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THE MID-INFRARED FREQUENCY STANDARD USING $^{14}N^{m}O(m=16,17,18)$ SPECTRAL LINES*

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Based on the global analysis of all available and reliable data for isotopic species $^{14}N^{m}O(m=16,17,18)$, the $^{14}N^{16}O$ rovibrational spectral lines are calculated with very high accuracy and completely agree with previous results. These lines with relative intensities can be achieved as an infrared frequency standard in the spectral range 1600–5600 cm^{-1}. The calculated rovibrational transitions of $^{14}N^{m}O(m=17,18)$ have the same accuracy as that for $^{14}N^{16}O$ although their data are rare due to their small natural abundance.

PACC: 3520P; 3320E

I. INTRODUCTION

Nitric Oxide is a well-known stable radical with $^2\Pi_{3/2}$ lying above $^2\Pi_{1/2}$ for 123 cm^{-1} in the ground state. As one of the poisonous pollutants in the atmosphere and a signal molecule in living bodies, it attracted attention of many spectroscopists. In 1950s, Burrus and Gordy *et al.*[1−5] first obtained the microwave spectrum of $^{14}N^{16}O$ in the ground state $X^2\Pi$. Shortly afterwards, Meerts, Dymanus[6], Lowe[7] and Neumann[8] measured the Λ-doubling transitions of $^{14}N^{16}O$ and $^{15}N^{16}O$ by molecular beam electric resonance and obtained accurate hyperfine parameters. In the far-infrared region, Mizushima[9] observed Zeeman effect of rotational energy levels of $^{14}N^{16}O$, while Brown *et al.*[10], Heuvel *et al.*[11] and Saleck *et al.*[12−13] analyzed magnetic dipole transitions between $X^2\Pi_{1/2}$ and $X^2\Pi_{3/2}$. Additionally, in the mid-infrared region, the laser magnetic resonance(LMR) spectroscopy technique was adopted to obtain the magnetic parameters of NO.[14−16] As for the vibrational bands of ^{14}NO in zero field, Henry *et al.*[17−21] made a complete investigation of high quality. Moreover, Hinz *et al.*[22] measured the rovibrational transitions($v = 1 \leftarrow 0$) of $^{14}N^{16}O$ accurately by heterodyne method, based on which the NIST (the National Institute of Standard and Technology, U.S.A.) published the atlas of $^{14}N^{16}O$ absorption spectrum between 1741 cm^{-1} and 1940 cm.$^{-1}$ [23] However, no systematic analysis of $^{14}N^{m}O(m=16,17,18)$ has been made except for our previous work.[24,25]

Taking all the previous experimental data available and reliable into account, we have made a successful global least-square fit and given a full set of $^{14}N^{16}O$ molecular constants with high accuracy.[24,25] In this paper we calculate the rovibrational transitions of $^{14}N^{16}O$ with very high accuracy and compare them with the previous results partly. The remarkable precision proves that the calculated transition frequencies can serve as an infrared frequency standard in the spectral range of 1600–5600 cm^{-1}. Using the isotopic scaling function, the spectra of $^{14}N^{m}O(m=17,18)$ can also be calculated as an additional frequency standard if required.

II. CALCULATION OF SPECTRUM

The global least-square fit was performed using Brown's effective Hamiltonian model.[26] The Hamiltonian used in the program has been detailed in our previous work.[24,25,27] It is expanded in $\boldsymbol{N}^2$ terms other than $\boldsymbol{R}^2$ terms. The former method has much superiority over the latter. For instance, the former eliminates the interaction between different electronic states, while the latter contains the electronic interaction since $\boldsymbol{N}^2 = (\boldsymbol{J}-\boldsymbol{S})^2$ and $\boldsymbol{R}^2 = (\boldsymbol{J}-\boldsymbol{L}-\boldsymbol{S})^2$.

The effective Hamiltonian is transformed into a matrix in the symmetric basis

$$|\Lambda; JM_J\Omega\pm\rangle = \frac{1}{\sqrt{2}}(|\Lambda; S\Sigma; JM_J\Omega\rangle \pm (-1)^{J-S+s} \cdot |-\Lambda; S-\Sigma; JM_J-\Omega\rangle), \quad (1)$$

where $s = 1$ for Σ^- state; $s = 0$ for other states.

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The vibrational energy of the effective Hamiltonian is expressed as

$$G(v+1/2) = \omega_e(v+1/2) - \omega_e x_e(v+1/2)^2 + \omega_e y_e(v+1/2)^3 + \cdots, \quad (2)$$

while the vibrational dependencies of the other parameters are defined as

$$P_v = P_e + \alpha_p(v+1/2) + \beta_p(v+1/2)^2 + \cdots, \quad (3)$$

The isotopic scaling function[28] is introduced by the following formula

$$P_e^i(v+1/2)^k(\boldsymbol{N}^2)^l \equiv \rho_i^{k/2} P_e^*(v+1/2)^k(\boldsymbol{N}^2)^l F(\Delta_{kl}), \quad (4)$$

where P_e^i is the scaled parameter for the isotopomer i, $\boldsymbol{N}^2$ the rotational operator of the effective Hamiltonian, ρ_i the ratio of the reduced mass of the reference isotopomer to the reduced mass of isotopomer i, $\boldsymbol{P}_e^*$ the equilibrium value for the reference isotopomer, and $F(\Delta_{kl})$ a function of Watson's dimensionless Δ_{kl} parameters[28] used to compensate for the small effect of the breakdown of the Born-Oppenheimer approximation,

$$F(\Delta_{kl}) = \frac{1+(m_e/m_a^i)\Delta_{kl}(a)+(m_e/m_b^i)\Delta_{kl}(b)}{1+(m_e/m_a^*)\Delta_{kl}(a)+(m_e/m_b^*)\Delta_{kl}(b)}, \quad (5)$$

where m_e is the mass of electron, and m_a and m_b are the atomic masses of atoms a and b. In the calculation, only the modification to parameters ω_e and B_e was considered while for other parameters, $F(\Delta_{kl})$ was set to be unit one.

The reduced mass ratios of NO used are listed in Table 1. The intensity of spectral lines is evaluated according to the following formula

$$I_{abs} = v_{mn}|R_{mn}|^2[\exp(-E_n/2kT) - \exp(-E_m/2kT)]. \quad (6)$$

Here v_{mn} is the transition frequency between states m and n, R_{mn} the transition possibility. E_m and E_n the energy levels of states m and n respectively, k the Boltzman constant, and T the temperature (T=300 K is set in the calculation).

