

Einstein A-coefficients for vib-rotational transitions in CO*

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Abstract. — Einstein A-coefficients for vib-rotational transitions in CO isotopomers, for vibrational quantum number v up to 20, rotational quantum number J up to 140, and Δv up to 4, are calculated. The change in J is governed by the selection rules $\Delta J = \pm 1$. These coefficients play an important role in astronomy, as CO is the most abundant molecule after H₂, and has been observed in almost all the astronomical objects.

Key words: ISM: molecules — molecular data

1. Introduction

Carbon monoxide has been observed in almost all the astronomical objects and is the most abundant molecule after H₂. Hence, it has been a molecule of great interest for astrophysicists. For its theoretical studies, one of the essential parameters is the Einstein A-coefficients for vib-rotational transitions. The Einstein A-coefficients for vib-rotational transitions for CO have been calculated by a number of authors, e.g., Chackerian & Tipping (1983), Hure & Roueff (1993) and Goorvitch & Chackerian (1994a, b). The reason, for recalculations for these coefficients has been either more accurate Dunham coefficients, derived from the accurate and large number of transitions in the higher vibrational states, were obtained, or more accurate electric dipole moment function (EDMF) from the experimental measurements or ab-initio calculations was obtained. Chackerian & Tipping (1983) used the Dunham coefficients derived by Dale et al. (1979), and the EDMF, used by them, was obtained by using the data from various accurate observations. Hure & Roueff (1993) used the energies which were in agreement often better than 0.01 cm⁻¹ with the laboratory data of Farrenq et al. (1991), Le Floch (1991a, b), Guelachvili et al. (1983), and the EDMF was that calculated by Cooper & Kirby (1987). Goorvitch & Chackerian (1994a, b) used the Dunham coefficients of Farrenq et al. (1991) and the EDMF experimentally derived by Chackerian et al. (1984).

Besides the accuracy of the Dunham coefficients and the EDMF, one more important aspect in the calcula-

tions is the accurate determination of the potential energy curve by using the values of the Dunham coefficients. Our (Chandra et al. 1995) recent calculations for the Einstein A-coefficients for the CS molecule showed that the Einstein A-coefficients, particularly for large J and/or large v are very sensitive to the potential energy curve. Various methods for determination of the potential energy curve have been suggested time to time (see, e.g., Chandra & Sharma 1995). Recently, Chandra & Maheshwari (1995), and Chandra & Sharma (1995) have proposed new methods for the calculation of the potential energy curve. These methods are very fast and the accuracy of the turning points in the potential energy curve is at least 10⁻⁷ Å, which is better than that of the other methods, used earlier.

In the present investigation, we have calculated Einstein A-coefficients for the vib-rotational transitions in the more abundant CO isotopomers. We have used the Dunham coefficient of Farrenq et al. (1991) and the EDMF of Chackerian et al. (1984). However, the potential energy curve, to which the calculations are more sensitive than other parameters, is calculated by using the methods of Chandra & Maheshwari (1995), and Chandra & Sharma (1995). Both of these methods produce the turning points of the same accuracy of at least 10⁻⁷ Å. The Dunham coefficients of Farrenq et al. (1991) are very accurate as these have been derived from the laboratory data available up to very high vibrational states ($v \leq 41$).

2. Method of calculation and results

The RKR potential for the molecule CO has been calculated with the help of the methods of Chandra & Maheshwari (1995), and Chandra & Sharma (1995) where the Dunham coefficients of Farrenq et al. (1991) are used.

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*Tables 2A, 2B, 2C and 2D are available only in electronic form via anonymous ftp 130.79.128.5 at the CDS

Table 1. Turning points (in Å) and potential energy (in cm^{-1}) for $^{12}\text{C}^{16}\text{O}$

