

# Collisional rates for asymmetrical top molecules\*

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**Abstract.** Collisional rate coefficients for rotational transitions in  $C_3H_2$  and  $SiC_2$  due to collisions with  $H_2$  molecules are calculated. The  $C_3H_2$  has two distinct species, ortho and para, whereas the  $SiC_2$  has only ortho specie due to spin statistics for the identical carbon nuclei. For ortho- and para- $C_3H_2$  we accounted for 47 and 48 energy levels, respectively. The calculations are done for the kinetic temperatures 30, 60, 90, and 120 K. For ortho- $SiC_2$ , we accounted for 40 energy levels and the calculations are done for the kinetic temperatures 25, 50, 75, 100, and 125 K. The results are reported here for the transitions in the upward direction. The values for the downward direction can easily be calculated with the help of the detailed equilibrium equation.

**Key words:** ISM: interstellar molecules — molecular data

## 1. Introduction

Since in most regions of interstellar space the excitation of molecules (and atoms) deviates strongly from that under LTE conditions, a quantitative interpretation of observed interstellar molecular lines requires the simultaneous solution of the set of rate equations and the radiative transfer equation for a large number of lines. (In the rate equations one has to account for many more lines than are usually observed.) If all lines of the molecule under consideration are optically thin, the problem reduces to the solution of the - then linear - rate equations. The rate equations describe the interplay between radiative and collisional

transitions and the solution yields the relative occupation numbers from which the line intensities follow. As input parameters one has to know the radiative and the collisional transition probabilities. While for purely rotational transitions the radiative transition probabilities are known for many molecules, the collisional rate coefficients present a problem in most cases. Since in interstellar molecular clouds hydrogen is predominantly in the form of  $H_2$ , one usually considers only collisions with  $H_2$  molecules. To reduce the complexity of the problem one accounts in most cases only for  $H_2$  molecules in the rotational ground state ( $J = 0$ ). To simplify the problem even further, one often considers collisions with He atoms assuming that the rate coefficients for collisions with  $H_2$  may be obtained from the results for He by rescaling the latter accounting for the difference of the reduced mass. - In actual NLTE calculations one has to account for a large number of energy levels, which is possible only if the corresponding collisional rate coefficients are known. The goal of such computations is to determine the physical parameters in molecular clouds, in particular the temperature and the density. This requires that the rate coefficients are known for a sufficiently large range of temperatures.

The calculation of the collisional rate coefficients is a difficult task, and the situation becomes even more difficult for the case of an asymmetrical top molecule colliding with  $H_2$  molecules. In the present investigation, we have accounted for the collisional transitions between the rotational energy levels in  $C_3H_2$  and  $SiC_2$  molecules, extending previous work by Green et al. (1987) and Palma & Green (1987).

## 2. Wave-functions for an asymmetrical top molecule

In an asymmetrical top molecule, all the three moments of inertia about the three principal inertial axes,  $a$ ,  $b$  and  $c$ , are unequal to one another. The axes are designated as  $a$ ,  $b$  and  $c$  so that the moments of inertia about them satisfy the condition:  $I_a < I_b < I_c$ . Obviously, an asymmetrical

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\* Tables 3A, 3B, 3C, 3D, 4A, 4B, 4C, 4D, 5A, 5B, 5C, 5D and 5E are available only in electronic form via anonymous ftp (130.79.128.5) at the CDS to cdsarc.u-strasbg.fr or via <http://cdsweb.u-strasbg.fr/Abstract.html>

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**Table 1. A)** Wave-functions for ortho levels of C<sub>3</sub>H<sub>2</sub>

