The $B^2\Sigma^+$-$X^2\Sigma^+$ Transition of $^{12}C^{17}O^+$: The 2-υ'' Progression

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Abstract: Three new bands of the $B^2\Sigma^+$–$X^2\Sigma^+$ system of $^{12}C^{17}O^+$ have been investigated using conventional spectroscopic techniques. The spectra were observed in a graphite hollow-cathode lamp by discharging molecular oxygen (enriched in about 45% of the $^{17}O_2$ isotope) under 1.0 Torr pressure. The rotational analysis of the 2–4, 2–5, and 2–6 bands was performed with the effective Hamiltonian of Brown (Brown et al., *J. Mol. Spectrosc.* 1979; 74: 294–318). Molecular constants were derived from a merge calculation, including both the current wavenumbers and the spectroscopic data published by the authors previously. The principal equilibrium constants for the ground state of $^{12}C^{17}O^+$ are $\omega_e = 2185.9658(84)$, $\omega_e x_e = 14.7674(11)$, $B_e = 1.927001(38)$, $\alpha_e = 1.8236(22) \times 10^{-2}$, $\gamma_e = -0.331(28) \times 10^{-4}$, $D_e = 6.041(12) \times 10^{-6}$, $\beta_e = 0.100(31) \times 10^{-7}$ cm^{-1}, and the equilibrium constants for the excited state are $\sigma_e = 45876.499(15)$, $\omega_e = 1712.201(12)$, $\omega_e x_e = 27.3528(39)$, $B_e = 1.754109(35)$, $\alpha_e = 2.8706(57) \times 10^{-2}$, $\gamma_e = -1.15(19) \times 10^{-4}$, $D_e = 7.491(20) \times 10^{-6}$, $\beta_e = 2.13(12) \times 10^{-7}$, $\gamma_e = 2.0953(97) \times 10^{-2}$, and $\alpha_{\gamma e} = -9.46(59) \times 10^{-4}$ cm^{-1}, respectively. Rydberg–Klein–Rees potential energy curves were constructed for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states of this molecule, and Franck–Condon factors were calculated for the vibrational bands of the B–X system.

Keywords: $B^2\Sigma^+$–$X^2\Sigma^+$ transition, $^{12}C^{17}O^+$ molecule, rotational analysis

INTRODUCTION

The CO$^+$ ion is one of the most studied diatomic molecules. The major reason for this interest is the wide variety of environments like comets, molecular clouds,

and stellar and planetary atmospheres in which CO^+ can be found. During the past decade, much laboratory work devoted to the $B^2\Sigma^+ - X^2\Sigma^+$ electronic transition has been done in several isotopic species of CO^+: $^{12}C^{16}O^+$, $^{13}C^{16}O^+$, $^{12}C^{18}O^+$, and $^{13}C^{18}O^+$. A complete set of experimental references to previous work on the CO^+ isotopomers was provided in a paper by Prasad and Reddy[1] and in our previous paper.[2] Since then, three works dealing with $^{12}C^{16}O^{+[3,4]}$ and $^{12}C^{18}O^{+[5]}$ been published by our laboratory. More recently, Szajna and Kępa[6] and Szajna et al.[7] reported the first observation of eight bands (0–1, 2, 3, 4 and 1–2, 3, 4, 5) of the $B^2\Sigma^+ - X^2\Sigma^+$ transition of $^{12}C^{17}O^+$ and derived an accurate set of spectroscopic constants for both electronic states.

In the current article, we report an extension of our previous work. We have recorded and analyzed three new bands (2–4, 2–5, and 2–6) of the first negative system, whose heads are located in the 40,472, 38,436, and 36,431 cm^{-1} regions, respectively. From a merge calculation of the current data with the previous measurements,[6,7] an improved set for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states constants was obtained. Also, Rydberg–Klein–Rees (RKR) potential energy curves for both states were calculated, and Franck–Condon factors for bands of the $B–X$ transition were provided.

MATERIALS AND METHODS

The description of our experimental conditions has been given previously.[5,6] Here we present a short summary and the details specific to this investigation. The CO^+ molecule was excited in a graphite hollow-cathode type lamp filled with a mixture of molecular oxygen, $^{16}O_2$ and $^{17}O_2$ (almost 1:1), under 1.0 Torr pressure. The lamp was operated at 500 V with 50 mA current. The emission from the lamp was observed with a 2-m Ebert plane grating spectrograph in the 10th order and recorded on the ORWO-WU-2 (Original Wolfen) plates. The plates were measured automatically using an interferometric comparator. The peak positions were determined by fitting a Gaussian lineshape function to each spectral feature. The CO^+ spectrum has been calibrated using atomic thorium lines.[8] The strong molecular lines have been observed with a maximum signal-to-noise ratio of 50:1 and have spectral width of 0.15–0.20 cm^{-1}. This limits the precision of our measurements of the strong and unblended molecular transitions to ± 0.005 cm^{-1}. However, some blended or faint lines have somewhat worse accuracy, 0.010–0.020 cm^{-1} (see Table 1).

