

## **Microwave and submillimeterwave spectra of CH<sub>2</sub>DI and CHD<sub>2</sub>I**

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**Supplementary material**

Table S1. Observed transitions with hyperfine structure of CH2DI in its ground state.

J+1	Ka	Kc	F1'	F'	J	Ka	Kc	F1	F	Obs[MHz]	Obs.-Calc.[MHz]
1	0	1	5/2	3/2	0	0	0	5/2	3/2	13557.5270	-0.0017
1	0	1	5/2	7/2	0	0	0	5/2	7/2	13557.5360	0.0004
1	0	1	5/2	5/2	0	0	0	5/2	5/2	13557.5510	-0.0008
1	0	1	7/2	7/2	0	0	0	5/2	5/2	13962.2080	0.0014
1	0	1	7/2	9/2	0	0	0	5/2	7/2	13962.2170	-0.0030
1	0	1	7/2	5/2	0	0	0	5/2	3/2	13962.2250	0.0010
1	0	1	3/2	3/2	0	0	0	5/2	5/2	14136.9820	-0.0032
1	0	1	3/2	5/2	0	0	0	5/2	7/2	14136.9910	0.0022
1	0	1	3/2	1/2	0	0	0	5/2	3/2	14136.9910	-0.0006
2	0	2	1/2	3/2	1	0	1	3/2	5/2	27844.0700	-0.0085
2	0	2	5/2	7/2	1	0	1	5/2	7/2	27902.7250	0.0191
2	0	2	3/2	1/2	1	0	1	5/2	3/2	28175.4450	0.0037
2	0	2	5/2	3/2	1	0	1	3/2	3/2	27323.2640	0.0110
2	0	2	7/2	9/2	1	0	1	7/2	9/2	27398.0020	0.0010
2	0	2	5/2	7/2	1	0	1	7/2	9/2	27398.0410	0.0194
2	0	2	3/2	5/2	1	0	1	3/2	5/2	27596.0060	0.0152
2	0	2	9/2	11/2	1	0	1	7/2	9/2	27770.0770	0.0035
2	0	2	7/2	7/2	1	0	1	5/2	7/2	27802.6870	0.0048
2	1	1	7/2	7/2	1	1	0	5/2	7/2	27556.9530	0.0041
2	1	1	5/2	7/2	1	1	0	5/2	7/2	27603.6450	0.0035
2	1	1	3/2	5/2	1	1	0	5/2	7/2	27744.0960	0.0007
2	1	1	7/2	9/2	1	1	0	7/2	9/2	27761.1370	-0.0172
2	1	1	5/2	7/2	1	1	0	7/2	9/2	27807.5660	0.0147
2	1	1	5/2	3/2	1	1	0	3/2	3/2	27896.0260	0.0354
2	1	1	9/2	11/2	1	1	0	7/2	9/2	27943.7490	0.0017
2	1	1	3/2	5/2	1	1	0	3/2	3/2	28036.4480	0.0087
2	1	1	1/2	3/2	1	1	0	3/2	5/2	28156.7450	0.0175
2	1	2	7/2	7/2	1	1	1	5/2	7/2	27362.8260	-0.0049
2	1	2	5/2	7/2	1	1	1	5/2	7/2	27409.6890	-0.0128
2	1	2	3/2	5/2	1	1	1	5/2	7/2	27550.7010	0.0095
2	1	2	7/2	9/2	1	1	1	7/2	9/2	27566.2980	0.0334
2	1	2	5/2	7/2	1	1	1	7/2	9/2	27613.1480	0.0207
2	1	2	5/2	7/2	1	1	1	3/2	5/2	27700.9480	0.0093
2	1	2	9/2	11/2	1	1	1	7/2	9/2	27749.5670	0.0222
2	1	2	3/2	5/2	1	1	1	3/2	5/2	27841.9500	0.0216
2	1	2	1/2	3/2	1	1	1	3/2	5/2	27962.6450	0.0252
10	0	10	19/2	21/2	9	1	9	17/2	19/2	28804.3160	-0.0020
10	0	10	17/2	19/2	9	1	9	15/2	17/2	28807.1210	0.0067
10	0	10	21/2	23/2	9	1	9	19/2	21/2	28808.3260	0.0125
10	0	10	23/2	25/2	9	1	9	21/2	23/2	28816.1410	0.0039
10	0	10	15/2	17/2	9	1	9	13/2	15/2	28818.8260	-0.0105
10	0	10	25/2	27/2	9	1	9	23/2	25/2	28824.0710	-0.0082

Table S2. Observed transitions with hyperfine structure of CHD2I in its ground state.