v	r_{min}	r_{max}	pot. energy	v	r_{min}	r_{max}	pot. energy
-	R_e	R_e	0.0000	20	0.9115891	1.5960224	38998.6766
0	1.0833117	1.1787672	1081.5857	21	0.9081211	1.6134756	40626.6001
1	1.0534226	1.2196100	3224.8568	22	0.9047982	1.6309782	42229.6144
2	1.0342213	1.2498865	5341.6478	23	0.9016101	1.6485461	43807.8009
3	1.0193930	1.2759139	7432.0247	24	0.8985475	1.6661943	45361.2396
4	1.0071103	1.2995223	9496.0550	25	0.8956024	1.6839371	46890.0081
5	0.9965406	1.3215471	11533.8078	26	0.8927673	1.7017887	48394.1814
6	0.9872218	1.3424533	13545.3543	27	0.8900356	1.7197625	49873.8318
7	0.9788664	1.3625314	15530.7670	28	0.8874012	1.7378720	51329.0276
8	0.9712811	1.3819774	17490.1202	29	0.8848588	1.7561305	52759.8334
9	0.9643289	1.4009315	19423.4901	30	0.8824033	1.7745513	54166.3090
10	0.9579086	1.4194984	21330.9539	31	0.8800304	1.7931478	55548.5091
11	0.9519425	1.4377586	23212.5907	32	0.8777358	1.8119337	56906.4825
12	0.9463702	1.4557764	25068.4807	33	0.8755161	1.8309228	58240.2716
13	0.9411431	1.4736037	26898.7056	34	0.8733677	1.8501297	59549.9117
14	0.9362215	1.4912839	28703.3478	35	0.8712878	1.8695691	60835.4299
15	0.9315727	1.5088537	30482.4908	36	0.8692735	1.8892565	62096.8449
16	0.9271692	1.5263443	32236.2189	37	0.8673224	1.9092080	63334.1657
17	0.9229877	1.5437834	33964.6167	38	0.8654323	1.9294409	64547.3909
18	0.9190083	1.5611953	35667.7691	39	0.8636015	1.9499730	65736.5076
19	0.9152138	1.5786016	37345.7608	40	0.8618281	1.9708235	66901.4905

The turning points (r_{min} and r_{max}) in the potential energy curve and the corresponding potential energy for $^{12}\text{C}^{16}\text{O}$ are given in Table 1. By using this potential energy curve, the Einstein A-coefficients are calculated with the help of the program LEVEL (Le Roy 1993). In the calculations, we used the value of the equilibrium nuclear separation, $R_e = 1.1283226$ Å and the dissociation energy 90674 cm^{-1} (Eidelsberg et al. 1987).

We calculated the A-coefficients for vibrational quantum number v up to 20, rotational quantum number J up to 140, and Δv up to 4. The numerical results are given in Tables 2A, 2B, 2C and 2D for $^{12}\text{C}^{16}\text{O}$, $^{12}\text{C}^{17}\text{O}$, $^{12}\text{C}^{18}\text{O}$ and $^{13}\text{C}^{16}\text{O}$, respectively, and are available in electronic form via anonymous ftp 130.79.128.5 at the CDS. In the Tables VL and JL are, respectively, the vibrational and rotational quantum numbers for the lower level, and VU and JU are the corresponding numbers for the upper level for a transition. The units of the Einstein A-coefficient, A , energy of the lower level, E and the frequency of the transition, freq, are s^{-1} , cm^{-1} and cm^{-1} , respectively. A part of the Table 2A for v up to 2 and J up to 10 is given, here, in the printed form.

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Table 2. A. Einstein A-coefficients, energy of lower level, and frequency of transition for C¹²O¹⁶

