.07^{-3}$	$8.15^{-4}$	5.83-4	$4.03^{-4}$	$2.54^{-4}$	$1.85^{-4}$	$1.76^{-4}$	$h\sigma$	$1.51^{-3}$	$1.24^{-3}$	$9.09^{-4}$	$5.89^{-4}$	$3.80^{-4}$	$2.41^{-4}$	$1.74^{-4}$	$1.86^{-4}$
$p\pi$				$1.63^{-2}$					$p\pi$							$1.07^{-2}$ $3.02^{-5}$	
$d\pi$				$8.46^{-5}$ $3.25^{-3}$					$d\pi$							$3.02^{-3}$ $6.38^{-4}$	
$f\pi$				$3.25^{\circ}$ $3.91^{-4}$					$f\pi$							$6.38^{-4}$ $1.46^{-4}$	
$g\pi$				$\frac{3.91}{4.93^{-3}}$					$g\pi$							8.86 <sup>-5</sup>	
$h\pi$	1./0	1.29	0.12	4.93	2.11	3.21	4.23	1.20	$h\pi$	1.95	1.31	1.04 -	0.10	2.19	0.19	0.00	9.28

$$P_{k'k}^{\Phi} = +R^{-1}\langle \phi_{k'}|\hat{L}_{x'}|\phi_k\rangle - \mu_k$$

[assuming that  $\varphi_k$  is an eigenstate of  $L_{z'}$  with eigenvalue  $\mu_k(h/2\pi)$ ]. The corresponding form for **A** is obtained simply by expressing the vector **s** in terms of its components on the x', y', z' axes:

$$A_{k'k}^{R} = i(\epsilon_{k'} - \epsilon_{k}) \langle \phi_{k'} | s_{z'} | \phi_{k} \rangle,$$
  

$$A_{k'k}^{\Theta} = i(\epsilon_{k'} - \epsilon_{k}) \langle \phi_{k'} | s_{x'} | \phi_{k} \rangle,$$

$$A_{k'k}^{\Phi} = i(\epsilon_{k'} - \epsilon_{k}) \langle \phi_{k'} | s_{y'} | \phi_{k} \rangle,$$

$$\mathbf{s} = \frac{1}{2} (f + \lambda) [\mathbf{r} - \frac{1}{4} (f + \lambda) \mathbf{R}],$$

$$\lambda \equiv \frac{M_A - M_B}{M_A + M_B}.$$
(B10)

Given the components of **P** and **A** by Eqs. (B9) and (B10), we can construct explicit solutions to the close-coupled equations for inelastic scattering in a finite manifold of molecular electronic states. The Schrödinger equation can be

Table 25. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=6.81\,\mathrm{keV/amu}$ 

Table 26. Single differential cross sections (in  $10^{-16} \text{ cm}^2$ ) at E = 7.13 keV/amu

