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PHOTOIONIZATION CROSS SECTIONS OF He AND H_2

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ABSTRACT

We combine accurate measurements at low energies and theoretical calculations at high energies to construct sets of photoionization cross sections of He and H_2 that should be reliable at all energies. We control the accuracy of the recommended cross section data by ensuring that they satisfy a range of oscillator strength sum rules. We provide accurate analytic formulae for the photoionization cross sections that have the proper asymptotic form. At high frequencies the cross sections for H_2 are 2.8 times those for H.

Subject headings: atomic data — molecular data — molecular processes — ultraviolet: general — X-rays: general

1. INTRODUCTION

The photoionization cross sections of H, H_2, and He are important parameters in the determination of the ionization structure of cosmic gas subjected to ultraviolet and X-ray radiation. The cross section for H is known analytically as a function of photon energy (Bethe & Salpeter 1967; Sobel'man 1991), but the values for He and H_2 are approximate. The representations commonly used for He and H_2 in calculations for astrophysical environments (Shapiro & Kang 1987; Cen 1992; Haiman, Thoul, & Loeb 1996) yield cross sections that are probably adequate at ultraviolet and extreme-ultraviolet wavelengths, but with the exception of the expressions given by Band et al. (1990) and Verner et al. (1993), they do not have the correct form at X-ray wavelengths.

We construct here cross sections for He and H_2 from a combination of experimental measurements and theoretical calculations, and we show that their accuracy can be controlled by requiring that they be consistent with oscillator strength moment sum rules and that they have the correct physical form at high energies.

2. SUM RULES

The electric dipole absorption oscillator strength of a transition from an initial state with eigenfunction $\Psi_0(\boldsymbol{r})$ and eigenvalue E_0 to a final state with eigenfunction $\Psi_n(\boldsymbol{r})$ and eigenvalue E_n is given by the expression

$$f_n = \tfrac{2}{3}(E_0 - E_n)\left|\left\langle 0\left|\sum_{i=1}^{N} \boldsymbol{r}_i\right|n\right\rangle\right|^2 , \quad (1)$$

where $\boldsymbol{r}_i$ is the position vector of electron i of an N-electron atomic or molecular system, and all quantities are in atomic units. Define the oscillator strength moment $S(k)$,

$$S(k) = \sum_n (E_0 - E_n)^k f_n + \int_0^\infty (I + \epsilon)^k \frac{df}{d\epsilon}\, d\epsilon , \quad (2)$$

where I is the ionization potential, ϵ is the energy of the ejected electron, and $df/d\epsilon$ is the differential oscillator strength for absorption into the ionization continuum. The differential oscillator strength is related to the photoionization cross section $\sigma(E)$ by

$$\sigma(E) = 4.03 \times 10^{-18} \frac{df}{d\epsilon}\ \mathrm{cm}^2 , \quad (3)$$

where $E = I + \epsilon$ is the photon energy.

The oscillator strengths satisfy the sum rules (Dalgarno & Lynn 1957; Bethe & Salpeter 1967)

$$S(-2) = \alpha , \quad (4)$$

where α is the electric dipole polarizability,

$$S(-1) = \tfrac{2}{3}\left\langle 0\left|\left(\sum_i^N \boldsymbol{r}_i\right)^2\right|0\right\rangle , \quad (5)$$

$$S(0) = N , \quad (6)$$

$$S(1) = \tfrac{4}{3}\left(E_0 + \tfrac{1}{2}\left\langle 0\left|\sum_{i\neq j}^N \boldsymbol{p}_i \cdot \boldsymbol{p}_j\right|0\right\rangle\right) , \quad (7)$$

$$S(2) = \frac{8\pi}{3}\left\langle 0\left|\sum_i^N \delta(\boldsymbol{r}_i)\right|0\right\rangle \text{ for He} , \quad (8)$$

and

$$S(2) = \frac{16\pi}{3}\langle 0|\delta(\boldsymbol{r}_{ia})|0\rangle \text{ for } H_2 , \quad (9)$$

where $\boldsymbol{r}_{ia}$ is the position vector of electron i relative to nucleus a. In equation (7) $\boldsymbol{p}_i$ is the momentum of electron i. If the Bethe logarithm K is known, the relationship

$$\sum_n f_n(E_n - E_0)^2 \ln(E_n - E_0) + \int \frac{df}{d\epsilon}(I + \epsilon)^2 \ln(I + \epsilon) d\epsilon = S(2) \ln 2K \quad (10)$$

can also be used.

3. PHOTOIONIZATION OF HELIUM

The values of the sum rules and of $S(2)\ln 2K$ (Drake 1996) are presented in column (2) of Table 1. Discussions of the consistency of the sum rules with the available data on the discrete and continuum oscillator strengths have been given by Dalgarno & Lynn (1957), Dalgarno & Stewart (1960), Migneron & Levinger (1965), Cooper (1996), and Berkowitz (1997).

The contributions from the discrete 1^1S–n^1P transitions can be obtained from the oscillator strengths listed by Drake (1996). We extrapolated them to $n > 7$ using the formula

$$f_n = \frac{(7-\mu)^3}{(n-\mu)^3} f_7 , \quad (11)$$

TABLE 1

HELIUM SUM RULES

Sum Rule (1)	Exact (2)	Discrete (3)	24.6–280 eV (4)	Resonances (5)	0.28–2 keV (6)	2–8 keV (7)	8–∞ keV (8)	Total (9)
$S(-2)$..........	1.3832	0.6495	0.7267	0.0027	0.0001	...	...	1.379
$S(-1)$..........	1.5050	0.5234	0.9678	0.0063	0.0015	...	...	1.499
$S(0)$	2	0.4229	1.5242	0.0147	0.025	...	...	1.987
$S(1)$	4.0837	0.3426	3.179	0.034	0.3996	0.03395	0.006	3.995
$S(2)$	30.33	0.28	9.853	0.08	9.035	4.396	5.686	29.33
$S(2)\ln 2K$......	111.5	−0.06	13.21	0.08	29.54	21.71	44.46	108.9

where $\mu = -0.012$ is the limiting value of the quantum defect for the ^1P series. Their contributions to the individual sums are given in column (3) of Table 1. The discrete oscillator strengths sum to 0.4229, in satisfactory agreement with an experimentally derived sum of 0.431 ± 0.02 (Chan et al. 1991).

