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On the Spectral Line Broadening due to Collisions with Hydrogen Atoms: An Empirical Formula for the C_{12} Constant

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Abstract: By inversion of reliable empirical (mostly astrophysical) impact widths of 84 NaI, CaI, CaII and FeI lines from atomic hydrogen plasmas, we calculated repulsive force constants C_{12} of the Lennard-Jones potential. Obtained values have been succesfully fitted with a simple analytical expression, depending on both effective principal and orbital quantum numbers. The new empirical formula allows the theoretical estimates based on Lennard-Jones potential to fit the original empirical hydrogen-impact widths with accuracy better than 20%.

1. Introduction

Broadening due to collisions with hydrogen atoms gives the largest contribution (about 90% in the case of Sun) to the Lorentzian component of the widths of spectral lines formed in photospheres of the Sun, Main Sequence stars of spectral classes F, G, K and of the majority of stars with high surface gravities. Detailed theoretical treatment of this type of broadening demands taking into consideration the three-body problem of the type $A^+ - e^- - H$ with important contribution of short-range repulsion and exchange effects. Due to large polarizability of hydrogen atom, well studied cases of collisional broadening in noble gases are of insufficient help. On the other hand, it is difficult to keep very reactive atomic hydrogen in laboratory conditions. It reduces possibility for laboratory width measurements to strongest, resonant lines only. Since astrophysical calculations also require data on the broadening of many non-resonant lines of the majority of chemical elements, it is convenient to choose such simple semiempirical approach (based on the empirical data from the solar spectrum), which would be able to guarantee high average accuracy for the large number of lines.

The simplest potential which describes collision with atomic hydrogen perturbers and is not to far from the physical reality in stellar atmospheres is the Lennard-Jones potential. It also allows use of the simple classical methods in line broadening calculations (Hindmarsh *et al.*, 1967).

2. Results

Starting from the experiments with noble gasses Hindmarsh *et al.* (1967) suggested empirical expression for the C_{12} repulsive force constant in the Lennard-Jones potential. In order to obtain a new expression appropriate for hydrogen plasma, we have inverted empirical (mostly astrophysical) impact widths of 84 lines of NaI, CaI, CaII and FeI with Lennard -Jones potential assumed. List of carefuly chosen reliable empirical material we have used is given in Table 1, with the sources of data indicated. (Accuracy B assumes uncertainty within 30% and C within 50%). All widths are taken at temperature of about 5000 K. Results we have obtained are successfuly fitted with the empirical formula:

$$\log C_{12} = -80.5 + 0.25\, l_u^2 + (3.5 - 0.5\, l_u)\, n_u^* \tag{1}$$

where l_u and n_u^* are the orbital and effective principal quantum numbers of the upper levels.

Table 1. Critically selected empirical hydrogen-impact widths and their ratios to the widths obtained using the new empirical expression for C_{12} constant.

UPPER LEVEL ORBITAL QUANTUM NUMBER= s

SOURCE OF DATA	METHOD	ACCU-RACY	SPEC-TRUM	TRANSITION	MULTI-PLET	WAVE-LENGTH	Wm*1.E9 [rad s-1 cm3]	Wm/Wth	MEAN
O'Nail & Smith (1980a)	experiment	B	CaI	4p3P0-5s3S	3	6141.9*	19.5	0.83	0.83
	solar	C					24.	1.03	1.03
Simmons & Blackwell(1982)	solar	C	FeI	z7D0-e7D	152	4235.94	18.5	1.02	1.02
Krsljanin(1990)	solar	B	NaI	3p2P0-4s2S	3	11397.*	29.3	0.97	0.86+0.14
				3p2P0-5s2S	5	6158.6*	126.9	0.95	
				3p2P0-6s2S	8	5151.9*	385.	0.67	

