OPACITY CROSS SECTIONS FOR He, C, N, O, and H^-

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1. INTRODUCTION

Peculiar stars frequently show enrichment in the abundance of He, C, N, and O, as well as of other elements, along with a deficiency of H, as compared to the solar photosphere. Most of these stars are giants or supergiants. In the atmosphere of these stars, Rayleigh scattering may be an important source of opacity. We have calculated Rayleigh-scattering cross sections for these elements and compared them with the corresponding absorption coefficients.

We also discuss some preliminary results on the effect of pressure ionization on H^- opacity and on the forbidden continuum produced by H^-.

2. RAYLEIGH-SCATTERING CROSS SECTIONS OF He, C, N, AND O

The Rayleigh-scattering cross section σ_λ for wavelength λ (in centimeters) can be written (e.g., see Griem, 1964, p. 35)

$$\sigma_\lambda = \frac{128\pi^5}{3} \frac{\alpha^2}{\lambda^4} . \tag{1}$$

Here the polarizability α (in cubic centimeters) is the sum of α_d, the contribution from the discrete excited levels, and α_c, the contribution from the continuum states. In the limiting case where the wavelength of the scattered light is longer than the longest wavelength emitted by the atom from a fixed state, we can write (Shore and Menzel, 1965; Bethe and Salpeter, 1957; Condon and Shortley, 1935)

$$\alpha_d = \frac{4}{3} a_0^3 \sum_i \frac{R_i^2 \mathcal{J}_i^2}{(2L+1) E_i} \left(1 + \frac{x^2}{\lambda^2 E_i^2} + \frac{x^4}{\lambda^4 E_i^4} + \dots \right) \tag{2}$$

and

$$\alpha_c = \frac{4 \times 10^{18}}{8.067} a_0^3 \int_{E_{ion}}^{\infty} \frac{a\, dE_i}{E_i^2} \left(1 + \frac{x^2}{\lambda^2 E_i^2} + \frac{x^4}{\lambda^2 E_i^4} + \dots \right) , \tag{3}$$

where

a_0 = the radius of the first Bohr orbit in centimeters,
a = the photoionization cross section in square centimeters,
E_i = the energy in Rydbergs of the i^{th} level with respect to the ground level,

R_i = the multiplet factor,
L = total orbital angular momentum of the initial state,
E_{ion} = the energy in Rydbergs corresponding to the series limit,
x = $4\pi a_0/\alpha'$, where α' is the fine-structure constant,
$\mathcal{J}_i$ = the radial factor defined in the dipole length formalism by

$$\mathcal{J}_i(\ell - \ell') = \sqrt{\ell_>}\,(-1)^{\ell_> - 1} \int_0^\infty R_{0\ell} R_{i\ell'}\, r\, dr \quad , \tag{4}$$

and in the dipole velocity formalism by

$$\mathcal{J}_i(\ell - \ell') = \sqrt{\ell_>}\,(-1)^{\ell_> - 1} \frac{2}{E_i} \int_0^\infty R_{i\ell'} \left\{ \frac{dR_{0\ell}}{dr} + \left[(\ell - \ell')(\ell_> + \ell - \ell') - 1\right] \frac{R_{0\ell}}{r} \right\} dr \quad . \tag{5}$$

Here, $\ell_>$ is the larger of the two orbital quantum numbers ℓ and ℓ' of the jumping electron, and $R_{0\ell}/r$ and $R_{i\ell'}/r$ are the radial wave functions for the initial and intermediate states, respectively.

We have assumed the atoms to be initially in the ground state. The energy values of various levels are taken from Moore (1949) for He, N, and O, and from Johansson (1966) for C. The photoionization cross sections for He are taken from Stewart and Webb (1963), for C from Praderie (1964), for N from Bates and Seaton (1949), and for O from Dalgarno, Henry, and Stewart (1964). The multiplet factors of different transitions have been calculated following the method of Shore and Menzel (1965). The radial factors have been calculated from equations (4) and (5) with wave functions of the form used by Praderie (1964) with slight modification. The wave functions used behave as $r^{\ell+1}$ near the origin.