From the continuity of the oscillator strength across the ionization threshold, we obtain from equation (11) a value of 1.84 for $df/d\epsilon$ at the spectral head, corresponding to a threshold photoionization cross section of 7.42×10^{-18} cm^2 at a photon energy of 24.587 eV. The value is in close agreement with several theoretical calculations and experimental measurements (Samson et al. 1994b). Samson et al. (1994b) recommend a threshold cross section of 7.40×10^{-18} cm^2, and Bizau & Wuilleumier (1995) recommend 7.42×10^{-18} cm^2.

Reliable measurements exist for photon energies up to 120 eV. Samson et al. (1994b) and Bizau & Wuilleumier (1995) extended them to 280 eV with an extrapolation based on several earlier sources of experimental data. The recommended values are listed in Table 2. They are in satisfactory agreement with theoretical calculations (Bell & Kingston 1971; Hino et al. 1993; Meyer & Greene 1994; Decleva, Lisini, & Venuti 1994; Tang & Shimamura 1995; Pont & Shakeshaft 1995; Venuti, Decleva, & Lisini 1996). We list in column (4) of Table 1 the contributions to the sum rules. In the same energy region are absorptions into doubly excited resonance states (*nsmp*), which introduce structural features into the variation of the cross section with photon energy. Although resonance parameters, energy, width, and profile have been calculated by a number of investigators (Ho 1995; Venuti et al. 1996; Sadeghpour & Cavagnero 1993; Sanchez & Martin 1991; Tang et al. 1992), explicit values for the resonant contributions to different oscillator sum rules have not been available. A recent calculation (Sadeghpour 1998) shows that they contribute negligibly for $m \geq 5$ and $n \geq 6$. The doubly excited state contributions to the sum rules obtained by integrating over the calculated resonance profiles are given in column (5) of Table 1. With their inclusion, the sum rules $S(-2)$ and $S(-1)$ to which higher energies yield negligible amounts are satisfied to within 0.5%.

The photoionization cross sections at higher energies are less certain. The measurements may be affected by the presence of impurities in the gas and, at energies above 1.5 keV, by Compton ionization (McCrary, Looney, & Atwater 1970; Samson, Greene, & Bartlett 1993; Samson et al. 1994a; see also § 5). From a review of the theoretical and experimental data, Samson et al. (1994b) have constructed a set of photoionization cross sections at energies between 280 eV and 8 keV. Subsequently, several calculations of the cross sections have been reported (Hino 1993; Andersson & Burgdoerfer 1993; Forrey et al. 1997) using different methods. The calculations are consistent with the limiting nonrelativistic form,

$$\frac{df}{d\epsilon} \sim \frac{2^{1/2} Z^2 S(2)}{\pi} E^{-7/2} \tag{12}$$

(Kabir & Salpeter 1957; Dalgarno & Stewart 1960), which, on using the value of $S(2)$ in Table 1 and converting from atomic units, becomes, for the photoionization cross section,

$$\sigma(E) \sim \frac{733.0}{E(\mathrm{keV})^{7/2}} \text{ barns} . \tag{13}$$

We constructed a set of cross sections by merging the high-energy data of Andersson & Burgdoerfer (1993) and Forrey et al. (1997), computed in the acceleration gauge, with the low-energy results of Samson et al. (1994b). The corresponding contributions to the sum rules are listed in columns (6), (7), and (8) of Table 1 for energies between 280 eV and 2 keV, 2 and 8 keV, and greater than 8 keV, respectively.

The sums of all the contributions are given in column (9). There are differences of up to 3% from the exact values that can be sensibly remedied only by increasing the cross sections in the lower energy region between 170 eV and 2 keV. We modified them accordingly so that a smoothly varying cross section results. It is illustrated in Figure 1 as the product of $E^{7/2}\sigma(E)$ with E in units of the ionization poten-

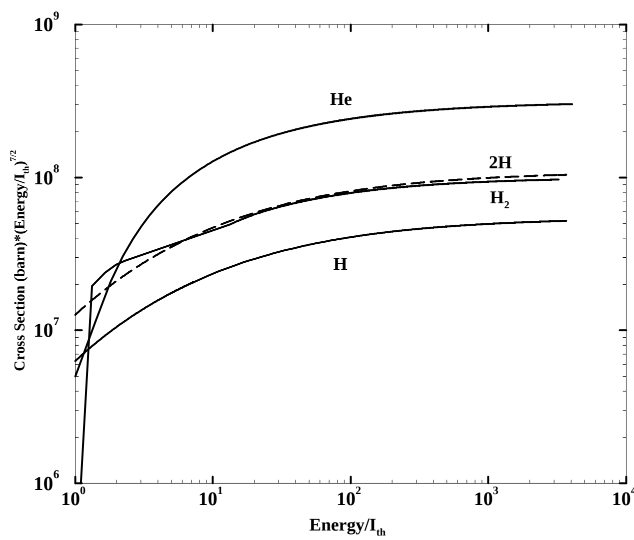

FIG. 1.—Recommended photoionization cross sections in the form $(E/I_{th})^{7/2}\sigma(E)$, where I_{th} is the respective ionization potential for H, He, and H_2. Also shown is $2 \times$ the hydrogen cross section.