No.	Level	$E(\text{cm}^{-1})$	$\epsilon_{J\tau}$	$g_{J\tau}^1$	$g_{J\tau}^3$	$g_{J\tau}^5$	$g_{J\tau}^7$	$g_{J\tau}^9$	$g_{J\tau}^{11}$
1	1 <sub>01</sub>	1.633	-	-0.707107					
2	1 <sub>10</sub>	2.245	+	0.707107					
3	2 <sub>12</sub>	4.480	-	-0.707107					
4	2 <sub>21</sub>	6.315	+	0.707107					
5	3 <sub>03</sub>	8.387	-	-0.676228	0.206677				
6	3 <sub>12</sub>	11.155	+	0.483241	-0.516216				
7	3 <sub>21</sub>	12.626	-	-0.206677	-0.676228				
8	4 <sub>14</sub>	13.419	-	-0.651603	0.274615				
9	3 <sub>30</sub>	13.530	+	0.516216	0.483241				
10	4 <sub>23</sub>	17.347	+	0.426209	-0.564221				
11	5 <sub>05</sub>	19.568	-	-0.629935	0.316322	-0.055880			
12	4 <sub>32</sub>	20.204	-	-0.274615	-0.651603				
13	4 <sub>41</sub>	22.394	+	0.564221	0.426209				
14	5 <sub>14</sub>	24.616	+	0.371915	-0.574031	0.179351			
15	6 <sub>16</sub>	26.834	-	-0.611098	0.343724	-0.091722			
16	5 <sub>23</sub>	28.511	-	-0.291406	-0.511000	0.392380			
17	5 <sub>32</sub>	31.083	+	0.344116	0.030181	-0.616987			
18	5 <sub>41</sub>	32.489	-	-0.135148	-0.372585	-0.585590			
19	6 <sub>25</sub>	33.006	+	0.331431	-0.567582	0.260776			
20	5 <sub>50</sub>	34.045	+	0.493217	0.411797	0.295229			
21	7 <sub>07</sub>	35.217	-	-0.594594	0.362415	-0.121998	0.015160		
22	6 <sub>34</sub>	38.044	-	-0.309498	-0.423776	0.473946			
23	6 <sub>43</sub>	41.962	+	0.366852	-0.062054	-0.601306			
24	7 <sub>16</sub>	42.513	+	0.299686	-0.553473	0.317154	-0.057179		
25	8 <sub>18</sub>	44.717	-	-0.580000	0.375444	-0.147684	0.028826		
26	6 <sub>52</sub>	44.976	-	-0.175415	-0.449741	-0.516684			
27	6 <sub>61</sub>	47.731	+	0.505543	0.417133	0.265380			
28	7 <sub>25</sub>	48.675	-	-0.318245	-0.345014	0.507768	-0.147840		
29	8 <sub>27</sub>	53.136	+	0.274154	-0.536222	0.356831	-0.099888		
30	7 <sub>34</sub>	53.688	+	0.336546	-0.148211	-0.521837	0.304065		
31	9 <sub>09</sub>	55.334	-	-0.566976	0.384631	-0.169517	0.042949	-0.004117	
32	7 <sub>43</sub>	57.440	-	-0.177015	-0.387188	-0.223015	0.518667		
33	7 <sub>52</sub>	59.706	+	0.261749	0.082995	-0.213490	-0.615647		
34	8 <sub>36</sub>	60.423	-	-0.323060	-0.279038	0.514355	-0.230670		
35	7 <sub>61</sub>	61.383	-	-0.117659	-0.315762	-0.421369	-0.457054		
36	7 <sub>70</sub>	63.933	+	0.477925	0.405972	0.285519	0.158914		
37	9 <sub>18</sub>	64.877	+	0.253141	-0.517977	0.384735	-0.138890	0.017558	
38	8 <sub>45</sub>	66.571	+	0.314342	-0.208485	-0.442017	0.402920		
39	10 <sub>1,10</sub>	67.068	-	-0.555254	0.391121	-0.188132	0.056975	-0.008766	
40	8 <sub>54</sub>	71.575	-	-0.202218	-0.391675	-0.095246	0.544634		
41	9 <sub>27</sub>	73.287	-	-0.325373	-0.223583	0.505360	-0.293416	0.051595	
42	8 <sub>63</sub>	75.524	+	0.319063	0.063310	-0.303806	-0.549447		
43	10 <sub>29</sub>	77.734	+	0.235518	-0.499801	0.404154	-0.173678	0.035017	
44	8 <sub>72</sub>	78.873	-	-0.135426	-0.357449	-0.452279	-0.386437		
45	11 <sub>0,11</sub>	79.919	-	-0.544627	0.395670	-0.204065	0.070554	-0.014334	0.001118
46	9 <sub>36</sub>	80.560	+	0.293570	-0.250434	-0.360834	0.454239	-0.120688	
47	8 <sub>81</sub>	82.372	+	0.473527	0.406192	0.291538	0.160579		

top molecule has no preferential axis, and therefore the treatment of the molecule can be done in six different representations (Chandra 1987). The rotational energy levels in an asymmetrical top molecule may be represented by  $J_\tau$  or  $J_{k_a, k_c}$ , where  $\tau$ ,  $k_a$  and  $k_c$  are sub-quantum numbers and are related through the relations:

$$\tau = k_a - k_c$$

and

$$k_a = \text{Int}\left[\frac{J + \tau + 1}{2}\right] \quad k_c = \text{Int}\left[\frac{J - \tau + 1}{2}\right].$$

