



Rotational quenching of H₂CO by molecular hydrogen – Suggestion on the work of Wiesenfeld & Faure

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MS received 2 May 2015; revised 20 April 2016; accepted 6 May 2016; published online 5 December 2016

Abstract. Wiesenfeld and Faure investigated rotational quenching of H₂CO by molecular hydrogen where they considered 40 rotational levels of *o*-H₂CO and 41 rotational levels of *p*-H₂CO. Data on energies of rotational levels of the molecule are fundamental in the investigation. We have found that the sequence of levels reported by Wiesenfeld and Faure is not as per convention of molecular physics. Their results are also available on the website: <http://home.strw.leidenuniv.nl/~moldata/datafiles/ph2co-h2.dat>, where the collisional transitions are shown even between the levels having equal energies. Data for such transitions should not be there.

Keywords. Interstellar matter: molecules; H₂CO molecule; quenching.

PACS No. 34.50.–s

1. Introduction

Molecules may be classified on the basis of their moments of inertia, computed about three mutually perpendicular principal inertial axes. The axes are named as *a*, *b* and *c* accordingly to the moments of inertia *I_a*, *I_b* and *I_c*, respectively, such that $I_a \leq I_b \leq I_c$. For example, the axis about which the moment of inertia is the minimum is named as the *a*-axis. The molecular constants *A*, *B* and *C* are expressed as

$$A = \frac{h}{8\pi^2 I_a}, \quad B = \frac{h}{8\pi^2 I_b}, \quad C = \frac{h}{8\pi^2 I_c},$$

where *h* denotes the Planck constant. Obviously, the constants *A*, *B* and *C* satisfy the relation $A \geq B \geq C$ and *A*, *B* and *C* are known as the rotational constants. Owing to the rotational motion, centrifugal distortions come in the picture, and we have centrifugal distortion constants besides the rotational constants.

Troscompt *et al* [1] investigated the collisional rate coefficients for *o*-H₂CO colliding with *o*-H₂ (in the ground state with rotational quantum number *J* = 1) and with *p*-H₂ (in the ground state with rotational quantum number *J* = 0). Using the values given in

column 3 of table 1, they calculated the rate coefficients for collisional transitions between 10 rotational levels only of *o*-H₂CO. No results were given for the *p*-H₂CO.

Wiesenfeld and Faure [2] have extended the work of Troscompt *et al* [1] where they have considered 40 rotational levels of *o*-H₂CO and 41 rotational levels of *p*-H₂CO. The rotational and centrifugal distortion constants used by them also are given in column 4 of table 1. Here, Wiesenfeld and Faure [2] have taken three centrifugal distortion constants, *D_J*, *D_{JK}* and *D_K*, besides the rotational constants.

Sharma *et al* [3] have calculated rate coefficients for collisional transitions between 23 levels in *o*-H₂CO and *p*-H₂CO due to collisions with He atom. They have used the rotational and centrifugal distortion constants reported by Brünken *et al* [4] and given in column 2 of table 1.

In such investigations, the energies of levels are fundamental data and are often calculated with high accuracy. We have calculated energies of rotational levels for isolated H₂CO, as the density in the interstellar medium is low.

Table 1. Molecular and centrifugal distortion constants.

