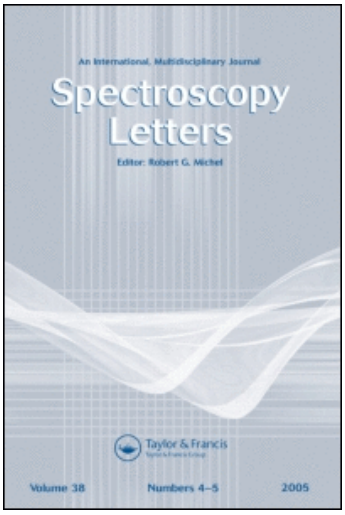

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Rotational Analysis of the 1–4 Band of the $B^2\Sigma^+$–$X^2\Sigma^+$ System of $^{14}C^{16}O^+$

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ABSTRACT High-resolution emission spectrum of the 1–4 band of the $B^2\Sigma^+$–$X^2\Sigma^+$ transition of $^{14}C^{16}O^+$ was observed for the first time by conventional emission spectroscopy. The band spectrum was excited in a water-cooled Geissler lamp filled with commercial gaseous carbon monoxide enriched in about 80% of the radiocarbon ^{14}C. A rotational analysis has been carried out and obtained molecular constants have been merged with previously published data for the $B^2\Sigma^+$–$A^2\Pi_i$ and $A^2\Pi_i$–$X^2\Sigma^+$ transitions. The principal equilibrium constants for the ground $X^2\Sigma^+$ state obtained from this work are $\omega_e = 2121.7726(98)$, $\omega_e x_e = 13.9055(27)$, $B_e = 1.815290(30)$, $\alpha_e = 1.6594(33) \times 10^{-2}$, and $\gamma_e = -0.377(73) \times 10^{-4}\,cm^{-1}$. Also, presently known experimental equilibrium molecular constants of the $X^2\Sigma^+$ states of the CO^+ isotopic molecules are summarized and isotopic dependence of the B_e and ω_e constants is discussed.

KEYWORDS $^{14}C^{16}O^+$ molecule, $B^2\Sigma^+$–$X^2\Sigma^+$ transition, equilibrium parameters, rotational analysis

INTRODUCTION

The emission spectrum of CO^+ has been known since the 1920s, and it still remains a subject of numerous experimental works. Four bands' systems in the visible and ultraviolet regions are known as a result of transition between the excited $A^2\Pi_i$, $B^2\Sigma^+$, $C^2\Delta_r$ states and the ground $X^2\Sigma^+$ state. The $B^2\Sigma^+$–$X^2\Sigma^+$ transition, designated as the first negative system, was extensively studied in a several isotopic species (see the literature[1–9] and references therein). However, only two papers about the B–X system of the $^{14}C^{16}O^+$ molecule have been published until now. In 1979, Dhumwad et al.[10] made some observations and presented isotope shifts and vibrational assignments of 15 bands of this system. Saaby Johansen and Middelboe[11] studied the CO^+ spectrum in the 210–250 nm wavelength interval and reported bands head isotope shifts in the $^{13}C^{16}O^+$ and $^{14}C^{16}O^+$ species.

In this article we report first-line positions and rotational analysis of the 1–4 band of the $B^2\Sigma^+$–$X^2\Sigma^+$ transition in the $^{14}C^{16}O^+$ molecule. The present data, when combined in merge calculations with previous results,[12–14] provided an improved set of molecular constants for $B^2\Sigma^+$ ($v = 0, 1$) and $X^2\Sigma^+$ ($v = 0, 1, 2, 4$) states. Next, some major vibrational and rotational

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equilibrium molecular parameters for the $B^2\Sigma^+$ an $X^2\Sigma^+$ states were obtained for the first time. Moreover, the isotopic dependence of the B_e rotational and ω_e vibrational constants for the ground $X^2\Sigma^+$ state of CO^+ isotopologues is analyzed and discussed.