The Rayleigh-scattering cross section can be expressed as

$$\sigma_\lambda = \frac{A}{\lambda^4} \left(1 + \frac{B}{\lambda^2} + \frac{C}{\lambda^4} + \ldots\right) \quad , \tag{6}$$

where A, B, C for different elements are as shown in Table 1. The fairly good agreement between the values obtained by length and by velocity formalisms gives us some confidence in the wave functions used and, hence, in the computed cross sections. The Rayleigh-scattering cross sections of H, He, C, N, and O are approximately in the ratio of 9 : 1 : 108 : 46 : 27 at long wavelengths. Figure 1 shows the variation of σ_λ with λ at short wavelengths.

It is worthwhile to compare the scattering cross sections of these elements with their corresponding photoionization cross sections at a few wavelengths and temperatures. The photoionization cross sections for C, N, and O have been extrapolated from the results given by Peach (1967); and for He, from Vardya (1964). The results are presented in Table 2, which shows that the Rayleigh scattering may be an important source of the opacity in the atmosphere of low-temperature peculiar stars. These cross sections should also be compared with electron scattering and with the absorption due to negative ions. Electron scattering should be negligible for low-temperature stars except at very long wavelengths and at very low pressures. The contribution from negative ions should be considered, though it is difficult to state its relative importance without the electron pressure being specified as well.

Table 1. Coefficients of Rayleigh-scattering formula [equation (6)]

Element		A	B	C
He	Length	6.138(-46)	0.483(-10)	0.191(-20)
	Velocity	5.472(-46)	0.473(-10)	0.184(-20)
C	Length	6.653(-44)	3.086(-10)	8.515(-20)
	Velocity	6.583(-44)	3.260(-10)	9.257(-20)
N	Length	2.819(-44)	2.034(-10)	3.485(-20)
	Velocity	2.897(-44)	2.032(-10)	3.449(-20)
O	Length	1.671(-44)	1.416(-10)	1.945(-20)
	Velocity	1.433(-44)	1.352(-10)	1.852(-20)

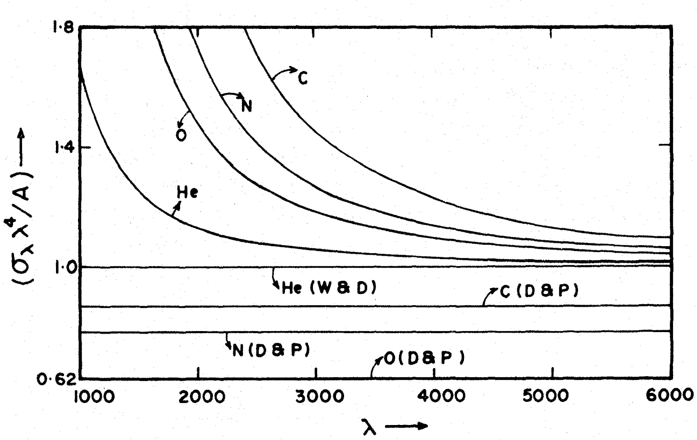

Figure 1. Departure of the Rayleigh-scattering cross section at short wavelengths from the $1/\lambda^4$ law is plotted as a function of λ(A). The ratios of the Rayleigh-scattering cross section for C, N, O, and He obtained from static polarizabilities to the corresponding A/λ^4 law are plotted as a comparison. D & P: computed by Dalgarno and Parkinson (1959); W & D: computed by Wikner and Das (1957).

Table 2. Comparison of Rayleigh-scattering and photoionization cross sections

Elements	Temperature (°K)	Wavelength (A)	Rayleigh-scattering cross section (cm^2)	Photoionization cross section (cm^2)
He	20160	3953	2.590(-28)	1.423(-22)
	10080	3953	2.590(-28)	1.281(-28)
	10080	7038	2.525(-29)	6.508(-28)
	7000	3953	2.590(-28)	6.594(-34)
	7000	7038	2.525(-29)	3.591(-33)
C	7000	4100	2.856(-26)	5.166(-24)
	4000	4100	2.856(-26)	2.453(-29)
	7000	6000	5.606(-27)	5.569(-24)
	4000	6000	5.606(-27)	2.453(-29)
N	7000	4192	1.028(-26)	9.795(-26)
	4000	4192	1.028(-26)	3.125(-32)
	7000	6000	2.303(-27)	8.814(-26)
	4000	6000	2.303(-27)	9.731(-33)
O	7000	4000	7.157(-27)	1.189(-25)
	4000	4000	7.157(-27)	1.135(-31)
	7000	6000	1.341(-27)	7.525(-26)
	4000	6000	1.341(-27)	1.724(-32)

