# FORMATION OF SO, SO<sup>+</sup>, AND S<sub>2</sub> BY RADIATIVE ASSOCIATION

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#### **ABSTRACT**

Rate coefficients for radiative association of SO, SO<sup>+</sup>, and S<sub>2</sub> are estimated. For temperatures ranging from 300 to 14,000 K, the direct radiative association rate coefficients are found to vary with temperature from  $1.73 \times 10^{-19}$  to  $7.29 \times 10^{-19}$  cm<sup>3</sup> s<sup>-1</sup> and from  $1.49 \times 10^{-21}$  to  $3.70 \times 10^{-19}$  cm<sup>3</sup> s<sup>-1</sup> for S<sub>2</sub> and SO, respectively. The rate coefficients for formation through the inverse predissociation for S<sub>2</sub> are found to vary from  $3.59 \times 10^{-18}$  to  $1.44 \times 10^{-20}$  cm<sup>3</sup> s<sup>-1</sup>. For SO<sup>+</sup>, the direct rate coefficient varies rapidly with temperature from  $3.62 \times 10^{-27}$  cm<sup>3</sup> s<sup>-1</sup> at 2000 K to  $2.34 \times 10^{-20}$  cm<sup>3</sup> s<sup>-1</sup> at 14,000 K. The direct radiative association rate coefficients increase with the increase in temperature, but the inverse predissociation rate coefficients decrease with the increase in temperature.

Subject headings: astrochemistry — atomic data — atomic processes — ISM: molecules

## 1. INTRODUCTION

Sulfur monoxide, SO, has been detected in high-mass star formation (Goldsmith et al. 1987), translucent molecular clouds (Turner 1995), dark clouds (e.g., Ohishi et al. 1992), diffuse clouds (Lucas & Liszt 2002), and in supernova remnant IC 443G (e.g., Turner et al. 1992). The observed abundances of the SO molecule cannot be reproduced by any gas-phase ionmolecule chemistry in such sources (e.g., Turner et al. 1992; Turner 2000; Lucas & Liszt 2002). In addition, the SO molecule is known to be present in circumstellar envelopes (e.g., Omont et al. 1993), extragalactic sources (e.g., Johansson 1991), and comets (Woodney et al. 2000). Liu (1998) has modeled the sulfur chemistry in SN 1987A and has proposed the radiative association reaction,  $S + O \longrightarrow SO + h\nu$ , as an alternative source of the SO molecule in SN 1987A. There have been no calculations and no measurements of the radiative association of S and O atoms.

The sulfoxide ion,  $SO^+$ , has been detected in shocked interstellar object IC 443G (Turner 1992), interstellar clouds of varied morphological types (Turner 1994, 1996), and in comet Halley (Marconi et al. 1991). The formation of the  $SO^+$  ion in interstellar sources has been discussed (e.g., Turner et al. 1992; Turner 2000 and references therein) on the basis of ion-molecule reactions and dissociative shocks. Radiative association of the ground-state  $S^+(^2P)$  ion and  $O(^3P)$  atom may be a source of the  $SO^+$  ion in an astronomical source in which sulfur ions and oxygen atoms are available in the gas phase. The rate coefficients of the reaction  $S^+ + O \longrightarrow SO^+ + h\nu$  are not known.

The sulfur dimer,  $S_2$ , has been observed in the UV spectra of comet IRAS-Araki-Alcock (A'Hearn et al. 1983), comet Hyakutake (Budzien & Feldman 1992), and comet Lee (Feldman et al. 1999), but the origin of the  $S_2$  molecule in these comets is unclear. In addition, spectroscopic observation of Io's Pele Plume against Jupiter (Spencer et al. 2000) and of Jupiter after the collision of comet Shoemaker-Levy 9 (Noll et al. 1995) by the *Hubble Space Telescope* revealed absorption due to the  $S_2$  molecule. Unsuccessful attempts have been made in the search for this species by Liszt (1978) in several clouds, and he only tentatively detected a line in Sgr B2OH. The abundance in this source and the upper limits in the others were estimated to be roughly  $4 \times 10^{-7}$ . How-

ever, the  $S_2$  molecule has been included in the sulfur chemistry proposed for dense interstellar clouds (Mitchell 1984), circumstellar envelopes (Nejad & Millar 1988), and for hot cores (Charnley 1997). Radiative association of two ground-state sulfur atoms may be a source of the  $S_2$  species in astronomical environments.

