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Rydberg-Klein-Rees $^1\Sigma^+$ Potential Curve Turning Points for the Isotopes of Carbon Monoxide

C. Chackerian, Jr. and D. Goorvitch

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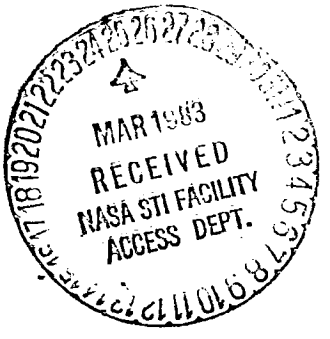

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ABS: First order RKR turning points were computed for (C-12)O16, (C-12)O17, (C-13)O16, (C-12)O18, and (C-13)O18 for vibrational levels up to v = 40. These turning points should be useful in the numerical computation of matrix elements of powers of the internuclear separation.

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Rydberg-Klein-Rees $^1\Sigma^+$ Potential Curve Turning Points for the Isotopes of Carbon Monoxide

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Rydberg-Klein-Rees $^1\Sigma^+$ potential curve turning points for the isotopes of carbon monoxide

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(Received

First order RKR turning points have been computed for $^{12}C^{16}O$, $^{12}C^{17}O$, $^{13}C^{16}O$, $^{12}C^{18}O$, and $^{13}C^{18}O$ for vibrational levels up to $v = 40$. These turning points should be useful in the numerical computation of matrix elements of powers of the internuclear separation.

I. INTRODUCTION

The carbon monoxide molecule is of interest to astronomers because it is found via high resolution infrared spectroscopy (1) in astrophysical sources and can be used to determine physical conditions and isotopic abundances in these sources. In addition, the CO laser which can be made to oscillate on high v, $\Delta v = 1$,

transitions (2) ($v \leq 37$) as well as $\Delta v = 2$ transitions (3) ($v \leq 16$) is a useful probe for a number of laboratory experiments. Further, this laser can be used as a stable local oscillator for heterodyne spectroscopy of high-temperature astrophysical sources in much the same way that the CO_2 laser has been used (4) for planetary spectroscopy. In this paper we present the results of first order RKR turning point calculations for the stable isotopes of electronic ground state carbon monoxide.

Values for state properties (diagonal) and transition (non-diagonal) matrix elements may be obtained for isotopic variants of molecules from corresponding values for the normal molecule using analytical techniques. For example, in the lowest order of approximation (harmonic-oscillator, Born-Oppenheimer) the ratio of intensities (normal species/isotopic species) for vibrational transitions ($\Delta v = 1$, $v \rightarrow v + 1$) is equal to $(\mu^*/\mu)^{1/2}$, where μ^* and μ are the reduced masses of the variant and normal isotopic species, respectively. However, the complexity of the formulae and the number of parameters required for determining accurate matrix elements for isotopic species increase rapidly as the magnitude of Δv or v values are increased. For the case of CO we advocate determining matrix elements (especially for the higher v levels involving $\Delta v > 1$ transitions) using wave functions obtained from numerical solution of the radial Schrödinger equation. To this end we have computed first order RKR potential function turning points for the stable isotopic species of CO.

II. DISCUSSION AND RESULTS

Previous work on the RKR potential of normal CO has been summarized by Huffaker. (5) We use Huffaker's notation to summarize the theory for the first order RKR method. The inner (r_-) and outer (r_+) classical turning points for rotationless levels with vibrational quantum number, v, are given by:

$$r_{\pm}(v) = C[(f^2 + f/g)^{1/2} \pm f] \tag{1}$$

where $C = (h/8\pi^2 c\mu)^{1/2}$ and μ is the reduced mass. The integrals f and g are given by Eqs. (2) and (3):

