Molecules in the Sun

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Abstract: In view of the already available reviews on the subject, the progress after 1972 is summarised. Newly identified species and molecular transitions are listed. How the studies of solar molecules can be helpful in understanding the solar atmosphere, in structuring better models and in deriving molecular parameters with some degree of confidence, is stated.

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1. Introduction

Broida and Moore (1957), Moore-Sitterly (1967) and Pande (1972) reviewed the progress in the field of solar molecules. As the subject continued to grow, transcending the 'solar barrier', it was realised that the Sun is only a representative star with molecular features and in fact reviews like 'Molecules in Stars' (Wurm 1957), 'Molecular Spectra in Stars' (Mallia 1974) and 'The Study of Small Molecules in Stellar Atmospheres' (Lambert 1977) may be presented. With the discovery of a myriad of molecular features in comets and the interstellar medium and the wealth of information gained from such studies, there can now be reviews like 'Molecules in Astronomy'. However, keeping in view the vastness of the subject and my limitations, the organisers of the present symposium have aptly decided to limit the discussions to the Sun only. Another review, on the same subject, is being prepared by Grevesse and Sauval for presentation during October 1990 at the Montpellier Colloquium on infrared spectra.

2. Studies of the Solar Molecules

Ever since Norman Lockyer suggested the presence of simple diatomic molecules CN and C_2 in 1878 (Meadows 1970, Brocklehurst *et al.* 1972) solar molecules have remained a subject of insatiable quests. The telluric molecules were studied with the help of solar spectroscopy (Herzberg 1965). Until 1928 only five molecules, i.e., C_2, CH, CN, NH and OH were known to be present in the Sun. By 1964 the list grew to eleven, including the molecules CaH, CO, MgH, SiH TiO and ZrO. The situation in 1967 and 1974 is compared in Table 1. One may immediately notice the addition of SiH in disk spectrum, CoH in spot spectrum and FeH in spot and disk spectrum as foreseen by Moore-Sitterly, though ZrO remains yet to be confirmed in identification.

As more and more spectral regions are becoming accessible with high quality low noise solar atlases, new molecular transitions are being discovered in the solar spectrum. Table 2 which should be treated as an addendum to Engvold and Hauge's (1974) compilation, lists several new transitions detected to date. Also presented in the same table are the molecular transitions expected to show up in later studies.

The difficult task of detecting molecular lines has now been made to look easy. Excellent resumes have been written by Schadee (1964), Sotirovski (1971) and Grevesse and Sauval (1973). These authors discuss the method of line coincidences and the computation of line intensities. The Russell-Bown formula for coincidences may now be supplemented with the Wavelength Coincidence Statistics (Hartoog *et al.* 1973) successfully employed in the case of the star R And (Cowley and Hensberge 1981). The normalisation procedure recommended by Whiting *et al.* (1980) and Larsson (1983) should be utilised for Hönl London factors. Based on the above, one may establish or refute the detection of certain species in the solar spectrum. O_2 and C_2 are no longer believed detected in the umbral spectrum and identification of CH^+ in the disk seems not secure (Sinha and Tripathi 1990a). Additional lines of the Swan bands of C_2, the violet bands of CN and the green bands of FeH have been detected in the disk spectrum (Porfireva 1981, 1982, 1983, 1987; Sinha and Mehrotra 1985). Thanks to sustained efforts for better molecular data (Berkeley News Letters), for better oscillator strengths (Lambert 1989) and for reliable estimates of elemental abundances (Grevesse 1989), the solar spectrum can now be understood with some confidence.

Several interesting aspects of molecules in the Sun include refining model atmospheres, identifying Fraunhofer lines, checking isotopic abundances, deriving oscillator strengths and molecular constants, checking departures from LTE and measuring magnetic fields in sunspots. Also, low-abundance elements, like Chlorine and Fluorine, may combine with Hydrogen to present detectable lines, thus leading to their abundance determinations.