3. PRESSURE IONIZATION AND H^- ABSORPTION

In the atmospheres of red dwarf stars, H^- is an important source of opacity. All the calculations that have been done (see, e.g., Geltman, 1962; John, 1960; Doughty and Fraser, 1964) are based on wave functions belonging to single atoms. This simple picture is not really valid, especially in the very cool red dwarf stars, where the densities are rather high. We have here attempted to compute approximately the effect of pressure ionization on the H^- opacity, making use of the strong-electrolyte approach of Debye.

The Hamiltonian, H, for a two-electron system, in atomic units (energy = 2 Ry), can be written as

$$H = -\frac{1}{2}(\nabla_1^2 + \nabla_2^2) - \frac{Z\exp(-r_1/\lambda_D)}{r_1} - \frac{Z\exp(-r_2/\lambda_D)}{r_2} + \frac{1}{r_{12}} , \qquad (7)$$

where subscripts 1 and 2 refer to electrons one and two, Z is the nuclear charge equal to unity for H^-, and λ_D is the Debye length, given by

$$\lambda_D^{-1} = \left(\frac{4\pi e^2}{KT} \Sigma N_a Z_a^2\right)^{1/2} a_0 , \qquad (8)$$

where T is the temperature, K the Boltzmann constant, e the charge of an electron, a_0 the radius of the first Bohr orbit, and N_a the number density of the species of charge $Z_a e$. Note that in equation (7) we have replaced the coulomb potential, Z/r, by the Debye potential, $Z \exp(-r/\lambda_D)/r$, to take into account the effect of other particles.

Let us assume that the ground-state wave function, ψ_d, is of the form

$$\psi_d = \frac{P(r_1)\, P(r_2)}{r_1 r_2} \quad , \tag{9}$$

where

$$P^2(r) = (\tfrac{1}{2})\, \beta^3 r^2 \exp(-\beta r) \quad , \tag{10}$$

so that P is normalized. The energy, E, of the system is then given by

$$E = \frac{\int \psi_d^* H \psi_d \, d\tau}{\int \psi_d^* \psi_d \, d\tau} = 2\mathcal{J} + F_0 \quad , \tag{11}$$

where

$$2\mathcal{J} = -\int_0^\infty P(r)\left[P''(r) + \frac{2 Z \exp(-r/\lambda_D)}{r} P(r)\right] dr \tag{12}$$

$$= \frac{1}{4}\beta^2 - \frac{Z\beta^3}{(\lambda_D^{-1} + \beta)^2} \quad , \tag{13}$$

and

$$F_0 = \int \frac{P^2(r_1)}{4\pi r_1^2}\left[\int \frac{1}{r_{12}} \frac{P^2(r_2)}{4\pi r_2^2}\, d\tau_2\right] d\tau_1 \tag{14}$$

$$= (\tfrac{5}{16})\, \beta \quad . \tag{15}$$

We have made use of equation (10) in deriving equations (13) and (15). Now we can write

$$E = \frac{1}{4}\beta^2 - \frac{Z\beta^2}{(\lambda_D^{-1} + \beta)^2} + \frac{5}{16}\beta \quad . \tag{16}$$

Minimizing the energy with respect to β gives

$$\beta^4 + \beta^3 (3\lambda_D^{-1} + \frac{5}{8} - 2Z) + \beta^2 (3\lambda_D^{-1} + \frac{15}{8} - 6Z)\lambda_D^{-1}$$
$$+ \beta(\lambda_D^{-1} + \frac{15}{8})\lambda_D^{-2} + \frac{5}{8}\lambda_D^{-3} = 0 \quad . \tag{17}$$

Equation (17) has no positive real root if

$$\lambda_D \le \frac{1}{2Z - 5/8} \quad . \tag{18}$$

This means that for the condition (18), the ground state merges with the continuum.

