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Molecular Column Densities In Selected Model Atmospheres*

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ABSTRACT

Molecular column densities are presented for 35 molecules in a variety of cool stellar model atmospheres. From an examination of the predicted column densities, we draw the following conclusions. 1) SiO ought to be visible in carbon stars which have been generated from triple-α burning, but will be absent from carbon stars generated from the CNO bi-cycle. 2) The variation in the observed relative strengths of TiO and ZrO is indicative of real differences in the ratio Ti/Zr. 3) The TiO/ZrO ratio shows a small variation as C/O is changed and as the effective temperature is changed. 4) The column density of silicon dicarbide (SiC_2) is sensitive to abundance, temperature, and gravity; hence all relationships between the strength of SiC_2 and other stellar parameters will show appreciable scatter. There is, however, a substantial luminosity effect present in the SiC_2 column densities. 5) Unexpectedly, SiC_2 is anti-correlated with C_2. 6) The presence of SiC_2 in a carbon star allows us to eliminate the possibility that these stars are both "hot" ($T_{eff} \geq 3000$ K) and have been produced through the CNO bi-cycle (so that C/H < solar).

I. INTRODUCTION

Molecules become more and more abundant in stellar atmospheres with decreasing temperature until they become sources both of the principal spectral features and the opacity. Molecules are particularly important in the red giant stars, in which knowledge of such physical parameters as the temperature-density structure and chemical composition is crucial to our understanding of stellar evolution. Any unravelling of the mysteries of these cool stars must therefore depend on an understanding of molecular formation and opacity.

Only in the last few years have model atmospheres for cool stars become available, and even these have been calculated under rather severe approximations. Recent reviews of the state of calculations for cool star atmospheres have been given by Fujita (1970), Vardya (1970) and Johnson (1972). In the present paper we present sets of molecular column densities predicted by theoretical atmospheric models.

We are especially concerned with the abundances of C, N and O, whose atoms are largely locked up in molecules whose bands usually can be observed. The ideal method for an abundance study is the use of synthetic spectra along with good model atmospheres to compare with the results of high dispersion observations. Since many of the most interesting red giant stars are very faint, such high dispersion observations are difficult to obtain. Photometric indices are, however, available for such molecules as CO, C_2, TiO, and CN for a wide variety of cool stars. It would be therefore very interesting, both as a check upon the model atmospheres and as a clue to the chemical composition of the stars, to try to compare the predictions of molecular column densities from the theoretical atmospheres with the interrelation among the band strengths observed in real stars.

Molecular number densities for cool star atmospheres have been given for various molecules by a number of workers, including Dolan (1965), Vardya (1966), Morris and Wyller (1967) and Scalo (1974). Of more direct relevance to our work is the previous study by Goon and Auman (1970) in which molecular column densities were computed for a number of molecules in stellar model atmospheres of various effective temperatures and surface gravities, and essentially solar composition. In a way, the present work can be regarded as an extension of their work to stars whose compositions differ significantly from that of the sun. In particular, we give column densities for a wide variety of molecules for stars which are both carbon deficient and carbon rich.

II. PROCEDURE

Over the past few years a large number of model atmospheres have been computed, and many have already been published (Johnson, 1974). These atmospheres were computed under the usual assumptions of hydrostatic equilibrium, and energy flux conservation (including transport both by radiation and convection). The geometry was that of a plane-parallel semi-infinite atmosphere.

Opacities included in these atmospheres were H, H^-, H_2, H_2^-, Rayleigh scattering from H and H_2, molecular opacities from H_2O, CO (the fundamental and first three overtone vibration-rotation bands), and CN (the red system). The molecular opacities were added as straight mean opacities. (All these opacities together are often designated "standard opacities" and abbreviated SO). Opacity contributions of the polyatomic molecules and free radicals NH_2, CH_2, SiC_2, HCN, and HCO in the approximations of Main and Bauer (1967) were

added in some models (designated P in the opacity column). A few models (T) included also the opacity of CH, NH, OH, and C_2 in the same approximation.

A mean opacity due to atomic lines was also included using the method and solar statistics of Mutschlecner and Keller (1970, 1972), called simply MK hereafter. In order to avoid overblanketing, most models were run with scaled amounts of MK opacity, either: (1) MK II, which has MK opacity at all wavelengths except for $\lambda = 1\mu m$, where we use 0.1 MK; or (2) MKC, which has 0.5 MK at all wavelengths except that all atomic line blanketing is neglected for $\lambda = 1\mu m$.

The atmospheres were calculated by a version of the ATLAS code, which has been used extensively in model atmosphere calculations. Since this code is already well documented in the literature (Kurucz, 1970) and our modifications to it have also been described (Johnson, 1974), we shall discuss only one aspect of the calculations in the present paper.

The molecular associative equilibrium equations were solved by a subroutine (STATEH) written by Beebe (1972). For these calculations, the equation of state routine normally included the 21 diatomic molecules of H, C, N, O, Si, and S; the additional diatomic molecules MgH, MgN, MgO, TiO, ZrH, ZrC, ZrO; and the 25 polyatomic molecules and radicals H_2O, HCN, HCO, HNO, NH_2, NH_3, CH_2, CH_3, CH_4, C_4, C_3, C_2N_2, CH_2O, CHNO, HCN, NCO, C_2H, C_2N, N_2H, NCN, N_3, C_2H_2, SiC_2, TiO_2, and ZrO_2. Ionization equilibrium was calculated by solving the equations for the neutral atom and first ion of the elements H, He, C, N, O, Na, Mg, Al, Si, S, K, Ca, and Fe.

Parameters of a number of selected model atmospheres are summarized in table 1, where the columns show, in order: model number, effective temperature, logarithm of the surface gravity, chemical composition, opacities, and an

identifying computer sequence number. In the chemical composition column, L refers to solar composition (Lambert, 1968, and his collaborators).

Cool star atmospheres are complex structures, and the assumptions on which these model atmospheres are based may not always be met. Convection, atmospheric inhomogeneities, gas flows, mechanical heating, departures from local thermodynamic equilibrium, opacity sources, grain formation, and extended atmospheres are all problems yet to be properly treated. Perhaps the largest failure of the present set of model atmospheres is in the treatment of atomic and molecular line blanketing. Solar line blanketing (or some fraction thereof) is used for all stars in the absence of observational data. Mean molecular opacities were used for simplicity; better approximations are slowly becoming available (Carbon, 1974; Querci, Querci, and Tsuji, 1974). The present models are therefore clearly to be regarded as an exploratory venture. They form a uniform set which should be of considerable use for various studies of cool stars.

III. RESULTS AND DISCUSSION

Table 2 contains the column densities for a selected number of molecules in our model atmospheres. We define the column density as

$$X \equiv \log N = \log \int_0^{\tau_\nu = 0.3} n(x)\, dx \qquad (1)$$

where $n(x)$ is the number density of a given molecule at depth x. For many models from an extensive set, column densities for 35 molecules are given.

We tabulate for all molecules the column densities at a wavelength of 1 micron so that the column densities for different molecules may be intercompared. For empirically determining the column density of a particular

molecule however, one measures molecular band depressions, so that it is important to tabulate each column density at the wavelengths that the particular molecule has substantial absorption features. Since the absorption coefficient is a function of wavelength, the depth (on a physical scale) at which $\tau_\nu = 0.3$ occurs must also depend on wavelength. We therefore tabulate the column densities (down to $\tau_\nu = 0.3$) for each molecule at a few appropriate frequencies.

The choice of the exact depth to which the integration (1) is to be taken is of course somewhat arbitrary. One is interested in the number of molecules "above the photosphere"; that is, above the range where most of the photospheric radiation arises. We have chosen the value $\tau_\nu = 0.3$ largely to conform with the results of Goon and Auman (1970). Several tests show however, that were we to continue the integration down to $\tau_\nu = 0.5$, the column density would most generally be raised about 0.2 in the logarithm, and the results would not strongly vary from molecule to molecule or model to model.

A thorough analysis of the large amount of data in table 2 is beyond the scope of this paper. We limit ourselves here to a discussion of some of the obvious trends in column densities of a few chosen model atmospheres.

As has already been noted (Alexander and Johnson 1972), our column densities agree almost exactly with those of Goon and Auman (1970) for similar models. However, the addition of opacities not used by previous workers to our models (CO, CN, polyatomic molecules, and atomic lines) alters the atmospheric structure and resultant column densities substantially. Such effects have been described as part of an attempt to use these column densities to deduce the C, N, and O abundances in Betelgeuse (Faÿ and Johnson, 1973).