Table 1. The reduced mass ratios μ^*/μ^i of ^{14}NO

	Mass of Nitrogen[a)]	Mass of Oxygen[a)]	μ^*/μ^{i} [b)]
$^{14}N^{16}O$	14.00307	15.99491	1.0000000000
$^{14}N^{17}O$	14.00307	16.99913	0.9724238635
$^{14}N^{18}O$	14.00307	17.99916	0.9480206429

a) in atomic mass unit;
b) μ^* and μ^i are the reduced masses of the reference molecule $^{14}N^{16}O$ and its isotopomer i respectively.

After the determination of molecular parameters by the global least-square fit, we calculate the rovibrational spectra of $^{14}N^{16}O$ for several bands(v=1–0, v=2–0, v=3–0), and compared the results with the mid-infrared frequency standard of NIST. The result of band v=1–0 is shown in Table 2. The remarkable agreement with the NIST implies our calculation is reliable and accurate.

Table 2. the calculated v=1–0 transition lines in the ground state (in unit of cm^{-1})[a)].

	$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ P_-				$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ P_+			
J	v_{cal}	v_{NIST}	Δv	I	v_{cal}	v_{NIST}	Δv	I
1.5								
2.5	1867.21230	1867.21225	0.5	0.37D+01	1867.21239	1867.21234	0.5	0.37D+01
3.5	1863.68298	1863.68293	0.5	0.47D+01	1863.68280	1863.68275	0.5	0.47D+01
4.5	1860.11813	1860.11808	0.5	0.49D+01	1860.11843	1860.11838	0.5	0.49D+01
5.5	1856.51900	1856.51894	0.6	0.47D+01	1856.51854	1856.51849	0.5	0.47D+01
6.5	1852.88429	1852.88424	0.5	0.44D+01	1852.88493	1852.88488	0.5	0.44D+01
7.5	1849.21648	1849.21643	0.5	0.40D+01	1849.21563	1849.21558	0.5	0.40D+01
8.5	1845.51281	1845.51275	0.6	0.35D+01	1845.51389	1845.51383	0.6	0.35D+01
9.5	1841.77740	1841.77733	0.7	0.30D+01	1841.77605	1841.77600	0.5	0.30D+01
10.5	1838.00561	1838.00555	0.6	0.26D+01	1838.00724	1838.00717	0.7	0.26D+01
11.5	1834.20363	1834.20355	0.8	0.21D+01	1834.20169	1834.20162	0.7	0.21D+01
12.5	1830.36451	1830.36444	0.7	0.18D+01	1830.36678	1830.36670	0.8	0.18D+01
13.5	1826.49690	1826.49681	0.9	0.14D+01	1826.49428	1826.49421	0.7	0.14D+01
14.5	1822.59120	1822.59113	0.7	0.11D+01	1822.59418	1822.59409	0.9	0.11D+01
15.5	1818.65881	1818.65872	0.9	0.87D+00	1818.65545	1818.65538	0.7	0.87D+00
16.5	1814.68723	1814.68715	0.8	0.66D+00	1814.69098	1814.69088	1.0	0.66D+00
17.5	1810.69084	1810.69074	1.0	0.50D+00	1810.68669	1810.68661	0.8	0.50D+00
18.5	1806.65400	1806.65393	0.7	0.37D+00	1806.65857	1806.65847	1.0	0.37D+00
19.5	1802.59432	1802.59421	1.1	0.27D+00	1802.58932	1802.58926	0.6	0.27D+00
20.5	1798.49279	1798.49274	0.5	0.19D+00	1798.49822	1798.49812	1.0	0.19D+00
21.5	1794.37043	1794.37034	0.9	0.13D+00	1794.36457	1794.36452	0.5	0.13D+00

Table 2. (*Continued*)

$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ P_-					$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ P_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
22.5	1790.20477	1790.20474	0.3	0.93D−01	1790.21108	1790.21099	0.9	0.93D−01
23.5	1786.02030	1786.02022	0.8	0.63D−01	1786.01355	1786.01353	0.2	0.63D−01
24.5	1781.79100	1781.79100	0.0	0.42D−01	1781.79821	1781.79814	0.7	0.42D−01
25.5	1777.54493	1777.54488	0.5	0.28D−01	1777.53727	1777.53730	−0.3	0.28D−01
26.5	1773.25246	1773.25251	−0.5	0.18D−01	1773.26058	1773.26054	0.4	0.18D−01
27.5	1768.94527	1768.94525	0.2	0.12D−01	1768.93669	1768.93678	−0.9	0.12D−01
28.5	1764.59007	1764.59020	−1.3	0.72D−02	1764.59910	1764.59910	0.0	0.72D−02
29.5	1760.22219	1760.22222	−0.3	0.45D−02	1760.21269	1760.21287	−1.8	0.45D−02
30.5	1755.80468	1755.80491	−2.3	0.27D−02	1755.81463	1755.81471	−0.7	0.27D−02
31.5	1751.37655	1751.37666	−1.1	0.16D−02	1751.36613	1751.36641	−2.8	0.16D−02
32.5	1746.89713	1746.89749	−3.6	0.95D−03	1746.90801	1746.90819	−1.8	0.95D−03
33.5	1742.40914	1742.40938	−2.4	0.55D−03	1742.39780	1742.39824	−4.4	0.55D−03
34.5	1737.86823			0.31D−03	1737.88003			0.31D−03
35.5	1733.32077			0.18D−03	1733.30851			0.18D−03
36.5	1728.71874			0.97D−04	1728.73146			0.98D−04
37.5	1724.11220			0.53D−04	1724.09902			0.53D−04
38.5	1719.44944			0.28D−04	1719.46308			0.28D−04
39.5	1714.78420			0.15D−04	1714.77010			0.15D−04
40.5	1710.06110			0.77D−05	1710.07566			0.77D−05
$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ Q_-					$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ Q_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
1.5	1875.81289	1875.81285	0.4	0.53D+01	1875.81283	1875.81279	0.4	0.53D+01
2.5	1875.72261	1875.72256	0.5	0.26D+01	1875.72285	1875.72280	0.5	0.26D+01
3.5	1875.59685	1875.59680	0.5	0.15D+01	1875.59625	1875.59620	0.5	0.15D+01
4.5	1875.43375	1875.43370	0.5	0.91D+00	1875.43494	1875.43489	0.5	0.91D+00
5.5	1875.23716	1875.23711	0.5	0.60D+00	1875.23509	1875.23505	0.5	0.60D+00
6.5	1875.00027	1875.00023	0.4	0.40D+00	1875.00356	1875.00351	0.5	0.40D+00
7.5	1874.73419	1874.73413	0.6	0.28D+00	1874.72929	1874.72924	0.5	0.28D+00
8.5	1874.42214	1874.42209	0.5	0.19D+00	1874.42908	1874.42902	0.6	0.19D+00
9.5	1874.08829	1874.08822	0.7	0.13D+00	1874.07883	1874.07879	0.4	0.13D+00
10.5	1873.69937	1873.69933	0.4	0.93D−01	1873.71187	1873.71178	0.9	0.93D−01
11.5	1873.29985	1873.29975	1.0	0.65D−01	1873.28376	1873.28374	0.2	0.65D−01
12.5	1872.83204	1872.83202	0.2	0.45D−01	1872.85228	1872.85217	1.1	0.45D−01
13.5	1872.36921	1872.36908	1.3	0.31D−01	1872.34420	1872.34419	0.1	0.31D−01
14.5	1871.82026	1871.82027	−0.1	0.21D−01	1871.85067	1871.85053	1.4	0.21D−01
15.5	1871.29671	1871.29654	1.7	0.14D−01	1871.26025	1871.26027	−0.2	0.14D−01
16.5	1870.66419	1870.66423	−0.4	0.97D−02	1870.70735	1870.70716	1.9	0.97D−02
17.5	1870.08264	1870.08242	2.2	0.65D−02	1870.03209	1870.03216	−0.7	0.65D−02
18.5	1869.36398	1869.36408	−1.0	0.43D−02	1869.42260			0.43D−02
19.5	1868.72726			0.28D−02	1868.65987			0.28D−02
20.5	1867.91979			0.18D−02	1867.99665			0.18D−02
21.5	1867.23078			0.12D−02	1867.14375			0.12D−02
22.5	1866.33177			0.72D−03	1866.42969			0.72D−03
23.5	1865.59337			0.45D−03	1865.48388			0.45D−03
24.5	1864.60008			0.28D−03	1864.72186			0.28D−03
25.5	1863.81516			0.17D−03	1863.68040			0.17D−03
26.5	1862.72484			0.10D−03	1862.87328			0.10D−03
27.5	1861.89623			0.59D−04	1861.73342			0.59D−04
28.5	1860.70615			0.34D−04	1860.88401			0.34D−04
29.5	1859.83663			0.20D−04	1859.64304			0.20D−04
39.5	1858.54409			0.11D−04	1858.75409			0.11D−04
31.5	1857.63639			0.62D−05	1857.40932			0.62D−05
32.5	1856.23873			0.34D−05	1856.48353			0.34D−05
33.5	1855.29550			0.19D−05	1855.03232			0.19D−05
34.5	1853.79010			0.10D−05	1854.07230			0.10D−05
35.5	1852.81393			0.53D−06	1852.51206			0.53D−06
36.5	1851.19821			0.27D−06	1851.52037			0.27D−06
37.5	1850.19162			0.14D−06	1849.84854			0.14D−06
38.5	1848.46304			0.71D−07	1848.82767			0.71D−07
39.5	1847.42851			0.35D−07	1847.04172			0.35D−07
40.5	1845.58458			0.17D−07	1845.99413			0.17D−07