For $\lambda_D >> 1$, equation (17) can be approximated to

$$(\beta + 3\lambda_D^{-1})(\beta + \frac{5}{8} - 2Z) = 0 \quad . \tag{19}$$

This gives the positive root for β as

$$\beta = 2Z - \frac{5}{8} \quad . \tag{20}$$

This is independent of λ_D. Thus, the ground-state wave function is not disturbed in the first-order perturbation. The shift, ΔE, of the ground-state energy due to pressure can be written as

$$\Delta E = E - E_{\lambda_D=\infty} = -\frac{Z\beta^3}{(\lambda_D^{-1} + \beta)^2} + \frac{Z\beta^3}{\beta^2} \simeq 2Z\lambda_D^{-1} \quad , \tag{21}$$

if higher powers are neglected.

The shift, ΔI, in the ionization energy in Rydbergs is then given by

$$\Delta I = -2\left(E - E_{\lambda_D=\infty}\right) \simeq -4Z\lambda_D^{-1} \quad . \tag{22}$$

If we let (N_{H^-}) and $(N_{H^-})_0$ be the number density of H^- ions when λ_D is finite and tends to infinity, respectively, then

$$\frac{N_{H^-}}{(N_{H^-})_0} = \exp\left(\frac{\Delta I}{KT}\right) = \exp\left(\frac{-4Z}{\lambda_D KT}\right) \quad . \tag{23}$$

The photoionization cross section, a_ν, in the dipole length formalism can be written as

$$a_\lambda = 6.812 \times 10^{-20}\, k(k^2 + I) \left| \int \psi_d (Z_1 + Z_2)\, \psi_c \, d\tau \right|^2 \, cm^2 \quad . \tag{24}$$

Here, ψ_d as given by equation (9) and

$$\psi_c = \frac{1}{\sqrt{2\pi}} \left[\exp(-r_1 + ikZ_2) + \exp(-r_2 + ikZ_1) \right] \tag{25}$$

defines the wavefunctions for the ground state of H$^-$ and for the continuum, respectively; k is the momentum (atomic units) of the ejected electron, and I is the electron affinity in Rydbergs.

With the help of equations (9) and (25), equation (24) reduces to

$$a_\lambda = 6.812 \times 10^{-20}\, k\,(k^2 + I) \frac{(4\beta)^2 \,(8\pi\beta^2)^3\, k^2}{(1 + \frac{\beta}{2})^6 \left(k^2 + \frac{\beta^2}{4}\right)^6} \quad . \tag{26}$$

If we let a_λ and $(a_\lambda)_0$ be the cross sections when λ_D is finite and tends to infinity, respectively, then,

$$\frac{a_\lambda}{(a_\lambda)_0} = \frac{k^3(k^2 + I)}{\left(k^2 + \frac{\beta^2}{4}\right)^6} \cdot \frac{\left(k_0^2 + \frac{\beta^2}{4}\right)^6}{k_0^3\left(k_0^2 + I_0\right)} \quad , \tag{27}$$

where k and k_0 are the momenta of the ejected electron, and I and I_0 the electron affinities when λ_D is finite and tends to infinity, respectively. As the wavelength, λ(A), of the absorbed photon is the same in the two cases, we have

$$k^2 + I = k_0^2 + I_0 = \frac{911.3}{\lambda} \quad . \tag{28}$$

This gives, with the help of equation (22),

$$k = (k_0^2 + 4Z\lambda_D^{-1})^{1/2} \simeq k_0 \left(1 + \frac{2Z\lambda_D^{-1}}{k_0^2}\right) \quad , \text{ if } k^2 >> 4Z\lambda_D^{-1} \quad . \tag{29}$$