J+1	Ka	Kc	F'	J	Ka	Kc	F	Obs[MHz]	Obs.-Calc.[MHz]
1	0	1	5/2	0	0	0	5/2	12597.3890	-0.0030
1	0	1	7/2	0	0	0	5/2	13001.7750	-0.0018
1	0	1	3/2	0	0	0	5/2	13176.5390	0.0001
2	0	2	5/2	1	0	0	3/2	25402.7410	-0.0058
2	0	2	7/2	1	0	0	7/2	25477.2720	-0.0044
2	0	2	5/2	1	0	0	7/2	25577.5050	-0.0040
2	0	2	3/2	1	0	0	3/2	25675.1100	-0.0005
2	0	2	9/2	1	0	0	7/2	25849.1130	0.0085
2	0	2	7/2	1	0	0	5/2	25881.6610	-0.0001
2	0	2	1/2	1	0	0	3/2	25923.0490	-0.0001
2	0	2	5/2	1	0	0	5/2	25981.8910	-0.0027
2	0	2	3/2	1	0	0	5/2	26254.2560	-0.0013
2	1	1	7/2	1	1	0	5/2	25636.8920	-0.0165
2	1	1	5/2	1	1	0	5/2	25683.6590	-0.0141
2	1	1	3/2	1	1	0	5/2	25824.7550	0.0228
2	1	1	7/2	1	1	0	7/2	25840.3850	-0.0042
2	1	1	5/2	1	1	0	7/2	25887.1380	-0.0158
2	1	1	5/2	1	1	0	3/2	25975.0290	-0.0030
2	1	1	9/2	1	1	0	7/2	26023.2530	-0.0055
2	1	1	3/2	1	1	0	3/2	26116.0900	-0.0011
2	1	1	1/2	1	1	0	3/2	26236.4900	-0.0059
2	1	2	7/2	1	1	1	5/2	25441.8340	0.0035
2	1	2	5/2	1	1	1	5/2	25488.4270	0.0063
2	1	2	3/2	1	1	1	5/2	25629.1170	0.0210
2	1	2	7/2	1	1	1	7/2	25645.9200	-0.0122
2	1	2	5/2	1	1	1	7/2	25692.5140	-0.0044
2	1	2	5/2	1	1	1	3/2	25780.6070	-0.0141
2	1	2	9/2	1	1	1	7/2	25828.2240	0.0091
2	1	2	3/2	1	1	1	3/2	25921.3000	0.0036
2	1	2	1/2	1	1	1	3/2	26041.2190	0.0118

Table S3. Observed rotational transitions of CH2DI in its ground state.

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*****
*
*           THE CHARACTERISTICS OF THE FIT ARE
*
*   NUMBER OF DATA POINTS      33053
*   NUMBER OF CONSTANTS         12
*   DEGREES OF FREEDOM         33041
*
*   CHISQUARE      N      STD      WEIGHT
*   rotational     333.7   135     .07740   1.000
*   GSCD-v3        5400.1  5221   6.31950  0.026
*   GSCD-v6sprime  18354.4 17491  4.63337  0.049
*   GSCD-v6dprime  11018.1 10206  4.17792  0.062
*   TOTAL          35106.4 33053   .78257
*   VARIANCE       1.0308
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*****
*
*   CALC.DATA   OBS.DATA   OBS-CALC   OBS.ERROR   CALC.ERROR   IDENTIFICATION
*
*****