VL	JL	VU	JU	A(Eins)	E(lower)	freq	VL	JL	VU	JU	A(Eins)	E(lower)	freq
0	0	0	1	7.67D-08	1081.5857	3.8450	0	1	0	2	7.36D-07	1085.4307	7.6899
0	2	0	3	2.66D-06	1093.1206	11.5345	0	3	0	4	6.53D-06	1104.6551	15.3787
0	4	0	5	1.30D-05	1120.0338	19.2222	0	5	0	6	2.28D-05	1139.2560	23.0651
0	6	0	7	3.65D-05	1162.3211	26.9070	0	7	0	8	5.47D-05	1189.2281	30.7479
0	8	0	9	7.81D-05	1219.9760	34.5877	0	9	0	10	1.07D-04	1254.5637	38.4261
0	1	1	0	3.42D+01	1085.4307	2139.4261	0	0	1	1	1.15D+01	1081.5857	2147.0811
0	2	1	1	2.26D+01	1093.1206	2135.5462	1	0	1	1	4.90D-08	3224.8568	3.8100
0	1	1	2	1.39D+01	1085.4307	2150.8560	0	3	1	2	2.03D+01	1104.6551	2131.6316
1	1	1	2	4.70D-07	3228.6668	7.6199	0	2	1	3	1.50D+01	1093.1206	2154.5956
0	4	1	3	1.92D+01	1120.0338	2127.6824	1	2	1	3	1.70D-06	3236.2867	11.4295
0	3	1	4	1.56D+01	1104.6551	2158.2997	0	5	1	4	1.85D+01	1139.2560	2123.6988
1	3	1	4	4.16D-06	3247.7162	15.2386	0	4	1	5	1.60D+01	1120.0338	2161.9682
0	6	1	5	1.81D+01	1162.3211	2119.6810	1	4	1	5	8.29D-06	3262.9548	19.0472
0	5	1	6	1.64D+01	1139.2560	2165.6010	0	7	1	6	1.78D+01	1189.2281	2115.6290
1	5	1	6	1.45D-05	3282.0020	22.8550	0	6	1	7	1.66D+01	1162.3211	2169.1979
0	8	1	7	1.75D+01	1219.9760	2111.5430	1	6	1	7	2.32D-05	3304.8571	26.6620
0	7	1	8	1.69D+01	1189.2281	2172.7588	0	9	1	8	1.73D+01	1254.5637	2107.4232
1	7	1	8	3.48D-05	3331.5190	30.4679	0	8	1	9	1.71D+01	1219.9760	2176.2835
0	10	1	9	1.71D+01	1292.9898	2103.2697	1	8	1	9	4.96D-05	3361.9869	34.2726
0	9	1	10	1.72D+01	1254.5637	2179.7719	1	9	1	10	6.80D-05	3396.2595	38.0760
0	1	2	0	8.34D-01	1085.4307	4256.2171	1	1	2	0	6.66D+01	3228.6668	2112.9810
0	0	2	1	2.83D-01	1081.5857	4263.8372	0	2	2	1	5.52D-01	1093.1206	4252.3022
1	0	2	1	2.24D+01	3224.8568	2120.5661	1	2	2	1	4.41D+01	3236.2867	2109.1361
2	0	2	1	2.18D-08	5341.6478	3.7750	0	1	2	2	3.42D-01	1085.4307	4267.5421
0	3	2	2	4.93D-01	1104.6551	4248.3176	1	1	2	2	2.71D+01	3228.6668	2124.3060
1	3	2	2	3.95D+01	3247.7162	2105.2566	2	1	2	2	2.09D-07	5345.4229	7.5499
0	2	2	3	3.70D-01	1093.1206	4271.1766	0	4	2	3	4.66D-01	1120.0338	4244.2634
1	2	2	3	2.92D+01	3236.2867	2128.0105	1	4	2	3	3.74D+01	3262.9548	2101.3424
2	2	2	3	7.53D-07	5352.9728	11.3245	0	3	2	4	3.87D-01	1104.6551	4274.7407
0	5	2	4	4.49D-01	1139.2560	4240.1398	1	3	2	4	3.04D+01	3247.7162	2131.6797
1	5	2	4	3.62D+01	3282.0020	2097.3938	2	3	2	4	1.85D-06	5364.2972	15.0986
0	4	2	5	3.99D-01	1120.0338	4278.2342	0	6	2	5	4.38D-01	1162.3211	4235.9470
1	4	2	5	3.13D+01	3262.9548	2135.3132	1	6	2	5	3.53D+01	3304.8571	2093.4110
2	4	2	5	3.68D-06	5379.3959	18.8722	0	5	2	6	4.09D-01	1139.2560	4281.6570
0	7	2	6	4.29D-01	1189.2281	4231.6850	1	5	2	6	3.19D+01	3282.0020	2138.9110
1	7	2	6	3.46D+01	3331.5190	2089.3940	2	5	2	6	6.42D-06	5398.2681	22.6450
0	6	2	7	4.17D-01	1162.3211	4285.0089	0	8	2	7	4.22D-01	1219.9760	4227.3540
1	6	2	7	3.24D+01	3304.8571	2142.4729	1	8	2	7	3.41D+01	3361.9869	2085.3431
2	6	2	7	1.03D-05	5420.9131	26.4169	0	7	2	8	4.24D-01	1189.2281	4288.2898
0	9	2	8	4.16D-01	1254.5637	4222.9542	1	7	2	8	3.29D+01	3331.5190	2145.9988
1	9	2	8	3.37D+01	3396.2595	2081.2583	2	7	2	8	1.53D-05	5447.3300	30.1879
0	8	2	9	4.31D-01	1219.9760	4291.4994	0	10	2	9	4.10D-01	1292.9898	4218.4857
1	8	2	9	3.33D+01	3361.9869	2149.4885	1	10	2	9	3.33D+01	3434.3356	2077.1399
2	8	2	9	2.18D-05	5477.5179	33.9576	0	9	2	10	4.38D-01	1254.5637	4294.6378
1	9	2	10	3.36D+01	3396.2595	2152.9419	2	9	2	10	2.99D-05	5511.4755	37.7260

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