Earlier we also considered the column densities for CO, CN and CH as a function of the column density of C_2 for a series of carbon star atmospheres

with the same effective temperature but increasing carbon overabundance (Fay, Warren, Johnson, and Honeycutt, 1974). It was there shown that column densities of CN increased in strength as C_2 increased, but CO was expected to decrease in strength. These relationships all held whether the carbon stars were carbon rich (C/H > solar) or carbon poor (C/H < solar). Interestingly, these interrelations for molecular column densities show exactly the same trend as observations of the band strengths of these same molecules.

Let us now consider tests provided by molecular bands for the different evolutionary models for carbon stars. Cosmically, of course, oxygen is more abundant than carbon, so that it is necessary to devise a scheme to increase the ratio C/O in stellar interiors. Two processes are envisioned for accomplishing this end. If stellar material is processed through the complete CNO bi-cycle, C/H decreases, but O/H drops even more, so that the ratio C/O rises from the original value of 0.6 to something in the range 2-5. On the other hand, carbon can be created through the triple-α process, increasing C/H while leaving O/H essentially unchanged. Either of these mechanisms will produce a carbon mixture in the interior of a star, and that material can be brought to the surface either by mixing or stripping the outer layers. The two carbon production mechanisms lead to basically different abundance mixtures. A carbon star generated from the CNO bi-cycle will be carbon-poor (C/H < solar) and one generated from the triple-α process will be carbon-rich (C/H > solar). We note that the number of oxygen-containing molecules will be radically different in the two cases. Most of the oxygen is locked up in CO anyway, and the rest is O I. In carbon-rich carbon stars, where the O/H ratio is still equal to the solar value, much more oxygen is available for the formation of oxygen containing molecules than in carbon-poor carbon stars, which are very deficient in oxygen.

We therefore consider briefly whether there are any oxygen-containing molecules whose presence or absence might help distinguish between the two mechanisms for forming carbon stars. The absorption coefficient for a strong line of TiO is about 10^{-16}, so that we require about 10^{16} molecules of TiO in the line of sight in order to produce an observable spectrum feature. We expect similar numbers to hold for ZrO. A perusal of column densities in table 2 indicates that while TiO and perhaps ZrO (even with solar abundances) are observable in S stars ($C/O \simeq 1.0$), the detection of either of these molecules in any carbon star would seem to require an enhancement in the abundance of the metallic element. It is possible that in hotter, very carbon-rich stars one might see TiO, but it is not expected to appear in a sufficiently wide variety of stars to be of any value. The molecule MgO also appears in too low a concentration in the carbon stars to be of help here. The molecule NO, whose strongest bands lie at 6 microns, might be helpful, but the situation here is more complicated, since N itself may be produced by the CNO bi-cycle. The only truly promising candidate for this type of study appears to be SiO. Unfortunately the first overtone vibration rotation bands of SiO fall at about 4 microns, where observations are difficult. This is, however, an otherwise excellent candidate. As table 2 shows, in the range 3000-3500 K, there is sufficient oxygen to produce a column density of SiO large enough to make an observable spectral feature for carbon-rich carbon stars, while in carbon-poor carbon stars there is usually insufficient SiO to produce an observable feature. We would argue strongly that the detection of SiO at 4 microns in a carbon star implies that the star in question is carbon-rich. We therefore urge that this key observation be undertaken in as many carbon stars as possible.

Next, let us look at the behavior of TiO and ZrO more closely. Both of these oxides are essentially unchanged by changes in the ratio C/O as long as

that ratio is less than 0.6. As C/O rises beyone 0.6 (the solar value), the column densities of the oxides drop rapidly. Apparently then, the oxide concentration is controlled by the concentration of the metal, and not by the excess oxygen until C/O gets very close to 1.0. This conclusion holds for all values of the ratio C/H from 10^{-2} to 10 times the solar value. We note that the behavior of titanium and zirconium oxides are remarkably similar.

Although the results for 3000 K are not nearly as complete in our grid as those for 3500 K, the models do indicate that the behavior ot TiO and ZrO is probably qualitatively similar to their behavior at 3500 K. Also the column densities of TiO and ZrO show little sensitivity to the values of surface gravity for temperatures $T \leq 3500$ K. The column densities for dwarfs are, however, slightly less, in agreement with observations. For $T \leq 4000$ K, there is some sensitivity to the surface gravity in the sense that the column density of the oxide increases as log g increases.

The earlier observations of Keenan (1954) are very interesting at this point. These show that for any given TiO strength one finds stars with a <u>wide</u> variety of ZrO strengths. On the basis of our atmospheres and column densities, this <u>large</u> observational difference can only be interpreted in terms of real abundance differences of Zr among these stars since the behaviors of TiO and ZrO are otherwise so similar.

Small differences between theoretical column densities of ZrO and TiO can arise from differences in structure. Consider models N10 through N15 with the parameters (3000/0.0/[L except C/H]/S0,T,MKC), where C/H is changed such that the ratio C/O varies from 1.0 to 5.0. While the strengths of both molecules fall as C/O is increased, the ZrO strengths fall slightly faster than those of TiO. We therefore predict a slight enhancement of ZrO relative to TiO as one moves from the carbon stars back through the CS to the S stars, even for a fixed Zr/Ti ratio. Second, compare the Zr/Ti ratio in two models with C/O = 1.05 (which might be CS stars or weak C stars), one with an effective

temperature of 3000 K and the other with 3500 K. For the 3000 K model, the difference in the column densities of TiO and ZrO (at 8000 Å) is a factor of 5, while it is a whole order of magnitude for the 3500 K model. In other words, as one goes to cooler temperatures there is a systematic enhancement of ZrO relative to TiO. This effect is of course well known in certain variable S stars where the ratio TiO/ZrO is a function of phase (Keenan, 1954), assumed to arise because of the slightly greater dissociation energy of TiO. Our results are in accord with that conclusion.

Since CN is a well known indicator of luminosity among G, K and M stars, it is worthwhile to look for a similar effect in the column densities. The observed effect, which is well studied in the violet system of CN (Keenan, 1941) and may hold for the red system as well (Wing and Warner 1966), is such that CN strength increases as luminosity increases. Although our temperature grid is quite coarse and we have not included the violet CN bands, we may still examine the CN bands at 0.74 μm. There, we see no significant luminosity effect at 3000 K or 5000 K. At 4000 K there is a substantial effect in that the column density of CN increases by a factor of 25 as log g decreases from 4.0 (model J4) to 0.0 (J6), in nice accord with observations. No such effect is observed or expected in carbon stars because CN also depends strongly on chemical composition, which likely varies from star to star.

Let us finally look at the predictions for the interesting triatomic molecule SiC_2. Examination of the column density of this molecule in a wide variety of cool stars allows us to conclude that SiC_2 is generally favored by cool temperatures, high ratios of C/O, high ratios of C/H, and large values of surface gravity. We make the following particular comments about the column densities. (1) Because of the special conditions required for the formation of the molecule, we expect that it will not be seen in most

carbon stars and not at all in M or S stars. (2) The molecule is of great interest because its abundance is sensitive to both temperature and surface gravity (as well as to chemical composition). We therefore expect that all relations between Merrill-Sanford bands (attributed to SiC_2) and other parameters of carbon stars (strengths of other molecular features, colors, temperatures, or luminosities) will contain a fair amount of scatter. The several parameters which control the strength of SiC_2 cannot be observationally determined without much difficulty. (3) Because of the strong dependence of SiC_2 on log g, we predict a substantial luminosity effect to be seen in the Merrill-Sanford bands. We note that as log g is increased from 0.0 to 3.0, the column density of SiC_2 rises from 10^{14} to 10^{17}. The lower of these values is insufficient to produce a spectral feature, while the higher is sufficient to produce a strong feature. Such a luminosity effect in carbon stars has already been reported (Peery, 1973). (4) The most striking and surprising result is the anti-correlation of SiC_2 with C_2, as seen from the carbon star models N10 through N15. As C/O or C/H is increased beyond the solar value, the column density of C_2 rises dramatically, as expected, while the column density of SiC_2 drops strongly. This is a totally unexpected result and not at all in accord with our intuitive feelings that SiC_2 must rise as carbon is increased. The result is also different from that predicted by applying the equations of molecular associative equilibrium to a slab of constant temperature and density (Fujita, 1970 and references contained therein). This effect clearly warrants additional investigation and will be treated separately in a subsequent paper.