Molecular lines are detected in the Flash Spectrum of the low chromosphere also during total eclipses of the Sun (Dunn *et al.* 1968) and in coronagraphic observations (Parker 1955). The fine effort of Thomas (1958) about understanding the low chromosphere with the help of CN lines, was somehow not followed up. We believe that the temperature determined by Blackwell (1955) depended on too few lines and involved some lines with weak or uncertain intensities.

3. Studies of the Solar Atmosphere

Since the molecules are known to be quite sensitive to their environs, it is only natural to enquire about what they say for the solar atmosphere. Studies of molecular lines at different centre to limb distances elicit information on temperature inhomogeneities (Withbroe 1968). The photosphere, spot and faculae, all have been subjects of continuous probes. Here, we concentrate upon work after 1972.

Hinkle and Lambert (1975) investigated the line forming mechanism in stars in general and in the Sun in particular. The excited electronic states seem to be populated by radiative excitation. Scattering rather than pure absorption seems to be the line forming mechanism in electronic transitions. Depth of formation and half widths, yield information on temperature, column density and the radial and tangential components of turbulent velocity (Sarychev 1982).

Tripathi *et al.* (1982a, b) investigated the different facula models in molecular lines. However, saturation was not accounted for in this study. Each molecule shall now be taken separately to see what has been learnt from its Sun-related studies.

CH

Drake and Ehzerivish (1984, 1985, 1986) investigated the $A^2\Delta - X^2\Pi$ transition at several centre to limb distances and calculated number densities in a photospheric model. It is shown that these lines are formed much below the temperature minimum. The importance of similar studies is highlighted by Pechinskaya (1976) and Erofeev and Solonskij (1982). Large turbulence velocities are deduced by Punetha and Joshi (1984b).

Table 1. Molecular transitions discovered in the Sun up till 1974

Engvold and Hauge (1974) and Mallia (1974)			Moore-Sitterly (1967)		
Disk	Spot	Possibly identified	Disk	Spot	Future work
	AlH	in disk			
C_2		FeH	C_2	C_2	C_2 (extend identifications when Berkeley monograph appears)
	CaH	in spot		CaH	
CH	CH	AlF	CH	CH	
CH^+		AlO			
CN	CN	BaO	CN	CN	SiH? (needs further study, may be present in disk spectrum; borderline case)
CO	CO	BeH	CO		
	CoH	BH			
	CuH	BO			
	H_2O	FeO			FeH, CoH (possibly present; further study needed)
	HCl	LaO			
	HF	MgH			
MgH	MgH	ND	MgH	MgH	
	MgO	O_2			
NH	NH	SiO	NH		
	NiH	VO			
OH	OH	ZrO	OH		
SH					
SiH	SiH			SiH	
SiH^+					
	SiO				
	TiO			TiO	
				ZrO	

CN

Tripathi and Sinha (1986) showed that the lines of the red system may serve as diagnostic tools for faculae.

Mount *et al.* (1973) and Mount and Linsky (1974a, 1975) studied photospheric spectra of the violet bands at various centre-to-limb positions by taking into account non-LTE effects and one- and multi-component model atmospheres and recommended a low carbon abundance which was found in agreement with similar analysis of CH lines (Mount and Linsky 1974b). It is believed that the uncertain choice of molecular data, such as dissociation energy and oscillator strengths played a crucial role in abundance determination which, however, is in surprising agreement with the studies of CO lines by Tsuji (1977a).

CN lines with different rotational quantum numbers are formed in about the same layers of the photosphere (Porfireva 1976). Contribution functions for the centre of the disk are slightly different from those at the limb. Earlier determination of turbulent velocity was improved to $\pm 2.1\,\mathrm{km\,s^{-1}}$ (Porfireva 1986).

CO

The molecule forms high in the photosphere and close to the lower chromosphere. It is considered to be a good probe for sensing temperature inhomogeneities, temperature minima and departures from LTE.