EXPERIMENTAL DETAILS

The 1–4 band, with origin at 39,045.9766(80) cm^{-1}, of the B–X system of $^{14}C^{16}O^+$ was accidentally observed while we were trying to measure the $A^1\Pi$–$X^1\Sigma^+$ (fourth-positive) system in the $^{14}C^{16}O$ neutral molecule spectrum. A water-cooled Geissler lamp, containing gaseous carbon monoxide enriched in about 80% of the radiocarbon ^{14}C at a total pressure of approximately 2.5 hPa, was operated at 3 kV and 100-mA A.C. The spectrum was observed with the 2-m Ebert plane grating spectrograph in the 10th order and recorded on the ORWO WU-2 plates. The atomic Th lines[15] emitted from a water-cooled hollow cathode lamp have been used for calibration of our CO^+ spectra. The peak positions were determined by the fitting of a Gauss line-shape function to each spectral feature. The strongest CO^+ lines have a spectral width of about 0.20 cm^{-1} and appear with a maximum signal-to-noise ratio of about 50:1. Therefore, the absolute accuracy and precision of measurements of unblended molecular lines are expected to be of the order of $\pm 0.005\ cm^{-1}$. Certain lines of both R and P branches of the $^{14}C^{16}O^+$ isotopologue could not be observed or measured because of being overlapped by some of the strongest lines of the $^{14}C^{16}O$ molecule (11–22 band of A–X). The accuracy of measurements of these lines is reduced to $\pm 0.020\ cm^{-1}$. A compressed portion of the low-resolution spectrum of the 1–4 band of the $B^2\Sigma^+$–$X^2\Sigma^+$ transition of $^{14}C^{16}O^+$ is presented in Fig. 1.

ANALYSIS AND RESULTS

In total, almost 90 lines belonging to the 1–4 band of $^{14}C^{16}O^+$ have been measured and their wavenumbers are provided in Table 1. We used the usual effective Hamiltonian for $^2\Sigma^+$ states[16] to reduce the experimental wavenumber data to molecular constants. The following energy level expression has been applied in the present work in a individual band fitting:

$$^2\Sigma^+_{e,f} = T_v + B_v x(x \mp 1) - D_v x^2 (x \mp 1)^2 \pm 0.5\gamma_v (x \mp 1), \quad (1)$$

where $x = (J + 0.5)$ and upper and lower signs ($\pm$ or $\mp$) refer to the e/f levels, respectively. T_v, B_v, D_v, and γ_v are the band origin, rotational constants, and the spin–rotation interaction constants, respectively. During calculations, the existence of very strong correlation between spin–rotation interaction parameters upper and lower state has been determined. For this reason, we have decided to fix the ground state constant γ_4 to the value recalculated from equilibrium parameters of $^{12}C^{16}O^+$ given by Bogey et al.[17] from microwave studies. A least squares fit wavenumbers data to the molecular parameters gives a satisfactory result, though only 54 lines (about 61% of the total) were used. The details of computation were as follows: standard deviation of the fit $\sigma = 2.01 \times 10^{-2}\ cm^{-1}$, the number of the calculated constants $n = 6$, and the number of degrees of freedom $f = 48$.

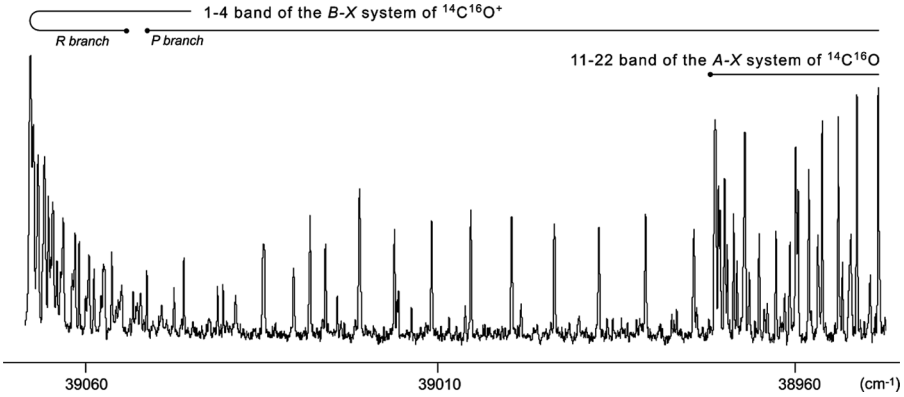

FIGURE 1 A compressed portion of the low-resolution spectrum of the 1–4 band of the $B^2\Sigma^+$–$X^2\Sigma^+$ system of $^{14}C^{16}O^+$. Part of the 11–22 band of the $A^1\Pi$–$X^1\Sigma^+$ system in the $^{14}C^{16}O$ is shown at right.