TABLE 2

TOTAL PHOTOIONIZATION CROSS SECTIONS OF He FROM 24.6 TO 300 eV

E(eV)	σ(Mbarn) (Samson et al. 1994a)	Bizau & Wuilleumier 1995	σ(Mbarn) (Present Work)
24.6	7.400	7.420	7.460
26	6.790	7.800	6.820
28	6.050	6.050	6.080
30	5.380	5.380	5.440
32	4.820	4.820	4.870
34	4.320	4.320	4.360
36	3.880	3.880	3.910
38	3.500	3.500	3.530
40	3.160	3.160	3.190
42	2.860	2.850	2.890
44	2.600	2.600	2.630
46	2.380	2.380	2.410
48	2.190	2.190	2.200
50	2.020	2.010	2.020
52	1.850	1.840	1.860
54	1.710	1.710	1.720
56	1.630	1.620	1.590
58	1.580	1.560	1.470
64	1.190	1.200	1.180
66	1.150	1.150	1.100
68	1.060	1.060	1.030
70	0.975	0.980	0.965
72	0.907	0.910	0.903
74	0.842	0.850	0.847
76	0.788	0.800	0.794
78	0.738	0.750	0.746
80	0.693	0.700	0.702
82	0.652	0.660	0.660
84	0.614	0.622	0.622
86	0.578	0.586	0.587
88	0.546	0.555	0.554
90	0.516	0.523	0.523
92	0.488	0.494	0.495
94	0.464	0.469	0.469
96	0.438	0.442	0.444
98	0.416	0.421	0.421
100	0.3930	0.3960	0.3990
105	0.3450	0.3470	0.3510
110	0.3060	0.3080	0.3100
115	0.2730	0.2760	0.2750
120	0.2440	0.2480	0.2450
125	0.2180	0.2280	0.2190
130	0.1960	0.2070	0.1970
135	0.1770	0.1870	0.1770
140	0.1600	0.1710	0.1600
145	0.1440	0.1550	0.1450
150	0.1310	0.1370	0.1320
155	0.1180	0.1240	0.1200
160	0.1080	0.1150	0.1090
165	0.0980	0.1040	0.1010
170	0.0894	0.0940	0.0920
175	0.0826	0.0870	0.0850
180	0.0760	0.0800	0.0782
185	0.0700	0.0730	0.0722
190	0.0643	0.0670	0.0667
195	0.0593	0.0620	0.0618
200	0.0550	0.0580	0.0574
205	0.0510	0.0530	0.0533
210	0.0474	0.0500	0.0497
215	0.0440	0.0460	0.0463
220	0.0409	0.0430	0.0433
225	0.0382	0.0397	0.0404
230	0.0356	0.0369	0.0379
235	0.0335	0.0340	0.0355
240	0.0315	0.0329	0.0333
245	0.0295	0.0309	0.0313
250	0.0277	0.0287	0.0295
255	0.0261	0.0267	0.0278
260	0.0245	0.0253	0.0262
270	0.0218	0.0227	0.0234
280	0.0194	0.0196	0.0209
300	0.0155	0.0162	0.0169

tial of helium. A detailed comparison with the recommendations of Samson et al. (1994b) and Bizau & Wuillemier (1994) is given in Table 2. The revised sum rules are presented in Table 3, where they are compared to those of Table 1. The agreement with the sum rules is now within 0.5%. If we use the recent experimental photoionization data of Azuma et al. (1995) in the range of energies 3–14 keV, we obtain results for the $S(k)$ sum rules that agree with the values given in Table 3 for $k < 2$, but the Azuma et al. (1995) data underestimate $S(2)$ and $S(2)\ln 2K$ by as much as 6%. The Azuma et al. (1995) photoionization data are obtained by subtracting the theoretical coherent and incoherent scattering cross sections compiled by Hubbell et al. (1975), which dominate for energies higher than about 5 keV, from the measured total attenuation cross sections. The data do not fit the asymptotic behavior with energy given in equation (13).

The modified photoionization cross sections are reproduced by the analytical formula

$$\sigma_{\mathrm{He}}(E) = \frac{733.0}{E(\mathrm{keV})^{7/2}}\left(1 + \sum_{n=1}^{6} \frac{a_n}{x^{n/2}}\right) \text{barns} , \qquad (14)$$

where $x = E/24.58$ eV and a_n are parameters given in Table 4. The resonance structures calculated by Sadeghpour (1997) may be superposed, but their effects are small.

The fit in equation (14) satisfies the oscillator strength sum rules very accurately and has the proper asymptotic form with energy. The expansion coefficients in Table 4 have alternating signs, suggestive of a decaying exponential form. We fitted the data alternatively to the following form:

$$\sigma_{\mathrm{He}}(E) = 7.4 \times 10^6[a_1 x^{-s} + (1 - a_1)x^{-(s+1)}] + \frac{733.0}{E(\mathrm{keV})^{7/2}} (1 + a_2 x^{-1/2} e^{-a_3 x^{-1/2}}) \text{ barns} , \qquad (15)$$

where the first two terms were suggested by Seaton (1958) for energies near threshold. The fitting parameters are given in Table 5. The four-term polynomial fit in $x^{-1/2}$ in place of the exponential term produces an alternating series whose

TABLE 3

VALUES OF SUM RULES FOR He

Value	$S(-2)$	$S(-1)$	$S(0)$	$S(1)$	$S(2)$	$S(2)\ln 2K$
Exact	1.383	1.505	2	4.084	30.3	111.5
Empirical	1.383	1.504	1.996	4.063	30.2	111.2