$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
$s\sigma$			$2.23^{-2}$	$2.21^{-2}$	$2.18^{-2}$	$2.14^{-2}$	$2.11^{-2}$	$2.06^{-2}$	sσ	$2.74^{-2}$	$2.72^{-2}$	$2.69^{-2}$	$2.65^{-2}$	$2.62^{-2}$	$2.57^{-2}$	$2.53^{-2}$	$2.47^{-2}$
$p\sigma$	$3.24^{-1}$	$3.23^{-1}$	$3.21^{-1}$	$3.18^{-1}$	$3.16^{-1}$	$3.13^{-1}$	$3.09^{-1}$	$3.05^{-1}$	$p\sigma$	$3.41^{-1}$	$3.39^{-1}$	$3.37^{-1}$	$3.35^{-1}$	$3.32^{-1}$	$3.29^{-1}$	$3.25^{-1}$	$3.21^{-1}$
$d\sigma$				$1.38^{-2}$					$d\sigma$							$1.44^{-2}$	
$f\sigma$		$1.08^{-2}$	$1.06^{-2}$	$1.05^{-2}$	$1.04^{-2}$	$1.02^{-2}$	$9.98^{-3}$		$f\sigma$	$1.20^{-2}$	$1.19^{-2}$	$1.18^{-2}$	$1.16^{-2}$	$1.15^{-2}$		$1.11^{-2}$	$1.09^{-2}$
$g\sigma$	$6.75^{-4}$	$6.73^{-4}$	$6.70^{-4}$	$6.67^{-4}$	$6.64^{-4}$	$6.61^{-4}$	$6.57^{-4}$	$6.54^{-4}$	$g\sigma$	$7.18^{-4}$	$7.14^{-4}$	$7.09^{-4}$	$7.04^{-4}$	$6.99^{-4}$	$6.93^{-4}$	$6.86^{-4}$	$6.79^{-4}$
$h\sigma$		$1.06^{-2}$		$1.05^{-2}$					$h\sigma$							$1.31^{-2}$	
$p\pi$				$1.03^{-1}$					$p\pi$							$1.14^{-1}$	
$d\pi$				$1.32^{-3}$					$d\pi$							$1.30^{-3}$	
$f\pi$	$1.14^{-1}$	$1.13^{-1}$	1.11	$1.09^{-1}$	$1.07^{-1}$	$1.05^{-1}$	$1.03^{-1}$	$9.99^{-2}$	$f \pi$	$1.27^{-1}$	$1.25^{-1}$	$1.24^{-1}$	$1.22^{-1}$	$1.20^{-1}$	$1.18^{-1}$	$1.15^{-1}$	$1.12^{-1}$
$g \pi$				$3.99^{-3}$					$g \pi$							$4.13^{-3}$	
$h\pi$	4.03 2	3.96 -2	3.88 2	$3.79^{-2}$	3.70 -2	3.60 2	3.49 2	3.37 -	$h\pi$	4.35 2	4.27	4.18 2	4.09 2	3.98 2	3.87 2	$3.74^{-2}$	3.62 -
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$				$1.84^{-2}$			$1.62^{-2}$	$1.54^{-2}$	$s\sigma$		$2.34^{-2}$						$1.81^{-2}$
$p\sigma$				$2.82^{-1}$					$p\sigma$							$2.69^{-1}$	
$d\sigma$				$1.22^{-2}$					$d\sigma$							$1.21^{-2}$	
$f\sigma$				$8.83^{-3}$					$f\sigma$							$8.96^{-3}$	
$g\sigma$				$6.44^{-4}$					$g\sigma$							$6.42^{-4}$	
$h\sigma$	$1.03^{-2}$	$1.02^{-2}$	$1.00^{-2}$	$9.85^{-3}$	$9.59^{-3}$	$9.25^{-3}$	$8.80^{-3}$	$8.24^{-3}$	$h\sigma$							$1.07^{-2}$	
$p\pi$	$9.27^{-2}$	$9.01^{-2}$	8.74 <sup>-2</sup>	$8.45^{-2}$ $1.06^{-3}$	8.16 <sup>-2</sup>	7.86	$7.55^{-2}$	7.24 <sup>-2</sup>	$p\pi$	$1.07^{-1}$	1.04	$1.00^{-1}$	$9.63^{-2}$	$9.23^{-2}$	8.81	$8.40^{-2}$ $9.31^{-4}$	7.98
$d\pi$	1.19	1.15	1.11	$1.06^{-3}$ $8.45^{-2}$	1.01	9.56	8.95	8.29	$d\pi$								
$f\pi$				$8.45^{-2}$ $3.43^{-3}$					$f\pi$							$7.75^{-2}$ $3.27^{-3}$	
$g\pi$	$3.70^{-2}$	3.62	$3.53^{\circ}$	$2.93^{-2}$	3.32	$3.20^{-3}$	3.07	$2.93^{\circ}$	$g\pi$	3.97	3.88	3.78	3.6/	3.54	3.41	$\frac{3.27}{2.93^{-2}}$	3.11
$h\pi$	3.20	3.14	3.03	2.93	2.85	2.80	2.11	2.78	$h\pi$	3.48	3.33	3.23	3.12	3.03	2.96	2.93	2.93
$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$1.46^{-2}$	$1.37^{-2}$	$1.28^{-2}$	$1.19^{-2}$	$1.09^{-2}$	$9.96^{-3}$	$8.97^{-3}$	$7.96^{-3}$	sσ	$1.70^{-2}$	$1.59^{-2}$	$1.48^{-2}$	$1.37^{-2}$	$1.26^{-2}$	$1.15^{-2}$	$1.04^{-2}$	$9.21^{-3}$
$p\sigma$	$2.32^{-1}$	$2.18^{-1}$	$2.04^{-1}$	$1.88^{-1}$	$1.71^{-1}$	$1.53^{-1}$	$1.35^{-1}$	$1.16^{-1}$	$p\sigma$	$2.45^{-1}$	$2.31^{-1}$	$2.15^{-1}$	$1.99^{-1}$	$1.81^{-1}$	$1.62^{-1}$	$1.43^{-1}$	$1.24^{-1}$
				2								2	0.00 - 3	-00-3			
$d\sigma$					$6.93^{-3}$				$d\sigma$								$4.97^{-3}$
dσ fσ	$7.63^{-3}$	$7.43^{-3}$	$7.23^{-3}$	$6.98^{-3}$	$6.63^{-3}$	$6.13^{-3}$	$5.44^{-3}$	$4.59^{-3}$	$d\sigma$ $f\sigma$	$8.40^{-3}$	$8.14^{-3}$	$7.89^{-3}$	$7.60^{-3}$	$7.24^{-3}$	$6.72^{-3}$	$6.00^{-3}$	$5.07^{-3}$
** **	$7.63^{-3}$ $6.46^{-4}$	$7.43^{-3}$ $6.43^{-4}$	$7.23^{-3}$ $6.35^{-4}$	$6.98^{-3}$ $6.18^{-4}$	$6.63^{-3}$ $5.88^{-4}$	$6.13^{-3}$ $5.41^{-4}$	$5.44^{-3}$ $4.79^{-4}$	$4.59^{-3}$ $4.02^{-4}$		$8.40^{-3}$ $6.41^{-4}$	$8.14^{-3}$ $6.40^{-4}$	$7.89^{-3}$ $6.36^{-4}$	$7.60^{-3}$ $6.25^{-4}$	$7.24^{-3}$ $6.03^{-4}$	$6.72^{-3}$ $5.66^{-4}$	$6.00^{-3}$ $5.12^{-4}$	$5.07^{-3}$ $4.40^{-4}$
$f\sigma$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup>	$7.23^{-3}$ $6.35^{-4}$ $5.72^{-3}$	$6.98^{-3}$ $6.18^{-4}$ $4.68^{-3}$	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup>	$6.13^{-3}$ $5.41^{-4}$ $2.77^{-3}$	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup>	$4.59^{-3}$ $4.02^{-4}$ $1.81^{-3}$	$f\sigma$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup>	$7.60^{-3}$ $6.25^{-4}$ $5.22^{-3}$	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup>	$6.00^{-3}$ $5.12^{-4}$ $2.00^{-3}$	$5.07^{-3}$ $4.40^{-4}$ $1.69^{-3}$
$f\sigma$ $g\sigma$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup>	$4.59^{-3}$ $4.02^{-4}$ $1.81^{-3}$ $3.90^{-2}$	$f\sigma$ $g\sigma$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup>	$8.14^{-3}$ $6.40^{-4}$ $7.87^{-3}$ $7.16^{-2}$	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup>	$7.60^{-3}$ $6.25^{-4}$ $5.22^{-3}$ $6.32^{-2}$	$7.24^{-3}$ $6.03^{-4}$ $3.88^{-3}$ $5.86^{-2}$	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup>	$6.00^{-3}$ $5.12^{-4}$ $2.00^{-3}$ $4.80^{-2}$	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup>	$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup>	fσ gσ hσ pπ dπ fπ	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup>	fσ gσ hσ pπ dπ fπ	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup>	fσ gσ hσ pπ dπ fπ	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup>	fσ gσ hσ pπ dπ fπ	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup>
f σ g σ h σ p π d π f π g π h π	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup> 1.000	f σ g σ h σ p π d π f π g π h π	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640 3.69 <sup>-3</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410 5.90 <sup>-3</sup> 7.96 <sup>-2</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640 3.18 <sup>-3</sup> 3.51 <sup>-2</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743 2.50 <sup>-3</sup> 2.47 <sup>-2</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup> 1.000	$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552 4.64 <sup>-3</sup> 5.23 <sup>-2</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640 3.69 <sup>-3</sup> 3.85 <sup>-2</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup>	1.000 1.69 <sup>-3</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000
$ f\sigma \\ g\sigma \\ h\sigma \\ p\pi \\ d\pi \\ f\pi \\ g\pi \\ h\pi $ $ \frac{\epsilon \text{(Ry)}}{s\sigma} $	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353 6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476 4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640 3.18 <sup>-3</sup> 3.51 <sup>-2</sup> 1.28 <sup>-3</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743  2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.67 <sup>-2</sup> 5.21 <sup>-4</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup>	$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$ $\epsilon \text{ (Ry)}$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552 4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640 3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.64 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.71 <sup>-3</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup> 1.17 <sup>-3</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640  3.18 <sup>-3</sup> 3.51 <sup>-2</sup> 1.28 <sup>-3</sup> 6.33 <sup>-4</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743  2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 3.47 <sup>-4</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup>	4.59 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup> 1.72 <sup>-4</sup>	$ \begin{array}{c} f\sigma \\ g\sigma \\ h\sigma \\ p\pi \\ d\pi \\ f\pi \\ g\pi \\ h\pi \end{array} $ $ \begin{array}{c} \epsilon \text{ (Ry)} \\ s\sigma \\ p\sigma \end{array} $	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.30 <sup>-3</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-4</sup>	5.07 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$ $\epsilon \text{ (Ry)}$ $s\sigma$ $p\sigma$ $d\sigma$ $f\sigma$ $g\sigma$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.64 <sup>-3</sup> 3.19 <sup>-4</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.71 <sup>-3</sup> 2.36 <sup>-4</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup> 1.59 <sup>-4</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup> 1.17 <sup>-3</sup> 9.37 <sup>-5</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640 3.18 <sup>-3</sup> 3.51 <sup>-2</sup> 1.28 <sup>-3</sup> 6.33 <sup>-4</sup> 4.62 <sup>-5</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743 2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 1.94 <sup>-5</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup> 8.70 <sup>-6</sup>	1.81 <sup>-3</sup> 4.02 <sup>-4</sup> 1.81 <sup>-3</sup> 3.90 <sup>-2</sup> 2.68 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup> 1.72 <sup>-4</sup> 5.76 <sup>-6</sup>	$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$ $e (Ry)$ $s\sigma$ $p\sigma$ $d\sigma$ $f\sigma$ $g\sigma$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup> 3.57 <sup>-4</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup> 2.70 <sup>-4</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup> 1.87 <sup>-4</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.30 <sup>-3</sup> 1.15 <sup>-4</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup> 5.91 <sup>-5</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup> 2.55 <sup>-5</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-4</sup>	1.000 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup> 6.41 <sup>-6</sup>
$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$ $e (Ry)$ $s\sigma$ $p\sigma$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.64 <sup>-3</sup> 3.19 <sup>-4</sup> 1.66 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.71 <sup>-3</sup> 2.36 <sup>-4</sup> 1.47 <sup>-3</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup> 1.59 <sup>-4</sup> 1.11 <sup>-3</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup> 9.37 <sup>-5</sup> 6.70 <sup>-4</sup>	6.63-3 5.88-4 3.65-3 5.48-2 4.62-4 2.85-2 2.04-3 3.07-2 0.640 3.18-3 3.51-2 1.28-3 6.33-4 4.62-5 3.76-4	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743 2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 3.47 <sup>-4</sup> 1.94 <sup>-5</sup> 2.29 <sup>-4</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup> 8.70 <sup>-6</sup> 1.56 <sup>-4</sup>	1.000 1.46 <sup>-3</sup> 1.000 1.000 1.72 <sup>-4</sup> 1.35 <sup>-2</sup> 1.33 <sup>-3</sup> 2.60 <sup>-2</sup> 1.000	f σ g σ h σ p π d π f π g π h π   ε (Ry)  σ σ σ σ σ σ σ σ σ σ σ σ σ σ σ σ σ σ σ	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup> 3.57 <sup>-4</sup> 1.69 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup> 2.70 <sup>-4</sup> 1.69 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup> 1.87 <sup>-4</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.30 <sup>-3</sup> 1.15 <sup>-4</sup> 8.48 <sup>-4</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup> 4.15 <sup>-4</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup> 2.55 <sup>-5</sup> 2.26 <sup>-4</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-4</sup> 1.08 <sup>-5</sup> 1.41 <sup>-4</sup>	1.000 1.69 <sup>-3</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup> 6.41 <sup>-6</sup> 1.86 <sup>-4</sup>