Thus,  $\tau$  can assume an integer value ranging from  $-J$  to  $+J$ . However,  $k_a$  and  $k_c$  can, independently, assume positive integer values ranging from 0 to  $J$ . In case of a planar asymmetrical top molecule, the electric dipole of the molecule lies in the  $ab$ -plane. When the electric dipole

**Table 1. B)** Wave-functions for ortho levels of C<sub>3</sub>H<sub>2</sub>

No.	Level	$E(\text{cm}^{-1})$	$\epsilon_{J\tau}$	$g_{J\tau}^0$	$g_{J\tau}^2$	$g_{J\tau}^4$	$g_{J\tau}^6$	$g_{J\tau}^8$	$g_{J\tau}^{10}$
1	0 <sub>00</sub>	0.000	+	1.000000					
2	1 <sub>11</sub>	1.729	+	1.000000					
3	2 <sub>02</sub>	4.468	+	0.827119	-0.397413				
4	2 <sub>11</sub>	6.027	-	0.000000	-0.707107				
5	2 <sub>20</sub>	6.747	+	0.562027	0.584861				
6	3 <sub>13</sub>	8.389	+	0.766296	-0.454307				
7	3 <sub>22</sub>	11.215	-	0.000000	-0.707107				
8	3 <sub>31</sub>	13.201	+	0.642488	0.541853				
9	4 <sub>04</sub>	13.419	+	0.718896	-0.479649	0.107382			
10	4 <sub>13</sub>	17.340	-	0.000000	-0.635216	0.310645			
11	5 <sub>15</sub>	19.568	+	0.683173	-0.490823	0.160406			
12	4 <sub>22</sub>	20.032	+	0.470746	0.222275	-0.582917			
13	4 <sub>31</sub>	21.441	-	0.000000	-0.310645	-0.635216			
14	4 <sub>40</sub>	22.621	+	0.511455	0.469606	0.385586			
15	5 <sub>24</sub>	24.617	-	0.000000	-0.584861	0.397413			
16	6 <sub>06</sub>	26.834	+	0.654761	-0.494988	0.199460	-0.029101		
17	5 <sub>33</sub>	28.538	+	0.487527	0.143014	-0.600588			
18	5 <sub>42</sub>	31.454	-	0.000000	-0.397413	-0.584861			
19	6 <sub>15</sub>	33.006	-	0.000000	-0.539835	0.445198	-0.101869		
20	5 <sub>51</sub>	33.902	+	0.543684	0.488507	0.336993			
21	7 <sub>17</sub>	35.217	+	0.631379	-0.495423	0.229268	-0.051692		
22	6 <sub>24</sub>	38.042	+	0.467641	0.064532	-0.571815	0.243966		
23	6 <sub>33</sub>	41.885	-	0.000000	-0.390129	-0.367525	0.461221		
24	7 <sub>26</sub>	42.513	-	0.000000	-0.501251	0.471081	-0.163799		
25	6 <sub>42</sub>	44.304	+	0.325435	0.207486	-0.110560	-0.625917		
26	8 <sub>08</sub>	44.717	+	0.611633	-0.493777	0.252481	-0.072993	0.007900	
27	6 <sub>51</sub>	45.793	-	0.000000	-0.237439	-0.408319	-0.52621		
28	6 <sub>60</sub>	47.814	+	0.496682	0.455820	0.347879	0.218773		
29	7 <sub>35</sub>	48.675	+	0.452248	0.007015	-0.530786	0.340519		
30	8 <sub>17</sub>	53.136	-	0.000000	-0.468041	0.483902	-0.213926	0.031800	
31	7 <sub>44</sub>	53.698	-	0.000000	-0.407106	-0.252299	0.520202		
32	9 <sub>19</sub>	55.334	+	0.594622	-0.490941	0.270828	-0.092671	0.015947	
33	7 <sub>53</sub>	57.623	+	0.386067	0.211407	-0.205920	-0.581705		
34	8 <sub>26</sub>	60.423	+	0.438239	-0.036789	-0.484223	0.400509	-0.087982	
35	7 <sub>62</sub>	60.778	-	0.000000	-0.288119	-0.463064	-0.450066		
36	7 <sub>71</sub>	63.886	+	0.497780	0.458054	0.351140	0.207351		
37	9 <sub>28</sub>	64.877	-	0.000000	-0.439270	0.488639	-0.254398	0.059624	
38	8 <sub>35</sub>	66.570	-	0.000000	-0.405374	-0.146845	0.525963	-0.193574	
39	10 <sub>0,10</sub>	67.068	+	0.579734	-0.487425	0.285498	-0.110612	0.024943	-0.002146
40	8 <sub>44</sub>	71.545	+	0.370380	0.158669	-0.278315	-0.445159	0.361396	
41	9 <sub>37</sub>	73.287	+	0.425919	-0.070707	-0.437671	0.436124	-0.150122	
42	8 <sub>53</sub>	75.155	-	0.000000	-0.261843	-0.328501	-0.0866310	0.562157	
43	8 <sub>62</sub>	77.309	+	0.262033	0.181832	-0.026777	-0.288719	-0.590365	
44	10 <sub>19</sub>	77.734	-	0.000000	-0.414146	0.488263	-0.286888	0.087661	-0.009638
45	8 <sub>71</sub>	79.290	-	0.000000	-0.219197	-0.369272	-0.412424	-0.381442	
46	11 <sub>1,11</sub>	79.919	+	0.566537	-0.483534	0.297340	-0.126851	0.034461	-0.004794
47	9 <sub>46</sub>	80.561	-	0.000000	-0.399157	-0.061842	0.502292	-0.290778	
48	8 <sub>80</sub>	82.397	+	0.477503	0.443387	0.351575	0.229650	0.114276	