$$f(v) = \int_{vo}^{v} [G(v) - G(v')]^{-1/2}\, dv' \tag{2}$$

$$g(v) = \int_{vo}^{v} B(v')[G(v) - G(v')]^{-1/2}\, dv' \tag{3}$$

where the quantities G(v) and B(v) express the vibrational energy and rotational constant as a function of the vibrational quantum number. Solutions to the above equations were obtained using a computer program (6) which we adopted for use with a CDC 7600 computer. The program was modified to accommodate Kaiser's correction (7) to the RKR method. This correction entails starting the integrations in Eqs. (2) and (3) at v_o, where $v_o \sim -1/2 - Y_{00}/Y_{10}$ and the Y's are Dunham constants. Values for the appropriate vibrational and rotational constants were obtained using the Dunham constants recently reported by Dale et al. (8) The accuracy of the RKR code was checked by comparing the analytic and numerical solutions of Eqs. (1)-(3)

for a harmonic oscillator. The largest error in the turning points occurs for the lowest vibrational level, $v = 0$. Here r_- is too large by 9 parts in 10^6 and r_+ is too small by the same amount. At $v = 10$ the error decreases to 2 parts in 10^6. As a further check we computed turning points for $^{12}C^{16}O$ using the same values (9) for $G(v)$ and $B(v)$ as were used by Kirschner and Watson. (10) In this case the differences in the two sets of calculations, for the first ten levels, are in the range of 0.4 - 4 parts in 10^7. For $v = 28$ the inner and outer turning points differed by 3 and 10 parts in 10^7, respectively.

Our results are presented in Table I. For completeness G and B values computed from Dunham constants are also included. The results for $^{12}C^{16}O$ are slightly different from the first order constants reported by Kirschner and Watson (10) principally because the spectroscopic and fundamental constants used for the two sets of calculations are different. Kirschner and Watson (11) have also computed second order RKR curves for $^{12}C^{16}O$. We have made a limited comparison of transition moment matrix elements ($\Delta v \leq 4$, $v \leq 11$) computed via a numerical solution of the radial Schrödinger equation using the first and second order RKR potential curves and found differences in the two calculations of less than 0.1%.

ACKNOWLEDGMENT

To Ms. Ellen Howell for assisting in some of the calculations.

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TABLE I. First order RKR turning points[a] for $^1\Sigma^+$ CO and its isotopes.

Isotope	v+1/2	$G(v)+Y_{00}$[b]	r(min)[c]	r(max)[c]	B(v)[b]
$^{12}C^{16}O$	0.5	1,081.7764	1.0833075	1.1787712	1.9225289
	1.5	3,225.0480	1.0534204	1.2196121	1.9050258
	2.5	5,341.8392	1.0342203	1.2498872	1.8875240
	3.5	7,432.2160	1.0193934	1.2759129	1.8700238
	4.5	9,496.2462	1.0071128	1.2995188	1.8525253
	5.5	11,533.9990	0.9965457	1.3215402	1.8350285
	6.5	13,545.5454	0.9872303	1.3424417	1.8175338
	7.5	15,530.9582	0.9788792	1.3625135	1.8000412
	8.5	17,490.3116	0.9712993	1.3819516	1.7825510
	9.5	19,423.6814	0.9643538	1.4008959	1.7650633
	10.5	21,331.1451	0.9579413	1.4194508	1.7475782
	11.5	23,212.7818	0.9519847	1.4376968	1.7300960
	12.5	25,068.6717	0.9464234	1.4556975	1.7126167
	13.5	26,898.8964	0.9412089	1.4735049	1.6951406
	14.5	28,703.5383	0.9363019	1.4911620	1.6776678
	15.5	30,482.6810	0.9316696	1.5087050	1.6601985
	16.5	32,236.4087	0.9272847	1.5261651	1.6427329
	17.5	33,964.8059	0.9231240	1.5435694	1.6252710
	18.5	35,667.9576	0.9191677	1.5609417	1.6078131
	19.5	37,345.9486	0.9153984	1.5783036	1.5903594
	20.5	38,998.8632	0.9118014	1.5956743	1.5729099