fσ   gσ   hσ   pπ   dπ   fπ   gπ   hπ     ε (Ry)     sσ   pσ   dσ   fσ   fσ   fσ   fσ   fσ   fσ   f	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.64 <sup>-3</sup> 3.19 <sup>-6</sup> 3.30 <sup>-2</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.11 <sup>-3</sup> 2.36 <sup>-4</sup> 1.47 <sup>-3</sup> 2.72 <sup>-2</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup> 1.59 <sup>-4</sup> 1.11 <sup>-3</sup> 2.21 <sup>-2</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup> 1.17 <sup>-3</sup> 9.37 <sup>-5</sup> 6.70 <sup>-4</sup> 1.82 <sup>-2</sup>	6.63 <sup>-3</sup> 5.88 <sup>-4</sup> 3.65 <sup>-3</sup> 5.48 <sup>-2</sup> 4.62 <sup>-4</sup> 2.85 <sup>-2</sup> 2.04 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640  3.18 <sup>-3</sup> 3.51 <sup>-2</sup> 1.28 <sup>-3</sup> 6.33 <sup>-4</sup> 4.62 <sup>-5</sup> 4.62 <sup>-6</sup> 1.52 <sup>-2</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743  2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 3.47 <sup>-4</sup> 1.94 <sup>-5</sup> 2.29 <sup>-4</sup> 1.30 <sup>-2</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup> 8.70 <sup>-6</sup> 1.156 <sup>-4</sup> 1.10 <sup>-2</sup>	1.000 1.46 <sup>-3</sup> 1.000 1.46 <sup>-3</sup> 1.000 1.72 <sup>-4</sup> 1.35 <sup>-2</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup> 1.72 <sup>-4</sup> 5.76 <sup>-6</sup> 1.92 <sup>-4</sup> 9.16 <sup>-3</sup>	fσ gσ hσ pπ dπ fπ gπ hπ ε (Ry) sσ pσ dσ fσ gσ hσ	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup> 3.57 <sup>-4</sup> 3.55 <sup>-2</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup> 2.70 <sup>-3</sup> 2.93 <sup>-2</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup> 1.87 <sup>-4</sup> 1.39 <sup>-3</sup> 2.38 <sup>-2</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.15 <sup>-4</sup> 1.49 <sup>-2</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup> 5.91 <sup>-5</sup> 4.15 <sup>-4</sup> 1.59 <sup>-2</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup> 2.55 <sup>-5</sup> 2.26 <sup>-4</sup> 1.34 <sup>-2</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-4</sup> 1.08 <sup>-5</sup> 1.41 <sup>-4</sup> 1.14 <sup>-2</sup>	1.000 1.69 <sup>-3</sup> 4.40 <sup>-4</sup> 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup> 6.41 <sup>-4</sup> 6.41 <sup>-4</sup> 9.45 <sup>-3</sup>
fσ   gσ   hσ   pπ   dπ   fπ   gπ   hπ	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.64 <sup>-3</sup> 3.19 <sup>-4</sup> 1.66 <sup>-3</sup> 3.30 <sup>-2</sup> 2.17 <sup>-4</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.716 <sup>-3</sup> 1.47 <sup>-3</sup> 2.72 <sup>-2</sup> 1.73 <sup>-4</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup> 1.11 <sup>-3</sup> 2.21 <sup>-2</sup> 1.36 <sup>-4</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup> 1.17 <sup>-3</sup> 9.37 <sup>-5</sup> 6.70 <sup>-4</sup> 1.82 <sup>-2</sup> 1.03 <sup>-4</sup>	6.63-3 5.88-4 3.65-3 5.48-2 4.62-4 2.85-2 2.04-3 3.07-2 0.640 3.18-3 3.51-2 1.28-3 6.33-4 4.62-5 7.45-5	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743  2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 3.47 <sup>-4</sup> 1.94 <sup>-5</sup> 2.29 <sup>-4</sup> 1.30 <sup>-2</sup> 5.11 <sup>-5</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup> 8.70 <sup>-6</sup> 1.56 <sup>-4</sup> 1.10 <sup>-2</sup> 3.47 <sup>-5</sup>	1.000 1.000 1.46 <sup>-3</sup> 1.000 1.46 <sup>-3</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup> 1.72 <sup>-4</sup> 5.76 <sup>-6</sup> 1.92 <sup>-4</sup> 9.16 <sup>-3</sup> 2.48 <sup>-5</sup>	f σ g σ h σ p π d π f π g π h π σ σ σ d σ f σ g σ h σ d π f σ σ g σ h σ d π d π d π d π d π d π d π d π d π d	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup> 3.57 <sup>-4</sup> 1.69 <sup>-3</sup> 3.55 <sup>-2</sup> 2.29 <sup>-4</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup> 2.70 <sup>-3</sup> 1.69 <sup>-3</sup> 2.93 <sup>-2</sup> 1.84 <sup>-4</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup> 1.87 <sup>-3</sup> 1.39 <sup>-3</sup> 2.38 <sup>-2</sup> 1.45 <sup>-4</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.30 <sup>-3</sup> 1.15 <sup>-4</sup> 8.48 <sup>-4</sup> 1.93 <sup>-2</sup> 1.11 <sup>-4</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup> 5.91 <sup>-5</sup> 4.15 <sup>-4</sup> 1.59 <sup>-2</sup> 8.17 <sup>-5</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743  2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup> 2.55 <sup>-5</sup> 2.26 <sup>-4</sup> 1.34 <sup>-2</sup> 5.71 <sup>-5</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-5</sup> 1.41 <sup>-4</sup> 1.14 <sup>-2</sup> 3.91 <sup>-5</sup>	1.000 1.69 <sup>-3</sup> 1.45 <sup>-3</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup> 6.41 <sup>-6</sup> 1.86 <sup>-4</sup> 9.45 <sup>-3</sup> 2.80 <sup>-5</sup>
f σ g σ h σ p π d π f π g π h π σ p σ d σ f σ g σ d σ f σ g σ h σ d π f π f π f π f π f π f π f π f π f π	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.64 <sup>-3</sup> 3.19 <sup>-4</sup> 1.66 <sup>-3</sup> 3.30 <sup>-2</sup> 2.17 <sup>-4</sup> 1.02 <sup>-2</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.716 <sup>-3</sup> 1.47 <sup>-3</sup> 2.72 <sup>-2</sup> 1.73 <sup>-4</sup> 7.68 <sup>-3</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup> 1.59 <sup>-4</sup> 1.11 <sup>-3</sup> 2.21 <sup>-2</sup> 1.36 <sup>-4</sup> 5.72 <sup>-3</sup>	0.552 3.99 <sup>-3</sup> 1.17 <sup>-3</sup> 9.37 <sup>-5</sup> 6.09 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552	6.63-3 5.88-4 3.65-3 5.48-2 4.62-4 2.85-2 2.04-3 3.07-2 0.640 3.18-3 3.51-2 1.28-3 6.33-4 4.62-5 3.76-4 1.52-2 7.45-5 2.79-3	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743  2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 3.47 <sup>-4</sup> 1.94 <sup>-5</sup> 2.29 <sup>-4</sup> 1.30 <sup>-2</sup> 5.11 <sup>-5</sup> 1.66 <sup>-3</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862 1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup> 8.70 <sup>-6</sup> 1.56 <sup>-4</sup> 1.10 <sup>-2</sup> 3.47 <sup>-5</sup> 8.08 <sup>-4</sup>	1.000 1.000 1.46 <sup>-3</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup> 1.72 <sup>-4</sup> 5.76 <sup>-6</sup> 1.92 <sup>-4</sup> 9.16 <sup>-3</sup> 2.48 <sup>-5</sup> 3.11 <sup>-4</sup>	$f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$ $g\pi$ $h\pi$ $e (Ry)$ $s\sigma$ $p\sigma$ $d\sigma$ $f\sigma$ $g\sigma$ $h\sigma$ $p\pi$ $d\pi$ $f\pi$	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup> 3.57 <sup>-4</sup> 1.69 <sup>-3</sup> 3.55 <sup>-2</sup> 2.29 <sup>-4</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410 6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup> 2.95 <sup>-3</sup> 2.93 <sup>-2</sup> 1.69 <sup>-3</sup> 2.93 <sup>-2</sup> 1.84 <sup>-4</sup> 8.62 <sup>-3</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup> 1.87 <sup>-4</sup> 1.39 <sup>-3</sup> 2.38 <sup>-2</sup> 1.45 <sup>-4</sup> 6.36 <sup>-3</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.30 <sup>-3</sup> 1.15 <sup>-4</sup> 8.48 <sup>-4</sup> 1.93 <sup>-2</sup> 1.11 <sup>-4</sup> 4.61 <sup>-3</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup> 4.15 <sup>-4</sup> 1.59 <sup>-2</sup> 8.17 <sup>-5</sup> 3.17 <sup>-3</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup> 2.55 <sup>-5</sup> 2.26 <sup>-4</sup> 1.34 <sup>-2</sup> 5.71 <sup>-5</sup> 1.94 <sup>-3</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-4</sup> 1.08 <sup>-5</sup> 1.41 <sup>-4</sup> 1.14 <sup>-2</sup> 3.91 <sup>-5</sup> 9.96 <sup>-4</sup>	1.000 1.69 <sup>-3</sup> 4.45 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup> 6.41 <sup>-6</sup> 1.86 <sup>-4</sup> 1.86 <sup>-3</sup> 4.91 <sup>-3</sup> 2.80 <sup>-5</sup> 4.01 <sup>-4</sup>
fσ   gσ   hσ   pπ   dπ   fπ   gπ   hπ	7.63 <sup>-3</sup> 6.46 <sup>-4</sup> 7.53 <sup>-3</sup> 6.93 <sup>-2</sup> 7.59 <sup>-4</sup> 5.53 <sup>-2</sup> 2.78 <sup>-3</sup> 2.82 <sup>-2</sup> 0.353  6.93 <sup>-3</sup> 9.75 <sup>-2</sup> 3.62 <sup>-3</sup> 3.19 <sup>-4</sup> 1.66 <sup>-3</sup> 3.30 <sup>-2</sup> 2.17 <sup>-4</sup> 1.02 <sup>-2</sup> 1.09 <sup>-3</sup>	7.43 <sup>-3</sup> 6.43 <sup>-4</sup> 6.69 <sup>-3</sup> 6.60 <sup>-2</sup> 6.86 <sup>-4</sup> 4.85 <sup>-2</sup> 2.61 <sup>-3</sup> 2.89 <sup>-2</sup> 0.410  5.90 <sup>-3</sup> 7.96 <sup>-2</sup> 2.93 <sup>-3</sup> 2.71 <sup>-3</sup> 2.36 <sup>-4</sup> 1.47 <sup>-3</sup> 2.72 <sup>-2</sup> 1.73 <sup>-6</sup> 8.58 <sup>-4</sup>	7.23 <sup>-3</sup> 6.35 <sup>-4</sup> 5.72 <sup>-3</sup> 6.27 <sup>-2</sup> 6.12 <sup>-4</sup> 4.16 <sup>-2</sup> 2.44 <sup>-3</sup> 2.97 <sup>-2</sup> 0.476  4.91 <sup>-3</sup> 6.29 <sup>-2</sup> 2.32 <sup>-3</sup> 1.88 <sup>-3</sup> 1.59 <sup>-4</sup> 1.11 <sup>-3</sup> 2.21 <sup>-2</sup> 1.36 <sup>-5</sup> 6.55 <sup>-4</sup>	6.98 <sup>-3</sup> 6.18 <sup>-4</sup> 4.68 <sup>-3</sup> 5.90 <sup>-2</sup> 5.36 <sup>-4</sup> 3.49 <sup>-2</sup> 2.25 <sup>-3</sup> 3.04 <sup>-2</sup> 0.552 3.99 <sup>-3</sup> 4.79 <sup>-2</sup> 1.78 <sup>-3</sup> 1.17 <sup>-3</sup> 9.37 <sup>-5</sup> 6.70 <sup>-4</sup> 1.82 <sup>-2</sup> 1.03 <sup>-4</sup>	0.640 3.18 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640 3.18 <sup>-3</sup> 3.07 <sup>-2</sup> 0.640 3.18 <sup>-3</sup> 3.51 <sup>-2</sup> 1.28 <sup>-3</sup> 6.33 <sup>-4</sup> 4.62 <sup>-5</sup> 3.76 <sup>-4</sup> 1.52 <sup>-5</sup> 7.45 <sup>-5</sup> 3.63 <sup>-4</sup>	6.13 <sup>-3</sup> 5.41 <sup>-4</sup> 2.77 <sup>-3</sup> 5.01 <sup>-2</sup> 3.91 <sup>-4</sup> 2.27 <sup>-2</sup> 1.82 <sup>-3</sup> 3.02 <sup>-2</sup> 0.743 2.50 <sup>-3</sup> 2.47 <sup>-2</sup> 8.52 <sup>-4</sup> 3.47 <sup>-4</sup> 1.94 <sup>-5</sup> 2.29 <sup>-4</sup> 1.30 <sup>-2</sup> 5.11 <sup>-6</sup> 5.16 <sup>-3</sup> 2.60 <sup>-4</sup>	5.44 <sup>-3</sup> 4.79 <sup>-4</sup> 2.15 <sup>-3</sup> 4.48 <sup>-2</sup> 3.26 <sup>-4</sup> 1.77 <sup>-2</sup> 1.58 <sup>-3</sup> 2.87 <sup>-2</sup> 0.862  1.94 <sup>-3</sup> 1.67 <sup>-2</sup> 5.21 <sup>-4</sup> 2.44 <sup>-4</sup> 8.70 <sup>-6</sup> 1.10 <sup>-2</sup> 3.47 <sup>-5</sup> 4.080 <sup>-4</sup> 1.68 <sup>-4</sup>	1.000 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 1.000 1.46 <sup>-3</sup> 1.06 <sup>-2</sup> 3.02 <sup>-4</sup> 1.72 <sup>-4</sup> 5.76 <sup>-6</sup> 1.92 <sup>-4</sup> 9.16 <sup>-3</sup> 2.48 <sup>-5</sup> 3.11 <sup>-4</sup> 8.93 <sup>-5</sup>	f σ g σ h σ p π d π f π g π h π σ σ σ d σ f σ g σ h σ d π f σ σ g σ h σ d π d π d π d π d π d π d π d π d π d	8.40 <sup>-3</sup> 6.41 <sup>-4</sup> 9.00 <sup>-3</sup> 7.57 <sup>-2</sup> 7.92 <sup>-4</sup> 6.32 <sup>-2</sup> 2.95 <sup>-3</sup> 2.98 <sup>-2</sup> 0.353 8.04 <sup>-3</sup> 1.05 <sup>-1</sup> 4.10 <sup>-3</sup> 4.01 <sup>-3</sup> 3.57 <sup>-4</sup> 1.69 <sup>-3</sup> 3.55 <sup>-2</sup> 2.29 <sup>-4</sup> 1.16 <sup>-2</sup> 1.20 <sup>-3</sup>	8.14 <sup>-3</sup> 6.40 <sup>-4</sup> 7.87 <sup>-3</sup> 7.16 <sup>-2</sup> 7.16 <sup>-4</sup> 5.57 <sup>-2</sup> 2.77 <sup>-3</sup> 3.06 <sup>-2</sup> 0.410  6.86 <sup>-3</sup> 8.59 <sup>-2</sup> 3.32 <sup>-3</sup> 2.95 <sup>-3</sup> 2.70 <sup>-4</sup> 1.69 <sup>-3</sup> 2.93 <sup>-2</sup> 1.84 <sup>-4</sup> 8.62 <sup>-3</sup> 9.50 <sup>-4</sup>	7.89 <sup>-3</sup> 6.36 <sup>-4</sup> 6.59 <sup>-3</sup> 6.74 <sup>-2</sup> 6.39 <sup>-4</sup> 4.80 <sup>-2</sup> 2.59 <sup>-3</sup> 3.16 <sup>-2</sup> 0.476  5.71 <sup>-3</sup> 6.83 <sup>-2</sup> 2.64 <sup>-3</sup> 2.04 <sup>-3</sup> 1.87 <sup>-4</sup> 1.39 <sup>-3</sup> 2.38 <sup>-2</sup> 1.45 <sup>-4</sup> 6.36 <sup>-3</sup> 7.28 <sup>-4</sup>	7.60 <sup>-3</sup> 6.25 <sup>-4</sup> 5.22 <sup>-3</sup> 6.32 <sup>-2</sup> 5.61 <sup>-4</sup> 4.04 <sup>-2</sup> 2.39 <sup>-3</sup> 3.25 <sup>-2</sup> 0.552  4.64 <sup>-3</sup> 5.23 <sup>-2</sup> 2.03 <sup>-3</sup> 1.15 <sup>-4</sup> 8.48 <sup>-4</sup> 1.93 <sup>-2</sup> 1.11 <sup>-4</sup> 4.61 <sup>-3</sup> 5.45 <sup>-4</sup>	7.24 <sup>-3</sup> 6.03 <sup>-4</sup> 3.88 <sup>-3</sup> 5.86 <sup>-2</sup> 4.84 <sup>-4</sup> 3.31 <sup>-2</sup> 2.18 <sup>-3</sup> 3.31 <sup>-2</sup> 0.640  3.69 <sup>-3</sup> 3.85 <sup>-2</sup> 1.49 <sup>-3</sup> 7.37 <sup>-4</sup> 5.91 <sup>-5</sup> 4.15 <sup>-4</sup> 1.59 <sup>-2</sup> 8.17 <sup>-5</sup> 4.17 <sup>-3</sup> 4.01 <sup>-4</sup>	6.72 <sup>-3</sup> 5.66 <sup>-4</sup> 2.75 <sup>-3</sup> 5.35 <sup>-2</sup> 4.10 <sup>-4</sup> 2.64 <sup>-2</sup> 1.95 <sup>-3</sup> 3.28 <sup>-2</sup> 0.743 2.89 <sup>-3</sup> 2.72 <sup>-2</sup> 1.01 <sup>-3</sup> 3.87 <sup>-4</sup> 2.55 <sup>-5</sup> 2.26 <sup>-4</sup> 1.34 <sup>-5</sup> 5.71 <sup>-5</sup> 5.71 <sup>-5</sup> 1.94 <sup>-3</sup> 2.88 <sup>-4</sup>	6.00 <sup>-3</sup> 5.12 <sup>-4</sup> 2.00 <sup>-3</sup> 4.80 <sup>-2</sup> 3.42 <sup>-4</sup> 2.05 <sup>-2</sup> 1.71 <sup>-3</sup> 3.15 <sup>-2</sup> 0.862 2.23 <sup>-3</sup> 1.84 <sup>-2</sup> 6.25 <sup>-4</sup> 2.45 <sup>-5</sup> 1.41 <sup>-4</sup> 1.14 <sup>-2</sup> 3.91 <sup>-5</sup>	1.000 1.69 <sup>-3</sup> 4.19 <sup>-2</sup> 2.81 <sup>-4</sup> 1.55 <sup>-2</sup> 1.45 <sup>-3</sup> 2.88 <sup>-2</sup> 1.000 1.69 <sup>-3</sup> 1.19 <sup>-2</sup> 3.60 <sup>-4</sup> 1.72 <sup>-4</sup> 6.41 <sup>-6</sup> 9.45 <sup>-3</sup> 2.80 <sup>-5</sup> 4.01 <sup>-4</sup> 1.06 <sup>-4</sup>

