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Excitation of Atomic Oxygen and Carbon by Collisions with Hydrogen Atoms[*]

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Cross sections are calculated for the excitation of fine-structure levels in neutral atomic oxygen and in both neutral and singly ionized carbon by collisions with neutral hydrogen atoms. The appropriate reaction rates are averaged over a Maxwell distribution of relative velocities, and the results are applied to a discussion of atomic cooling processes in the interstellar medium.

I. INTRODUCTION

THE excitation of fine-structure levels of relatively abundant atoms by collisions with atomic hydrogen has been proposed as a possibly important cooling process in the interstellar medium.[1] In particular, a process involving atomic oxygen

$$\mathrm{O}(^3P_2)+\mathrm{H}\rightarrow \mathrm{O}(^3P_{1,0})+\mathrm{H}$$

has been discussed in this connection,[2,3] and also in regard to the upper atmosphere.[4] No explicit calculations of the cross section for this process have been published. However, Breig and Lin[5] have considered the production of this transition by electron impact.

A somewhat similar process involving singly ionized carbon has been considered by Dalgarno and Rudge[6];

$$\mathrm{C}^+(^2P_{1/2})+\mathrm{H}\rightarrow \mathrm{C}^+(^2P_{3/2})+\mathrm{H}.$$

These authors have estimated the cross section for this process and, on that basis, have estimated the cooling rate to be expected. However, there does not appear to be any good reason to ignore a reaction involving neutral carbon:

$$\mathrm{C}(^3P_0)+\mathrm{H}\rightarrow \mathrm{C}(^3P_{1,2})+\mathrm{H}.$$

(The ground state of singly ionized oxygen is a $4S$ state, so there are no levels of this type to be considered.)

Processes involving oxygen and carbon atoms are of interest because these are the most abundant elements with energy levels in the range of a few hundredths of an electron volt or less above their ground state.[7] Low-energy processes are important because the temperature of the interstellar gas is estimated to be about 125°K.[1] The transition energies for the three reactions listed above are given in Table I. It is apparent from the table that it will be energetically possible for excitation of transitions involving these levels to occur in the interstellar gas, although in the case of oxygen, the effective cross section will be quite substantially reduced since only a relatively small portion of the gas will be able to produce an excitation.

After an excitation takes place, the atom will subsequently lose its energy, mainly by magnetic dipole radiation. Collisional de-excitation is probably unimportant (except for the $^3P_1\rightarrow {}^3P_0$ transition in carbon, which seems to be unimportant anyway as a source of cooling), since if the number density of the interstellar gas is 10 cm^{-3}, and the de-excitation cross section is $100a_0^2$, the mean free time between collisions at a temperature of 125°K should be in excess of 2×10^8 sec. For comparison, the lifetime for a magnetic dipole transition with an energy of 5×10^{-3} eV (58°K) can be estimated to be about 7×10^6 sec. Thus the radiative lifetime is short compared to the time between collisions. Therefore, the population of these excited states will not be in thermal equilibrium with the ground state. We may conclude that essentially all of the excited atoms radiate.

The contribution of excitations produced by atom-atom collisions to the cooling of the interstellar medium can be compared with that produced by other mechanisms of excitation. This will be done briefly in Sec. V. The conclusion may, however, be anticipated here: We find that atom-atom collisions dominate for temperatures of the medium below 1000°K.

TABLE I. Lowest energy levels in ionized and neutral carbon, and in neutral oxygen. Energies are measured in degrees Kelvin.

Atom	State	Energy above ground state (°K)
C$^+$	$^2P_{1/2}$	0
C$^+$	$^2P_{3/2}$	92
C	$^3P_0$	0
C	$^3P_1$	23
C	$^3P_2$	62
O	$^3P_2$	0
O	$^3P_1$	228
O	$^3P_0$	326

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[1] N. H. Dieter and W. M. Goss, Rev. Mod. Phys. **38**, 256 (1966).

[2] A. Burgess, G. V. Field, and R. W. Michie, Astrophys. J. **131**, 529 (1960).

[3] G. B. Field, in *Interstellar Matter in Galaxies*, edited by L. Woltjer (W. A. Benjamin, Inc., New York, 1962), p. 183.

[4] D. R. Bates, Proc. Phys. Soc. (London) **64B**, 805 (1951).

[5] E. L. Breig and C. C. Lin, Phys. Rev. **151**, 67 (1966).

[6] A. Dalgarno and M. R. H. Rudge, Astrophys. J. **140**, 800 (1966).

[7] L. H. Aller, *Abundance of the Elements* (Interscience Publishers, Inc., New York, 1961), pp. 179 ff.

The cross sections for the three processes previously mentioned will be computed using procedures developed in a study of sensitized fluorescence in alkali-metal–rare-gas mixtures.[8] This method, which has been studied in detail elsewhere,[9] enables computation of cross sections in an approximation which satisfies the requirements of unitarity, and is exact in certain interesting limiting cases. The most serious approximation we make concerns the interaction between the atoms. In the cases we consider here, the interaction of longest range capable of producing a transition between fine-structure levels is the Van der Waals interaction, and it is this which will be treated here. Of course, the interaction of oxygen and carbon atoms with hydrogen atoms is more complicated than this, particularly at short range; and it is hoped to consider the interaction in a more detailed way in subsequent work. However, the cross sections we compute are considerably larger than πR_0^2, where R_0 is the effective atomic radius. This indicates that collisions at relatively large distances are effective in producing transitions; and we may expect that our simple treatment of the interaction is reasonably adequate in this region.

