Pure Rotation Spectrum of NNO in the Far Infrared Region

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The pure rotational spectrum of NNO has been observed as an impurity in the NO spectrum which has been recorded with a high resolution Fourier transform spectrometer. The observed high-*J* transitions in the ground vibrational state were analyzed by a least-squares fit together with the available millimeter and submillimeter wave data. It has been proved that the highly precise data of Maki et al. [3] can be used as a wavenumber standard for the far infrared.

Recently Maki and coworkers have revised the spectroscopic parameters of the NNO molecule intending to supply a good wavenumber standard in the infrared region [1–3]. They have measured the vibration-rotation transitions of this molecule in the infrared region with high precision by using heterodyne technique. They have provided also a very accurate set of the constants for the ground state [3]. However, to the best of our knowledge, the pure rotational transitions in the far infrared (FIR) have not been measured yet. In the course of our meaurements of NO [4], we have accidentally found the spectrum of NNO in the region from 20 to 50 cm^{-1} as an impurity. By analyzing these data together with the available millimeter (mmw) and submillimeter (sub-mmw) wave data [5, 6] up to 552 GHz, we have confirmed the ground state constants of [3].

The measurement has been carried out with a Bruker IFS 120 HR vacuum Michelson spectrometer at the molecular spectroscopy laboratory, Physikalisch-Chemisches Institut, Universität Giessen. The sample of NO was sublimated at a low temperature, in order to prevent contamination by water, and was transfered at a total pressure of about 150 Pa into the 1.8 m long cell sealed with polyethylene windows. The total pressure was around 156 Pa. The spectrum was recorded in the region from 20 to 90 cm^{-1}, using a myler beamsplitter and InSb detector at liq. He temperature. Small amounts of water, which presumably came out of the cell wall, have been detected. In addition to the NO spectrum very regularly spaced lines were observed, whose separation indicated NNO to be the carrier caused by a small impurity in the NO gas.

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Table 1. Measured transitions of NNO in the ground state.

$J'-J''$	Observed	Obs-Calc	Unit
24–23	20.10268	–0.00012	cm^{-1} [a]
25–24	20.93954	0.00000	cm^{-1} [a]
26–25	21.77625	0.00006	cm^{-1} [a]
27–26	22.61283	0.00010	cm^{-1} [a]
28–27	23.44908	–0.00007	cm^{-1} [a]
29–28	24.28544	–0.00002	cm^{-1} [a]
30–29	25.12173	0.00008	cm^{-1} [a]
31–30	25.95782	0.00012	cm^{-1} [a]
32–31	26.79374	0.00012	cm^{-1} [a]
33–32	27.62954	0.00013	cm^{-1} [a]
34–33	28.46510	0.00003	cm^{-1} [a]
35–34	29.30064	0.00007	cm^{-1} [a]
36–35	30.13594	0.00001	cm^{-1} [a]
37–36	30.97119	0.00005	cm^{-1} [a]
38–37	31.80625	0.00006	cm^{-1} [a]
39–38	32.64120	0.00013	cm^{-1} [a]
40–39	33.47586	0.00006	cm^{-1} [a]
41–40	34.31028	–0.00008	cm^{-1} [a]
42–41	35.14466	–0.00007	cm^{-1} [a]
43–42	35.97887	–0.00008	cm^{-1} [a]
44–43	36.81301	0.00005	cm^{-1} [a]
45–44	37.64684	0.00003	cm^{-1} [a]
46–45	38.48049	0.00004	cm^{-1} [a]
47–46	39.31394	0.00004	cm^{-1} [a]
48–47	40.14717	0.00002	cm^{-1} [a]
49–48	40.98036	0.00016	cm^{-1} [a]
50–49	41.81312	0.00007	cm^{-1} [a]
51–50	42.64565	–0.00003	cm^{-1} [a]
52–51	43.47817	0.00007	cm^{-1} [a]
53–52	44.31021	–0.00008	cm^{-1} [a]
55–54	45.97391	–0.00010	cm^{-1} [a]
57–56	47.63681	0.00002	cm^{-1} [a]
5– 4	125613.69600	–0.00111	MHz [b]
6– 5	150735.04600	0.00308	MHz [b]
7– 6	175855.62300	–0.00558	MHz [b]
8– 7	200975.25600	–0.07138	MHz [c]
10– 9	251211.55700	–0.00068	MHz [b]
12–11	301442.70000	–0.02022	MHz [b]
15–14	376777.75300	0.00822	MHz [d]
16–15	401885.80200	0.01432	MHz [d]
17–16	426991.80800	0.00456	MHz [d]
18–17	452095.67000	0.00467	MHz [d]
19–18	477197.24700	0.00033	MHz [d]
20–19	502296.42300	0.00228	MHz [d]
21–20	527393.05100	–0.00977	MHz [d]
22–21	552487.03600	–0.00411	MHz [d]

[a] Present work: estimated uncertainty of 3 MHz.
[b] From [5]: estimated uncertainty of 10 kHz.
[c] From [5]: estimated uncertainty of 100 kHz.
[d] From [6]: estimated uncertainty of 10 kHz.

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Table 2. The rotational and centrifugal distortion constants of NNO in the ground vibrational state[a]

	Present work		Maki et al. [3]
	Combined fit	FIR only	
B/MHz	12561.63365 (25)	12561.646 (31)	12561.63395 (10)
D/kHz	5.27882 (51)	5.273 (17)	5.27915 (12)
H/MHz	−0.17 (40)	−1.9 (29)	−4.921 (138)

[a] Numbers in the parentheses are the standard deviation in units of the last digit quoted.

The spectrum was calibrated using the water lines in the recorded spectrum, the positions of which are listed by Guelachvili and Rao [7], and some sub-mmw lines of NO which were measured by coherent radiation sources [8]. In the recorded region we have identified 77 standard lines, and the fit of those to an non-linear calibration equation,

$$\nu = a\,\nu_{\exp} + b/\nu_{\exp}, \qquad (1)$$

resulted in a standard deviation of 2.3 MHz, which represents the accuracy of the present measurements. The non-linear part in (1) represents the diffraction effect at the aperture of the radiation source which gives a significant effect at long wavelengths [9].

The measured transition wavenumbers of the NNO lines are summarized in Table 1 together with the mmw and sub-mmw data from [5] and [6] which were included in the present analysis. The constants obtained from the weighted least-squares fit are listed in Table 2. We have used the weight reciprocally proportional to the square of the estimated experimental uncertainties: 10 kHz for most of the mmw and sub-mmw lines and 3 MHz for the FIR data. The constants resulting from this fit are listed in Table 2, together with the constants given by Maki and coworkers [3] and the constants obtained from FIR data only.

The present constants agree within one standard deviation with those of [3]. The constants obtained from the FIR only are also in a good agreement with those obtained from the combined fit. The heterodyne measurements of Maki and coworkers are very precise; the uncertainties for the three constants B, D, and H are smaller than those of the present work. From the present result we conclude that the transition frequencies calculated from the ground state constants reported in [3] should be used as a wavenumber standard in the FIR region with an accuracy better than 0.0001 cm^{-1}.

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