reduced to one-dimensional (radial) equations by using a partial wave expansion. The total wave function is written as

$$\Psi(\mathbf{r},\mathbf{R}) = \sum_{k} \exp[i(m_e/M)(-i\nabla_R)\cdot\mathbf{s}_k]\phi_k(\mathbf{r};\mathbf{R})F_k(\mathbf{R}),$$

where M is the reduced mass of the nuclei. Then the partial wave expansion of nuclear wave function in symmetric-top eigenfunctions takes the form

$$F_k(\mathbf{R}) = R^{-1} \sum_{J=\Lambda_k} \sum_{M_J=-J}^{J} G_k^{JM_J}(R) Y_{JM_J}^{\Lambda_k}.$$
 (B11)

Here, the electronic basis state  $\varphi_k$  is the eigenstate of  $L_{z'}$  with eigenvalue  $\Lambda_k$ . The functions  $Y_{JM_J}^{\Lambda_k}$  satisfy the differential equations

$$\left[ (\sin \Theta)^{-1} \frac{\partial}{\partial \Theta} \sin \Theta \frac{\partial}{\partial \Theta} + (\sin \Theta)^{-2} \left( \frac{\partial}{\partial \Phi} - i \Lambda_k \cos \Theta \right)^2 - \Lambda_k^2 \right] Y_{JM_J}^{\Lambda_k} = -J(J+1) Y_{JM_J}^{\Lambda_k}$$
(B12)

and

Table 27. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at  $E=7.45\,\mathrm{keV/amu}$ 

Table 28. Single differential cross sections (in  $10^{-16}$  cm<sup>2</sup>) at E = 7.76 keV/amu

- 7.43	KC V/aiiiu	L							- 7.70	Ke v/aiii	u						
$\epsilon$ (Ry)				0.016			0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018		0.024	0.028
$s\sigma$	$3.29^{-2}$	$3.26^{-2}$	$3.22^{-2}$	$3.18^{-2}$	$3.13^{-2}$	$3.08^{-2}$	$3.02^{-2}$	$2.95^{-2}$	$s\sigma$	$3.92^{-2}$		$3.83^{-2}$	$3.78^{-2}$	$3.72^{-2}$		$3.58^{-2}$	$3.50^{-2}$
$p\sigma$	$3.58^{-1}$	$3.56^{-1}$	$3.54^{-1}$	$3.51^{-1}$	$3.48^{-1}$	$3.45^{-1}$	$3.41^{-1}$	$3.37^{-1}$	$p\sigma$	$3.74^{-1}$	$3.72^{-1}$	$3.70^{-1}$	$3.67^{-1}$	$3.64^{-1}$	$3.61^{-1}$	$3.57^{-1}$	$3.52^{-1}$
$d\sigma$	$1.58^{-2}$	$1.58^{-2}$	$1.57^{-2}$	$1.56^{-2}$	$1.55^{-2}$	$1.54^{-2}$			$d\sigma$		$1.65^{-2}$						$1.59^{-2}$
$f\sigma$				$1.26^{-2}$			$1.21^{-2}$		$f\sigma$		$1.36^{-2}$						$1.27^{-2}$
$g\sigma$				$7.59^{-4}$					$g\sigma$		$8.44^{-4}$						
$h\sigma$				$1.69^{-2}$ $1.42^{-1}$					$h\sigma$	2.15	$2.15^{-2}$ $1.72^{-1}$	2.14	2.14	2.14	2.13	2.12	2.11 2
$p\pi$				$1.42^{-3}$ $1.42^{-3}$					$p\pi$	1.74	$1.72^{-1}$ $1.51^{-3}$	1.69	1.66	1.62	1.58	1.54	1.49
$d\pi$ $f\pi$	1.47	1.40	1.44	$1.42$ $1.35^{-1}$	1.40	1.3/	1.33	1.32	$d\pi$ $f\pi$		$1.51$ $1.53^{-1}$						
$g\pi$	1.40 1.70 <sup>-3</sup>	1.39 4.75 <sup>-3</sup>	1.37	$4.66^{-3}$	1.33	1.51 4.53 <sup>-3</sup>	$1.20$ $1.46^{-3}$	1.24	$g\pi$	5.21 <sup>-3</sup>	$5.17^{-3}$	5 12 <sup>-3</sup>	5.06 <sup>-3</sup>	1.47	1.44 1.01 <sup>-3</sup>	1.41 4.82 <sup>-3</sup>	1.36 4.73 <sup>-3</sup>
$\overset{s}{h}\overset{n}{\pi}$				$4.35^{-2}$					$\overset{s}{h}\pi$	$4.88^{-2}$	$4.79^{-2}$	$4.68^{-2}$	$4.57^{-2}$	$4.44^{-2}$	$4.31^{-2}$	$4.16^{-2}$	$4.01^{-2}$
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)		0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$	$2.87^{-2}$	$2.79^{-2}$	$2.70^{-2}$	$2.59^{-2}$	$2.49^{-2}$	$2.37^{-2}$	$2.24^{-2}$	$2.11^{-2}$	$s\sigma$		$3.30^{-2}$						$2.47^{-2}$
$p\sigma$				$3.12^{-1}$					$p\sigma$		$3.41^{-1}$						
$d\sigma$				$1.42^{-2}$					$d\sigma$		$1.56^{-2}$						
$f\sigma$				$1.08^{-2}$ $6.78^{-4}$					$f\sigma$		$1.23^{-2}$ $7.50^{-4}$						
$g\sigma$				$1.56^{-2}$					$g\sigma$		$2.08^{-2}$						
$h\sigma$	1.04	1.02	1.60	$1.36^{-1}$ $1.10^{-1}$	1.51	0.04-2	0.20-2	0.05-2	$h\sigma = p\pi$		$1.38^{-1}$						
$p\pi$ $d\pi$				$1.10$ $1.15^{-3}$					$d\pi$		$1.36$ $1.29^{-3}$						
$f\pi$				$1.07^{-1}$					$f\pi$		$1.29^{-1}$						
$g\pi$	$4.28^{-3}$	$4.17^{-3}$	$4.06^{-3}$	$3.93^{-3}$	$3.79^{-3}$	$3.64^{-3}$	$3.48^{-3}$	$3.31^{-3}$	$g\pi$	$4.62^{-3}$	$4.50^{-3}$	$4.37^{-3}$	$4.22^{-3}$	$4.06^{-3}$	$3.89^{-3}$	$3.71^{-3}$	$3.52^{-3}$
$\overset{s}{h}\pi$	$3.68^{-2}$	$3.54^{-2}$	$3.40^{-2}$	$3.27^{-2}$	$3.17^{-2}$	$3.09^{-2}$	$3.05^{-2}$	$3.06^{-2}$	$\overset{s}{h}\pi$	$3.85^{-2}$	$3.69^{-2}$	$3.54^{-2}$	$3.39^{-2}$	$3.27^{-2}$	$3.19^{-2}$	$3.14^{-2}$	$3.14^{-2}$
$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	$\epsilon$ (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$1.98^{-2}$	$1.85^{-2}$	$1.71^{-2}$	$1.58^{-2}$	$1.44^{-2}$	$1.31^{-2}$	$1.18^{-2}$	$1.05^{-2}$	sσ	$2.30^{-2}$	$2.13^{-2}$	$1.97^{-2}$	$1.80^{-2}$	$1.64^{-2}$	$1.49^{-2}$	$1.34^{-2}$	$1.19^{-2}$
$p\sigma$		$2.43^{-1}$	$2.27^{-1}$	$2.10^{-1}$	$1.91^{-1}$	$1.72^{-1}$	$1.52^{-1}$	$1.32^{-1}$	$p\sigma$	$2.70^{-1}$	$2.55^{-1}$	$2.38^{-1}$	$2.20^{-1}$	$2.01^{-1}$	$1.81^{-1}$	$1.60^{-1}$	$1.39^{-1}$
$d\sigma$				$9.62^{-3}$					$d\sigma$		$1.22^{-2}$						
$f\sigma$				$8.27^{-3}$					$f\sigma$		$9.70^{-3}$						
$g\sigma$				$6.29^{-4}$					$g\sigma$		$6.46^{-4}$						
$h\sigma$				$6.47^{-3}$					$h\sigma$		$1.33^{-2}$						
$p\pi$	$8.32^{-2}$	$7.80^{-2}$	$7.29^{-2}$	$6.78^{-2}$	$6.26^{-2}$	$5.71^{-2}$	$5.12^{-2}$	$4.48^{-2}$	$p\pi$		$8.54^{-2}$						
$d\pi$	8.22-4	7.44	6.64	$5.83^{-4}$ $4.63^{-2}$	5.04	4.28	3.57	2.94	$d\pi$		$7.72^{-4}$ $7.15^{-2}$						
$f\pi$				$4.63^{-2}$ $2.53^{-3}$					$f\pi$		$7.15^{-2}$ $3.11^{-3}$						
$g\pi$				$3.44^{-2}$					$g \pi h \pi$		$3.11^{-2}$ $3.30^{-2}$						
$-h\pi$	5.11	3.20	3.32	3.44	3.33	3.33	3.42	3.13	$-n\pi$	3.20	3.30	3.43	3.00	3.72	3.70	3.07	3.42
$\epsilon$ (Ry)		0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
$s\sigma$	$9.21^{-3}$	$7.88^{-3}$	$6.57^{-3}$	$5.34^{-3}$			$2.54^{-3}$	$1.92^{-3}$	$s\sigma$		$8.96^{-3}$				$3.75^{-3}$	$2.88^{-3}$	$2.17^{-3}$
$p\sigma$	$1.12^{-1}$	$9.21^{-2}$	$7.36^{-2}$	$5.67^{-2}$	$4.20^{-2}$	$2.98^{-2}$	$2.02^{-2}$		$p\sigma$	$1.18^{-1}$	$9.81^{-2}$	$7.89^{-2}$	$6.12^{-2}$	$4.55^{-2}$	$3.24^{-2}$	$2.21^{-2}$	$1.44^{-2}$
$d\sigma$				$2.30^{-3}$					$d\sigma$		$4.20^{-3}$						
$f\sigma$	$4.45^{-3}$	$3.25^{-3}$	$2.20^{-3}$	$1.41^{-3}$	$8.29^{-4}$	$4.38^{-4}$	$2.52^{-4}$	$1.73^{-4}$	$f\sigma$	$4.96^{-3}$	$3.61^{-3}$	$2.41^{-3}$	$1.52^{-3}$	$9.06^{-4}$	$4.93^{-4}$	$2.68^{-4}$	$1.75^{-4}$
$g\sigma$	$3.92^{-4}$	$3.04^{-4}$	$2.16^{-4}$	$1.37^{-4}$	$7.41^{-5}$	$3.32^{-5}$	$1.37^{-5}$	$7.20^{-6}$	$g\sigma$	$4.23^{-4}$	$3.35^{-4}$	$2.45^{-4}$	$1.61^{-4}$	$9.12^{-5}$	$4.27^{-5}$	$1.75^{-5}$	$8.26^{-6}$
$h\sigma$	$1.57^{-3}$	$1.81^{-3}$	$1.70^{-3}$	$1.13^{-3}$	$5.21^{-4}$	$2.38^{-4}$	$1.36^{-4}$	$1.70^{-4}$	$h\sigma$	$1.33^{-3}$	$1.78^{-3}$	$1.96^{-3}$	$1.47^{-3}$	$7.11^{-4}$	$2.78^{-4}$	$1.44^{-4}$	$1.52^{-4}$
$p\pi$				$2.05^{-2}$					$p\pi$		$3.38^{-2}$ $2.00^{-4}$						
$d\pi$				$1.19^{-4}$					$d\pi$								
$f\pi$				$5.11^{-3}$ $6.00^{-4}$					$f\pi$		$1.09^{-2}$ $1.13^{-3}$						
$g\pi$				$6.00^{-4}$ $1.02^{-2}$					$g\pi$		$1.13^{-3}$ $2.44^{-2}$						
$h\pi$	2.74 -	2.20 2	1.00 2	1.02	5.38	2.10	4.02	0.38	$h\pi$	3.00 2	2.44	1.80 2	1.1/ 2	0.40	2.05	0./1	8.50

$$-i\frac{\partial}{\partial\Phi}Y_{JM_{J}}^{\Lambda_{k}} = M_{J}Y_{JM_{J}}^{\Lambda_{k}}, \tag{B13}$$

where J is the total angular momentum,  $M_J$  its (laboratory frame) z-axis component, and  $\Lambda_k$  is the body-fixed component. In this representation, the angular components of  $\mathbf{P}$  and  $\mathbf{A}$  by couple states  $\varphi_k$  that have different  $\Lambda_k$  but are diagonal in J,  $M_J$ , and a system of coupled radial equations arises for each J, which may be written as

$$\left\{ \frac{1}{2M} \left[ -i \frac{d}{dR} \mathbf{1} + \mathbf{P}^R + \mathbf{A}^R \right]^2 + \frac{J(J+1) - \Lambda_k}{2MR^2} \mathbf{1} + \frac{1}{2M} \left[ \mathbf{D} \right] \right\}$$

$$-\mathbf{Q}]\bigg\}G_{k}^{JM_{J}}(R) = [\mathbf{1}E - \mathbf{U}(R)]G_{k}^{JM_{J}}(R), \qquad (B14)$$

where

$$D_{k'k} = (P_{k'k}^{\Theta} + A_{k'k}^{\Theta})^2 + (\tilde{P}_{k'k}^{\Phi} + A_{k'k}^{\Phi})^2,$$

$$U_{k'k}(R) = (\epsilon_k + Z_A Z_B / R) \delta_{k'k},$$
(B15)

