Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information: Methane dimer rovibrational states and Raman transition moments

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I. MOLECULAR SYMMETRY GROUP OF THE METHANE DIMER

TABLE I. Character table of the molecular symmetry group of the methane dimer. The table was generated using the GAP program according to instructions of Ref. [1].

G_{576}[a]	$\hat{E}$	(14)(23)	(14)(23)(58)(67)	(243)	(243)(58)(67)	(243)(687)	(234)(687)	(34)(78)(9,10)	(1423)(78)(9,10)	(1423)(5867)(9,10)	(15)(26)(37)(48)	(1548)(2637)	(15)(264837)	(15)(26)(38)(47)(9,10)	(1547)(2638)(9,10)	(15)(264738)(9,10)	
R[b]	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	
K_R[c]	1	6	9	16	48	32	32	36	72	36	12	36	96	12	36	96	$g_{\rm ns}$[d]
$X_1(1)$	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	15
$X_2(1)$	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	1	1	1	10
$X_3(1)$	1	1	1	1	1	1	1	−1	−1	−1	1	1	1	−1	−1	−1	15
$X_4(1)$	1	1	1	1	1	1	1	1	1	1	−1	−1	−1	−1	−1	−1	10
$X_5(2)$	2	2	2	−1	−1	2	−1	.	.	.	.	.	.	2	2	−1	1
$X_6(2)$	2	2	2	−1	−1	2	−1	.	.	.	.	.	.	−2	−2	1	1
$X_7(2)$	2	2	2	−1	−1	−1	2	.	.	.	−2	−2	1	.	.	.	0
$X_8(2)$	2	2	2	−1	−1	−1	2	.	.	.	2	2	−1	.	.	.	2
$X_9(2)$	4	4	4	1	1	−2	−2	.	.	.	.	.	.	.	.	.	10
$X_{10}(6)$	6	2	−2	3	−1	.	.	−2	.	2	.	.	.	.	.	.	15
$X_{11}(6)$	6	2	−2	3	−1	.	.	2	.	−2	.	.	.	.	.	.	15
$X_{12}(9)$	9	−3	1	.	.	.	.	−1	1	−1	−3	1	.	3	−1	.	3
$X_{13}(9)$	9	−3	1	.	.	.	.	−1	1	−1	3	−1	.	−3	1	.	6
$X_{14}(9)$	9	−3	1	.	.	.	.	1	−1	1	−3	1	.	−3	1	.	3
$X_{15}(9)$	9	−3	1	.	.	.	.	1	−1	1	3	−1	.	3	−1	.	6
$X_{16}(12)$	12	4	−4	−3	1	.	.	.	.	.	.	.	.	.	.	.	6

[a] Zero characters are labeled with "." to enhance readability.
[b] Class index.
[c] Number of elements in class Cl.[R].
[d] Spin statistical weight.

II. T_{d}(M) CHARACTER TABLE

TABLE II. Characters and irrep decomposition of the rotational functions of methane in the T_{d}(M) molecular symmetry group [2].

	E	(123)	(14)(23)	$[(1423)]^*$	$[(23)]^*$	Irreps
	1	8	3	6	6	
j_k^{M}	$2j^{\mathrm{M}}+1$	$\sum_{m=-j^{\mathrm{M}}}^{j^{\mathrm{M}}} D^{j^{\mathrm{M}}*}_{m,m}(0,0,\frac{2\pi}{3})$	$\sum_{m=-j^{\mathrm{M}}}^{j^{\mathrm{M}}} D^{j^{\mathrm{M}}*}_{m,m}(\frac{\pi}{3},\pi,0)$	$\sum_{m=-j^{\mathrm{M}}}^{j^{\mathrm{M}}} D^{j^{\mathrm{M}}*}_{m,m}(\frac{\pi}{6},\frac{\pi}{2},-\frac{\pi}{6})$	$\sum_{m=-j^{\mathrm{M}}}^{j^{\mathrm{M}}} D^{j^{\mathrm{M}}*}_{m,m}(0,\pi,0)$	
0	1	1	1	1	1	A_1
1	3	0	-1	1	-1	F_1
2	5	-1	1	-1	1	$\mathrm{E}\oplus\mathrm{F}_2$
3	7	1	-1	-1	-1	$\mathrm{A}_2\oplus\mathrm{F}_1\oplus\mathrm{F}_2$
4	9	0	1	1	1	$\mathrm{A}_1\oplus\mathrm{E}\oplus\mathrm{F}_1\oplus\mathrm{F}_2$
5	11	-1	-1	1	-1	$\mathrm{E}\oplus 2\mathrm{F}_1\oplus\mathrm{F}_2$

