

## LETTER TO THE EDITOR

## An Improved Set of Rotational Constants for HF

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HF is an important gas for use as an absolute wavenumber standard and as a laser medium. Rotational constants for the ground vibrational level of HF were published by Jennings *et al.* (1, 2) and by Hedderich

TABLE I

Observed Pure Rotational Transitions of HF (in  $\text{cm}^{-1}$ )

$J'$	$J''$	$v = 0$ / $\text{cm}^{-1}$	$v = 1$ / $\text{cm}^{-1}$	$v = 2$ / $\text{cm}^{-1}$
1	0	41.1109832(17) <sup>a</sup>		
2	1	82.1711179(13) <sup>a</sup>		
3	2	123.12967(-1) <sup>a</sup>		
4	3	163.93616(0) <sup>a</sup>		
5	4	204.54045(1) <sup>b</sup>		
6	5	244.89283(0) <sup>b</sup>		
7	6	284.94444(23) <sup>b</sup>		
13	12	516.28061(-14) <sup>c</sup>	496.68517(-5) <sup>c</sup>	
14	13	552.92047(9) <sup>c</sup>	531.89851(-3) <sup>c</sup>	
15	14	588.89912(6) <sup>c</sup>	566.46812(-11) <sup>c</sup>	544.59319(22) <sup>c</sup>
16	15	624.17735(11) <sup>c</sup>	600.35572(-2) <sup>c</sup>	577.12112(-17) <sup>c</sup>
17	16	658.71685(4) <sup>c</sup>	633.52402(12) <sup>c</sup>	608.94862(22) <sup>c</sup>
18	17	692.48118(2) <sup>c</sup>	665.93707(7) <sup>c</sup>	640.03793(-146) <sup>c</sup>
19	18	725.43521(-3) <sup>c</sup>	697.56091(8) <sup>c</sup>	670.36020(-50) <sup>c</sup>
20	19	757.54563(5) <sup>c</sup>	728.36279(5) <sup>c</sup>	699.8808(5) <sup>f</sup>
21	20	788.78038(3) <sup>c</sup>	758.31128(-36) <sup>c</sup>	728.5675(0) <sup>f</sup>
22	21	819.10934(0) <sup>c</sup>	787.37827(21) <sup>c</sup>	756.3966(35) <sup>f</sup>
23	22	848.50403(0) <sup>c</sup>	815.5344(2) <sup>f</sup>	783.3306(12) <sup>f</sup>
24	23	876.93760(1) <sup>c</sup>	842.7524(-15) <sup>f</sup>	809.3482(-20) <sup>f</sup>
25	24	904.38479(-7) <sup>c</sup>		
26	25	930.82215(-20) <sup>c</sup>		
27	26	956.22816(-13) <sup>d</sup>		
28	27	980.58255(0) <sup>c</sup>		
29	28	1003.86689(22) <sup>c</sup>		
31	30	1047.1570(-17) <sup>c</sup>		
32	31	1067.1377(-1) <sup>e</sup>		
33	32	1085.98903(0) <sup>d</sup>		

Note. Observed – calculated in parentheses.

<sup>a</sup> Tunable far infrared spectroscopy (1).

<sup>b</sup> Fourier transform spectroscopy (1).

<sup>c</sup> Fourier transform spectroscopy (our work).

<sup>d</sup> Diode laser heterodyne spectroscopy (2).

<sup>e</sup> Diode laser spectroscopy (1).

<sup>f</sup> Vacuum grating spectroscopy (6).

TABLE II  
Rotational Constants of HF

constant	$v = 0$	$v = 1$	$v = 2$
	/cm <sup>-1</sup>	/cm <sup>-1</sup>	/cm <sup>-1</sup>
$B_v$	20.559 729 9 (3)	19.787 476 7 (20)	19.034 974 (18)
10 <sup>3</sup> $D_v$	2.119 904 (12)	2.063 778 (57)	2.010 26 (14)
10 <sup>6</sup> $H_v$	0.163 495 (37)	0.159 05 (32)	0.153 76 (41)
10 <sup>10</sup> $L_v$	-0.149 87 (41)	-0.156 3 (71)	-0.141 4 (37)
10 <sup>14</sup> $M_v$	0.105 6 (15)	0.170 (54)	

Note. One standard deviation in parentheses.

*et al.* (3). The molecular constants were determined from measurements that covered the spectral range from 40 to 1100 cm<sup>-1</sup>.

After submittal of Ref. (3), another spectrum was found containing additional pure rotational HF transitions. From this new set of pure rotational transitions the rotational constants for the ground vibrational level of HF were calculated more accurately. In addition, rotational constants for the first and second vibrational levels were obtained.

The rotational emission spectrum of HF was accidentally recorded during an attempt to measure the infrared spectrum of CaF<sub>2</sub>. Solid CaF<sub>2</sub> was heated in an alumina tube furnace to about 1600 K (for details of the system see Ref. (4)). HF was produced by the reaction of hot CaF<sub>2</sub> with water, which is always present in the system. The spectrum was observed with the McMath Fourier transform spectrometer of the National Solar Observatory at Kitt Peak. The unapodized resolution was 0.0053 cm<sup>-1</sup> with a liquid helium cooled As:Si detector and a KCl beamsplitter. The upper wavenumber limit (1300 cm<sup>-1</sup>) was set by a wedged InSb filter while the lower limit (500 cm<sup>-1</sup>) was given by the transmission of the KCl beamsplitter and by the detector response.

The data analysis was done by using PC-DECOMP, a spectral analysis program, developed by J. W. Brault. The signal-to-noise ratio for the strong rotational lines of ground state HF was better than 1000 and the resulting resolution-enhanced linewidth was 0.0005 cm<sup>-1</sup>. The HF lines (3) were used for absolute calibration ( $\pm 0.0002$  cm<sup>-1</sup>) of the spectrum. The line positions are listed in Table I.

The energy levels of HF were fit to the expression (5)

$$E_v(J) = G_v + B_v J(J+1) - D_v [J(J+1)]^2 + H_v [J(J+1)]^3 + L_v [J(J+1)]^4 + M_v [J(J+1)]^5.$$

Rovibrational transitions reported by Guelachvili (6) and Goddon *et al.* (8) were included in the fit as were some pure rotational lines reported by Sengupta *et al.* (7). The rotational constants obtained from this fit are shown in Table II and the  $v = 1 \leftarrow 0$  and  $v = 2 \leftarrow 0$  band origins are 3961.42245(2) and 7750.79445(51) cm<sup>-1</sup>, respectively.

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