TABLE 4

FITTING PARAMETERS FOR HELIUM PHOTOIONIZATION CROSS SECTION: EQUATION (14)

a_1	a_2	a_3	a_4	a_5	a_6
−4.7416	14.8200	−30.8678	37.3584	−23.4585	5.9133

TABLE 5

FITTING PARAMETERS FOR HELIUM PHOTOIONIZATION CROSS SECTION: EQUATION (15)

a_1	s	a_2	a_3
7.3861	3.9119	−3.2491	1.1783

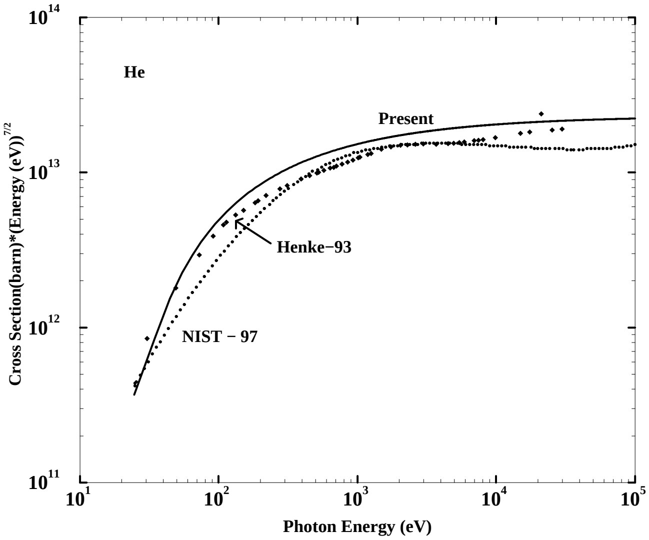

FIG. 2.—Recommended photoionization cross section for He in the form $E^{7/2}\sigma(E)$. Also shown are the data of Henke et al. (1993) and NIST (1997). The NIST results do not asymptotically tend to a constant. (According to a note on X-ray attenuation databases at NIST 1997, the photoabsorption results given there for helium are unreliable.)

coefficients are approximately equal to the expansion coefficients for the exponential, $-a_3$, $a_3^2/2$, $-a_3^3/3!$.

Double photoionization of helium $\nu + \mathrm{He} \rightarrow \mathrm{He}^{2+} + 2e$ is included in the sum rules. It has received considerable attention (Ishihara, Hino, & McGuire 1991; Levin et al. 1991, 1993; Bartlett et al. 1992; Dalgarno & Sadeghpour 1992; Andersson & Burgdoerfer 1993; Kornberg & Miraglia 1993; Hino 1993; Hino et al. 1993; Proulx & Shakeshaft 1993; Berrah et al. 1993; Teng & Shakeshaft 1993, 1994; Fan, Sadeghpour, & Dalgarno 1994; Azuma et al. 1995; Sadeghpour 1996), because it provides a direct measure of the effect of electron correlation. At high energies, the ratio of the cross sections for double to single ionization tends to a constant value of 0.0164 (Dalgarno & Sadeghpour 1992; Forrey et al. 1995). As the energy decreases below 1 keV, the ratio increases to a maximum of about 0.04 at 120 eV and then decreases sharply to zero at the threshold of 79.0 eV (Samson, Bartlett, & He 1992).

In Figure 2 we show also the data from Henke, Gullikson, & Davis (1993) and NIST (1997). We believe that in the energy range from threshold to 600 eV, our cross sections have an uncertainty of less than 2%. The error in the photoabsorption cross sections at higher energies should be no more than 5% at any energy, and it is on average less than 2%.

4. PHOTOIONIZATION OF MOLECULAR HYDROGEN

Samson & Haddad (1994) have measured the photoabsorption cross sections of H_2 at photon energies between 18 and 113 eV to within an uncertainty of $\pm 3\%$. There have been earlier measurements down to the threshold energy of 15.4 eV (Cook & Metzger 1964; Lee, Carlson, & Judge 1976). The threshold region is complicated by the presence of autoionizing resonances arising from vibrationally excited Rydberg states whose detailed structure has not been fully analyzed (Dehmer & Chupka 1976; Dehmer et al. 1992; Jungen, Pratt, & Ross 1995). Theoretical calculations (Ford, Docken, & Dalgarno 1975; Flannery, Tai, & Albritton 1977; Cacelli, Moccia, & Rizzo 1993) yield an average cross section increasing from 1×10^{-18} cm^2 at threshold to 1×10^{-17} cm^2 at 18 eV, where it agrees with the measurements of Samson & Haddad (1994). The increasing average cross section is a reflection of the Franck-Condon overlap of the initial $v'' = 0$ vibrational wave function of H_2 with the final v' vibrational wave function of H_2^+. The Franck-Condon factors maximize at $v' = 2$.

Samson & Haddad (1994) have measured the cross sections between 18 and 113 eV and recommend cross sections out to 300 eV, which they believe to be uncertain by no more than 4%. Theoretical calculations (Ford et al. 1975; Flannery et al. 1977; O'Neill & Reinhardt 1978) do not extend beyond 37 eV, except for the evaluation of Cooper (1974) and Sadeghpour & Dalgarno (1993) of the high-energy limiting nonrelativistic formula

$$\sigma_{\mathrm{H}_2}(E) \sim \frac{45.6}{E(\mathrm{keV})^{7/2}}\ \text{barns}\ . \tag{16}$$

We attempt to make use of the sum rules to extend the cross sections of Samson & Haddad (1994) to the high-energy region. Sum rules for H_2 have been obtained within the Born-Oppenheimer approximation over an extended range of internuclear distance R by Wolniewicz (1993). The sums vary slowly with R in the Franck-Condon region, which extends from $1a_0$ to $2a_0$, and the vibrational averages for $v'' = 0$ do not differ importantly from the values at the equilibrium internuclear distance of $1.4a_0$. The sum rules are given in Table 6. The value of ln $2K$ calculated by Wolniewicz (1993) makes use of an approximate representation of $S(k)$ as a function of k (Dalgarno 1960; Garcia 1966; Bishop & Cheung 1978) of uncertain accuracy.