Radiative association plays an important role in the formation of simple molecules found in supernovae (Liu 1998 and references therein) and in the early universe (Stancil & Dalgarno 1997; Babb & Kirby 1998; Bennett et al. 2003). In addition, this process has been included in the chemical models proposed for stellar atmospheres (e.g., Clegg et al. 1983; Glassgold & Mamon 1992), interstellar clouds (e.g., Bates & Herbst 1988), and fast neutral winds around protostars (Glassgold et al. 1991).

In this paper, we present theoretical estimates of the rate coefficients for radiative association of S and O atoms ( $k_{SO}$ ) to form the SO molecule, of the S<sup>+</sup> ion and O atom ( $k_{SO}$ <sup>+</sup>) to form the SO<sup>+</sup> ion, and between two S atoms ( $k_{S_2}$ ) to form the S<sub>2</sub> molecule for temperatures in the 300–14,000 K range.

## 2. METHOD OF CALCULATION

The radiative association rate coefficient k is defined as the formation rate of the AB molecule in the reaction  $A + B \longrightarrow AB + h\nu$  by the expression dn(AB)/dt = kn(A)n(B), where n is the number density of each species (A, B, and AB).

Radiative association processes can be divided into two classes: "direct radiative association" and "inverse predissociation" (preassociation; e.g., Babb & Dalgarno 1995). The direct radiative association is the process in which two particles approach along a particular potential in a particular state, which can emit a photon, leaving a molecule in a bound state. In this process, a semiclassical description of the nuclear motion is valid for collision of massive reactants or strong stabilizing transitions (Zygelman & Dalgarno 1988). A convenient method for estimating the rate coefficients has been proposed by Bates (1951). Here we follow the notation as given by Dalgarno et al. (1990), in which the rate coefficient for a Maxwellian velocity distribution is given by

$$k_d(T) = \left(\frac{8}{\mu\pi}\right)^{1/2} \left(\frac{1}{k_{\rm B}T}\right)^{3/2} I(T),$$
 (1)

where

$$I(T) = \int_0^\infty \sigma(E) \exp\left(-\frac{E}{k_{\rm B}T}\right) E dE, \qquad (2)$$

 $k_{\rm B}$  is the Boltzmann constant, and  $\sigma(E)$  is the collision cross section at an energy E of relative motion of two species, given by

$$\sigma(E) = 4\pi \frac{g_1}{g} \left(\frac{\mu}{2E}\right)^{1/2} \int_{r_c}^{\infty} J(r, E) A(r) dr.$$
 (3)

Here

$$J(r,E) = \int_0^\infty \frac{b \, db}{\sqrt{1 - V_{\Lambda'S}(r)/E - b^2/r^2}},\tag{4}$$

 $g_1$  is the statistical weight of the state through which the colliding particles unite, g is the statistical weight of the colliding pair,  $\mu$  is the reduced mass of the colliding particles in units of the electron's mass,  $r_c$  is the minimum distance of approach, b is the impact parameter,  $V_{\Lambda'S}$  is the molecular potential energy curve of the excited state through which two species approach each other, r is the internuclear distance, and A(r) is the probability of radiative transition from the initial state to a lower electronic state, given by

$$A(r) = 2.03 \times 10^{-6} \frac{2 - \delta_{0,\Lambda' + \Lambda''}}{2 - \delta_{0,\Lambda'}} \nu(r)^3 D(r)^2, \tag{5}$$

where  $\nu(r)$  is the transition frequency at r in cm<sup>-1</sup>, D(r) is the electric dipole transition moment of electronic transition (in a.u.), and  $\Lambda'$  and  $\Lambda''$  are the projection quantum numbers of the initial and final state, respectively.