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	CALC.DATA	OBS.DATA	OBS-CALC	OBS.ERROR	CALC.ERROR	J'	Ka	Kc	J''	Ka	Kc			
1	27630.733528	27630.717000	-.016528	.0300	.00079	2	1	2	0	1	1	0		+
2	27825.015743	27825.010000	-.005743	.0290	.00079	2	1	1	0	1	1	0		+
3	27728.112025	27728.093000	-.019025	.0300	.00079	2	0	2	0	1	0	1		-
4	28814.251857	28814.334000	.082143	.0340	.00494	10	0	10	0	9	1	9		*****
5	28064.715115	28064.676000	-.039115	.0300	.00467	5	1	5	0	6	0	6		----
6	33711.138255	33711.036000	-.102255	.0300	.01310	20	2	19	0	21	1	20		*****
7	31301.909439	31301.860000	-.049439	.0430	.01316	22	2	20	0	23	1	23		---
8	30670.625395	30670.703000	.077605	.0440	.01419	28	1	28	0	27	2	25		+++++++
9	35206.450116	35206.335000	-.115116	.0930	.02184	37	3	34	0	38	2	37		----
10	26761.510200	26761.506000	-.004200	.0290	.00971	23	1	22	0	23	1	23		+
11	29083.256198	29083.280000	.023802	.0300	.01038	24	1	23	0	24	1	24		+
12	31500.721229	31500.735000	.013771	.0300	.01107	25	1	24	0	25	1	25		+
13	34013.752682	34013.748000	-.004682	.0290	.01178	26	1	25	0	26	1	26		+
14	36622.186378	36622.177000	-.009378	.0300	.01250	27	1	26	0	27	1	27		+
15	39325.845945	39325.842000	-.003945	.0290	.01326	28	1	27	0	28	1	28		+
16	263203.802917	263203.703000	-.099917	.0310	.00619	19	0	19	0	18	0	18		*****
17	264175.503350	264175.413000	-.090350	.0300	.00614	19	1	18	0	18	1	17		*****
18	262334.277735	262334.185000	-.092735	.0300	.00613	19	1	19	0	18	1	18		*****
19	263324.155157	263324.083000	-.072157	.0300	.00596	19	2	17	0	18	2	16		*****
20	263252.469162	263252.379000	-.090162	.0310	.00595	19	2	18	0	18	2	17		*****
21	263259.343129	263259.274000	-.069129	.0300	.00569	19	3	16	0	18	3	15		*****
22	263258.823988	263258.737000	-.086988	.0310	.00569	19	3	17	0	18	3	16		*****
23	263234.911265	263234.851000	-.060265	.0300	.00536	19	4	15	0	18	4	14		*****
24	263207.442969	263207.427000	-.015969	.0300	.00504	19	5	14	0	18	5	13		+

