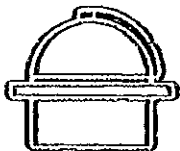


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CALCULATIONS OF IONIZATION
EQUILIBRIA FOR OXYGEN

--- ° --- NSG-438

Scientific Report #7

By

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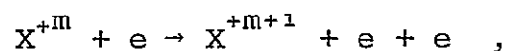
November 1965

INTRODUCTION

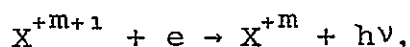
Recent calculations by Burgess (1964a, 1964b, 1965a, 1965b) have indicated that dielectronic recombination is important in the study of ionization equilibria of the solar corona. Burgess and co-workers have carried out calculations for iron and calcium. The present paper studies the effect of including the dielectronic recombination process in calculations of the ionization equilibria for oxygen.

To facilitate the calculation of dielectronic recombination rates, Burgess (1964b) presented a formula accurate to roughly 20% when applied to a plasma of low density and high temperature. More recently, Burgess (1965b) has published a revised version of this expression, which is more accurate by a few percent than the original one and is in a more compact form. The calculations discussed here have employed the formula given in 1964. The small differences in the values of the dielectronic recombination rates that result from use of the newer expression do not justify a recalculation.

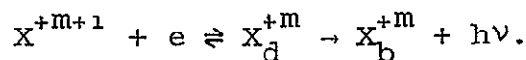
At coronal temperatures the ionization equilibrium is determined by collisional ionization,



radiative recombination,



and dielectronic recombination,



Here X^{+m} represents an ion of charge $+m$. In the dielectronic recombination process the electron, e , is first captured in a radiationless transition to the doubly excited state X_d^{+m} ; this capture may be followed by a radiative stabilizing transition to a bound state X_b^{+m} . In this latter transition the principal quantum number, n , of the outer electron does not change. Furthermore, n must be rather large for the dielectronic recombination process to be effective. Hence, the stabilizing transition is effectively a transition between an excited state of X^{+m+1} , which is the series limit for the outer electron with principal quantum number n , and the ground state of X^{+m+1} .

The recombination and ionization rates are proportional to a rate coefficient, the proper ion population, and the electron density, N_e . Hence, if $q(X^{+m})$, $\alpha_r(X^{+m})$, and $\alpha_d(X^{+m})$ are respectively the rate coefficients of collisional ionization, radiative recombination, and dielectronic recombination, the ionization equilibrium may be expressed as

$$N_e N(X^{+m}) q(X^{+m}) = N_e N(X^{+m+1}) \alpha_r(X^{+m}) + N_e N(X^{+m+1}) \alpha_d,$$

if one assumes a steady state situation. If simplified, this expression becomes

$$\frac{N(X^{+m+1})}{N(X^{+m})} = \frac{\alpha_r(X^{+m})}{\alpha_r(X^{+m}) + \alpha_d(X^{+m})} \quad (1)$$

RATE COEFFICIENTS OF IONIZATION AND RECOMBINATION

The Burgess (1964b) expression for the dielectronic recombination rate coefficient is

$$\alpha_d = \sum_d 1.0053 \times 10^{-8} f(d,b) T^{-3/2} (\Delta W_d)^{1/2} (m+2)^2 A(x) B(m+1) e^{-1.4388 \frac{\Delta W_d}{T} \left(1 + 0.015 \frac{(m+1)^3}{(m+2)^2} \right)^{-1}}, \quad (2)$$

where the summation is over those excited levels of X^{+m+1} from which radiative transitions to the ground level of X^{+m+1} are possible. $f(d,b)$ is the oscillator strength of the transition and ΔW_d is the excitation energy of the X^{+m+1} level in cm^{-1} . $A(x)$ and $B(m+1)$ are functions tabulated by Burgess. They are reproduced here in Table 1. The quantity x is given by the expression

$$x = 9.113 \times 10^{-6} \frac{\Delta W_d}{m+2}.$$

Burgess finds that this expression for α_d is accurate to within 20% provided $x > 0.05$ and

$$T \geq 0.286 \Delta W_d \left(1 + 0.015 \frac{(m+1)^3}{(m+2)^2} \right)^{-1} \quad (3)$$

However, Burgess (1965b) points out that in comparison with the radiative rate, the dielectronic one becomes small for temperatures less than this minimum value. Hence errors in α_d in this temperature range will be unimportant.

