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THE CONTINUOUS ABSORPTION COEFFICIENT OF ATOMIC AND MOLECULAR NEGATIVE IONS

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SUMMARY

The continuous absorption coefficient of the free–free transitions of 17 atomic and molecular negative ions are reported for the temperature and wavelength ranges $100 \leqslant T(\mathrm{K}) \leqslant 15\,000$, $0{\cdot}5 \leqslant \lambda(\mu) \leqslant 10$. We give an analytical expression for some molecular negative ions of astrophysical interest.

In an earlier paper (**1**) we considered free–free absorption of 17 atomic and molecular negative ions near the infrared threshold, the present paper is an attempt to improve the accuracy absorption coefficients of these ions away from threshold. We use Dalgarno & Lane's method (**2**) which determines the continuous absorption coefficient $k_\lambda(T)$ from momentum-loss cross-sections by the expression

$$k_\lambda(T) = 4{\cdot}876\times 10^{-3}\, T^{-5/2}\lambda^3(1-\exp(-\alpha/\lambda T))$$
$$\times \int_0^\infty \exp(-\beta E_0)\sqrt{E_0 E_1}\{E_1 Q_\mathrm{d}(E_0)+E_0 Q_\mathrm{d}(E_1)\}\, dE_0 \text{ cm}^4 \text{ per dyne} \qquad (1)$$
$$(\alpha = 14\,388,\ \beta = 11\,605/T,\ \lambda(\mu) = 1{\cdot}240/(E_1-E_0)).$$

The absorption coefficient $k_\lambda(T)$, at temperature $T(\mathrm{K})$ and wavelength $\lambda(\mu)$, is given in units per unit electron pressure per neutral atom or molecule and includes the stimulated emission; the momentum-loss cross-section $Q_\mathrm{d}(E)$ must be expressed in units cm^2, the energy E being in electron volts.

We adopted the momentum-loss cross-section data from Keiffer's recent report (**3**), this tabulates the most reliable data available from experimental and theoretical sources. Our results are given in Tables I and II, for wavelengths greater than 10 μ the tables given in the previous paper (**1**) should be used, alternatively a good estimate can be obtained with

$$k_\lambda(T) = 10^{-3}\,\lambda^3 k_{10}(T) \quad (\lambda \geqslant 10). \qquad (2)$$

An estimate of the errors that arise from approximation (1) can be obtained by considering results for the negative ions N^- and O^-. Geltman (**4**) has calculated the absorption coefficients of these negative ions using the more accurate procedure of evaluating matrix elements directly with wave functions; the same wave functions were used to determine the momentum-loss cross-sections in Kieffer's report. Our results agree within a few per cent with those of Geltman for $\lambda \geqslant 1{\cdot}5\ \mu$ but underestimate the cross-section by 10–15 per cent at 1 μ and 30–40 per cent at 0·5 μ.

TABLE I

The continuous absorption coefficient of atomic negative ions in units 10^{-26} cm^4 per dyne

	γ (μ)	T (K) 100	500	1000	2500	5000	7500	10 000	12 500	15 000
He^-	10·0	106·0	44·1	34·1	23·5	17·3	14·2	12·2	10·9	9·78
	5·0	33·1	10·8	8·16	5·78	4·30	3·54	3·04	2·72	2·44
	2·5	11·0	2·94	2·00	1·39	1·06	0·876	0·756	0·679	0·609
	1·5	4·98	1·21	0·756	0·484	0·370	0·310	0·269	0·243	0·218
	1·0	2·67	0·620	0·366	0·214	0·159	0·134	0·118	0·107	0·0961
	0·75	1·72	0·389	0·224	0·122	0·0880	0·0740	0·0650	0·0596	0·0535
	0·5	0·931	0·205	0·114	0·0579	0·0388	0·0319	0·0281	0·0263	0·0233
Ne^-	10·0	8·59	5·51	5·36	4·81	4·09	3·61	3·28	3·05	2·95
	5·0	2·65	1·32	1·26	1·17	1·01	0·898	0·817	0·763	0·737
	2·5	0·865	0·347	0·298	0·277	0·247	0·222	0·203	0·190	0·184
	1·5	0·386	0·139	0·109	0·0941	0·0854	0·0778	0·0719	0·0676	0·0659
	1·0	0·205	0·0691	0·0514	0·0405	0·0363	0·0335	0·0313	0·0296	0·0292
	0·75	0·132	0·0427	0·0307	0·0228	0·0198	0·0183	0·0172	0·0164	0·0164
	0·5	0·0707	0·0220	0·0153	0·0105	0·0086	0·0078	0·0074	0·0071	0·0074
Ar^-	10·0	108·0	10·0	2·76	2·23	3·83	5·03	6·23	7·16	7·90
	5·0	36·0	3·17	0·901	0·591	0·955	1·26	1·56	1·79	1·97
	2·5	12·4	1·04	0·295	0·164	0·236	0·316	0·387	0·445	0·493
	1·5	5·71	0·472	0·133	0·0641	0·0850	0·112	0·138	0·159	0·177
	1·0	3·09	0·254	0·0703	0·0304	0·0374	0·0491	0·0606	0·0704	0·0782
	0·75	2·00	0·164	0·0450	0·0184	0·0211	0·0273	0·0337	0·0392	0·0436
	0·5	1·09	0·0885	0·0243	0·0094	0·0096	0·0120	0·0147	0·0171	0·0189
Kr^-	10·0	446·0	62·6	20·8	4·15	3·52	5·40	7·28	8·87	10·5
	5·0	146·0	18·1	6·27	1·26	0·925	1·37	1·82	2·23	2·62
	2·5	50·0	5·69	1·95	0·408	0·257	0·351	0·459	0·559	0·656
	1·5	22·9	2·52	0·843	0·178	0·104	0·131	0·168	0·203	0·236
	1·0	12·4	1·34	0·443	0·0928	0·0512	0·0610	0·0757	0·0902	0·104
	0·75	8·04	0·863	0·284	0·0592	0·0315	0·0356	0·0431	0·0507	0·0580
	0·5	4·36	0·465	0·153	0·320	0·0162	0·0168	0·0194	0·0223	0·0225