25	263175.142285	263175.122000	-.020285	.0300	.00479	19	6	13	0	18	6	12	0		-	
26	263137.544247	263137.556000	.011753	.0290	.00468	19	7	12	0	18	7	11	0		+	
27	263094.471964	263094.518000	.046036	.0300	.00476	19	8	11	0	18	8	10	0		++++++	
28	263045.850006	263045.938000	.087994	.0320	.00503	19	9	10	0	18	9	9	0		*****	
29	262991.645915	262991.759000	.113085	.0330	.00549	19	10	9	0	18	10	8	0		*****	
30	262931.848104	262931.989000	.140896	.0360	.00609	19	11	8	0	18	11	7	0		*****	
31	262866.456366	262866.641000	.184634	.0500	.00685	19	12	7	0	18	12	6	0		*****	
32	262795.477373	262795.557000	.079627	.0310	.00782	19	13	7	0	18	13	6	0		*****	
33	262718.922376	262719.046000	.123624	.0300	.00915	19	14	5	0	18	14	4	0		*****	
34	262636.805954	262636.948000	.142046	.0360	.01100	19	15	5	0	18	15	4	0		*****	
35	346114.003047	346113.968000	-.035047	.0330	.00715	25	0	25	0	24	0	24	0		---	
36	345023.700794	345023.635000	-.065794	.0300	.00708	25	1	25	0	24	1	24	0		*****	
37	346235.043114	346234.981000	-.062114	.0300	.00687	25	2	24	0	24	2	23	0		*****	
38	346397.753753	346397.709000	-.044753	.0300	.00688	25	2	23	0	24	2	22	0		-----	
39	346262.817986	346262.838000	.020014	.0440	.00654	25	3	23	0	24	3	22	0		+	
40	346264.871202	346264.811000	-.060202	.0290	.00654	25	3	22	0	24	3	21	0		*****	
41	346228.024219	346227.996000	-.028219	.0300	.00616	25	4	21	0	24	4	20	0		--	
42	346190.166321	346190.163000	-.003321	.0300	.00578	25	5	20	0	24	5	19	0		+	
43	346146.778816	346146.765000	-.013816	.0290	.00551	25	6	19	0	24	6	18	0		+	
44	346096.793823	346096.817000	.023177	.0300	.00542	25	7	18	0	24	7	17	0		+	
45	346039.800590	346039.812000	.011410	.0300	.00556	25	8	17	0	24	8	16	0		+	
46	345975.617727	345975.660000	.042273	.0300	.00592	25	9	16	0	24	9	15	0		+++++	
47	345904.160215	345904.213000	.052785	.0310	.00646	25	10	15	0	24	10	14	0		+++++++	
48	345825.389165	345825.458000	.068835	.0310	.00715	25	11	14	0	24	11	13	0		*****	
49	345739.290233	345739.387000	.096767	.0300	.00800	25	12	13	0	24	12	12	0		*****	
50	345645.863389	345645.969000	.105611	.0300	.00914	25	13	12	0	24	13	11	0		*****	
51	345545.117694	345545.230000	.112306	.0300	.01076	25	14	11	0	24	14	10	0		*****	
52	345437.068454	345437.164000	.095546	.0500	.01315	25	15	11	0	24	15	10	0		+++++++	
53	345321.735602	345321.815000	.079398	.0500	.01658	25	16	9	0	24	16	8	0		+++++++	
54	621069.436630	621069.325000	-.111630	.1550	.01129	45	0	45	0	44	0	44	0		-	
55	619593.477848	619593.680000	.202152	.1730	.01142	45	1	45	0	44	1	44	0		+++	
56	623873.805972	623873.970000	.164028	.1660	.01131	45	1	44	0	44	1	43	0		++	
57	621793.524042	621793.581000	.056958	.1560	.01121	45	2	44	0	44	2	43	0		+	
58	622699.069640	622699.217000	.147360	.1620	.01115	45	2	43	0	44	2	42	0		++	
59	622015.692394	622015.477000	-.215394	.1650	.01078	45	3	43	0	44	3	42	0		----	
60	622053.932010	622053.723000	-.209010	.1650	.01077	45	3	42	0	44	3	41	0		----	
61	621932.458037	621932.076000	-.382037	.2110	.01054	45	4	41	0	44	4	40	0		-----	
62	637636.044022	637635.953000	-.091022	.1540	.01174	46	1	45	0	45	1	44	0		+	
63	636479.335131	636478.823000	-.512131	.2930	.01159	46	2	44	0	45	2	43	0		-----	
64	648413.672620	648413.774000	.101380	.1590	.01217	47	0	47	0	46	0	46	0		+	
65	646933.411533	646933.525000	.113467	.1600	.01235	47	1	47	0	46	1	46	0		+	
66	649232.600803	649232.516000	-.084803	.1540	.01211	47	2	46	0	46	2	45	0		+	
67	649486.617783	649486.220000	-.397783	.2150	.01165	47	3	45	0	46	3	44	0		-----	
68	649534.007922	649534.079000	.071078	.1550	.01164	47	3	44	0	46	3	43	0		+	
69	649307.629731	649307.828000	.198269	.1640	.01130	47	5	42	0	46	5	41	0		++++	
70	649216.198854	649215.868000	-.330854	.2050	.01134	47	6	41	0	46	6	40	0		-----	
71	771059.796906	771059.916000	.119094	.1560	.01673	56	0	56	0	55	0	55	0		+	
72	769633.754849	769634.004000	.249151	.1690	.01712	56	1	56	0	55	1	55	0		+++++	