An expression for the collisional ionization rate coefficient is given by Seaton (1964):

$$q(X^{+m}) = 2.0 \times 10^{-8} \frac{\zeta}{I_m^2} T^{1/2} 10^{-50.40 I_m / T}, \quad (4)$$

where I_m is the ionization potential of X^{+m} and ζ is the number of electrons in the shell from which ionization takes place. This formula is supposedly accurate to within a factor of 2.

The calculations presented here employ Seaton's (1959) expression for the rate coefficient for radiative recombination to all levels:

$$\alpha_r = 5.20 \times 10^{-14} (m+1) \lambda^{1/2} \{0.4288 + \frac{1}{2} \ln \lambda + 0.469 \lambda^{-1/3}\} \quad (5)$$

where $\lambda = 157890 \frac{(m+1)^2}{T}$

THE CALCULATIONS

Equations (1), (2), (4), and (5) have been programmed for computation on an IBM 7094 computer. Calculations of the dielectronic recombination rates require oscillator strengths for permitted transitions to ground levels of oxygen ions and excitation energies of the upper levels of these transitions. Oscillator strengths of most resonance lines have been taken from tabulated values given by Varsavsky (1962). When available, empirical excitation energies given by Moore (1949) are employed. For other transitions, radial quantum integrals and excitation energies come from tables of Kelly (1964) and calculations performed with a

Hartree-Fock computer program written by C. Froese (1964). The corresponding oscillator strengths follow from computations based on tabulated line and multiplet factors (Shore and Menzel, 1965). Ionization potentials have been obtained from Moore (op.cit.).

Both empirical and theoretical excitation energies are available for certain levels. When compared, the theoretical values are found to be systematically lower than the empirical ones by a nearly constant amount for a given ion. A correction factor to shift the theoretical values into agreement with the experimental ones can thus be derived. This factor is then applied to the excitation energies of levels for which only theoretical values are available. The adopted excitation energies and f-values are tabulated in Table 2.

From these data, equation (1) has been calculated for each stage of ionization. The resulting relative ion populations, $N(O^{+m})/N_{\text{tot}}$, where

$$N_{\text{tot}} = \sum_{m=0}^7 N(O^{+m}),$$

are plotted versus $\log T$ in Figures 1 and 2. Dielectronic recombination has been included only in the calculations yielding the results displayed in Figure 1. The plotted values are also tabulated in Table 3 for convenience in actual use of the numbers. For a given ion an asterisk marks the relative ion population corresponding to the temperature for which the equality holds in equation (3).

DISCUSSION

A comparison of Figures 1 and 2 shows that the inclusion of dielectronic recombination in the calculations alters the relative ionization equilibrium populations by a rather large amount. As noted by Burgess and Seaton (1964) for certain ions of iron, the temperature corresponding to the maximum abundance of a given ion has a higher value when the dielectronic recombination process is included. The ion abundances obtained here for oxygen, like those calculated by Burgess (1965a) for iron and calcium, show much flatter maxima than do those calculated only from collisional ionization and recombination rates.

The computer program described above can readily be applied to the calculation of ionization equilibria of other elements, provided the necessary excitation energies and oscillator strengths are known. At present, calculations are proceeding for silicon and nitrogen.

ACKNOWLEDGEMENTS

This work has been supported by NASA Grant Nsg-438 and Contract NONr 1866(48) of the Office of Naval Research. I wish to thank Dr. L. Goldberg for suggesting the problem. Discussions with him, Dr. B. Shore, Dr. C. Froese, and Mrs. A. Dupree on various aspects of the calculations were very helpful.