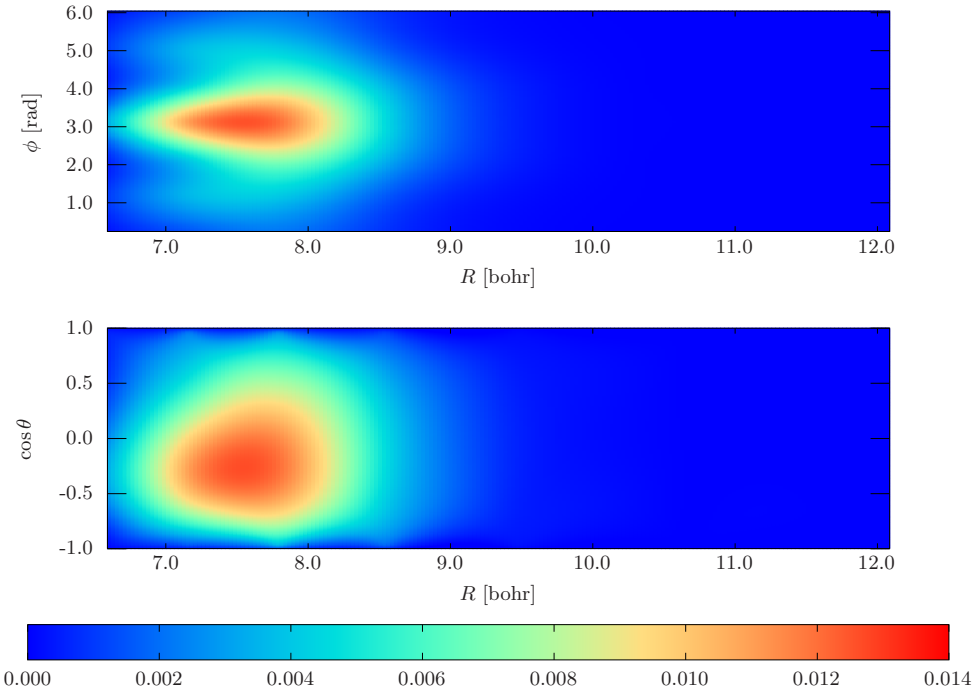

FIG. 1. 2D cut of the wave function of the ground state, $[1, 0]$, of the ortho-meta spin isomer corresponding to the J0.2 (from the 6-fold degenerate J0.2–7) state (Table V).