73	774859.906361	774859.849000	-.057361	.1560	.01660	56	1	55	0	55	1	54	0		+	
74	774019.569402	774019.629000	.059598	.1530	.01649	56	2	54	0	55	2	53	0		+	
75	772376.318179	772376.220000	-.098179	.1570	.01657	56	2	55	0	55	2	54	0		-	
76	772916.175748	772916.215000	.039252	.1530	.01583	56	3	53	0	55	3	52	0		+	
77	772804.244776	772804.278000	.033224	.1530	.01585	56	3	54	0	55	3	53	0		+	
78	772693.294672	772693.237000	-.057672	.1560	.01557	56	4	53	0	55	4	52	0		+	
79	772696.100526	772696.011000	-.089526	.1590	.01557	56	4	52	0	55	4	51	0		+	
80	772574.117259	772574.161000	.043741	.1530	.01545	56	5	51	0	55	5	50	0		+	
81	772458.418117	772458.460000	.041883	.1530	.01556	56	6	50	0	55	6	49	0		+	
82	788538.984113	788538.959000	-.025113	.1550	.01707	57	1	56	0	56	1	55	0		+	
83	786022.699953	786022.680000	-.019953	.1540	.01705	57	2	56	0	56	2	55	0		+	
84	787743.508681	787743.436000	-.072681	.1580	.01697	57	2	55	0	56	2	54	0		+	
85	786473.060110	786473.063000	.002890	.1540	.01629	57	3	55	0	56	3	54	0		+	
86	786595.075164	786594.923000	-.152164	.1660	.01627	57	3	54	0	56	3	53	0		--	
87	786360.093169	786360.137000	.043831	.1530	.01599	57	4	54	0	56	4	53	0		+	
88	786363.264007	786363.279000	.014993	.1540	.01598	57	4	53	0	56	4	52	0		+	
89	786237.330972	786237.327000	-.003972	.1540	.01586	57	5	52	0	56	5	51	0		+	
90	786118.732149	786118.501000	-.231149	.1800	.01598	57	6	51	0	56	6	50	0		----	
91	785993.390136	785993.733000	.342864	.1860	.01645	57	7	50	0	56	7	49	0		+++++	
92	878194.254114	878194.422000	.167886	.1550	.02145	64	1	64	0	63	1	63	0		+++	
93	879488.893839	879488.570000	-.323839	.2280	.02087	64	0	64	0	63	0	63	0		-----	
94	881062.423797	881062.215000	-.208797	.1600	.02427	64	9	55	0	63	9	54	0		----	
95	881233.455531	881233.417000	-.038531	.1540	.02146	64	8	56	0	63	8	55	0		+	
96	881322.947787	881322.923000	-.024787	.1560	.02011	64	2	63	0	63	2	62	0		+	
97	881389.765345	881390.319000	.553655	.3410	.01960	64	7	57	0	63	7	56	0		+++++	
98	881534.510081	881534.813000	.302919	.1760	.01859	64	6	58	0	63	6	57	0		+++++	
99	881674.655130	881674.507000	-.148130	.1680	.01828	64	5	59	0	63	5	58	0		--	
100	881824.269371	881824.365000	.095629	.1530	.01844	64	4	61	0	63	4	60	0		+	
101	881831.312726	881831.428000	.115274	.1540	.01844	64	4	60	0	63	4	59	0		+	
102	881947.523055	881947.613000	.089945	.1530	.01894	64	3	62	0	63	3	61	0		+	
103	882161.332379	882161.567000	.234621	.1600	.01896	64	3	61	0	63	3	60	0		+++++	
104	883625.735442	883625.969000	.233558	.1580	.02018	64	2	62	0	63	2	61	0		+++++	
105	884045.377570	884045.325000	-.052570	.1590	.02012	64	1	63	0	63	1	62	0		+	
106	893001.639965	893001.568000	-.071965	.1620	.02143	65	0	65	0	64	0	64	0		+	
107	894653.613815	894653.459000	-.154815	.1550	.02527	65	9	56	0	64	9	55	0		--	
108	894827.563441	894827.475000	-.088441	.1550	.02217	65	8	57	0	64	8	56	0		+	
109	894986.696444	894986.675000	-.021444	.1540	.02009	65	7	58	0	64	7	57	0		+	
110	895134.318319	895134.521000	.202681	.1610	.01896	65	6	59	0	64	6	58	0		++++	
111	895277.728179	895277.874000	.145821	.1550	.01860	65	5	60	0	64	5	59	0		++	
112	895431.420360	895431.377000	-.043360	.1580	.01876	65	4	62	0	64	4	61	0		+	
113	895439.255205	895439.360000	.104795	.1540	.01876	65	4	61	0	64	4	60	0		+	
114	895555.465897	895555.261000	-.204897	.1820	.01929	65	3	63	0	64	3	62	0		---	
115	895785.817128	895785.663000	-.154128	.1750	.01933	65	3	62	0	64	3	61	0		--	
116	897294.267558	897294.365000	.097442	.1530	.02064	65	2	63	0	64	2	62	0		+	
117	897651.921518	897652.273000	.351482	.1760	.02054	65	1	64	0	64	1	63	0		*****	
118	1033512.872038	1033513.058000	.185962	.1530	.02917	75	2	73	0	74	2	72	0		++++	
119	1033152.687273	1033152.913000	.225727	.1550	.02829	75	1	74	0	74	1	73	0		++++	
120	1031613.017407	1031613.208000	.190593	.1540	.02712	75	3	72	0	74	3	71	0		++++	