TABLE 1 The Wavenumbers (in cm^{-1}) of the 1–4 Band of the $B^2\Sigma^+$–$X^2\Sigma^+$ System of the $^{14}C^{16}O^+$ Molecule[a]

J	$R_{11ee}(J)$		$R_{22ff}(J)$		$P_{11ee}(J)$		$P_{22ff}(J)$	
0.5	39,049.199	(−13)	39,052.21	[b]				
1.5	39,052.21	[b]	39,054.89	[b]	[c]		39,038.74	[b]
2.5	39,054.89	[b]	39,057.35	[b]	39,038.74	[b]	39,034.76	[b]
3.5	39,057.35	[b]	39,059.54	[b]	39,034.76	[b]	39,030.51	[b]
4.5	39,059.54	[b]	39,061.51	[b]	39,030.51	[b]	39,026.02	[b]
5.5	39,061.51	[b]	39,063.177	(−11)	39,026.02	[b]	39,021.27	[b]
6.5	39,063.262	(−6)	39,064.626	(−24)	39,021.27	[b]	39,016.242	(−15)
7.5	39,064.717	(−14)	39,065.815	(−32)	39,016.302	(−18)	39,010.992	(−4)
8.5	39,065.924	(−30)	39,066.743	(−37)	39,011.058	(−12)	39,005.470	(−11)
9.5	39,066.858	(−29)	39,067.42	[b]	39,005.554	(−12)	38,999.714	(−1)
10.5	39,067.54	[b]	39,067.82	[b]	38,999.804	(−4)	38,993.687	(−2)
11.5	39,067.95	[b]	39,067.96	[b]	38,993.783	(−13)	38,987.403	(−8)
12.5	39,068.10	[b]	39,067.82	[b]	38,987.505	(−24)	38,980.850	(−28)
13.5	39,067.99	[b]	39,067.45	[b]	38,980.964	(−43)	38,974.090	(−1)
14.5	39,067.62	[b]	[c]		38,974.215	(−15)	[c]	
15.5	39,066.998	(−17)	[c]		38,967.163	(−34)	[c]	
16.5	39,066.136	(0)	[c]		[c]		[c]	
17.5	39,064.990	(−6)	39,063.389	(−16)	38,952.31	[b]	38,944.414	(−34)
18.5	39,063.607	(−14)	39,061.661	(−34)	38,944.587	(−23)	38,936.338	(−27)
19.5	39,061.934	(−6)	39,059.752	(−3)	38,936.522	(−17)	[c]	
20.5	39,060.014	(−16)	39,057.535	(−14)	38,928.194	(−5)	[c]	
21.5	39,057.819	(−17)	39,055.046	(−31)	38,919.602	(−12)	38,910.568	(−15)
22.5	39,055.26	[b]	39,052.333	(−4)	38,910.788	(−8)	38,901.455	(−7)
23.5	39,052.67	[b]	39,049.344	(−14)	[c]		[c]	
24.5	39,049.647	(−30)	[c]		[c]		38,882.439	(−18)
25.5	39,046.332	(−19)	[c]		38,882.682	(−35)	38,872.50	[b]
26.5	39,042.832	(−17)	[c]		38,872.77	[b]	[c]	

[a]Numbers in parentheses are one standard deviation in the last digit.
[b]Denotes lines not used in evaluation of molecular constants.
[c]Denotes unmeasured lines.

In the merge fit[18,19] we used simultaneously present measured lines together with previously published data for the $B^2\Sigma^+$–$A^2\Pi_i$ (0–0, 0–1, 1–0 bands),[12] and for the $A^2\Pi_i$–$X^2\Sigma^+$ (0–2, 1–0, 2–0, 2–1, 3–0, 4–0, 4–2, 6–1 bands)[13,14] transitions. The estimated variance of this merging $\sigma_M^2 = 1.37$, the number of the calculated constants $n = 61$, and the number of degrees of freedom $f_M = 47$. The value of variance is satisfactory and lies inside the 95% confidence limits. Table 2 presents the constant values derived for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states.

