The application of a vacuum ultraviolet Fourier transform spectrometer and synchrotron radiation source to measurements of: V. The β(11,0) band of NO

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The β(11,0) band of NO was measured at high resolution (0.06 cm^{-1}) by the vacuum ultraviolet Fourier transform spectrometer from Imperial College, London, using synchrotron radiation at the Photon Factory, KEK, Japan, as a continuum light source. Such resolution facilitates a line by line analysis of the NO β(11,0) band which yields accurate rotational line positions and term values as well as the photoabsorption cross sections. The molecular constants of the $B(11)$ $^2\Pi_r$ level are found to be $T_0 = 55\,983.203 \pm 0.017$ cm^{-1}, $A = 47.977 \pm 0.024$, $B_v = 1.010\,77 \pm 0.000\,37$ cm^{-1}, $D_v = (6.7 \pm 0.8) \times 10^{-6}$ cm^{-1} and $A_D = 0.0438 \pm 0.0035$ cm^{-1}. The sum of the line strengths for all rotational transitions of the NO β(11,0) band is determined as 3.04×10^{-16} cm^2 cm^{-1}, corresponding to a band oscillator strength of $(3.44 \pm 0.21) \times 10^{-4}$. © *2002 American Institute of Physics.* [DOI: 10.1063/1.1520535]

I. INTRODUCTION

The absorption of ultraviolet solar radiation between 175 and 205 nm in the middle atmosphere[1–4] is dominated by the Schumann–Runge bands of O_2. Despite this the predissociation of NO, produced by radiation in approximately the same region, 183 to 195 nm, is still a significant photochemical process requiring improved laboratory investigation for reasons given in earlier publications.[5–8] Initial work[9] on acquiring high resolution photoabsorption cross sections of NO was conducted at Imperial College (IC) using their vacuum ultraviolet Fourier transform spectrometer (VUV FTS) and a gaseous arc source. It was not possible with this source to record spectra with adequate signal-to-noise ratios for the weaker lines, and we therefore transported the IC VUV FTS to Photon Factory, KEK, Japan to make use of the 12-B beam line of the synchrotron source. This combination has yielded high resolution NO absorption spectra throughout the region 160–195 nm. The results of measurements of line positions and cross sections for several of the bands have already been published.[5–8] This paper will address the data gathered over the β(11,0) ($B\,^2\Pi_r – X\,^2\Pi_r$) band of NO.

The first measurements of the vacuum ultraviolet spectra of NO were made by Leifson,[10] who photographed the absorption bands of the molecule in 1926. An extensive review of early experimental work on the electronic spectrum of NO is given by Miescher and Huber.[11] The β bands of NO were studied extensively by Miescher and his co-workers. The (5,0) to (19,0) bands of the β system were examined in absorption by Herzberg *et al.*[12] with a reciprocal dispersion of 0.63 Å/mm, and the rotational constants of these bands were presented. A complete line list based on their observations[13] of the β band with $v' = 5 - 19$ and the δ bands with $v' = 0 - 2$ is available together with the homogeneous perturbations between $B\,^2\Pi$ and $C\,^2\Pi$ states. A later paper[14] extended these analyses up to $v' = 24$.