Because of the nuclear motion, the near-threshold photoionization cross sections cannot be transformed directly into the electronic differential oscillator strengths that enter into the sum rules. Absorption occurs preferentially into the $v' = 2$ level of H_2^+ once it becomes energetically accessible. As the photon energy exceeds the vibrational energies, the

TABLE 6

VALUES OF SUM RULES FOR H_2

Sum Rule[a]	Exact	Discrete	15.4–18 eV	18–115 eV	115–300 eV	300–∞ eV	Total
$S(-2)$	5.180	3.784	0.315	1.018	...	...	5.117
$S(-1)$	3.036	1.884	0.195	0.900	0.003	...	2.982
$S(0)$	2	0.943	0.121	0.873	0.014	0.002	1.954
$S(1)$	1.701	0.474	0.075	0.981	0.088	0.041	1.659
$S(2)$	3.851	0.239	0.047	1.359	0.577	1.578	3.800
$S(2)\ln(2K)$......	8.911	−0.163	−0.022	0.638	1.108	7.405	8.966

[a] These are the values of the electronic sum rules evaluated at the equilibrium separation. The value of $S(2)\ln 2K$ is an *approximate estimate*.

sums over the vibrational energy levels approach unity and the relationship (3) can be applied to the cross section data. We assume that the relationship is valid for photon energies above 18 eV.

Estimates of the contributions of photoionization to the sum rules below 18 eV can be obtained from the calculations of Ford et al. (1975). After correcting for the Franck-Condon overlap, we infer a nearly constant electronic oscillator strength $df/d\epsilon$ of 2.7 at threshold, where ϵ is measured in atomic units. This modified value is a factor of 1.7 times that of atomic hydrogen.

Values of the discrete oscillator strengths of the transitions from the ground state to the $B^1\Sigma_u^+$, $C^1\Pi_u^+$, and $B'^1\Sigma_u^+$ states have been calculated by O'Neill & Reinhardt (1978), Dressler & Wolniewicz (1985), and Komasa & Thakkar (1994) and the transition energies by Rothenberg & Davidson (1967). The sum of the oscillator strengths at the equilibrium separation is the same factor of 1.7 times the $1s$–$2p$ oscillator strength of H. We make little error in assuming that the other discrete oscillator strengths of H_2 are 1.7 times those for H. For the transitions we adopt a mean transition energy of 15.2 eV. The resulting discrete contributions to the sums $S(k)$ and $S(2)\ln 2K$ are given in Table 6 with the contributions of $df/d\epsilon$ between threshold and 18 eV.

For energies between 18 and 300 eV, we initially adopted the cross sections recommended by Samson & Haddad (1994), and for higher energies, cross sections with the same shape as for the hydrogen atom but scaled in magnitude to match the correct asymptotic form (eq. [16]). The resulting values of $S(2)$ and $S(2)\ln 2K$ were too small. To achieve agreement with the sum rules, we raised the cross section at 300 eV from 1.54×10^{-21} cm^2 to 1.75×10^{-21} cm^2 and connected the cross sections smoothly to the measurements at 113 eV and to the asymptotic limit at high energies. The revised sums are listed in Table 6. The agreement is close, though, for $S(-2)$ partly fortuitous. The cross sections at high energies should be reliable. They are about 2.8 times those for atomic hydrogen, in agreement with the measurements of Crasemann et al. (1974) at 5.4 and 8.4 keV.

Table 7 is a list of our recommended cross sections from 100 to 300 eV compared to those suggested by Samson & Haddad (1994).

The cross sections for the photoionization of H_2 may be represented analytically by

$$\sigma_{H_2}(E) = 10^8(-37.895 + 99.723x - 87.227x^2 + 25.400x^3) \text{ barns for } 15.4 < E < 18 \text{ eV} , \quad (17)$$

$$\sigma_{H_2}(E) = 2 \times 10^7(0.071x^{-s} - 0.673x^{-(s+1)} + 1.977x^{-(s+2)} - 0.692x^{-(s+3)}) \text{ barns for } 18 < E < 85 \text{ eV} , \quad (18)$$

$$\sigma_{H_2}(E) = 45.57(1 - 2.003/x^{0.5} - 4.806/x + 50.577/x^{1.5} - 171.044/x^2 + 231.608/x^{2.5} - 81.885/x^3)/E(\text{keV})^{3.5} \text{ barns for } E > 85 \text{ eV} , \quad (19)$$

where $x = E(\text{eV})/15.4$ and $s = 0.252$. We do not attempt to reproduce the structures near threshold introduced by the presence of resonance states. Figure 1 shows the resulting cross section in the form $x^{7/2}\sigma(E)$ as a function of the scaled energy x and compares it to the similar cross sections for H and He. Above 20 eV, the possible error in the cross sections for H_2 should not exceed 5%.

TABLE 7

TOTAL PHOTOIONIZATION CROSS SECTIONS OF H_2 FROM 100 TO 300 eV

E(eV)	σ(Mbarn) (Samson & Haddad 1994)	σ(Mbarn) (Present Work)
100......	0.04790	0.04762
105......	0.04130	0.04122
110......	0.03570	0.03598
115......	0.03160	0.03163
120......	0.02710	0.02797
125......	0.02380	0.02485
130......	0.02110	0.02219
135......	0.01860	0.01989
140......	0.01650	0.01789
145......	0.01480	0.01615
150......	0.01330	0.01462
160......	0.01080	0.01208
170......	0.00895	0.01009
180......	0.00755	0.00849
190......	0.00640	0.00721
200......	0.00545	0.00617
210......	0.00470	0.00531
220......	0.00403	0.00460
230......	0.00350	0.00401
240......	0.00308	0.00351
250......	0.00270	0.00309
260......	0.00240	0.00273
270......	0.00213	0.00243
280......	0.00190	0.00216
290......	0.00171	0.00194
300......	0.00154	0.00174

The fraction of ionizations that produce H^+ ions is important in astrophysics. Double photoionization,

$$H_2 + \nu \rightarrow H^+ + H^+ + 2e^- , \quad (20)$$

has a vertical threshold of 51.4 eV. The cross section has been measured by Dujardin et al. (1987) and Kossmann et al. (1989a, 1989b), and calculations have been reported by Le Rouzo (1986). At 110 eV, the measured ratio of double to single ionization is 0.038. The asymptotic ratio is predicted to be 0.0225 (Sadeghpour & Dalgarno 1993).