Parameter	Value (MHz) ^a	Value (cm ⁻¹) ^b	Value (cm ⁻¹) ^c
<i>A</i>	2.819705578×10^5	9.405525	9.405525
<i>B</i>	3.883398715×10^4	1.295431	1.295431
<i>C</i>	3.400424349×10^4	1.134191	1.134191
<i>D_J</i>	70.32100×10^{-3}		2.51×10^{-6}
<i>D_{JK}</i>	1321.101×10^{-3}		4.31×10^{-5}
<i>D_K</i>	19.39089		6.48×10^{-4}
<i>d₁</i>	-10.43798×10^{-3}		
<i>d₂</i>	-2.501461×10^{-3}		
<i>H_J</i>	3.92×10^{-9}		
<i>H_{JK}</i>	7.453×10^{-6}		
<i>H_{KJ}</i>	10.72×10^{-6}		
<i>H_K</i>	4.021×10^{-3}		
<i>h₁</i>	32.33×10^{-9}		
<i>h₂</i>	47.87×10^{-9}		
<i>h₃</i>	15.946×10^{-9}		
<i>L_{JJK}</i>	-94.0×10^{-12}		
<i>L_{JK}</i>	0.33×10^{-9}		
<i>L_{KKJ}</i>	-4.52×10^{-9}		
<i>L_K</i>	-0.59×10^{-6}		
<i>l₂</i>	-0.307×10^{-12}		
<i>l₃</i>	-0.427×10^{-12}		
<i>l₄</i>	-0.1375×10^{-12}		

^aReported by Brünken *et al* [4] and used in the present work.

^bReported by Troscompt *et al* [1].

^cReported by Wiesenfeld and Faure [2].

2. Energies of rotational levels

For an asymmetric top molecule, rotational levels are denoted by J_{k_a, k_c} or J_τ , where J stands for the rotational quantum number, and k_a and k_c are the projections of J on the symmetry axis in the case of prolate and oblate symmetric top molecules, respectively. The pseudoquantum number τ is expressed as $\tau = k_a - k_c$ and can assume values from $-J$ to $+J$ with the step size of 1. The value of τ increases with the increase of energy. Wiesenfeld and Faure [2] have given two sets of energy levels: (i) Used by them in their investigation (denoted by MOLSCAT) and (ii) experimental values taken from Bocquet *et al* [5] (denoted by Experimental).

The energies of the levels used by Wiesenfeld and Faure [2] need to be modified due to the following observations, based on the conventions followed in molecular physics [3]:

- (i) Level 7_{44} can never be higher than 7_{43} level.
- (ii) Level 6_{43} can never be higher than 6_{42} level.
- (iii) Level 5_{42} can never be higher than 5_{41} level.

- (iv) Level 4_{41} can never be higher than 4_{40} level.

However, equal energies are given for levels 5_{42} and 5_{41} , and for levels 4_{41} and 4_{40} .

3. Calculations

In order to look into the details, we have performed two sets of calculations:

- (a) By using the molecular and centrifugal distortion constants given in column 2 of table 1. The results are marked as ‘Present1’.
- (b) By using the molecular and centrifugal distortion constants given in column 4 of table 1. These are the rotational and centrifugal distortion constants reported by Wiesenfeld and Faure [2]. We have done the calculations independently and the results are marked as ‘Present2’. The results given by Wiesenfeld and Faure [2] are marked as ‘MOLSCAT’.

The results are given in table 2 for *o*-H₂CO and in table 3 for *p*-H₂CO. The sequences of energy levels are according to the convention being followed in molecular physics. The other two sets of data (MOLSCAT and Experimental) are the same as given by Wiesenfeld and Faure [2].

4. Discussion

Both the results, marked as Present1 and Present2, support our observations (i)–(iv), as expected. As the values marked as Present2 are obtained by using the constants given by Wiesenfeld and Faure [2], it appears that they have taken the values, marked MOLSCAT, from some other source.

The discrepancies in the energies of Wiesenfeld and Faure [2] can be visualized easily in the following manner. For example, for levels 7_{44} and 7_{43} , the values of τ are 0 and 1, respectively, and therefore level 7_{43} must always be higher than level 7_{44} . But, for the values used by them the situation is reverse. Again, for levels 6_{43} and 6_{42} , the values of τ are 1 and 2, respectively, and therefore level 6_{42} must be higher than level 7_{44} . But, for the values used by them the situation is reverse. In view of the above, the investigation of Wiesenfeld and Faure need to be modified.