TABLE 1

Burgess A(x) and B(m+1) Functions

x	A(x)	m+1	B(m+1)
0	1.13	1	2.07
1	1.00	2	2.80
2	0.88	3	2.99
3	0.77	4	3.00
4	0.67	5	2.93
5	0.58	6	2.82
6	0.51	7	2.70
7	0.44	8	2.60
8	0.39	9	2.50
9	0.34	10	2.42
10	0.31	11	2.34
11	0.28	12	2.26
12	0.25 ₅	13	2.18
13	0.23 ₅	14	2.11
14	0.21	15	2.05
15	0.19	16	1.98
16	0.17 ₅	17	1.92
17	0.16	18	1.88
18	0.14 ₅	19	1.82
19	0.13	20	1.78
20	0.12		
21	0.11		

This table should not be used for $x < 0.05$.

TABLE 2
Excitation Energies and Oscillator Strengths for
Dielectronic Recombination Stabilizing Transitions

Ion (X^{+m})	Transition	Excitation Energy (cm^{-1})	f	Refer- ence	
O I	$1s^2 2s^2 2p^2 \text{ ms } ^4P_{1/2, 3/2, 5/2} n\ell \rightarrow 1s^2 2s^2 2p^3 \text{ } ^4S_{3/2}^o n\ell$				
	3s	185,300	0.166	1	
	4s	238,700	0.0242	1	
	5s	257,800	0.00705	1	
	6s	267,500	0.00290	1	
	7s	271,900	0.00146	1	! <br/ ∞
	8s	275,000	0.00085	1	
	$1s^2 2s^2 2p^2 \text{ md } ^4P_{1/2, 3/2, 5/2} n\ell \rightarrow 1s^2 2s^2 2p^3 \text{ } ^4S_{3/2}^o n\ell$				
	3d	232,500	0.500	1	
	4d	255,100	0.240	1	
	5d	265,500	0.105	1	
	6d	271,500	0.0515	1	
	7d	274,900	0.0288	1	
	8d	277,100	0.0177	1	
	$1s^2 2s 2p^4 \text{ } ^4P n\ell \rightarrow 1s^2 2s^2 2p^3 \text{ } ^4S_{3/2}^o n\ell$	120,000	0.77	3	
O II	$1s^2 2s^2 2p \text{ ms } ^3P_1^o n\ell \rightarrow 1s^2 2s^2 2p^2 \text{ } ^3P_0 n\ell$				
	3s	267,400	0.107	1	

TABLE 2 (Continued)

Ion(X^{+m})	Transition	Excitation Energy (cm^{-1})	f	Refer- ence	
	4s	356,800	0.0167	1	
	5s	392,200	0.00517	1	
	6s	409,800	0.00221	1	
	7s	419,700	0.00115	1	
	8s	426,200	0.00067	1	
	$1s^2 2s^2 2p \cdot md \ ^3D_1^o nl \rightarrow 1s^2 2s^2 2p^2 \ ^3P_o nl$				
	3d	327,300	0.528	1	
	4d	379,300	0.161	1	
	5d	402,500	0.0561	1	
	6d	415,200	0.0252	1	
	7d	422,800	0.0137	1	
	8d	427,700	0.00838	1	
	$1s^2 2s^2 2p \cdot md \ ^3P_1^o nl \rightarrow 1s^2 2s^2 2p^2 \ ^3P_o nl$				
	3d	329,600	0.177	1	
	4d	380,700	0.0537	1	
	5d	405,100	0.0188	1	
	6d	418,500	0.00845	1	
	7d	426,300	0.00460	1	
	8d	431,500	0.00282	1	
	$1s^2 2s 2p^3 \ ^3D_1^o nl \rightarrow 1s^2 2s^2 2p^2 \ ^3P_o nl$	120,100	0.117	1	
	$\ ^3P_1^o$	142,383	0.231	1	

TABLE 2 (Continued)