Table 2. (*Continued*)

$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ R_-					$^2\Pi_{3/2}$–$^2\Pi_{3/2}$ R_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
1.5	1884.32320	1884.32316	0.4	0.53D+01	1884.32329	1884.32325	0.4	0.39D+01
2.5	1887.63648	1887.63643	0.5	0.26D+01	1887.63630	1887.63625	0.5	0.51D+01
3.5	1890.91248	1890.91242	0.6	0.15D+01	1890.91276	1890.91271	0.5	0.54D+01
4.5	1894.15192	1894.15187	0.5	0.91D+00	1894.15149	1894.15145	0.4	0.53D+01
5.5	1897.35315	1897.35310	0.5	0.60D+00	1897.35373	1897.35368	0.5	0.50D+01
6.5	1900.51798	1900.51793	0.5	0.40D+00	1900.51722	1900.51717	0.5	0.46D+01
7.5	1903.64352	1903.64347	0.5	0.28D+00	1903.64448	1903.64443	0.5	0.42D+01
8.5	1906.73303	1906.73298	0.5	0.19D+00	1906.73185	1906.73181	0.4	0.37D+01
9.5	1909.78206	1909.78200	0.6	0.13D+00	1909.78345	1909.78340	0.5	0.32D+01
10.5	1912.79559	1912.79553	0.6	0.93D−01	1912.79395	1912.79390	0.5	0.27D+01
11.5	1915.76738	1915.76733	0.5	0.65D−01	1915.76927	1915.76921	0.6	0.23D+01
12.5	1918.70435	1918.70429	0.6	0.45D−01	1918.70220	1918.70215	0.5	0.18D+01
13.5	1921.59828	1921.59822	0.6	0.31D−01	1921.60069	1921.60063	0.6	0.15D+01
14.5	1924.45816	1924.45809	0.7	0.21D−01	1924.45547	1924.45542	0.5	0.12D+01
15.5	1927.27367	1927.27362	0.5	0.14D−01	1927.27663	1927.27655	0.8	0.92D+00
16.5	1930.05599	1930.05591	0.8	0.97D−02	1930.05276	1930.05271	0.5	0.71D+00
17.5	1932.79262	1932.79257	0.5	0.65D−02	1932.97612	1932.79604	0.8	0.53D+00
18.5	1935.49692	1935.49684	0.8	0.43D−02	1935.49315	1935.49310	0.5	0.39D+00
19.5	1938.15425	1938.15420	0.5	0.28D−02	1938.15830	1938.15820	1.0	0.29D+00
20.5	1940.78013	1940.78003	1.0	0.18D−02	1940.77583	1940.77578	0.5	0.21D+00
21.5	1943.35778			0.12D−02	1943.36235			0.15D+00
22.5	1945.90484			0.72D−03	1945.90002			0.10D+00
23.5	1948.40244			0.45D−03	1948.40752			0.69D−01
24.5	1950.87029			0.28D−03	1950.86499			0.46D−01
25.5	1953.28752			0.17D−03	1953.29309			0.31D−01
26.5	1955.67578			0.10D−03	1955.67000			0.20D−01
27.5	1958.01229			0.59D−04	1958.01832			0.13D−01
28.5	1960.32056			0.34D−04	1960.31435			0.80D−02
29.5	1962.57602			0.20D−04	1962.58249			0.50D−02
30.5	1964.80391			0.11D−04	1964.79729			0.30D−02
31.5	1966.97795			0.62D−05	1966.98484			0.18D−02
32.5	1969.12505			0.34D−05	1969.11805			0.11D−02
33.5	1971.21733			0.19D−05	1971.22460			0.63D−03
34.5	1973.28321			0.10D−05	1973.27586			0.36D−03
35.5	1975.29334			0.53D−06	1975.30097			0.20D−03
36.5	1977.27756			0.27D−06	1977.26989			0.11D−03
37.5	1979.20515			0.14D−06	1979.21313			0.61D−04
38.5	1981.10727			0.71D−07	1981.09929			0.33D−04
39.5	1982.95190			0.35D−07	1982.06019			0.17D−04
40.5	1984.77144			0.17D−07	1984.06319			0.90D−05
$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ P_-					$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ P_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
1.5	1871.06628	1871.06637	−0.9	0.87D+01	1871.05442	1871.05451	−0.9	0.87D+01
2.5	1867.65918	1867.65926	−0.8	0.10D+02	1867.67100	1867.67108	−0.8	0.10D+02
3.5	1864.24149	1864.24157	−0.8	0.10D+02	1864.22975	1864.22983	−0.8	0.10D+02
4.5	1860.76612	1860.76619	−0.7	0.97D+01	1860.77775	1860.77783	−0.8	0.97D+01
5.5	1857.27980	1857.27986	−0.6	0.91D+01	1857.26830	1857.26836	−0.6	0.91D+01
6.5	1853.73629	1853.73635	−0.6	0.83D+01	1853.74763	1853.74769	−0.6	0.83D+01
7.5	1850.18125	1850.18130	−0.5	0.74D+01	1850.17011	1850.17015	−0.4	0.74D+01
8.5	1846.56976	1846.56980	−0.4	0.65D+01	1846.58069	1846.58072	−0.3	0.65D+01
9.5	1842.94595	1842.94597	−0.2	0.56D+01	1842.93527	1842.93528	−0.1	0.56D+01
10.5	1839.26665	1839.26666	−0.1	0.48D+01	1839.27706	1839.27707	−0.1	0.48D+01
11.5	1835.57406	1835.57406	0.0	0.40D+01	1835.56394	1835.56393	0.1	0.40D+01
12.5	1831.82718	1831.82716	0.2	0.33D+01	1831.83699	1831.83698	0.1	0.33D+01
13.5	1828.06590	1828.06586	0.4	0.26D+01	1828.05642	1828.05638	0.4	0.26D+01
14.5	1824.25171	1824.25164	0.7	0.21D+01	1824.26084	1824.26079	0.5	0.21D+01