We have looked into the website: <http://home.strw.leidenuniv.nl/~moldata/datafiles/ph2co-h2.dat> also and have found the following. The energies used in the work of Wiesenfeld and Faure [2] are not given there. Experimental energies are given, where the

Table 2. Energies of rotational levels of *o*-H₂CO in cm⁻¹.

No.	<i>J</i>	<i>k_a</i>	<i>k_c</i>	<i>τ</i>	Present1	Present2	MOLSCAT ^a	Experimental ^a
1	1	1	1	0	10.531751	10.538966	10.53897	10.53900
2	1	1	0	1	10.692740	10.700206	10.70021	10.70010
3	2	1	2	-1	15.226402	15.236713	15.23672	15.23690
4	2	1	1	0	15.709351	15.720433	15.72044	15.72020
5	3	1	3	-2	22.266783	22.281705	22.28172	22.28220
6	3	1	2	-1	23.232610	23.249123	23.24914	23.24870
7	4	1	4	-3	31.651014	31.672018	31.67205	31.67290
8	4	1	3	-2	33.260498	33.284264	33.28429	33.28350
9	5	1	5	-4	43.376635	43.405136	43.40518	43.40670
10	5	1	4	-3	45.790272	45.823120	45.82316	45.82200
11	6	1	6	-5	57.440655	57.477996	57.47805	57.48040
12	6	1	5	-4	60.818421	60.862188	60.86224	60.86050
13	7	1	7	-6	73.839601	73.887034	73.88710	73.89070
14	7	1	6	-5	78.340616	78.397137	78.39720	78.39490
15	3	3	1	2	88.177203	88.238084	88.23817	88.23820
16	3	3	0	3	88.177224	88.238106	88.23819	88.23830
17	8	1	8	-7	92.569578	92.628252	92.62834	92.63370
18	4	3	2	1	97.889884	97.957518	97.95762	97.95760
19	4	3	1	2	97.890036	97.957672	97.95777	97.95780
20	8	1	7	-6	98.351635	98.422744	98.49283	98.41970
21	5	3	3	0	110.032390	110.108442	110.10856	110.10860
22	5	3	2	1	110.033000	110.109058	110.10917	110.10920
23	9	1	9	-8	113.626339	113.697279	113.69738	113.70560
24	9	1	8	-7	120.845294	120.932806	120.93290	120.92900
25	6	3	4	-1	124.605706	124.691824	124.69196	124.69200
26	6	3	3	0	124.607534	124.693671	124.69380	124.69380
27	10	1	10	-9	137.005355	137.089444	137.08956	137.10020
28	7	3	5	-2	141.610898	141.708712	141.70886	141.70889
29	7	3	4	-1	141.615462	141.713328	141.71348	141.71350
30	10	1	9	-8	145.814359	145.920057	145.92017	145.91530
31	8	3	6	-3	161.049051	161.160171	161.16034	161.16051
32	8	3	5	-2	161.059080	161.170319	161.17049	161.17059
33	11	1	11	-10	162.701890	162.799851	162.79999	162.81450
34	11	1	10	-9	173.250451	173.376064	173.37619	173.37041
35	9	3	7	-4	182.921208	183.047217	183.04741	183.04781
36	9	3	6	-3	182.941233	183.067489	183.06768	183.06790
37	12	1	12	-11	190.711080	190.823457	190.82361	190.84309
38	12	1	11	-10	203.143955	203.291131	203.29127	203.28461
39	10	3	8	-5	207.228293	207.370744	207.37096	207.37180
40	10	3	7	-4	207.265399	207.408328	207.40854	207.40891

^aTaken from Wiesenfeld and Faure [2].

energies of 4₄₁ and 4₄₀ are the same (155.1694 cm⁻¹); 5₄₂ and 5₄₁ are the same (167.3146 cm⁻¹); 6₄₃ and 6₄₂ are the same (181.8899 cm⁻¹); 7₄₄ and 7₄₃ are the same (198.8960 cm⁻¹). We tried to understand the reason for the discrepancy, but could not find it. Each of the two calculations in §3 gives the results as per the conventions of molecular physics.