Xe^-	10·0	2032·0	230·0	72·1	14·3	13·2	18·8	23·5	27·4	28·7
	5·0	673·0	68·1	22·2	4·41	3·43	4·75	5·91	6·84	7·18
	2·5	231·0	21·7	7·01	1·46	0·936	1·21	1·49	1·71	1·79
	1·5	106·0	9·71	3·07	0·639	0·369	0·447	0·541	0·611	0·644
	1·0	57·4	5·18	1·62	0·332	0·179	0·204	0·240	0·269	0·286
	0·75	37·2	3·34	1·04	0·211	0·108	0·117	0·134	0·150	0·160
	0·5	20·2	1·80	0·558	0·113	0·0531	0·0529	0·0586	0·0651	0·0681
Li^-	10·0	3154·0	4183·0	2500·0	323·0	50·0	20·0	10·0	5·9	3·7
	5·0	723·0	957·0	650·0	91·0	20·0	7·2	3·1	1·8	1·2
	2·5	210·0	266·0	185·0	30·0	8·7	3·2	1·4	0·79	0·52
	1·5	95·1	113·0	77·0	13·0	4·6	1·8	0·77	0·44	0·29
	1·0	51·1	59·0	40·0	6·5	2·7	1·1	0·48	0·28	0·18
	0·75	32·9	37·0	25·0	4·1	1·7	0·72	0·33	0·20	0·13
	0·5	17·8	20·0	13·0	2·1	0·94	0·40	0·19	0·12	0·08
Na^-	10·0	2818·0	3528·0	2377·0	762·0	269·0	165·0	129·0	113·0	106·0
	5·0	604·0	744·0	553·0	190·0	69·0	43·0	33·0	29·0	27·0
	2·5	173·0	191·0	139·0	49·0	19·0	12·0	8·9	7·5	6·9
	1·5	75·8	78·0	55·0	19·0	7·5	4·8	3·5	2·9	2·6
	1·0	40·4	40·0	27·0	8·9	3·7	2·4	1·7	1·4	1·2
	0·75	26·0	25·0	17·0	5·4	2·2	1·5	1·1	0·83	0·71
	0·5	14·1	13·0	9·0	2·8	1·1	0·74	0·53	0·40	0·34
Cs^-	10·0	124613·0	14171·0	6789·0	1850·0	410·0	297·0	248·0	229·0	264·0
	5·0	41701·0	3933·0	1698·0	500·0	104·0	71·0	62·0	59·0	63·0
	2·5	14150·0	1189·0	473·0	151·0	27·0	18·0	16·0	16·0	18·0
	1·5	6494·0	532·0	201·0	63·0	11·0	6·5	6·2	6·2	7·1
	1·0	3514·0	284·0	105·0	32·0	5·0	2·9	2·9	3·0	3·6
	0·75	2275·0	183·0	66·0	20·0	2·9	1·6	1·7	1·8	2·3
	0·5	1235·0	99·0	35·0	10·0	1·3	0·79	0·78	0·90	1·3