Cross section measurements of the β bands were performed at low resolution in the presence of Ar by Bethke[15] in the wavelength region 170 nm to 230 nm. The addition of the argon buffer gas ensured that the rotational lines were broadened beyond the instrumental resolution, allowing the true cross section to be presented. The same technique was applied for the (0,0) through (4,0) bands of the β system by Hasson and Nicholls.[16] Later investigators used "Hook" technique to measure the (3,0) through (5,0) bands of the β system.[17] Cieslik[18] made low resolution measurements of NO with a low pressure of NO gas, and used the equivalent width and curve of growth method to obtain band oscillator strengths including the β (9,0) band. Cooper,[19] and more recently Luque and Crosley[20] have produced electronic transition moments for the β band via *ab initio* calculation and selective laser excitation, respectively. Chan *et al.*[21] used the
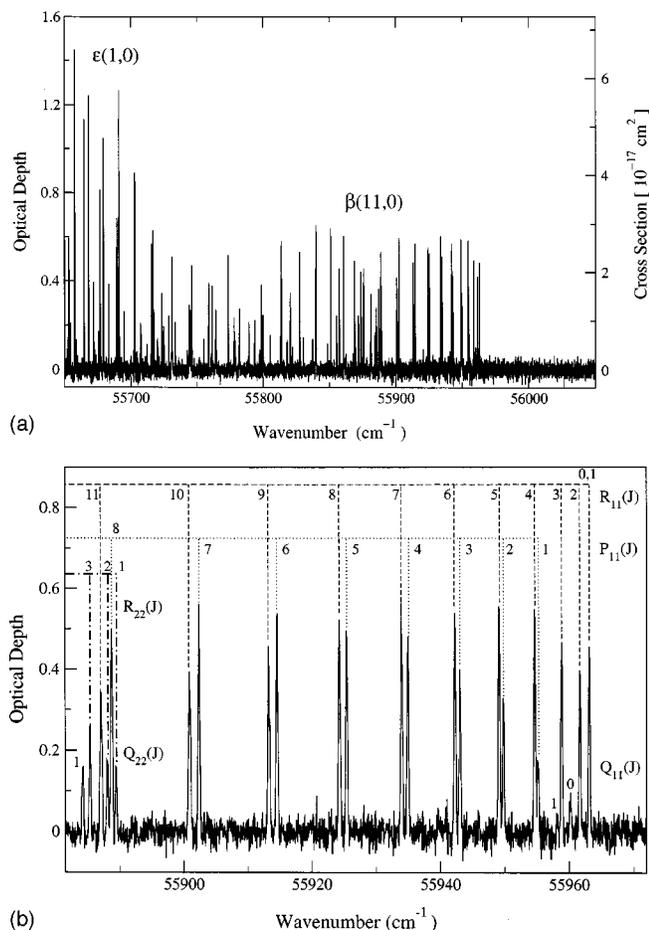
FIG. 1. The $\beta(11, 0)$ band at 0.150 Torr of NO with 4.50 cm pathlength is shown in (a) together with a portion of the $\varepsilon(1, 0)$ band. An expanded portion of the spectrum with the rotational assignments is displayed in (b).

high resolution dipole (e,e) technique to obtain the band oscillator strengths.

This paper present the analysis for the $\beta(11,0)$ band around 179 nm recorded using the VUV FTS with a synchro-

tron background source. Accurate line positions and strengths are presented together with rotational term values for the $B\ ^2\Pi_r\ (v=11)$ level. The oscillator strength of the band has been determined from line by line measurements, a process made possible by the approximate matching of instrumental resolution to the Doppler widths of the rotational transitions.

II. EXPERIMENT

Details of the experimental procedures for recording high resolution FT spectra of NO between 160–198 nm have been described in our earlier publications.[5] Only a brief description of the experimental conditions with respect to the recording of the $\beta(11,0)$ band will be given here. An absorption cell with optical path length of 4.50 cm was used, which was filled with 0.150 torr of NO at 295 K. The column density of NO in this experiment was 2.21×10^{16} mol cm^{-2}. A total of 296 scans, corresponding to above 13.5 hours of integration time, with a resolution of 0.06 cm^{-1} have been coadded. The signal-to-noise ratio in the continuum background was about 66. The resonance line of Hg I at 184.8 nm was used as reference wave number in the previous papers.[5,6] However, in this wavelength region we have no convenient absolute reference. From the calibration constant in the previous papers, we estimate the uncertainty in the absolute values as 0.02 cm^{-1}. Relative uncertainties for the strong lines are better than 0.01 cm^{-1}.

III. RESULTS AND DISCUSSION

The absorption spectra at around 179 nm were converted to optical depth by taking the logarithms of the intensity and fitting a smooth continuum to the regions between the lines. The absorption lines were fitted to Voigt profiles using the spectral reduction routine *XGREMLIN*,[22] a UNIX implemen-

TABLE I. Observed wave numbers of the $\beta(11,0)$ band of NO,[a] cm^{-1}.