of the molecule is along the  $a$ -axis of inertia, the molecule is known as  $a$ -type asymmetrical top molecule, and when it is along the  $b$ -axis of inertia, the molecule is said to be  $b$ -type asymmetrical top molecule. In case the electric dipole lies in between the  $a$  and  $b$  axes, it can be resolved into two components along the two axes, and such molecule has both  $a$  and  $b$  type transitions. In an  $a$ -type asymmetrical

top molecule, the rotational energy levels are grouped into two distinct categories:

$(k_a, k_c)$ : (odd, even) or (odd, odd) one category  
(even, even) or (even, odd) another category

**Table 2.** Wave-functions for ortho levels of SiC<sub>2</sub>

No.	Level	$E(\text{cm}^{-1})$	$\epsilon_{J\tau}$	$g_{J\tau}^0$	$g_{J\tau}^2$	$g_{J\tau}^4$	$g_{J\tau}^6$	$g_{J\tau}^8$	$g_{J\tau}^{10}$
1	0 <sub>00</sub>	0.000	+	1.000000					
2	1 <sub>01</sub>	0.787	+	1.000000					
3	2 <sub>02</sub>	2.357	+	0.999583	0.020428				
4	3 <sub>03</sub>	4.701	+	0.997932	0.045452				
5	2 <sub>21</sub>	7.788	-	0.000000	-0.707107				
6	2 <sub>20</sub>	7.793	+	0.028889	-0.706812				
7	4 <sub>04</sub>	7.805	+	0.993927	0.077808	0.000857			
8	3 <sub>22</sub>	10.148	-	0.000000	-0.707107				
9	3 <sub>21</sub>	10.171	+	0.064278	-0.705644				
10	5 <sub>05</sub>	11.654	+	0.986385	0.116259	0.002504			
11	4 <sub>23</sub>	13.292	-	0.000000	-0.707030	-0.010411			
12	4 <sub>22</sub>	13.359	+	0.110043	-0.702736	-0.010391			
13	6 <sub>06</sub>	16.230	+	0.974474	0.158655	0.005368	0.000040		
14	5 <sub>24</sub>	17.216	-	0.000000	-0.706812	-0.020428			
15	5 <sub>23</sub>	17.370	+	0.164448	-0.697183	-0.020343			
16	7 <sub>07</sub>	21.517	+	0.958119	0.202263	0.009672	0.000136		
17	6 <sub>25</sub>	21.917	-	0.000000	-0.706371	-0.032245	-0.000273		
18	6 <sub>24</sub>	22.218	+	0.224483	-0.688316	-0.032014	-0.000273		
19	7 <sub>26</sub>	27.389	-	0.000000	-0.705615	-0.045896	-0.000732		
20	8 <sub>08</sub>	27.502	+	0.938122	0.244385	0.015471	0.000330	1.87D-06	
21	7 <sub>25</sub>	27.913	+	0.286321	-0.675978	-0.045430	-0.000733		
22	4 <sub>41</sub>	29.574	-	0.000000	-0.010411	0.707030			
23	4 <sub>40</sub>	29.574	+	0.000413	-0.010422	0.707030			