II. METHOD OF CALCULATION

The method we will use to calculate the cross section for excitation was developed in Ref. 8. We will review the procedure briefly here. The impact-parameter method is employed. We assume that the interaction between the colliding systems which produces the transitions of interest can be represented by some effective potential V_{eff}. The amplitude of the ith excited level will be denoted a_i. These quantities satisfy the coupled differential equations

$$\frac{da_i}{dt}=-\frac{i}{\hbar}\sum_j \langle i|V_{\text{eff}}|j\rangle a_j(t)e^{-i\omega_{ji}t}, \tag{1}$$

in which

$$\hbar\omega_{ji}=E_j-E_i \tag{2}$$

is the energy difference between states i and j.

A useable exact solution of Eq. (1) is not known. An approximate solution which has many desirable properties is the following: Let the $a_i(t)$ be regarded as the components of a vector $\mathbf{a}$. We put

$$\mathbf{a}(t)=\exp\left[-i\int_{-\infty}^{t}\mathbf{Q}(t')dt'\right]\mathbf{a}(-\infty), \tag{3}$$

where $\mathbf{Q}(t)$ is a matrix whose elements are

$$\hbar Q_{ij}=\langle i|V_{\text{eff}}|j\rangle e^{-i\omega_{ji}t}. \tag{4}$$

The approximate solution (3) becomes exact if and only if $\mathbf{Q}(t)$ and

$$\int_{-\infty}^{t}\mathbf{Q}(t')dt'$$

commute. This condition is satisfied only in a limited number of cases. However, as an approximation, it has the desirable features of (a) reproducing first-order perturbation theory when the interaction is weak, (b) giving an exact solution when

$$\left[\mathbf{Q}(t),\int_{-\infty}^{t}\mathbf{Q}(t')dt'\right]=0,$$

and (c) preserving the normalization of the state vector $\mathbf{a}$ no matter what the interaction is. The last property makes it possible to compute cross sections using interactions which are singular at small distances without having to impose an arbitrary cutoff.

Cross sections are found as follows: Let

$$M_{ij}=\int_{-\infty}^{t}Q_{ij}(t')dt'. \tag{5}$$

We wish to calculate $\exp(-i\mathbf{M})$. To do this, we find, by standard procedures, a unitary matrix $\mathbf{U}$ which diagonalizes $\mathbf{M}$:

$$\mathbf{M}_D=\mathbf{U}^{+}\mathbf{M}\mathbf{U}. \tag{6}$$

The matrix $\mathbf{U}$ is formed from the normalized eigenvectors of $\mathbf{M}$. The diagonalized matrix $\mathbf{M}_D$ is exponentiated according to the prescription

$$[\exp(-iM_D)]_{ij}=\delta_{ij}\exp[-i(M_D)_{ii}], \tag{7}$$

and then the reverse transformation is applied to e^{-iM_D};

$$\exp(-i\mathbf{M})=\mathbf{U}\exp(-i\mathbf{M}_D)\mathbf{U}^{+}. \tag{8}$$

The components of $\mathbf{a}$ are now available, and the cross section for the transition from state j to state i is obtained from

$$\begin{aligned}\sigma_{i,j}&=\int_0^\infty\int_0^{2\pi}|a_i(\infty)|^2pdpd\varphi\\&=\int_0^\infty\int_0^{2\pi}|[\exp(-iM)]_{ij}|^2pd\,pd\,\varphi\end{aligned} \tag{9}$$

(assuming that the atom was in state j for $t=-\infty$). Here, p is the impact parameter, and ϕ is the azimuthal angle.

III. OXYGEN-HYDROGEN COLLISIONS

We discuss the calculation of the cross sections for the $J=2$ to $J=1$, and $J=2$ to $J=0$ transitions in atomic oxygen in detail. The calculations concerning the other processes mentioned in the Introduction are quite similar, and we discuss only those features in which they differ from the present case.

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[8] J. Callaway and E. Bauer, Phys. Rev. **140,** A1072 (1965).

[9] J. Callaway and J. Q. Bartling, Phys. Rev. **150,** 69 (1966).

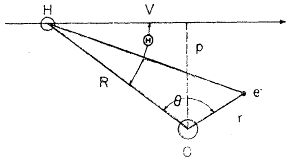

FIG. 1. Coordinate system for collision of a hydrogen atom H with an oxygen atom O. For convenience, only one of the electrons of the oxygen atom is shown. The polar axis is opposite in direction to the velocity v of H.

The interaction between oxygen and hydrogen atoms is undoubtedly quite complex at short range. We consider here only the interaction of longest range: the asymptotic Van der Waals interaction, which is proportional to R^{-6}. The contribution of a possible quadrupole moment of the oxygen atom will be ignored. Effects due to elastic scattering of the atoms are also disregarded, and the relative velocity is assumed to be unchanged during the interaction. A partial correction for the difference in speed after excitation is applied at the end of the calculation. For the present purposes, the four electrons of the oxygen atom in the 1s and 2s states may be neglected, and the effective potential which produces transitions between the levels of interest may be written

$$V_{\text{eff}}=\sum_i v(x_i)\,, \tag{10}$$

where the sum runs over the four electrons in 2p states. The function $v(x_i)$ may be expressed as

$$v(x_i)=-\tfrac{1}{2}(\alpha_{\text{H}}e^2r_i^2/R^6)(3\cos^2\theta_i+1)\,. \tag{11a}$$