Table 29. Single differential cross sections (in  $10^{-16}\,\mathrm{cm^2}$ ) at  $E=8.08\,\mathrm{keV/amu}$ 

Table 30. Single differential cross sections (in  $10^{-16} \,\mathrm{cm^2}$ ) at  $E = 8.40 \,\mathrm{keV/amu}$ 

= 8.08	keV/amu	l							= 8.40	keV/amu	1						
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$4.63^{-2}$	$4.58^{-2}$	$4.53^{-2}$	$4.47^{-2}$	$4.40^{-2}$	$4.32^{-2}$	$4.23^{-2}$	$4.12^{-2}$	sσ	$5.43^{-2}$	$5.38^{-2}$	$5.31^{-2}$	$5.24^{-2}$	$5.15^{-2}$	$5.06^{-2}$	$4.95^{-2}$	$4.83^{-2}$
$p\sigma$	$3.89^{-1}$	$3.87^{-1}$	$3.85^{-1}$	$3.83^{-1}$	$3.79^{-1}$	$3.76^{-1}$	$3.72^{-1}$	$3.67^{-1}$	$p\sigma$	$4.05^{-1}$	$4.03^{-1}$	$4.00^{-1}$	$3.98^{-1}$	$3.95^{-1}$	$3.91^{-1}$	$3.87^{-1}$	$3.82^{-1}$
$d\sigma$	$1.72^{-2}$	$1.72^{-2}$	$1.71^{-2}$	$1.71^{-2}$	$1.70^{-2}$	$1.69^{-2}$	$1.68^{-2}$	$1.66^{-2}$	$d\sigma$	$1.78^{-2}$	$1.78^{-2}$	$1.77^{-2}$	$1.76^{-2}$	$1.76^{-2}$	$1.75^{-2}$	$1.74^{-2}$	$1.72^{-2}$
$f\sigma$	$1.44^{-2}$	$1.43^{-2}$	$1.42^{-2}$	$1.41^{-2}$	$1.40^{-2}$	$1.38^{-2}$	$1.37^{-2}$	$1.35^{-2}$	$f\sigma$	$1.51^{-2}$	$1.50^{-2}$	$1.49^{-2}$	$1.48^{-2}$	$1.47^{-2}$	$1.45^{-2}$	$1.44^{-2}$	$1.42^{-2}$
$g\sigma$					$8.92^{-4}$				$g\sigma$	$1.02^{-3}$	$1.01^{-3}$	$9.97^{-4}$	$9.86^{-4}$	$9.72^{-4}$	$9.57^{-4}$	$9.41^{-4}$	$9.22^{-4}$
$h\sigma$	$2.66^{-2}$	$2.66^{-2}$	$2.66^{-2}$	$2.66^{-2}$	$2.66^{-2}$	$2.66^{-2}$	$2.65^{-2}$	$2.64^{-2}$	$h\sigma$		$3.22^{-2}$						
$p\pi$	$2.02^{-1}$	$1.99^{-1}$	$1.96^{-1}$	$1.92^{-1}$	$1.88^{-1}$	$1.83^{-1}$	$1.78^{-1}$	$1.72^{-1}$	$p\pi$	$2.33^{-1}$	$2.30^{-1}$	$2.26^{-1}$	$2.21^{-1}$	$2.16^{-1}$	$2.11^{-1}$	$2.04^{-1}$	$1.98^{-1}$
$d\pi$					$1.50^{-3}$				$d\pi$		$1.62^{-3}$						
$f\pi$					$1.61^{-1}$				$f\pi$		$1.83^{-1}$						
$g\pi$					$5.43^{-3}$				$g\pi$		$6.16^{-3}$						
$h\pi$	5.09-2	4.99-2	4.88-2	4.76-2	$4.62^{-2}$	4.48-2	4.32-2	4.15-2	$h\pi$	5.25-2	$5.15^{-2}$	5.03-2	4.90-2	4.76-2	4.61-2	4.44-2	4.26-2
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$					$3.43^{-2}$				$s\sigma$	$4.69^{-2}$	$4.54^{-2}$	$4.38^{-2}$	$4.19^{-2}$	$3.99^{-2}$	$3.78^{-2}$	$3.55^{-2}$	$3.32^{-2}$
$p\sigma$					$3.32^{-1}$				$p\sigma$		$3.70^{-1}$						
$d\sigma$					$1.55^{-2}$				$d\sigma$		$1.69^{-2}$						
$f\sigma$					$1.23^{-2}$				$f\sigma$		$1.39^{-2}$						
$g\sigma$	$8.30^{-4}$	$8.11^{-4}$	$7.90^{-4}$	$7.69^{-4}$	$7.48^{-4}$	$7.27^{-4}$	$7.07^{-4}$	$6.89^{-4}$	$g\sigma$	$9.02^{-4}$	$8.80^{-4}$	$8.56^{-4}$	$8.31^{-4}$	$8.04^{-4}$	$7.78^{-4}$	$7.52^{-4}$	$7.28^{-4}$
$h\sigma$	$2.63^{-2}$	$2.61^{-2}$	$2.58^{-2}$	$2.55^{-2}$	$2.49^{-2}$	$2.41^{-2}$	$2.31^{-2}$	$2.17^{-2}$	$h\sigma$	$3.23^{-2}$	$3.21^{-2}$	$3.19^{-2}$	$3.16^{-2}$	$3.11^{-2}$	$3.03^{-2}$	$2.92^{-2}$	$2.78^{-2}$
$p\pi$	$1.66^{-1}$	$1.59^{-1}$	$1.52^{-1}$	$1.44^{-1}$	$1.36^{-1}$	$1.27^{-1}$	$1.19^{-1}$	$1.10^{-1}$	$p\pi$		$1.82^{-1}$						
$d\pi$					$1.17^{-3}$				$d\pi$	$1.43^{-3}$	$1.39^{-3}$	$1.34^{-3}$	$1.28^{-3}$	$1.22^{-3}$	$1.15^{-3}$	$1.08^{-3}$	$1.00^{-3}$
$f\pi$					$1.24^{-1}$				$f\pi$	$1.61^{-1}$	$1.56^{-1}$	$1.50^{-1}$	$1.44^{-1}$	$1.36^{-1}$	$1.28^{-1}$	$1.20^{-1}$	$1.10^{-1}$
$g \pi$					$4.37^{-3}$				$g \pi$	$5.44^{-3}$	$5.29^{-3}$	$5.11^{-3}$	$4.92^{-3}$	$4.72^{-3}$	$4.49^{-3}$	$4.26^{-3}$	$4.01^{-3}$
$h\pi$	3.98 -	3.81 2	3.64 -	3.48 2	$3.35^{-2}$	3.25 2	3.19 2	3.19 2	$h\pi$	4.08 -	$3.89^{-2}$	3.71 2	3.54 2	3.39 -	3.28 -	3.22 2	3.22 2
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$	$2.66^{-2}$	$2.46^{-2}$	$2.26^{-2}$	$2.06^{-2}$	$1.87^{-2}$	$1.68^{-2}$	$1.51^{-2}$	$1.34^{-2}$	$s\sigma$	$3.07^{-2}$	$2.83^{-2}$	$2.58^{-2}$	$2.34^{-2}$	$2.11^{-2}$	$1.90^{-2}$	$1.69^{-2}$	$1.50^{-2}$
$p\sigma$					$2.11^{-1}$				$p\sigma$		$2.78^{-1}$						
$d\sigma$					$1.04^{-2}$				$d\sigma$		$1.39^{-2}$						
$f\sigma$					$9.23^{-3}$				$f\sigma$		$1.14^{-2}$						
$g\sigma$					$6.31^{-4}$				$g\sigma$		$6.88^{-4}$						
$h\sigma$					$8.63^{-3}$				$h\sigma$		$2.33^{-2}$						
$p\pi$					$7.19^{-2}$				$p\pi$		$1.03^{-1}$						
$d\pi$					$5.42^{-4}$				$d\pi$		$8.32^{-4}$						
$f\pi$					$4.92^{-2}$				$f\pi$		$8.91^{-2}$						
$g \pi$					$2.56^{-3}$				$g \pi$		$3.49^{-3}$						
$h\pi$	3.25-2	3.37-2	3.54-2	3.72-2	$3.88^{-2}$	3.96-2	3.91-2	3.68-2	$h\pi$	3.28-2	$3.41^{-2}$	3.60-2	3.81-2	4.01-2	4.14	4.13	3.93-2
$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
$s\sigma$					$5.46^{-3}$				$s\sigma$		$1.13^{-2}$						
$p\sigma$	$1.25^{-1}$	$1.04^{-1}$	$8.41^{-2}$	$6.56^{-2}$	$4.91^{-2}$	$3.52^{-2}$	$2.41^{-2}$	$1.58^{-2}$	$p\sigma$	$1.32^{-1}$	$1.10^{-1}$	$8.92^{-2}$	$7.00^{-2}$	$5.27^{-2}$	$3.80^{-2}$	$2.61^{-2}$	$1.72^{-2}$
$d\sigma$	$5.80^{-3}$	$4.70^{-3}$	$3.72^{-3}$	$2.89^{-3}$	$2.18^{-3}$	$1.56^{-3}$	$1.02^{-3}$	$6.02^{-4}$	$d\sigma$	$6.43^{-3}$	$5.22^{-3}$	$4.15^{-3}$	$3.22^{-3}$	$2.45^{-3}$	$1.77^{-3}$	$1.18^{-3}$	$7.09^{-4}$
$f\sigma$	$5.53^{-3}$	$4.05^{-3}$	$2.68^{-3}$	$1.64^{-3}$	$9.71^{-4}$	$5.44^{-4}$	$2.91^{-4}$	$1.79^{-4}$	$f\sigma$	$6.16^{-3}$	$4.56^{-3}$	$3.01^{-3}$	$1.80^{-3}$	$1.04^{-3}$	$5.89^{-4}$	$3.18^{-4}$	$1.87^{-4}$
$g\sigma$					$1.10^{-4}$				$g\sigma$		$3.93^{-4}$						
$h\sigma$					$9.88^{-4}$				$h\sigma$		$1.31^{-3}$						
$p\pi$					$1.84^{-2}$				$p\pi$		$3.84^{-2}$						
$d\pi$					$1.00^{-4}$				$d\pi$		$2.13^{-4}$						
$f\pi$					$4.36^{-3}$				$f\pi$		$1.38^{-2}$						
$g \pi$					$5.23^{-4}$				$g \pi$		$1.29^{-3}$						
$h\pi$	$3.27^{-2}$	$2.69^{-2}$	$2.01^{-2}$	$1.33^{-2}$	$7.48^{-3}$	$3.27^{-3}$	$9.22^{-4}$	$1.27^{-4}$	$h\pi$	$3.53^{-2}$	$2.94^{-2}$	$2.23^{-2}$	$1.50^{-2}$	$8.64^{-3}$	$3.94^{-3}$	$1.22^{-3}$	$1.91^{-4}$

and

$$\begin{split} Q_{kk'} &= \delta_{\Lambda_{k'}\Lambda_{k} \pm 1} R^{-1} [(J \mp \Lambda_{k})(J \pm \Lambda_{k} + 1)]^{1/2} \\ &\times [(P_{k'k}^{\Theta} + A_{k'k}^{\Theta}) \pm i(\widetilde{P}_{k'k}^{\Phi} + A_{k'k}^{\Phi})] \end{split} \tag{B16}$$

with

$$\tilde{P}_{k'k} = R^{-1} \langle \phi_{k'} | \hat{L}_{x'} | \phi_k \rangle. \tag{B17}$$