ANALYSIS AND CALCULATIONS

All bands of the $B^2\Sigma^+ - X^2\Sigma^+$ system form a simple and regular structure, that is, four main branches: double R (R_{11ee}, R_{22ff}) and double P (P_{11ee}, P_{22ff}) (two weak satellite branches, $^{Q}R_{21fe}$ and $^{Q}P_{12ef}$, were not observed). Because B_v constants for the excited state are smaller than for the ground state, the

Table 1. The wavenumbers (in cm^{-1}) of the $B^2\Sigma^+ - X^2\Sigma^+$ system of the $^{12}C^{17}O^+$ molecule for (a) 2−4, (b) 2−5, and (c) 2−6 bands

J	$R_{11ee}(J)$		$R_{22ff}(J)$		$P_{11ee}(J)$		$P_{22ff}(J)$	
(a) 2−4 band[a]								
0.5	40457.099	(−4)	40460.139	b				
1.5	40460.139	b	40462.850	b	40450.050	(−12)	40446.047	b
2.5	40462.850	b	40465.234	b	40446.047	b	40441.696	b
3.5	40465.234	b	40467.259	(−4)	40441.696	b	40437.024	b
4.5	40467.326	b	40468.974	(−8)	40437.024	b	40432.052	b
5.5	40469.054	(−2)	40470.378	(−5)	40432.052	b	40426.726	b
6.5	40470.465	(−2)	40471.447	(−9)	40426.726	b	40421.052	(−2)
7.5	40471.562	(−11)	40472.188	b	40421.118	(−8)	40415.082	(−2)
8.5	40472.325	b	40472.618	b	40415.155	(−3)	40408.792	(−3)
9.5	40472.710	b	40472.710	b	40408.878	(−11)	40402.158	(−11)
10.5	40472.849	b	40472.480	b	40402.244	(−13)	40395.232	(−9)
11.5	40472.618	b	40471.884	b	40395.332	(−11)	40387.951	(0)
12.5	40472.022	b	40470.980	(−2)	40388.063	(−5)	40380.353	(−2)
13.5	40471.143	(−6)	40469.729	(−15)	40380.472	(−3)	40372.415	(−10)
14.5	40469.903	(−6)	40468.165	(−9)	40372.547	(−7)	40364.163	(−9)
15.5	40468.346	(−4)	40466.282	(−13)	40364.309	(−1)	40355.592	(−2)
16.5	40466.461	(−6)	40464.048	(−18)	40355.734	(−4)	40346.680	(0)
17.5	40464.229	(−4)	40461.451	(−4)	40346.833	(−5)	40337.432	(−8)
18.5	40461.654	(−7)	40458.552	(−10)	40337.603	(−6)	40327.884	(12)
19.5	40458.754	(−4)	40455.288	(−5)	40328.043	(−7)	c	
20.5	40455.511	(−7)	40451.717	(−14)	c		40307.752	(−10)
21.5	40451.945	(−6)	40447.785	(−11)	40307.941	(−1)	40297.174	(−5)
22.5	40448.017	(−3)	40443.494	(−9)	40297.380	(−8)	40286.292	(−8)

(*continued*)

