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On the oscillator strength and the dissociation energy of CN molecules

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Abstract. We compute the equivalent widths of CN red system in the solar spectrum and compare them with the observational data, in order to choose between various published oscillator strengths (f_{0-0}) and values of dissociation energy (D_0^0). It is found that the Holweger & Müller (1974) photospheric model, along with $f_{0-0} = 1.9 \times 10^{-3}$ and $7.66 < D_0^0$ (CN) < 7.76 eV, gives results consistent with the red system observed in the photospheric spectrum. The same range of dissociation energy can also be used for the violet system without involving increased UV opacity.

Key words : CN molecules—solar spectrum

1. Introduction

We have a program to test different facular models with the help of molecular lines (Tripathi, Sinha & Pande 1982; Tripathi, Pande & Sinha 1982). However, when we look into the laboratory parameters like the dissociation energy and oscillator strength of the molecules CN, some contrasting values are obtained. Grevesse & Sauval (1973) obtain $7.5 < D_0^0$ (CN) < 8.4 eV, whereas Larsson, Siegbahn & Ågren (1983) get D_0^0 (CN) $= 7.00$ eV correctable to $7.4 < D_0^0$ (CN) < 7.7 eV from *ab initio* calculations. Also the latter authors give f_{0-0} value for the red system of the molecules CN which is a factor of about two higher than that due to Lavendy, Gandara & Robbe (1984) and Sneden & Lambert (1982). Uncertain value of D_0^0 (CN) has recently been reported from a recent laboratory investigation (Lambert *et al.* 1984).

The importance of the accuracies involved in these parameters can be realized from the following. The line strength of a weakly saturated CN line is given as

$$S \propto N(C).N(N) f_{v',v''} 10^{D_0^0(CN).\theta} \qquad ...(1)$$

where the symbols have their usual meaning (Grevesse & Sauval 1973). For the solar photosphere, if the dissociation energy is changed by about 0.3 eV only, the

line strength will be changed by a factor of two. Clearly, we need a good pair of oscillator strength and dissociation energy for use in a standard model atmosphere. To achieve this objective we use the red and the violet systems of the CN molecules as observed in the solar spectrum and put the D_0^0 and $f_{v'v''}$ value for the $(0-0)$ band given by Sneden & Lambert (1982) to test. Because of its extensive nature, we prefer Sneden & Lambert's (1982) investigation to that of Lavendy, Gandara & Robbe (1984).

2. Formulation and calculations

The important factors for the model based calculation of equivalent width are given as under. The abundance of the carbon and nitrogen atoms for the Holweger & Müller's (1974) model and the oscillator strength for the violet system are from Lambert (1978). In different investigations (Lambert 1978: Sauval *et al.* 1984; Sinha 1984), Holweger & Müller's (1974) photospheric model is found better than others. Schadee (1964) and Kovacs (1969) provide the source for the rotational line strengths. The different normalizations for these factors were accounted for. Molecular constants are from Huber & Herzberg (1979) and opacities from Tsuji (1966). The observed equivalent widths were taken from Grevesse & Sauval (1973) and Lambert (1968).

3. Results and discussions

About 70 lines for the red system were taken from Grevesse & Sauval (1973) for investigation. In figures 1a, b the theoretical results based upon D_0^0 (CN) = 7.66 eV are plotted against the observed values of equivalent widths. The small scatter $\simeq 20\%$ is an argument in favour of the value of $f_{0-0} = 1.9 \times 10^{-3}$ due to Sneden & Lambert (1982).

In figures 2a, b we fit a straight line with slope 45° between the calculated and the observed values of equivalent widths. The small deviations in the calculated

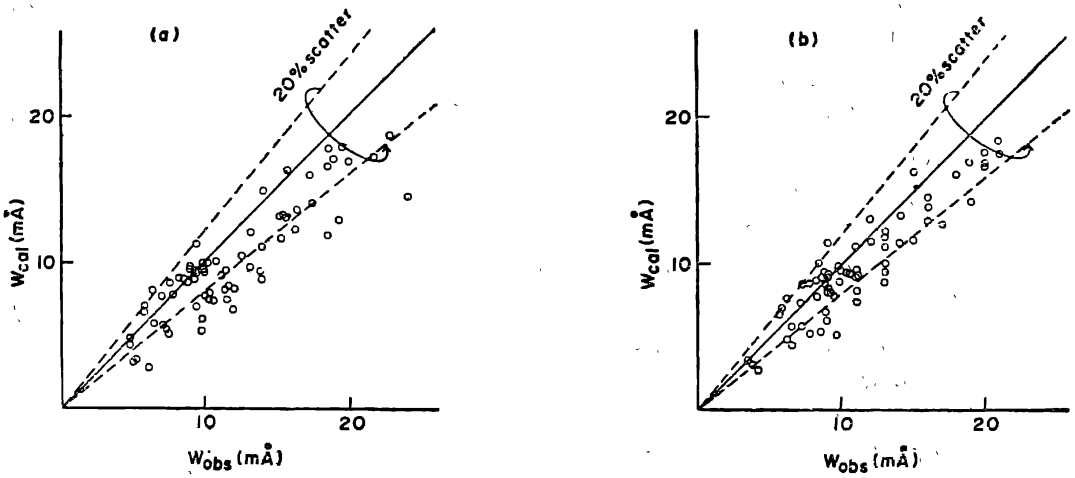

Figure 1. Calculated and observed equivalent widths of the lines of the (0—0) band of the red system of CN molecules. D_0^0 (CN) = 7.66 eV was used in calculations. Figure (a) uses the observations from Grevesse & Sauval (1973) whereas figure (b) uses those of Lambert (1968).