Noyes and Hall (1972) studied the centre-to-limb variation of lines at 4.66μm and obtained temperatures as low as 3500 K near the limb. Under LTE, this indicates the presence of material at low temperature in the quiet upper photosphere. Evidence is also found to show that the material with 3500 K brightness temperature may exist in intergranular lanes. Also five minute oscillations in intensity with amplitudes corresponding to several hundred degrees in brightness temperature are also found. Ayres (1978), Ayres and Testerman (1981) and Ayres *et al.* (1986) studied the above behaviour and suggest future areas of research. Similar conclusions were arrived at by Muchmore and Ulmschneider (1984, 1985) and Muchmore *et al.* (1988). Kalkofen (1985) argues that the bi-stable character of bifurcated models is only postulated through the assumption concerning the opacity sources and the effect of mechanical waves, which are allowed to destroy CO molecules, without heating the gas. Also, the role of metallic lines towards cooling seems underestimated.

Tsuji (1977a,b) carefully tried to determine the rotational temperature of first overtone bands of CO and argues in favour of a single component model due to Vernazza *et al.* (1976).

MgH

Several possibilities, e.g., presence of umbral dots (Lambert *et al.* 1971), role of blurring and stray light (Sinha 1982), influence of lateral influx of the photospheric radiation (Yun and Kim 1983) and the possibility of rapid photodissociation (Dutta *et al.* 1983) have been suggested to explain smaller than predicted equivalent widths.

Table 2. Molecular transitions discovered in the Sun in and after 1974

Molecule	Transition	Reference	Remarks	Future Work
C_2	$A^1\Pi_u - X^1\Sigma_g^+$	Lambert and Mallia (1974)	disk	disk and/or facula
		Brault *et al.* (1982)	disk	detailed investigations needed on AlH^+ ($A^2\Pi - X^2\Sigma$) C_2 ($b^3\Sigma_g - a^3\Pi_u$), ($D^1\Sigma_u^+ - X^1\Sigma_g^+$)
CH	Vib-rot	Sauval and Grevesse (1985),	disk	CaH^+
		Grevesse *et al.* (1987)	disk	CH^+ ($b^3\Sigma - a^3\Pi$)
CO	Vib-rot	Grevesse *et al.* (1987)	disk	CO^+ H_2^+
	$A^1\Pi - X^1\Sigma^+$	Jordan *et al.* (1977)	spot & flare	MgH^+ ($A^1\Sigma - X^1\Sigma$)
		Sandlin *et al.* (1986)	disk & spot	NH ($c^1\Pi - a^1\Delta$) NH^+
CrH	$^6\Sigma - ^6\Sigma$	Engvold *et al.* (1980)	disk & spot	OH^+ ($A^3\Pi_i - X^3\Sigma^-$) PH($A^3\Pi_i - X^3\Sigma$)
FeH	$^4\Delta - ^4\Delta$	Carroll *et al.* (1976)	disk & spot	SH ($A^2\Sigma^+ - X^2\Pi_i$)
		Wing *et al.* (1977)	spot	SH^+ ($A^2\Sigma^+ - X^2\Pi_i$)
		Wöhl *et al.* (1983)	spot	SiH^+ ($A^1\Pi - X^1\Sigma$)
H_2	$B^1\Sigma_u^+ - X^1\Sigma_g^+$	Jordan *et al.* (1977)	disk & spot	spot CO_2
		Brueckner *et al.* (1978)	disk & spot	MgH (vib-rot)
		Sandlin *et al.* (1986)	disk & spot	MgH^+($A^1\Sigma^+ - X^1\Sigma^+$)
		Bartoe *et al.* (1979)	spot & flare	NO (vib-rot) $A^2\Sigma^+ - X^2\Pi_{1/2}$)
	$C^1\Pi_u - X^1\Sigma_g^+$	Bartoe *et al.* (1979)	spot	O_2 ($B^3\Sigma_u - X^3\Sigma_g$) PH ($A^3\Pi_i - X^3\Sigma^-$) PO ($B^3\Sigma^+ - X^2\Pi$)
NH	Vib-rot	Grevesse *et al.* (1987)	disk	SH ($A^2\Sigma - X^2\Pi$)
OH	Vib-rot	Grevesse *et al.* (1987)	disk	SiH (vib-rot)
	$A^2\Sigma - X^2\Pi$	Moore *et al.* (1981)	disk	SiO ($A^1\Pi - X^1\Sigma^+$)
SiO	Vib-rot	Glenar *et al.* (1983)	spot	
	$A^1\Pi - X^1\Sigma$	Moore *et al.* (1981)	disk	
	$G^1\Pi - X^1\Sigma$	Sandlin *et al.* (1986)	disk & spot	

