

LETTER TO THE EDITOR

Spectroscopic Constants and Term Values for the $X^2\Pi_i$ State of OH ($v = 0-10$)

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The OH free radical is widely observed in flames, the upper atmosphere, comets, the interstellar medium, the sun, and cool stars. The most recent spectroscopic constants for $v = 0-3$ of the $X^2\Pi$ state are available from the comprehensive analysis of Mélen *et al.* (1). For higher vibrational levels $v < 11$, the best work is that of Abrams *et al.* (2). A few higher vibrational levels ($v = 11-13$) are known from the analysis of Copeland *et al.* (3) of the $B^2\Sigma^+-X^2\Pi_i$ system.

In the course of our work on hot water vapor, we have also detected the Meinel system of OH. Starting with our detection of hot water in the spectrum of a sunspot (4), we have reported on a series of laboratory thermal emission spectra (5–8). Unfortunately at 1800 K, the laboratory samples are not a very good match for the sunspot at 3000 K and therefore we have very recently investigated the emission from an oxyacetylene torch, similar to the one used by Flaud *et al.* (9) in their pioneering work on hot water. The new spectra of hot water now closely match those of the sunspot. In order to make a hot water

line-list, it was necessary to identify and eliminate the OH Meinel lines. For this purpose it is convenient to use HITRAN (10), which uses the intensities of Goldman *et al.* (11) and line positions generated from the spectroscopic constants of Mélen *et al.* (1) and Abrams *et al.* (2). Apart from one minor typographical error (the q_M constant for $v = 0$ is -0.3505×10^{-16} and not $+0.3505 \times 10^{-16} \text{ cm}^{-1}$) the constants of Mélen *et al.* (1) are very reliable but those of Abrams *et al.* (2) are not. Indeed the constants of Abrams *et al.* do not always reproduce their own data, particularly at the high J values needed for our torch spectrum.

We therefore refitted all of the excellent data of Abrams *et al.* (2), holding fixed the spectroscopic constants for $v = 0-3$ to the values of Mélen *et al.* (1). Because OH spectrum is of such utility, we provide the revised constants (Table 1) and a new set of term values (available at <http://www.ulb.ac.be/cpm/>). The term values were limited to $J = 30.5$ as no lines with J values higher than 19.5 were

TABLE 1
 Molecular Constants for the $X^2\Pi_i$ State of OH (cm^{-1})

	$v = 4$	$v = 5$	$v = 6$	$v = 7$	$v = 8$	$v = 9$	$v = 10$
$T^* \times 10^{-3}$	13.29461572(25)	16.21059933(29)	18.96299370(34)	21.54917835(35)	23.96464104(40)	26.20244717(42)	28.25254020(74)
$A \times 10^{-2}$	-1.4008254(60)	-1.4028821(73)	-1.4043956(78)	-1.4050384(82)	-1.4043057(91)	-1.4014107(97)	-1.395059(17)
$B \times 10^{-1}$	1.5736987(10)	1.5045764(11)	1.4348655(12)	1.3639385(13)	1.2908903(22)	1.2145252(22)	1.1332467(53)
$D \times 10^3$	1.782340(96)	1.768599(90)	1.76174(11)	1.77204(11)	1.80091(35)	1.85734(31)	1.9547(10)
$H \times 10^7$	1.1502(25)	1.0898(20)	0.8594(26)	0.6808(28)	0.336(15)	-0.184(12)	-0.986(56)
$L \times 10^{11}$	-1.9**	-2.0**	-2.1**	-2.2**	-2.3**	-2.4**	-2.5**
$\gamma \times 10$	-0.9678(11)	-0.9053(15)	-0.8373(14)	-0.7595(17)	-0.6687(22)	-0.5513(25)	-0.4077(53)
$\gamma_D \times 10^5$	2.402(56)	2.509(89)	2.711(80)	2.84(11)	3.48(17)	4.15(18)	6.50(50)
$q \times 10^2$	-3.15691(79)	-2.9691(10)	-2.77662(98)	-2.5714(11)	-2.3546(17)	-2.1156(19)	-1.8498(35)
$q_D \times 10^5$	1.3879(41)	1.3739(68)	1.3840(56)	1.3885(85)	1.422(14)	1.4337(17)	1.4111(37)
$q_H \times 10^9$	-2.3**	-2.2**	-2.1**	-2.0**	-1.9**	-1.8**	-1.7**
$q_L \times 10^{13}$	3.3**	3.0**	2.7**	2.4**	2.1**	1.8**	1.5**
$p \times 10$	1.9142(11)	1.7949(12)	1.6642(13)	1.5205(13)	1.3635(17)	1.1684(18)	0.9273(32)
$p_D \times 10^5$	-5.319(79)	-5.73(11)	-5.86(11)	-6.38(13)	-7.63(20)	-8.18(22)	-8.67(46)
$p_H \times 10^9$	4.65**	4.6**	4.5**	4.4**	4.3**	4.2**	4.1**

* Zero energy is the F_{ie} (1.5) level of $v = 0$.

** Extrapolated value from Mélen *et al.* (1).

Uncertainties are on the last two given decimals.

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Supplementary data for this article are available on IDEAL (<http://www.idealibrary.com>) and as part of the Ohio State University Molecular Spectroscopy Archives (http://msa.lib.ohio-state.edu/jmsa_hp.htm).



observed. These can also be found online at <http://www.idealibrary.com> and http://msa.lib.ohio-state.edu/jmsa_hp.htm.

In contrast to Abrams *et al.* (2), the $^2\Pi$ Hamiltonian of Brown *et al.* (12) was used in our work along with a partial list of matrix elements provided by Amiot *et al.* (13). The necessary additional higher order matrix elements were generated by algebraic matrix multiplication using the Maple program. Mélen *et al.* (1) also used Brown's effective Hamiltonian and we checked our term values against theirs. The main difference between our analysis and that of Abrams *et al.* (2) lies in the values of the spin-orbit constants A . Our constants now agree well with those derived by Copeland *et al.* (3) for the higher v levels.

Cosby *et al.* also found a problem with the ground state constants of OH and carried out a refit of the existing data (14).

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