

ON THE GF-VALUES FOR SOME DIATOMIC MOLECULAR SPECTRA

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ABSTRACT. In view of rich structure of the energy levels and the variety of transition types which are observable, molecules are the useful tool for investigation of physical parameters of stellar atmospheres, interstellar and circumstellar matter, such as gas density, its temperature, chemical and isotopic composition, ionization degree, radiation field density, kinematics, etc. The success of investigations is defined to a considerable extent by the amount and reliability of spectral information used. The molecular radiative coefficients must be calculated for a huge number of spectral lines, involving rather weak lines. These calculations are performed using spectral line lists containing such parameters as positions of line centres, lower level energies, transition probabilities, and, in a number of cases, broadening parameters.

Key words: Molecular spectra: Molecular bands: Oscillator strengths.

At present several scientific teams are engaged in the creation of such lists. The most complete lists for diatomic molecules are prepared by Kurucz (1993). These lists contain more than fifteen million lines belonging to various electronic spectra H₂, CH, OH, NH, MgH, SiH, C₂, CO, CN, TiO. Only a small part of lower level energies and transition frequencies are from laboratory data, all values gf are calculated. The functions of electronic transition moments needed for such calculations were taken from quantum-chemical researches or proper experimental measures.

The most of Kurucz' calculations were made more than fifteen years ago. Since then a large amount of results, both experimental and theoretical, have been obtained extending and refining our knowledge about the structure of energy levels for molecules indicated and their radiative properties. Therefore, refining and extension of Kurucz's data base are supposed, and the first step must be the analysis of all information available on spectral and radiative properties of astrophysically important diatomic molecules for selection of the most reliable values.

We do such a work for some molecular systems, commonly used for determining the abundances of the

light elements (C,N,O) and isotopic ratio ¹²C/¹³C in the late-type star atmospheres, on the base of information and program units containing in the RADEN data bank (Moscow) and program complex "MOLEC" (Kiev).

The most reliable information about electronic transition moments for relatively light molecules can be obtained from quantum-chemical calculations controlled by lifetime measurements. Note that for the light molecules, taking into account of vibrational-rotational interaction is rather essential. The influence of rotation on vibronic wave function can be taken into account in the solution of Schredinger's nuclear equation with effective interatomic potential, involving the rotation energy. We have calculated the gf-values for some rotational lines according to the normalization rule from (Whiting et al. 1980) and have compared them with the Kurucz's data.

In Table 1. we compare the Kurucz's values of gf with our ones calculated in a) R-centroids approximation, using the data from Kuznetsova (1987); b) with ab-initio calculation of $f_{\nu'\nu''}$, controlled by lifetime measurements and c) those as b) but with rotational correction of $f_{\nu'\nu''}$. The asterisk in a) means the constant S_e for the system (see Kuznetsova (1987)). The data used for ab-initio calculations are taken from papers (Hetteema and Yarkony (1994) for CH, Kirby and Goldfield (1991) for NH, Arnold and Landhoff (1978) for C₂, Kirby et al. (1979) for MgH, Larsson (1987) for SiH). We noted that Kurucz's list for Swan C₂ system ($D^3\Pi - A^3\Pi$) included only one lambda component of ¹²C₂ but two lambda components of ¹³C¹²C lines with the same values of gf. In the case of homonuclear molecule ¹²C¹²C the statistical weight of level must be twice as much as for heteronuclear ¹³C¹²C (even-odd alternation). For Swan system ¹²C₂ lines of Kurucz's list we can double the gf-values. Note that our value $f_{00}=2.91E-02$ for C₂($D^3\Pi - A^3\Pi$) system almost the same as $f_{00}=2.8E-02$ in Grevesse et al. (1991).

The isotopic ratio ¹²C/¹³C is often determined from the spectra of the CN red system near 8000 Å. We have noted that positions of ¹³CN lines in Kurucz's list are displaced on 0.7-0.8 Å in the violet relative the

Table 1. $\lg gf$ -value

	wavelength (Å)	Kurucz's value, 1993	our values a)	b)	c)
CH($A^2\Delta - X^2\Pi$)					
(0-0) R _{1c} (10.5)	4248.941	-1.30	-1.40*	-1.43	-1.44
(1-1) R _{2d} (10.5)	4247.562	-1.36	-1.38*	-1.49	-1.50
(2-2) R _{2d} (11.5)	4262.594	-1.39	-1.35*	-1.51	-1.53
(0-1) Q _{1c} (16.5)	4835.268	-2.49	-3.17*	-2.55	-2.66
(3-4) Q _{1c} (11.5)	4835.224	-2.32	-3.87*	-2.51	-2.58
NH($A^3\Pi - X^3\Sigma^-$)					
(0-0) Q ₃ (24)	3365.196	-0.41	-0.71*	-0.69	-0.80
C ₂ ($D^3\Pi - A^3\Pi$)					
(0-0) P ₁ (45)	5135.57	0.03	0.37	0.42	0.40
(0-0) P ₂ (44)	5135.58	0.02	0.36	0.41	0.39
(0-0) P ₃ (43)	5135.68	0.01	0.35	0.40	0.38
MgH($A^2\Pi - X^2\Sigma^+$)					
(1-0) P ₂ (15.5)	4835.216	-1.42	-1.01*	-1.26	-1.26
(2-1) P ₂ (23.5)	4835.314	-0.95	-0.53*	-0.52	-0.58
SiH($A^2\Delta - X^2\Pi$)					
(1-3) R ₂₁ (28.5)	4835.285	-4.90	-4.72	-5.15	-4.71

observed wavelengths (Wyller 1966). The gf -values for CN ($A^2\Pi - X^2\Sigma^+$) lines of Kurucz are approximately the same as our ones.

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References

Arnold J.O., Landhoff S.R.: 1978, *JQSRT*, **19**, 461.
Grevesse N., Lambert D.L., Sauval A.J., van Dishoek E.F., Farmer S.V., Norton R.H.: 1991, *As.Ap.*, **242**, 488.

Hetteima H., Yarkony D.R.: 1994, *J.Chem.Phys.*, **100(12)**, 8991.

Kirby K.P., Goldfield E.M.: 1991, *J.Chem.Phys.*, **94(2)**, 1271.

Kirby K.P., Saxon R.P., Lin B.: 1979, *Ap.J.*, **231(2)**, 637.

Kurucz R.L.: 1993, *Molecules in the Stellar Environment*, IAU Coll.No 146, Copenhagen, p. 282

Kuznetsova L.A.: 1987, *Spectrosc. Lett.*, **20(9)**, 665.

Larsson M.: 1987, *J.Chem.Phys.*, **86(9)**, 5018.

Whiting E.E., Schadee A., Tatum J.B., Hougen J.T., Nicholls R.W.: 1980, *J.Mol.Spectrosc.*, **80**, 249.

Wyller A.A.: 1966, *Ap.J.*, **143**, 828.