The effective temperature of the N irregular variables is at present poorly known. Angular diameter measurements of two of these have provided the following effective temperatures: 3140 K for 19 Psc (Lasker, Bracker and

Kunkel, 1973) and 2580 K for X Cnc (Bartholdi, Evans, Mitchell, Silverberg, Wells and Wiant, 1972). Spectral scans, however, show that the emergent flux curves of both of these stars are very similar, and it is therefore difficult to imagine that their effective temperatures can differ by 600 K. Our models allow us to make one firm statement. If the effective temperature of the N irregular stars are as high as 3000 K, the column density of SiC_2 is too low to produce the observed spectral features for a carbon-poor carbon star. We are thus able to eliminate the alternative that the N stars are both "hot" (effective temperature $\geq$ 3000 K) and that the surface material was produced by processing through the CNO b-cycle. At the moment, however, we are not able to distinguish between the other three logical alternatives of carbon-poor and "cool" ($T_{eff} < 3000$ K), carbon-rich and "cool", and carbon-rich and "hot".

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TABLE 1

CHARACTERISTICS OF SELECTED MODEL ATMOSPHERES

Model No.	T_{eff} (K)	Log g	Chemical Composition	Opacities	Seq.No.
J1	5000	4.0	L	SO,P,MK II	214052
J2	5000	2.0	L	SO,P,MK II	213160
J3	5000	0.0	L	SO,P,MK II	745457
J4	4000	4.0	L	SO,P,MK II	214091
J5	4000	2.0	L	SO,P,MK II	214101R
J6	4000	0.0	L	SO,P,MK II	214106
J7	4000	-2.0	L	SO,P,MK II	214871
J8	3500	4.0	L	SO,P,MK II	215776
J9	3000	2.0	L	SO,P,MK II	214879
J10	3000	0.0	L	SO,P,MK II	V0112
J13	3500	0.0	C/H=3.55E-5, N/H=4.04E-4 O/H=5.89E-4, C/O=0.060	SO,P,MK II	745456
J14	3000	0.0	C/H=3.55E-5, N/H=4.04E-4 O/H=5.89E-4, C/O=0.060	SO,P,MK II	214050
J15	3000	-2.0	C/H=3.55E-5, N/H=4.04E-4 O/H=5.89E-4, C/O=0.060	SO,P,MK II	214053
J16	3500	0.0	C/H=3.55E-5, N/H=9.57E-4 O/H=3.55E-5, C/O=1.00	SO,P,MK II	215450R
J17	3000	0.0	C/H=3.55E-5, N/H=9.57E-4 O/H=3.55E-5, C/O=1.00	SO,P,MK II	215462
J18	3500	0.0	C/H=3.55E-5, N/H=9.57E-4 O/H=3.55E-5, C/O=1.00	SO,P,MKC	671223R
J19	3500	2.0	C/H=3.55E-5, N/H=9.86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	214072R
J20	3500	0.0	C/H=3.55E-5, N/H=9.86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	214051R

TABLE 1 (continued)

Model No.	Teff (K)	Log g	Chemical Composition	Opacities	Seq.No.
J21	3000	2.0	C/H=3.55E-5, N/H=9.86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	214102R
J22	3000	0.0	C/H=3.55E-5, N/H=9.86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	214107R
J23	2500	0.0	C/H=3.55E-5, N/H=9.86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	V0508
J24	2000	0.0	C/H=3.55E-5, N/H=9,86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	V0510
J30	3000	1.0	L*	SO,P,MK	156121
J31	2800	1.0	L*	SO,P,MK	156139
J32	2500	1.0	L*	SO,P,MK	167390
J35	2300	1.0	L*	SO,P,MK	156719
K1	3500	0.0	L	SO,P,MKC	V1526R
K3	3500	0.0	C/H=3.55E-5, N/H=4.04E-4 O/H=5.89E-4, C/O=0.06	SO,P,MKC	213344
K4	3500	0.0	C/H=3.55E-6, N/H=4.04E-4 O/H=5.89E-4, C/O=0.006	SO,P,MKC	213376
K9	3500	0.0	C/H=3.55E-5, N/H=9.57E-4 O/H=3.55E-5, C/O=1.00	SO,P,MKC	213012
K12	3500	0.0	C/H=3.55E-5, N/H=9.75E-4 O/H=1.78E-5, C/O=2.00	SO,P,MKC	213041
K15	3500	0.0	C/H=3.55E-4, N/H=4.96E-4 O/H=1.78E-4, C/O=2.00	SO,P,MKC	670638
K16	3500	0.0	C/H=7.10E-4, N/H=9.92E-4 O/H=3.55E-4, C/O=2.00	SO,P,MKC	670646
K18	3500	0.0	C/H=3.55E-3, N/H=4.96E-3 O/H=1.78E-3, C/O=2.00	SO,P,MKC	157903
K20	3500	0.0	C/H=3.55E-3, N/H=1.00E-2 O/H=1.78E-3, C/O=2.00	SO,P,MKC	159379R
K23	3500	0.0	C/H=3.55E-4, N/H=8.15E-4 O/H=7.10E-5, C/O=5.00	SO,P,MKC	213112

TABLE 1 (continued)

Model No.	T_{eff} (K)	Log g	Chemical Composition	Opacities	Seq.No.
K24	3500	0.0	C/H=3.55E-3, N/H=8.15E-4 O/H=7.10E-4, C/O=5.00	SO,P,MKC	213173
K26	3500	0.0	C/H=3.55E-2, N/H=8.15E-4 O/H=7.10E-4, C/O=50.0	SO,P,MKC	213381
**K27	3500	0.0	C/H=3.55E-2, N/H=8.15E-4 O/H=7.10E-4, C/O=50.0	SO,P,MKC	215725
K28	3500	4.0	C/H=3.55E-5, N/H=9.86E-4 O/H=7.10E-6, C/O=5.00	SO,P,MK II	214092
N12	3000	0.0	C/H=7.10E-4, C/O=1.20†	SO,T,MKC	V0528
N4	3000	2.0	C/H=7.10E-4, C/O=1.20	SO,T,MKC	V0541
N10	3000	0.0	C/H=2.95E-3, C/O=5.00	SO,T,MKC	V0524
N11	3000	0.0	C/H=1.18E-3, C/O=2.00	SO,T,MKC	V0525
N13	3000	0.0	C/H=6.18E-4, C/O=1.05	SO,T,MKC	04121
N14	3000	0.0	C/H=5.95E-4, C/O=1.01	SO,T,MKC	V0530
N15	3000	0.0	C/H=5.89E-4, C/O=1.00	SO,T,MKC	V0532
N20	3500	0.0	C/H=7.10E-4, C/O=1.20	SO,T,MKC	V0516b

*These models have L only for C, N, and O. Metal abundances are as in: Goldberg, Müller, and Aller (1960).

**K27 has exactly the same parameters as K26 except He/H=3.00 in K27.

†All N-models have L composition except for carbon, which is shown.

TABLE 2

MOLECULAR COLUMN DENSITIES

(X = log N)

