

# ABSORPTION OF RADIATION BY AN ATMOSPHERE OF H, H<sup>+</sup> AND H<sub>2</sub><sup>+</sup>—SEMI-CLASSICAL TREATMENT

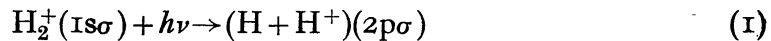
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(Received 1951 September 28)

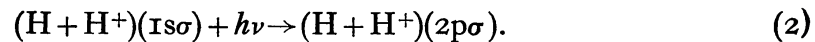
## *Summary*

Calculations are carried out on the absorption of an atmosphere of H, H<sup>+</sup> and H<sub>2</sub><sup>+</sup> using the accurate quantal dipole moment but treating the nuclei as classical particles. Absorption coefficients are tabulated for wave numbers between 500 cm<sup>-1</sup> and 26 000 cm<sup>-1</sup>, and for temperatures between 2 500 deg. K and 12 000 deg. K. The relative importance of bound-free and free-free transitions is also determined.

1. *Introduction.*—Some time ago Wildt (1) suggested that a significant contribution to the opacity of stellar atmospheres might arise from bound-free absorption by H<sub>2</sub><sup>+</sup> ions,



and from free-free absorption by colliding H atoms and H<sup>+</sup> ions



The present paper is devoted to the investigation of these two processes on the assumption that the nuclei behave as classical particles.

2. *Basis of calculations.*—The absorption coefficient  $\kappa(\nu, T)$  associated with (1) and (2) together is related to the photon emissivity,  $j(\nu, T)$ , due to the inverse processes, by the well-known equation

$$\kappa(\nu, T) = (c^2/8\pi\nu^2) \{ \exp(h\nu/kT) - 1 \} j(\nu, T), \quad (3)$$

$\nu$  being the frequency of the radiation,  $T$  the temperature,  $h$  Planck's constant, and  $k$  Boltzmann's constant. Formulae from which  $j(\nu, T)$  may be obtained have been developed elsewhere (2). On introducing  $\gamma(\nu, T) d\nu$ , the rate coefficient giving the photon emission in the frequency range  $\nu$  to  $\nu + d\nu$ , we see that

$$j(\nu, T) = n(\text{H})n(\text{H}^+)\gamma(\nu, T), \quad (4)$$

the  $n$ 's being the concentrations of the substances indicated. Further, if  $R$  is the internuclear distance corresponding to the frequency  $\nu$ , and  $\gamma(R, T) dR$  is the rate coefficient giving the photon emission from H atoms and H<sup>+</sup> ions whose separation lies between  $R$  and  $R + dR$ , then

$$\gamma(\nu, T) = \gamma(R, T) / (d\nu/dR). \quad (5)$$

Now from the earlier paper (2) just mentioned

$$\gamma(R, T) = 4\pi g A(R) R^2 \exp \{ -U(2p\sigma | R) / kT \}, \quad (6)$$

where  $g$  is the ratio of the statistical weight of the repulsive potential energy curve  $U(2p\sigma | R)$  to the sum of the statistical weights of this curve and of the attractive potential energy curve  $U(1s\sigma | R)$ , and where  $A(R)$  is the Einstein

spontaneous transition probability. Denoting the dipole moment involved by  $D(R)$ , writing

$$x(1s\sigma | R, T)^2 = -U(1s\sigma | R)/kT, \quad (7)$$

$$x(2p\sigma | R, T)^2 = -U(2p\sigma | R)/kT, \quad (8)$$

and using the relations

$$A(R) = \frac{64\pi^4\nu^3}{3hc^3} D(R), \quad (9)^*$$

$$h\nu = U(2p\sigma | R) - U(1s\sigma | R), \quad (10)$$

we find

$$\kappa(\nu, T) = \frac{32\pi^4g}{3hc} \left\{ \nu \frac{d\nu}{dR} \right\} R^2 D(R) [\exp \{x(1s\sigma | R, T)^2\} - \exp \{x(2p\sigma | R, T)^2\}] n(H)n(H^+). \quad (11)$$