The obtained individual rotational constants were fitted to the usual power series of the $(\upsilon + ½)$ argument, relations to obtain the equilibrium parameters

TABLE 2 Molecular Constants (in cm^{-1}) of the $B^2\Sigma^+$ and $X^2\Sigma^+$ States of the $^{14}C^{16}O^+$ Molecule[a,b]

	$B^2\Sigma^+$			$X^2\Sigma^+$		
υ	B_υ	$D_\upsilon \times 10^6$	$\gamma_\upsilon \times 10^2$	B_υ	$D_\upsilon \times 10^6$	$\gamma_\upsilon \times 10^3$
0	1.639281(27)	6.569(30)	1.9530(88)	1.806979(27)	5.197(31)	[8.3625]
1	1.612916(33)	6.793(39)	1.897(15)	1.790335(38)	5.426(52)	[8.3147]
2				1.773558(31)	5.357(40)	[8.2465]
3				—	—	—
4				1.739860(62)	5.250(88)	[8.0490]

[a]1σ in parentheses.
[b]Values in squares brackets were fixed during the fit.

TABLE 3 Equilibrium Molecular Constants (in cm^{-1}) of the $B^2\Sigma^+$ State of the $^{14}C^{16}O^+$ Molecule[a,b]

σ_e	ω_e	$\omega_e x_e$	$\omega_e y_e \times 10^3$	B_e	$\alpha_e \times 10^2$	$D_e \times 10^6$	$\beta_e \times 10^7$	$\gamma_e \times 10^2$	$\alpha_{\gamma e} \times 10^4$
45,876.1644(42)	1662.1772(46)	[−25.9641]	[0.3477]	1.652464(44)	2.6365(43)	6.457(49)	2.24(50)	1.981(16)	−5.6(18)

[a] 1σ in parentheses.
[b] Values in squares brackets were fixed during the fit to values recalculated from $^{12}C^{16}O^+$[4] parameters.

of the $B^2\Sigma^+$ and $X^2\Sigma^+$ states. Because only two vibrational levels have been observed in the excited state, the equilibrium rotational constants were determined from the exact fit of data, providing values featured in Table 3. Also, essential vibrational equilibrium constants (i.e., σ_e and ω_e) were determined from the $v' = 0$ and 1 vibrational level position, which were calculated as 45,643.3957(25) cm^{-1} and 47,254.7747(38) cm^{-1}, respectively (related to the $X^2\Sigma^+$, $v = 0$ level). Prior to the present work there haven't been any experimental equilibrium constants for the $B^2\Sigma^+$ state of the $^{14}C^{16}O^+$ ion. However, the present value of the B–X system origin $\sigma_e = 45{,}876.1644(42)$ cm^{-1} can be compared with corresponded values: $\sigma_e = 45{,}876.724(48)$ cm^{-1} of $^{12}C^{16}O^+$[4] and $\sigma_e =$ 45,876.4530(32) cm^{-1} of $^{13}C^{16}O^+$.[2] Vibrational equilibrium constants of the $B^2\Sigma^+$ state of $^{14}C^{16}O^+$ are presented in Table 3.

Main ground state equilibrium vibrational constants, ω_e and $\omega_e x_e$, have been derived on the basis $v = 0$, 1, 2, 4 level positions and $\omega_e y_e$ constant fixed to the value recalculated from $^{12}C^{16}O^+$ parameters.[4] The results are featured in the sixth column of Table 4. The present main rotational equilibrium constants are compatible with the recent results derived from $A^2\Pi_i$–$X^2\Sigma^+$ transition investigation.[14] This is not surprising because experimental material dealing with the A–X transition[14] has been used in our global fit. For example, their $B_e = 1.815337(52)$ cm^{-1} constant compares with our value of 1.815290(30) cm^{-1} and their $\alpha_e = 1.6707(32) \times 10^{-2}$ cm^{-1} compares with our value of $1.6594(33) \times 10^{-2}$ cm^{-1}. However, presently obtained D_v constants do not show significant variation with v and give the following equilibrium parameter: $D_e = 5.285\ (54) \times 10^{-6}\ cm^{-1}$.