121	1031158.757971	1031158.963000	.205029	.1560	.02669	75	3	73	0	74	3	72	0		++++	
122	1031060.709703	1031060.950000	.240297	.1590	.02612	75	4	71	0	74	4	70	0		++++++	
123	1031039.869975	1031039.963000	.093025	.1530	.02609	75	4	72	0	74	4	71	0		+	
124	1030663.687409	1030664.009000	.321591	.1920	.02766	75	6	69	0	74	6	68	0		++++++	
125	1030485.737625	1030485.760000	.022375	.1560	.03062	75	7	68	0	74	7	67	0		+	
126	1030297.415633	1030297.260000	-.155633	.1530	.03537	75	8	67	0	74	8	66	0		--	
127	1030202.813176	1030203.012000	.198824	.1560	.02835	75	2	74	0	74	2	73	0		++++	
128	1027608.407069	1027608.503000	.095931	.1550	.03117	75	0	75	0	74	0	74	0		+	
129	1026566.499295	1026566.705000	.205705	.1540	.03177	75	1	75	0	74	1	74	0		+++++	
130	1044551.547831	1044551.711000	.163169	.1550	.02780	76	4	73	0	75	4	72	0		+++	
131	1044574.351267	1044574.664000	.312733	.1680	.02783	76	4	72	0	75	4	71	0		+++++++	
132	1254118.846194	1254118.810000	-.036194	.3630	.10900	92	0	92	0	91	0	91	0		+	
133	1260813.942613	1260813.990000	.047387	.1630	.10396	92	1	91	0	91	1	90	0		+	
134	1262703.347503	1262703.410000	.062497	.3100	.10576	92	2	90	0	91	2	89	0		+	
135	1271093.818978	1271093.510000	-.308978	.3050	.11288	93	2	92	0	92	2	91	0		--	

Table S4. Observed rotational transitions of CHD2I in its ground state.

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*****
*
* THE CHARACTERISTICS OF THE FIT ARE
*
* NUMBER OF DATA POINTS 28194
* NUMBER OF CONSTANTS 12
* DEGREES OF FREEDOM 28182
* CHISQUARE N STD WEIGHT
* rotational 263.5 151 .04153 1.000
* GSCD-v3 3181.2 3009 7.25473 0.020
* GSCD-v6sprime 17539.8 16605 4.52227 0.052
* GSCD-v6dprime 8874.2 8429 4.06798 0.064
* TOTAL 29858.6 28194 .44002
* VARIANCE 1.0293
*
*****

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*****
*
* CALC.DATA OBS.DATA OBS-CALC OBS.ERROR CALC.ERROR IDENTIFICATION
*
*****