The cross section for dissociative ionization,

$$H_2 + \nu \rightarrow H + H^+ + e^- , \quad (21)$$

is complicated by the contribution of resonance states (He at al. 1995). It has been measured by Browning & Fryar (1973), Strathdee & Browning (1976, 1979), Ito et al. (1988), Chung et al. (1993), Latimer et al. (1995), and Ito, Hall, & Ukai (1996) for energies up to 124 eV. Its ratio to the total photoionization cross section increases from zero at the threshold of 18.08 eV to 0.284 at 76 eV and then decreases slowly to 0.258 at 124 eV.

5. COMPTON IONIZATION

At high energies Compton ionization is a more efficient source of ionization than photoionization. In Compton ionization, the photon is not absorbed but scattered, and it shares energy and momentum with the ejected electron. At high energies the bound energies of electrons in atoms or molecules can be ignored, and the cross sections are those for scattering by free electrons. The nonrelativistic limit of the Compton ionization cross section is the Thompson cross section (Jackson 1975, p. 679):

$$\sigma_T(E) = \pi r_e^2\left(\frac{4}{3} + \cos\theta_c + \frac{\cos^3\theta_c}{3}\right) , \quad (22)$$

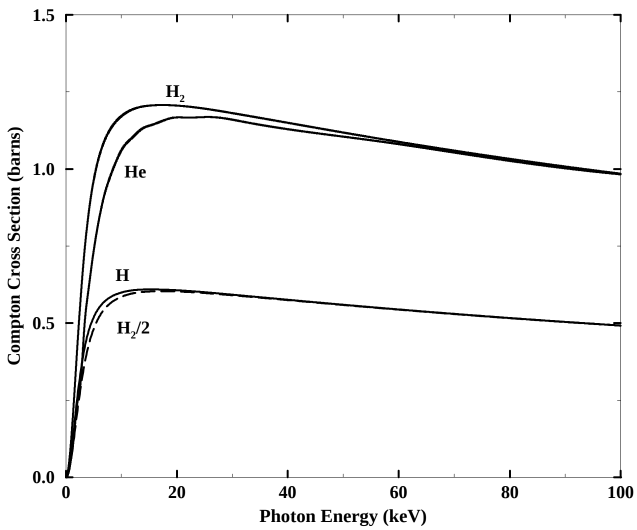

FIG. 3.—Compton ionization cross sections for H, He, and H_2 from the compilation of Hubbell et al. (1975). For comparison, the H_2 cross section per electron is also plotted. It converges to the hyrdogen atom cross section at high photon energies.

where $x = E/I_{\rm th}$, $\cos\theta_c = 1 - (c^2/E)[x/(1-x)]$, $r_e = e^2/m_e c^2$ is the classical electron radius, c is the speed of light and $r_e^2 = 0.07940775$ barns. The inclusion of retardation effects causes the cross sections to diminish with increasing energy where they are accurately represented by the Klein-Nishina (1929) formula.

Tables of the Compton ionization cross sections for all the elements have been compiled by Hubbell et al. (1975), where they are referred to as incoherent scattering cross sections. We reproduce in Figure 3 the Compton cross sections for H, H_2, and He. At high photon energies the Compton cross sections for He and H_2 become similar as the ratio of the binding energies of the electrons to the photon energy decreases. The Compton cross sections become larger than the corresponding photoionization cross sections at 2.8, 6.5, and 3.1 keV for H, He, and H_2, respectively. The ratio of the H_2 to H Compton cross sections is close to 2 (Hubbell et al. 1975).

It is also possible to eject two electrons in the Compton process. There have been recent calculations (Andersson & Burgdoerfer 1993; Suric et al. 1994; Hino, Bergstrom, & Macek 1994) and experiments (Spielberger et al. 1995) that obtained the double Compton total cross sections of He for energies in the 10 keV range. The emerging theme from both theory and experiment is that the double-to-single Compton ionization ratio does not differ significantly from 0.016, the asymptotic value of the double-to-single photoionization ratio.