TABLE I—*continued*

	λ (μ)	T (K) 100	500	1000	2500	5000	7500	10 000	12 500	15 000
Hg^-	10·0	16·1	33·9	147·0	308·0	196·0	139·0	97·0	72·0	57·0
	5·0	8·45	15·1	38·3	73·0	46·0	35·0	24·0	18·0	14·0
	2·5	7·69	7·73	9·6	16·0	11·0	8·4	5·9	4·4	3·5
	1·5	2·32	1·71	2·3	4·8	3·5	3·0	2·1	1·5	1·3
	1·0	0·798	0·480	0·77	1·9	1·4	1·3	0·91	0·68	0·55
	0·75	0·412	0·203	0·37	1·0	0·78	0·73	0·51	0·38	0·31
	0·5	0·178	0·652	0·15	0·46	0·34	0·33	0·23	0·17	0·14
N^-	10·0	19·8	11·9	11·5	10·7	9·99	9·49	9·04	8·62	8·25
	5·0	6·14	2·85	2·71	2·62	2·48	2·36	2·26	2·15	2·06
	2·5	2·01	0·754	0·648	0·624	0·606	0·584	0·559	0·536	0·513
	1·5	0·901	0·304	0·240	0·214	0·210	0·205	0·198	0·190	0·183
	1·0	0·481	0·153	0·114	0·0934	0·0899	0·0884	0·0861	0·0832	0·0803
	0·75	0·309	0·0950	0·0688	0·0528	0·0490	0·0483	0·0472	0·0459	0·0445
	0·5	0·166	0·0491	0·0344	0·0244	0·0212	0·0205	0·0201	0·0196	0·0191
O^-	10·0	20·1	10·9	9·86	8·38	7·41	6·91	6·54	6·22	5·97
	5·0	6·26	2·61	2·32	2·05	1·84	1·72	1·63	1·55	1·49
	2·5	2·05	0·693	0·556	0·489	0·450	0·425	0·405	0·387	0·371
	1·5	0·924	0·281	0·207	0·169	0·157	0·150	0·144	0·138	0·133
	1·0	0·494	0·142	0·0992	0·0739	0·0673	0·0647	0·0626	0·0603	0·0583
	0·75	0·318	0·0885	0·0600	0·0420	0·0396	0·0355	0·0344	0·0333	0·0323
	0·5	0·171	0·0461	0·0302	0·0196	0·0160	0·0152	0·0147	0·0143	0·0139

TABLE II

The continuous absorption coefficient of molecular negative ions in units 10^{-26} cm^4 per dyne

	λ (μ)	T (K) 100	500	1000	2500	5000	7500	10 000	12 500	15 000
H_2^-	10·0	153·0	79·7	67·9	54·6	42·7	34·8	29·3	24·6	20·9
	5·0	47·4	19·3	16·2	13·4	10·6	8·69	7·29	6·13	5·21
	2·5	15·6	5·22	3·92	3·19	2·59	2·14	1·80	1·52	1·30
	1·5	7·02	2·13	1·46	1·09	0·894	0·750	0·638	0·542	0·463
	1·0	3·76	1·07	0·695	0·470	0·380	0·322	0·277	0·237	0·203
	0·75	2·41	0·668	0·419	0·265	0·207	0·176	0·152	0·130	0·112
	0·5	1·30	0·347	0·210	0·123	0·0893	0·0748	0·0647	0·0558	0·0482
N_2^-	10·0	53·8	45·1	43·5	35·1	36·7	29·1	35·3	29·5	19·7
	5·0	16·1	10·6	10·1	8·57	9·03	7·53	8·77	6·99	4·87
	2·5	5·07	2·69	2·33	2·02	2·17	2.01	2·13	1·67	1·23
	1·5	2·22	1·05	0·845	0·717	0·774	0·702	0·691	0·602	0·469
	1·0	1·18	0·529	0·408	0·335	0·341	0·291	0·308	0·271	0·206
	0·75	0·758	0·337	0·263	0·207	0·190	0·153	0·167	0·148	0·108
	0·5	0·420	0·186	0·137	0·0890	0·0711	0·0582	0·0659	0·0588	0·0439
O_2^-	10·0	61·5	30·4	25·6	20·7	17·0	13·8	11·6	10·1	9·21
	5·0	18·8	7·13	6·11	5·11	4·24	3·45	2·90	2·52	2·30
	2·5	6·19	1·94	1·53	1·22	1·03	0·850	0·718	0·628	0·573
	1·5	2·81	0·806	0·587	0·418	0·352	0·297	0·255	0·224	0·205
	1·0	1·51	0·405	0·279	0·177	0·147	0·127	0·111	0·0982	0·0901
	0·75	0·967	0·250	0·167	0·0978	0·0789	0·0691	0·0612	0·0546	0·0502
	0·5	0·520	0·129	0·0829	0·0444	0·0339	0·0298	0·0267	0·0240	0·0222
CO^-	10·0	212·0	61·5	58·2	53·7	44·9	42·9	24·4	23·1	25·0
	5·0	69·7	15·1	13·7	13·6	12·2	10·0	6·24	6·18	6·21
	2·5	23·7	4·01	3·24	3·20	2·88	2·41	1·73	1·54	1·48
	1·5	10·8	1·62	1·22	1·15	0·917	0·907	0·590	0·500	0·512
	1·0	5·86	0·889	0·643	0·478	0·378	0·367	0·236	0·215	0·232
	0·75	3·78	0·524	0·345	0·236	0·192	0·196	0·129	0·120	0·132
	0·5	2·03	0·255	0·161	0·106	0·0830	0·0850	0·0557	0·0525	0·0596