The inverse predissociation involves a "crossing" or coupling of the incoming potential—through a spin interaction or through the action of the nuclear kinetic energy operator—with an intermediate bound state that radiates to a lower bound state. In this work, we follow the notation as given by Brzozowski et al. (1976), in which the rate coefficient is given by

$$k_p(T) = \hbar^3 \left(\frac{2\pi}{\mu k_{\rm B} T}\right)^{3/2} \frac{g_1}{g} \sum_{J,v'} (2J+1) \frac{\tau_{\rm rad}^J - \tau_{\rm exp}^J}{\left(\tau_{\rm rad}^J\right)^2} \exp\left(-\frac{E_{v'J}}{k_{\rm B} T}\right), \tag{6}$$

where  $\mu$  denotes the reduced mass,  $g_1$  is the statistical weight of the state through which the colliding particles unite, g is the statistical weight of the colliding pair,  $E_{v'J}$  is the energy of the level v'J above the dissociation limit, J is the rotational quantum number,  $\tau_{\rm rad}^{J}$  is the radiative lifetime, and  $\tau_{\rm exp}^{J}$  is the experimental measured (total) lifetime.

#### 3. RADIATIVE ASSOCIATION

## 3.1. Sulfur Monoxide (SO)

Direct radiative association of S( $^3P$ ) and O( $^3P$ ) atoms, both in their ground state, can occur through the approach along the A  $^3\Pi$  state, which radiates to the ground X  $^3\Sigma^-$  state of the SO molecule in a time less than 35.6  $\mu$ s from v'=0. The statistical weight factor is  $g_1/g=6/81$ .

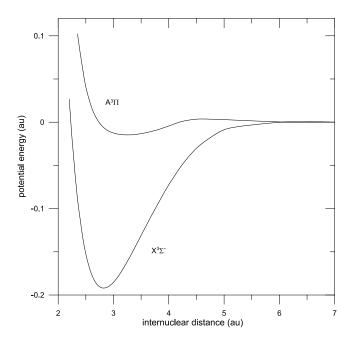


Fig. 1.—The  $X^3\Sigma^-$  and  $A^3\Pi$  potentials of the SO molecule.

The potential energy curves of the  $X^3\Sigma^-$  and  $A^3\Pi$  electronic states calculated by Borin & Ornellas (2000) using the internally contracted multireference configuration-interaction (ICMRCI) method were adopted for  $r>2.2a_0$  (Fig. 1). The short-range form  $V(r)=a\exp(-br)+c$  was fitted smoothly to the ab initio potentials (Dalgarno et al. 1996), where a,b, and c are, respectively,  $2.9483\times 10^4$ , 5.37391, and -0.6551 for the  $A^3\Pi$  state and  $2.4708\times 10^5$ , 6.32717, and -0.8285 for the  $X^3\Sigma^-$  state. The variation of electronic moments with internuclear distance for the A-X transition are from Borin & Ornellas (2000) for  $1.2 \le r \le 2.6$  Å. For r<1.2 Å, the transition moments are fitted to the form  $D(r)=ar+br^2$  (Dalgarno et al. 1996), where a and b are 0.37794 and -0.13303, respectively. At long range, the function  $D(r)=c\exp(-dr)$  is utilized (Stancil & Dalgarno 1997), where c and d are  $-1.37766\times 10^6$  and 3.964833, respectively (values in a u)

The rate coefficients for approach along the excited  $A^3\Pi$  state are displayed in Table 1 for temperatures in the range 300–14,000 K. The rate coefficients increase with temperature and are fitted to the form

$$k_{\rm SO} = \alpha \left(\frac{T}{300}\right)^{\beta} \exp\left(-\frac{\gamma}{T}\right) \, \mathrm{cm}^3 \, \mathrm{s}^{-1},$$
 (7)

where,  $\alpha$ ,  $\beta$ , and  $\gamma$  are, respectively,  $1.114 \times 10^{-19}$ , 0.2761, and 1297.9 for  $300 \le T \le 2000$  K and  $3.113 \times 10^{-20}$ , 0.6454, and 18.728 for T > 2000 K.