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REFERENCES

Andersson, L. R., & Burgdoerfer, J. 1993, Phys. Rev. Lett., 71, 50
Azuma, Y., Berry, H. G., Gemmell, D. S., Suleiman, J., Westerlind, M., Sellin, I., Woicek, J. C., & Kirkland, J. P. 1995, Phys. Rev. A, 51, 447
Band, I. M., Trzhaskovshaya, M. B., Verner, D. A., & Yakovlev, D. G. 1990, A&A, 237, 267
Bartlett, R. J., Walsh, P. J., He, Z. X., Chung, Y., Lee, E.-M., & Samson, J. A. R. 1992, Phys. Rev. A, 46, 5574
Bell, K. L., & Kingston, A. E. 1971, J. Phys. B, 4, 1308
Berkowitz, J. 1997, J. Phys. B, 30, 881
Berrah, N., Heiser, F., Wehlitz, R., Levin, J., Whitfield, S. P., Viefhaus, J., Sellin I. A., & Becker, U. 1993, Phys. Rev. A, 48, R1733
Bethe, H. A., & Salpeter, E. E. 1967, Quantum Mechanics of One- and Two-Electron Systems (New York: Plenum)
Bishop, D. M., & Cheung, L. M. 1978, J. Phys. B, 11, 3133
Bizau, J. M., & Wuilleumier, F. J. 1995, J. Electron Spectrosc. Rel. Phenom., 71, 205
Browning R., & Fryar J. 1973, J. Phys. B, 6, 364
Cacelli, I., Moccia, R., & Rizzo, A. 1993, J. Chem. Phys., 98, 8742
Cen, R. 1992, ApJS, 78, 341
Chan, W. V., Cooper, G., & Brion, C. E. 1991, Phys. Rev. A, 44, 186
Chung, Y. M., Lee, E.-M. Masuoka, T., & Samson, J. A. R. 1993, J. Chem. Phys., 99, 885
Cook, G. R., & Metzger, P. H. 1964, J. Opt. Soc. Am., 54, 968
Cooper, J. W. 1974, Phys. Rev. A, 9, 2236
———. 1996, Radiat. Phys. Chem. 47, 927
Crasemann, B., Koblas, P. E., Wang, T.-C., Birdseye, H. E., & Chen, M. H. 1974, Phys. Rev. A, 9, 1143
Dalgarno, A. 1960, Proc. Phys. Soc. London, 76, 422
Dalgarno, A., & Lynn, N. 1957, Proc. Phys. Soc. London, 70, 802
Dalgarno, A., & Sadeghpour, H. R. 1992, Phys. Rev. A, 46, R3591
Dalgarno, A., & Stewart, A. L. 1960, Proc. Phys. Soc. London, 76, 49
Decleva, F., Lisini, A., & Venuti, M. 1994, J. Phys. B, 27, 4867
Dehmer, P. M., & Chupka, W. A. 1976, J. Chem. Phys., 65, 2243
Dehmer, J. L., Dehmer, P. M., West, J. B., Hayes, M. A., Siggel, M. R. F., & Parr, A. C. 1992, J. Chem. Phys., 97, 7911
Drake, G. W. F. 1996, in Atomic, Molecular and Optical Physics Handbook, ed. G. W. F. Drake (New York: AIP)
Dressler, K., & Wolniewicz, L. 1985, J. Chem. Phys., 82, 4720
Dujardin, G., Besnard, M. J., Hellner, L., & Malinowsky, Y. 1987, Phys. Rev. A, 35, 5012
Fan, Z., Sadeghpour, H. R., & Dalgarno, A. 1994, Phys. Rev. A, 50, 3174
Flannery, M. R., Tai, H., & Albritton, D. L. 1977, At. Data Nucl. Data Tables 20, 563
Ford, A. L., Docken, K. K., & Dalgarno, A. 1975, ApJ, 195, 819
Forrey, R. C., Sadeghpour, H. R., Baker, J. D., Morgan, J. D., & Dalgarno, A. 1995, Phys. Rev. A, 51, 2112
Forrey, R. C., Yan, Z.-C., Sadeghpour, H. R., & Dalgarno, A. 1997, Phys. Rev. Lett., 78, 3662
Garcia, J. D. 1966, Phys. Rev., 14, 66
Haiman, Z., Thoul, A. A., & Loeb, A. 1996, ApJ, 464, 523
He, Z. X., Cutler, J. N., Southworth, S. H., Hughey, L. R., & Samson, J. A. R. 1995, J. Chem. Phys., 103, 3912
Henke, B. L., Gullikson, E. M., & Davis, J. C. 1993, At. Data Nuc. Data Tables, 54, 181
Hino, K. 1993, Phys. Rev. A, 47, 4845
Hino, K., Bergstrom, P. M., & Macek, J. H. 1994, Phys. Rev. Lett., 72, 1620
Hino, K., Ishihara, T., Shimizu, F., Toshima, N., & McGuire, J. H. 1993, Phys. Rev. A, 48, 1271
Ho, Y. K. 1995, Chinese J. Phys., 34, 9
Hubbell, J. H., et al. 1975, J. Phys. Chem. Ref. Data, 4, 471
Ishihara, T., Hino, K., & McGuire, J. H. 1991, Phys. Rev. A, 44, R6980
Ito, K., Hall, R. I., & Ukai, M. 1996, J. Chem. Phys., 104, 9449
Ito, K., Lablanquie, P., Guyon, P.-M., & Nenner, I. 1988, Chem. Phys. Lett., 151, 121
Jackson, J. D. 1975, Classical Electrodynamics (New York: Wiley)
Jungen, Ch., Pratt, S. T., & Ross, S. C. 1995, J. Phys. Chem., 99, 1700
Kabir, P. K., & Salpeter, E. E. 1957, Phys. Rev., 108, 1256
Klein, O., & Nishina, Y. 1929, Z. Phys., 52, 853
Komasa, J., & Thakkar, A. J. 1994, Chem. Phys. Lett., 222, 65
Kornberg, M. A., & Miraglia, J. E. 1993, Phys. Rev. A, 48, 3714
Kossman, H., Schwarzkopf, O., Kammerburg, B., Braun, W., & Schmidt, V. 1989a, J. Phys. B, 22, L411
Kossman, H., Schwarzkopf, O., Kammerburg, B., & Schmidt, V. 1989b, Phys. Rev. Lett., 63, 2040
Latimer, C. J., Dunn, R. F., O'Neill, F. P., MacDonald, M. A., & Kouchi, N. 1995, J. Chem. Phys., 102, 722
Lee, L. C., Carlson, R. W., & Judge, D. L. 1976, J. Quant. Spectrosc. Radiat. Transfer 16, 873
Le Rouzo, H. 1986, J. Phys. B, 19, 677
Levin, J. C., et al. 1991, Phys. Rev. Lett., 67, 968
———. 1993, Phys. Rev. A, 47, R16
McCrary, J. H., Looney, L. D., & Atwater, H. F. 1970, J. Appl. Phys., 41, 3570
Meyer, K. W., & Greene, C. H. 1994, Phys. Rev. A, 50, R3573
Migneron, R., & Levinger, J. S. 1965, Phys. Rev., 139, 646
NIST Standard Reference Database 66. 1997, FFAST database, NIST X-ray attenuation databases
O'Neill, S. V., & Reinhardt, W. P. 1978, J. Chem. Phys., 69, 2126