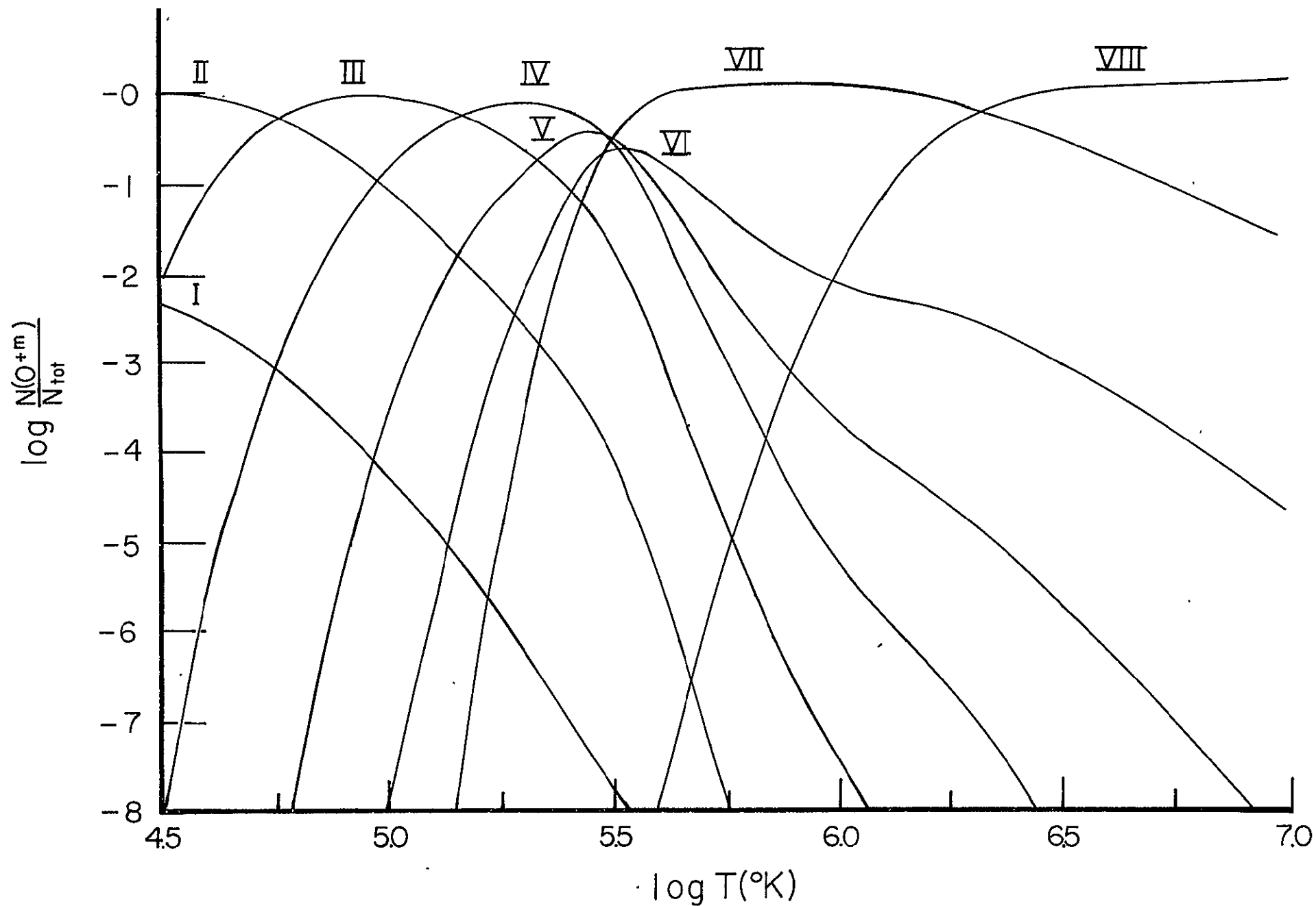
Ion(X^{+m})	Transition	Excitation Energy (cm^{-1})	f	Refer- ence
O III	$1s^2 2s^2 ms \ ^2S_{1/2} n\ell \rightarrow 1s^2 2s^2 2p \ ^2P_{1/2}^o n\ell$			
	3s	357,600	0.0501	1
	4s	485,800	0.00824	1
	5s	539,400	0.00267	1
	6s	566,900	0.00117	1
	7s	582,900	0.00062	1
	8s	592,900	0.00038	1
	$1s^2 2s^2 md \ ^2D_{3/2} n\ell \rightarrow 1s^2 2s^2 2p \ ^2P_{1/2}^o n\ell$			
	3d	419,500	0.504	1
	4d	510,600	0.111	1
	5d	552,000	0.0352	1
	6d	574,400	0.0154	1
	7d	587,900	0.00839	1
	8d	596,700	0.00508	1
	$1s^2 2s 2p^2 \ ^2S_{1/2} n\ell \rightarrow 1s^2 2s^2 2p \ ^2P_{1/2}^o n\ell$	164,400	0.0470	1
	$\ ^2P_{1/2, 3/2}$	180,600	0.464	1
	$\ ^2D_{3/2}$	127,000	0.182	1
	$1s^2 2s 2p \ ^3P mp \ ^2S_{1/2} n\ell \rightarrow 1s^2 2s^2 2p \ ^2P_{1/2}^o n\ell$			
	$\ ^2P_{1/2, 3/2}$			

