MOLECULES IN THE SOLAR PHOTOSPHERE

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Abstract. A consideration of the dissociation equilibrium of diatomic molecules in the Utrecht Reference Photosphere leads us to conclude that SH, SiO, CS, HF and HCl may show up in enough concentrations in the solar atmosphere. The number above photosphere for these molecules is comparable with or more than that of MgH.

For late-type stars the variation of molecular abundance with spectral class has been studied (e.g. TSUJI, 1964; DOLAN, 1965; VARDYA, 1966). A similar investigation has been carried out by us for the Utrecht Reference Photospheric (URP) model of HEINTZE *et al.* (1964), with the aim of investigating the presence of certain new molecules in the photosphere. Throughout this paper this model has been assumed.

The following species were included in our investigation: H, H^-, H^+, CH, OH, SiH, MgH, SH, OH^-, BH, PH, AlH, BeH, LiH, NH, HF, HCl, HI, HBr, H_2, H_2^+, O, O^-, O^+, CO, NO, AlO, ZrO, BO, SiO, MgO, CaO, PO, LiO, SO, OH^+, O_2, O_2^+, N, N^+, CN, NS, SiN, PN, MgN, AlN, N_2, C, C^+, CP, SiC, CS, CCl, C_2, Si, Si^+, SiF, Mg, Mg^+, MgF, Al, Al^+, AlCl, AlF, S, S^-, S^+, S_2, B, B^+, BF, P, P^+, Be, Be^+, BeF, Li, Li^+, Br, Br^-, Br^+, I, I^-, I^+, Cl, Cl^-, Cl^+, NaCl, KCl, F, F^-, F^+, Zr, Zr^+, Na, Na^+, Ca, Ca^+, K and K^+.

'Reduced' or simplified equations were obtained from detailed equilibrium equations. These former contain the minimum number of terms necessary to describe free partial pressure of any element as a function of optical depth τ_0 at 5000 Å. The equilibrium constants are taken from tables by GLUSHKO *et al.* (1962). The tables by TATUM (1966) have been used for CN and CH as they are based on latest information about the dissociation energy of these molecules. They have been used also for C_2 at temperatures greater than 6000 K.

In case of Mg as a representative case, the equilibrium equation is:

$$P(\mathrm{Mg}) = p(\mathrm{Mg})\left[1 + \frac{K(\mathrm{Mg})}{p(\mathrm{e})} + \frac{p(\mathrm{H})}{K(\mathrm{MgH})} + \frac{p(\mathrm{O})}{K(\mathrm{MgO})} + \frac{p(\mathrm{N})}{K(\mathrm{MgN})} + \frac{p(\mathrm{F})}{K(\mathrm{MgF})}\right]. \quad (1)$$

Here p's denote partial pressures and P the total fictitious pressure of the element obtainable from abundance and URP gas pressure with assumed He/H ratio of 1/16 (VARDYA, 1961). The quantities K's denote dissociation, ionization or detachment constants as the case may be.

Assuming that molecular formation does not affect appreciably the value of $p(\mathrm{H})$ we have $P(\mathrm{H}) \approx p(\mathrm{H})$ which can be obtained from the value of gas pressure for each τ_0 in URP with the accepted He/H ratio. Accepted abundances then give fictitious total pressure of each element at various τ_0. Abundances have been taken from

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ALLER (1961) except in some cases in which MULLER's (1966) data was used. For F, Cl, Br, I and B abundances prevailing in the solar system in general (ALLER, 1961) have been used (see Table I).

As an initial solution for H, C, N, and O the group I[a] by DE JAGER and NEVEN (1957) (DJN), was adopted after applying abundance correction. This group holds for the higher dissociation energy of C_2 i.e. 6.25 eV, later established by SCHADEE (1964). Combination of URP and DJN gives $p(H)$, $p(C)$, $p(N)$, $p(O)$ and $p(e)$ at various optical depths at 5000 Å. Plotting the logarithms of $p(H)/K(MgH)$, $p(O)/K(MgO)$ and $p(N)/K(MgN)$ as a function of τ_0, each curve showed an inflection point corresponding to a maximum at $\tau_0 \approx 0.02$ where the value of each term was found to be significantly less than unity. The plot of $\log K(Mg)/p(e)$ against optical depth also showed an inflection but now corresponding to a minimum. A study of similar curves for various elements leads us to conclude that the ionization term can be neglected for ionization potentials greater than 11 eV. In case of Mg the ionization term is significant.