J	$R_{11}(J)_e$	$R_{11}(J)_f$	$P_{11}(J)_e$	$P_{11}(J)_f$	$Q_{11}(J)$	$R_{22}(J)$	$P_{22}(J)$	$Q_{22}(J)$
0.5	55 963.189b				55 960.197			
1.5	55 963.081b		55 955.192		55 958.141	55 889.419		55 884.309
2.5	55 961.617		55 949.825			55 888.067	55 875.791B	55 880.817
3.5	55 958.868		55 943.046			55 885.367	55 868.886B	55 875.791B
4.5	55 954.695		55 934.927			55 881.278	55 860.643B	55 869.843
5.5	55 949.150		55 925.433			55 875.791B	55 851.035B	
6.5	55 942.250		55 914.574			55 868.886B	55 840.009B	
7.5	55 933.957		55 902.328			55 860.643B	55 827.666B	
8.5	55 924.296		55 888.739			55 851.035B	55 813.910B	
9.5	55 913.269		55 873.763			55 840.009B	55 798.859b	
10.5	55 900.863		55 857.435			55 827.666B	55 782.390b	
11.5	55 887.083		55 839.691b			55 813.910B	55 764.493	
12.5	55 871.921		55 820.598			55 798.735b	55 745.290	
13.5	55 855.368		55 800.149			55 782.029b	55 724.606	
14.5	55 837.441		55 778.251	55 778.503		55 763.932		
15.5	55 818.136	55 818.360	55 755.026	55 755.317		55 744.002		
16.5	55 797.408	55 797.698	55 730.471b	55 730.629b				
17.5			55 704.451	55 704.726				

[a]Absolute values of the wave numbers are subject to the calibration uncertainty of 0.02 cm^{-1}. Lines followed by B are blends observed as a single line, and by b are blends observed as an incompletely resolved complex.

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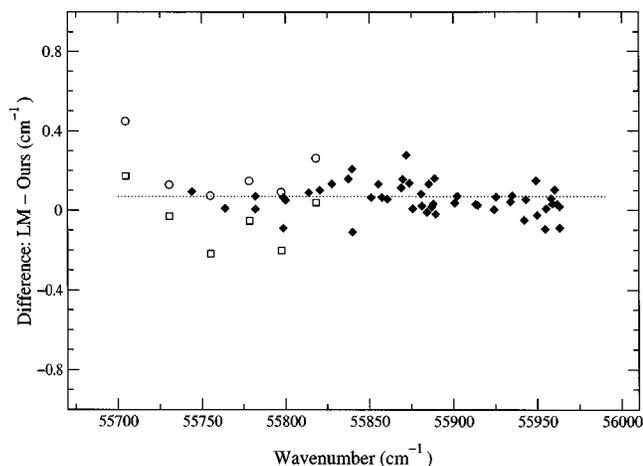
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FIG. 2. Differences in the observed line positions between our results and Lagerqvist and Miescher (Ref. 13). The differences are given by the solid diamonds whereas the dotted horizontal line represents the average shift of $+0.069$ cm^{-1}. Differences of the separated lines by Λ-type doubling are compared with those of the unseparated lines, and they are presented by squares and circles.

tation of the *GREMLIN*[23] program. Line parameters are determined through a nonlinear least-squares iterative fitting procedure. The Voigt profile should represent the convolution of a Gaussian due to Doppler broadening with a Lorentzian due to predissociation, but, as with the Photon Factory spectra previously analyzed, the best-fit Gaussian had a full width at half maximum of 0.175 cm^{-1} which is considerably greater than the 0.12 cm^{-1} expected for Doppler width in our experimental conditions. This anomalous Gaussian width is considered to be due to drifts in alignment of the synchrotron beam and external optics which cause very small wave number shifts over the long observation periods.[24]

A. Line positions and molecular constants

Figure 1(a) shows the Fourier transform spectrum of the $\beta(11,0)$ and a portion of the $\epsilon(1,0)$ bands near 179 nm. As can be seen, the $\beta(11,0)$ band is considerably weaker than the $\epsilon(1,0)$ band. The high J lines of the $\beta(11,0)$ band overlap heavily with the $\epsilon(1,0)$ band. Figure 1(b) is an expanded portion of the spectrum showing details of the rotational structure of the $\beta(11,0)$ band. We observed 73 lines of the $\beta(11,0)$ band and these lines were assigned to six main branches ($R_{11}, P_{11}, Q_{11}, R_{22}, P_{22}, Q_{22}$). These lines are tabulated in Table I. Partly resolved complexes and entirely blended lines have been labeled with b and B, respectively. Approximately one quarter of the lines observed exhibited structure consistent with full or partial blending either with lines of the same branch or lines of different J quantum number. Where Λ-type doubling was observed, we have assumed the f component has the higher energy although there is no internal evidence to verify this assumption. From previous analyses[5–8] we know the frequency calibration to be good to an uncertainty of 0.02 cm^{-1} while for the strongest lines the relative uncertainty is 0.01 cm^{-1}. Differences in the observed line positions between present results and those of Lagerqvist and Miescher[13] are plotted in Fig. 2, where differences of the separated lines by Λ-type doubling are presented by open circles and squares. The average shift of $+0.069$ cm^{-1} is entirely consistent with the claimed uncertainties of their measurements, 0.1 cm^{-1}.