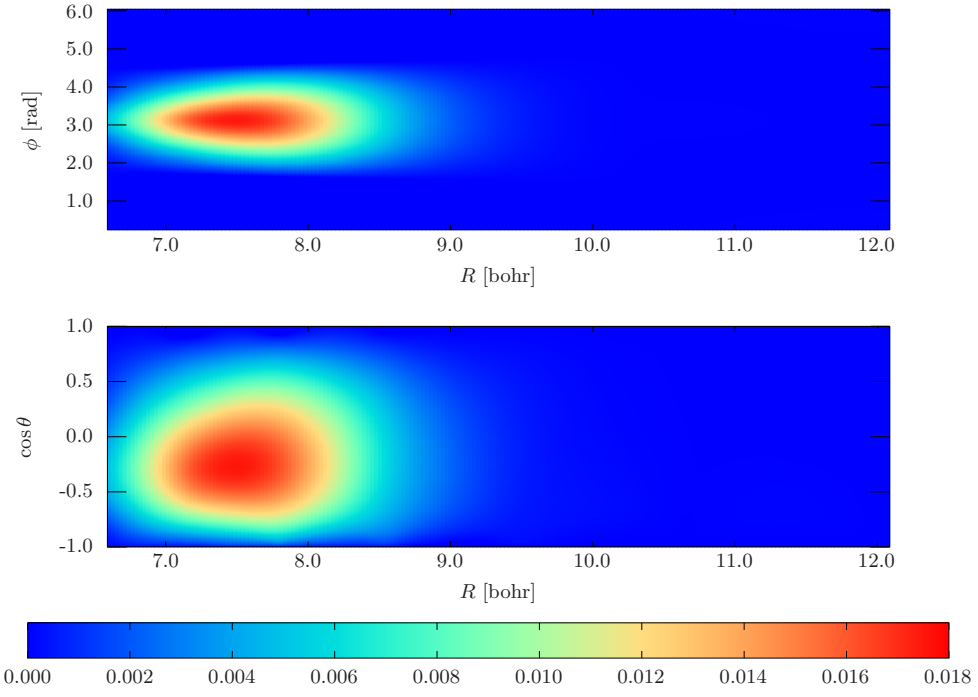

FIG. 2. 2D cut of the wave function of the ground state, $[1, 1]$, of the ortho-ortho spin isomer corresponding to the J0.8 (from the 9-fold degenerate J0.8–16) state (Table V).

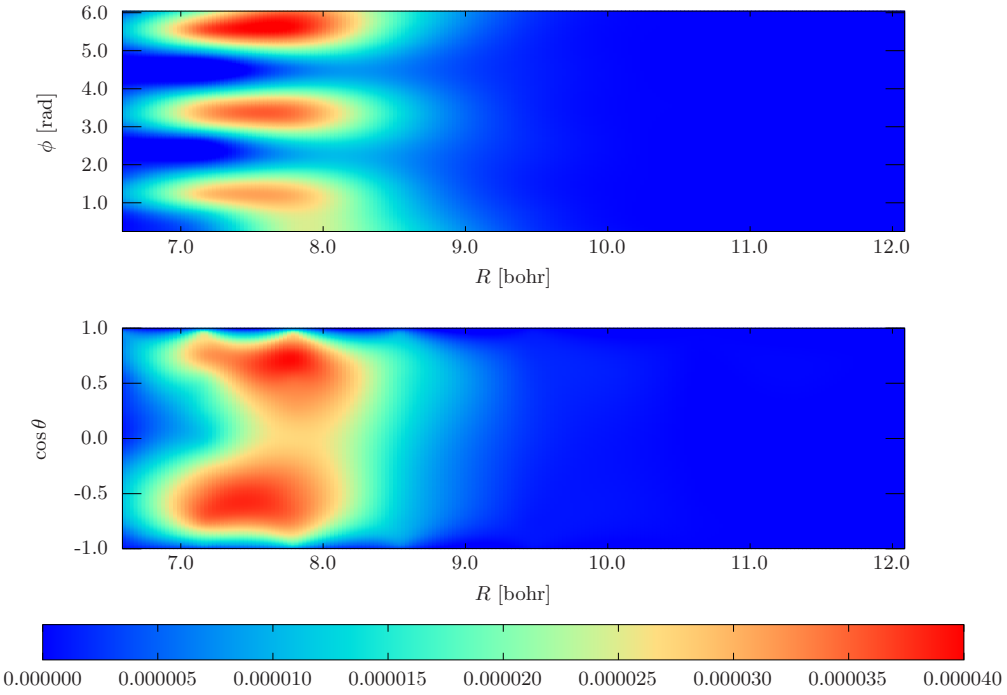

FIG. 3. 2D cut of the wave function of the ground state, $[2, 0]$, of the meta-para spin isomer corresponding to the J1.83 (from the 4-fold degenerate J1.83–86) state (Table V).