This formula can of course be derived directly using classical statistics to obtain the distribution of internuclear distances. On taking  $g$  to equal  $\frac{1}{2}$ , and substituting for the fundamental physical constants, we have

$$\kappa(\nu, T) = 2.51 \times 10^{-42} \left\{ \nu \frac{d\nu}{dR} \right\} R^2 D(R) [\exp \{x(1s\sigma | R, T)^2\} - \exp \{x(2p\sigma | R, T)^2\}] n(H)n(H^+) \text{ cm}^{-1}, \quad (12)$$

where  $R$  and  $D(R)$  are in the appropriate atomic units ( $a_0$  and  $a_0^2 e^2$  respectively),  $n(H)$  and  $n(H^+)$  are particle numbers per  $\text{cm}^3$ , and the other quantities are in any self-consistent set of units. The stimulated transitions are of course included in  $\kappa(\nu, T)$  as negative absorptions.

An asymptotic expression suitable for use at low frequencies can be derived. From elementary perturbation theory (3) we have that as  $R$  tends to infinity

$$\nu/c \sim (8/3)(R - 3/2R) \exp(-R) \text{ Rydbergs}^\dagger, \quad (13)$$

so

$$\nu \frac{d\nu}{dR} \sim R(2R^2 - 3)/(2R^3 - 2R^2 - 3R - 3). \quad (14)$$

Noting also (4) that

$$D(R) \sim \frac{1}{4}R^2, \quad (15)$$

we see on expanding the exponentials in (12) that

$$\kappa(\nu, T) \sim 6.28 \times 10^{-43} \left( \frac{h\nu}{kT} \right) \left\{ \frac{R^5(2R^2 - 3)}{2R^3 - 2R^2 - 3R - 3} \right\} n(H)n(H^+) \text{ cm}^{-1}, \quad (16)$$

the units being as specified above. From (13)  $R$  is approximately

$$- \ln(3\nu/8c) + \ln R, \quad (17)$$

so that the value appropriate to any chosen  $\nu$  can be found rapidly by iteration.

For certain purposes it is desirable to be able to separate the contributions from bound-free and free-free absorption. This can readily be done, for, as can be seen from the earlier paper (2), the fraction of the total due to the former is given by

$$r_B(\nu, T) = \Phi \{x(1s\sigma | R, T)\} - 2\pi^{-\frac{1}{2}} x(1s\sigma | R, T) \exp \{-x(1s\sigma | R, T)^2\}, \quad (18)$$

where  $\Phi$  is the error integral. At low frequencies  $r_B(\nu, T)$  is clearly very small. An asymptotic expression can be obtained, but it is of little interest and need not be given.

\* The orbital degeneracy factor is omitted as it equals unity for the transition under discussion.

† 1 Rydberg =  $109\,677.58 \text{ cm}^{-1}$ .

All the functions appearing in (12) and (18) are known with some precision; thus the potential energy curves have been evaluated in the course of a recent quantal study of the two-centre problem (5), and the dipole moment has been calculated (6) from electronic wave-functions made available by this investigation. A number of convenient values of the wave number  $\nu/c$  covering the range  $500\text{ cm}^{-1}$  to  $26000\text{ cm}^{-1}$  were chosen, and the corresponding values of  $R$ ,  $U(1s\sigma|R)$ ,  $U(2p\sigma|R)$ ,  $\nu/(d\nu/dR)$  and  $D(R)$  were computed by inverse interpolation and numerical differentiation. The figures obtained (which are displayed in Table I) were then used in (12) and (18) to determine  $\kappa(\nu, T)$  and