OH

The anomalous weakening of the pure rotation line of OH is attributed to the increased source function owing to the nearby Mg emission lines (Deming *et al.* 1984a). The $v = 0R_{22}(24.5)e$ line strengthens at the solar limb, contrary to expectations based on one dimensional photospheric models (Deming *et al.* 1984b).

SiO

Observed line widths suggest an upper limit of 0.5 km s^{-1} for the microturbulent velocity in sunspot umbrae. Also, it is supposed to yield better umbral models (Glenar *et al.* 1983).

Until recently, photospheric models HM (Holweger and Müller 1974) and MACKKL (Maltby *et al.* 1986) could be considered fairly good representations of the solar photosphere (Sinha and Tripathi 1990a). Grevesse *et al.* (1987) report that the strongest pure rotation lines of OH cannot be accounted for by the HM model; also for CO they find $W_{(obs)} > W_{pred}$ for the strongest lines and $W_{(obs)} < W_{pred}$ for the fainter lines in their study. W is equivalent width. An attempt to construct a model yielded better fits for CO observations but increased the disagreement in the case of OH. Perhaps with a set of a great number of very high-quality data from ATMOS (Atmospheric Trace Molecule Spectroscopy) being avaiilable, the problems related to non-LTE effects, thermal bifurcation etc. can be examined with an unprecedented level of confidence. Further work is in progress.

Regarding better sunspot models with conventional techniques, we suggested a simultaneous study of photosphere and umbra in the C_2, MgH and TiO lines around 5200 Å (Sinha and Tripathi 1990b,c). The method automatically accounts for scattered photospheric radiation. It will also help in a study of the evolution of a pore into a large sunspot during different cycles of solar activity.

4. Excitation Temperature

The molecular spectrum of the Sun allows one to determine temperatures of the line-forming layers in terms of vibration temperature, rotation temperature and electronic temperature which, in the case of LTE and under the assumption of thin layer formation of lines, should be equal (Pande 1972). However, it is extremely important to use cautiously the assumptions and the method involved (Cowley 1964; Sinha 1979a). Analysing

CO lines, Sarychev (1978) clearly demonstrated that allowance must be made for (i) the optically thick layer of line formation and (ii) the possibility of re-emission in lines. A neglect of these may lead to high values of rotational temperatures and a false rise in temperature towards the limb. Such an affect was noticed by Sinha (1979b) in C_2 lines and a possible solution to the problem was provided (Sinha 1984b). Persi (1975) suggested a numerical method for the analysis of the solar photospheric spectrum. Sarychev (1980), later revised his own calculations to deduce T = 4510 K.

High quality spectra obtained in a balloon-borne experiment enabled Goldman *et al.* (1973) to determine the excitation temperature as 4500 K from CO vibration–rotation lines. Also from an analysis of the fourth positive system of the same molecule an effort has been made to determine the solar minimum temperature (Macris and Petropoulos 1985).