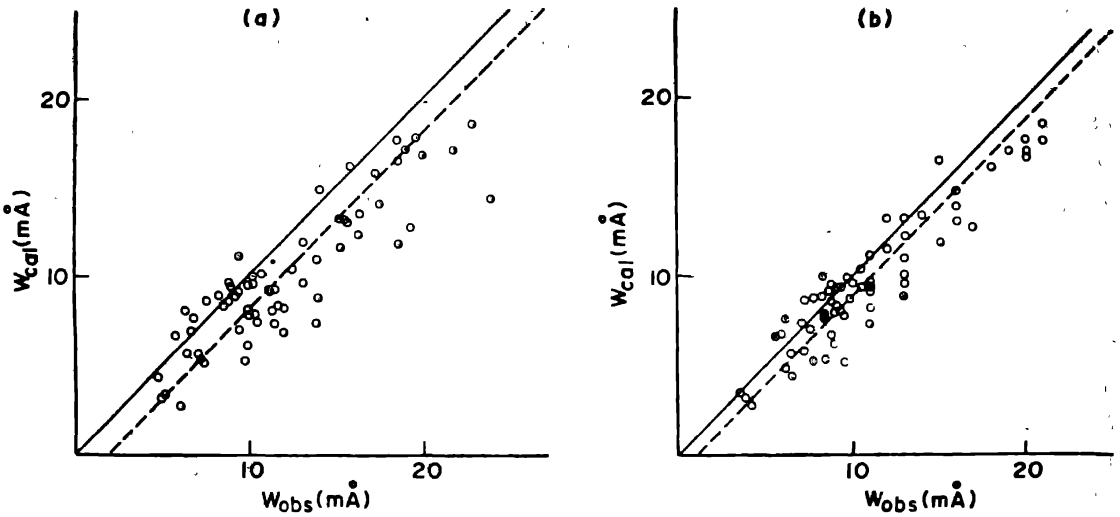

Figure 2. Same as figure 1. The distance between the dotted line and the solid line is a measure of the needed change in the dissociation energy (*cf.* text).

and the observed values of the equivalent widths can be removed by slightly changing the dissociation energy. The amount of the needed change in D_0^0 can be assesed with the help of the intersection of the dotted line with the x-axis; the principle involved being a shift of the dotted line in such a way that it coincides with the solid line. The same objective can also be achieved by obtaining an average value of (W_{cal}/W_{obs}) which in ideal case should be 1. The average values are 0.854 ± 0.17 in case of observations from Grevesse & Sauval (1973) and 0.905 ± 0.15 in case of Lambert (1968). These values yield $\Delta D_0^0 = 0.08$ eV and 0.05 eV respectively for the above two cases. Another value of D_0^0 close to these changes is 7.76 eV (Huber & Herzberg 1979). We repeated the calculations for D_0^0 (CN) = 7.76 eV and the results are plotted in figures 3a and 3b. The average value of (W_{cal}/W_{obs}) is now 1.064 ± 0.21 and 1.127 ± 0.19 in case of observations from Grevesse & Sauval (1973) and Lambert (1968) respectively. The shift of points in figure 3b to the other side of the 45° line (as compared with figure 1b) tends to indicate that 7.76 eV is a slightly large dissociation energy. Thus it appears that within the scatter involved in the solar observations the dissociation energies used here represent the upper and the lower limits of D_0^0 and therefore $7\,66 < D_0^0\,(CN) < 7.76$ eV.

It is heartening to find the value of $f_{0-0} = 2.54 \times 10^{-3}$ (for the red system) from a recent effort of *ab initio* calculations by H. J. Werner, P. J. Hay & D. C. Cartwright (1984, personal communication). However, the D_0^0 (CN) given by these authors as 7.0 eV is rather low.

In figures 4a, b we present the results for the $\Delta v = 0$ sequences of the violet system with D_0^0 (CN) = 7.66 eV and D_0^0 (CN) = 7.76 eV respectively. The observed values are from Grevesse & Sauval (1973). These figures further support our viewpoint regarding the dissociation energy. We believe that the discrepancy reported by Grevesse & Sauval (1973) and quoted by Sneden & Lambert (1982) in favour of increased UV opacity can alternatively be explained as follows.