The rotational term values of the $v=11$ level of the $B\ ^2\Pi$ state [upper level of the $\beta(11,0)$ band] can be obtained by adding the term values of the $X(0)$ levels to the wave numbers of the observed lines. The rotational term values of the $X(0)$ levels relative to the level $\Omega=\frac{1}{2}$, $J=0.5$, e are given by Amiot *et al.*[25] The term values obtained for the upper level are averaged, and the results are listed in Table II,

TABLE II. The term values of $B(11)\ ^2\Pi$ level of NO,^{a} cm^{-1}.

| J | F_1, $^2\Pi_{1/2}$ | | F_2, $^2\Pi_{3/2}$ | |
	e	f	e	f
0.5	$55\,960.200 \pm 0.004$	$55\,960.218 \pm 0.012$		
1.5	$55\,963.176 \pm 0.022$	$55\,963.200 \pm 0.025$	$56\,009.264 \pm 0.058$	$56\,009.264 \pm 0.058$
2.5	$55\,968.100 \pm 0.012$	$55\,968.135 \pm 0.028$	$56\,014.368 \pm 0.062$	$56\,014.368 \pm 0.062$
3.5	$55\,975.033 \pm 0.003$	$55\,975.080 \pm 0.013$	$56\,021.628 \pm 0.066$	$56\,021.629 \pm 0.067$
4.5	$55\,983.926 \pm 0.006$	$55\,983.985 \pm 0.011$	$56\,030.926 \pm 0.054$	$56\,030.927 \pm 0.054$
5.5	$55\,994.796 \pm 0.004$	$55\,994.866 \pm 0.012$	$56\,042.309 \pm 0.002$	$56\,042.310 \pm 0.002$
6.5	$56\,007.630 \pm 0.013$	$56\,007.711 \pm 0.002$	$56\,055.744 \pm 0.008$	$56\,055.746 \pm 0.009$
7.5	$56\,022.459 \pm 0.015$	$56\,022.551 \pm 0.001$	$56\,071.199 \pm 0.019$	$56\,071.201 \pm 0.020$
8.5	$56\,039.241 \pm 0.012$	$56\,039.344 \pm 0.003$	$56\,088.768 \pm 0.058$	$56\,088.772 \pm 0.060$
9.5	$56\,058.006 \pm 0.001$	$56\,058.120 \pm 0.016$	$56\,108.377 \pm 0.056$	$56\,108.382 \pm 0.059$
10.5	$56\,078.724 \pm 0.021$	$56\,078.848 \pm 0.006$	$56\,129.990 \pm 0.044$	$56\,129.997 \pm 0.046$
11.5	$56\,101.420 \pm 0.021$	$56\,101.554 \pm 0.007$	$56\,153.718 \pm 0.036$	$56\,153.727 \pm 0.039$
12.5	$56\,126.094 \pm 0.011$	$56\,126.238 \pm 0.003$	$56\,179.422 \pm 0.023$	$56\,179.432 \pm 0.020$
13.5	$56\,152.694 \pm 0.048$	$56\,152.848 \pm 0.035$	$56\,207.188$	$56\,207.199$
14.5	$56\,181.276 \pm 0.041$	$56\,181.439 \pm 0.028$	$56\,236.828$	$56\,236.840$
15.5	$56\,211.848 \pm 0.003$	$56\,212.019 \pm 0.008$	$56\,268.493$	$56\,268.509$
16.5	$56\,244.337 \pm 0.029$	$56\,244.767 \pm 0.019$	$56\,301.740$	$56\,301.759$
17.5	$56\,278.782$	$56\,279.252$		

^{a}Absolute values of the wave numbers are subject to the calibration uncertainty of 0.02 cm^{-1}.

TABLE III. Molecular constants of the $B(11)$ $^2\Pi$ level of NO, cm^{-1}.

	Our work	HLM[a]	LM[b]
T_0^{c}	55 983.203±0.017		55 984
A	47.977±0.024		
B_v	1.010 77±0.000 37	1.010	1.009
D_v, 10^{-6}	6.7±0.8		
A_D	0.0438±0.0035		

[a]HLM: Herzberg *et al.* (Ref. 12).
[b]LM: Lagerqvist and Miescher (Ref. 13).
[c]The value of T_0 is subject to the calibration uncertainty of 0.02 cm^{-1}.

with the standard deviation shown as an estimated error.