TABLE I

Element	Log N	Mean of the I.A.U. Symp. values of log N	Species in the reduced equations	Element	Log N	Mean of the I.A.U. Symp. values of log N	Species in the reduced equations
H	12.00		H	Be	2.36	1.33, 2.34	Be, Be^+
C	8.72	8.60	C, CO	Li	0.96	1.54, 1.17	Li, Li^+
N	7.98	7.83	N, N_2	I	1.35		I
O	8.96	8.92	O, CO	Br	2.65		Br
Si	7.50	7.45	Si, Si^+	Cl	6.25		Cl
Mg	7.40		Mg, Mg^+	Zr	2.23	2.65	Zr, Zr^+
Al	6.20		Al, Al^+	Ca	6.15	6.31, 6.04	Ca, Ca^+
S	7.30		S, S^+	Na	6.30	5.44, 6.46	Na, Na^+
B	2.88		B, B^+	K	4.70		K, K^+
P	5.34		P, P^+	F	6.00		F

The role of $p(F)/K(MgF)$ in Equation (1) was estimated differently because the free partial pressure of F as a function of τ_0 is not obtainable from URP and DJN. We assumed $p(F) \approx P(F)$, i.e. F has maximum partial pressure obtainable from assumed abundance. Also $p(H) = P(H)$ and that $\log p(F)/K(MgF)$ and $\log p(H)/K(MgH)$ have inflection points corresponding to maximum at the same optical depth. Then, at inflection point

$$\left[\log \frac{p(MgF)}{p(MgH)}\right]_{max} = \left[\log \frac{P(F)}{P(H)} \cdot \frac{K(MgH)}{K(MgF)}\right]_{max} \approx \bar{4}.56 \text{ as } \left[\log \frac{K(MgH)}{K(MgF)}\right]_{max} = 2.56.$$

Thus, finally Equation (1) reduces to

$$P(Mg) = p(Mg)\left[1 + \frac{K(Mg)}{p(e)}\right]. \tag{2}$$

In the same manner reduced equations for various other elements were obtained. These were fed back into the detailed equilibrium equations for H, C, N and O using latest dissociation constants from GLUSHKO *et al.* (1962) and TATUM (1966). This was done because in DJN approximate dissociation constants were used in some cases. Thus, we obtained reduced equations for these elements also (see last column of Table I). These enabled us to calculate the free partial pressures of various diatomic molecules as a function of optical depth.

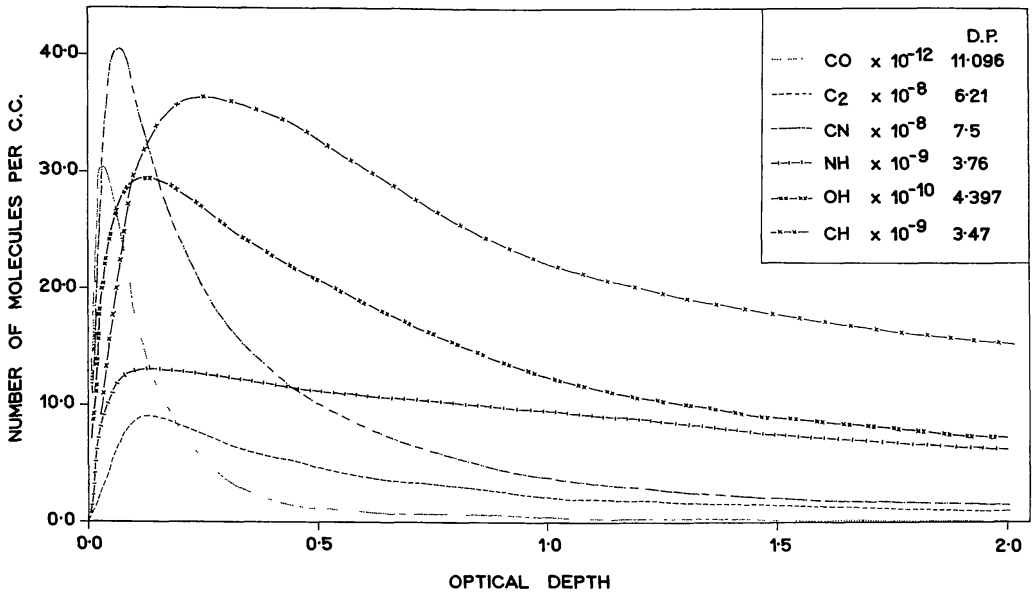

Fig. 1. Behaviour of CO, C_2, CN, NH, OH and CH with optical depth in URP. The concentrations are to be obtained by multiplying the ordinate scale by various factors, e.g., in case of CO a factor of 10^{12} is needed.