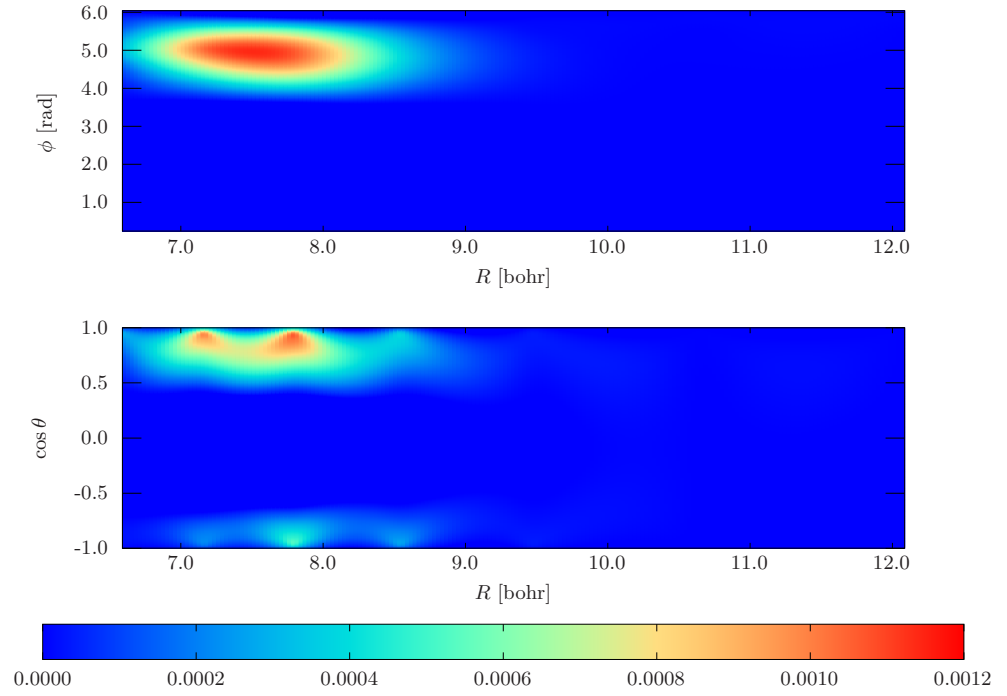

FIG. 4. 2D cut of the wave function of the ground state, $[2, 1]$, of the ortho-para spin isomer corresponding to the J1.93 (from the 12-fold degenerate J1.93–104) state (Table V).

TABLE III. $U^{(\Omega)}_{\omega\sigma,\alpha}$ matrix elements for $\Omega = 2$.

(ω,σ)	α:	xx	xy	xz	yy	yz	zz
(0,0)		$-\frac{1}{\sqrt{3}}$	0	0	$-\frac{1}{\sqrt{3}}$	0	$-\frac{1}{\sqrt{3}}$
(2,−2)		$\frac{1}{2}$	$-\frac{\mathrm{i}}{2}$	0	$-\frac{1}{2}$	0	0
(2,−1)		0	0	$\frac{1}{2}$	0	$-\frac{\mathrm{i}}{2}$	0
(2,0)		$-\frac{1}{\sqrt{6}}$	0	0	$-\frac{1}{\sqrt{6}}$	0	$\sqrt{\frac{2}{3}}$
(2,1)		0	0	$-\frac{1}{2}$	0	$-\frac{\mathrm{i}}{2}$	0
(2,2)		$\frac{1}{2}$	$\frac{\mathrm{i}}{2}$	0	$-\frac{1}{2}$	0	0

TABLE IV. $[U^{(\Omega)}_{\omega\sigma,\alpha}]^{-1}$ matrix elements for $\Omega = 2$.

α	(ω,σ):	(0,0)	(2,−2)	(2,−1)	(2,0)	(2,1)	(2,2)
xx		$-\frac{1}{\sqrt{3}}$	$\frac{1}{2}$	0	$-\frac{1}{\sqrt{6}}$	0	$\frac{1}{2}$
xy		0	$\frac{\mathrm{i}}{2}$	0	0	0	$-\frac{\mathrm{i}}{2}$
xz		0	0	$\frac{1}{2}$	0	$\frac{1}{2}$	0
yy		$-\frac{1}{\sqrt{3}}$	$-\frac{1}{2}$	0	$-\frac{1}{\sqrt{6}}$	0	$-\frac{1}{2}$
yz		0	0	$\frac{\mathrm{i}}{2}$	0	$\frac{\mathrm{i}}{2}$	0
zz		$-\frac{1}{\sqrt{3}}$	0	0	$\sqrt{\frac{2}{3}}$	0	0

TABLE V. Computed $J = 0$ and $J = 1$ rovibrational states of the $(CH_4)_2$. The energies are referenced to the ZPVE (94.25 cm^{-1}).