The remainder of  $P^{\Phi}$  has been absorbed in the rotational kinetic energy. Q, which couples states with  $\Lambda$  values that

differ by  $\pm 1$ , is the angular or Coriolis coupling; D is diagonal in  $\Lambda(\Lambda_{k'} = \Lambda_k)$  and represents a small correction to the rotation kinetic energy. Equation (B14) can be reduced to the conventional form

$$\left\{ \frac{1}{2M} \left[ -i \frac{d}{dR} \mathbf{1} + \mathbf{P}^R + \mathbf{A}^R \right]^2 + \frac{K(K+1)}{2MR^2} \mathbf{1} + \frac{\sqrt{K(K+1)}}{MR} \right] \times \left[ \mathbf{P}^{\Theta} + \mathbf{A}^{\Theta} \right] \right\} \mathbf{G}(R) = \left[ \mathbf{1}E - \mathbf{U}(R) \right] \mathbf{G}(R), \tag{B18}$$

TABLE 31. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at E TABLE 32. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at E= 8.72 keV/amu

=9.04 keV/amu

$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ				$6.09^{-2}$					sσ		$7.22^{-2}$						
$p\sigma$				$4.12^{-1}$					$p\sigma$	$4.34^{-1}$	$4.32^{-1}$	$4.30^{-1}$	$4.27^{-1}$	$4.23^{-1}$	$4.20^{-1}$	$4.15^{-1}$	$4.10^{-1}$
$d\sigma$				$1.82^{-2}$					$d\sigma$		$1.87^{-2}$						
$f\sigma$				$1.57^{-2}$					$f\sigma$		$1.71^{-2}$						
$g\sigma$				$1.07^{-3}$					$g\sigma$		$1.17^{-3}$						
$h\sigma$				$3.83^{-2}$					$h\sigma$		$4.42^{-2}$						
$p\pi$				$2.53^{-1}$					$p\pi$		$2.98^{-1}$						
$d\pi$				$1.65^{-3}$					$d\pi$		$1.77^{-3}$						
$f\pi$				$1.95^{-1}$					$f\pi$		$2.16^{-1}$						
$g \pi$				$6.58^{-3}$					$g \pi$		$7.39^{-3}$						
$h\pi$	$5.38^{-2}$	$5.27^{-2}$	$5.15^{-2}$	$5.01^{-2}$	$4.86^{-2}$	$4.70^{-2}$	$4.53^{-2}$	$4.34^{-2}$	$h\pi$	$5.47^{-2}$	$5.36^{-2}$	$5.23^{-2}$	$5.09^{-2}$	$4.93^{-2}$	$4.76^{-2}$	$4.58^{-2}$	4.38 <sup>-2</sup>
ε (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$	$5.46^{-2}$	$5.28^{-2}$	$5.08^{-2}$	$4.86^{-2}$	$4.63^{-2}$	$4.37^{-2}$	$4.11^{-2}$	$3.82^{-2}$	$s\sigma$	$6.29^{-2}$	$6.09^{-2}$	$5.86^{-2}$	$5.60^{-2}$	$5.33^{-2}$	$5.03^{-2}$	$4.72^{-2}$	$4.39^{-2}$
$p\sigma$	$3.91^{-1}$	$3.84^{-1}$	$3.77^{-1}$	$3.68^{-1}$	$3.59^{-1}$	$3.48^{-1}$	$3.36^{-1}$	$3.22^{-1}$	$p\sigma$		$3.98^{-1}$						
$d\sigma$				$1.71^{-2}$					$d\sigma$		$1.80^{-2}$						
$f\sigma$	$1.49^{-2}$	$1.47^{-2}$	$1.45^{-2}$	$1.43^{-2}$	$1.40^{-2}$	$1.37^{-2}$	$1.34^{-2}$	$1.30^{-2}$	$f\sigma$		$1.58^{-2}$						
$g\sigma$				$8.98^{-4}$					$g\sigma$		$1.03^{-3}$						
$h\sigma$				$3.83^{-2}$					$h\sigma$		$4.54^{-2}$						
$p\pi$				$1.86^{-1}$					$p\pi$		$2.34^{-1}$						
$d\pi$				$1.34^{-3}$					$d\pi$		$1.51^{-3}$						
$f\pi$				$1.57^{-1}$					$f\pi$		$1.85^{-1}$						
$g \pi$				$5.34^{-3}$					$g \pi$		$6.27^{-3}$						
$h\pi$	$4.14^{-2}$	$3.95^{-2}$	$3.75^{-2}$	$3.57^{-2}$	$3.41^{-2}$	$3.29^{-2}$	$3.21^{-2}$	$3.21^{-2}$	$h\pi$	$4.18^{-2}$	$3.97^{-2}$	$3.76^{-2}$	$3.57^{-2}$	$3.40^{-2}$	$3.27^{-2}$	$3.19^{-2}$	$3.17^{-2}$
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	<i>ϵ</i> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$	$3.53^{-2}$	$3.24^{-2}$	$2.95^{-2}$	$2.66^{-2}$	$2.39^{-2}$	$2.13^{-2}$	$1.89^{-2}$	$1.67^{-2}$	$s\sigma$	$4.04^{-2}$	$3.70^{-2}$	$3.35^{-2}$	$3.01^{-2}$	$2.69^{-2}$	$2.39^{-2}$	$2.11^{-2}$	$1.85^{-2}$
$p\sigma$				$2.51^{-1}$					$p\sigma$		$3.01^{-1}$						
$d\sigma$	$1.52^{-2}$	$1.46^{-2}$	$1.39^{-2}$	$1.30^{-2}$	$1.21^{-2}$	$1.09^{-2}$	$9.72^{-3}$	$8.41^{-3}$	$d\sigma$	$1.58^{-2}$	$1.52^{-2}$	$1.46^{-2}$	$1.37^{-2}$	$1.28^{-2}$	$1.17^{-2}$	$1.05^{-2}$	$9.12^{-3}$
$f\sigma$				$1.13^{-2}$					$f\sigma$		$1.32^{-2}$						
$g\sigma$				$6.82^{-4}$					$g\sigma$		$7.67^{-4}$						
$h\sigma$				$2.19^{-2}$					$h\sigma$		$3.72^{-2}$						
$p\pi$				$9.26^{-2}$					$p\pi$		$1.25^{-1}$						
$d\pi$				$6.77^{-4}$					$d\pi$		$9.06^{-4}$						
$f\pi$				$7.41^{-2}$					$f\pi$		$1.08^{-1}$						
$g \pi$				$3.12^{-3}$					$g \pi$		$3.96^{-3}$						
$h\pi$	$3.27^{-2}$	$3.42^{-2}$	$3.62^{-2}$	$3.87^{-2}$	$4.11^{-2}$	$4.28^{-2}$	$4.32^{-2}$	$4.16^{-2}$	$h\pi$	$3.24^{-2}$	$3.39^{-2}$	$3.62^{-2}$	$3.90^{-2}$	$4.18^{-2}$	$4.40^{-2}$	$4.49^{-2}$	4.38 <sup>-2</sup>
<i>ϵ</i> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
$s\sigma$	$1.46^{-2}$	$1.25^{-2}$	$1.06^{-2}$	$8.64^{-3}$	$6.86^{-3}$	$5.30^{-3}$	$4.02^{-3}$	$3.01^{-3}$	$s\sigma$	$1.61^{-2}$	$1.39^{-2}$	$1.17^{-2}$	$9.57^{-3}$	$7.61^{-3}$	$5.88^{-3}$	$4.45^{-3}$	$3.32^{-3}$
$p\sigma$	$1.38^{-1}$	$1.15^{-1}$	$9.41^{-2}$	$7.43^{-2}$	$5.63^{-2}$	$4.08^{-2}$	$2.82^{-2}$	$1.86^{-2}$	$p\sigma$	$1.44^{-1}$	$1.21^{-1}$	$9.90^{-2}$	$7.85^{-2}$	$5.99^{-2}$	$4.37^{-2}$	$3.03^{-2}$	$2.01^{-2}$
$d\sigma$				$3.58^{-3}$					$d\sigma$		$6.34^{-3}$						
$f\sigma$				$2.00^{-3}$					$f\sigma$		$5.75^{-3}$						
$g\sigma$				$2.36^{-4}$					$g\sigma$		$4.46^{-4}$						
$h\sigma$				$2.39^{-3}$					$h\sigma$		$8.13^{-4}$						
$p\pi$				$2.61^{-2}$					$p\pi$		$4.33^{-2}$						
$d\pi$				$1.41^{-4}$					$d\pi$		$2.26^{-4}$						
$f\pi$				$7.55^{-3}$					$f\pi$		$1.73^{-2}$						
$g \pi$				$8.30^{-4}$					$g \pi$		$1.45^{-3}$						
$h\pi$	$3.78^{-2}$	$3.18^{-2}$	$2.45^{-2}$	$1.68^{-2}$	$9.86^{-3}$	$4.66^{-3}$	$1.55^{-3}$	$2.79^{-4}$	$h\pi$	$4.02^{-2}$	$3.43^{-2}$	$2.67^{-2}$	$1.86^{-2}$	$1.11^{-2}$	$5.44^{-3}$	$1.93^{-3}$	$3.91^{-4}$

Table 33. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at E Table 34. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at E=9.36 keV/amu