Table 2. (*Continued*)

$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ P_-					$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ P_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
15.5	1820.42187	1820.42181	0.6	0.16D+01	1820.41310	1820.41302	0.8	0.16D+01
16.5	1816.54069	1816.54059	1.0	0.13D+01	1816.54908	1816.54900	0.8	0.13D+01
17.5	1812.64254	1812.64244	1.0	0.95D+00	1812.63453	1812.63442	1.1	0.95D+00
18.5	1808.69473	1808.69460	1.3	0.71D+00	1980.70233	1808.70223	1.0	0.71D+00
19.5	1804.72856	1804.72845	1.1	0.52D+00	1804.72136	1804.72121	1.5	0.52D+00
20.5	1800.71454	1800.71437	1.7	0.37D+00	1800.72132	1800.72120	1.2	0.37D+00
21.5	1796.68073	1796.68059	1.4	0.26D+00	1796.67436	1796.67417	1.9	0.26D+00
22.5	1792.60094	1792.60074	2.0	0.18D+00	1792.60688	1792.60674	1.4	0.18D+00
23.5	1788.49989	1788.49976	1.3	0.13D+00	1788.49439	1788.49418	2.1	0.13D+00
24.5	1784.34383	1784.35462	2.1	0.85D−01	1784.35990	1784.35976	1.4	0.86D−01
25.5	1780.18702	1780.18689	1.3	0.57D−01	1780.18238	1780.18217	1.1	0.37D−01
26.5	1775.97718	1775.97697	2.1	0.37D−01	1775.98137	1775.98126	1.1	0.37D−01
27.5	1771.74310	1771.74300	1.0	0.24D−01	1771.73934	1771.73914	2.9	0.24D−01
28.5	1767.46901	1767.46882	1.9	0.15D−01	1767.47232	1767.47224	0.8	0.15D−01
29.5	1763.16918	1763.16913	0.5	0.95D−02	1763.16631	1763.16614	1.7	0.95D−02
30.5	1758.83138	1758.83123	1.5	0.58D−02	1758.83381	1758.83380	0.1	0.58D−02
31.5	1754.46635	1754.46638	−0.3	0.35D−02	1754.46436	1754.46423	1.3	0.35D−02
32.5	1750.06538	1750.06530	0.8	0.21D−02	1750.06692	1750.06701	−0.9	0.21D−02
33.5	1745.63568	1745.63584	−1.6	0.12D−02	1745.63458	1745.63454	0.4	0.12D−02
34.5	1741.17210	1741.17211	−0.1	0.70D−03	1741.17276	1741.17298	−2.2	0.71D−03
35.5	1736.67829			0.40D−03	1736.67807			0.40D−03
36.5	1732.15264			0.22D−03	1732.15241			0.22D−03
37.5	1727.59527			0.12D−03	1727.59594			0.12D−03
38.5	1723.00810			0.66D−04	1723.00700			0.66D−04
39.5	1718.38773			0.35D−04	1718.38928			0.35D−04
40.5	1713.73959			0.19D−04	1713.73760			0.19D−04
$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ Q_-					$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ Q_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
0.5	1876.06439	1876.06447	−0.8	0.30D+01	1876.08812	1876.08821	−0.9	0.30D+01
1.5	1876.04862	1876.04870	−0.8	0.10D+01	1876.00121	1876.00129	−0.8	0.10D+01
2.5	1875.90386	1875.90393	−0.7	0.51D+00	1875.97483	1875.97491	−0.8	0.51D+00
3.5	1875.86670	1875.86678	−0.8	0.30D+00	1875.77235	1875.77242	−0.7	0.30D+00
4.5	1875.60670	1875.60675	−0.5	0.19D+00	1875.72419	1875.72426	−0.7	0.19D+00
5.5	1875.54726	1875.54732	−0.6	0.12D+00	1875.40691	1875.40696	−0.5	0.12D+00
6.5	1875.17299	1875.17302	−0.3	0.84D−01	1875.33586	1875.33590	−0.4	0.84D−01
7.5	1875.08993	1875.08997	−0.4	0.59D−01	1874.90493	1874.90495	−0.2	0.59D−01
8.5	1874.60273	1874.60273	0.0	0.41D−01	1874.80942	1874.80944	−0.2	0.41D−01
9.5	1874.49429	1874.49430	−0.1	0.30D−01	1874.26637	1874.26635	0.2	0.30D−01
10.5	1873.89584	1873.89580	0.4	0.21D−01	1874.14446	1874.14445	0.1	0.21D−01
11.5	1873.75990	1873.75989	0.1	0.15D−01	1873.49112	1873.49106	0.6	0.15D−01
12.5	1873.05219	1873.05209	1.0	0.11D−01	1873.34055	1873.34053	0.2	0.11D−01
13.5	1872.88636	1872.88632	0.4	0.76D−02	1872.57901	1872.57889	1.2	0.76D−02
14.5	1872.07158	1872.07141	1.7	0.54D−02	1872.39727	1872.39722	0.5	0.54D−02
15.5	1871.87323			0.38D−02	1871.52984			0.38D−02
16.5	1870.95377			0.26D−02	1871.31420			0.26D−02
17.5	1870.72014			0.18D−02	1870.34334			0.18D−02
18.5	1869.69852			0.12D−02	1870.09099			0.12D−02
19.5	1869.42671			0.83D−03	1869.01926			0.83D−03
20.5	1868.30553			0.56D−03	1868.72727			0.56D−03
21.5	1867.99263			0.37D−03	1867.55730			0.37D−03
22.5	1866.77453			0.24D−03	1867.22274			0.24D−03
23.5	1866.41757			0.15D−03	1865.95719			0.15D−03
24.5	1865.10524			0.98D−04	1865.57710			0.98D−04
25.5	1864.70128			0.62D−04	1864.21864			0.61D−04
26.5	1863.29736			0.38D−04	1863.79010			0.38D−04
27.5	1862.84351			0.23D−04	1862.34137			0.23D−04
28.5	1861.35064			0.14D−04	1861.86150			0.14D−04