Table 1. Continued

J	R_{11ee} (J)		R_{22ff} (J)		P_{11ee} (J)		P_{22ff} (J)	
23.5	40443.754	(-5)	40438.886	(-3)	40286.511	(-9)	40275.038	(-16)
24.5	40439.162	(-7)	40433.925	(-6)	40275.285	(-1)	40263.505	(-15)
25.5	40434.198	(-9)	40428.628	(0)	40263.745	(-15)	40251.585	(-6)
26.5	40428.927	(-13)	40422.975	(-3)	40251.836	(-5)	40239.358	(-3)
27.5	40423.262	(-12)	40416.978	(-1)	40239.605	(-9)	40226.791	(-10)
28.5	40417.280	(-6)	40410.594	b	40227.069	(-18)		c
29.5	40410.954	(-5)				c	40200.651	b
30.5					40200.895	(-12)		
(b) 2−5 band[a]								
0.5	38418.920	(-3)	38421.988	b				
1.5	38421.988	b	38424.766	b	38411.906	b	38407.999	b
2.5	38424.766	b	38427.239	(-2)	38407.999	b	38403.753	b
3.5	38427.281	(-9)	38429.438	(-1)	38403.753	b	38399.223	b
4.5	38429.517	(-13)	38431.359	(-6)	38399.223	b	38394.424	b
5.5	38431.424	(-4)	38432.980	(-4)	38394.424	b	38389.339	b
6.5	38433.056	(-6)	38434.299	(-10)	38389.339	b	38383.909	(-2)
7.5	38434.408	(-2)	38435.359	(-7)	38383.969	(-4)	38378.238	(-3)
8.5	38435.451	(-6)	38436.090	b	38378.307	(-4)	38372.273	(-2)
9.5	38436.194	b	38436.553	b	38372.353	(0)	38366.028	(-2)
10.5	38436.677	b	38436.728	b	38366.112	(-3)	38359.484	(-4)
11.5	38436.896	b	38436.553	b	38359.586	(-2)	38352.663	(-1)
12.5	38436.728	b	38436.194	b	38352.774	(-4)		c
13.5	38436.340	b	38435.451	(-8)	38345.659	(-6)	38338.145	(-6)
14.5	38435.624	(-2)	38434.442	(-4)	38338.262	(-8)	38330.441	(-2)
15.5	38434.620	(-2)	38433.131	(-4)	38330.584	(0)	38322.457	(1)
16.5	38433.315	(-7)	38431.516	(-11)	38322.610	(-4)	38314.174	(-3)

17.5	38431.718	(−7)	38429.630	(−10)	38314.342	(−5)	38305.609	(−3)
18.5	38429.836	(−7)	38427.416	(−2)	38305.778	(0)	38296.749	(5)
19.5	38427.643	(−11)	38424.906	(−1)	38296.927	(−3)	38287.588	(−1)
20.5	38425.144	(−8)	38422.090	(−7)	38287.777	(−1)	38278.135	(−1)
21.5	38422.344	(−7)	38418.968	*b*	38278.339	(−1)	38268.390	(0)
22.5	38419.233	(−2)	38415.574	(−5)	38268.605	(−2)	38258.351	(−2)
23.5	38415.821	(−7)	38411.851	(−5)	*c*		38248.014	(−3)
24.5	38412.112	(−3)	*c*		38248.243	(0)	38237.376	(0)
25.5	*c*		38403.467	(−11)	38237.620	(−1)	38226.442	(0)
26.5	38403.768	(−1)	38398.826	(−5)	38226.692	(−3)	38215.208	(0)
27.5	8399.127	(−5)	38393.873	(0)	38215.473	(1)	38203.679	(4)
28.5	*c*		38388.602	(1)	38203.942	(−6)	*c*	
29.5	38388.924	(−1)	38383.021	(−5)	*c*		38179.701	(0)
30.5	38383.348	(0)	38377.115	(0)	38179.999	(−4)		
31.5	38377.478	*b*						
(c) 2−6 band*a*								
0.5			36413.394	*b*				
1.5	36413.394	*b*	36416.227	*b*	36403.328	*b*	*c*	
2.5	36416.227	*b*	36418.876	*b*	*c*		36395.352	*b*
3.5	36418.876	*b*	36421.166	(−15)	36395.352	*b*	36390.937	*b*
4.5	36421.249	(−3)	36423.294	(−13)	36390.937	*b*	36386.360	*b*
5.5	36423.375	*b*	36425.119	(−9)	36386.360	*b*	36381.484	*b*
6.5	36425.215	(−1)	36426.732	(−11)	36381.484	*b*	36376.311	(−7)
7.5	36426.842	(−24)	36428.063	(−2)	36376.391	(−13)	36370.940	(−4)
8.5	36428.174	(−5)	36429.155	(−8)	36371.035	*b*	36365.314	(−5)
9.5	36429.263	(−2)	36429.976	(−2)	36365.402	(−2)	36359.432	(−11)
10.5	36430.118	(−12)	36430.540	*b*	36359.541	(−8)	36353.309	(−6)

