

Addition to "Indirect Rotational Spectroscopy of HCO+"

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After publication, we learned that pure rotational transitions in the $1\nu_1$ vibrationally excited state of HCO⁺ had been measured by Warner in his Ph.D. thesis and by Hirao et al., so our combination differences and fit results should be compared to the results from this work.

Additionally, a 1 MHz error was found in the calculation of all of the vibrationally excited combination differences as a result of a single transcription error in the $J=3\leftarrow 2$ excited state transition³ used in determining the combination differences. The corrected values are reported in Table 1.

Table 1. Summary of the Corrected Rotational Transitions in the $1\nu_1$ Vibrationally Excited State and a Comparison of Those to Previously Determined Values^a

J'-J"	frequency	previous	calc - prev
1-0	88485.7(19)	$88480.748(100)^b$	5.0
2-1	176956.4(16)	176959.485 ^c	-3.1
4-3	353901.7(9)	$353903.215(30)^d$	-1.5
5-4	442365.0(11)	$442364.230(30)^d$	0.8
6-5	530814.3(13)	530815.436 ^c	-1.1
7-6	619256.7(16)	$619254.813(30)^d$	1.9
8-7	707677.4(19)	$707680.392(30)^d$	-3.0
9-8	796092.7(19)	$796090.220(20)^d$	2.5
10-9	884478.9(24)	884482.326 ^c	-3.4

^aThe comparison column is the difference between our calculated combination difference and the previously calculated or observed value. All the values are in MHz. ^bWarner. ¹ ^cHirao et al. calculated. ² ^dHirao et al. observed. ²

Excluding the $J=1\leftarrow 0$ transition, all previous values are within 2σ of our determined frequencies.

The differences between the B and D constants in this paper and those in Hirao et al. arise from the inclusion of a sextic distortion constant. When the sextic distortion constant is not included, the B and D constants (B = 44240.511(41) MHz and D = 82.13(30) kHz) are in good agreement with those of Hirao et al. (B = 44240.52774(118) MHz and D = 82.0571(87) kHz).

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■ REFERENCES

(1) Warner, H. The Microwave Spectroscopy of Ions and Other Transient Species in DC Glow and Extended Negative Glow Discharges. Ph.D. thesis, University of Wisconsin—Madison, 1988.

(2) Hirao, T.: Yu. S.: Amano, T. Sub-millimeter Spectroscopy of

(2) Hirao, T.; Yu, S.; Amano, T. Sub-millimeter Spectroscopy of HCO⁺ in the Excited Vibrational States. *J. Mol. Spectrosc.* **2008**, 248, 26–40

(3) Hirota, E.; Endo, Y. Microwave Spectroscopy of HCO⁺ and DCO⁺ in the Excited Vibrational States. *J. Mol. Spectrosc.* **1988**, *127*, 527–534.

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