= 9.68 keV/amu

		-															
$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028	$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$8.35^{-2}$	$8.27^{-2}$	$8.17^{-2}$	$8.05^{-2}$	$7.92^{-2}$	7.77-2	$7.61^{-2}$	$7.42^{-2}$	sσ	$9.49^{-2}$	$9.39^{-2}$	$9.28^{-2}$	$9.15^{-2}$	$9.00^{-2}$	8.83-2	$8.64^{-2}$	8.43 <sup>-2</sup>
$p\sigma$	$4.48^{-1}$	$4.46^{-1}$	$4.44^{-1}$	$4.41^{-1}$	$4.37^{-1}$	$4.33^{-1}$	$4.29^{-1}$	$4.24^{-1}$	$p\sigma$		$4.60^{-1}$						
$d\sigma$				$1.90^{-2}$					$d\sigma$		$1.95^{-2}$						
$f\sigma$	1.07	1.00	1.07	$1.85^{-2}$	1.00	1.01	1.,,	1.,,	$f\sigma$		$2.12^{-2}$						
$g\sigma$				$1.22^{-3}$					$g\sigma$		$1.32^{-3}$						
$h\sigma$				$5.08^{-2}$					$h\sigma$		$5.64^{-2}$						
$p\pi$				$3.23^{-1}$					$p\pi$		$3.76^{-1}$						
$d\pi$				$1.82^{-3}$					$d\pi$		$1.96^{-3}$						
$f\pi$				$2.28^{-1}$					$f\pi$		$2.52^{-1}$						
$g \pi$				$7.89^{-3}$					$g \pi$		$8.86^{-3}$						
$h\pi$	5.52-2	5.41 <sup>-2</sup>	5.28-2	$5.13^{-2}$	4.97-2	$4.80^{-2}$	4.61 <sup>-2</sup>	4.40 <sup>-2</sup>	$h\pi$	5.55-2	5.43 <sup>-2</sup>	5.30-2	5.15 <sup>-2</sup>	4.98-2	4.80-2	4.61 <sup>-2</sup>	4.40 <sup>-2</sup>
<b>ε</b> (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093	<b>ε</b> (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
$s\sigma$	$7.20^{-2}$	$6.97^{-2}$	$6.70^{-2}$	$6.41^{-2}$	$6.10^{-2}$	$5.75^{-2}$	$5.39^{-2}$	$5.00^{-2}$	$s\sigma$	$8.19^{-2}$	$7.92^{-2}$	$7.62^{-2}$	$7.29^{-2}$	$6.93^{-2}$	$6.54^{-2}$	$6.12^{-2}$	$5.68^{-2}$
$p\sigma$	$4.18^{-1}$	$4.11^{-1}$	$4.03^{-1}$	$3.95^{-1}$	$3.85^{-1}$	$3.73^{-1}$	$3.60^{-1}$	$3.46^{-1}$	$p\sigma$	$4.31^{-1}$	$4.24^{-1}$	$4.16^{-1}$	$4.07^{-1}$	$3.97^{-1}$	$3.85^{-1}$	$3.72^{-1}$	$3.58^{-1}$
$d\sigma$	$1.86^{-2}$	$1.84^{-2}$	$1.83^{-2}$	$1.81^{-2}$	$1.78^{-2}$	$1.76^{-2}$	$1.72^{-2}$	$1.68^{-2}$	$d\sigma$		$1.88^{-2}$						
$f\sigma$	$1.74^{-2}$	$1.72^{-2}$	$1.69^{-2}$	$1.66^{-2}$	$1.62^{-2}$	$1.59^{-2}$	$1.55^{-2}$	$1.51^{-2}$	$f\sigma$	$1.93^{-2}$	$1.90^{-2}$	$1.86^{-2}$	$1.82^{-2}$	$1.78^{-2}$	$1.74^{-2}$	$1.69^{-2}$	$1.64^{-2}$
$g\sigma$				$1.04^{-3}$					$g\sigma$		$1.17^{-3}$						
$h\sigma$				$5.25^{-2}$					$h\sigma$		$5.92^{-2}$						
$p\pi$				$2.35^{-1}$					$p\pi$		$2.95^{-1}$						
$d\pi$				$1.47^{-3}$					$d\pi$		$1.68^{-3}$						
$f\pi$				$1.86^{-1}$					$f\pi$		$2.17^{-1}$						
$g \pi$				$6.31^{-3}$					$g \pi$		$7.46^{-3}$						
$h\pi$	$4.19^{-2}$	$3.97^{-2}$	$3.75^{-2}$	$3.55^{-2}$	$3.37^{-2}$	$3.22^{-2}$	$3.14^{-2}$	$3.12^{-2}$	$h\pi$	$4.17^{-2}$	$3.95^{-2}$	$3.72^{-2}$	$3.51^{-2}$	$3.31^{-2}$	$3.16^{-2}$	$3.07^{-2}$	$3.05^{-2}$
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305	<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
$s\sigma$	$4.60^{-2}$	$4.20^{-2}$	$3.79^{-2}$	$3.40^{-2}$	$3.02^{-2}$	$2.67^{-2}$	$2.35^{-2}$	$2.05^{-2}$	$s\sigma$	$5.22^{-2}$	$4.75^{-2}$	$4.28^{-2}$	$3.82^{-2}$	$3.39^{-2}$	$2.98^{-2}$	$2.60^{-2}$	$2.26^{-2}$
$p\sigma$	$3.30^{-1}$	$3.12^{-1}$	$2.93^{-1}$	$2.72^{-1}$	$2.49^{-1}$	$2.25^{-1}$	$2.00^{-1}$	$1.75^{-1}$	$p\sigma$	$3.41^{-1}$	$3.23^{-1}$	$3.03^{-1}$	$2.81^{-1}$	$2.58^{-1}$	$2.34^{-1}$	$2.08^{-1}$	$1.82^{-1}$
$d\sigma$	$1.64^{-2}$	$1.58^{-2}$	$1.52^{-2}$	$1.44^{-2}$	$1.35^{-2}$	$1.24^{-2}$	$1.12^{-2}$	$9.80^{-3}$	$d\sigma$	$1.69^{-2}$	$1.63^{-2}$	$1.57^{-2}$	$1.50^{-2}$	$1.41^{-2}$	$1.30^{-2}$	$1.18^{-2}$	$1.05^{-2}$
$f\sigma$				$1.31^{-2}$					$f\sigma$		$1.54^{-2}$						
$g\sigma$				$7.53^{-4}$					$g\sigma$		$8.75^{-4}$						
$h\sigma$				$3.60^{-2}$					$h\sigma$		$5.38^{-2}$						
$p\pi$				$1.09^{-1}$					$p\pi$		$1.52^{-1}$						
$d\pi$				$7.40^{-4}$					$d\pi$		$1.00^{-3}$						
$f\pi$				$9.03^{-2}$					$f\pi$		$1.29^{-1}$						
$g \pi$				$3.48^{-3}$					$g \pi$		$4.53^{-3}$						
$h\pi$	$3.19^{-2}$	$3.35^{-2}$	$3.59^{-2}$	$3.90^{-2}$	$4.22^{-2}$	$4.50^{-2}$	$4.64^{-2}$	$4.57^{-2}$	$h\pi$	$3.12^{-2}$	$3.28^{-2}$	$3.55^{-2}$	$3.88^{-2}$	$4.24^{-2}$	$4.57^{-2}$	$4.76^{-2}$	$4.75^{-2}$
<b>ε</b> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000	<b>ε</b> (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
$s\sigma$				$1.05^{-2}$					$s\sigma$	$1.96^{-2}$	$1.67^{-2}$	$1.41^{-2}$	$1.16^{-2}$	$9.23^{-3}$	$7.14^{-3}$	$5.38^{-3}$	$4.00^{-3}$
$p\sigma$	$1.51^{-1}$	$1.27^{-1}$	$1.04^{-1}$	$8.27^{-2}$	$6.35^{-2}$	$4.66^{-2}$	$3.25^{-2}$	$2.16^{-2}$	$p\sigma$	$1.57^{-1}$	$1.32^{-1}$	$1.09^{-1}$	$8.68^{-2}$	$6.69^{-2}$	$4.95^{-2}$	$3.47^{-2}$	$2.32^{-2}$
$d\sigma$				$4.35^{-3}$					$d\sigma$		$7.50^{-3}$						
$f\sigma$				$2.59^{-3}$					$f\sigma$		$7.13^{-3}$						
$g\sigma$				$2.84^{-4}$					$g\sigma$		$4.98^{-4}$						
$h\sigma$				$2.42^{-3}$					$h\sigma$		$1.36^{-3}$						
$p\pi$				$2.92^{-2}$					$p\pi$		$4.84^{-2}$						
$d\pi$				$1.49^{-4}$					$d\pi$		$2.39^{-4}$						
		1 00-2	1 24-2	0.14 - 3	c ac-3	4 21 - 3	$2.64^{-3}$	$1.42^{-3}$	$f\pi$	$3.04^{-2}$	$2.15^{-2}$	$1.48^{-2}$	$1.01^{-2}$	$6.83^{-3}$	$4.59^{-3}$	$2.90^{-3}$	$1.60^{-3}$
$f\pi$	$2.73^{-2}$								<i>J ''</i>								
$g \pi$	$1.82^{-3}$	$1.52^{-3}$	$1.22^{-3}$	$9.41^{-4}$	$6.97^{-4}$	$4.99^{-4}$	$3.45^{-4}$	$2.24^{-4}$	$g\pi$	$1.90^{-3}$	$1.58^{-3}$	$1.28^{-3}$	$9.94^{-4}$	$7.40^{-4}$	$5.31^{-4}$	$3.68^{-4}$	$2.40^{-4}$
9	$1.82^{-3}$	$1.52^{-3}$	$1.22^{-3}$		$6.97^{-4}$	$4.99^{-4}$	$3.45^{-4}$	$2.24^{-4}$	5	$1.90^{-3}$		$1.28^{-3}$	$9.94^{-4}$	$7.40^{-4}$	$5.31^{-4}$	$3.68^{-4}$	$2.40^{-4}$

Table 35. Single differential cross sections (in  $10^{-16}\,\mathrm{cm}^2$ ) at  $E=10.0\,\mathrm{keV/amu}$ 

$\epsilon$ (Ry)	0.010	0.012	0.013	0.016	0.018	0.021	0.024	0.028
sσ	$1.07^{-1}$	$1.06^{-1}$	$1.05^{-1}$	$1.03^{-1}$	$1.02^{-1}$	$9.96^{-2}$	$9.75^{-2}$	9.51-2
$p\sigma$	$4.75^{-1}$	$4.73^{-1}$	$4.70^{-1}$	$4.67^{-1}$	$4.63^{-1}$	$4.59^{-1}$	$4.55^{-1}$	$4.50^{-1}$
$d\sigma$	$2.00^{-2}$	$1.99^{-2}$	$1.99^{-2}$	$1.98^{-2}$	$1.97^{-2}$	$1.97^{-2}$	$1.96^{-2}$	$1.95^{-2}$
$f\sigma$	$2.45^{-2}$	$2.43^{-2}$	$2.40^{-2}$	$2.37^{-2}$	$2.34^{-2}$	$2.31^{-2}$	$2.27^{-2}$	$2.23^{-2}$
$g\sigma$	$1.39^{-3}$	$1.38^{-3}$	$1.37^{-3}$	$1.36^{-3}$	$1.34^{-3}$	$1.33^{-3}$	$1.31^{-3}$	$1.29^{-3}$
$h\sigma$	$6.20^{-2}$	$6.23^{-2}$	$6.26^{-2}$	$6.30^{-2}$	$6.34^{-2}$	$6.38^{-2}$	$6.43^{-2}$	$6.48^{-2}$
	$4.25^{-1}$	$4.18^{-1}$	$4.11^{-1}$	$4.03^{-1}$	$3.93^{-1}$	$3.83^{-1}$	$3.71^{-1}$	$3.58^{-1}$
$p\pi$	$2.09^{-3}$	$2.07^{-3}$	$2.05^{-3}$	$2.02^{-3}$	$1.99^{-3}$	$1.96^{-3}$	$1.92^{-3}$	$1.88^{-3}$
$d\pi$		$2.07$ $2.71^{-1}$	$2.68^{-1}$	$2.65^{-1}$	$2.61^{-1}$	$2.57^{-1}$	$2.52^{-1}$	
$f\pi$	$2.73^{-1}$	2./1		2.65	2.61			$2.47^{-1}$
$g\pi$	$9.78^{-3}$	$9.67^{-3}$	$9.55^{-3}$	$9.42^{-3}$	$9.26^{-3}$	$9.08^{-3}$	$8.88^{-3}$	$8.66^{-3}$
$h\pi$	$5.55^{-2}$	$5.42^{-2}$	$5.29^{-2}$	$5.14^{-2}$	$4.97^{-2}$	$4.78^{-2}$	$4.58^{-2}$	$4.37^{-2}$
$\epsilon$ (Ry)	0.033	0.038	0.044	0.051	0.059	0.069	0.080	0.093
sσ	$9.24^{-2}$	$8.94^{-2}$	$8.60^{-2}$	$8.23^{-2}$	$7.82^{-2}$	$7.38^{-2}$	$6.90^{-2}$	$6.40^{-2}$
$p\sigma$	$4.43^{-1}$	$4.36^{-1}$	$4.28^{-1}$	$4.19^{-1}$	$4.09^{-1}$	$3.97^{-1}$	$3.84^{-1}$	$3.69^{-1}$
$d\sigma$	$1.94^{-2}$	$1.92^{-2}$	$1.91^{-2}$	$1.89^{-2}$	$1.86^{-2}$	$1.84^{-2}$	$1.81^{-2}$	$1.77^{-2}$
$f\sigma$	$2.18^{-2}$	$2.14^{-2}$	$2.09^{-2}$	$2.03^{-2}$	$1.98^{-2}$	$1.92^{-2}$	$1.86^{-2}$	$1.80^{-2}$
$g\sigma$	$1.27^{-3}$	$1.24^{-3}$	$1.21^{-3}$	$1.18^{-3}$	$1.15^{-3}$	$1.11^{-3}$	$1.07^{-3}$	$1.02^{-3}$
$h\sigma$	$6.54^{-2}$	$6.60^{-2}$	$6.65^{-2}$	$6.70^{-2}$	$6.74^{-2}$	$6.76^{-2}$	$6.74^{-2}$	$6.67^{-2}$
$p\pi$	$3.43^{-1}$	$3.28^{-1}$	$3.10^{-1}$	$2.92^{-1}$	$2.72^{-1}$	$2.52^{-1}$	$2.30^{-1}$	$2.09^{-1}$
	$1.83^{-3}$	$1.77^{-3}$	$1.71^{-3}$	$1.64^{-3}$	$1.56^{-3}$	$1.48^{-3}$	$1.38^{-3}$	$1.28^{-3}$
$d\pi$		$2.34^{-1}$	$2.26^{-1}$	$2.17^{-1}$	$2.07^{-1}$	$1.46$ $1.96^{-1}$	$1.83^{-1}$	$1.70^{-1}$
$f\pi$	$2.41^{-1}$	$8.12^{-3}$						$5.81^{-3}$
$g\pi$	$8.41^{-3}$		$7.81^{-3}$	$7.47^{-3}$	$7.10^{-3}$	$6.69^{-3}$	$6.26^{-3}$	
$h\pi$	$4.14^{-2}$	$3.90^{-2}$	$3.67^{-2}$	$3.45^{-2}$	$3.25^{-2}$	$3.09^{-2}$	$2.98^{-2}$	$2.96^{-2}$
<b>ε</b> (Ry)	0.108	0.125	0.145	0.168	0.195	0.226	0.263	0.305
sσ	$5.88^{-2}$	$5.35^{-2}$	$4.81^{-2}$	$4.29^{-2}$	$3.78^{-2}$	$3.31^{-2}$	$2.88^{-2}$	$2.49^{-2}$
$p\sigma$	$3.52^{-1}$	$3.34^{-1}$	$3.13^{-1}$	$2.91^{-1}$	$2.67^{-1}$	$2.42^{-1}$	$2.16^{-1}$	$1.89^{-1}$
$d\sigma$	$1.73^{-2}$	$1.68^{-2}$	$1.62^{-2}$	$1.55^{-2}$	$1.46^{-2}$	$1.36^{-2}$	$1.24^{-2}$	$1.11^{-2}$
$f\sigma$	$1.74^{-2}$	$1.67^{-2}$	$1.61^{-2}$	$1.53^{-2}$	$1.45^{-2}$	$1.36^{-2}$	$1.26^{-2}$	$1.14^{-2}$
$g\sigma$	$9.81^{-4}$	$9.37^{-4}$	$8.94^{-4}$	$8.52^{-4}$	$8.12^{-4}$	$7.72^{-4}$	$7.29^{-4}$	$6.76^{-4}$
$h\sigma$	$6.52^{-2}$	$6.26^{-2}$	$5.87^{-2}$	$5.31^{-2}$	$4.57^{-2}$	$3.66^{-2}$	$2.63^{-2}$	$1.61^{-2}$
	$1.88^{-1}$	$1.67^{-1}$	$1.47^{-1}$	$1.29^{-1}$	$1.13^{-1}$	$9.77^{-2}$	$8.45^{-2}$	$7.25^{-2}$
$p\pi$	$1.17^{-3}$	$1.07$ $1.06^{-3}$	$9.42^{-4}$	$8.22^{-4}$	$7.03^{-4}$	$5.90^{-4}$	$4.85^{-4}$	$3.91^{-4}$
$d\pi$	1.1/		9.42	1.00-1	7.03	5.90 7.51 <sup>-2</sup>	4.85 5.07 <sup>-2</sup>	$4.58^{-2}$
$f\pi$	$1.56^{-1}$	$1.40^{-1}$	$1.24^{-1}$	$1.08^{-1}$	$9.13^{-2}$	$7.51^{-2}$	$5.97^{-2}$	4.58
$g\pi$	$5.34^{-3}$	$4.86^{-3}$	$4.39^{-3}$	$3.92^{-3}$	$3.48^{-3}$	$3.06^{-3}$	$2.67^{-3}$	$2.31^{-3}$
$h\pi$	$3.03^{-2}$	$3.20^{-2}$	$3.48^{-2}$	$3.84^{-2}$	$4.24^{-2}$	$4.61^{-2}$	$4.87^{-2}$	$4.91^{-2}$
$\epsilon$ (Ry)	0.353	0.410	0.476	0.552	0.640	0.743	0.862	1.000
$s\sigma$	$2.14^{-2}$	$1.83^{-2}$	$1.54^{-2}$	$1.26^{-2}$	$1.01^{-2}$	$7.81^{-3}$	$5.89^{-3}$	$4.36^{-3}$
$p\sigma$	$1.63^{-1}$	$1.37^{-1}$	$1.13^{-1}$	$9.08^{-2}$	$7.04^{-2}$	$5.23^{-2}$	$3.70^{-2}$	$2.48^{-2}$
$d\sigma$	$9.61^{-3}$	$8.07^{-3}$	$6.57^{-3}$	$5.18^{-3}$	$3.99^{-3}$	$3.00^{-3}$	$2.16^{-3}$	$1.43^{-3}$
$f\sigma$	$9.83^{-3}$	$7.88^{-3}$	$5.63^{-3}$	$3.43^{-3}$	$1.75^{-3}$	$8.20^{-4}$	$4.32^{-4}$	$2.57^{-4}$
$g\sigma$	$6.09^{-4}$	$5.26^{-4}$	$4.31^{-4}$	$3.32^{-4}$	$2.38^{-4}$	$1.54^{-4}$	$8.40^{-5}$	$3.66^{-5}$
$h\sigma$	$7.59^{-3}$	$2.39^{-3}$	$9.59^{-4}$	$1.93^{-3}$	$2.73^{-3}$	$1.99^{-3}$	$7.70^{-4}$	$2.96^{-4}$
$p\pi$	$6.14^{-2}$	$5.10^{-2}$	$4.13^{-2}$	$3.25^{-2}$	$2.73$ $2.51^{-2}$	$1.93^{-2}$	$1.51^{-2}$	$1.21^{-2}$
	$3.11^{-4}$	$2.46^{-4}$	$1.96^{-4}$	$1.56^{-4}$	$1.25^{-4}$	$9.78^{-5}$	$7.47^{-5}$	$5.65^{-5}$
$d\pi$	2.11	$2.46$ $2.39^{-2}$	1.70	1.50	$7.43^{-3}$	$4.98^{-3}$	$3.18^{-3}$	$1.79^{-3}$
$f\pi$	$3.37^{-2}$	2.39 2	$1.64^{-2}$	$1.10^{-2}$	7.43	4.98	3.18 <sup>3</sup>	1.79
$g \pi$	$1.97^{-3}$	$1.65^{-3}$	$1.34^{-3}$	$1.05^{-3}$	$7.83^{-4}$	$5.63^{-4}$	$3.91^{-4}$	$2.57^{-4}$
	4 2	4 4 2	2 2 2	2 42-2	4 2	0.02	2 2 2	0 = -1
$h\pi$	$4.67^{-2}$	$4.13^{-2}$	$3.34^{-2}$	$2.42^{-2}$	$1.53^{-2}$	$8.09^{-3}$	$3.29^{-3}$	$8.79^{-4}$