Table 1. Continued

J	$R_{11ee}(J)$		$R_{22ff}(J)$		$P_{11ee}(J)$		$P_{22ff}(J)$	
11.5	36430.732	b	36430.308	b	36353.426	(−10)	36346.935	(0)
12.5	36431.016	b	36430.895	b	36347.043	(−4)	36340.285	(−18)
13.5	36431.143	b	36430.732	b	36340.409	(−15)	36333.407	(−11)
14.5	36430.895	b	36430.275	b	36333.545	(−6)	36326.274	(−7)
15.5	36430.463	(0)	36429.567	(−1)	36326.413	(−10)	36318.880	(−9)
16.5	36429.760	(−1)	36428.590	(−3)	36319.034	(−8)	36311.207	b
17.5	36428.808	(−14)	36427.360	(−3)	36311.366	b	36303.346	(−2)
18.5	36427.567	(−1)	36425.845	(−14)	36303.512	(−5)	36295.183	(−5)
19.5	36426.067	(−13)	36424.096	(0)	36295.377	(−5)	36286.786	(−10)
20.5	36424.332	(−4)	36422.077	(−8)	36286.976	(−5)	36278.110	(−3)
21.5	36422.310	(−2)	36419.750	b	36278.317	(−5)		c
22.5	36420.023	(−6)	36417.221	(−6)		c	36260.005	(−9)
23.5	36417.483	(−4)	36414.404	(−16)	36260.215	(−7)	36250.552	(−1)
24.5	36414.652	(−10)	36411.285	(−4)	36250.807	(−18)	36240.858	(−9)
25.5	36411.577	(−4)	36407.927	(−7)	36241.096	(0)	36230.883	(−1)
26.5	36408.217	(−2)	36404.293	b	36231.146	(5)	36220.644	(−13)
27.5	36404.582	(−3)	36400.367	(3)	36220.924	(0)	36210.156	(−10)
28.5	36400.681	(−2)			36210.448	(−4)	36199.400	(−10)
29.5					36199.669	b	36188.395	(−5)
30.5					36188.682	(−8)	36177.074	b
31.5					36177.423	b	36165.521	b
32.5					36165.841	b		

^{a}Numbers in parentheses denote observed minus calculated (final constants) values in units of the last quoted digit.

^{b}Denotes lines not used in evaluation of molecular constants.

^{c}Denotes unmeasured lines.

bands head is formed in the R branch and bands are degraded to the red. Figure 1 shows a compressed spectrum of the 2–4 band for $^{12}C^{17}O^+$. For the vibrational assignments of the bands, the information about bands of the major $^{12}C^{16}O^+$ isotope has been used. The rotational assignments were made by predicting the line positions using the rotational and vibrational equilibrium constants by Szajna et al.[4] The observed, $\sim$350 line positions for the 2–4, 2–5, and 2–6 bands of the first negative transition are provided in Table 1. The observed rotational lines positions were fitted to the following customary energy level expression for each vibrational level of a $^2\Sigma^+$ state[9–11]:

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

where $x = (J + 0.5)$ and upper and lower signs ($\pm$ or $\mp$) refer to the e/f levels, respectively. Definition of molecular constants and their physical meaning are generally known and will not be discussed here. The molecular parameters T_v, B_v, D_v, and γ_v have been determined for both states, but the γ_v ($v = 4, 5, 6$) constants for the ground state were fixed to the values recalculated from microwave studies.[12] This procedure had to be applied due to the large correlation between spin-rotation interaction constants for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states. It is understandable because both electronic states of CO$^+$ belong to the Hund's (b) coupling case. In this way, the very precise values of the γ_v ($v = 0, 1, 2$) constants for the $B^2\Sigma^+$ state have been extracted. The statistical data of individual bands fit are presented in Table 2.
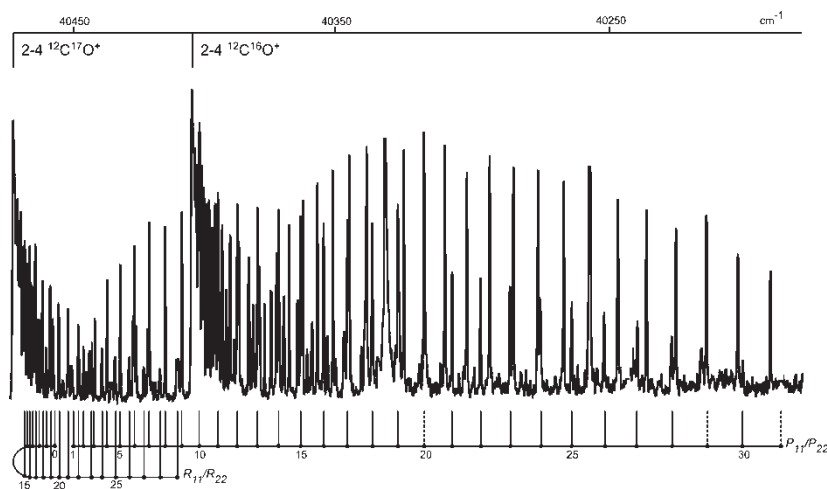