The effective Hamiltonian operator, suitable for the description of the $^2\Pi$ state, can be found in Hougen[26] and Zare *et al.*[27] The matrix elements used in this work for the calculation of rotational energy levels are the same as those in Amiot *et al.*[28] and Stark *et al.*[29] The parameters included in the description of the $^2\Pi$ state are the band origin T_0; the rotational parameters B, and D; and the spin–orbit parameters A and A_D. In our analysis, we have performed least-squares fittings to the rovibronic term values. Table III summarizes the molecular constants obtained for the $v=11$ level of the B $^2\Pi$ state. The molecular parameters determined by Herzberg *et al.*[12] and Lagerqvist and Miescher[13] are included for comparison. Our molecular parameters were determined with high accuracy and the agreement between our values and those of earlier work is excellent.

B. The integrated cross sections and oscillator strengths

The fitting procedure employed under *XGREMLIN*[22] also evaluates integrated areas for the lines fitted. These are unaffected by the anomalous widths of the lines, provided

that the residuals of the fit are comparable with the noise levels in the observed spectrum. This was found to be the case when the Gaussian contribution of the Voigt profile was held constant at 0.175 cm^{-1}, and the integrated cross sections derived from the areas and the total column density of NO are given in Table IV. These cross sections depend on the temperature, which was 295 K in this case. The integrated cross sections of blended lines have been separated by using branching ratios observed for other transitions together with the Boltzmann population distribution. The values listed in Table IV can be divided by the fractional populations of the rotational levels to obtain values proportional to the line oscillator strengths. The integrated cross sections of R_{11} branch lines are plotted in Fig. 3.

The uncertainties in the integrated cross sections arise from noise and the errors in the measurement of path length and pressure. The relative importance of these components in the uncertainty can be evaluated by making measurements at different sample gas pressures and path lengths, as was done for a band previously analyzed.[6] These measurements showed that noise made the dominant contribution to the uncertainty and that because photon noise is evenly distributed throughout an FT spectrum the typical uncertainty for a single point in a cross section was $\pm 1.70\times 10^{-18}$ cm^2 for all points on the linear portion of the curve of growth. Points from partly saturated lines were subject to a slightly larger error. The uncertainty of a strong (but unsaturated) unblended line of integrated cross section 3×10^{-17} cm^2 cm^{-1} is 5.6%. Weaker lines have errors many times larger associated with them, but since most of the total integrated cross section for the band is contributed by strong lines the total error was taken to be 6%.

The band oscillator strength of a (v',v'') band is given by

TABLE IV. Integrated cross sections of lines of the $\beta(11,0)$ band of NO in units of 10^{-18} cm^2 cm^{-1}.[a]

J	$R_{11}(J)_e$	$R_{11}(J)_f$	$P_{11}(J)_e$	$P_{11}(J)_f$	$Q_{11}(J)$	$R_{22}(J)$	$P_{22}(J)$	$Q_{22}(J)$
0.5	2.27b				1.20			
1.5	3.75b		2.49		0.37	2.07		2.23
2.5	5.68		4.27			2.25	2.02B	1.71
3.5	6.30		5.39			3.44	2.76B	1.46
4.5	7.73		6.69			4.56	3.72B	1.02
5.5	8.25		7.12			4.62B	3.83B	
6.5	7.87		7.74			4.42B	3.72B	
7.5	7.76		7.75			4.63B	3.65B	
8.5	7.78		7.73			4.54B	4.05B	
9.5	6.94		7.67			4.16B	3.87b	
10.5	7.01		7.04			3.51B	3.17b	
11.5	5.76		6.22b			3.37B	3.38	
12.5	4.10		5.23			2.97b	2.91	
13.5	3.88		3.99			2.67b	2.18	
14.5	2.65		2.58	0.77		1.72		
15.5	1.47	0.79	2.10	0.80		1.12		
16.5	0.81	0.52	1.56b	0.67b				
17.5			0.95	0.51				
Total[b]	91.33		89.27		1.57	50.04	39.25	6.43
Extended[c]	95.77		95.46		1.57	54.56	50.19	6.43

[a]Lines followed by B are blends observed as a single line, and by b are blends observed as an incompletely resolved complex.
[b]Total cross section for observed lines.
[c]Total cross section after correction of higher J lines.