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{12}C^{16}O$	21.5	40,626.7854	0.9083634	1.6130716	1.5554649
(cont.)	22.5	42,229.7979	0.9050727	1.6305119	1.5380246
	23.5	43,807.9822	0.9019191	1.6480106	1.5205890
	24.5	45,361.4181	0.8988932	1.6655821	1.5031584
	25.5	46,890.1831	0.8959867	1.6832403	1.4857329
	26.5	48,394.3522	0.8931920	1.7009986	1.4683126
	27.5	49,873.9974	0.8905020	1.7188700	1.4508979
	28.5	51,329.1872	0.8879105	1.7368673	1.4334887
	29.5	52,759.9861	0.8854116	1.7550030	1.4160853
	30.5	54,166.4542	0.8829998	1.7732898	1.3986878
	31.5	55,548.6463	0.8806700	1.7917405	1.3812965
	32.5	56,906.6117	0.8784172	1.8103679	1.3639114
	33.5	58,240.3935	0.8762370	1.8291852	1.3465327
	34.5	59,550.0281	0.8741250	1.8482059	1.3291606
	35.5	60,835.5442	0.8720769	1.8674442	1.3117953
	36.5	62,096.9625	0.8700886	1.8869146	1.2944369
	37.5	63,334.2950	0.8681561	1.9066324	1.2770855
	38.5	64,547.5440	0.8662755	1.9266139	1.2597415
	39.5	65,736.7018	0.8644427	1.9468762	1.2424048
	40.5	66,901.7495	0.8626537	1.9674374	1.2250757

$Y_{00} = 0.19005\ cm^{-1}$; $v_o = -0.500088$; $C = 1.5680368 \times 10^{-8}\ cm^{1/2}$.

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{12}C^{17}O$	0.5	1,068.0314	1.0835760	1.1784263	1.8739663
	1.5	3,184.3259	1.0538510	1.2189640	1.8571236
	2.5	5,274.8090	1.0347465	1.2489994	1.8402823
	3.5	7,339.5443	1.0199886	1.2748087	1.8234423
	4.5	9,378.5968	1.0077615	1.2982103	1.8066040
	5.5	11,392.0333	0.9972378	1.3200341	1.7897674
	6.5	13,379.9218	0.9879585	1.3407418	1.7729328
	7.5	15,342.3322	0.9796378	1.3606218	1.7561002
	8.5	17,279.3358	0.9720840	1.3798688	1.7392698
	9.5	19,191.0055	0.9651608	1.3986218	1.7224419
	10.5	21,077.4158	0.9587677	1.4169843	1.7056164
	11.5	22,938.6425	0.9528279	1.4350363	1.6887936
	12.5	24,774.7625	0.9472811	1.4528411	1.6719737
	13.5	26,585.8543	0.9420793	1.4704500	1.6551567
	14.5	28,371.9971	0.9371831	1.4879058	1.6383429
	15.5	30,133.2710	0.9325602	1.5052442	1.6215324
	16.5	31,869.7571	0.9281833	1.5224962	1.6047253
	17.5	33,581.5367	0.9240294	1.5396885	1.5879218
	18.5	35,268.6913	0.9200787	1.5568447	1.5711221
	19.5	36,931.3027	0.9163142	1.5739860	1.5543263
	20.5	38,569.4522	0.9127209	1.5911313	1.5375345