Figure 1. A compressed portion of the low-resolution spectrum of the $B^2\Sigma^+ - X^2\Sigma^+$ system of CO$^+$ shows the isotopic shift between $^{12}C^{17}O^+$ and $^{12}C^{16}O^+$. Some lines of the R and P branches are marked with their N'' values.

Table 2.   Individual band fits in the $B^2\Sigma^+ - X^2\Sigma^+$ system of $^{12}C^{17}O^+$

Band	Band origin (cm^{-1})	n^a	J_{max}	f^b	$\sigma^c \times 10^2$ (cm^{-1})
2–4	40453.7306(17)	114	30.5	79	0.85
2–5	38415.5442(12)	115	31.5	82	0.50
2–6	36406.9140(24)	115	32.5	73	0.85

^{a}Total number of observed lines.
^{b}Number of degrees of freedom of the fit for the individual band analysis.
^{c}Standard deviation of the fit for the individual band analysis.

Then the global merge calculations[13,14] were performed by combining current and previous experimental data[6,7] and calculating all constants. The final fit gave the molecular constants for the $B^2\Sigma^+$ ($v = 0, 1, 2$) and $X^2\Sigma^+$ ($v = 1, 2, 3, 4, 5,$ and 6) states of $^{12}C^{17}O^+$, reported in Table 3.

The molecular constants for the different vibrational levels enabled us to determine equilibrium parameters for the ground and excited states of $^{12}C^{17}O^+$ (Table 4). The results were compared with the values recalculated from $^{12}C^{16}O^{+[4]}$ and from $^{13}C^{16}O^{+[2]}$ isotopes with using usual isotopic relationships.[15] The current σ_e, ω_e, and $\omega_e x_e$ constants for $B^2\Sigma^+$ have been extracted on the basis of 0–1, 2, 3, 4, 1–2, 3, 4, 5, and 2–4, 5, 6 bands origins and $\omega_e y_e$ and $\omega_e z_e$ constants recalculated from equilibrium parameters of the $^{13}C^{16}O^{+[2]}$ and fixed in calculations. For the recalculations, the usual isotopic relationships $\omega_e y_e^i = \rho^3 \omega_e y_e$ and $\omega_e z_e^i = \rho^4 \omega_e z_e$[15] have been used. The ρ coefficient is defined as follows: $\rho = (\mu/\mu^i)^{1/2}$, where μ and μ^i are the reduced masses of $^{13}C^{16}O^+$ and $^{12}C^{17}O^+$, respectively. In this same manner, the $\omega_e y_e$ constants for the $X^2\Sigma^+$ state have been determined. The B_e constants were used to determine the equilibrium bond lengths

Table 3.   Molecular constants^{a,b} of the $B^2\Sigma^+$ and $X^2\Sigma^+$ states of $^{12}C^{17}O^+$

	$B^2\Sigma^+$			$X^2\Sigma^+$		
v	B_v	$D_v \times 10^6$	$\gamma_v \times 10^2$	B_v	$D_v \times 10^6$	$\gamma_v \times 10^3$
0	1.739727(15)	7.605(12)	2.0520(41)			
1	1.710792(15)	7.800(11)	1.9492(30)	1.899566(15)	6.049(11)	[8.822]
2	1.681628(15)	8.033(13)	1.8632(43)	1.881223(15)	6.076(11)	[8.746]
3				1.862757(15)	6.066(11)	[8.647]
4				1.844277(14)	6.098(11)	[8.526]
5				1.825696(15)	6.090(13)	[8.381]
6				1.807078(20)	6.098(20)	[8.213]

^{a}In cm^{-1}, one standard deviation in parentheses.
^{b}Values in square brackets were fixed during the fit.