The coordinate system is shown in Fig. 1. However, as mentioned in Ref. 8, we may ignore the portion of the interaction potential which is spherically symmetric since that can not produce a transition among the levels of interest to us. Thus, we may write

$$v(x_i)=(-\alpha_{\text{H}}e^2r_i^2/R^6)P_2(\cos\theta_i)\,, \tag{11b}$$

in which θ_i is polar angle of the position vector of electron i with respect to the vector of length R connecting the nuclei of the colliding atoms and α_{H} is the polarizability of hydrogen. We require the matrix elements of V_{eff} between wave functions representing the states of interest. These are linear combinations of determinantal wave functions; however, the calculation can be performed quite simply in terms of the wave functions for the states of two p electrons in L-S coupling as given by Slater.[10] Since we are concerned with states of $J=2, 1, 0$, the matrix Q of Eq. (4) is 9×9. The spin sums and angular integrations required in the calculation of Q may be performed readily, and we find

$$Q_{ij}=-\frac{\alpha_{\text{H}}e^2\langle r^2\rangle}{\hbar R^6}\sum_n c_{ij}^{(n)}Y_{2n}(\Theta,\Phi)e^{-i\omega_{ji}t}. \tag{12}$$

The states i, j here refer to two-particle wave functions characterized by the quantum numbers J, m_J. The quantities $c_{ij}^{(n)}$ are numerical coefficients. The $Y_{2,n}$ are normalized spherical harmonics which depend on the angles specifying the orientation of the vector R connecting the colliding atoms. Finally, $\langle r^2\rangle$ is the average of r^2 for a single 2p electron. This quantity was computed using the wave functions of Clementi *et al.*[11] We obtained $\langle r^2\rangle=1.974a_0^2$. The integration over time can now be done using Eq. (16) of Ref. 8. The elements of the Hermitian matrix M can be expressed as

$$M_{ij}=\frac{3\pi}{160}\,\frac{\alpha_{\text{H}}e^2\langle r^2\rangle}{\hbar vp^5}S_{ij}. \tag{13}$$

The matrix S has the form

$$\begin{bmatrix}
1 & 0 & -5(6)^{-1/2} & 0 & 0 & \frac{1}{3}F_2(x_1) & (2^{1/2}/6)F_1(x_1) & 0 & (-3^{1/2}/9)F_1(x_2)\\
 & -\frac{1}{2} & 0 & -\frac{5}{2} & 0 & F_3(x_1) & (2^{1/2}/6)F_2(x_1) & \frac{1}{6}F_1(x_1) & 0\\
 & & -1 & 0 & 5(6)^{-1/2} & (-6^{1/2}/18)F_2(x_1) & 0 & (6^{1/2}/18)F_2(x_1) & (8^{1/2}/3)F_3(x_2)\\
 & & & -\frac{1}{2} & 0 & -\frac{1}{6}F_1(x_1) & (-2^{1/2}/6)F_2(x_1) & -F_3(x_1) & 0\\
 & & & & -1 & 0 & (2^{1/2}/6)F_1(x_1) & \frac{1}{3}F_2(x_1) & (3^{1/2}/9)F_1(x_2)\\
 & & & & & -\frac{1}{2} & 0 & \frac{5}{2} & (3^{1/2}/9)F_2(x_3)\\
 & & & & & & 1 & 0 & 0\\
 & & & & & & & -\frac{1}{2} & (-3^{1/2}/9)F_2(x_3)\\
 & & & & & & & & 0
\end{bmatrix}, \tag{14}$$

in which we have

$$\begin{aligned}
F_1(x)&=e^{-x}(x^3+6x^2+15x+15)\,,\\
F_2(x)&=e^{-x}(x^3+3x^2+3x)\,,\\
F_3(x)&=\tfrac{1}{2}e^{-x}(x^3+2x^2+3x+3)\,,\\
x_i&=\omega_ip/v\,,\\
\omega_1&=E(J=1)/\hbar\,,\\
\omega_2&=E(J=0)/\hbar\,,\\
\omega_3&=[E(J=1)-E(J=0)]/\hbar.
\end{aligned} \tag{15}$$

Energies are measured with respect to the ground state ($J=2$). The order of states used in writing the matrix S above is ($J=2, m_J=2$), (2,1), (2,0), (2, −1), (2, −2), (1,1), (1,0), (1, −1), and (0,0). An inessential dependence on ϕ has been suppressed.

In general, the matrix M must be exponentiated numerically. However, in the limit $x_i=0$ (for all i), it is

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[10] J. C. Slater, *Quantum Theory of Atomic Structure* (McGraw-Hill Book Company, Inc., New York, 1960), Vol. II, p. 202.

[11] E. Clementi, C. C. J. Roothaan, and M. Yoshimine, Phys. Rev. **127**, 1618 (1962).

possible to make use of the fact that $F_2(0)=0$, and perform the exponentiation analytically. This limit corresponds to the case where the energy differences between the states may be neglected, and is approached when the relative velocity of the colliding atoms becomes large. We will refer to this as the $\omega=0$ approximation. Although the $\omega=0$ approximation will not be good over the entire range of energies of interest to us, it is interesting to give the explicit results in that case, since a closed formula for the excitation cross section can be obtained.