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{12}C^{17}O$	21.5	40,183.2207	0.9092858	1.6082983	1.5207470
(cont.)	22.5	41,772.6881	0.9059973	1.6255028	1.5039639
	23.5	43,337.9332	0.9028451	1.6427601	1.4871852
	24.5	44,879.0333	0.8998200	1.660842	1.4704113
	25.5	46,396.0637	0.8969137	1.6774886	1.4536422
	26.5	47,889.0974	0.8941187	1.6949865	1.4368780
	27.5	49,358.2047	0.8914281	1.7125902	1.4201190
	28.5	50,803.4527	0.8888355	1.7303123	1.4033653
	29.5	52,224.9050	0.8863352	1.7481649	1.3866170
	30.5	53,622.6208	0.8839217	1.7661602	1.3698744
	31.5	54,996.6549	0.8815900	1.7843103	1.3531375
	32.5	56,347.0570	0.8793353	1.8026276	1.3364065
	33.5	57,673.8711	0.8771532	1.8211246	1.3196815
	34.5	58,977.1349	0.8750393	1.8398142	1.3029628
	35.5	60,256.8792	0.8729894	1.8587098	1.2862504
	36.5	61,513.1276	0.8709997	1.8778251	1.2695446
	37.5	62,745.8955	0.8690661	1.8971745	1.2528454
	38.5	63,955.1895	0.8671849	1.916773	1.2361531
	39.5	65,141.0071	0.8653523	1.9366374	1.2194677
	40.5	66,303.3354	0.8635643	1.9567839	1.2027895

Y_{00} = 0.18544 cm^{-1}; v_o = -0.500087; C = 1.5480564×10^{-8} $cm^{1/2}$.

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{13}C^{16}O$	0.5	1,057.7276	1.0837804	1.1781686	1.8379720
	1.5	3,153.7950	1.0541777	1.2184782	1.8216135
	2.5	5,244.5474	1.0351455	1.2483333	1.8052562
	3.5	7,270.0464	1.0204396	1.2739801	1.7889003
	4.5	9,290.3552	1.0082531	1.2972282	1.7725459
	5.5	11,285.5384	0.9977623	1.3189037	1.7561931
	6.5	13,255.6622	0.9885103	1.3394660	1.7398422
	7.5	15,200.7942	0.9802128	1.3592022	1.7234933
	8.5	17,121.0038	0.9726787	1.3783060	1.7071464
	9.5	19,016.3615	0.9657725	1.3969156	1.6908018
	10.5	20,886.9395	0.9593942	1.4151341	1.6744596
	11.5	22,732.8113	0.9534672	1.4330409	1.6581199
	12.5	24,554.0516	0.9479315	1.4506990	1.6417830
	13.5	26,350.7364	0.9427394	1.4681595	1.6254488
	14.5	28,122.9425	0.9378517	1.4854647	1.6091177
	15.5	29,870.7477	0.9332360	1.5026503	1.5927897
	16.5	31,594.2305	0.9288654	1.5197468	1.5764649
	17.5	33,293.4699	0.9247168	1.5367808	1.5601436
	18.5	34,968.5451	0.9207706	1.5537757	1.5438259
	19.5	36,619.5353	0.9170098	1.5707524	1.5275119
	20.5	38,246.5198	0.9134196	1.5877298	1.5112017

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{13}C^{16}O$	21.5	39,849.5772	0.9099869	1.6047250	1.4948955
(cont.)	22.5	41,428.7852	0.9067002	1.6217539	1.4785935
	23.5	42,984.2208	0.9035494	1.6388314	1.4622958
	24.5	44,515.9593	0.9005252	1.6559714	1.4460026
	25.5	46,024.0743	0.8976193	1.6731870	1.4297139
	26.5	47,508.6372	0.8948244	1.6904912	1.4134300
	27.5	48,969.7172	0.8921335	1.7078961	1.3971510
	28.5	50,407.3801	0.8895403	1.7254139	1.3808770
	29.5	51,821.6887	0.8870392	1.7430564	1.3646082
	30.5	53,212.7017	0.8846247	1.7608354	1.3483447
	31.5	54,580.4737	0.8822919	1.7787627	1.3320867
	32.5	55,925.0545	0.8800360	1.7968503	1.3158343
	33.5	57,246.4885	0.8778526	1.8151103	1.2995877
	34.5	58,544.8143	0.8757375	1.8335550	1.2833470
	35.5	59,820.0643	0.8736865	1.8521973	1.2671123
	36.5	61,072.2635	0.8716959	1.8710504	1.2508839
	37.5	62,301.4299	0.8697617	1.8901281	1.2346618
	38.5	63,507.5731	0.8678802	1.9094448	1.2184462
	39.5	64,690.6937	0.8660477	1.9290159	1.2022372
	40.5	65,850.7833	0.8642604	1.9488573	1.1860351

Y_{00} = 0.18185 cm^{-1}; v_o = -0.500086; C = 1.5330829×10^{-8} $cm^{1/2}$.