Molecule	λ(μm)	MODEL NO. J1	J2	J3	J4	J5	J6	J7	J8	J9	J10	J13	J14
H	1.00	24.41	25.32	26.17	24.48	25.13	25.98	26.92	24.41	25.04	25.36	25.41	25.36
H^-	1.00	16.12	16.12	16.10	16.00	15.74	15.67	15.60	15.98	15.40	14.20	14.51	14.20
H_2	1.00	21.55	21.35	21.05	23.14	22.19	21.70	21.46	23.97	24.35	23.67	22.07	23.62
	2.27	21.70	21.43	21.09	23.22	22.04	20.60	19.34	24.04	24.14	23.36	22.31	23.73
C_2	1.00	15.65	15.85	15.64	12.93	15.11	16.09	16.28	10.71	8.51	7.89	10.07	4.81
	0.74	15.57	15.82	15.63	12.23	13.58	15.24	16.03	10.03	6.85	5.81	8.02	2.94
	0.58	15.60	15.84	15.62	11.57	13.01	14.72	15.58	9.36	6.07	4.91	7.24	2.15
N_2	1.00	18.51	18.32	18.14	20.06	20.20	20.05	19.85	20.27	20.82	21.00	21.61	21.68
	3.45	18.52	18.33	18.14	20.15	20.23	20.07	19.86	20.39	20.62	21.52	21.95	22.27
O_2	1.00	14.75	14.79	14.56	15.86	15.06	15.04	15.03	16.43	17.02	16.64	15.79	17.49
S_2	1.00	14.04	14.71	14.39	10.90	15.38	15.89	15.58	8.88	10.13	12.63	15.43	10.69
	0.31	13.76	14.13	13.81	10.13	14.22	15.00	14.76	7.93	9.93	8.62	14.36	7.89
CH	1.00	17.42	17.40	17.14	16.22	16.95	17.30	17.30	15.21	13.84	12.85	13.84	11.32
	0.42	17.08	17.05	16.75	14.52	14.40	14.89	15.39	13.30	11.14	9.62	10.73	8.24
	3.78	17.59	17.44	17.16	17.20	17.65	17.76	17.56	14.98	12.11	16.03	16.88	14.45
NH	1.00	17.20	16.99	16.71	17.81	17.47	17.15	16.94	17.73	17.34	16.52	17.22	16.85
	3.18	17.35	17.06	16.75	18.15	17.78	17.54	17.20	17.11	16.04	17.78	18.49	17.91
	0.37	16.91	16.61	16.17	16.77	15.93	15.53	15.23	16.51	15.33	14.62	15.20	14.96
OH	1.00	18.42	18.34	18.08	19.67	18.81	18.56	18.45	20.29	20.68	20.07	19.01	20.49
	2.74	18.57	18.44	18.12	19.76	19.07	18.73	18.17	19.37	18.52	20.22	19.55	20.69
	0.31	17.58	17.43	17.14	18.47	17.12	16.33	15.90	19.09	19.13	19.15	17.14	19.30
MgH	1.00	15.29	14.18	12.98	16.97	15.70	14.40	13.09	17.53	17.16	15.90	15.04	15.90
	0.51	15.17	14.09	12.85	16.44	14.81	13.46	12.10	16.99	16.17	14.91	13.87	14.85
	6.46	15.21	14.04	12.85	17.01	15.74	14.14	12.38	16.57	15.15	16.17	15.49	16.56
SiH	1.00	15.15	14.34	13.21	16.07	15.24	14.47	13.36	16.00	15.08	14.21	14.39	13.77
	0.40	14.92	14.09	12.87	15.13	13.82	12.97	12.10	14.52	12.47	11.51	12.63	11.12

TABLE 2 (continued)

Molecule	λ(μm)	J15	J16	J17	J18	J19	J20	J21	J22	J23	J24	J30	J31
H	1.00	25.48	25.41	25.36	25.41	24.72	25.38	23.82	24.92	24.89	23.71	24.75	24.77
H^-	1.00	12.81	14.54	14.22	14.54	14.72	14.50	13.18	13.39	13.91	12.73		
H_2	1.00	21.92	21.99	23.75	21.99	22.79	21.83	23.27	22.85	25.13	25.67	23.07	23.64
	2.27	22.01	22.31	23.86	22.31	23.13	22.40	24.09	23.20	25.31	25.99	22.96	23.46
C_2	1.00	6.49	13.78	12.43	13.78	16.07	15.05	16.21	16.57	16.41	12.97	8.24	6.62
	0.74	4.52	12.84	11.90	12.84	16.05	14.79	15.92	16.54	15.66	11.88	8.00	6.37
	0.58	3.23	12.42	11.64	12.42	15.99	14.75	17.01	16.45	15.33	11.22	6.68	4.99
N_2	1.00	21.77	22.01	22.06	22.01	21.42	21.97	20.70	21.62	22.22	22.65	20.39	20.46
	3.45	22.51	22.39	22.62	22.39	22.00	22.36	22.27	22.67	22.78	23.15	20.51	20.47
O_2	1.00	15.84	11.79	9.32	11.79	6.94	9.68	-0.17	2.99	-0.80	-2.79		
S_2	1.00	16.01	17.07	19.65	17.07	17.89	16.83	18.18	18.68	19.89	17.86		
	0.31	12.70	15.93	18.73	15.93	17.06	15.60	17.93	17.85	18.22	12.33		
CH	1.00	11.27	15.73	15.21	15.73	17.17	16.28	16.65	16.79	17.10	14.60	12.85	12.12
	0.42	7.99	13.62	13.66	13.62	16.56	15.02	17.25	16.24	15.22	11.16	10.95	10.11
	3.78	15.04	17.12	16.85	17.12	17.70	17.17	18.43	17.54	18.50	17.25	13.38	12.34
NH	1.00	15.97	17.45	17.03	17.45	17.44	17.41	15.68	16.33	16.25	14.72	16.22	16.16
	3.18	17.72	18.73	18.54	18.73	18.94	18.71	18.92	18.59	18.12	16.56	16.47	16.04
	0.37	13.98	15.42	15.14	15.42	16.32	15.52	16.13	15.25	14.15	11.45	15.09	14.99
OH	1.00	18.80	16.93	16.34	16.93	14.82	15.75	11.39	12.73	11.86	10.91	19.56	20.08
	2.74	19.26	18.03	17.99	18.03	17.41	17.39	16.99	17.08	14.98	13.14	19.57	19.31
	0.31	17.80	14.19	13.00	14.19	12.10	12.40	10.83	10.00	8.52	6.24	18.91	19.23
MgH	1.00	14.04	14.96	15.95	14.96	15.94	14.79	15.39	15.06	16.85	17.68		
	0.51	12.99	13.81	14.95	13.81	15.26	13.75	15.62	14.50	13.35	0.71		
	6.46	14.92	15.33	16.53	15.33	16.50	15.29	17.31	16.15	17.42			
SiH	1.00	13.11	14.38	15.12	14.38	15.12	14.26	14.55	14.23	15.91	16.31	13.98	13.53
	0.40	10.85	12.74	13.85	12.74	14.33	12.72	14.38	13.38	14.29	14.97	12.53	11.86

TABLE 2 (continued)

Molecule	λ(μm)	J32	J35	K1	K3	K4	K9	K12	K15	K16	K18	K20	K23
H	1.00	24.68	24.49	25.67	25.65	25.65	25.64	25.57	25.12	24.80	23.97	23.84	24.92
H^-	1.00			14.92	14.79	14.76	14.86	14.78	14.00	13.50	12.07	11.82	13.63
H_2	1.00	24.22	24.51	23.12	23.26	23.40	22.80	22.35	21.57	21.09	19.95	19.79	21.26
	2.27	24.04	24.25	22.91	23.32	23.60	22.92	22.76	21.66	21.17	20.09	20.01	21.70
C_2	1.00	4.90	3.85	12.55	8.35	5.52	13.81	15.26	16.50	16.65	17.04	16.92	16.62
	0.74	4.61	3.47	9.55	5.58	2.91	12.62	15.05	16.45	16.65	17.08	16.95	16.61
	0.58	3.31	3.18	8.57	4.78	2.19	12.23	15.01	16.44	16.70	17.25	17.11	16.66
N_2	1.00	20.54	20.61	21.20	21.94	21.95	22.29	22.19	21.41	21.41	21.34	21.52	21.45
	3.45	20.11	20.15	21.35	22.36	22.44	22.65	22.58	21.88	22.00	22.37	22.72	22.06
O_2	1.00			16.11	17.05	17.23	11.76	10.48	10.08	9.72	8.16	7.76	8.49
S_2	1.00			16.03	13.40	13.69	18.34	17.54	16.84	16.40	15.40	15.29	16.54
	0.31			10.58	9.20	13.66	17.93	16.64	16.52	16.15	15.37	15.29	16.26
CH	1.00	11.35	10.82	15.33	13.25	11.86	16.00	16.56	16.75	16.55	16.00	15.82	16.62
	0.42	9.12	8.43	11.19	9.67	8.69	13.81	15.41	16.28	16.32	16.74	16.80	16.37
	3.78	8.44	7.36	18.09	16.73	15.95	17.32	17.40	18.15	18.15	18.42	18.25	18.16
NH	1.00	16.05	15.85	17.23	17.51	17.46	17.76	17.68	16.81	16.53	15.62	15.55	16.60
	3.18	13.92	13.39	18.11	18.83	18.84	19.06	19.05	18.47	18.69	18.68		18.66
	0.37	14.53	13.94	15.10	15.43	15.43	15.66	15.73	15.65	15.96	16.70	17.07	16.03
OH	1.00	20.39	20.35	19.56	20.16	20.32	17.24	16.38	15.80	15.37	13.99	13.71	14.85
	2.74	16.42	15.54	19.68	20.36	20.54	18.34	17.98	18.51	18.26	17.65	17.52	18.17
	0.31	18.43	17.71	18.99	19.07	18.33	14.25	12.57	12.98	13.05	13.68	13.69	12.53
MgH	1.00			15.80	15.99	16.11	15.71	15.35	14.45	13.89	12.50	12.30	14.07
	0.51			14.84	14.87	14.85	14.56	14.31	14.05	13.75	13.16	13.11	13.92
	6.46			15.91	16.34	16.52	15.98	15.69	14.99	14.52	13.24	13.09	14.91
SiH	1.00	12.94	12.55	14.98	14.91	14.83	14.98	14.70	13.86	13.34	11.97	11.75	13.50
	0.40	11.13	10.72	12.77	12.31	12.33	13.47	13.23	13.04	13.04	12.65	12.88	13.19