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	CALC.DATA	OBS.DATA	OBS-CALC	OBS.ERROR	CALC.ERROR														
1	25709.446012	25709.500000	.053988	.0380	.00048	2	1	2	0	1	1	1	0						+++++
2	256931.141815	256931.137000	-.004815	.0150	.00382	20	1	20	0	19	1	19	0						
3	257825.947304	257825.913000	-.034304	.0150	.00347	20	0	20	0	19	0	19	0		*****				
4	258012.511053	258012.522000	.010947	.0160	.00335	20	2	18	0	19	2	17	0						+
5	257924.329371	257924.293000	-.036371	.0170	.00314	20	3	18	0	19	3	17	0		*****				
6	257925.418871	257925.384000	-.034871	.0170	.00314	20	3	17	0	19	3	16	0		*****				
7	257901.742789	257901.768000	.025211	.0200	.00294	20	4	16	0	19	4	15	0						++++
8	257877.381387	257877.375000	-.006387	.0150	.00275	20	5	15	0	19	5	14	0						+
9	257849.496641	257849.490000	-.006641	.0150	.00265	20	6	14	0	19	6	13	0						+
10	257780.789879	257780.806000	.016121	.0150	.00288	20	8	13	0	19	8	12	0						+++
11	257739.579635	257739.599000	.019365	.0150	.00320	20	9	11	0	19	9	10	0						++++
12	322109.284036	322109.254000	-.030036	.0150	.00397	25	0	25	0	24	0	24	0		*****				
13	323475.633239	323475.608000	-.025239	.0160	.00437	25	1	24	0	24	1	23	0		-----				
14	321048.563140	321048.562000	-.001140	.0160	.00434	25	1	25	0	24	1	24	0						+
15	322478.397563	322478.376000	-.021563	.0160	.00385	25	2	23	0	24	2	22	0		-----				
16	322270.926065	322270.916000	-.010065	.0150	.00377	25	2	24	0	24	2	23	0						-
17	322314.967870	322314.951000	-.016870	.0150	.00355	25	3	23	0	24	3	22	0						---
18	322318.299838	322318.285000	-.014838	.0150	.00355	25	3	22	0	24	3	21	0						--
19	322283.333334	322283.344000	.010666	.0160	.00331	25	4	21	0	24	4	20	0						+
20	322283.312588	322283.310000	-.002588	.0150	.00331	25	4	22	0	24	4	21	0						+
21	322250.999255	322250.992000	-.007255	.0150	.00309	25	5	21	0	24	5	20	0						+
22	322215.167133	322215.156000	-.011133	.0160	.00298	25	6	19	0	24	6	18	0						-
23	322215.167133	322215.149000	-.018133	.0160	.00298	25	6	20	0	24	6	19	0						---
24	322174.461671	322174.465000	.003329	.0150	.00302	25	7	19	0	24	7	18	0						+