TABLE I  
Data on  $1s\sigma-2p\sigma$  transition of  $\text{H}_2^+$

Wave number $\nu/c$ ( $\text{cm}^{-1}$ )	Internuclear distance $R$ (atomic units)	$-\nu/(d\nu/dR)$ (atomic units)	Potentials		Dipole moment $D(R)$ (atomic units)
			$-U(1s\sigma R)$ (Rydbergs)	$+U(2p\sigma R)$ (Rydbergs)	
500	8.633	1.15	0.00315	0.00141	17.4
1 000	7.839	1.16	.00583	.00329	14.2
1 500	7.367	1.17 <sub>6</sub>	.00843	.00525	12.5
2 000	7.026	1.18 <sub>8</sub>	.01097	.00727	11.3
2 500	6.760	1.19 <sub>7</sub>	.01346	.00933	10.4
3 000	6.541 <sub>6</sub>	1.20 <sub>6</sub>	.01592	.01143	9.7 <sub>7</sub>
3 500	6.354 <sub>8</sub>	1.21 <sub>5</sub>	.01834	.01357	9.1 <sub>8</sub>
4 000	6.191 <sub>9</sub>	1.22 <sub>2</sub>	.02074	.01573	8.7 <sub>0</sub>
5 000	5.917 <sub>8</sub>	1.23 <sub>6</sub>	.02545	.02014	7.9 <sub>2</sub>
6 000	5.691 <sub>2</sub>	1.24 <sub>9</sub>	.03004	.02467	7.3 <sub>1</sub>
7 000	5.497 <sub>8</sub>	1.26 <sub>1</sub>	.03451	.02931	6.8 <sub>0</sub>
8 000	5.328 <sub>8</sub>	1.27 <sub>1</sub>	.03891	.03403	6.3 <sub>7</sub>
9 000	5.178 <sub>3</sub>	1.28 <sub>0</sub>	.04322	.03884	6.0 <sub>0</sub>
10 000	5.042 <sub>9</sub>	1.28 <sub>9</sub>	.04744	.04374	5.6 <sub>8</sub>
12 000	4.806 <sub>6</sub>	1.30 <sub>4</sub>	.05560	.05381	5.1 <sub>4</sub>
14 000	4.604 <sub>8</sub>	1.31 <sub>5</sub>	.06347	.06418	4.7 <sub>1</sub>
16 000	4.428 <sub>6</sub>	1.32 <sub>5</sub>	.07100	.07488	4.3 <sub>6</sub>
18 000	4.272 <sub>0</sub>	1.33 <sub>8</sub>	.07828	.08584	4.0 <sub>5</sub>
20 000	4.131 <sub>2</sub>	1.34 <sub>0</sub>	.08527	.09708	3.7 <sub>9</sub>
22 000	4.003 <sub>2</sub>	1.34 <sub>5</sub>	.09200	.10859	3.5 <sub>6</sub>
24 000	3.885 <sub>9</sub>	1.35 <sub>1</sub>	.09847	.12035	3.3 <sub>6</sub>
26 000	3.777 <sub>6</sub>	1.35 <sub>6</sub>	0.10470	0.13236	3.1 <sub>8</sub>

$r_B(\nu, T)$  at various temperatures between 2500 deg. K and 12000 deg. K. Tables II and III contain the final results. Those in the former table may be a few per cent in error (particularly at the lower wave numbers) because of possible slight inaccuracies in the original data; those in the latter should be correct to the number of decimal places given. It is difficult to assess the extent of the uncertainties introduced by the assumption that the movement of the nuclei is strictly classical. The de Broglie wave-length of a proton near the maximum of the Maxwellian distribution at 2500 deg. K (the lowest temperature considered) is about one atomic unit, which is certainly not negligible compared with the internuclear separations of importance; but in spite of this the classical treatment of the free states should actually be quite successful since the use of the Winans-Stueckelberg  $\delta$ -function (7) gives a fair representation of the photo-dissociation of even light molecules (8). The quantization of the bound states is unlikely to be very important owing to the large number involved. We consider

TABLE II \*

*Absorption coefficient in units 10<sup>-89</sup> cm<sup>-1</sup>/(H atom/cm<sup>3</sup>)/(H<sup>+</sup> ion/cm<sup>3</sup>)*