TABLE 2 (continued)

Molecule	λ(μm)	K24	K26	K27	K28	N12	N4	N10	N11	N13	N14	N15	N20
H	1.00	24.19	23.31	23.31	24.01	25.01	24.36	23.77	24.43	25.38	25.60	25.62	25.41
H^-	1.00	12.31	10.73	11.06	15.14	13.55	14.01	11.35	12.52	14.22	14.67	14.87	14.53
H_2	1.00	20.15	18.90	18.89	23.42	22.45	22.76	20.11	21.27	23.35	24.29	25.08	22.01
	2.27	20.38	19.65	19.74	23.81	22.11	22.25	20.63	21.35	22.70	23.72	24.21	21.42
C_2	1.00	17.63	18.65	18.54	16.54	17.36	17.54	17.65	17.57	17.02	16.32	14.34	16.64
	0.74	17.67	18.70	18.59	16.33	17.33	17.63	18.07	17.77	16.90	16.06	13.66	16.55
	0.58	17.86	18.99	18.91	16.66	17.00	17.14	16.71	16.66	16.51	15.78	13.38	16.51
N_2	1.00	20.72	19.84	19.81	20.88	20.62	20.00	19.34	20.02	21.01	21.27	21.44	20.79
	3.45	21.50	20.79	20.59	21.52	21.40	18.85	20.33	20.92	21.68	21.89	22.05	20.97
O_2	1.00	7.24	3.24	4.21	5.09	7.43	6.83	4.12	5.94	8.29	8.72	9.25	12.00
S_2	1.00	15.53	14.16	14.07	18.30	18.06	17.76	15.70	16.86	19.02	19.92	20.51	17.23
	0.31	15.53	14.66	14.14	17.74	17.45	17.27	15.84	16.67	18.04	18.86	18.55	16.78
CH	1.00	16.42	16.16	16.23	17.75	17.20	17.60	16.12	16.72	17.41	17.38	16.57	17.07
	0.42	17.40	16.04	16.85	17.72	16.59	17.00	15.98	16.38	16.42	16.14	14.63	16.25
	3.78	18.76	18.94	18.96	18.41	18.47	16.43	18.64	18.72	18.23	18.12	18.22	18.49
NH	1.00	15.43	14.02	14.26	17.48	16.05	16.19	14.10	15.15	16.58	16.88	16.89	16.81
	3.18	18.28	17.70	17.43	18.88	18.12	14.12	17.62	17.89	18.37	18.48	18.54	17.94
	0.37	16.71	17.04	15.73	17.23	15.03	16.10	15.60	15.38	15.01	14.99	14.45	15.38
OH	1.00	13.64	10.99	11.50	14.26	14.83	14.73	12.01	13.51	15.67	16.24	16.90	16.97
	2.74	17.37	16.72	16.90	17.29	17.95	11.66	16.91	17.72	17.60	17.69	18.41	18.23
	0.31	13.62	14.76	11.85	12.63	12.47	13.50	12.88	12.65	12.33	12.50	12.35	13.28
MgH	1.00	12.72	11.21	11.29	16.77	14.96	15.54	12.46	13.76	15.79	16.46	17.05	14.97
	0.51	13.60	12.75	12.32	16.70	13.70	13.88	10.20	11.52	14.11	15.41	15.98	14.17
	6.46	13.64	12.65	12.68	17.44	15.84	16.56	14.25	15.04	16.33	16.87	17.53	15.14
SiH	1.00	12.19	10.69	10.87	15.92	14.15	14.71	11.72	12.97	14.96	15.62	16.19	14.38
	0.40	12.23	7.61	7.88	15.73	12.81	10.34	10.14	11.64	13.40	14.46	14.86	13.14

TABLE 2 (continued)

Molecule	λ(μm)	J1	J2	J3	J4	J5	J6	J7	J8	J9	J10	J13	J14
SH	1.00	15.96	16.25	15.92	14.50	16.38	16.38	16.16	13.49	13.48	14.18	15.65	13.21
	3.78	16.14	16.28	15.94	15.26	16.73	16.70	16.37	13.39	12.40	16.60	17.05	15.73
	0.37	15.65	15.86	15.41	13.37	14.86	14.80	14.44	12.29	11.51	11.74	13.69	10.92
CN	1.00	16.67	16.70	16.47	15.87	16.97	17.40	17.43	14.80	13.87	13.56	15.13	12.37
	0.74	16.64	16.68	16.46	15.52	16.27	16.96	17.28	14.42	12.85	12.34	13.91	11.25
SiN	1.00	14.22	13.44	12.30	15.46	15.10	14.45	13.40	15.27	14.71	14.48	15.36	14.37
	0.40	14.11	13.32	12.14	14.66	14.11	13.64	12.86	13.92	12.28	11.88	13.86	11.85
CO	1.00	20.62	20.84	20.71	21.07	21.64	22.19	22.45	21.20	21.74	21.92	20.96	20.92
	3.45	20.64	20.85	20.71	21.29	21.81	22.25	22.46	21.32	21.55	22.55	21.68	21.56
NO	1.00	16.21	16.13	15.88	17.31	16.98	16.82	16.68	17.54	17.88	17.58	17.82	18.37
	6.46	16.13	16.02	15.81	17.34	17.02	16.55	16.08	16.63	15.37	16.84	18.30	18.94
MgO	1.00	13.25	12.29	11.10	15.22	13.98	12.86	11.65	15.98	16.14	15.29	14.22	15.72
	0.51	13.16	12.23	11.02	14.86	13.34	12.10	10.95	15.59	15.44	14.76	13.41	15.08
SiO	1.00	16.92	16.31	15.34	19.46	18.61	17.99	17.45	20.11	20.71	20.85	19.84	20.89
	8.90	16.82	16.25	15.31	19.45	18.61	17.98	17.45	19.82	19.92	20.92	19.87	20.99
SO	1.00	13.53	13.94	13.65	12.26	14.20	14.40	14.26	11.45	11.92	12.91	14.31	12.42
	8.90	13.29	13.73	13.53	12.16	14.18	14.35	14.30	10.80	10.50	10.87	14.68	12.67
TiO	1.00	12.05	11.03	9.86	15.57	13.84	12.47	11.43	16.80	17.50	17.46	15.01	17.64
	8.90	11.94	10.95	9.79	15.56	13.83	12.46	11.43	16.63	16.86	17.47	15.02	17.68
	0.74	12.04	11.03	9.85	15.57	13.80	12.40	11.41	16.78	17.30	17.36	14.96	17.45
ZrO	1.00	10.47	9.47	8.34	14.13	12.66	11.46	10.82	14.81	15.40	15.56	14.05	15.59
	0.63	10.48	9.46	8.35	14.11	12.65	11.44	10.82	14.69	15.12	15.18	13.99	15.17
CS	1.00	15.50	16.01	15.76	12.83	16.10	16.84	16.87	10.89	10.51	11.84	13.96	9.34
	0.26	14.98	15.42	14.91	10.60	13.49	14.57	15.05	8.20	7.07	6.56	10.97	4.72
	8.90	15.31	15.88	15.70	12.52	16.06	16.79	16.88	9.65	7.93	12.34	14.80	9.85
NS	1.00	12.94	13.22	12.91	11.27	13.62	13.72	13.47	9.81	9.64	10.66	13.47	9.99
	0.26	12.33	12.42	11.74	9.37	11.50	11.74	11.42	7.33	6.36	6.21	10.81	6.08
	8.90	12.72	13.01	12.78	11.05	13.59	13.67	13.51	8.73	7.35	11.06	14.10	10.41

TABLE 2 (continued)