We would like to state that the energies of rotational levels reported here are calculated for isolated H₂CO.

Acknowledgements

The authors are grateful to the learned referee for constructive suggestions. Suresh Chandra is grateful to the Founder President Dr Ashok K Chauhan for his full support and encouragements. Financial support from the Department of Science & Technology, New Delhi in the form of research project is thankfully acknowledged.

Table 3. Energies of rotational levels of p -H₂CO in cm⁻¹.

No.	J	k_a	k_c	τ	Present1	Present2	MOLSCAT ^a	Experimental ^a
1	0	0	0	0	0.000000	0.000000	0.00000	0.00000
2	1	0	1	-1	2.427932	2.429610	2.42961	2.42960
3	2	0	2	-2	7.281363	7.286388	7.28640	7.28640
4	3	0	3	-3	14.555436	14.565455	14.56547	14.56550
5	4	0	4	-4	24.242883	24.259509	24.25953	24.25970
6	5	0	5	-5	36.334084	36.358878	36.35891	36.35920
7	2	2	1	1	40.012543	40.040207	40.04024	40.04020
8	2	2	0	2	40.014914	40.042588	40.04262	40.04260
9	3	2	2	0	47.295064	47.327762	47.32780	47.32780
10	3	2	1	1	47.306916	47.339665	47.33970	47.33970
11	6	0	6	-6	50.817182	50.851634	50.85168	50.85240
12	4	2	3	-1	57.002990	57.042365	57.04241	57.04250
13	4	2	2	0	57.038519	57.078052	57.07810	57.07800
14	7	0	7	-7	67.678306	67.723809	67.72387	67.72520
15	5	2	4	-2	69.134519	69.182187	69.18225	69.18240
16	5	2	3	-1	69.217299	69.265349	69.26541	69.26520
17	6	2	5	-3	83.687401	83.744940	83.74502	83.74530
18	6	2	4	-2	83.852559	83.910890	83.91097	83.91060
19	8	0	8	-8	86.901916	86.959738	86.95982	86.96210
20	7	2	6	-4	100.658943	100.727879	100.72797	100.72860
21	7	2	5	-3	100.955104	101.025531	101.02562	101.02500
22	9	0	9	-9	108.471308	108.542560	108.54265	108.54640
23	8	2	7	-5	120.046005	120.127807	120.12792	120.12910
24	8	2	6	-4	120.536892	120.621294	120.62140	120.62030
25	10	0	10	-10	132.369253	132.454864	132.45497	132.46091
26	9	2	8	-6	141.845010	141.941076	141.94120	141.94321
27	9	2	7	-5	142.610531	142.710867	142.71099	142.70931
28	4	4	1	3	155.062082	155.168731	155.16894	155.16940
29	4	4	0	4	155.062082	155.168731	155.16894	155.16940
30	11	0	11	-11	158.578752	158.679436	158.67956	158.68851
31	10	2	9	-7	166.051952	166.163592	166.16374	166.16690
32	10	2	8	-6	167.188620	167.306950	167.30709	167.30440
33	5	4	2	2	167.198855	167.313979	167.31421	167.31461
34	5	4	1	3	167.198857	167.313980	167.31421	167.31461
35	6	4	3	1	181.764099	181.889355	181.88961	181.88989
36	6	4	2	2	181.764106	181.889362	181.88960	181.88989
37	12	0	12	-12	187.083795	187.200034	187.20017	187.21330
38	11	2	10	-8	192.662400	192.790825	192.79099	192.79581
39	11	2	9	-7	194.283000	194.421488	194.42165	194.41750
40	7	4	4	0	198.758417	198.895445	198.89574	198.89600
41	7	4	3	1	198.758445	198.895472	198.89572	198.89600

^aTaken from Wiesenfeld and Faure [2].

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