24	5 <sub>42</sub>	33.512	-	0.000000	-0.020428	0.706812			
25	5 <sub>41</sub>	33.512	+	0.001238	-0.020478	0.706810			
26	8 <sub>27</sub>	33.629	-	0.000000	-0.704441	-0.061322	-0.001491	-9.08D-06	
27	9 <sub>09</sub>	34.179	+	0.915870	0.282980	0.022653	0.000664	6.90D-06	
28	8 <sub>26</sub>	34.463	+	0.346182	-0.660609	-0.060603	-0.001503	-9.24D-06	
29	6 <sub>43</sub>	38.240	-	0.000000	-0.032246	0.706306	0.009593		
30	6 <sub>42</sub>	38.240	+	0.002769	-0.032403	0.706296	0.009593		
31	9 <sub>28</sub>	40.631	-	0.000000	-0.702740	-0.078416	-0.002640	-0.000030	
32	10 <sub>0,10</sub>	41.543	+	0.892835	0.316956	0.030999	0.001178	0.000018	-2.89D-08
33	9 <sub>27</sub>	41.868	+	0.401203	-0.643029	-0.077622	-0.002690	-0.000031	
34	7 <sub>44</sub>	43.761	-	0.000000	-0.045900	0.705384	0.018054		
35	7 <sub>43</sub>	43.761	+	0.005302	-0.046300	0.705348	0.018054		
36	10 <sub>29</sub>	48.387	-	0.000000	-0.700406	-0.097022	-0.004268	-0.000072	-3.44D-07
37	11 <sub>0,11</sub>	49.594	+	0.870196	0.346057	0.040250	0.001905	0.000040	3.47D-07
38	8 <sub>45</sub>	50.076	-	0.000000	-0.061334	0.703903	0.027556	0.000210	
39	8 <sub>44</sub>	50.078	+	0.009185	-0.062220	0.703795	0.027554	0.000210	
40	10 <sub>28</sub>	50.125	+	0.449816	-0.624074	-0.096670	-0.004429	-0.000076	-4.11D-07

whereas in a *b*-type asymmetrical top molecule, the rotational energy levels are grouped into the following two categories:

$(k_a, k_c)$ : (even, odd) or (odd, even) one category  
 (even, even) or (odd, odd) another category

This grouping of energy levels is independent of the aforesaid representations. Spectroscopists generally use *I*<sup>r</sup> representation in which the *a*-axis of inertia is used as the preferential direction (Sharma & Chandra 1996; Chandra & Rashmi 1998). However, for calculations of the collisional rate coefficients, the direction of the electric

dipole of the molecule is generally taken as the preferential direction (Green et al. 1987; Palma & Green 1987). Consequently, for collisional transitions in an *a*-type asymmetrical top molecule, one has to use *I*<sup>r</sup> representation, whereas in the *b*-type asymmetrical top molecule, one has to use *II*<sup>r</sup> representation.

