

THE SUN AS A LABORATORY SOURCE FOR IR MOLECULAR SPECTROSCOPY

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Abstract. The infrared solar spectrum is used to refine our knowledge of molecular constants of CH and CO and to test the accuracy of transition probabilities and dissociation energies of a few diatomic molecules.

Key words: : infrared: stars – molecular data – Sun: atmosphere

1. Introduction

In the past the Sun itself has proven to serve as a good laboratory source for atomic as well as molecular spectroscopy. Let us only quote two different investigations related to the CO molecule and based on the IR solar spectrum: the pioneering determination of the spectroscopic constants by Goldberg and Müller (1953) and the relative transition probabilities derived by Tsuji (1977). As accurate molecular data are still lacking for a few molecular species of astrophysical interest, we use the many molecular transitions present in the solar infrared spectrum to refine our knowledge. A summary of the advantages and disadvantages of using the solar spectrum is shown in Table I.

The spectroscopic data are deduced from infrared solar spectra recorded by the *ATMOS* experiment onboard the Space Shuttle in April/May 1985 (Spacelab 3 flight; Farmer and Norton, 1989) and from ground-based observations obtained at Kitt Peak (Delbouille *et al.*, 1981).

2. Spectroscopic Constants

2.1. CH X²Π

The *ATMOS* solar spectra show the vibration-rotation lines of the 1-0, 2-1 and 3-2 bands to much higher N'' -values (>30) than laboratory spectra ($N'' = 9$). The 4-3 band, which was not seen in the laboratory (in the days of our investigation), even shows up in the solar spectrum (Fig. 1).

We used solar wavenumbers together with laboratory wavenumbers to refine the molecular constants of the CH ground state (Mélen *et al.*, 1989).

2.2. CO X¹Σ

Over 2000 new very high J'' -value solar lines ($J''_{\max} = 133$) for v'' -values up to 19 of the fundamental and first-overtone bands, never seen in the laboratory ($J''_{\max} = 94$), clearly appear on the *ATMOS* solar IR spectra (σ 1350–4360 cm⁻¹) (Fig. 2).

TABLE I
The Sun – a very good source for spectroscopic studies

ADVANTAGES
<ul style="list-style-type: none"> - very stable source (permanent!) - high temperature (high-excitation lines which are not seen in the laboratory) - good representative model of the photospheric layers <ul style="list-style-type: none"> - accurate determination of the physical conditions (T, P, N) - equilibrium conditions (LTE): Boltzmann, Saha, Guldberg-Waage laws are valid
DISADVANTAGES
<ul style="list-style-type: none"> - broad solar lines as compared to IR laboratory lines - large wavelength shifts <ul style="list-style-type: none"> - relative motion Sun/observer - rotation of the Sun - Einstein gravitational redshift - convective motions (intensity-dependent shift!) <ul style="list-style-type: none"> - about 0.003 cm^{-1} between strong and weak CO lines - gradual violet shift from strong to weak lines - very accurate laboratory line positions needed to convert to rest wavelengths

Combining the new solar wavenumbers with the available laboratory data (14000 measurements) has permitted to derive a new set of 31 spectroscopic constants which allows to predict wavenumbers with high accuracy from low to high J'' -values (Farrenq *et al.*, 1991).

2.3. OTHER MOLECULES

New molecular transitions, never observed in the laboratory, have been measured in the IR solar spectrum such as pure rotation lines of NH ($X^3\Sigma, v = 0, 1$) near $600\text{--}900 \text{ cm}^{-1}$ (see Fig. 3, from Geller *et al.*, 1991).

3. Transition Probabilities and Dissociation Energies

The line absorption coefficient of a molecule AB depends on the line oscillator strength, f_{vJ} , on the dissociation energy, D_0^0 , and on the number densities of the relevant atoms, N_A and N_B . From this well-known relationship in the solar photosphere, one can derive a very useful relation: $\Delta \log f_{vJ} \approx -\Delta D_0^0$ (eV)

3.1. C₂ PHILLIPS SYSTEM (A ¹Π_u - X ¹Σ_g⁺)

Both the dissociation energy of C₂ and the transition probability of the Phillips system are still rather uncertain. The combined use of C₂ (Swan and Phillips sys-

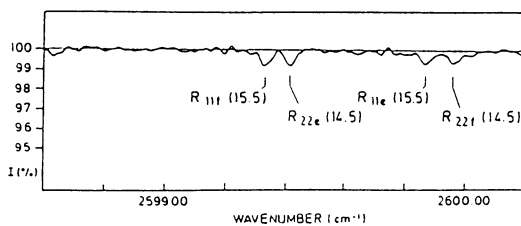


Fig. 1. Lines of the 4-3 band of CH in the *ATMOS* IR spectrum.

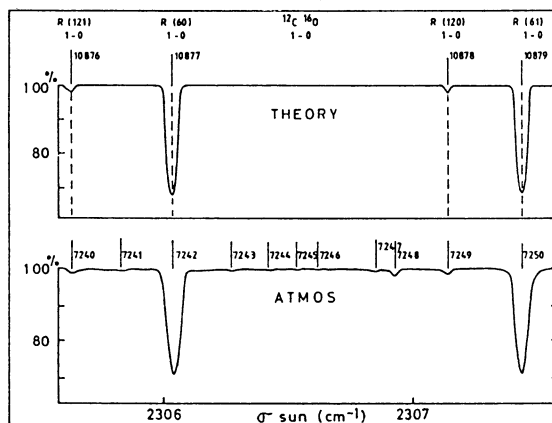


Fig. 2. $^{12}\text{C}^{16}\text{O}$ lines of the 1-0 band with $J'' = 60, 61, 120$ and 121 in the IR solar spectrum (*ATMOS*).