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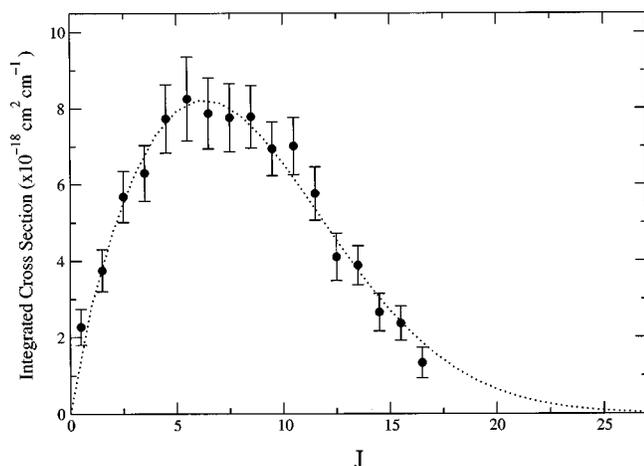
FIG. 3. The integrated cross sections of the R_{11} branch lines.

$$f(v',v'') = \frac{mc^2}{\pi e^2} \frac{1}{\tilde{N}(v'')} \int \sigma(\nu) d\nu, \tag{1}$$

in which $\tilde{N}(v'')$ is the fractional Boltzmann population of the absorbing vibrational level—in this case since $v''=0$ this quantity is unity—and the integration of the cross section $\sigma(\nu)$ is performed over all of the rotational lines belonging to the (11,0) band. The total integrated cross sections of observed lines for each branch are presented in Table IV. Observations of the rotational lines are mostly limited to $J \leqslant 19.5$. The effects from higher J lines cannot be ignored. We extended the sum to $J=33.5$ by using the Boltzmann distribution and these value are presented in Table IV as "Extended." The integrated cross section of the β(11,0) band was found to be 3.04×10^{-16} cm^2 cm^{-1}, meaning that the oscillator strength for the band is $(3.44 \pm 0.21) \times 10^{-4}$. Our value for the band oscillator strength of the β(11,0) band happens to agree well with the value quoted by Bethke[15] of 3.6×10^{-4}, although his estimated uncertainty was as high as 20% because of overlapping with the strong ϵ(1,0) band. The calculated value by Laux and Kruger[30] agree well with ours

though their values for $v' \geqslant 6$ are regarded as approximate. Our value is also in good agreement with Gallusser and Dressler[31] whose theoretical analysis produced an oscillator strength of 3.6×10^{-4}. While the β(11,0) band was visible in the raw data of Cieslik,[18] it was too weak and too overlapped with the strong ϵ(1,0) band to derive reasonable band oscillator strength from the absorption signal. Chan et al.[21] report a value of 6.48×10^{-4} although no evidence of the β(11,0) band was seen in their Fig. 2. The band oscillator strengths from the FT measurements are summarized in Table V under FTS/VUV, and compared with the previous results. We would like to postpone our discussion on band oscillator strengths of band systems of NO in the wavelength region 160–195 nm until after the analyses of all these bands are completed.

IV. SUMMARY

This work provides the first absorption measurements of the β(11,0) band of NO free of problems arising from inadequate spectral resolution, achieved by using the combination of a VUV FT spectrometer and a synchrotron radiation source. Accurate rotational line positions and term values as well as the photoabsorption integrated cross sections are provided.

ACKNOWLEDGMENTS

TABLE V. A comparison of band oscillator strengths (10^{-3}) for selected NO bands.[a]

Main band	γ(3,0)	β(6,0)	β(9,0)	δ(1,0)	ϵ(1,0)	β(11,0)
FTS/UVU[b]	**0.269**	**0.048**	**0.265**	**5.4**	**2.88**	**0.344**
Bethke[c]	0.36	0.046	0.36	5.8	4.6	0.36
Chan et al.	0.36	0.037	0.31	6.0	4.6	0.65
Cieslik[e]	0.31		0.36	5.6	6.5	
Luque and Crosley[f]	**0.36**				**3.7**	
Laux and Kruger[g]	**0.34**	0.043	0.16			**0.34**
Gallusser and Dressler[h]		**0.040**	**0.35**	**6.1**		**0.36**
Blended band	β(6,0)	γ(3,0)		β(10,0)	β(11,0) γ(5,0)	ϵ(1,0)

[a]Values in bold are obtained for a single band.
[b]Present work for the β(11,0) band, and our published works (Refs. 5–8).
[c]Bethke (Ref. 15).
[d]Chan et al. (Ref. 21).
[e]Cieslik (Ref. 18).
[f]Luque and Crosley (Ref. 20).
[g]Laux and Kruger (Ref. 30).
[h]Gallusser and Dressler (Ref. 31).

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