GROUND STATE EQUILIBRIUM PARAMETERS OF CO^+

Carbon and oxygen have three natural, most abundant isotopes: ^{12}C, ^{13}C, ^{14}C, and ^{16}O, ^{17}O, ^{18}O, respectively. Accordingly, nine different isotopologues of CO^+ can be anticipated. Until now information about the ground state of CO^+ is known for

TABLE 4 Equilibrium Molecular Constants (in cm^{-1}) of the $X^2\Sigma^+$ State of the CO^+ Isotopic Molecules[a,b]

Constant	$^{12}C^{16}O^+$[4]	$^{12}C^{17}O^+$[8]	$^{13}C^{16}O^+$[2]	$^{12}C^{18}O^+$[5]	$^{14}C^{16}O^+$[c]	$^{13}C^{18}O^+$[9]
ω_e	2214.2219(79)	2185.9658(84)	2164.8473(63)	2160.7469(36)	2121.7726(98)	2110.039(4)
$\omega_e x_e$	15.1509(31)	14.7674(11)	14.4873(18)	14.44090(56)	13.9055(27)	13.738(2)
$\omega_e y_e \times 10^3$	−2.21(30)	[−1.302]	−0.970(15)	[−1.257]	[−1.945]	−3.2(2)
B_e	1.976949(26)	1.927001(38)	1.889648(30)	1.882791(22)	1.815290(30) 1.815337(52)[d]	1.79468(2)
$\alpha_e \times 10^2$	1.8948(18)	1.8236(22)	1.7771(18)	1.78041(64)	1.6594(33) 1.6707(32)[d]	1.6440(3)
$\gamma_e \times 10^4$	−0.332(26)	−0.331(28)	−0.241(23)	—	−0.377 (73)	—
$D_e \times 10^6$	6.3009(97)	6.041(12)	5.6758(88)	5.841(71)	5.285 (54) 5.17(10)[d]	—
$\beta_e \times 10^7$	0.308(33)	0.100(31)	0.0740(23)	1.71(48)	— 0.87(65)[d]	—
$\delta_e \times 10^8$	—	—	—	2.25(77)	—	—

[a] 1σ in parentheses.
[b] Values in squares brackets were fixed during the fit to values recalculated from $^{12}C^{16}O^+$[4] and $^{13}C^{16}O^+$[2] isotope parameters.
[c] This work.
[d] After Ostrowska-Kopeć and Piotrowska-Domagała.[14]

the following six isotopic species: $^{12}C^{16}O^+$, $^{12}C^{17}O^+$, $^{12}C^{18}O^+$, $^{13}C^{16}O^+$, $^{13}C^{18}O^+$, and $^{14}C^{16}O^+$. Using experimental data from this work and from previous studies,[2,4,5,8,9] the reduced mass relationship of the B_e and ω_e constants for the $X^2\Sigma^+$ state of the CO^+ isotopologue has been examined. These constants show a relatively high isotopic dependence and they have the most crucial meaning while trying to calculate possible deviations from Born-Oppenheimer (B-O) approximation.

The reduced mass dependence B_e constants are graphically presented in Fig. 2a. A linear course of B_e against a $1/\mu$ argument implies that to model the isotopic dependence of the Y_{kl} Dunham parameter[20] the following expression can be used:

$$Y_{kl} = \mu^{-(k+2l)/2} U_{kl}, \qquad (2)$$

where U_{kl} is an isotopically invariant parameter and μ is a reduced mass of CO^+ isotopologue. This simple formula is obligatory when the Born-Oppenheimer approximation holds strictly, which is quite well fulfilled for molecules with relatively large reduced masses (like CO^+). Fitting isotopic B_e data (see Table 4) to Eq. (2) gives a value for U_{01} for the $X^2\Sigma^+$ state of 13.55468(48) cm^{-1}. The present U_{01} constant is in excellent agreement with those given by Bogey et al.;[17] that is, 13.55468 cm^{-1} (recalculated from $U_{01}^e = 406{,}358.4535(710)$ MHz value), obtained from microwave spectrum of CO^+.

In this same manner we examined isotopic dependence of the main vibrational constant of the $X^2\Sigma^+$ state: ω_e (Y_{10}). From the fitting experimental data to the relationship $Y_{10} = \mu^{-1/2} U_{10}$, derived from Eq. (2), we obtained value of $U_{10} = 5797.797(27)$ cm^{-1}. This isotopically invariant parameter has been determined for the first time and cannot be compared with previous results. The isotopic values of ω_e constants in function of a $\mu^{-1/2}$ argument are plotted in Fig. 2b.