Equation (27) can now be approximated to

$$\frac{a_\lambda}{(a_\lambda)_0} \simeq 1 + 6 Z \lambda_D^{-1} \left[\frac{1}{k_0^2} - \frac{4}{k_0^2 + (\beta^2/4)} \right] . \tag{30}$$

The ratio of absorption coefficients, $K_\lambda = a_\lambda N_{H^-}$ with and without pressure effect, can now be written as

$$\frac{K_\lambda}{(K_\lambda)_0} = \left\{ 1 + 2 Z \lambda_D^{-1} \left[\frac{3}{k_0^2} - \frac{12}{k_0^2 + (\beta^2/4)} - \frac{2}{KT} \right] \right\} . \tag{31}$$

The behavior of the ratio $a_\lambda/(a_\lambda)_0$ as a function of k_0^2 (and λ) is shown in Figure 2, and that of $K_\lambda/(K_\lambda)_0$ in Figure 3, for three values of λ_D at T = 4737°K.

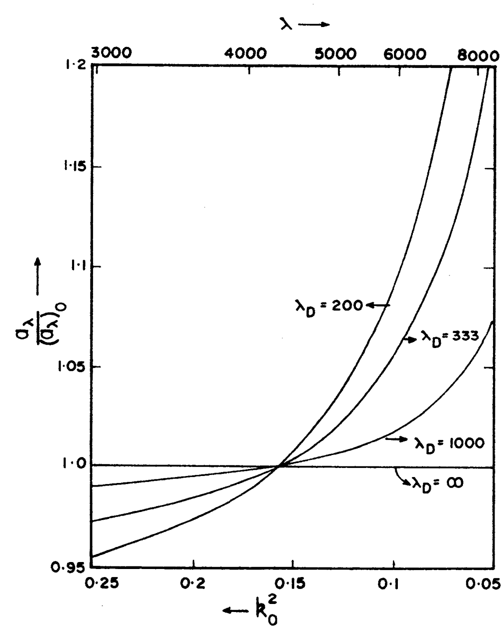

Figure 2. Photodetachment cross section of H^- at various values of λ_D, relative to that at $\lambda_D = \infty$, as a function of λ(A).

The horizontal line, for which these ratios are unity, corresponds to $\lambda_D = \infty$, i.e., no pressure effect. The pressure ionization decreases the absorption coefficient of H^- at short wavelengths and increases it at long wavelengths. The critical value of the wavelength at which the ratio becomes unity is independent of pressure in the first approximation but shifts to shorter wavelengths with increasing temperatures.

The results obtained here are rather crude, and attempts are being made to improve them by using better wavefunctions for the ground state of H^-, though we do not expect any drastic qualitative change in the results.

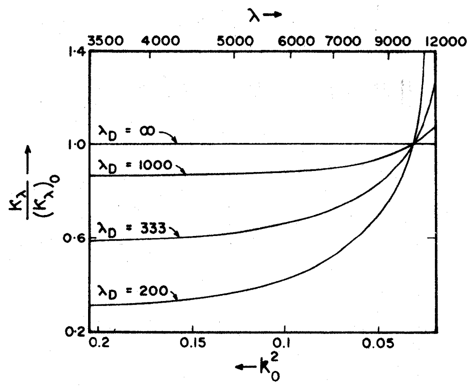

Figure 3. Absorption coefficient of H^- at various values of λ_D, relative to that at $\lambda_D = \infty$, as a function of λ(A).

4. FORBIDDEN CONTINUUM PRODUCED BY H^-

Recently, Weinberg and Berry (1966) considered the photodetachment of electrons from H^- due to local electric fields in an ionized plasma and computed the cross section for detachment, using a binary collision model. This is essentially equivalent to considering the effect of pressure on the photodetachment cross sections. We have looked into this interesting investigation but find that we disagree with their results. With the help of Dr. Weinberg, we are investigating this discrepancy.

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DISCUSSION

Auman: How high a pressure do you have to have before the influence of pressure ionization on the H^- opacity appears to be important? Do you have numerical values?

Vardya: At about 6000 A and with an electron number density of about 2×10^{17} cm^{-3} and a temperature of about 4700°K, the ratio of absorption coefficient with and without pressure ionization effect is about 0.4.