Label	$\tilde{\nu}$ [cm^{-1}]	Assignment	Symm.	Label	$\tilde{\nu}$ [cm^{-1}]	Assignment	Symm.
$J0.n$				$J1.n$			
1	0.00	$[[0,0]_0,0]_{00}$	$X_1(1)$	1	0.24	$[[0,0]_0,1]_{10}$	$X_2(1)$
2–7	8.99	$[[1,0]_1,1]_{00}$	$X_{11}(6)$	2–7	9.12	$[[1,0]_1,0]_{10}$	$X_{10}(6)$
8–16	18.04	$[[1,1]_L,L]_{00}$ $(L=0,2)$	$X_{15}(9)$	8–13	9.80	$[[1,0]_1,1]_{10}$	$X_{11}(6)$
17–25	19.32	$[[1,1]_1,1]_{00}$	$X_{12}(9)$	14–19	9.91	$[[1,0]_1,2]_{10}$	$X_{10}(6)$
26–34	19.37	$[[1,1]_L,L]_{00}$ $(L=0,2)$	$X_{15}(9)$	20–28	18.10	$[[1,1]_0,1]_{10}$	$X_{12}(9)$
35–40	31.43	$[[2,0]_2,2]_{00}$	$X_{11}(6)$	29–37	18.65	$[[1,1]_1,0]_{10}$	$X_{15}(9)$
41–44	31.73	$[[2,0]_2,2]_{00}$	$X_9(2)$	38–46	18.74	$[[1,1]_2,1]_{10}$	$X_{12}(9)$
45–56	32.17	$[[2,1]_L,L]_{00}$ $(L=1,2,3)$	$X_{16}(12)$	47–55	18.90	$[[1,1]_1,2]_{10}$	$X_{15}(9)$
57	32.93	$[[0,0]_0,0]_{00}$	$X_1(1)$	56–64	18.95	$[[1,1]_1,1]_{10}$	$X_{12}(9)$
58–66	38.44	$[[2,1]_3,3]_{00}$	$X_{14}(9)$	65–73	19.64	$[[1,1]_2,2]_{10}$	$X_{15}(9)$
67–75	38.88	$[[2,1]_1,1]_{00}$	$X_{15}(9)$	74–82	19.74	$[[1,1]_2,3]_{10}$	$X_{12}(9)$
76–84	40.47	$[[2,1]_2,2]_{00}$	$X_{12}(9)$	83–86	22.52	$[[2,0]_2,L]_{10}$ $(L=1,2,3)$	$X_9(2)$
85–96	40.52	$[[2,1]_L,L]_{00}$ $(L=1,2,3)$	$X_{16}(12)$	87–92	31.29	$[[2,0]_2,1]_{10}$	$X_{10}(6)$
97–105	42.19	$[[2,1]_2,2]_{00}$	$X_{12}(9)$	93–104	31.67	$[[2,1]_j,\Lambda]_{10}$ (mixed)	$X_{16}(12)$
106–114	42.43	$[[2,1]_1,1]_{00}$	$X_{14}(9)$	105–110	31.82	$[[2,0]_2,2]_{10}$	$X_{11}(6)$
115–123	43.57	$[[2,1]_3,3]_{00}$	$X_{15}(9)$	111–114	31.97	$[[2,0]_2,L]_{10}$ $(L=1,2,3)$	$X_9(2)$
124–129	45.14	$[[1,0]_1,1]_{00}$	$X_{11}(6)$	115–120	32.20	$[[2,0]_2,3]_{10}$	$X_{10}(6)$
				121–132	32.45	$[[2,1]_j,\Lambda]_{10}$ (mixed)	$X_{16}(12)$
				133	33.15	$[[0,0]_0,1]_{10}$	$X_2(1)$

TABLE VI. Computed $J = 2$ and $J = 3$ rovibrational states of the $(CH_4)_2$. The energies are referenced to the ZPVE (94.25 cm^{-1}).