When the breakdown of the B-O approximation must be taken into account, some new term should be added in Eq. (2).[21] In these conditions, the Dunham coefficients can be written as:

$$Y_{kl} = \mu^{-(k+2l)/2} U_{kl} \left(1 + \frac{m_e}{M_A}\Delta_{kl}^A + \frac{m_e}{M_B}\Delta_{kl}^B\right), \qquad (3)$$

where M_A, M_B, are the atomic masses, m_e is the electron mass, and $\Delta_{kl}^A, \Delta_{kl}^B$ are dimensionless and isotopically invariant coefficients. Equation (3) has been used by Bogey et al.[17] for study of the B-O approximation breakdown in the CO^+ molecule. However, only Δ_{01} coefficients can be significantly determined: $\Delta_{01}^C = -0.296(36)$ and $\Delta_{01}^O = -1.060(28)$, respectively.

An attempt to determine the Δ_{01} and Δ_{10} coefficients, from Eq. (3), gives no satisfactory results. The precision and isotopic variation of the present studied B_e constants (Table 4) have been not sufficient to calculate small B-O approximation breakdown parameters. We believe that higher precision of determination of the wavenumbers (in the range of fourth decimal place) gives the opportunity for future studying the B-O approximation in the CO^+ molecule.

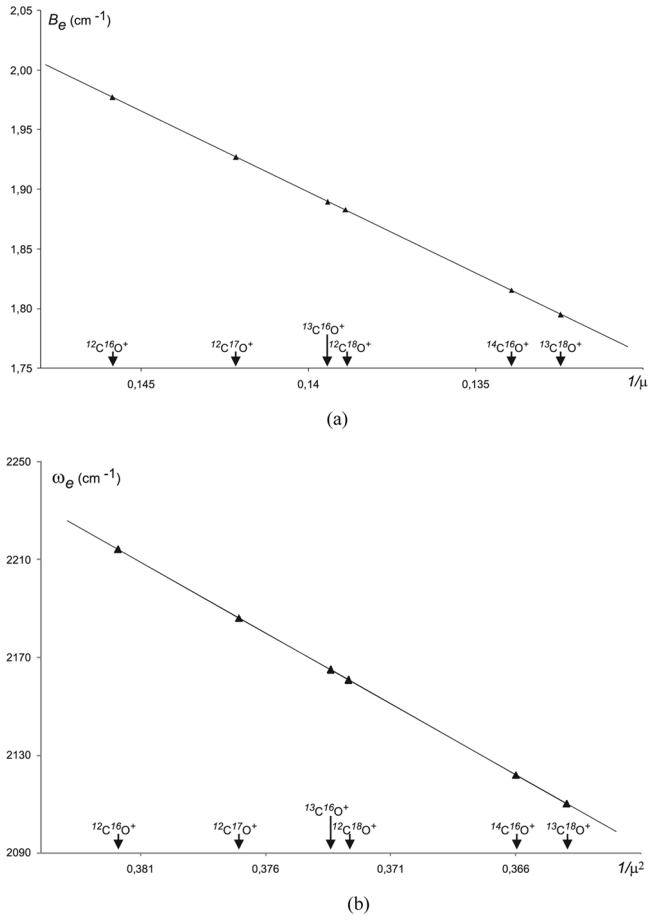

FIGURE 2 **Experimental values of the B_e (a) and ω_e (b) equilibrium constants of the $X^2\Sigma^+$ state for six isotopologues of CO^+. Standard deviation was impossible to show because of scale of the plot (for details see Table 4).**

CONCLUSION

We have investigated the rotational structure of the 1–4 band of the $B^2\Sigma^+$–$X^2\Sigma^+$ electronic transitions

of $^{14}C^{16}O^+$ for the first time. The present results have been merged with previous data for the $B^2\Sigma^+$–$A^2\Pi_i$ and $A^2\Pi_i$–$X^2\Sigma^+$ transitions of this isotopologue. In this way, a set of molecular constants for the $B^2\Sigma^+$ ($v = 0,1$) and $X^2\Sigma^+$ ($v = 0, 1, 2, 4$) states has been obtained. Prior to the present work, there has been no information about vibrational equilibrium parameters of the ground and excited states of $^{14}C^{16}O^+$. Our investigation derived the first values of the following constants for the $X^2\Sigma^+$ state: $\omega_e = 2121.7726(98)$ and $\omega_e x_e = 13.9055(27)$ cm^{-1}. Moreover, the isotopic dependence of the B_e rotational constants of the $X^2\Sigma^+$ state has been analyzed, and isotopically invariant parameter $U_{01} = 13.55468(48)$ cm^{-1} has been determined.

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