$\nu/c$ (cm <sup>-1</sup> )	Temperature in 10 <sup>3</sup> deg. K									
	2.5	3	3.5	4	5	6	7	8	10	12
500	1.14	0.94	0.80	0.69	0.55	0.46	0.39	0.34	0.270	0.226
1 000	1.61	1.32	1.12	0.97	0.77	.63	.54	.47	.38	.31
1 500	1.97	1.60	1.35	1.17	0.92	.76	.64	.56	.44	.37
2 000	2.28	1.83	1.53	1.32	1.03	.85	.72	.63	.50	.41
2 500	2.56	2.04	1.69	1.45	1.13	.92	.78	.68	.54	.44
3 000	2.84	2.23	1.84	1.56	1.21	0.99	.83	.72	.57	.47
3 500	3.1	2.42	1.97	1.67	1.28	1.04	.88	.76	.60	.49
4 000	3.4	2.60	2.10	1.77	1.35	1.09	.92	.79	.62	.51
5 000	4.0	2.98	2.36	1.96	1.47	1.17	.98	.84	.66	.54
6 000	4.8	3.4	2.63	2.15	1.57	1.25	1.04	.89	.69	.57
7 000	5.6	3.9	2.91	2.33	1.67	1.31	1.08	.92	.71	.58
8 000	6.7	4.4	3.2	2.53	1.77	1.37	1.12	.95	.73	.59
9 000	7.9	5.0	3.5	2.74	1.87	1.43	1.16	.97	.74	.60
10 000	9.3	5.6	3.9	2.95	1.97	1.48	1.19	0.99	.75	.61
12 000	13.0	7.2	4.7	3.4	2.18	1.58	1.25	1.03	.77	.62
14 000	18.1	9.3	5.7	4.0	2.40	1.69	1.30	1.06	.78	.62
16 000	25.1	11.9	7.0	4.7	2.64	1.80	1.36	1.09	.78	.62
18 000	35	15.2	8.4	5.4	2.91	1.91	1.41	1.11	.79	.61
20 000	47	19.3	10.2	6.3	3.2	2.03	1.46	1.14	.79	.61
22 000	64	24.3	12.2	7.3	3.5	2.16	1.52	1.16	.79	.60
24 000	86	31	14.6	8.4	3.8	2.29	1.57	1.18	.79	.59
26 000	114	38	17.3	9.6	4.2	2.42	1.63	1.21	0.79	0.58

\* At wave numbers below 500 cm<sup>-1</sup> the asymptotic formula (16) may be used.

TABLE III

*Fraction of total absorption due to bound-free transitions*

$\nu/c$ (cm <sup>-1</sup> )	Temperature in 10 <sup>3</sup> deg. K									
	2.5	3	3.5	4	5	6	7	8	10	12
500	0.059	0.046	0.037	0.031	0.022	0.017	0.014	0.011	0.008	0.006
1 000	.135	.107	.087	.072	.053	.041	.033	.027	.020	.015
1 500	.214	.171	.141	.118	.088	.069	.056	.046	.034	.026
2 000	.291	.236	.196	.166	.125	.098	.080	.067	.049	.038
2 500	.363	.298	.250	.214	.162	.129	.105	.088	.065	.050
3 000	.430	.357	.303	.260	.200	.159	.131	.110	.082	.064
3 500	.490	.413	.353	.305	.237	.190	.157	.132	.099	.077
4 000	.546	.464	.400	.349	.273	.221	.183	.155	.116	.091
5 000	.640	.556	.486	.429	.342	.280	.234	.200	.151	.120
6 000	.715	.632	.561	.501	.406	.336	.284	.243	.186	.148
7 000	.775	.696	.625	.564	.464	.388	.331	.285	.220	.176
8 000	.822	.748	.680	.619	.517	.437	.375	.326	.254	.204
9 000	.859	.792	.727	.667	.564	.482	.417	.364	.286	.232
10 000	.888	.827	.767	.709	.607	.524	.456	.400	.317	.258
12 000	.929	.881	.829	.777	.680	.597	.526	.467	.375	.309
14 000	.954	.917	.874	.829	.739	.658	.586	.525	.428	.356
16 000	.970	.942	.906	.867	.786	.708	.638	.577	.476	.400
18 000	.980	.959	.930	.897	.824	.751	.683	.622	.519	.440
20 000	.987	.970	.947	.919	.854	.786	.721	.661	.558	.476
22 000	.991	.978	.960	.936	.879	.816	.754	.695	.593	.510
24 000	.994	.984	.969	.949	.898	.841	.782	.726	.625	.541
26 000	0.996	0.988	0.976	0.959	0.914	0.862	0.806	0.752	0.653	0.569

therefore that the results presented are probably accurate at the higher temperatures and lower frequencies and that they are probably correct to well within one part in ten even at the lower temperature and higher frequencies. Quantal calculations in the former region would be very laborious. Though still very formidable in the latter region they have, nevertheless, been undertaken by Dr R. A. Buckingham\* and Mr S. Reed and should show clearly the range of validity of the classical approximation. The two investigations are essentially supplementary and together should provide reliable data at all temperatures and frequencies of interest.

The application of the absorption cross-section data to stellar atmospheres is being carried out by Professor B. Strömgren.

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1951 September 26.*

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\* I wish to thank Dr Buckingham for informing me of this work and for helpful discussions.