UPPER LEVEL ORBITAL QUANTUM NUMBER= p

SOURCE OF DATA	METHOD	ACCU-RACY	SPEC-TRUM	TRANSITION	MULTI-PLET	WAVE-LENGTH	Wm*1.E9 [rad s-1 cm3]	Wm/Wth	MEAN
Simmons & Blackwell(1982)	solar	C	FeI	a5F-z5D0	15	5269.54	5.43	0.94	1.01+0.13
						5328.04	5.46	0.94	
						5371.49	4.97	0.85	
						5397.13	4.91	0.85	
						5405.78	5.49	0.94	
						5434.78	5.49	0.96	
				a3F-y5F0	39	4531.15	7.12	1.03	
				a3F-z5G0	41	4383.55	5.99	0.84	
						4415.13	6.85	0.93	
						4404.75	6.75	0.93	
				a3F-z3G0	42	4271.76	6.85	0.94	
				a3F-y3F0	43	4045.82	7.92	1.04	
						4071.74	6.66	0.84	
				a5P-z5P0	60	8688.63	6.72	1.08	
						8387.78	6.87	1.09	
						8327.06	7.44	1.17	
				a5P-y5D0	62	6430.85	7.63	1.11	
				a3P-z3P0	111	6421.36	7.25	0.97	
				a3H-z5G0	168	6494.99	8.07	1.11	
				a3H-z3G0	169	6252.56	7.02	0.94	
				b3F-y3F0	207	6065.49	9.73	1.21	
						6137.70	10.13	1.27	
						6230.73	10.04	1.28	

Table 1. (Continued.)

SOURCE OF DATA	METHOD	ACCU-RACY	SPEC-TRUM	TRANSITION	MULTI-PLET	WAVE-LENGTH	Wm*1.E9 [rad s-1 cm3]	Wm/Wth	MEAN
Ayres (1977)	solar	C	CaI	4s21S-4p1P0	2	4226.73	28.	3.18)	
			CaII	4s2S-4p2P0	1	3945.2*	17.	1.07	1.16+0.09
				3d2D-4p2P0	2	8579.1*	20.	1.25	
O'Neil & Smith (1980b)	experiment	B	FeI	a5D-z7F0	2	4461.65	6.4	1.20	0.99+0.10
				a5D-z7P0	3	4258.32	6.2	1.14	
				a5D-z5D0	4	3906.48	6.8	1.19	
						3930.30	5.2	0.92	
						3886.28	5.1	0.90	
				a5D-z5F0	5	3733.32	6.0	1.01	
						3745.56	6.2	1.05	
						3705.57	6.2	1.05	
						3719.94	6.0	1.03	
				a5D-z5P0	6	3465.86	6.9	1.10	
						3526.04	7.7	1.25	
						3490.60	6.8	1.11	
				a5D-z3F0	7	3180.76	6.4	0.94	
						3214.40	6.4	0.95	
				a5D-z3D0	8	3226.73	6.9	1.03	
						3265.05	6.1	0.92	
				a5D-z3P0	11	3007.28	7.4	1.01	
				a5F-z5D0	15	5434.53	6.4	1.09	
						5455.61	6.2	1.06	
						5497.52	5.4	0.92	
						5405.78	6.2	1.06	
						5446.92	5.8	0.99	
						5506.78	4.8	0.83	
						5371.49	5.6	0.96	
						5429.70	5.1	0.88	
						5501.47	5.0	0.87	
						5328.04	5.0	0.86	
						5397.13...	5.0	0.87	
				a5F-y5D0		3849.97	6.2	0.90	
						3865.53	6.1	0.89	
						3898.01	6.0	0.88	
						3840.44	6.1	0.89	
						3872.50	6.1	0.90	
						3917.19	6.2	0.92	
						3834.22	6.6	0.97	
						3878.02	6.1	0.91	
						3940.88	6.1	0.92	
						3825.88	6.7	1.00	
						3887.05	6.6	0.98	
						3820.43	7.2	1.09	
Lemaire et al. (1985)	experiment	B	NaI	3s2S-3p2P0	1	5891.8*	13.9	1.47	1.47
Krsljanin(1990)	solar	B	NaI	3s2S-3p2P0	1	5891.8*	7.80	0.82	0.94+0.19
				4s2S-4p2P0		22070.*	43.3	1.21	
				4s2S-5p2P0	18	10747.*	130.	1.02	
				4s2S-6p2P0	19	8650.3*	330.	0.73	

UPPER LEVEL ORBITAL QUANTUM NUMBER= d

SOURCE OF DATA	METHOD	ACCU-RACY	SPEC-TRUM	TRANSITION	MULTI-PLET	WAVE-LENGTH	Wm*1.E9 [rad s-1 cm3]	Wm/Wth	MEAN
Krsljanin(1990)	solar	B	NaI	3p2P0-3d2D	4	8191.1*	20.6	0.96	0.97+0.15
				3p2P0-4d2D	6	5686.4*	63.1	1.02	
				3p2P0-5d2D	9	4981.4*	216.	1.21	
				4p2P0-4d2D		23370.*	56.2	0.90	
				4p2P0-5d2D		14776.*	130.	0.74	