In the limit of $\omega=0$, the matrix M may be partitioned into a 5×5 and a 4×4 matrix. This corresponds to the fact that in this limit, transitions with $\Delta m_J=\pm1$ are forbidden.

$$M=\begin{pmatrix} M_5 & 0 \\ 0 & M_4 \end{pmatrix}. \tag{16}$$

The 5×5 submatrix M_5 contains the states (2,2), (2,0), (2, −2), (1,0), and (0,0), and M_4 contains (2,1), (2, −1), (1,1), and (1, −1). Then

$$e^{-iM}=\begin{pmatrix} e^{-iM_5} & 0 \\ 0 & e^{-iM_4} \end{pmatrix}. \tag{17}$$

The unitary matrices U_5 and U_4 which are required for the construction of the exponentiated matrices are

$$U_5=\begin{bmatrix} a & b & 0 & a & -b \\ -a/3^{1/2} & b/3^{1/2} & {\tfrac{2}{3}}^{1/2} & a/3^{1/2} & b/3^{1/2} \\ b & -a & 0 & b & a \\ -b & -a & 0 & b & -a \\ -{\tfrac{2}{3}}^{1/2}a & {\tfrac{2}{3}}^{1/2}b & -{\tfrac{1}{3}}^{1/2} & {\tfrac{2}{3}}^{1/2}a & {\tfrac{2}{3}}^{1/2}b \end{bmatrix}, \tag{18}$$

$$U_4=\begin{bmatrix} \tfrac{1}{2} & -{\tfrac{1}{2}}^{1/2} & 0 & \tfrac{1}{2} \\ \tfrac{1}{2} & 0 & {\tfrac{1}{2}}^{1/2} & -\tfrac{1}{2} \\ \tfrac{1}{2} & {\tfrac{1}{2}}^{1/2} & 0 & \tfrac{1}{2} \\ -\tfrac{1}{2} & 0 & {\tfrac{1}{2}}^{1/2} & \tfrac{1}{2} \end{bmatrix}. \tag{19}$$

In the above matrices,

$$a=(2^{1/2}-1)^{1/2}/2^{5/4},\quad b=(2^{1/2}+1)^{1/2}/2^{5/4}. \tag{20}$$

The calculation of the exponential matrices can now be performed without difficulty. We find

$$e^{-iM_5}=\begin{bmatrix} A & -B/6^{1/2} & 0 & -B/2^{1/2} & -B/3^{1/2} \\ & C & -B/6^{1/2} & 0 & D/(18)^{1/2} \\ & & A & B/2^{1/2} & -B/3^{1/2} \\ & & & A & 0 \\ & & & & E \end{bmatrix}, \tag{21}$$

$$e^{-iM_4}=\begin{bmatrix} F & -\tfrac{1}{2}B & -\tfrac{1}{4}D & -\tfrac{1}{2}B \\ & F & \tfrac{1}{2}B & -\tfrac{1}{4}D \\ & & F & \tfrac{1}{2}B \\ & & & F \end{bmatrix}. \tag{22}$$

In these matrices, we have

$$\begin{aligned} A&=e^{id}\cos5d\,, \\ B&=ie^{id}\sin5d\,, \\ C&=\tfrac{1}{6}(e^{6id}+4e^{-2id}+e^{-4id})\,, \\ D&=e^{6id}-2e^{-2id}+e^{-4id}\,, \\ E&=\tfrac{1}{3}(e^{6id}+e^{-2id}+e^{-4id})\,, \\ F&=\tfrac{1}{4}(e^{6id}+2e^{-2id}+e^{-4id})\,, \\ d&=\frac{3\pi}{160}\frac{\alpha_{\mathrm{H}}e^2\langle r^2\rangle}{\hbar vp^5}\,. \end{aligned} \tag{23}$$

The exponential matrices are symmetric but not Hermitian.

The transition amplitudes can be immediately found from the appropriate elements. The integration over impact parameter p is accomplished with the aid of Eq. (19) of Ref. 8. To obtain cross sections for the transtiton from J to J', we sum over the partial cross sections from m_J to $m_{J'}$, then average over the initial m_J. The result for the J to J' transition will be labeled $\sigma_{J',J}$. We find

$$\sigma_{1,2}/a_0^2=C\left(\frac{27\pi}{160}\frac{e^2\langle r^2\rangle}{\hbar a_0^2 v}\right)^{2/5}, \tag{24}$$

$$\begin{aligned} \sigma_{0,2}&=(4/9)\sigma_{1,2}\,, \\ \sigma_{0,1}&=0\,, \\ C&=\frac{\pi^2(1+4^{2/5}+5^{2/5})}{50\Gamma(7/5)\sin\frac{1}{5}\pi}=1.76\,. \end{aligned} \tag{25}$$

The quantity a_0 is the Bohr radius of hydrogen. We have inserted the value of the polarizability of hydrogen: $\alpha_{\mathrm{H}}=\frac{9}{2}a_0^3$.

It is convenient, with regard to the construction of thermal averages of the collision cross section which will be considered below, to measure the speed v which appears in the above formulas in terms of a temperature. Therefore, we will define a temperature T through the equation

$$\tfrac{1}{2}\mu v^2=KT\,, \tag{26}$$

in which K is Boltzmann's constant and μ is the reduced mass of the colliding atoms. In the present case,

$$\mu^{-1}=m_{\mathrm{H}}^{-1}+m_{\mathrm{O}}^{-1}. \tag{27}$$

The cross sections given above can then be expressed numerically as

$$\begin{aligned} \sigma_{1,2}/a_0^2&=87.11T^{-1/5}\,, \\ \sigma_{0,2}/a_0^2&=38.72T^{-1/5}\,, \end{aligned} \tag{28}$$

where T is in degrees Kelvin.

We now wish to consider the excitation cross sections without the approximation $\omega=0$. Numerical computations were made for this case using the full matrix of

Eq. (14). The operations of matrix diagonalization, exponentiation, and integration of the transition probability to determine the cross section were performed on an IBM 7040. Some features of the results deserve comment.