TABLE II—*continued*

	λ (μ)	T (K) 100	500	1000	2500	5000	7500	10 000	12 500	15 000
CO_2^-	10·0	3518·0	465·0	192·0	49·9	19·8	15·8	15·1	13·5	14·6
	5·0	1166·0	129·0	52·5	13·6	5·23	4·06	3·81	3·42	3·74
	2·5	400·0	39·3	15·1	3·96	1·46	1·09	0·971	0·895	0·956
	1·5	184·0	17·3	6·35	1·61	0·589	0·421	0·363	0·344	0·343
	1·0	99·5	9·15	3·29	0·804	0·293	0·200	0·173	0·156	0·152
	0·75	64·5	5·87	2·09	0·497	0·179	0·120	0·102	0·088	0·084
	0·5	35·0	3·15	1·11	0·259	0·091	0·058	0·046	0·040	0·038
H_2O^-	10·0	59160·0	4906·0	1247·0	163·0	25·0				
	5·0	19867·0	1539·0	394·0	53·0	8·2				
	2·5	6850·0	503·0	126·0	18·5	3·2				
	1·5	3153·0	227·0	55·2	8·4					
	1·0	1708·0	122·0	29·2						

We find that the coefficients of molecular negative ion absorption are roughly the same magnitude for most of the ions in Table II, but at low temperatures H_2O^- and CO_2^- are much more efficient absorbers. The absorption coefficient of H_2^- was underestimated in earlier calculations by Sommerville (5).

In cool stars, the role of H_2^- in opacity calculations is well known. According to Tsuji (6), other molecules with a high abundance are N_2 and CO in carbon-rich stars and H_2O, CO and N_2 in oxygen-rich dwarfs. Auman (7) has shown the importance of H_2O absorption in model atmosphere calculations of late-type stars and Vardya (8) has discussed the possibility that the bound–free transitions of H_2O^-, if it exists as a stable negative ion, may contribute to the opacity of these stars. From results in Table II, we find that the free–free transitions of H_2O^- may also be a significant source of absorption regardless of the stability of H_2O^-. For molecules of astrophysical interest (H_2^-, N_2^-, CO^- and H_2O^-) we fitted results to a Gingerich-type formula

$$k_\lambda(T) = 10^{-26} \sum_{n=0}^{2} \{a_n\lambda^2 + b_n + c_n\lambda^{-1} + d_n\lambda^{-2}\} \left(\frac{5040 \cdot 2}{T(\mathrm{K})}\right)^{(n+q)/2} \quad (3)$$

suitable for model atmosphere computations. The relevant parameters are given

TABLE III

Parameters for molecular negative ion absorption coefficients using a Gingerich-type expression

$$k_\lambda(T) = 10^{-26} \sum_{n=0}^{2} \{a_n\lambda^2 + b_n + c_n\lambda^{-1} + d_n\lambda^{-2}\} \left(\frac{5040 \cdot 2}{T(\mathrm{K})}\right)^{(n+q)/2} \text{ cm}^4 \text{ per dyne}$$

	H_2^-	N_2^-	CO^-	H_2O^-
q	1	0	−2	3
a_0	0·4612	0·3064	−0·3272	−0·5344
a_1	0·006916	0·02011	0·4099	0·7476
a_2	−0·03981	0·01569	0·4301	0·01036
b_0	0·2403	1·5304	−3·0951	−15·702
b_1	−1·0119	−2·4375	5·9763	25·875
b_2	0·3508	0·6750	−3·0779	−6·8465
c_0	0·03423	−2·0031	6·3007	35·961
c_1	0·9102	3·3677	−11·995	−55·697
c_2	−0·3048	−0·9343	5·9642	14·595
d_0	−0·06184	0·6201	−2·2828	−22·757
d_1	−0·2181	−1·0768	4·3311	34·072
d_2	0·07262	0·3049	−2·1299	−8·6890

in Table III. The fit is based on the ' best ' estimate of the cross-section, that is results at 1 μ and 0·5 μ were scaled up by factors 1/0·85 and 1/0·65, respectively.

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