Label	$\tilde{\nu}$ [cm^{-1}]	Assignment	Symm.	Label	$\tilde{\nu}$ [cm^{-1}]	Assignment	Symm.
$J2.n$				$J3.n$			
1	0.73	$[[0,0]_0,2]_{20}$	$X_1(1)$	1	1.49	$[[0,0]_0,3]_{30}$	$X_2(1)$
2–7	9.44	$[[1,0]_1,1]_{20}$	$X_{11}(6)$	2–7	10.00	$[[1,0]_1,2]_{30}$	$X_{10}(6)$
8–13	10.29	$[[1,0]_1,2]_{20}$	$X_{10}(6)$	8–13	11.02	$[[1,0]_1,3]_{30}$	$X_{11}(6)$
14–19	10.55	$[[1,0]_1,3]_{20}$	$X_{11}(6)$	14–19	11.46	$[[1,0]_1,4]_{30}$	$X_{10}(6)$
20–28	18.28	$[[1,1]_2,0]_{20}$	$X_{15}(9)$	20–28	18.66	$[[1,1]_2,1]_{30}$	$X_{12}(9)$
29–37	19.01	$[[1,1]_1,1]_{20}$	$X_{12}(9)$	29–37	19.58	$[[1,1]_2,2]_{30}$	$X_{15}(9)$
38–46	19.10	$[[1,1]_2,1]_{20}$	$X_{12}(9)$	38–46	19.61	$[[1,1]_1,2]_{30}$	$X_{15}(9)$
47–55	19.22	$[[1,1]_0,2]_{20}$	$X_{15}(9)$	47–55	19.95	$[[1,1]_0,3]_{30}$	$X_{12}(9)$
56–64	19.31	$[[1,1]_1,2]_{20}$	$X_{15}(9)$	56–64	20.00	$[[1,1]_1,3]_{30}$	$X_{12}(9)$
65–73	19.80	$[[1,1]_2,2]_{20}$	$X_{15}(9)$	65–73	20.57	$[[1,1]_2,3]_{30}$	$X_{12}(9)$
74–82	19.92	$[[1,1]_1,3]_{20}$	$X_{12}(9)$	74–82	20.58	$[[1,1]_2,4]_{30}$	$X_{15}(9)$
83–91	20.27	$[[1,1]_2,3]_{20}$	$X_{12}(9)$	83–91	21.16	$[[1,1]_1,4]_{30}$	$X_{15}(9)$
92–100	20.50	$[[1,1]_2,4]_{20}$	$X_{15}(9)$	92–100	21.58	$[[1,1]_2,5]_{30}$	$X_{12}(9)$
101–104	22.98	$[[2,0]_2,L]_{20}$ $(L=0,1,2,3,4)$	$X_9(2)$	101–104	23.66	$[[2,0]_2,L]_{30}$ $(L=1,2,4)$	$X_9(2)$
105–108	26.68	$[[2,0]_2,L]_{20}$ $(L=0,1,2,3,4)$	$X_9(2)$	105–108	27.40	$[[2,0]_2,L]_{30}$ $(L=2,3)$	$X_9(2)$
109–114	29.86	$[[2,0]_2,0]_{20}$	$X_{11}(6)$	109–114	30.46	$[[2,0]_2,1]_{30}$	$X_{10}(6)$
115–120	29.87	$[[2,0]_2,1]_{20}$	$X_{10}(6)$	115–120	30.50	$[[2,0]_2,2]_{30}$	$X_{11}(6)$
121–126	31.54	$[[2,0]_2,2]_{20}$	$X_{11}(6)$	121–126	32.03	$[[2,0]_2,3]_{30}$	$X_{10}(6)$
127–138	31.93	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{16}(12)$	127–138	32.40	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{16}(12)$
139–144	32.38	$[[2,0]_2,3]_{20}$	$X_{10}(6)$	139–142	33.14	$[[2,0]_2,L]_{30}$ $(L=1,3,5)$	$X_9(2)$
145–148	32.42	$[[2,0]_2,4]_{20}$	$X_9(2)$	143–148	33.20	$[[2,0]_2,4]_{30}$	$X_{11}(6)$
149–160	32.54	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{16}(12)$	149–160	33.27	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{16}(12)$
161–172	33.04	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{16}(12)$	161	33.85	$[[0,0]_0,3]_{30}$	$X_2(1)$
173–178	33.06	$[[2,0]_2,4]_{20}$	$X_{11}(6)$	162–173	33.87	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{16}(12)$
179	33.19	$[[0,0]_0,2]_{20}$	$X_1(1)$	174–179	34.13	$[[2,0]_2,5]_{30}$	$X_{10}(6)$
180–191	35.72	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{16}(12)$	180–191	36.12	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{16}(12)$
192–195	36.02	$[[2,0]_2,L]_{20}$ $(L=0,1,2)$	$X_9(2)$	192–195	36.75	$[[2,0]_2,L]_{30}$ $(L=1,2,3)$	$X_9(2)$
196–207	36.74	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{16}(12)$	196–207	36.81	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{16}(12)$
208–216	38.44	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	208–219	37.59	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{16}(12)$
217–225	38.46	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	220–228	38.84	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
226–234	38.53	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	229–237	38.84	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
235–243	38.60	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	238–246	38.92	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
244–252	38.84	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	247–255	38.97	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
253–261	39.22	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	259–264	39.38	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
262–270	39.32	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	265–273	39.55	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
271–279	39.35	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	274–282	39.56	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
280–288	39.80	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	283–291	39.75	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
289–297	39.99	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	292–300	40.01	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
298–306	40.13	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	301–309	40.04	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
307–315	40.21	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	310–318	40.06	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
316–324	40.43	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	319–327	40.14	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
325–333	40.64	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{15}(9)$	328–336	40.57	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
334–345	40.96	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{16}(12)$	337–345	40.58	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
346–349	41.15	$[[2,0]_2,L]_{20}$ $(L=3,4)$	$X_9(2)$	346–354	40.80	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
350–358	41.20	$[[2,1]_j,\Lambda]_{20}$ (mixed)	$X_{12}(9)$	355–363	40.97	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{15}(9)$
				364–372	41.12	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$
				373–381	41.38	$[[2,1]_j,\Lambda]_{30}$ (mixed)	$X_{12}(9)$