Table 2. (*Continued*)

$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ Q_-					$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ Q_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
29.5	1860.84403			0.83D−05	1860.32513			0.83D−05
30.5	1859.26481			0.49D−05	1859.79109			0.49D−05
31.5	1858.70264			0.28D−05	1858.16966			0.28D−05
32.5	1857.03963			0.16D−05	1857.57867			0.16D−05
33.5	1856.41915			0.90D−06	1855.87470			0.90D−06
34.5	1854.67485			0.50D−06	1855.22406			0.50D−06
35.5	1853.99337			0.27D−06	1853.44004			0.27D−06
36.5	1852.17025			0.15D−06	1852.72708			0.15D−06
37.5	1851.42515			0.78D−07	1850.86544			0.78D−07
38.5	1849.52560			0.41D−07	1850.08757			0.41D−07
39.5	1848.71432			0.21D−07	1848.15070			0.21D−07
40.5	1846.74071			0.11D−07	1847.30537			0.11D−07
$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ R_-					$^2\Pi_{1/2}$–$^2\Pi_{1/2}$ R_+			
J	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I	$v_{\rm cal}$	$v_{\rm NIST}$	Δv	I
0.5	1881.04672	1881.04680	−0.8	0.89D+01	1881.03491	1881.03499	−0.8	0.89D+01
1.5	1884.29330	1884.29337	−0.7	0.10D+02	1884.30504	1884.30517	−1.3	0.10D+02
2.5	1887.52907	1887.52914	−0.7	0.11D+02	1887.51743	1887.51750	−0.7	0.11D+02
3.5	1890.70728	1890.70734	−0.6	0.11D+02	1890.71879	1890.71885	−0.6	0.11D+02
4.5	1893.87416	1893.87421	−0.5	0.10D+02	1893.86281	1893.86286	−0.5	0.10D+02
5.5	1896.98396	1896.98399	−0.3	0.94D+01	1896.99514	1896.99517	−0.3	0.94D+01
6.5	1900.08166	1900.08169	−0.3	0.86D+01	1900.07068	1900.07070	−0.2	0.86D+01
7.5	1903.12290	1903.12290	0.0	0.77D+01	1903.13367	1903.13367	0.0	0.77D+01
8.5	1906.15107	1906.15106	0.1	0.68D+01	1906.14053	1906.14051	0.2	0.68D+01
9.5	1909.12348	1909.12344	0.4	0.59D+01	1909.13377	1909.13373	0.4	0.59D+01
10.5	1912.08168	1912.08163	0.5	0.50D+01	1912.07164	1912.07158	0.6	0.50D+01
11.5	1914.98491	1914.98482	0.9	0.42D+01	1914.99468	1914.99461	0.7	0.42D+01
12.5	1917.87265	1917.87255	1.0	0.34D+01	1917.86315	1917.86304	1.1	0.34D+01
13.5	1920.70623	1920.70609	1.4	0.28D+01	1920.71544	1920.71532	1.2	0.28D+01
14.5	1923.52293	1923.52278	1.5	0.22D+01	1923.51400	1923.51383	1.7	0.22D+01
15.5	1926.28631	1926.28611	2.0	0.17D+01	1926.29496	1926.29478	1.8	0.17D+01
16.5	1929.03137	1929.03116	2.1	0.13D+01	1929.02301	1929.02278	2.3	0.13D+01
17.5	1931.72393	1931.72365	2.8	0.10D+01	1931.73200	1931.73175	2.5	0.10D+01
18.5	1934.39667	1934.39639	2.8	0.76D+00	1934.38888	1934.38857	3.1	0.76D+00
19.5	1937.01770	1937.01736	3.4	0.56D+00	1937.02520	1937.02489	3.1	0.56D+00
20.5	1939.61743	1939.61708	3.5	0.40D+00	1939.61021	1939.60982	3.9	0.40D+00
21.5	1942.16622			0.29D+00	1942.17316			0.29D+00
22.5	1944.69221			0.20D+00	1944.68554			0.20D+00
23.5	1947.16798			0.14D+00	1947.17439			0.14D+00
24.5	1949.61950			0.93D−01	1949.61336			0.94D−01
25.5	1952.02147			0.62D−01	1952.02736			0.62D−01
26.5	1954.39778			0.41D−01	1954.39213			0.41D−01
27.5	1956.72515			0.26D−01	1956.73055			0.26D−01
28.5	1959.02549			0.17D−01	1959.02032			0.17D−01
29.5	1961.27747			0.11D−01	1961.28241			0.11D−01
30.5	1963.50111			0.65D−02	1963.49639			0.65D−02
31.5	1965.67689			0.39D−02	1965.68140			0.39D−02
32.5	1967.82310			0.23D−02	1967.81879			0.24D−02
33.5	1969.92190			0.14D−02	1969.92600			0.14D−02
34.5	1971.98994			0.80D−03	1971.98603			0.80D−03
35.5	1974.01098			0.46D−03	1974.01471			0.45D−03
36.5	1976.00013			0.25D−03	1975.99659			0.26D−03
37.5	1977.94265			0.14D−03	1977.94602			0.14D−03
38.5	1979.85220			0.76D−04	1979.84900			0.76D−04
39.5	1981.71544			0.41D−04	1981.71848			0.41D−04
40.5	1983.54468			0.21D−04	1983.54180			0.21D−04

Table 2. (*Continued*)