The theoretical  $A^{3}\Pi$  potential energy curve exhibits a repulsive hump at a nuclear separation of approximately  $4.5a_{0}$ , and for nuclear separations less than  $4.5a_{0}$  it contains an attractive well with a depth of  $\simeq 0.5$  eV. Because of the barrier, the rate coefficient drops rapidly at low temperatures.

Martin (1932) reported an abrupt termination of the  $B^3\Sigma^ X^3\Sigma^-$  bands of the SO molecule related to the vibrational states v'=0,1,2, and 3 at the rotational levels n'=66,53,39, and 6, respectively, which was attributed to a predissociation. However, there are insufficient data to determine reliably the preassociation rate coefficient for the SO molecule. Thus, we are

 $\label{table 1}$  Radiative Association Rate Coefficients of S=O, S^+=O, and S=S

Т (К)	S-O $(d)$ $(10^{-20} \text{ cm}^3 \text{ s}^{-1})$	$S^{+}$ -O (d) (cm <sup>3</sup> s <sup>-1</sup> )	S-S(d) ( $10^{-19} \text{ cm}^3 \text{ s}^{-1}$ )	S-S (p) (cm <sup>3</sup> s <sup>-1</sup> )
300	0.15		1.73	3.59E-18
700	2.20		2.12	1.15E-18
1100	4.90		2.36	6.11E-19
1500	7.32		2.53	3.91E-19
2000	9.84	3.62E - 27	2.71	2.58E-19
2500	11.94	3.23E-25	2.86	1.86E-19
3000	13.74	3.04E - 24	2.99	1.42E-19
4000	16.79	4.08E - 23	3.26	9.30E-20
5000	19.41	1.98E-22	3.52	6.68E - 20
6500	22.87	9.14E - 22	3.96	4.52E-20
8500	26.99	3.40E - 21	4.64	3.03E - 20
10500	30.81	8.27E - 21	5.46	2.21E-20
12500	34.39	1.59E - 20	6.44	1.71E-20
14000	36.97	2.34E-20	7.29	1.44E-20

Notes.—The missing values for S<sup>+</sup>-O denote rate coefficients less than  $2 \times 10^{-27}$  cm<sup>3</sup> s<sup>-1</sup>. (d) Direct association. (p) Preassociation.

not assured that preassociation is negligible (e.g., Borin & Ornellas 1999; Archer et al. 2000).

A comparison of direct radiative association rate coefficients of the SO molecule (this work) with those of SiO (Andreazza et al. 1995) shows that  $k_{\rm SiO}$  is 3 orders of magnitude larger than  $k_{\rm SO}$  at 2000 K. In contrast to the SiO molecule, the direct radiative association of the S and O atoms through the  $A^3\Pi$  state is a relatively unimportant source of the SO molecule in Type II supernovae (SN 1987A) and in other dust-poor astrophysical environments.

## 3.2. Sulfoxide Ion (SO<sup>+</sup>)

Direct radiative association of the sulfur ion  $S^+(^4S)$  and oxygen atom  $O(^3P)$  will occur preferentially through the approach in the repulsive  $1\ ^4\Sigma^+$  state, which irradiates to the  $a\ ^4\Pi$  state. The statistical weight factor is  $g_1/g=4/36$ . The approach along the  $^2\Sigma^+$  potential energy curve is inhibited by a large potential barrier at  $r\simeq 2.25\ \text{Å}$  (Cossart et al. 1983).

The potential energy curves of the 1  $^4\Sigma^+$  and a  $^4\Pi$  states calculated by Ornellas & Borin (1998) by means of the ICMRCI method are used for  $r>2.2a_0$  (Fig. 2). For  $r<2.2a_0$  we used the short-range forms  $V(r)=70.26\exp{(-2.24593r)}-2.291026$  and  $V(r)=1428.2\exp{(-3.751263r)}-2.36052$  for the 1  $^4\Sigma^+$  and a  $^4\Pi$  states, respectively. The transition dipole moments for the system 1  $^4\Sigma^+-a$   $^4\Pi$  are from Ornellas & Borin (1998) for  $r>2.2a_0$ . At short range, we used the function  $D(r)=0.219987r-0.074544r^2$ .