TABLE VII. Computed $J = 4, 5$, and 6 rovibrational states of the $(CH_4)_2$. The energies are referenced to the ZPVE (94.25 cm^{-1}).

Label	$\tilde{\nu}$[cm^{-1}]	Assignment	Symm.	Label	$\tilde{\nu}$[cm^{-1}]	Assignment	Symm.
$J4.n$				$J5.n$			
1	2.43	$[[0,0]_0,4]_{40}$	$X_1(1)$	1	3.65	$[[0,0]_0,5]_{50}$	$X_2(1)$
2–7	10.79	$[[1,0]_1,3]_{40}$	$X_{11}(6)$	2–7	11.82	$[[1,0]_1,4]_{50}$	$X_{10}(6)$
8–13	12.00	$[[1,0]_1,4]_{40}$	$X_{10}(6)$	8–13	13.21	$[[1,0]_1,5]_{50}$	$X_{11}(6)$
14–19	12.61	$[[1,0]_1,5]_{40}$	$X_{11}(6)$	14–19	14.01	$[[1,0]_1,6]_{50}$	$X_{10}(6)$
20–28	19.25	$[[1,1]_2,2]_{40}$	$X_{15}(9)$	20–28	20.09	$[[1,1]_2,3]_{50}$	$X_{12}(9)$
29–37	20.38	$[[1,1]_1,3]_{40}$	$X_{12}(9)$	29–37	21.39	$[[1,1]_1,4]_{50}$	$X_{15}(9)$
38–46	20.38	$[[1,1]_2,3]_{40}$	$X_{12}(9)$	38–46	21.42	$[[1,1]_2,4]_{50}$	$X_{15}(9)$
47–55	20.92	$[[1,1]_0,4]_{40}$	$X_{15}(9)$	47–55	22.13	$[[1,1]_0,5]_{50}$	$X_{12}(9)$
56–64	20.95	$[[1,1]_1,4]_{40}$	$X_{15}(9)$	56–64	22.15	$[[1,1]_1,5]_{50}$	$X_{12}(9)$
65–73	21.57	$[[1,1]_2,4]_{40}$	$X_{15}(9)$	65–73	22.80	$[[1,1]_2,5]_{50}$	$X_{12}(9)$
74–82	22.05	$[[1,1]_2,5]_{40}$	$X_{12}(9)$	74–82	23.47	$[[1,1]_2,6]_{50}$	$X_{15}(9)$
83–91	22.30	$[[1,1]_1,5]_{40}$	$X_{12}(9)$	83–91	23.70	$[[1,1]_1,6]_{50}$	$X_{15}(9)$
92–100	22.92	$[[1,1]_2,6]_{40}$	$X_{15}(9)$	92–100	24.51	$[[1,1]_2,7]_{50}$	$X_{12}(9)$
101–104	24.56	$[[2,0]_2,L]_{40}$ $(L=2,3,4,5,6)$	$X_9(2)$	101–104	25.69	$[[2,0]_2,L]_{50}$ $(L=3,6)$	$X_9(2)$
105–108	28.36	$[[2,0]_2,L]_{40}$ $(L=2,3,4,5,6)$	$X_9(2)$	105–108	29.56	$[[2,0]_2,L]_{40}$ $(L=4,5)$	$X_9(2)$
109–114	31.25	$[[2,0]_2,2]_{40}$	$X_{11}(6)$	109–114	32.22	$[[2,0]_2,3]_{50}$	$X_{10}(6)$
115–120	31.34	$[[2,0]_2,3]_{40}$	$X_{10}(6)$	115–120	32.41	$[[2,0]_2,4]_{50}$	$X_{11}(6)$
121–126	32.80	$[[2,0]_2,4]_{40}$	$X_{11}(6)$	121–126	33.87	$[[2,0]_2,5]_{50}$	$X_{10}(6)$
127–138	33.10	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{16}(12)$	127–138	34.03	$[[2,1]_j,\Lambda]_{50}$ (mixed)	$X_{16}(12)$
139–142	34.10	$[[2,0]_2,L]_{40}$ $(L=2,4,6)$	$X_9(2)$	139–142	35.31	$[[2,0]_2,7]_{50}$	$X_9(2)$
143–154	34.20	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{16}(12)$				
155–160	34.29	$[[2,0]_2,5]_{40}$	$X_{10}(6)$	$J6.n$			
161	34.74	$[[0,0]_0,4]_{40}$	$X_1(1)$	1	5.10	$[[0,0]_0,6]_{60}$	$X_1(1)$
162–173	34.94	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{16}(12)$	2–7	13.08	$[[1,0]_1,5]_{60}$	$X_{11}(6)$
174–179	35.42	$[[2,0]_2,5]_{40}$	$X_{11}(6)$	8–13	14.68	$[[1,0]_1,6]_{60}$	$X_{10}(6)$