	$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ P_-		$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ P_+		$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ Q_-	
J	$v_{\rm cal}$	I	$v_{\rm cal}$	I	$v_{\rm cal}$	I
0.5						
1.5					1995.71645	0.27D−02
2.5	1987.32701	0.74D−03	1987.36249	0.74D−03	1995.83732	0.35D−02
3.5	1984.17495	0.11D−02	1984.12786	0.11D−02	1996.08881	0.37D−02
4.5	1980.98823	0.13D−02	1981.04672	0.13D−02	1996.30385	0.37D−02
5.5	1977.97696	0.14D−02	1977.90733	0.14D−02	1996.69512	0.35D−02
6.5	1974.88415	0.13D−02	1974.96460	0.13D−02	1997.00013	0.32D−02
7.5	1972.00840	0.12D−02	1971.91748	0.12D−02	1997.52610	0.29D−02
8.5	1969.00593	0.11D−02	1969.10690	0.11D−02	1997.91527	0.25D−02
9.5	1966.25849	0.98D−03	1966.14793	0.99D−03	1998.56938	0.22D−02
10.5	1963.34174	0.85D−03	1963.46140	0.84D−03	1999.03550	0.18D−02
11.5	1960.71373	0.70D−03	1960.58550	0.71D−03	1999.80995	0.15D−02
12.5	1957.87723	0.58D−03	1958.01345	0.57D−03	2000.34475	0.12D−02
13.5	1955.35846	0.46D−03	1955.21482	0.46D−03	2001.23078	0.97D−03
14.5	1952.59613	0.36D−03	1952.74656	0.36D−03	2001.82519	0.77D−03
15.5	1950.17549	0.28D−03	1950.01889	0.28D−03	2002.81338	0.58D−03
16.5	1947.48084	0.21D−03	1947.64293	0.21D−03	2003.45780	0.44D−03
17.5	1945.14657	0.15D−03	1944.97964	0.16D−03	2004.53836	0.33D−03
18.5	1942.51295	0.11D−03	1942.68403	0.11D−03	2005.22293	0.24D−03
19.5	1940.25298	0.80D−04	1940.07843	0.80D−04	2006.38592	0.17D−03
20.5	1937.67375	0.56D−04	1937.85105	0.56D−04	2007.10073	0.12D−03
21.5	1935.47593	0.38D−04	1935.29656	0.39D−04	2008.33628	0.84D−04
22.5	1932.94459	0.26D−04	1933.12532	0.26D−04	2009.07158	0.58D−04
23.5	1930.79695	0.17D−04	1930.61557	0.17D−04	2010.37001	0.38D−04
24.5	1928.30727	0.11D−04	1928.48861	0.11D−04	2011.11634	0.26D−04
25.5	1926.19813	0.72D−05	1926.01753	0.73D−05	2012.46834	0.16D−04
26.5	1923.74424	0.46D−05	1923.92339	0.45D−05	2013.21661	0.11D−04
27.5	1921.66235	0.28D−05	1921.48533	0.28D−05	2014.61330	0.66D−05
28.5	1919.23880	0.17D−05	1919.41300	0.17D−05	2015.35487	0.41D−05
29.5	1917.17342	0.10D−05	1917.00271	0.10D−05	2016.78784	0.25D−05
30.5	1914.77520	0.61D−06	1914.94173	0.61D−06	2017.51460	0.15D−05
31.5	1912.71614	0.35D−06	1912.55445	0.36D−06	2018.97597	0.87D−06
32.5	1910.33872	0.20D−06	1910.49491	0.20D−06	2019.68030	0.51D−06
33.5	1908.27636	0.11D−06	1908.12633	0.11D−06	2021.16270	0.29D−06
34.5	1905.91567	0.63D−07	1906.05890	0.63D−07	2021.83752	0.16D−06
35.5	1903.84098	0.34D−07	1903.70518	0.34D−07	2023.33411	0.90D−07
36.5	1901.49339	0.18D−07	1901.62111	0.18D−07	2023.97284	0.50D−07
37.5	1899.39788	0.97D−08	1899.27887	0.97D−08	2025.47728	0.26D−07
38.5	1897.06025	0.51D−08	1897.16994	0.50D−08	2026.07382	0.14D−07
39.5	1894.93597	0.26D−08	1894.83622	0.26D−08	2027.58024	0.72D−08
40.5	1892.60553	0.13D−08	1892.69473	0.13D−08	2028.12898	0.37D−08
	$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ Q_+		$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ R_-		$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ R_+	
J	$v_{\rm cal}$	I	$v_{\rm cal}$	I	$v_{\rm cal}$	I
0.5			2000.71456	0.56D−02	2000.72640	0.56D−02
1.5	1995.69270	0.27D−02	2004.22676	0.43D−02	2004.20316	0.43D−02
2.5	1995.87295	0.35D−02	2007.75119	0.36D−02	2007.78640	0.36D−02
3.5	1996.04132	0.37D−02	2011.40444	0.31D−02	2011.35783	0.31D−02
4.5	1996.36323	0.37D−02	2015.02202	0.27D−02	2015.07978	0.27D−02
5.5	1996.62389	0.35D−02	2018.81111	0.23D−02	2018.74252	0.23D−02
6.5	1997.08324	0.32D−02	2022.51784	0.19D−02	2022.59689	0.19D−02
7.5	1997.43114	0.29D−02	2026.43544	0.16D−02	2026.34633	0.16D−02
8.5	1998.02209	0.25D−02	2030.22616	0.13D−02	2030.32486	0.13D−02
9.5	1998.45071	0.22D−02	2034.26314	0.11D−02	2034.15533	0.11D−02
10.5	1999.16602	0.18D−02	2038.13172	0.85D−03	2038.24810	0.85D−03
11.5	1999.66758	0.15D−02	2042.27747	0.66D−03	2042.15309	0.67D−03
12.5	2000.49896	0.12D−02	2046.21707	0.51D−03	2046.34887	0.51D−03
13.5	2001.06474	0.98D−03	2050.45984	0.39D−03	2050.32123	0.39D−03
14.5	2002.00305	0.76D−03	2054.46308	0.29D−03	2054.60785	0.29D−03
15.5	2002.62369	0.59D−03	2058.79034	0.21D−03	2058.64006	0.21D−03

Table 2. (*Continued*)