A model-based study of C_2, CH, CN, CO, NH and OH lines at different centre-to-limb positions lead Khlystov (1972) to conclude that the temperature varies within ±100 K towards the solar limb. Pande *et al.* (1980) observed that the rotational temperature appears unchanged towards the limb. Similar conclusions are drawn by Porfireva (1973). Molecular line formation and the rotational temperature of TiO has been critically examined by Boyer and Sotirovski (1973) and Boyer (1978). The observed rotational temperature of TiO was found in agreement with calculations in Zwaan's (1974) sunspot model (Sinha 1977). Extending his earlier work, Boyer (1980) examined four sunspot models and gave his own. He also suggests that coherent scattering is more likely to be the line-forming mechanism for TiO lines.

Model testing and model structuring with the help of rotational temperature has been an interesting area of study (Webber 1971; Dubey and Tripathi 1979; Sinha *et al.* 1979 and Punetha and Joshi 1984a). However, Khlystov (1974), on the basis of theoretical calculations believes that the excitation temperatures of molecules cannot be used to determine the physical conditions in the solar atmosphere because of a large scatter found in the observations.

A low temperature of 1740 ± 100 K for FeH lines, recently, led Mulchaey (1989) to suggest that the molecule is probably present in higher layers of sunspots than previously studied molecules or else the rotational temperature is non-thermal.

5. Abundances of Elements

Data from a large number of pure and unblended molecular lines are used to derive elemental abundances. In a recent compilation Grevesse (1989) critically reviewed the abundances.

The C, N, O and Na to Ca abundances have been determined by Lambert (1978) and Lambert and Luck (1978). Analysis of pure rotation and vibration-rotation spectra of the hydroxyl radical yields $\log N(O) = 8.92 \pm 0.035$ (Goldman *et al.* 1983, Sauval *et al.* 1984, Grevesse *et al.* 1984). Similar analysis of high quality data on NH and CH yields $\log N(N) = 8.00 \pm 0.05$ (Grevesse *et al.* 1990) and $\log N(C) = 8.60 \pm 0.05$ (Grevesse *et al.* 1990). Other carbon indicators are also utilised in the investigation.

Isotopic abundances of Carbon and Oxygen have been determined by Harris *et al.* (1987). The $^{13}C/^{12}C$, $^{18}O/^{16}O$ and $^{17}O/^{16}O$ ratios are expected to be determined with unsurpassed accuracy (Grevasse *et al.* 1987). Isotopic lines of SH and SiO are predicted observable for abundance analyses (Pande and Joshi 1978; Joshi *et al.* 1979; Joshi and Pande 1979).

6. Derivation of Molecular Parameters

Derivation of parameters like oscillator strengths and dissociation energies from the solar spectrum, though model dependent and abundance dependent, often help in arriving at acceptable values. A critical and exhaustive compilation was made by Grevesse and Sauval (1973) and it was rightly indicated that the only estimates for MgH could be in error. Similar conclusions were drawn for CH^+ (Grevasse and Sauval 1971). The oscillator strength for the (O-O) band of the Phillips system has been a subject of controversy in recent years. Solar estimates were arrived at by Lambert and Mallia (1974), Brault *et al.* (1982) and Sinha (1984a). In a recent paper Grevesse *et al.* (1990) revised Brault *et al.*'s (1982) estimates and find them in agreement with other investigations. Analyses of CH lines (Sauval and Grevesse 1985, Chmielewski 1984), CN lines (Sneden and Lambert 1982, Sinha and Tripathi 1986, Erdelyi-Mendes and Barbuy 1989), MgH lines (Sinha 1981) and TiO lines (Lambert and Mallia 1972) for dissociation energy and oscillator strength estimates are available.

7. Effect of Magnetic Fields and Oscillation Spectrum of the Sun

Since spots are known to possess strong magnetic fields, molecular lines are expected to be influenced. Polarisation of the red system of CN lines has been studied by Harvey (1973) and new features in the oscillatory spectrum of the Sun have been detected by Kneer *et al.* (1982).

8. Conclusions

In the above summary we have been able to show the diverse fields in which molecular lines may be of use. We believe that flash spectrum with waxing and waning of the solar crescent at the time of third and fourth contact during total solar eclipses can be of some help in structuring the lower chromosphere with precision.

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