Rotational wave-functions for an asymmetric top molecule can be expressed as linear combinations of wave-functions for a symmetric top molecule (Chandra & Rashmi 1998; Chandra et al. 1984):

$$\psi_{J\tau M}(\alpha, \beta, \gamma) = \sqrt{\frac{2J+1}{8\pi^2}} \sum_{K=-J}^J g_{J\tau}^K D_{MK}^J(\alpha, \beta, \gamma).$$

Values of the expansion coefficients  $g_{J\tau}^K$  depend on the representation (Chandra 1987). The  $C_3H_2$  is a  $b$ -type asymmetrical top molecule, and therefore  $II'$  representation is used. We have accounted for 47 and 48 rotational energy levels for ortho- and para- $C_3H_2$ , and for the rotational constants for the molecule,  $A = 35092.508332$  MHz,  $B = 32212.946832$  MHz, and  $C = 16749.028632$  MHz, the wave-functions are given in Tables 1A and 1B, respectively. The  $SiC_2$  is an  $a$ -type asymmetrical top molecule, and therefore  $I'$  representation is used. For ortho- $SiC_2$ , we have accounted for 40 rotational energy levels, and for the rotational constants for the molecule,  $A = 52473.6664$  MHz,  $B = 13158.65426$  MHz, and  $C = 10441.61928$  MHz, the wave-functions for one category are given in Table 2. The wave-functions for the second category of  $SiC_2$  are not reported here as these levels do not exist due to the spin statistics for the identical carbon nuclei. The coefficients with negative value of  $K$  are related to those with positive value of  $K$  through the relation

$$g_{J\tau}^{-K} = \epsilon_{J\tau} g_{J\tau}^K$$

where the value of  $\epsilon_{J\tau}$  for the levels is given in the table for wave-functions. Thus, the coefficients with negative value of  $K$  can be obtained.

### 3. Collisional rate coefficients

Collisional rate coefficient for the rotational transition  $J\tau \rightarrow J'\tau'$  at kinetic temperature  $T$ , averaged over the Maxwellian distribution is given by

$$C(J\tau \rightarrow J'\tau'|T) = \left(\frac{8kT}{\pi\mu}\right)^{1/2} \left(\frac{1}{kT}\right)^2 \int_0^\infty \sigma(J\tau \rightarrow J'\tau'|E) E e^{-E/kT} dE$$

where the cross section  $\sigma(J\tau \rightarrow J'\tau'|E)$  for the transition is given by

$$\sigma(J\tau \rightarrow J'\tau'|E) = (2J' + 1) \sum_{LMM'} S(J, \tau, J', \tau'|L, M, M') q(L, M, M'|E).$$

Here, the sum is finite, limited by triangle inequalities on  $J$ ,  $J'$  and  $L$ , and each of  $M$  and  $M'$  can independently assume the values ranging from  $-L$  to  $+L$ . The interaction potential is expressed in terms of spherical harmonics, and therefore, the scattering cross section is expressed here in terms of a parameter  $q(L, M, M'|E)$  (Hutson & Green 1995). The spectroscopic coefficients,  $S(J, \tau, J', \tau'|L, M, M')$ , depend on the wave-functions of the molecule and on angular momentum coupling factors:

$$S(J, \tau, J', \tau'|L, M, M') = \sum_{p, p', q, q'} g_{J\tau}^p g_{J\tau}^q g_{J'\tau'}^{p'} g_{J'\tau'}^{q'} (-1)^{p'+q'} \begin{pmatrix} J & L & J' \\ -p & M & p' \end{pmatrix} \begin{pmatrix} J & L & J' \\ -q & M' & q' \end{pmatrix}.$$

**Table 3. A)** Collisional rate coefficient ( $\text{cm}^3 \text{s}^{-1}$ ) for transitions in ortho- $C_3H_2$  at 30 K

Transition	Rate	$l$	$u$
1(0, 1) $\Rightarrow$ 1(1, 0)	7.800D-12	1	2
1(0, 1) $\Rightarrow$ 2(1, 2)	3.041D-11	1	3
1(0, 1) $\Rightarrow$ 2(2, 1)	1.666D-11	1	4
1(0, 1) $\Rightarrow$ 3(0, 3)	3.489D-12	1	5
1(1, 0) $\Rightarrow$ 2(1, 2)	2.409D-12	2	3
1(1, 0) $\Rightarrow$ 2(2, 1)	1.143D-11	2	4
1(1, 0) $\Rightarrow$ 3(0, 3)	4.431D-11	2	5
2(1, 2) $\Rightarrow$ 2(2, 1)	1.217D-11	3	4
2(1, 2) $\Rightarrow$ 3(0, 3)	9.661D-12	3	5