$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ Q_+			$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ R_-		$^2\Pi_{3/2}$–$^2\Pi_{1/2}$ R_+	
J	$v_{\rm cal}$	I	$v_{\rm cal}$	I	$v_{\rm cal}$	I
16.5	2003.65931	0.44D−03	2062.84959	0.15D−03	2063.00471	0.15D−03
17.5	2004.32504	0.33D−03	2067.24834	0.11D−03	2067.08907	0.11D−03
18.5	2005.44806	0.24D−03	2071.35587	0.75D−04	2071.51860	0.74D−04
19.5	2006.14898	0.17D−03	2075.81291	0.50D−04	2075.64740	0.51D−04
20.5	2007.34947	0.12D−03	2079.96108	0.34D−04	2080.12865	0.34D−04
21.5	2008.07574	0.84D−04	2084.46327	0.22D−04	2084.29433	0.22D−04
22.5	2009.34391	0.57D−04	2088.64465	0.15D−04	2088.81424	0.14D−04
23.5	2010.08589	0.39D−04	2093.17908	0.92D−05	2093.00953	0.93D−05
24.5	2011.41225	0.25D−04	2097.38656	0.58D−05	2097.55537	0.57D−05
25.5	2012.16065	0.17D−04	2101.94071	0.35D−05	2101.77334	0.36D−05
26.5	2013.53608	0.10D−04	2106.16755	0.22D−05	2106.33280	0.21D−05
27.5	2014.28205	0.67D−05	2110.72937	0.13D−05	2110.56694	0.13D−05
28.5	2015.69790	0.41D−05	2114.96929	0.76D−06	2115.12823	0.75D−06
29.5	2016.43304	0.25D−05	2119.52724	0.43D−06	2119.37248	0.44D−06
30.5	2017.88117	0.15D−05	2123.77443	0.25D−06	2123.92435	0.24D−06
31.5	2018.59763	0.88D−06	2128.31755	0.14D−06	2128.17313	0.14D−06
32.5	2020.07041	0.51D−06	2132.56664	0.76D−07	2132.70491	0.75D−07
33.5	2020.76083	0.29D−06	2137.08456	0.40D−07	2136.95309	0.41D−07
34.5	2022.25115	0.16D−06	2141.33066	0.22D−07	2141.45469	0.21D−07
35.5	2022.90872	0.91D−07	2145.81356	0.11D−07	2145.69761	0.11D−07
36.5	2024.41000	0.49D−07	2150.05224	0.59D−08	2150.15949	0.58D−08
37.5	2025.02836	0.27D−07	2154.49085	0.29D−08	2154.39292	0.30D−08
38.5	2026.53450	0.14D−07	2158.71810	0.15D−08	2158.80609	0.15D−08
39.5	2027.10781	0.73D−08	2163.10369	0.71D−09	2163.02625	0.72D−09
40.5	2028.61317	0.37D−08	2167.31591	0.35D−09	2167.38220	0.34D−09
$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ P_-			$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ P_+		$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ Q_-	
J	$v_{\rm cal}$	I	$v_{\rm cal}$	I	$v_{\rm cal}$	I
1.5	1751.16272	0.28D−02	1751.17455	0.28D−02	1756.14506	0.13D−02
2.5	1747.54447	0.21D−02	1747.52090	0.21D−02	1755.78915	0.17D−02
3.5	1743.74952	0.18D−02	1743.78468	0.18D−02	1755.37473	0.18D−02
4.5	1739.89601	0.16D−02	1739.84947	0.16D−02	1754.73659	0.18D−02
5.5	1735.82184	0.14D−02	1735.87951	0.14D−02	1754.08931	0.17D−02
6.5	1731.73644	0.12D−02	1731.66796	0.12D−02	1753.17313	0.15D−02
7.5	1727.38934	0.10D−02	1727.46826	0.10D−02	1752.29802	0.14D−02
8.5	1723.07664	0.86D−03	1722.98768	0.86D−03	1751.10960	0.12D−02
9.5	1718.46487	0.71D−03	1718.56339	0.72D−03	1750.01321	0.10D−02
10.5	1713.93052	0.58D−03	1713.82291	0.58D−03	1748.55971	0.85D−03
11.5	1709.06397	0.47D−03	1709.18013	0.47D−03	1747.24981	0.70D−03
12.5	1704.31447	0.37D−03	1704.19032	0.37D−03	1745.53948	0.56D−03
13.5	1699.20434	0.29D−03	1699.33588	0.29D−03	1744.02479	0.45D−03
14.5	1694.24679	0.22D−03	1694.10846	0.22D−03	1742.06666	0.34D−03
15.5	1688.90521	0.16D−03	1689.04967	0.17D−03	1740.35657	0.26D−03
16.5	1683.74709	0.12D−03	1683.59713	0.12D−03	1738.16017	0.20D−03
17.5	1678.18683	0.87D−04	1678.34159	0.88D−04	1736.26442	0.15D−03
18.5	1672.83578	0.63D−04	1672.67688	0.62D−04	1733.83957	0.10D−03
19.5	1667.06991	0.43D−04	1667.23226	0.44D−04	1731.76806	0.75D−04
20.5	1661.53360	0.30D−04	1661.36851	0.30D−04	1729.12459	0.52D−04
21.5	1655.57524	0.20D−04	1655.74237	0.20D−04	1726.88714	0.36D−04
22.5	1649.86113	0.13D−04	1649.69265	0.13D−04	1724.03472	0.24D−04
23.5	1643.72326	0.87D−05	1643.89238	0.88D−05	1721.64093	0.16D−04
24.5	1637.83857	0.56D−05	1637.66952	0.56D−05	1718.58897	0.10D−04
25.5	1631.53383	0.35D−05	1631.70213	0.35D−05	1716.04809	0.68D−05
26.5	1625.48541	0.22D−05	1625.31857	0.22D−05	1712.80559	0.42D−05
27.5	1619.02603	0.13D−05	1619.19071	0.13D−05	1710.12643	0.27D−05
28.5	1612.82028	0.80D−06	1612.65843	0.80D−06	1706.70191	0.16D−05
29.5	1606.21796	0.47D−06	1606.37629	0.47D−06	1703.89280	0.98D−06
30.5	1599.86086	0.28D−06	1599.70672	0.27D−06	1700.29429	0.57D−06
31.5	1593.12675	0.16D−06	1593.27604	0.16D−06	1697.36303	0.34D−06
32.5	1586.62379	0.88D−07	1586.48002	0.87D−07	1693.59803	0.19D−06

Table 2. (*Continued*)