Figure 1 shows that the effective depths of formation for various molecules are different and as such the concept of a single molecular layer is an oversimplification. However, this has been realized before by SCHADEE (1968). Saturation effects in the theory of line formation have then to be accounted for differently in various cases. The approach for this may be that given by PANDE and SITNIK (1965) or some variation of it. All the information obtained from molecular lines such as rotational or other temperatures and abundances using elementary theory of curve of growth will then need revision.

The molecules LiH, BH, BF, MgF, LiF and other diatomic molecules of F except HF are, perhaps, not present in significant amounts in the solar photosphere. MOORE *et al.* (1966) indicated that most probably F may be absent in solar atmosphere though there is some evidence of MgF and BH being present in the solar photosphere (BROIDA and MOORE, 1957).

We find that SH, SiO and CS occur in significant concentration (cf. Figure 2). The number of these molecules above photosphere is comparable or of an order of magnitude greater than that of MgH detected by LABORDE (1961). For SH we have

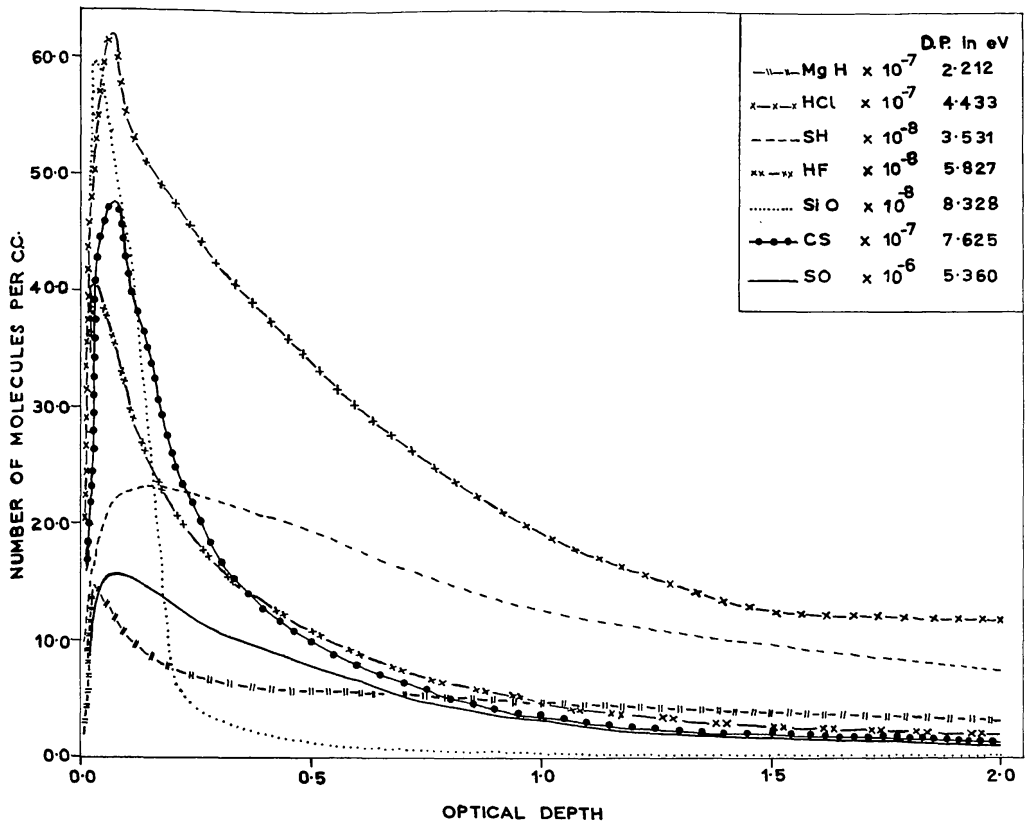

Fig. 2. Behaviour of MgH, HCl, SH, HF, SiO, CS and SO with optical depth in URP.

compared the wave numbers obtained by RAMSAY (1952) in the laboratory for $^2\Sigma$–$^2\Pi_i(a)$ transition with the solar absorption line wavelengths given by MOORE *et al.* (1966). The coincidences are within ± 0.02 Å to ± 0.05 Å for most of the lines and may be a pointer to the presence of SH in the solar photosphere.

We further find that HCl and HF also form in amounts comparable to MgH for the accepted values of abundances of Cl and F, i.e., those valid for the solar system in general. However, if they are lesser, then this conclusion may not hold.

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