The partial cross sections (transitions between states of specific m_J and $m_{J'}$) which do not vanish when $\omega=0$ remain large throughout the range of parameters we consider. However, as a function of velocity, such cross sections exhibit broad maxima with increasing velocity, followed by a slow decrease, instead of the monotonic decrease predicted by Eq. (24). For relatively high velocities, the cross section does approach the value given in Eq. (24). This behavior is illustrated in Fig. 2 for such a transition ($J=2$, $m_J=2$ to $J=1$, $m_J=0$).

There are two other kinds of partial cross sections to be considered: (a) those which have a nonzero matrix element in first-order perturbation theory if $\omega\neq 0$. An example of this type is that for the transition (2, 2 to 1, 1), which is shown in Fig. 2. Typically, these range from 10 to 20% of the large cross sections, and decrease somewhat more rapidly with increasing velocity. (b) Nearly an order of magnitude smaller than these are the partial cross sections which vanish in first-order perturbation theory, such as (2, 2 to 2, -1), also shown in Fig. 2. These make a negligible contribution to the total cross section. The cross sections for the transitions $(2,0\rightarrow 1,0)$ and $(1,0\rightarrow 0,0)$ are found to vanish.

Cross sections computed according to our procedure have one important defect. No account has been taken of the change in velocity of the incident particle during the encounter. As a result, the cross sections do not vanish automatically when the kinetic energy of the particle is below the threshold for excitation. It seems to us that a reasonable way to correct for this difficulty is to multiply the cross sections computed as described above by v_f/v_i, where v_f and v_i are the final and the initial relative velocities of the colliding atoms. This ratio is given by

$$v_f/v_i=(1-E_{\text{exc}}/\tfrac{1}{2}\mu v_i^2)^{1/2}, \tag{29}$$

in which E_{exc} is the excitation energy for the transition and μ is the reduced mass of the colliding particles. This factor, which can be derived from very general considerations, is present in all theories in which the motion of the colliding particles is treated quantum-mechanically. We believe that it is probably the most important quantum correction to the impact-parameter method. Cross sections including this factor of v_f/v_i will be referred to as corrected cross sections, as compared to those obtained directly from Eq. (9). Corrected and uncorrected cross sections for oxygen are given in Table II. The corrected cross sections are shown in Fig 3.

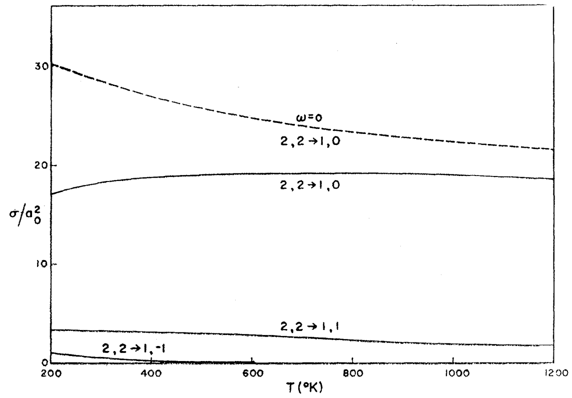

FIG. 2. Some partial cross sections for oxygen. The partial cross section for the transitions $(2,2\rightarrow 1,1)$, $(2,2\rightarrow 1,0)$, and $(2,2\rightarrow 1,-1)$ are shown as a function of velocity (as measured by the velocity temperature T). The result of the $\omega=0$ approximation is shown for the $(2,2\rightarrow 1,0)$ transition.

We now discuss the calculation of the cooling rate of the interstellar gas due to the excitation processes previously described. It is convenient to begin by obtaining a thermally averaged effective cross section.

TABLE II. Cross section for excitation of fine-structure levels in oxygen. The uncorrected cross sections are those obtained by numerical integration of Eq. (9); corrected cross sections include a factor of v_f/v_i.

Uncorrected cross sections				Corrected cross sections		
T (°K),	σ_{12}/a_0^2,	σ_{02}/a_0^2,	σ_{01}/a_0^2	σ_{12}/a_0^2,	σ_{02}/a_0^2,	σ_{01}/a_0^2
200	18.81	4.81	5.47			3.90
300	19.69	5.64	3.67	9.65		3.01
400	20.17	6.15	2.51	13.22	2.65	2.18
500	20.40	6.57	1.77	15.04	3.87	1.59
600	20.45	6.83	1.29	16.10	4.62	1.18
800	20.28	7.23	0.80	17.14	5.57	0.75
1000	19.94	7.42	0.60	17.52	6.09	0.57
1200	19.57	7.47	0.50	17.61	6.37	0.47

Since we are actually interested in a reaction rate, we define

$$\bar{v}\sigma_{\text{eff}}=\int P(v_i)v_i\sigma_{\text{corr}}(v)d^3v_i. \tag{30}$$

In this equation, $P(v_i)$ is the Maxwellian distribution of relative (initial) velocities of the colliding particles

$$P(v)=(\mu/2\pi K\Theta)^{3/2}e^{-\mu v^2/2K\Theta} \tag{31}$$

and $\bar{v}$ is the average velocity for such a distribution;

$$\bar{v}=(8K\Theta/\pi\mu)^{1/2}. \tag{32}$$

In addition, μ is, as before, the reduced mass, and Θ is the temperature of the medium. The cross section which appears above is the corrected one which contains the multiplicative factor of v_f/v_i. The calculations are simplified by introducing the velocity temperature T defined by Eq. (26). We then introduce the quantities y and a;

$$a=E_{\text{exc}}/K\Theta, \quad y=T/\Theta-a. \tag{33}$$

With these substitutions, we find

$$\sigma_{\text{eff}}=e^{-a}\int_0^\infty e^{-y}[y(y+a)]^{1/2}\sigma_{\text{uncorr}}(y+a)dy. \quad (34)$$

Note that we have introduced the uncorrected cross section. To compute these effective cross sections, we made a polynomial fit to the uncorrected cross sections given in Table II. Beyond the range of temperatures given there, we have used the formulas obtained in the $\omega=0$ approximation. The results are given in Table III as a function of the temperature of the medium.