180–191	36.86	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{16}(12)$	14–19	15.65	$[[1,0]_1,7]_{60}$	$X_{11}(6)$
192–195	37.73	$[[2,0]_2,L]_{40}$ $(L=3,4,5)$	$X_9(2)$	20–28	21.16	$[[1,1]_2,4]_{60}$	$X_{15}(9)$
196-207	37.84	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{16}(12)$	29–37	22.65	$[[1,1]_1,5]_{60}$	$X_{12}(9)$
208–219	38.71	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{16}(12)$	38–46	22.69	$[[1,1]_2,5]_{60}$	$X_{12}(9)$
220–228	39.38	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	47–55	23.58	$[[1,1]_1,6]_{60}$	$X_{15}(9)$
229–237	39.43	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	56–64	23.60	$[[1,1]_0,6]_{60}$	$X_{15}(9)$
238–246	39.59	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	65–73	24.27	$[[1,1]_2,6]_{60}$	$X_{15}(9)$
247–255	39.61	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	74–82	25.13	$[[1,1]_2,7]_{60}$	$X_{12}(9)$
256–264	40.14	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	83–91	25.34	$[[1,1]_1,7]_{60}$	$X_{12}(9)$
265–273	40.42	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	92–100	26.35	$[[1,1]_2,8]_{60}$	$X_{15}(9)$
274–282	40.43	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	101–104	27.04	$[[2,0]_2,2]_{60}$	$X_9(2)$
283–291	40.52	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	105–108	31.00	$[[2,0]_2,L]_{60}$ $(L=3,4)$	$X_9(2)$
292–300	40.84	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	109–114	33.39	$[[2,0]_2,2]_{60}$	$X_{11}(6)$
301–309	40.91	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	115–120	33.71	$[[2,0]_2,3]_{60}$	$X_{10}(6)$
310–318	41.03	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	121–132	35.18	$[[2,1]_j,\Lambda]_{60}$ (mixed)	$X_{16}(12)$
319–327	41.07	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	133–138	35.22	$[[2,0]_2,4]_{60}$	$X_{11}(6)$
328–336	41.45	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	139–150	36.70	$[[2,1]_j,\Lambda]_{60}$ (mixed)	$X_{16}(12)$
337–345	41.54	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	151–154	36.75	$[[2,0]_2,L]_{60}$ $(L=4,6)$	$X_9(2)$
346–354	41.72	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{15}(9)$	155	37.17	$[[0,0]_0,6]_{60}$	$X_1(1)$
355–363	41.84	$[[2,1]_j,\Lambda]_{40}$ (mixed)	$X_{12}(9)$	156–161	37.21	$[[2,0]_2,5]_{60}$	$X_{10}(6)$
				162–173	37.78	$[[2,1]_j,\Lambda]_{60}$ (mixed)	$X_{16}(12)$
				174–179	38.72	$[[2,0]_2,6]_{60}$	$X_{11}(6)$

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