Molecule	λ(μm)	J15	J16	J17	J18	J19	J20	J21	J22	J23	J24	J30	J31
SH	1.00	14.97	16.36	17.58	16.36	17.12	16.22	16.41	16.69	17.40	15.31		
	3.78	16.47	17.08	17.93	17.08	17.62	17.03	18.35	17.47	18.40	18.05		
	0.37	12.58	14.95	16.32	14.95	16.40	14.87	16.78	15.93	15.57	11.16		
CN	1.00	13.25	17.27	16.45	17.27	18.10	17.90	17.60	18.28	18.29	16.48	13.43	12.59
	0.74	12.06	16.57	15.98	16.57	18.05	17.51	17.33	18.22	17.72	15.69	13.30	12.45
SiN	1.00	14.64	15.57	15.90	15.57	15.65	15.50	14.99	15.23	16.55	17.56		
	0.40	12.51	14.19	14.75	14.19	14.96	14.20	14.84	14.46	15.25	16.86		
CO	1.00	21.03	20.89	20.93	20.89	19.58	20.20	18.87	19.78	20.39	20.81	21.32	21.38
	3.45	22.05	21.16	21.49	21.16	20.15	20.48	20.45	20.86	20.95	21.32	21.44	21.40
NO	1.00	17.56	16.04	14.47	16.04	13.24	14.94	8.92	11.05	9.08	7.73	17.12	17.34
	6.46	18.52	17.02	17.22	17.02	15.78	16.42	15.59	16.66	16.67		17.51	16.65
MgO	1.00	13.94	12.08	11.61	12.08	10.24	10.82	6.75	7.98	7.49	7.99		
	0.51	13.35	10.65	9.78	10.65	8.83	8.79	7.13	6.71	2.47	-11.84		
SiO	1.00	20.60	17.49	18.25	17.49	15.38	16.09	13.98	14.61	16.09	19.34		
	8.90	20.64	17.61	18.40	17.61	16.32	16.50	16.17	15.95	16.19	19.36		
SO	1.00	14.25	13.03	12.70	13.03	10.92	11.81	7.26	9.08	7.49	5.01		
	8.90	14.61	13.36	13.08	13.36	12.44	12.59	11.88	11.29	8.40	5.79		
TiO	1.00	16.35	12.47	13.86	12.47	11.08	10.94	9.53	10.18	11.35	13.81		
	8.90	16.53	12.54	14.03	12.54	11.82	11.23	11.99	11.32	11.52	13.89		
	0.74	16.52	12.25	13.45	12.25	10.95	10.29	9.22	10.02	11.06	13.69		
ZrO	1.00	15.13	11.45	13.13	11.45	9.99	9.83	8.92	9.43	11.12	14.56		
	0.63	15.02	11.22	12.71	11.22	9.87	9.31	9.51	9.29	10.85	14.52		
CS	1.00	12.85	16.58	17.71	16.58	18.39	17.30	19.05	19.41	20.30	18.13		
	0.26	7.63	14.88	16.55	14.88	17.75	16.12	18.82	18.78	18.77	13.56		
	8.90	13.68	16.74	17.79	16.74	18.43	17.35	19.68	19.47	20.66	18.62		
NS	1.00	12.63	14.40	14.40	14.40	14.42	14.33	12.61	13.70	13.08	10.27		
	0.26	8.25	12.04	11.69	12.04	12.88	12.14	12.12	11.87	9.99	3.37		
	8.90	13.28	14.71	14.68	14.71	15.08	14.81	15.34	14.69	13.87	10.99		

TABLE 2 (continued)

Molecule	λ (μm)	J32	J35	K1	K3	K4	K9	K12	K15	K16	K18	K20	K23
SH	1.00			16.22	14.87	14.46	17.07	16.70	15.90	15.41	14.16	13.97	15.57
	3.78			17.33	17.12	17.24	17.48	17.33	17.06	16.76	16.26	16.09	17.02
	0.37			13.05	12.15	12.59	15.91	15.48	15.18	15.07	14.78	14.84	15.23
CN	1.00	11.74	11.19	16.10	14.35	12.93	17.38	18.08	18.30	18.36	18.47	18.48	18.37
	0.74	11.56	10.96	14.37	12.73	11.40	16.52	17.72	18.20	18.36	18.55	18.56	18.36
SiN	1.00			15.41	15.63	15.50	16.01	15.83	15.01	14.74	14.00	13.98	14.84
	0.40			13.27	13.14	13.25	14.66	14.54	14.31	14.49	14.58	14.94	14.58
CO	1.00	21.46	21.53	22.22	21.20	20.21	21.16	20.80	21.37	21.35	21.22	21.09	20.77
	3.45	21.03	21.07	22.79	21.92	20.95	21.46	21.10	22.16	22.29	22.67	22.55	21.68
NO	1.00	17.41	17.22	17.57	18.45	18.54	16.11	15.43	14.81	14.62	13.73	13.61	14.02
	6.46	12.91	11.03	17.67	18.80	18.94	17.18	16.81	16.73	16.97	18.21	17.07	16.91
MgO	1.00			14.80	15.44	15.62	12.53	11.58	10.92	10.44	9.00	8.72	9.94
	0.51			14.42	14.80	14.74	10.88	9.31	10.02	10.12	10.91	11.10	9.60
SiO	1.00			20.50	20.91	21.03	18.05	16.82	16.34	15.97	14.91	14.72	15.48
	8.90			20.51	20.94	21.09	18.20	17.33	17.47	17.29	16.74	16.58	16.86
SO	1.00			14.49	13.68	13.40	13.39	12.46	11.90	11.49	10.18	9.92	10.97
	8.90			15.06	15.06	15.73	14.03	13.57	14.04	14.19	14.22	14.01	13.57
TiO	1.00			16.81	17.21	17.36	13.38	11.87	11.21	10.75	9.52	9.32	10.28
	8.90			16.81	17.21	17.36	13.43	12.18	12.09	11.84	11.18	10.09	11.42
	0.74			16.80	17.17	17.26	13.17	11.23	11.02	10.74	9.67	9.46	10.28
ZrO	1.00			15.12	15.55	15.70	12.46	10.78	10.14	9.70	8.56	8.38	9.25
	0.63			15.12	15.41	15.45	12.34	10.28	10.16	9.86	8.82	8.64	9.40
CS	1.00			15.53	12.22	10.46	17.14	17.84	18.18	18.06	17.83	17.73	18.07
	0.26			8.68	6.64	8.63	15.90	16.99	17.93	17.87	17.81	17.73	17.83
	8.90			17.03	15.44	14.50	17.35	17.88	18.27	18.16	17.98	17.88	18.18
NS	1.00			13.48	12.26	11.69	14.78	14.64	13.81	13.54	12.74	12.70	13.63
	0.26			7.89	7.60	9.64	12.44	12.42	12.31	12.31	12.57	12.67	12.42
	8.90			15.74	14.63	14.70	15.40	15.34	14.84	14.90	14.88	14.95	14.91

TABLE 2 (continued)