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{12}C^{18}O$	0.5	1,055.7186	1.0838202	1.1781177	1.8309808
	1.5	3,147.8417	1.0542416	1.2183826	1.8147158
	2.5	5,412.7457	1.0352236	1.2482023	1.7984520
	3.5	7,256.4922	1.0205280	1.2738173	1.7821895
	4.5	9,273.1437	1.0083495	1.2970353	1.7659286
	5.5	11,264.7647	0.9978651	1.3186818	1.7496693
	6.5	13,231.4208	0.9886185	1.3392157	1.7334118
	7.5	15,173.1794	0.9803255	1.3589238	1.7171562
	8.5	17,090.1094	0.9727953	1.3779995	1.7009028
	9.5	18,982.2809	0.9658925	1.3965811	1.6846515
	10.5	20,849.7658	0.9595171	1.4147714	1.6684027
	11.5	22,692.6370	0.9535926	1.4326499	1.6521563
	12.5	24,510.9689	0.9480592	1.4502794	1.6359126
	13.5	26,304.8369	0.9428690	1.4677108	1.6196718
	14.5	28,074.3175	0.9379829	1.4849866	1.6034338
	15.5	29,819.4880	0.9333687	1.5021423	1.5871990
	16.5	31,540.4265	0.9289993	1.5192085	1.5709675
	17.5	33,237.2114	0.9248518	1.5362116	1.5547393
	18.5	34,090.9217	0.9209065	1.5531751	1.5385146
	19.5	36,558.6361	0.9171464	1.5701197	1.5222936
	20.5	38,183.4334	0.9135568	1.5870643	1.5060765

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{12}C^{18}O$	21.5	39,784.3918	0.9101246	1.6040260	1.4898633
(cont.)	22.5	41,361.5887	0.9068383	1.6210207	1.4736542
	23.5	42,915.1006	0.9036878	1.6380631	1.4574494
	24.5	44,445.0026	0.9006638	1.6551672	1.4412490
	25.5	45,951.3680	0.8977580	1.6723460	1.4250531
	26.5	47,434.2679	0.8949631	1.6896125	1.4088619
	27.5	48,893.7711	0.8922722	1.7069786	1.3926756
	28.5	50,329.9434	0.8896789	1.7244566	1.3764942
	29.5	51,742.8473	0.8871777	1.7420582	1.3603179
	30.5	53,132.5417	0.8847630	1.7597951	1.3441470
	31.5	54,499.0809	0.8824300	1.7776790	1.3279814
	32.5	55,842.5147	0.8801739	1.7957219	1.3118214
	33.5	57,162.8878	0.8779903	1.8139357	1.2956671
	34.5	58,460.2390	0.8758750	1.8323328	1.2795186
	35.5	59,734.6007	0.8738239	1.8509259	1.2633761
	36.5	60,985.9985	0.8718331	1.8697280	1.2472398
	37.5	62,214.4508	0.869898	1.8887529	1.2311097
	38.5	63,419.9677	0.8680173	1.9080148	1.2149861
	39.5	64,602.5506	0.8661849	1.9275289	1.1988690
	40.5	65,762.1917	0.8643979	1.9473111	1.1827587

Y_{00} = 0.18112 cm^{-1}; v_o = -0.500086; C = 1.53015729×10^{-8} $cm^{1/2}$.