TABLE 2 (Continued)

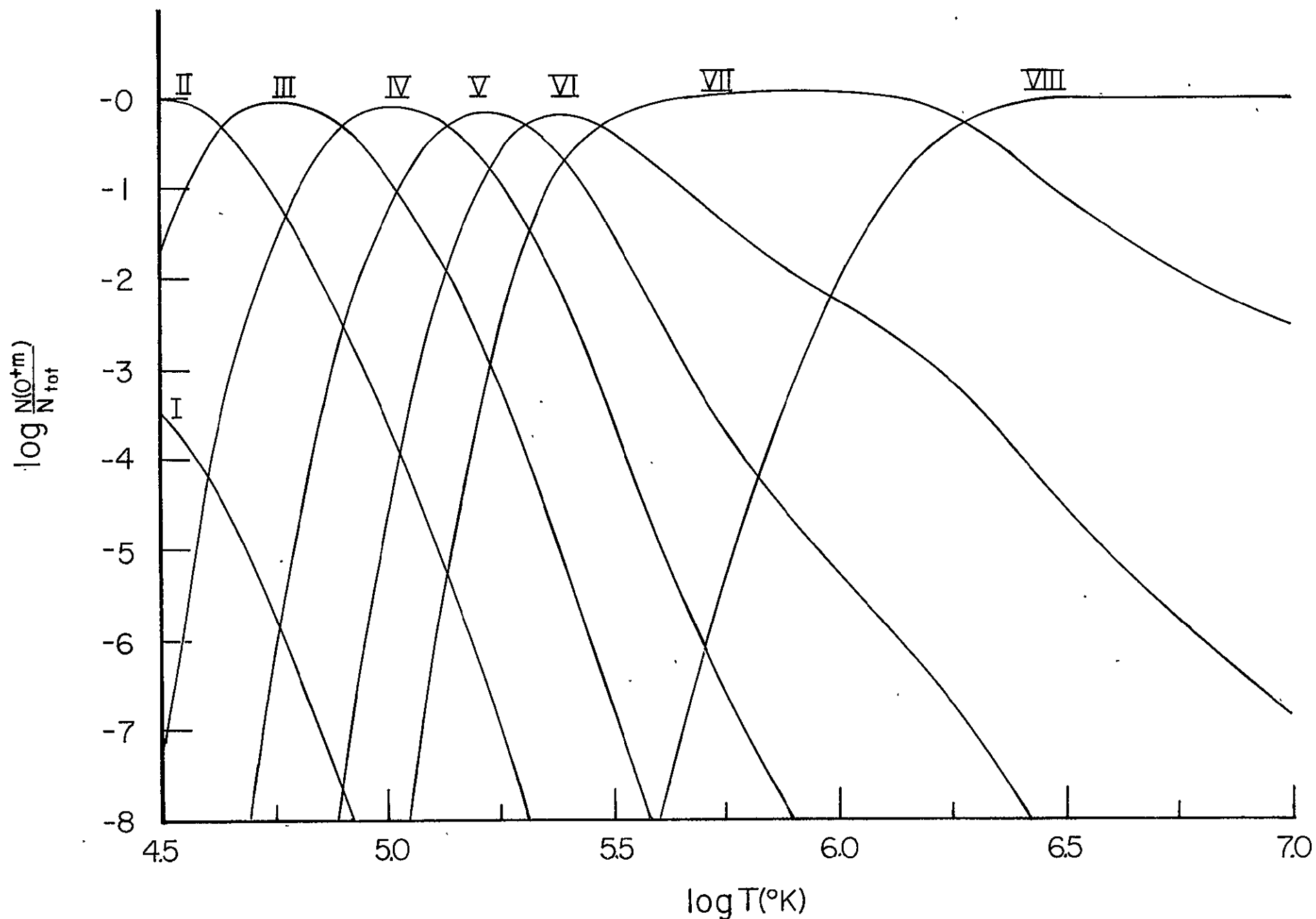
Ion (X^{+m})	Transition	Excitation Energy (cm^{-1})	f	Refer- ence	
	$^2D_{3/2}$				
	3p	492,900	0.0387	1	
		467,300	0.110	1	
		482,700	0.190	1	
	4p	590,100	0.0103	2	
		575,300	0.0309	2	
		584,600	0.0515	2	
	5p	630,000	0.0396	2	
	6p	649,500	0.0204	2	
	$1s^2 2s 2p \ ^1P \ mp \ ^2S_{1/2} n\ell \rightarrow 1s^2 2s^2 2p \ ^2P_{1/2}^o n\ell$				
	$^2P_{1/2, 3/2}$				
	$^2D_{3/2}$				
	3p	554,500	0.0145	1	
		549,800	0.0432	1	
		547,300	0.0716	1	
	4p	656,700	0.0346	2	
	5p	701,900	0.0147	2	
	6p	726,100	0.0075	2	