The resulting rate coefficient for approach along the  $1~^4\Sigma^+$  state is listed in Table 1 for temperatures up to 2000 K. Because the transition dipole moment is not large ( $\simeq 0.01~\text{a.u.}$ ) at  $3.25a_0$  and increases linearly up to about 0.12 a.u. as the distances gets shorter, and the potential energy curve of the  $1~^4\Sigma^+$  state is repulsive at nuclear separations inside  $5.0a_0$  (e.g., Ornellas & Borin 1998), the rate coefficient is very small. It varies rapidly with temperature from  $3.62 \times 10^{-27}~\text{cm}^3~\text{s}^{-1}$  at 2000 K to  $2.34 \times 10^{-20}~\text{cm}^3~\text{s}^{-1}$  at 14,000 K.

The direct radiative association of the  $S^+$  ion and O atom through the 1  $^4\Sigma^+$  state is an unimportant source of  $SO^+$  in Type II supernovae and other astronomical objects.

The photofragment spectroscopy of the SO<sup>+</sup> ion in Cosby (1984) indicates that the vibrational levels (v' = 7–12) of the  $b^4\Sigma^-$  state are predissociated. He proposes that a spin-orbit coupling between the  $b^4\Sigma^-$  and repulsive  $I^4\Sigma^+$  states leads to the

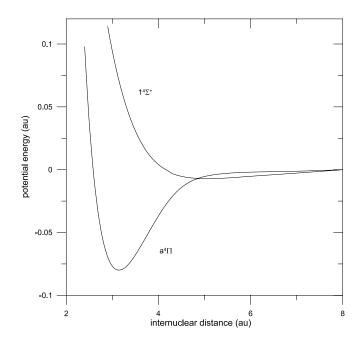


Fig. 2.—The a  $^4\Pi$  and 1  $^4\Sigma^+$  potentials of the SO $^+$  ion.

predissociation. However, as pointed out by Ornellas & Borin (1998), according to Figure 3 of Cosby's study, these two states cross near v'=12, and an effective coupling would be expected to occur only for v'=12. For the other vibrational levels, this effect would be practically negligible. In this sense, a definite understanding of these processes has not yet been achieved. However, a preassociation rate coefficient larger than the direct radiative association rate coefficient is expected for the  $\mathrm{SO}^+$  ion.

## 3.3. Sulfur Dimers (S<sub>2</sub>)

Direct radiative association of two sulfur atoms, both in their ground states, is possible through the  $B''^{3}\Pi$  state followed by radiative decay to the ground  $X^{3}\Sigma_{g}^{-}$  state at a time of the order of 25.5  $\mu$ s from v'=0. The statistical weight factor is  $g_{1}/g=6/81$ .

The ab initio potential energy curves for the B''  $^3\Pi$  and  $X^3\Sigma_g^-$  states have been calculated by Pradhan & Partridge (1996) by means of the ICMRCI approach. To improve the quality of B''  $^3\Pi$  and  $X^3\Sigma_g^-$  potentials for large r, we used the Hulbert & Hirschfelder (1941) function. For the  $X^3\Sigma_g^-$  state, the relevant molecular constants are extracted from Huber & Herzberg (1979), and those for the B''  $^3\Pi$  state are taken from ab initio calculations of Pradhan & Partridge (1996; Fig. 3). These potentials are in good agreement with ICMRCI curves (Pradhan & Partridge 1996). The transition dipole moments for the B''-X system calculated by Pradhan & Partridge (1996) were adopted for  $2.9a_0 \le r \le 7.0a_0$ . For  $r < 2.9a_0$ , the short-range form  $D(r) = 0.597309r - 0.167199r^2$  was used, and for  $r > 7.0a_0$ , the function  $D(r) = 1.379819 \exp{(-0.628119r)}$  was used.

The direct radiative association rate coefficients through the  $B''\,^3\Pi$  state for the  $S_2$  molecule at temperatures ranging from 300 to 14,000 K are listed in Table 1. The rate coefficients increase with an increase of the temperature and are fitted to relation (7), where  $\alpha$ ,  $\beta$ , and  $\gamma$  are  $1.374\times 10^{-19},\,0.3339,\, and <math display="inline">-78.801$  for  $300\leq T\leq 7100$  K and  $2.233\times 10^{-20},\,0.8957,\, and <math display="inline">-306.69$  for T>7100 K, respectively.