TABLE I. Continued

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{13}C^{18}O$	0.5	1,031.0569	1.0843121	1.1774931	1.7464085
	1.5	3,074.7503	1.0550299	1.2172086	1.7312597
	2.5	5,094.3902	1.0361873	1.2465945	1.7161121
	3.5	7,090.0336	1.0216184	1.2718188	1.7009657
	4.5	9,061.7390	1.0095386	1.2946684	1.6858206
	5.5	11,009.5661	0.9991344	1.3159591	1.6706771
	6.5	12,933.5761	0.9899546	1.3361445	1.6555351
	7.5	14,833.8313	0.9817181	1.3555080	1.6403940
	8.5	16,710.3957	0.9742363	1.3742408	1.6252566
	9.5	18,563.3345	0.9673752	1.3924794	1.6101203
	10.5	20,392.7142	0.9610360	1.4103254	1.5949861
	11.5	22,198.6026	0.9551430	1.4278570	1.5798542
	12.5	23,981.0686	0.9496371	1.4451363	1.5647246
	13.5	25,740.1821	0.9444708	1.4622136	1.5495976
	14.5	27,476.0141	0.9396055	1.4791304	1.5344732
	15.5	29,188.6365	0.9350094	1.4959218	1.5193516
	16.5	30,878.1216	0.9306556	1.5126177	1.5042328
	17.5	32,544.5425	0.9265214	1.5292441	1.4891172
	18.5	34,187.9725	0.9225874	1.5458239	1.4740046
	19.5	35,808.4850	0.9188368	1.5623774	1.4588954
	20.5	37,406.1535	0.9152550	1.5789229	1.4437895
	21.5	38,981.0510	0.9118290	1.5954771	1.4286872
	22.5	40,533.2501	0.9085476	1.6120552	1.4135886

TABLE I. Concluded

Isotope	v+1/2	$G(v)+Y_{00}$ [b]	r(min) [c]	r(max) [c]	B(v) [b]
$^{13}C^{18}O$	23.5	42,062.8226	0.9054006	1.6286716	1.3984938
(cont.)	24.5	43,569.8390	0.9023790	1.6453395	1.3834029
	25.5	45,054.3685	0.8994746	1.6620717	1.3683161
	26.5	46,516.4788	0.8966800	1.6788801	1.3532334
	27.5	47,956.2352	0.8939886	1.6957765	1.3381551
	28.5	49,373.7009	0.8913942	1.7127722	1.3230812
	29.5	50,768.9361	0.8888911	1.7298782	1.3080118
	30.5	52,141.9979	0.8864740	1.7471056	1.2929472
	31.5	53,492.9400	0.8841382	1.7644652	1.2778874
	32.5	54,821.8120	0.8818791	1.7819680	1.2628325
	33.5	56,128.6590	0.8796923	1.7996251	1.2477828
	34.5	57,413.5214	0.8775737	1.8174478	1.2327382
	35.5	58,676.4342	0.8755195	1.8354475	1.2176990
	36.5	59,917.4266	0.8735259	1.8536362	1.2026653
	37.5	61,136.5213	0.8715892	1.8720261	1.1876371
	38.5	62,333.7345	0.8697061	1.8906301	1.1726146
	39.5	63,509.0747	0.8678729	1.9094615	1.1575985
	40.5	64,662.5426	0.8660863	1.9285346	1.1425875

Y_{00} = 0.17269 cm^{-1}; v_o = -0.500084; C = 1.4943176×10^{-8} $cm^{1/2}$.

[a] Computed using Dunham constants from Ref. (8).

[b] Units are wavenumbers (cm^{-1}).

[c] Units are Angstroms (Å).

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16. Abstract

First order RKR turning points have been computed for $^{12}C^{16}O$, $^{12}C^{17}O$, $^{13}C^{16}O$, $^{12}C^{18}O$, and $^{13}C^{18}O$ for vibrational levels up to $v = 40$. These turning points should be useful in the numerical computation of matrix elements of powers of the internuclear separation.

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