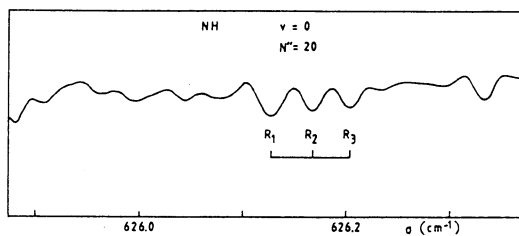


Fig. 3. First detection of pure rotation lines of NH ($X^3\Sigma v = 0$) in the IR solar spectrum near 626 cm^{-1} (*ATMOS* spectra).

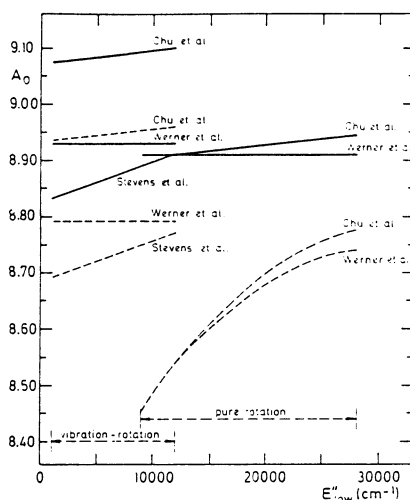


Fig. 4. The solar abundance of oxygen A_{O} must be independent of the excitation potential of OH lines (such as for Werner *et al.*'s EDMF). Results for two different photospheric models: Holweger-Müller 1974 (full lines) and Vernazza *et al.* 1976 (dashed lines) are shown. See Grevesse *et al.* (1984) for all references.

tems) together with other indicators of the solar abundance of carbon has enabled us (Grevesse *et al.*, 1991) to derive $D_0^0 \simeq 6.23$ eV and f_{00} (Phillips system) = 2.28×10^{-3} in agreement with the most recent theoretical result of Langhoff *et al.* (1990), but 50% larger than the most recent experimental result (Bauer *et al.*, 1986).

3.2. THE CN RED SYSTEM

The dissociation energy of CN is still a matter of debate. Combining the recent theoretical results for the transition probability that is supposed to be accurate, together with solar abundances of C and N derived independently, the solar intensities of our infrared CN lines are reproduced with $D_0^0 \simeq 7.75$ eV (Grevesse and Sauval, 1992), in agreement with two very recent measurements (Costes *et al.*, 1990; Huang *et al.*, 1992), and ruling out lower values of D_0^0 often used in the recent past.

3.3. TEST OF THE ELECTRIC DIPOLE MOMENT FUNCTION (EDMF) OF OH

We showed (Sauval *et al.*, 1984; Grevesse *et al.*, 1984) how sensitive the solar vibration-rotation and pure rotation lines are to the EDMF (Fig. 4).

Those lines have been remeasured in the *ATMOS* solar infrared spectra up to high rotational excitation.

The new EDMF of Nelson *et al.* (1990) leads to a very good agreement between observations and predictions from low to high N'' values.

3.4. CO $X^1\Sigma^+$

In the high resolution and low noise *ATMOS* solar spectra (Farmer and Norton, 1989) more than 7000 vibration-rotation lines of the fundamental $^1\Sigma^+$ state of four isotopic species of carbon monoxide ($^{12}\text{C}^{16}\text{O}$, $^{13}\text{C}^{16}\text{O}$, $^{12}\text{C}^{18}\text{O}$ which is about 500 times less abundant than $^{12}\text{C}^{16}\text{O}$; and eventually, for the first time in the solar photospheric spectrum, $^{12}\text{C}^{17}\text{O}$ which is about 2500 times less abundant than $^{12}\text{C}^{16}\text{O}$) are detected in the spectral range σ 1350–2328 cm^{-1} (fundamental bands, from 1-0 to 20-19) and σ 3410–4360 cm^{-1} (first overtone bands, from 2-0 to 14-12).

The dissociation energy of CO is known with high accuracy. But solar CO lines are extremely sensitive to the photospheric temperature structure. The available transition probabilities (Chackerian and Tipping, 1983) for medium and high J'' -values observed in the *ATMOS* solar IR spectrum might not have the accuracy required for a precise comparison between observations and predictions. Abundances derived from the fundamental and first overtone bands slightly disagree. Very accurate transition probabilities are urgently needed up to high J'' -values for the different isotopes present in the solar infrared spectrum.

3.5. OTHER MOLECULES

We have also tested the EDMF for vibration-rotation spectra of CH ($X^2\Pi$ 1-0, 2-1, 3-2, 4-3 bands) and of NH ($X^3\Sigma$ 1-0, 2-1 bands) and for pure rotation spectra of NH ($X^3\Sigma$, $v = 0, 1$) (see Grevesse *et al.*, 1990, 1991).

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