Table 4. Equilibrium molecular constants of the $B^2\Sigma^+$ and $X^2\Sigma^+$ states of $^{12}C^{17}O^+$

Constant	$B^2\Sigma^+$		$X^2\Sigma^+$	
	This work[a,b]	Recalculated[c]	This work[a,b]	Recalcuatedc
σ_e	45876.499(15)	45876.453		
ω_e	1712.201(12)	1712.229	2185.9658(84)	2185.9643
$\omega_e x_e$	27.3528(39)	27.3597	14.7674(11)	14.7665
$\omega_e y_e$	[0.3356]	0.3356	[−0.001302]	−0.001302
$\omega_e z_e \times 10^3$	[3.015]	3.015		
B_e	1.754109(35)	1.753957	1.927001(38)	1.926888
$\alpha_e \times 10^2$	2.8706(57)	2.8462	1.8236(22)	−.8237
$\gamma_e \times 10^4$	−1.15(19)	−3.01	−0.331(28)	−0.315
$D_e \times 10^6$	7.491(20)	7.474	6.041(12)	5.985
$\beta_e \times 10^7$	2.13(12)	1.93	0.100(31)	0.288
$\gamma_e \times 10^2$	2.0953(97)	2.1382		
$\alpha_{\gamma e} \times 10^4$	−9.46(59)	−9.82		

[a]In cm^{-1}, one standard deviation in parentheses.
[b]Values in square brackets were fixed during the fit.
[c]Values recalculated from $^{12}C^{16}O^{+[4]}$ and $^{13}C^{16}O^{+[2]}$ isotope parameters.

$r_e = 1.168849(12)$ Å and $r_e = 1.115182(11)$ Å for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states, respectively.

The $B(v)$ and $G(v)$ expansions of Table 4 were subsequently used to determine RKR potential curves for the $B^2\Sigma^+$ and $X^2\Sigma^+$ states. Energies and turning points up to the $v' = ''2$ and $v = 6$ vibrational levels obtained

Table 5. Vibrational terms values and RKR turning points of the $B^2\Sigma^+$ and $X^2\Sigma^+$ states of $^{12}C^{17}O^+$

v	$B^2\Sigma^+$		$X^2\Sigma^+$	
	$G(v) + Y_{00}$ (cm^{-1})[a]	r_{min}, r_{max}	$G(v) + Y_{00}$ (cm^{-1})	r_{min}, r_{max}
0	848.3482	1.12003, 1.22649	1089.347[b]	1.0709[b], 1.1649[b]
1	2506.9523	1.08883, 1.27575	3245.7736	1.04169, 1.20529
2	4113.9667	1.06932, 1.31385	5372.6539	1.02292, 1.23534
3			7469.9798	1.00844, 1.26125
4			9537.7436	0.99646, 1.28483
5			11575.9374	0.98618, 1.30689
6			13584.5535	0.97712, 1.32789

[a]Values expressed above minimum of $B^2\Sigma^+$, which is 45876.499(15) cm^{-1}.
[b]Theoretically determined for unobserved in this work, $v'' = 0$ vibrational level: $Y_{00}(B^2\Sigma^+) = -0.9564$ cm^{-1}, $Y_{00}(X^2\Sigma^+) = 0.0560$ cm^{-1}.

Table 6. Franck–Condon factors for the $B^2\Sigma^+$–$X^2\Sigma^+$ transition of $^{12}C^{17}O^+$

v/v''	0	1	2
0	5.3411E-01	3.1661E-01	1.1027E-01
1	3.3714E-01	6.1629E-02	2.7073E-01
2	1.0391E-01	3.1713E-01	1.2306E-02
3	2.1156E-02	2.1366E-01	1.5592E-01
4	3.2305E-03	7.1889E-02	2.5433E-01
5	3.9720E-04	1.6012E-02	1.3988E-01
6	3.9957E-05	2.6724E-03	4.4644E-02

from the RKR fit are collected in Table 5. The $B^2\Sigma^+$ and $X^2\Sigma^+$ potential energy curves were used to calculate the Franck–Condon factors for the bands involving $v' = 0$ to 2 and $v'' = 0$ to 6 vibrational levels (Table 6).

CONCLUSION

We have investigated the $B^2\Sigma^+$–$X^2\Sigma^+$ electronic transitions of $^{12}C^{17}O^+$ in the near ultraviolet spectral region. The observed spectrum has been classified as 2–4, 2–5, and 2–6 new bands of this system. The current data have been combined with our previous data,[6,7] and precise spectroscopic constants for the $B^2\Sigma^+$ state have been obtained. Especially, $\omega_e x_e = 27.3528(39)$ cm^{-1} and $\gamma_e = -1.15(19) \times 10^{-4}$ cm^{-1} constants have been derived for the first time. Also, RKR potential curves for both states and Franck–Condon factors for the vibrational bands of the B–X system have been calculated.

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