In addition to the direct radiative association, inverse predissociation might occur following approach along the  $1\,{}^{1}\Pi_{u}$  state of  $S_{2}$ , which crosses the excited  $B\,{}^{2}\Sigma_{u}^{-}$  state. The former state undergoes inverse predissociation into vibrational levels of the

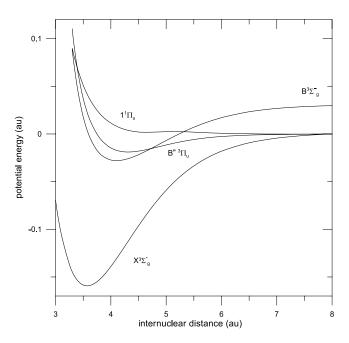


Fig. 3.—The  $X^{3}\Sigma_{a}^{-}$ ,  $B''^{3}\Pi_{u}$ ,  $B^{3}\Sigma_{a}^{-}$ , and  $1^{1}\Pi_{u}$  potentials of the S<sub>2</sub> molecule.

latter—caused by spin-forbidden interactions—which radiates

to the ground  $X^{3}\Sigma_{g}^{-}$  state and forms the S<sub>2</sub> molecule. The onset of predissociation of the  $B^{3}\Sigma_{u}^{-}$  state is very sudden. The break off in emission occurs around J = 0 for v = 10and at higher *J* for v = 8-9 levels.

Emission from lower J(J < 10) for v = 10, from J = 36, 37, and 38 for v = 9, as well as from J = 59, 60, and 62 for v = 8has been studied (Green & Western 1997; Quick & Weston 1981), and the lifetime was less than 3 ns, compared to a lifetime of 32 ns for lower, nonpredissociated levels (Quick & Weston 1981; Matsumi et al. 1985).

In order to evaluate the preassociation rate coefficient for energy levels above the dissociation limit (v = 0, J < 10; v = 9, J = 38; v = 8, J = 59, 60, and 62), we take the experimentally measured (total) lifetimes of the predissociation levels (3 ns) from Quick & Weston (1981) as well as the lifetime for lower, nonpredissociated levels. The latter constitutes the radiative lifetime (32 ns). The energy levels are calculated using the molecular constant extracted from Huber & Herzberg (1979) and the dissociation energy ( $D_e$ ), taken as 35,999 cm<sup>-1</sup> (Ricks & Barrow 1969).

The preassociation rate coefficients are listed in Table 1. They can be represented by formula (7), where  $\alpha = 4.492 \times 10^{-18}$ ,  $\beta =$ -1.4896, and  $\gamma = 67.166$ . These rate coefficients decrease with an increase in temperature, and for lower temperatures they are larger than those for direct radiative association. However, these rate coefficients are a lower limit, since  $\tau_{exp}$  < 3 ns. Uncertainties in  $\tau_{\rm rad}$ ,  $\tau_{\rm exp}$ , and  $E_{NJ}$  (from the uncertainty in  $D_e$ ) make the value of  $k_p$  very uncertain.

At 298 K, the preassociation rate coefficient associated with the lower rotational levels of the  $B^{3}\Sigma_{u}^{-}$ , v=10 level was experimentally deduced by Fair & Thrush (1969) to be  $8.3 \times 10^{-19}$  cm<sup>3</sup>  $s^{-1}$ . For this level and for the same temperature, we obtain a lower limit of  $5.9 \times 10^{-19}$  cm<sup>3</sup> s<sup>-1</sup>, which is consistent with laboratory measurements.

A direct comparison of the rate coefficients of the SO molecule with those of the  $S_2$  molecule shows that S + O reaction is slower than that of S + S. At 2000 K the rate coefficient of the SO molecule is approximately 5.4 times smaller than that of the corresponding of the S2 molecule. Small amounts of S2 molecules can be formed by radiative association in Type II supernovae and other hostile environments.

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