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Absolute Rovibrational Intensities for the $X^1\Sigma^+$ v=3←0 Band of $^{12}C^{16}O$ Obtained with Kitt Peak and BOMEM FTS Instruments

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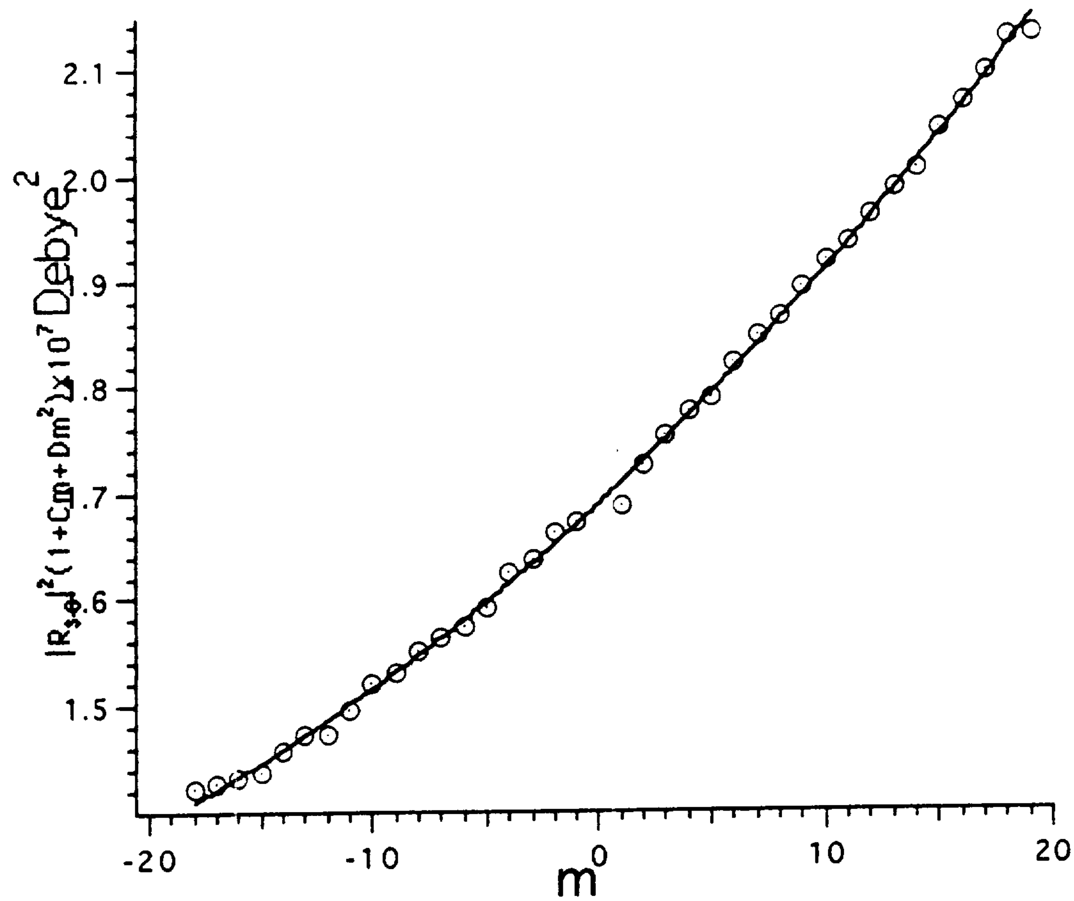
This work was initiated to compare absolute line intensities retrieved with the Kitt Peak FTS and Ames BOMEM FTS. Since thermal contamination[1] can be a problem using the BOMEM instrument if proper precautions are not taken it was thought that measurements done at 6300 cm^{-1} would more easily result in satisfactory intercomparisons. Very recent measurements[2,3] of the CO 3←0 band line intensities confirms results reported here that the intensities listed in HITRAN for this band are on the order of 6-7% too low. All of the infrared intensities in the current HITRAN tabulation are based on the electric dipole moment function reported fifteen years ago[4]. The latter in turn was partly based on intensities for the 3←0 band reported thirty years ago[5]. We have, therefore, redetermined the electric dipole moment function of ground electronic state CO using techniques discussed in Ref. The experimental conditions employed for our experiments are given in Table 1.

Table 1. Experimental Conditions.

Spectrum[a]	Path (M)	P(Torr)	T(K)	Res. (cm^{-1})
KP13	73	3.11	294.2	0.020
KP14	73	6.71	294.3	0.020
KP21	1.5	401.4	297.8	0.020
KP23	1.5	298.2	298.0	0.020
KP24	1.5	204.6	297.9	0.020
AMES010	207	0.732	296.0	0.016
AMES011	207	0.732	296.0	0.008

[a] Kitt Peak interferograms are double-sided and Ames interferograms single-sided.

Using these spectra individual line intensities, S_{obs}, were obtained via non-linear least-squares fitting of line profiles. Shown in the Figure is a plot of the reduced intensity versus m for the five Kitt Peak spectra averaged together.



The reduced intensity is given by the following equations.

$$S_{red}(m) = \frac{S_{obs}\left(3.27368x10^{-4}\right)Q_{vr}(T)T}{\sigma L(m)} e^{hcE''/kT}$$

$$S_{red}(m) = \left|R_{3-0}\right|^2 \bullet \left(1 + Cm + Dm^2\right)$$

Therefore a fit, quadratic in m, to these data gives the rotationless transition moment R and the Herman-Wallis intensity parameters, C and D.

Table 2 compares the intensity factors obtained by various groups. The last row in the table gives C and D parameters calculated via numerical wave functions obtained using an electric dipole moment function consistent with the rotationless transition moment given in the first row of the table. The agreement of these parameters with the results of Picqué *et al.* [3] is striking.

Table 2. Intensity Parameters for the 3←0 Band of $^{12}C^{16}O$.

Reference	$\lvert R \rvert^2 \times 10^7 (D^2)$	C	D
This work (KP)	1.7129(19)	0.01169(8)	0.000136(7)
This work (Ames)	1.7035(81)	0.01406(33)	0.000085(24)
Toth *et al.* [5]	1.85(10)	0.0118(7)	0.00018(10)
Bouanich *et al.* [6]	1.75(6)	0.0118(7)[b]	0.00018(10)[b]
Picqué *et al.* [3]	1.68(10)	0.01202(15)	0.000105(15)
Henningsen *et al.* [2]	1.68(17)	0.01323	
Calc. this work		0.011968	0.00010406

[a]Uncertainties for the last digits indicated represent one standard deviation.[b]Adopted from Ref. (5).

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