Molecule	λ(μm)	K24	K26	K27	K28	N12	N4	N10	N11	N13	N14	N15	N20
SH	1.00	14.36	12.89	13.02	17.70	16.48	16.75	14.06	15.30	17.32	18.00	14.80	16.37
	3.78	16.60	15.76	15.77	18.35	17.55	15.09	16.61	17.19	17.93	18.42	18.94	17.24
	0.37	15.19	15.31	14.10	17.51	15.76	16.67	15.09	15.44	16.19	16.66	16.41	15.46
CN	1.00	18.47	18.51	18.47	18.08	18.23	18.05	17.72	18.03	18.23	17.99	17.03	18.05
	0.74	18.54	18.59	18.55	17.83	18.17	18.22	18.38	18.39	18.02	17.65	16.41	17.92
SiN	1.00	13.80	12.59	12.67	15.87	14.71	14.71	12.84	13.82	15.31	15.77	16.17	14.95
	0.40	13.87	10.05	10.19	15.70	13.55	10.92	11.50	12.68	13.94	14.71	15.14	13.97
CO	1.00	21.04	20.16	20.16	19.04	21.79	21.15	20.54	21.20	22.16	22.41	22.59	22.17
	3.45	22.67	22.49	22.31	19.69	23.05	20.00	22.81	22.96	23.08	23.16	23.29	22.88
NO	1.00	12.96	10.44	10.97	12.07	12.89	12.36	10.55	11.84	13.48	13.75	13.99	15.44
	6.46	16.24	15.33	15.46	14.35	15.72	14.48	15.36	15.49	15.50	15.62	16.07	16.01
MgO	1.00	8.64	5.94	6.36	9.87	10.11	10.10	7.19	8.76	10.96	11.52	12.21	12.11
	0.51	11.06	10.10	9.12	9.77	7.70	7.11	3.65	4.96	7.74	9.07	9.82	10.33
SiO	1.00	14.54	12.29	12.49	15.04	16.29	15.91	13.62	14.99	17.22	18.08	19.49	17.38
	8.90	16.71	15.41	15.12	15.84	18.38	17.63	16.91	17.84	18.79	19.17	19.90	18.13
SO	1.00	9.83	7.18	7.66	10.34	11.11	10.84	8.29	9.79	11.97	12.55	13.09	13.04
	8.90	14.16	13.28	12.84	11.86	14.55	13.59	13.76	14.48	14.73	14.79	15.03	14.50
TiO	1.00	9.14	6.71	6.87	11.01	11.74	11.66	8.54	10.17	12.83	13.71	14.98	12.31
	8.90	11.19	9.98	9.65	11.87	13.33	13.27	11.40	12.50	14.02	14.68	15.53	12.86
	0.74	9.30	6.86	7.03	10.63	11.65	12.06	9.92	10.92	12.38	13.09	14.48	12.01
ZrO	1.00	8.18	5.85	5.93	9.90	10.89	10.72	7.75	9.34	12.00	13.01	14.47	11.22
	0.63	8.44	6.11	6.19	10.17	10.48	10.50	6.67	8.44	11.35	12.55	14.22	10.99
CS	1.00	18.16	18.00	17.83	18.79	19.39	19.18	18.36	18.88	19.74	19.90	19.28	18.51
	0.26	18.15	18.31	17.87	18.43	18.73	18.27	17.60	18.19	19.00	18.94	17.56	18.25
	8.90	18.36	18.45	18.22	18.90	19.47	19.39	18.72	19.08	19.79	19.94	19.54	18.57
NS	1.00	12.54	11.15	11.34	14.42	13.31	13.21	11.37	12.40	13.87	14.20	14.14	13.76
	0.26	12.51	12.88	11.52	13.46	11.25	10.74	9.43	10.39	11.46	11.36	9.99	11.80
	8.90	14.55	13.86	13.56	15.20	14.74	14.65	13.73	14.39	15.00	15.17	15.39	14.34

TABLE 2 (continued)

Molecule	λ(μm)	J1	J2	J3	J4	J5	J6	J7	J8	J9	J10	J13	J14
SiS	1.00	13.77	13.47	12.35	13.25	15.12	14.87	13.91	12.33	12.48	13.98	15.23	12.58
	14.30	13.39	13.08	12.06	12.45	14.25	14.18	13.59	11.03	10.50	10.76	13.99	9.54
	0.31	13.37	12.95	11.87	12.13	13.96	13.93	13.43	10.50	10.29	9.64	13.77	8.79
H_2O	1.00	15.71	14.49	13.10	18.66	16.16	14.54	13.24	20.33	20.67	19.45	16.16	19.54
	2.74	15.79	14.54	13.11	18.68	16.26	14.66	13.03	19.85	19.85	19.46	16.31	19.58
	6.46	15.62	14.35	13.02	18.67	16.19	14.23	12.43	19.97	19.92	19.46	16.29	19.56
HCN	1.00	14.79	13.69	12.33	15.63	15.15	14.31	13.17	15.33	14.60	13.37	13.15	12.24
	0.82	14.77	13.68	12.33	15.40	14.84	14.13	13.07	15.30	14.09	12.52	12.18	11.40
	3.18	14.83	13.70	12.34	16.10	15.33	14.38	13.18	14.87	13.14	15.15	14.63	13.74
HCO	1.00	14.93	13.95	12.62	15.95	15.05	14.32	13.27	16.34	15.80	14.43	13.04	13.44
	0.63	14.96	13.94	12.62	15.70	14.60	13.90	13.05	16.08	15.33	13.79	12.18	12.76
	3.78	14.99	13.96	12.61	16.18	15.30	14.40	13.30	16.33	15.05	15.26	14.19	14.30
HNO	1.00	10.69	9.48	8.09	12.56	10.72	9.30	8.02	13.24	12.71	10.98	10.49	11.78
	0.51	10.53	9.37	7.99	12.02	9.72	8.04	6.70	12.59	11.58	10.05	9.17	10.75
	2.74	10.80	9.55	8.11	12.69	10.92	9.45	7.75	11.78	9.53	11.31	11.21	12.18
CH_2	1.00	13.54	12.39	10.99	13.65	12.80	11.89	10.73	13.41	11.72	9.62	9.22	8.14
	0.40	13.30	12.05	10.63	12.10	10.30	9.44	8.71	11.79	9.05	6.81	6.21	5.36
C_2H	1.00	13.52	12.64	11.31	12.45	13.04	12.77	11.83	11.23	9.10	7.58	7.93	4.57
	0.51	13.30	12.58	11.13	10.74	10.52	10.89	10.80	9.53	6.19	4.20	4.64	1.42
NH_2	1.00	13.71	12.38	10.96	15.64	13.73	12.10	10.72	16.30	15.51	13.58	12.93	13.93
	0.63	13.74	12.33	10.95	15.42	13.39	11.66	10.21	16.03	15.03	12.97	12.09	13.26
TiO_2	1.00	4.44	2.45	0.17	9.41	6.15	3.64	1.64	11.51	12.15	11.53	7.52	11.92
	0.51	4.40	2.44	0.15	9.32	5.96	3.43	1.54	11.40	11.84	11.40	7.29	11.62
ZrO_2	1.00	5.49	3.52	1.37	11.01	8.10	6.19	4.97	12.74	13.55	13.22	9.94	13.45
	0.51	5.48	3.52	1.37	10.95	8.00	6.17	4.97	12.63	13.33	13.09	9.80	13.18
SiC_2	1.00	9.68	8.28	6.11	9.08	9.58	8.98	7.41	7.76	5.35	4.37	4.90	0.91
	0.51	9.58	8.27	6.11	7.44	7.40	7.67	6.97	5.74	1.73	0.02	1.84	-3.10

TABLE 2 (continued)

Molecule	λ(μm)	J15	J16	J17	J18	J19	J20	J21	J22	J23	J24	J30	J31
SiS	1.00	15.50	16.09	18.63	16.09	16.95	15.87	17.83	17.63	20.30	21.18		
	14.30	12.84	15.22	18.15	15.22	16.51	14.99	17.98	17.20	19.58	20.24		
	0.31	11.79	14.80	17.95	14.80	16.03	14.52	17.65	16.88	19.06	19.92		
H_2O	1.00	16.16	13.89	15.22	13.89	13.25	12.53	11.54	11.20	12.94	14.02	18.95	19.90
	2.74	16.21	14.41	15.73	14.41	14.84	13.58	15.18	13.98	13.77	15.10	18.96	19.65
	6.46	16.22	14.34	15.73	14.34	14.63	13.52	15.17	14.16	14.80		18.96	19.75
HCN	1.00	11.30	15.24	16.64	15.24	17.70	15.84	19.02	18.12	20.81	21.30	13.15	12.96
	0.82	10.38	14.76	16.41	14.76	17.52	15.63	18.52	17.88	20.46	20.99	13.02	12.82
	3.18	13.64	15.61	16.92	15.61	17.79	15.96	19.51	18.20	20.99	21.81	13.50	12.80
HCO	1.00	11.64	12.93	13.48	12.93	13.02	12.18	12.12	11.88	13.31	13.47	14.13	14.38
	0.63	10.88	12.14	12.82	12.14	12.89	11.47	12.91	11.74	12.63	12.66	14.07	14.32
	3.78	13.16	13.45	14.33	13.45	13.88	12.73	14.54	13.42	14.09	14.78	14.29	14.44
HNO	1.00	9.08	8.72	7.98	8.72	7.35	7.55	3.28	4.14	3.39	2.37		
	0.51	8.00	6.65	5.72	6.65	5.66	4.85	3.75	2.64	-3.02			
	2.74	10.04	9.99	10.17	9.99	10.38	9.33	10.11	9.28	7.15	5.20		
CH_2	1.00	6.24	11.00	12.18	11.00	14.00	11.50	14.70	13.30	15.80	14.80	9.65	9.43
	0.40	3.30	9.00	10.96	9.00	13.40	10.20	14.50	12.80	13.90	12.30	8.05	7.77
C_2H	1.00	4.43	11.60	12.55	11.60	15.64	12.95	17.61	16.46	18.90	17.75	7.77	6.81
	0.51	1.10	10.10	11.94	10.10	15.47	12.56	17.74	16.36	16.67	1.36	5.50	4.40
NH_2	1.00	11.19	13.07	14.18	13.07	14.54	12.92	13.94	13.10	15.07	14.91	13.33	13.77
	0.63	10.45	12.23	13.54	12.23	14.41	12.19	14.75	12.95	14.31	13.95	13.28	13.71
TiO_2	1.00	9.60	2.63	3.85	2.63	0.00	0.04	-3.75	-2.90	-2.39	0.55		
	0.51	9.59	1.61	2.08	1.61	-1.59	-2.31	-3.36	-4.38	-8.15			
ZrO_2	1.00	11.69	4.70	6.59	4.70	2.00	2.00	-0.70	-0.10	1.30	5.80		
	0.51	11.63	4.00	5.28	4.00	0.70	0.00	-0.40	-1.30	-3.50			
SiC_2	1.00	1.80	8.61	10.25	8.61	12.87	10.10	15.58	14.21	17.75	19.07	4.59	3.10
	0.51	-1.78	7.41	9.92	7.41	12.76	9.84	15.65	14.16	15.86	4.87	1.75	-0.11