Pont, M., & Shakeshaft, R. 1995, J. Phys. B., 28, L571
Proulx, D., & Shakeshaft, R. 1993, Phys. Rev. A, 48, R875
Rothenberg, S., & Davidson, E. R. 1967, J. Mol. Spectrosc., 22, 1
Sadeghpour, H. R. 1996, Canadian J. Phys., 74, 727
———. 1998, in preparation
Sadeghpour, H. R., & Cavagnero, M. 1993, J. Phys. B, 26, L271
Sadeghpour, H. R., & Dalgarno, A. 1993, Phys. Rev. A, 47, R2458
Samson, J. A. R., Bartlett, R. J., & He, Z. X. 1992, Phys. Rev. A, 46, 7277
Samson, J. A. R., & Haddad, G. N. 1994, J. Opt. Soc. Am. B, 11, 277
Samson, J. A. R., He, Z. X., Bartlett, R. T., & Sagurton, M. 1994a, Phys. Rev. Lett., 72, 3329
Samson, J. A. R., He, Z. X., Yin, L., & Haddad, G. N. 1994b, J. Phys. B, 27, 887
Samson, J. A. R., Greene, C. H., & Bartlett, R. J. 1993, Phys. Rev. Lett., 71, 201
Sanchez, I., & Martin, F. 1991, Phys. Rev. A, 44, 7318
Seaton M. J. 1958, Rev. Mod. Phys., 30, 979
Shapiro, P. R., & Kang, H. 1987, ApJ, 318, 32
Spielberger, L., et al. 1995, Phys. Rev. Lett., 74, 4615
Sobel'man, I. 1991, Atomic Spectra & Radiative Transitions (Berlin: Springer)
Strathdee, S., & Browning, R. 1976, J. Phys. B, 9, L505
———. 1979, J. Phys. B, 12, 1789
Suric, T., Pisk, K., Logan, B., & Pratt, R. 1994, Phys. Rev. Lett., 73, 790
Tang, J.-Z., & Shimamura, I. 1995, Phys. Rev. A, 52, R3413
Tang, J.-Z., Watanabe, S., Matsuzawa, M., & Lin, C. D. 1992, Phys. Rev. Lett., 69, 1633
Teng, Z., & Shakeshaft, R. 1993, Phys. Rev. A, 47, R3487
———. 1994, Phys. Rev. A, 49, 3597
Venuti, M., Decleva, F., & Lisini, A. 1996, J. Phys. B, 29, 5315
Verner, D. A. Yakovlev, D. G., Band, I. M., & Trzhasovskaya, M. B. 1993, At. Data. Nucl. Data Tables, 55, 233
Wolniewicz, L. 1993, J. Chem. Phys., 99, 1851

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ERRATUM

In the paper "Photoionization Cross Sections of He and H_2" by M. Yan, H. R. Sadeghpour, and A. Dalgarno (ApJ, 496, 1044 [1998]), the analytic representation of the H_2 photoionization cross sections (eqs. [17]–[19]) is given incorrectly. The cross sections for H_2 may be represented analytically by

$$
\begin{aligned}
\sigma_{\mathrm{H}_2}(E) &= 10^7(1 - 197.448x^{-0.5} + 438.823x^{-1} - 260.481x^{-1.5} + 17.915x^{-2}) \text{ barns} \\
&\quad \text{for } 15.4 < E < 18 \text{ eV} , \\
\sigma_{\mathrm{H}_2}(E) &= (-145.528 + 351.394x^{0.5} - 274.294x + 74.320x^{1.5})/E(\mathrm{keV})^{3.5} \text{ barns} \\
&\quad \text{for } 18 < E < 30 \text{ eV} , \\
\sigma_{\mathrm{H}_2}(E) &= (65.304 - 91.762x^{0.5} + 51.778x - 9.364x^{1.5})/E(\mathrm{keV})^{3.5} \text{ barns} \\
&\quad \text{for } 30 < E < 85 \text{ eV} , \\
\sigma_{\mathrm{H}_2}(E) &= 45.57(1 - 2.003x^{-0.5} - 4.806x^{-1} + 50.577x^{-1.5} - 171.044x^{-2} \\
&\quad +231.608x^{-2.5} - 81.885x^{-3})/E(\mathrm{keV})^{3.5} \text{ barns} \\
&\quad \text{for } E > 85 \text{ eV} .
\end{aligned}
$$

The sum rules and the tabulated photoionization cross sections in Tables 6 and 7 are correct. The errors were drawn to our attention by the paper of J. Wilms, A. Allen, and R. McCray (ApJ, 542, 914 [2000]).

We point out that our recommended cross sections are constructed from the best available experimental and calculated data and modified to ensure that several sum rules are satisfied and to conform to the correct physical high-energy limit. We emphasize that the asymptotic ratio of the nonrelativistic photoionization cross sections of H_2 and H is given exactly as

$$\frac{\sigma_{\mathrm{H}_2}}{\sigma_{\mathrm{H}}} = 4\pi\langle\delta(\boldsymbol{r}_{1a})\rangle , \tag{2}$$

where $\langle\delta(\boldsymbol{r}_{1a})\rangle$ is the delta function matrix element at the position of nucleus a for electron 1. The numerical value of the ratio of cross sections is $\sigma_{\mathrm{H}_2}/\sigma_{\mathrm{H}} = 2.833$ at high energies. As noted by us and by Wilms, Allen, and McCray, where molecular hydrogen contributes to the total photoabsorption, this excess of the ratio over 2 can be important.