The cooling rate can be obtained quite simply from the effective cross section. As was pointed out in the Introduction, the lifetime for collisional de-excitation is considerably longer than that for radiation. We are concerned with a gas in which the average density is perhaps 10 cm^{-3}. Then if we consider a transition with a cross section of 2.5×10^{-15} cm^2 and a relative velocity of 2×10^5 cm/sec, the mean free time is 2×10^8 sec. The radiative lifetime for the transition ${}^3P_1\rightarrow{}^3P_2$, as determined from the calculations of Pasternack[12] is 10^4 sec. Thus, if an atom is excited, it will almost always radiate. Hence, the cooling rate due to a particular transition will be just the rate at which energy is transferred to excited states by collision. This is, for a transition from state j to state i,

TABLE III. Thermal averaged effective cross section and cooling rates for transitions in oxygen. These quantities are given as functions of the temperature Θ of the medium. Cooling rates are based on the assumptions $n_{\text{H}}=10$ cm^{-3}, $n_{\text{O}}/n_{\text{H}}=9\times10^{-4}$.

Θ (°K)	$\sigma_{1,2}/a_0^2$	$\sigma_{0,2}/a_0^2$	$\Lambda_{1,2}$ (10^{-25} erg/ sec cm^3)	$\Lambda_{0,2}$ (10^{-25} erg/ sec cm^3)
50	0.446	0.023	0.037	0.003
75	1.78	0.174	0.182	0.026
100	3.47	0.474	0.41	0.080
125	5.14	0.857	0.68	0.162
150	6.64	1.27	0.96	0.26
200	9.04	2.05	1.51	0.49
300	12.03	3.27	2.47	0.96
400	13.65	4.05	3.24	1.38
600	15.10	4.91	4.39	2.04
800	15.58	5.30	5.22	2.54
1000	15.70	5.48	5.89	2.94
1200	15.66	5.56	6.43	3.26

$$\sigma_{i,j}=E_{\text{exc}}n_0n_H\bar{v}\sigma_{i,j}, \quad (35)$$

where $\sigma_{i,j}$ is the effective cross section just discussed, n_H is the density of hydrogen, and n_0 is the density of oxygen. The ratio of these densities has been estimated to be[7]

$$n_0/n_H=9\times10^{-4}.$$

Cooling rates have been calculated in this way for the $J=2$ to $J=1$ and $J=0$ transitions, and are given in Table III. Their significance will be discussed in Sec. V.

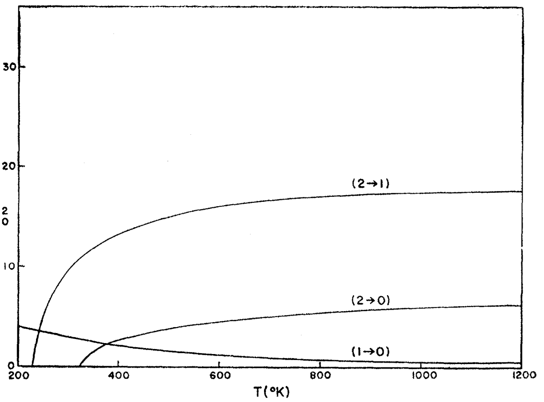

FIG. 3. Corrected cross sections for oxygen. The cross sections for the transitions $(J=2\rightarrow J=1)$, $(2\rightarrow0)$, and $(1\rightarrow0)$, corrected by a factor of v_f/v_i are shown as a function of velocity as measured by the kinetic temperature T.

IV. CARBON-HYDROGEN COLLISIONS

We now turn to the excitations produced in collisions between carbon and hydrogen atoms. In the case of neutral carbon, our attention will be focused on the $J=0$ to $J=2$ transition. It will be seen from Table I that this transition has a much lower excitation energy than was the case for the transitions we have considered in oxygen. The other possible transition from the ground state, that connecting $J=0$ with $J=1$, has a cross section which vanishes in the $\omega=0$ approximation, and on detailed computation turns out to be about 10% of that for $J=0$ to $J=2$. Consequently, it may be ignored in applications to the interstellar medium.

The computation of the cross section proceeds exactly as in Sec. III. It is necessary to change the radial matrix element, which turns out to be substantially larger in the present case: $\langle r^2\rangle=3.748a_0^2$. The sum over final states leads to a difference of a factor of 5, since in carbon, $J=0$ is the ground state. In the $\omega=0$ approximation, we therefore obtain

$$\sigma_{2,0}/a_0^2=3.90\left(\frac{27\pi e^2\langle r^2\rangle}{160hva_0^2}\right)^{2/5}=249.5T^{-1/5}. \quad (36)$$

Numerical calculations of the cross section have been made just as described in the case of oxygen, and the results are tabulated in Table IV.

TABLE IV. Corrected cross sections for ionized and neutral carbon.

T (°K)	$\sigma_{3/2,1/2}/a_0^2$	T (°K)	$\sigma_{2,0}/a_0^2$
100	24.52	75°	32.22
200	64.85	100°	49.14
300	70.90	150°	60.74
400	72.24	200°	64.68
500	71.81	400°	65.88
600	71.25	600°	63.75
800	69.50		
1000	67.67		
1200	66.04		

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[12] S. Pasternack, Astrophys. J. 92, 129 (1940).