These spectroscopic coefficients are obviously independent of collision dynamics. Thus, the rate coefficient is given by

$$C(J\tau \rightarrow J'\tau'|E) = (2J' + 1) \sum_{LMM'} S(J, \tau, J', \tau'|L, M, M') Q(L, M, M'|T)$$

where

$$Q(L, M, M'|T) = \left(\frac{8kT}{\pi\mu}\right)^{1/2} \left(\frac{1}{kT}\right)^2 \int_0^\infty q(L, M, M'|E) E e^{-E/kT} dE.$$

Now, owing to symmetries of  $g_{J\tau}^K$ ,  $S(L, M, M') = S(L, M', M)$ , so that only the real part of  $Q(L, M, M')$  is required, and the cross sections are real. - Green et al. (1987) calculated the  $Q(L, M, M'|T)$  for  $C_3H_2$ . These calculations were based on a potential energy surface describing the interaction of  $C_3H_2$  with He and used the infinite order sudden approximation (IOSA) according to Green (1979). They derived the  $Q(L, M, M'|T)$  for  $L \leq 25$ ,  $M' \leq M \leq 8$  and  $T = 30, 60, 90$ , and  $120$  K. Despite the larger parameter space for which the  $Q(L, M, M'|T)$  were calculated, Green et al. give the state-to-state rate coefficients only for  $T = 60$  K and for transitions between the lowest 20 energy levels of ortho- $C_3H_2$  and the lowest 22 of para- $C_3H_2$ . - Similar calculations were performed by Palma & Green (1987) for  $SiC_2$ . They computed the  $Q(L, M, M'|T)$  for  $L \leq 25$ ,  $M' \leq M \leq 6$  and  $T = 25, 50, 75, 100$ , and  $125$  K. State-to-state coefficients were given only for  $T = 100$  K and for transitions between the lowest 18 energy levels.

As mentioned in the introduction, in astrophysical applications, i.e. for actual NLTE calculations, one needs to know the state-to-state rate coefficients for a large number of transitions in a sufficiently large range of temperatures. We therefore extended the work of Green et al. and Palma and Green, respectively, by using the  $Q(L, M, M'|T)$  computed by them to calculate state-to-state rate coefficients for an extended set of transitions and for all temperatures for which the  $Q(L, M, M'|T)$  were given.

#### 4. Results

The calculations are made for the upward transitions  $J\tau \rightarrow J'\tau'$ . For ortho- $\text{C}_3\text{H}_2$ , we accounted for 47 energy levels given in Table 1A. The calculations are done for the kinetic temperatures 30, 60, 90, and 120 K, and the results are presented in Tables 3A, 3B, 3C, and 3D, respectively. For para- $\text{C}_3\text{H}_2$ , we accounted for 48 energy levels given in Table 1B. For this case also, the calculations are done for the kinetic temperatures 30, 60, 90, and 120 K, and the results are presented in Tables 4A, 4B, 4C, and 4D, respectively. For ortho- $\text{SiC}_2$ , we accounted for 40 energy levels given in Table 2. The calculations are done for the kinetic temperatures 25, 50, 75, 100, and 125 K, and the results are presented in Tables 5A, 5B, 5C, 5D, and 5E, respectively. The rate coefficient for the corresponding downward transition  $J'\tau' \rightarrow J\tau$  can easily be calculated with the help of the detailed equilibrium equation

$$C(J'\tau' \rightarrow J\tau) = \frac{2J+1}{2J'+1} \exp\left[\frac{hc[E(J'\tau') - E(J\tau)]}{kT}\right] C(J\tau \rightarrow J'\tau')$$

where the energy  $E$  of the energy level is in  $\text{cm}^{-1}$ . The Tables 3A, 3B, 3C, 3D, 4A, 4B, 4C, 4D, 5A, 5B, 5C, 5D and 5E are available only in electronic form via anonymous ftp. However, a part of the Table 3A is given in printed

form in order to have the information about the content of the tables. There we have given (i) transition, (ii) collisional rate coefficient (in  $\text{cm}^3 \text{s}^{-1}$ ), (iii) lower energy level number( $l$ ) of the transition (according to the table of wave-functions), and (iv) upper energy level number( $u$ ) of the transition.

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