by taking into account that the angular momentum of heavy particles K is much greater than that of electron system  $\Lambda$ , i.e.,  $K \approx J \gg \Lambda$ .

### 9. References

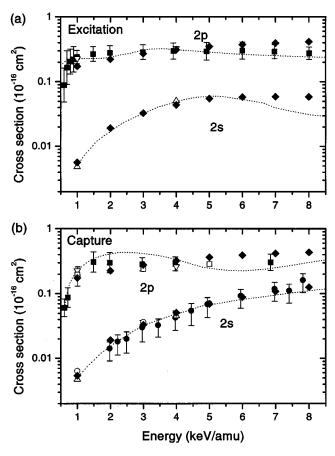


Fig. 6. Cross section comparison (hydrogen–proton system) for: (a) excitation to 2s and 2p levels and (b) capture into 2s and 2p levels of atomic hydrogen in collisions with slow protons. Solid squares with error bars, measured values of Barnett<sup>23</sup>; solid circles with error bars, measured values of Morgan *et al.*<sup>24</sup>; dotted lines, the triple-center close-coupling calculations of McLaughlin *et al.*<sup>17</sup>; open triangles, the double-center close-coupling calculations of Toshima<sup>10</sup>; open circles, molecular orbital close-coupling calculations of Kimura *et al.*<sup>25</sup>; solid diamonds, present calculations with basis set C.

<sup>&</sup>lt;sup>1</sup>M. Kimura and N. F. Lane, Adv. At. Mol. Opt. Phys. 26, 79 (1989).

<sup>&</sup>lt;sup>2</sup>B. H. Bransden and M. R. C. McDowell, *Charge Exchange and the Theory of Ion–Atom Collisions* (Oxford Science, Oxford, 1992).

<sup>&</sup>lt;sup>3</sup>H. B. Gilbody, Adv. At. Mol. Opt. Phys. **33**, 149 (1994).

<sup>&</sup>lt;sup>4</sup>H. B. Gilbody, *Proceedings XIX ICPEAC Invited Papers, British Columbia, Canada*, edited by L. J. Dube, J. B. Mitchell, J. W. McConkey, and C. E. Brion (AIP, New York, 1995), Vol. 360, p. 19.

<sup>&</sup>lt;sup>5</sup>S. Zou, L. Pichl, M. Kimura, and T. Kato, Phys. Rev. A 66, 042707 (2002).

<sup>&</sup>lt;sup>6</sup>M. Pieksma, S. Y. Ovchinnikov, J. van Eck, W. B. Westerveld, and A. Niehaus, Phys. Rev. Lett. **73**, 46 (1994).

<sup>&</sup>lt;sup>7</sup> M. B. Shah, J. Geddes, B. M. McLaughlin, and H. B. Gilbody, J. Phys. B. 31, L757 (1998).

<sup>&</sup>lt;sup>8</sup>M. B. Shah and H. B. Gilbody, J. Phys. B **14**, 2361 (1981).

<sup>&</sup>lt;sup>9</sup> M. B. Shah, D. S. Elliot, and H. B. Gilbody, J. Phys. B. **20**, 2481 (1987).

<sup>&</sup>lt;sup>10</sup>N. Toshima, Phys. Rev. A **59**, 1981 (1999).

<sup>&</sup>lt;sup>11</sup> A. Kolakowska, M. S. Pindzola, and D. R. Schultz, Phys. Rev. A **59**, 3588 (1999).

<sup>&</sup>lt;sup>12</sup>E. Y. Sidky and C. D. Lin, Phys. Rev. A **65**, 012711 (2001).

<sup>&</sup>lt;sup>13</sup> V. Sethu Raman, W. R. Thorson, and C. F. Lebeda, Phys. Rev. A 8, 1316 (1973)

<sup>&</sup>lt;sup>14</sup>W. R. Thorson and J. B. Delos, Phys. Rev. A **18**, 117 (1978); **18**, 135 (1978).

<sup>&</sup>lt;sup>15</sup> W. R. Thorson and G. Bandarage, Phys. Rev. A **37**, 692 (1988); G. Bandarage and W. R. Thorson, *ibid.* **37**, 716 (1988).

<sup>&</sup>lt;sup>16</sup>T. G. Winter and C. D. Lin, Phys. Rev. **29**, 3071 (1984).

<sup>&</sup>lt;sup>17</sup>B. M. McLaughlin, T. G. Winter, and J. F. McCann, J. Phys. B 30, 1043 (1997)

<sup>&</sup>lt;sup>18</sup>W. Fritsch and C. D. Lin, Phys. Rev. A 27, 3361 (1983).

- <sup>19</sup>S. Y. Ovchinnkov and J. H. Macek, 18th International Conference on Physics of Electronic and Atomic Collisions (Aarhus), edited by T. Andersen, B. Fastrup, F. Folkmann, and H. Knudsen (IFA Print, Aarhus, 1993), Abstracts p. 676.
- <sup>20</sup> M. Pieksma, S. Y. Ovchinnikov, and J. H. Macek, J. Phys. B **31**, 1267 (1998).
- <sup>21</sup>J. B. Delos, Rev. Mod. Phys. **53**, 287 (1981).
- <sup>22</sup> W. R. Thorson, M. Kimura, J. H. Choi, and S. K. Knudson, Phys. Rev. A 24, 1768 (1981).
- <sup>23</sup> C. F. Barnett, Oak Ridge National Laboratory Report No. 6086, July, 1990, unpublished; The data were extracted from the publication by McLaughlin *et al.*<sup>17</sup>
- <sup>24</sup>T. J. Morgan, J. Stone, and R. Mayo, Phys. Rev. A 22, 1460 (1980).
- <sup>25</sup> M. Kimura and W. R. Thorson, Phys. Rev. A **24**, 1780 (1981).

- <sup>26</sup>W. L. Fite, R. F. Stebbings, D. G. Hummer, and R. T. Brackmann, Phys. Rev. **119**, 663 (1960).
- $^{27}\mathrm{J}.$  Rankin and W. R. Thorson, Phys. Rev. A 18, 1990 (1978).
- <sup>28</sup> D. R. Bates and T. R. Carson, Proc. R. Soc., London Ser. A **234**, 207 (1956).
- <sup>29</sup>G. Hunter and H. O. Pritchard, J. Chem. Phys. **46**, 2146 (1967).
- $^{30}$  K. Helfrich and H. Hartmann, Theor. Chem. Acta 16, 263 (1970).
- <sup>31</sup>M. Aubert, N. Bessis, and G. Bessis, Phys. Rev. A **10**, 51 (1974).
- <sup>32</sup>L. I. Ponomarev and L. N. Somov, J. Comput. Phys. **20**, 183 (1976).
- <sup>33</sup>T. G. Winter, M. D. Duncan, and N. F. Lane, J. Phys. B 10, 285 (1977)
- <sup>34</sup> J. Rankin and W. R. Thorson, J. Comput. Phys. **32**, 437 (1979).
- <sup>35</sup>D. S. F. Crothers and J. F. McCann, J. Phys. B **16**, 3229 (1983).