TABLE 2 (Continued)

Ion(X^{+m})	Transition	Excitation Energy (cm^{-1})	f	Refer- ence
O IV	$1s^2 2s \text{ mp } ^1P_1^o n\ell \rightarrow 1s^2 2s^2 ^1S_0 n\ell$			
	2p	158,800	0.731	1
	3p	580,800	0.591	1
	4p	737,900	0.159	1
	5p	802,500	0.0622	1
	6p	839,600	0.0304	1
	7p	860,900	0.0171	1
	8p	874,400	0.0107	1
O V	$1s^2 \text{ mp } ^2P_{1/2,3/2}^o n\ell \rightarrow 1s^2 2s ^2S_{1/2} n\ell$			
	2p	96,600	0.199	1
	3p	666,200	0.309	1
	4p	863,400	0.0857	1
	5p	954,100	0.0365	1
	6p	1,003,100	0.0189	1
	7p	1,032,600	0.0111	1
	8p	1,051,700	0.00709	1
O VI	$1s \text{ mp } ^1P_1^o n\ell \rightarrow 1s^2 ^1S_0 n\ell$			
	2p	4,629,200	0.702	2
	3p	5,368,600	0.147	2
	4p	5,628,100	0.0512	2



Relative Ion Populations for Oxygen Including Dielectronic Recombination. Each curve is labeled with the conventional Roman numeral expression for $m + 1$.



Relative Ion Populations for Oxygen Without Dielectronic Recombination. The labeling convention of Figure 1 is employed here also.

TABLE 2 (Continued)

Ion (X^{+m})	Transition	Excitation Energy (cm^{-1})	f	Refer- ence
O VII	5p	5,748,500	0.0315	2
	6p	5,814,000	0.0106	2
	$mp \ ^2P_{1/2, 3/2}^o \ n\ell \rightarrow 1s \ ^2S_{1/2} \ n\ell$			
	2p	5,271,900	0.417	2
	3p	6,247,000	0.0797	2
	4p	6,588,000	0.0301	2
	5p	6,746,000	0.0123	2
	6p	6,832,000	0.00622	2