TABLE 2 (continued)

Molecule	λ(μm)	J32	J35	K1	K3	K4	K9	K12	K15	K16	K18	K20	K23
SiS	1.00			15.83	14.55	14.15	17.23	16.53	15.80	15.35	14.36	14.24	15.51
	14.30			16.14	15.58	15.26	17.24	16.57	15.93	15.49	14.54	14.43	15.67
	0.31			11.45	10.41	12.92	16.67	15.49	15.38	15.03	14.32	14.23	15.15
H_2O	1.00	20.80	21.15	18.73	18.54	18.71	14.76	13.47	12.61	12.04	10.38	10.09	11.57
	2.74	19.56	19.72	18.73	18.55	18.73	15.09	14.38	14.63	14.27	13.30	13.11	14.10
	6.46	19.67	19.58	18.73	18.55	18.73	15.04	14.25	14.09	13.86	12.78	12.65	13.85
HCN	1.00	12.82	12.95	14.52	13.25	12.11	15.94	16.44	16.34	16.27	16.15	16.16	16.30
	0.82	12.68	12.83	13.63	12.39	11.27	15.59	16.23	16.18	16.04	15.96	15.97	16.06
	3.18	11.39	11.82	15.49	15.02	14.06	16.23	16.52	16.51	16.49	16.48		16.52
HCO	1.00	14.63	14.78	14.63	13.71	12.78	13.53	13.01	13.18	12.95	12.22	11.99	12.40
	0.63	14.55	14.67	13.99	13.09	12.14	12.89	12.32	13.21	13.17	12.59	12.35	12.61
	3.78	13.47	13.34	15.46	14.63	13.79	13.99	13.54	14.55	14.59	14.73	14.52	14.00
HNO	1.00			10.61	11.66	11.86	9.15	8.28	7.29	6.91	5.49	5.29	6.34
	0.51			9.75	10.57	10.59	6.94	5.41	6.12	6.48	8.39	8.99	5.90
	2.74			10.85	12.09	12.31	10.43	10.04	10.17	10.08	9.73	9.79	9.91
CH_2	1.00	9.20	9.11	11.00	9.38	8.21	11.81	12.13	11.90	11.60	10.70	10.50	11.70
	0.40	7.55	7.48	7.70	6.26	5.20	9.94	11.11	11.40	11.40	11.10	11.20	11.50
C_2H	1.00	5.83	5.38	10.78	7.08	4.54	12.19	13.63	14.60	14.63	14.86	14.72	14.57
	0.51	4.23	4.13	6.48	3.28	1.03	10.75	13.40	14.55	14.62	14.90	14.78	14.54
NH_2	1.00	14.18	14.39	13.38	13.98	14.13	13.86	13.49	12.29	11.84	10.56	10.46	11.97
	0.63	14.10	14.27	12.86	13.41	13.52	13.23	12.81	12.31	12.04	10.93	10.82	12.17
TiO_2	1.00			10.89	11.06	11.09	3.63	1.44	0.68	0.13	-1.59	-1.92	-0.97
	0.51			10.89	10.99	10.71	2.64	-1.07	-0.37	-0.25	0.88	1.15	-1.37
ZrO_2	1.00			12.60	12.76	12.82	5.94	3.45	2.70	2.20	0.60	0.40	1.10
	0.51			12.60	12.61	12.35	5.33	1.42	1.80	1.90	2.60	2.80	0.80
SiC_2	1.00	1.39	0.56	7.78	4.08	1.46	9.30	10.91	12.04	12.11	12.47	12.35	11.93
	0.51	-0.71	-0.87	3.34	-0.32	-2.70	8.23	10.77	12.02	12.11	12.48	12.35	11.91

TABLE 2 (continued)

Molecule	λ(μm)	K24	K26	K27	K28	N12	N4	N10	N11	N13	N14	N15	N20
SiS	1.00	14.51	13.25	13.14	17.64	17.03	16.98	14.69	15.83	18.01	19.18	20.12	16.23
	14.30	14.77	13.72	13.53	17.48	17.21	17.33	15.29	16.21	18.09	19.21	20.15	16.30
	0.31	14.51	13.65	13.20	17.14	16.46	16.59	14.84	15.65	17.18	18.79	19.58	15.70
H_2O	1.00	10.02	7.09	7.54	14.06	12.77	13.61	8.92	10.89	14.12	15.30	16.86	13.89
	2.74	13.15	12.02	12.22	15.94	15.06	10.89	13.04	14.27	15.46	16.21	17.44	14.82
	6.46	12.82	11.52	11.77	15.40	14.65	15.22	13.12	13.72	15.28	16.17	17.44	14.33
HCN	1.00	16.11	15.82	15.71	19.00	17.46	18.15	15.87	16.65	18.06	18.67	18.71	16.33
	0.82	15.89	15.38	15.43	18.44	17.25	18.05	16.02	16.55	17.90	18.56	18.63	16.23
	3.17	16.43	16.31	16.14	19.16	17.60	17.51	16.33	16.95	18.13	18.71	18.79	16.42
HCO	1.00	12.05	10.48	10.72	13.82	13.80	14.42	11.35	12.63	14.59	15.20	15.86	14.24
	0.63	12.43	10.84	11.10	14.12	13.33	14.19	9.94	11.49	13.93	14.56	15.09	13.89
	3.78	14.87	14.44	14.40	14.85	15.75	12.72	15.02	15.51	15.88	16.15	16.54	15.40
HNO	1.00	4.73	1.61	2.31	7.53	5.79	6.43	2.29	4.16	6.81	7.50	8.18	8.14
	0.51	8.19	7.48	6.23	7.42	2.90	2.86	-2.09	-0.46	2.97	4.55	5.02	5.93
	2.74	8.86	7.84	8.09	11.15	9.42	2.57	7.71	8.88	9.12	9.23	10.11	9.42
CH_2	1.00	11.12	10.47	10.55	15.93	13.30	14.70	11.16	12.27	14.06	14.65	14.53	12.44
	0.40	11.22	7.49	7.80	15.78	12.30	11.20	9.90	11.28	12.97	13.82	13.28	11.64
C_2H	1.00	15.33	15.95	15.77	17.38	16.65	17.70	15.80	16.21	16.98	17.00	15.80	15.32
	0.51	15.42	16.18	15.95	17.35	16.37	17.37	14.66	15.39	16.65	16.75	15.39	15.29
NH_2	1.00	10.37	8.56	8.83	15.94	12.39	13.55	9.36	10.92	13.42	14.28	14.99	12.44
	0.63	10.73	8.92	9.18	16.25	11.92	13.31	7.89	9.73	12.76	13.67	14.39	12.15
TiO_2	1.00	-2.54	-6.66	-6.06	0.07	0.55	0.98	-4.20	-1.75	2.15	3.42	5.32	2.64
	0.51	0.61	-0.18	-2.36	-0.03	-2.19	-2.56	-8.23	-6.02	-1.60	0.70	3.12	0.62
ZrO_2	1.00	-0.28	-4.19	-3.74	2.11	3.00	3.30	-1.57	0.80	4.71	6.09	8.32	4.63
	0.51	2.26	0.33	-0.74	2.02	0.70	0.30	-4.99	-2.81	1.57	4.07	6.92	3.00
SiC_2	1.00	12.86	13.42	13.18	14.75	14.33	15.37	13.40	13.81	14.88	16.10	16.65	13.24
	0.51	12.87	13.46	13.21	14.73	14.20	15.23	12.49	13.24	14.75	16.10	16.65	13.24