M E A N 1.03 + 0.17

* mean for the multiplet

For more crude estimations one can neglect dependence on l and find C_{12} in the form proposed by Kielkopf (1972):

$$\log C_{12} = -79.5067 + 18.2710 \log n_{\rm u}^{*} \tag{2}$$

(In both formulas C_{12} is given in units $\mathrm{cm}^{12}\,\mathrm{s}^{-1}$.)

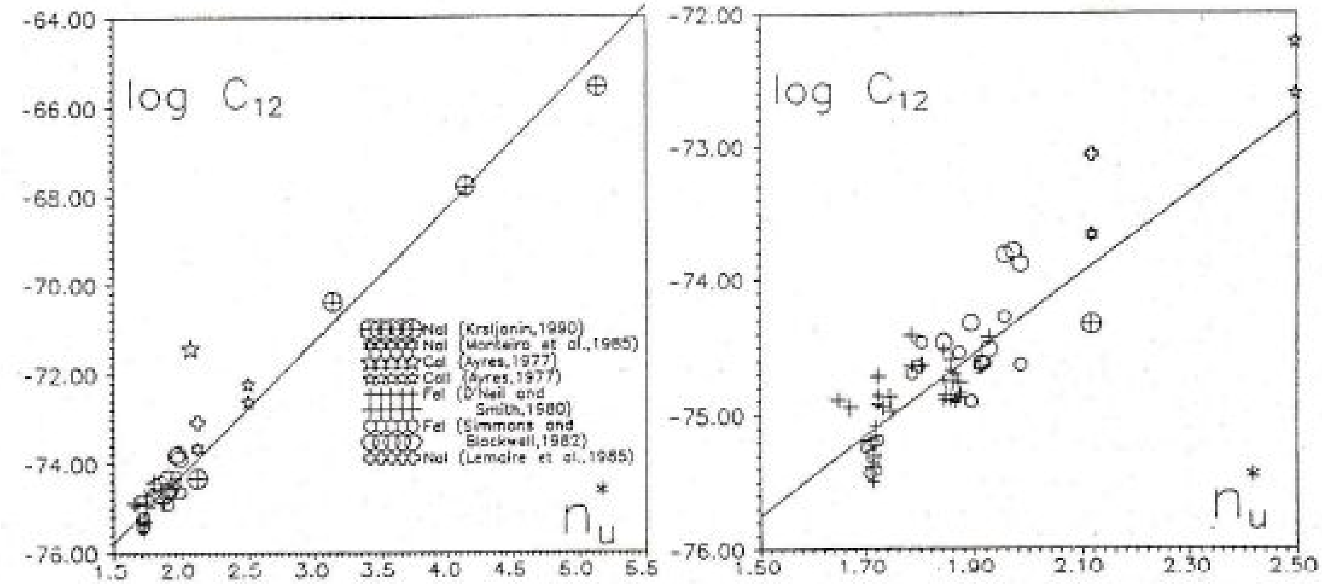

Fig. 1. Values of C_{12} constant obtained from the empirical hydrogen-impact widths (for $l = 1$), as a function of $n_{\rm u}^{*}$. Formula (1) is presented by a straight line.

Empirical and theoretical (1) values of C_{12}, for $l = 1$, are shown in Fig.1., for all (left) and for small (right) values of $n_{\rm u}^{*}$, respectively. Average ratio of the 84 empirical to the corresponding theoretical (obtained in accordance with Hindmarsh *et al.* (1967) and using formula (1)) widths is 1.03 ± 0.17 (Table 1.). Half-width obtained for NaI D-lines using this approach is $9.5 \times 10^{-9}\ \mathrm{rad\,s^{-1}\,cm^{3}}$, while *ab initio* calculation of the Newcastle group (Monteiro *et al.*, 1985) gives the value 10% larger. Ratios of the half-widths obtained using formula (1) to the ones obtained by Gomez *et al.*, (1987) with old formula for C_{12}, are 1.35, 0.85, 0.72, for $l = 0, 1, 2$ respectively.

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