- References: 1 Kelly (1964)
 2 Froese (1964)
 3 Varsavsky (1962)

TABLE 3a

Relative Ion Populations $\left(\log \frac{N(O^{+m})}{N_{\text{tot}}} \right)$

(dielectronic recombination included in the calculations)

log T	Stage of Ionization (m + 1)							
	I	II	III	IV	V	VI	VII	VIII
4.0	- 0.006	- 1.85	-16.21					
4.1	- 0.17	- 0.48	-11.09	-30.59				
4.2	- 0.95	- 0.05	- 7.65	-22.51				
4.3	- 1.75	- 0.008	- 5.21	-16.39	-34.11			
4.4	- 2.18	- 0.003	- 3.39	-11.67	-25.32			
4.5	- 2.41	- 0.005	- 2.08	- 8.20	-18.73	-35.59		
4.6	- 2.61	- 0.03	- 1.16	- 5.68	-13.87	-27.10		
4.7	- 2.89	- 0.15	- 0.54	- 3.83	-10.22	-20.56	-33.06	
4.8	- 3.30	- 0.41	- 0.21	- 2.52	- 7.48	-15.48	-25.00	
4.9	- 3.81*	- 0.77	- 0.09	- 1.60	- 5.38	-11.49	-18.63	
5.0	- 4.35	- 1.17	- 0.09	- 0.94	- 3.75	- 8.32	-13.54	
5.1	- 4.92	- 1.60*	- 0.19	- 0.49	- 2.50	- 5.81	- 9.48	
5.2	- 5.56	- 2.09	- 0.40	- 0.25	- 1.58	- 3.85	- 6.27	-29.11
5.3	- 6.26	- 2.63	- 0.70*	- 0.17	- 0.94	- 2.36	- 3.75	-21.64
5.4	- 7.05	- 3.26	- 1.11	- 0.25*	- 0.55	- 1.27	- 1.83	-15.76
5.5	- 8.11	- 4.16	- 1.79	- 0.64	- 0.54*	- 0.70	- 0.57	-11.33
5.6	- 9.67	- 5.55	- 2.98	- 1.58	- 1.13	- 0.83	- 0.12	- 8.34
5.7	-11.37	- 7.08	- 4.30	- 2.66	- 1.90	- 1.23	- 0.03	- 6.21

TABLE 3a (Continued)

log T	Stage of Ionization (m + 1)							
	I	II	III	IV	V	VI	VII	VIII
5.8	-12.97	- 8.49	- 5.52	- 3.65	- 2.62	- 1.61	- 0.01	- 4.53
5.9	-14.44	- 9.78	- 6.61	- 4.53	- 3.24	- 1.94	- 0.006	- 3.19
6.0	-15.80	-10.95	- 7.58	- 5.28	- 3.76	- 2.19	- 0.006	- 2.12
6.1	-17.03	-11.99	- 8.42	- 5.92	- 4.17	- 2.35	- 0.02	- 1.30
6.2	-18.21	-12.98	- 9.21	- 6.50	- 4.53	- 2.47*	- 0.09	- 0.73
6.3	-19.41	-13.99	-10.02	- 7.10	- 4.92	- 2.63	- 0.23*	- 0.38
6.4	-20.66	-15.04	-10.87	- 7.76	- 5.36	- 2.85	- 0.42	- 0.21
6.5	-21.94	-16.13	-11.77	- 8.44	- 5.84	- 3.12	- 0.63	- 0.12
6.6	-23.25	-17.25	-12.68	- 9.16	- 6.34	- 3.42	- 0.85	- 0.07
6.7	-24.58	-18.38	-13.61	- 9.89	- 6.87	- 3.73	- 1.07	- 0.04
6.8	-25.92	-19.52	-14.56	-10.63	- 7.41	- 4.07	- 1.29	- 0.02
6.9	-27.28	-20.68	-15.52	-11.39	- 7.96	- 4.42	- 1.51	- 0.01
7.0	-28.63	-21.84	-16.48	-12.15	- 8.52	- 4.78	- 1.72	- 0.008