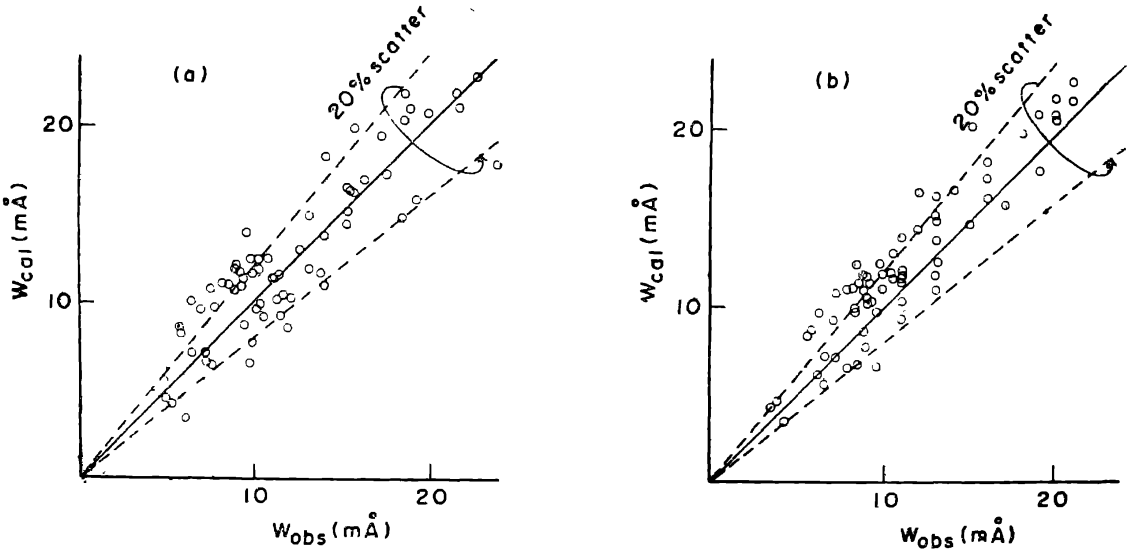

Figure 3. Same as figure 1 but for D_0^0 (*CN*) = 7.76 eV.

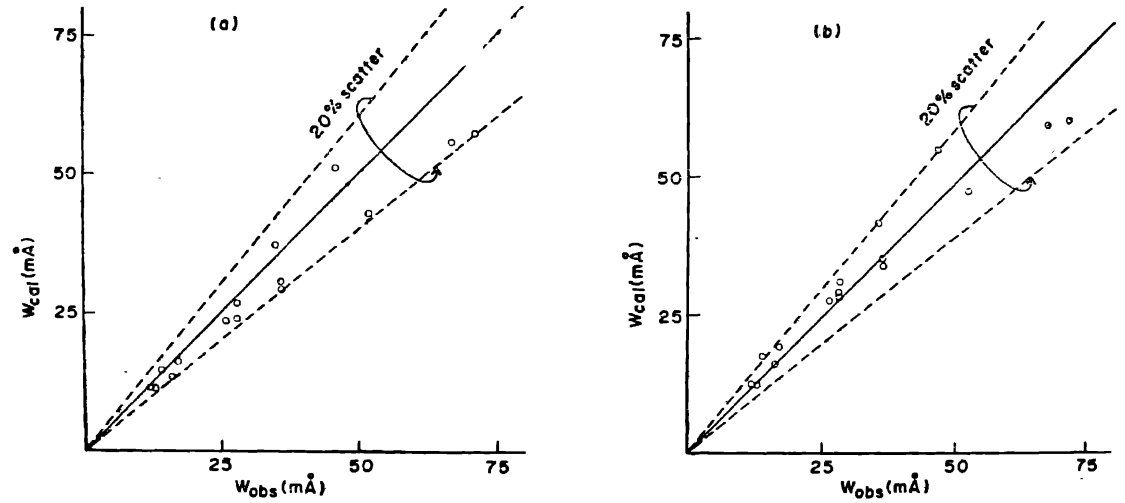

Figure 4. Calculated and observed equivalent widths of the lines of the $\Delta v = 0$ sepuences of the violet system of CN molecules. Figure 4a uses D_0^0 (CN) = 7.66 eV and figure 4b D_0^0 (CN) = 7.76 eV. Observed values are from Grevesse & Sauval (1973).

For their calculations Grevesse & Sauval (1973) adopt elemental abundances of carbon and nitrogen derived by Lambert (1968). It may be noted that the values for the oscillator strengths used in both the investigations are practically the same whereas those of D_0^0 are very much different (Lambert: 7.5 eV; Grevesse & Sauval: 7.89 eV). A high value for D_0^0 leads to large CN concentrations and thus to large calculated equivalent widths. If D_0^0 = 7.89 eV is to be used together with the quoted values of oscillator strengths, then a reanalysis of Lambert's (1968) work would lead to lower C and N abundances than those used by Grevesse & Sauval (1973).

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