It may be that a significant portion of the carbon in the interstellar gas is in the form of C^+ since the ionization potential of carbon is lower than that of hydrogen. Dalgarno and Rudge[6] assumed that almost all the carbon is in this form, and calculated the cooling rate to be expected. However, they used different abundance figures. We have repeated these calculations by our methods. We find that the cross section for the $J=\frac{1}{2}$ to $J=\frac{3}{2}$ transition in this system is not much different from the $J=2$ to $J=0$ transition in neutral carbon.

The effective interaction between carbon ions and hydrogen atoms is, in the framework of our approximations,

$$V_{\rm eff}=-\tfrac{1}{2}\alpha_{\rm H}F^2\,, \tag{37}$$

where F is the electric field at the hydrogen atom produced by the carbon ion. We denote the coordinate of the single $2p$ electron by r, and treat the nucleus plus the four electrons in $1s$ and $2s$ shells as a core of charge $+2$. Then $V_{\rm eff}$ may be expanded in the form, valid when R, the separation between the nuclei of the particles, is much larger than r;

$$V_{\rm eff}=-\frac{\frac{1}{2}\alpha_{\rm H}e^2}{R^4}\left[1-\frac{4r\cos\theta}{R}-(6\cos^2\theta-4)\frac{r^2}{R^2}+\cdots\right]. \tag{38}$$

The leading term in this expression which depends on the coordinates of the $2p$ electron is proportional to R^{-5}; however, this cannot cause transitions between states of the same parity since it is odd under inversion. Hence, we may drop the first two terms in the expansion, as well as the spherically symmetric part of the third term. $V_{\rm eff}$ reduces to

$$V_{\rm eff}=2\alpha_H e^2r^2P_2(\cos\theta)/R^6\,. \tag{39}$$

Transitions between P states of $J=\frac{1}{2}$ and $J=\frac{3}{2}$ have already been considered using this method in Ref. 8 in the $\omega=0$ approximation. Comparison of Eq. (39) with that paper indicates that expression of Ref. 8 for the $\frac{1}{2}\rightarrow\frac{3}{2}$ cross section may be adopted here provided that the interaction strength is multiplied by a factor of 2. Thus

$$\sigma_{3/2,1/2}/a_0^2=3.90\left(\frac{27\pi e^2\langle r^2\rangle}{80\hbar v a_0^2}\right)^{2/5}=288T^{-1/5}\,. \tag{40}$$

The radial matrix element was computed to be $2.689a^2{}_0$ using Clementi's wave functions.[13] This may be compared with Eq. (36).

We have also made numerical calculations of the cross section as described in Sec. III. In the case of ionized carbon, these are somewhat more rapid, since the matrix M which is to be exponentiated is only 6×6. Instead of Eqs. (13) and (14), we have

$$M_{ij}=\frac{3\pi}{80}\frac{\alpha_{\rm H}e^2\langle r^2\rangle}{\hbar v\rho^5}S_{ij}\,, \tag{41}$$

in which the matrix S is given by

$$S=\begin{bmatrix} 1 & 0 & 5(3)^{-1/2} & 0 & (6^{1/2}/9)F_2(x) & (-6^{1/2}/9)F_1(x) \\ & -1 & 0 & 5(3)^{-1/2} & -(8^{1/2}/3)F_3(x) & (2^{1/2}/9)F_2(x) \\ & & -1 & 0 & -(2^{1/2}/9)F_2(x) & (-8^{1/2}/3)F_3(x) \\ & & & 1 & -(6^{1/2}/9)F_1(x) & (-6^{1/2}/9)F_2(x) \\ & & & & 0 & 0 \\ & & & & & 0 \end{bmatrix}. \tag{42}$$

The order of states in Eq. (42) is $(\frac{3}{2},\frac{3}{2})$, $(\frac{3}{2},\frac{1}{2})$, $(\frac{3}{2},-\frac{1}{2})$, $(\frac{3}{2},-\frac{3}{2})$, $(\frac{1}{2},\frac{1}{2})$, and $(\frac{1}{2},-\frac{1}{2})$.

This matrix was exponentiated numerically, and the cross sections found by numerical integration. They are listed in Table IV, where they may be compared with corresponding ones for neutral carbon.

Effective cross sections may be computed by a thermal average, as was also done for oxygen. These results are listed, for both neutral and ionized carbon, in Table V. It will be seen that the cross sections are slightly larger for ionized carbon. In order to compute the cooling rate for transitions in carbon, we require both the total abundance of carbon and the fraction which is ionized. The total abundance is reasonably well determined (relative to hydrogen) to be[7]

$$n_C/n_H=4\times10^{-4}.$$

However, we must guess at the proportion ionized. Fortunately, the near equality of the cross sections in the two cases indicates that the uncertainty due to lack of knowledge of the ionization is not too large. (Ionized carbon does tend to contribute somewhat more to the cooling rate than an equal amount of neutral carbon because the transition energy is higher by a factor of $\frac{4}{3}$.) We give estimated cooling rates in Table V, under two assumptions: (a) that all of the carbon is neutral and (b) that all is singly ionized. The actual situation will correspond to some average of these results. The cooling rates due to oxygen and carbon atoms are compared in Fig. 4.

V. DISCUSSION AND CONCLUSIONS

The principal conclusion of this work is that if van de-Waals's interactions are considered, the cross sections for the production of transitions between some finer

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[13] E. Clementi, *Tables of Atomic Functions* (International Business Machines Corporation, New York, 1965).