$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ P_-			$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ P_+		$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ Q_-	
J	$v_{\rm cal}$	I	$v_{\rm cal}$	I	$v_{\rm cal}$	I
33.5	1579.76845	0.48D−07	1579.90604	0.49D−07	1690.55190	0.11D−06
34.5	1573.12464	0.27D−07	1572.99387	0.26D−07	1686.62738	0.59D−07
35.5	1566.15806	0.14D−07	1566.28138	0.14D−07	1683.47313	0.33D−07
36.5	1559.37796	0.75D−08	1559.26274	0.74D−08	1679.39555	0.17D−07
37.5	1552.30956	0.38D−08	1552.41606	0.39D−08	1676.13942	0.93D−08
38.5	1545.39726	0.20D−08	1545.30011	0.20D−08	1671.91474	0.48D−08
39.5	1538.23592	0.99D−09	1538.32311	0.10D−08	1668.56248	0.25D−08
40.5	1531.19510	0.49D−09	1531.11847	0.49D−09	1664.19619	0.12D−08
$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ Q_+			$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ R_-		$^2\Pi_{1/2}$–$^2\Pi_{3/2}$ R_+	
J	$v_{\rm cal}$	I	$v_{\rm cal}$	I	$v_{\rm cal}$	I
1.5	1756.12134	0.13D−02	1764.38974	0.34D−03	1764.42517	0.34D−03
2.5	1755.82473	0.17D−02	1767.41436	0.51D−03	1767.36733	0.51D−03
3.5	1755.32729	0.18D−02	1770.21531	0.58D−03	1770.27373	0.59D−03
4.5	1754.79591	0.18D−02	1773.00406	0.60D−03	1772.93452	0.60D−03
5.5	1754.01812	0.17D−02	1775.52600	0.57D−03	1775.60635	0.57D−03
6.5	1753.25619	0.15D−02	1778.08181	0.52D−03	1777.99101	0.52D−03
7.5	1752.20308	0.14D−02	1780.33098	0.46D−03	1780.43182	0.46D−03
8.5	1751.21642	0.12D−02	1782.65794	0.40D−03	1782.54752	0.40D−03
9.5	1749.89450	0.10D−02	1784.64240	0.33D−03	1784.76190	0.33D−03
10.5	1748.69031	0.85D−03	1786.74555	0.27D−03	1786.61749	0.27D−03
11.5	1747.10731	0.70D−03	1788.47481	0.22D−03	1788.61087	0.22D−03
12.5	1745.69388	0.56D−03	1790.35993	0.17D−03	1790.21648	0.17D−03
13.5	1743.85848	0.44D−03	1791.84466	0.13D−03	1791.99491	0.13D−03
14.5	1742.24489	0.35D−03	1793.51801	0.98D−04	1793.36162	0.97D−04
15.5	1740.16641	0.26D−03	1794.76965	0.71D−04	1794.93153	0.72D−04
16.5	1738.36226	0.20D−03	1796.23777	0.52D−04	1796.07107	0.51D−04
17.5	1736.05040	0.14D−03	1797.26821	0.36D−04	1797.43905	0.37D−04
18.5	1734.06554	0.11D−03	1798.53772	0.25D−04	1798.36343	0.25D−04
19.5	1731.53015	0.74D−04	1799.35905	0.17D−04	1799.53609	0.17D−04
20.5	1729.37445	0.52D−04	1800.43648	0.12D−04	1800.25739	0.11D−04
21.5	1726.62531	0.36D−04	1801.06073	0.75D−05	1801.24117	0.76D−05
22.5	1724.30851	0.24D−04	1801.95240	0.49D−05	1801.77131	0.48D−05
23.5	1721.35517	0.16D−04	1802.39134	0.31D−05	1802.57237	0.31D−05
24.5	1718.88671	0.11D−04	1803.10324	0.19D−05	1802.92296	0.19D−05
25.5	1715.73838	0.67D−05	1803.36828	0.12D−05	1803.54710	0.12D−05
26.5	1713.12729	0.43D−05	1803.90599	0.71D−06	1803.72932	0.70D−06
27.5	1709.79274	0.26D−05	1804.00806	0.41D−06	1804.18190	0.42D−06
28.5	1707.04760	0.16D−05	1804.37675	0.24D−06	1804.20641	0.24D−06
29.5	1703.53511	0.96D−06	1804.32623	0.14D−06	1804.49237	0.14D−06
30.5	1700.66399	0.58D−06	1804.53057	0.78D−07	1804.36927	0.76D−07
31.5	1696.98132	0.33D−06	1804.33727	0.42D−07	1804.49305	0.43D−07
32.5	1693.99176	0.19D−06	1804.38148	0.23D−07	1804.23187	0.23D−07
33.5	1690.14615	0.11D−06	1804.05464	0.12D−07	1804.19744	0.12D−07
34.5	1687.04515	0.60D−07	1803.94245	0.65D−08	1803.80711	0.64D−08
35.5	1683.04333	0.32D−07	1803.49072	0.33D−08	1803.61797	0.33D−08
36.5	1679.83739	0.18D−07	1803.22541	0.17D−08	1803.10687	0.17D−08
37.5	1675.68554	0.92D−08	1802.65689	0.83D−09	1802.76609	0.85D−09
38.5	1672.38066	0.48D−08	1802.24130	0.42D−09	1802.14206	0.41D−09
39.5	1668.08451	0.24D−08	1801.56358	0.20D−09	1801.65226	0.20D−09
40.5	1664.68622	0.13D−08	1801.00013	0.95D−10	1800.92262	0.94D−10

a) the Δv is in unit $10^{-4}\,\mathrm{cm}^{-1}$, I is the relative intensity. The subscription $+/-$ of P, Q and R refers to parity.

Ⅲ. CONCLUSION AND DISSCUSION

We have performed a global least-square analysis of all previous data for NO and determined the molecular parameters with very high precision. With these parameters, the rovibrational transitions for the ground states of $^{14}N^{16}O$ were calculated to serve as infrared frequency standard in the range 1600–5600 cm^{-1}. The transition frequencies are listed in Table 2 with their related intensities. From Table 2 we can draw conclusion that the precision of the transition frequency is remarkably high. Most of the residuals between v_{cal} and v_{NIST} are of the order of 10^{-5} cm^{-1}. The reliability and high quality of the calculation are due to the following facts:

(1) The spectrum of NO has been measured and remeasured using different spectroscopic techniques. We compared their qualities and removed the unreliable raw data.

(2) The program has introduced an advanced isotopic scaling function, which considered the breakdown of Born-Oppenheimer approximation. With the function, the spectral data of different isotopomers of NO can make significant contribution to the accuracy for determining the molecular parameter of $^{14}N^{16}O$.

(3) The effects of off-diagonal matrix elements are taken into account in the calculation, namely the interactions between the states of different quantum number $\boldsymbol{J}$ have been considered. In our calculation the Hamiltonian matrix was truncated at $\Delta \boldsymbol{J} = \pm 3$ to guarantee the accuracy of the calculation.

With the aid of isotopic scaling function, the possible transition frequencies of $^{14}N^{17}O$ and $^{14}N^{18}O$ can also be calculated. Since their natural abundance is rare, this work seems quite meaningful and valuable because there are few experimental data for $^{14}N^{17}O$ and $^{14}N^{18}O$. The calculated frequencies have the same precision as that of $^{14}N^{16}O$. Due to limited space, they are omitted in this paper. However, a list of the transitions of $^{14}N^{17}O$ and $^{14}N^{18}O$ can be supplied on request.

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