TABLE 3b

Relative Ion Populations $\left(\log \frac{N(O^{+m})}{N_{\text{tot}}} \right)$

(radiative recombination and collisional ionization only included in the calculations)

log T	Stage of Ionization (m + 1)							
	I	II	III	IV	V	VI	VII	VIII
4.0	- 0.006	- 1.85	-16.21					
4.1	- 0.17	- 0.48	-11.08	-30.59				
4.2	- 0.98	- 0.05	- 7.64	-22.50				
4.3	- 1.96	- 0.005	- 5.18	-16.33	-34.04			
4.4	- 2.78	- 0.001	- 3.22	-11.41	-24.98			
4.5	- 3.48	- 0.01	- 1.66	- 7.46	-17.73	-34.07		
4.6	- 4.20	- 0.15	- 0.53	- 4.41	-12.02	-24.51		
4.7	- 5.27	- 0.74	- 0.09	- 2.41	- 7.89	-17.30	-29.80	
4.8	- 6.50	- 1.55	- 0.05	- 1.12	- 4.88	11.81	-21.33	
4.9	- 7.79	- 2.49	- 0.28	- 0.33	- 2.70	- 7.64	-14.78	
5.0	- 9.28	- 3.67	- 0.88	- 0.09	- 1.33	- 4.67	- 9.89	
5.1	-10.84	- 4.95	- 1.67	- 0.18	- 0.50	- 2.54	- 6.21	
5.2	-12.51	- 6.37	- 2.67	- 0.61	- 0.17	- 1.15	- 3.57	-26.41
5.3	-14.31	- 7.95	- 3.89	- 1.34	- 0.27	- 0.39	- 1.79	-19.68
5.4	-16.28	- 9.71	- 5.33	- 2.38	- 0.78	0.19	- 0.74	-14.67
5.5	-18.35	-11.57	- 6.92	- 3.61	- 1.57	- 0.39	- 0.25	-11.01
5.6	-20.37	-13.41	- 8.51	- 4.89	- 2.47	- 0.79	- 0.08	- 8.30
5.7	-22.24	-15.09	- 9.96	- 6.07	- 3.32	- 1.22	- 0.03	- 6.20

TABLE 3b (Continued)

log T	Stage of Ionization (m + 1)							
	I	II	III	IV	V	VI	VII	VIII
5.8	-23.91	-16.58	-11.25	- 7.11	- 4.08	- 1.61	- 0.01	- 4.53
5.9	-25.43	-17.92	-12.39	- 8.03	- 4.74	- 1.96	- 0.005	- 3.19
6.0	-26.81	-19.13	-13.41	- 8.84	- 5.32	- 2.27	- 0.006	- 2.10
6.1	-28.10	-20.25	-14.35	- 9.59	- 5.86	- 2.56	- 0.03	- 1.23
6.2	-29.39	-21.38	-15.30	-10.35	- 6.43	- 2.90	- 0.13	- 0.59
6.3	-30.77	-22.59	-16.34	-11.22	- 7.10	- 3.37	- 0.38	- 0.23
6.4	-32.21	-23.87	-17.45	-12.16	- 7.86	- 3.94	- 0.74	- 0.09
6.5	-33.62	-25.13	-18.54	-13.08	- 8.62	- 4.51	- 1.13	- 0.03
6.6	-34.96	-26.34	-19.58	-13.96	- 9.33	- 5.05	- 1.48	- 0.01
6.7	-36.23	-27.49	-20.57	-14.78	- 9.99	- 5.54	- 1.80	- 0.007
6.8	-37.43	-28.60	-21.52	-15.56	-10.60	- 5.99	- 2.09	- 0.004
6.9		-29.67	-22.42	-16.31	-11.19	- 6.41	- 2.34	- 0.002
7.0		-30.70	-23.31	-17.03	-11.74	- 6.81	- 2.58	- 0.001

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Calculations of ionization equilibria are performed for oxygen. These include the processes of collisional ionization, radiative recombination, and dielectronic recombination. The effects of including dielectronic recombination in the calculations are discussed.		

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