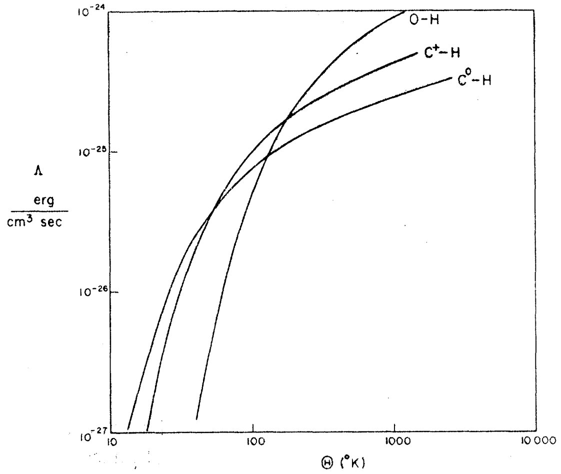

FIG. 4. Cooling rates due to oxygen-hydrogen and carbon-hydrogen collisions are shown as a function of the temperature of the interstellar gas Θ. The density of the gas is assumed to be 10 cm^{-3}. The curve labeled C^0-H is computed under the assumption that all the carbon is neutral; that labeled C^+-H assumes that all is ionized.

structure levels of oxygen and both neutral and singly ionized carbon atoms by collisions with neutral hydrogen atoms are of the order of 5×10^{-16} cm^2 and 2×10^{-15} cm^2, respectively, for the range of relative velocities of interest in astrophysical applications. These cross sections are large enough so that the cooling processes they produce are probably of substantial importance in the determination of the equilibrium temperature of the interstellar medium.

It appears that the possibility of relatively large cross sections for low-energy transitions in encounters between neutral atoms has perhaps not been appreciated. The leading term in the interaction between such atoms is often the van der Waals interaction, and this appears to be sufficiently strong and of sufficient range to produce large cross sections. It is certain that the simple asymptotic formula we have used for the interaction is inadequate for close encounters; however, in such cases, details of the interaction are relatively unimportant as long as it is strong.

Note that electron excitation of these transitions is probably substantially less important than that due to collisions with neutral hydrogen. The cross sections for electron excitation of fine-structure transitions in neutral oxygen have been carefully calculated by Breig and Lin.[5] If we assume that the electron temperature is 10^4°K or less and that the fractional abundance of free electrons relative to hydrogen is 2×10^{-4}, the cooling rate due to electron induced transitions in oxygen is down by a factor of 20 or more with respect to that due to collisions with neutral hydrogen (at 125°K). Similarly, electron-induced excitation of other elements may be expected to be relatively less important compared to the processes we consider if the abundance of free electrons is in fact of the order stated.

TABLE V. Thermal average effective cross section for ionized and neutral carbon, and cooling rates due to carbon, assuming (a) that all carbon is neutral, and (b) that all carbon is singly ionized.

Θ	$\sigma_{3/2,1/2}/a_0^2$	$\sigma_{2,0}/a_0^2$	Λ (10^{-25} erg/sec cm^3) Neutral C	Λ (10^{-25} erg/sec cm^3) Ionized C
50	22.3	32.5	0.33	0.33
75	36.5	44.3	0.55	0.67
100	45.8	50.9	0.73	0.97
125	52.0	54.8	0.88	1.2
150	56.2	57.2	1.0	1.5
200	61.2	59.7	1.2	1.8
300	65.2	60.7	1.5	2.4
400	66.3	60.1	1.7	2.8
600	65.7	58.0	2.0	3.4
800	64.3	55.9	2.3	3.8
1000	62.7	54.1	2.5	4.2
1200	61.3	52.6	2.6	4.5

Another cooling process which may be of some importance is the excitation of rotational levels of the neutral hydrogen molecule by collisions with hydrogen atoms.[14] Since the excitation energy for the lowest rotational transition in H_2 ($J=0$ to $J=2$) is roughly twice that of the processes we have considered here, such excitations would not be an important source of cooling in a gas with a temperature in the neighborhood of 100°K. The calculations of the cooling rate due to excitation of H_2 are extremely uncertain because there are as yet no observations of these molecules in the interstellar gas. The calculations reported in Ref. 14 indicate that cooling due to molecular excitation will be smaller than that due to atomic excitations for temperatures less than 1000°K if the number of hydrogen molecules present is 10^{-2} of the number of hydrogen atoms.

The question whether the calculated cooling rate is consistent with the energy input must also be considered. A more detailed discussion of the processes involved in the heating of the interstellar gas can be found in Ref. 1. The principal sources of heating are believed to be cloud-cloud collisions and ionization by low-energy cosmic rays. On an average basis, the energy input from these two sources is estimated to be about 4.6×10^{-26} erg/cm^3 sec for a density of 10 cm^{-3}. This would be consistent with our estimates of the cooling if the temperature were in the range 60 to 75°K in which case carbon atoms would be the most important source of cooling. The cooling rates are rapidly increasing functions of temperature below about 200°K, and if the gas temperature is as high as 125°K, as estimated in Ref. 1, the total cooling rate will be larger by a factor of 3 or more than estimated energy input. Since the cooling due to collisions is proportional to the square of the density, while the heating processes considered above are proportional to the density, it might be necessary to revise downward the estimated density. Alternatively, it may be necessary to reinvestigate possible heating processes.

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[14] K. Takayanagi and S. Nishimura, Publ. Astronom. Soc. Japan 12, 77 (1960).