25	322128.352001	322128.357000	.004999	.0150	.00324	25	8	18	0	24	8	17	0			+	
26	322076.599924	322076.627000	.027076	.0150	.00360	25	9	17	0	24	9	16	0		+++++++		
27	322019.089743	322019.120000	.030257	.0150	.00403	25	10	16	0	24	10	15	0		*****		
28	321955.763986	321955.795000	.031014	.0150	.00444	25	11	15	0	24	11	14	0		*****		
29	321886.595774	321886.636000	.040226	.0150	.00478	25	12	14	0	24	12	13	0		*****		
30	321811.575737	321811.619000	.043263	.0150	.00499	25	13	13	0	24	13	12	0		*****		
31	321730.705322	321730.749000	.043678	.0150	.00507	25	14	12	0	24	14	11	0		*****		
32	321643.993162	321644.044000	.050838	.0150	.00503	25	15	11	0	24	15	10	0		*****		
33	321551.452997	321551.501000	.048003	.0150	.00503	25	16	10	0	24	16	9	0		*****		
34	321453.102435	321453.130000	.027565	.0150	.00538	25	17	9	0	24	17	8	0		+++++++		
35	321348.962182	321348.980000	.017818	.0150	.00653	25	18	8	0	24	18	7	0		+++		
36	321239.055557	321239.032000	-.023557	.0150	.00875	25	19	7	0	24	19	6	0		-----		
37	321123.408166	321123.360000	-.048166	.0210	.01210	25	20	6	0	24	20	5	0		*****		
38	641475.849577	641475.447000	-.402577	.2430	.01326	50	0	50	0	49	0	49	0		-----		
39	642998.170785	642997.429000	-.741785	.4350	.01238	50	4	47	0	49	4	46	0		-----		
40	643000.809828	643000.067000	-.742828	.4360	.01238	50	4	46	0	49	4	45	0		-----		
41	643087.685312	643087.627000	-.058312	.2300	.01261	50	3	48	0	49	3	47	0			+	
42	643191.775874	643191.518000	-.257874	.2420	.01263	50	3	47	0	49	3	46	0		---		
43	644190.474668	644190.920000	.445332	.2710	.01320	50	2	48	0	49	2	47	0			+++++	
44	644918.689860	644918.480000	-.209860	.2310	.01317	50	1	49	0	49	1	48	0		--		
45	640207.353617	640206.717000	-.636617	.3320	.01347	50	1	50	0	49	1	49	0		-----		
46	628780.085310	628779.691000	-.394310	.2430	.01258	49	0	49	0	48	0	48	0		-----		
47	627499.642864	627499.027000	-.615864	.3230	.01276	49	1	49	0	48	1	48	0		-----		
48	632126.837823	632126.284000	-.553823	.2740	.01248	49	1	48	0	48	1	47	0		*****		
49	631354.627204	631354.730000	.102796	.2310	.01252	49	2	47	0	48	2	46	0			+	
50	629929.991793	629929.519000	-.472793	.2690	.01245	49	2	48	0	48	2	47	0		-----		
51	630401.439477	630401.621000	.181523	.2370	.01197	49	3	46	0	48	3	45	0			+	
52	630307.164906	630307.295000	.130094	.2340	.01195	49	3	47	0	48	3	46	0			+	
53	630221.862370	630221.524000	-.338370	.2540	.01173	49	4	45	0	48	4	44	0		-----		
54	630219.568766	630219.634000	.065234	.2300	.01173	49	4	46	0	48	4	45	0			+	
55	630128.624742	630128.506000	-.118742	.2330	.01159	49	5	44	0	48	5	43	0			+	
56	630043.449879	630043.524000	.074121	.2300	.01159	49	6	43	0	48	6	42	0			+	
57	629954.939581	629955.027000	.087419	.2290	.01182	49	7	43	0	48	7	42	0			+	
58	629638.748682	629638.697000	-.051682	.2400	.01450	49	10	40	0	48	10	39	0			+	
59	629512.876578	629513.290000	.413422	.2370	.01617	49	11	38	0	48	11	37	0			+++++	
60	629376.070841	629376.424000	.353159	.2310	.01828	49	12	37	0	48	12	36	0			+++++	
61	772441.836731	772442.099000	.262269	.2770	.02087	60	1	59	0	59	1	58	0			++	
62	769922.952290	769922.966000	.013710	.2310	.02058	60	2	59	0	59	2	58	0			+	
63	772292.171300	772292.205000	.033700	.2290	.02103	60	2	58	0	59	2	57	0			+	
64	770840.631777	770840.778000	.146223	.2340	.01980	60	3	57	0	59	3	56	0			+	
65	770588.208925	770588.294000	.085075	.2320	.01970	60	3	58	0	59	3	57	0			+	
66	770488.682817	770488.823000	.140183	.2330	.01927	60	4	57	0	59	4	56	0			+	
67	770356.870675	770356.964000	.093325	.2300	.01906	60	5	56	0	59	5	55	0			+	
68	770240.525360	770240.227000	-.298360	.2620	.01919	60	6	55	0	59	6	54	0		---		
69	770125.059974	770125.054000	-.005974	.2330	.01986	60	7	54	0	59	7	53	0			+	
70	770003.193449	770003.277000	.083551	.2310	.02128	60	8	53	0	59	8	52	0			+	
71	769871.557591	769871.895000	.337409	.2310	.02357	60	9	52	0	59	9	51	0			+++++	
72	769728.436639	769728.690000	.253361	.2300	.02679	60	10	51	0	59	10	50	0			+++	

73	780648.597010	780648.337000	-.260010	.2300	.02204	61	0	61	0	60	0	60	0		---	
74	779585.958935	779585.751000	-.207935	.2340	.02264	61	1	61	0	60	1	60	0		--	
75	793256.382025	793255.954000	-.428025	.2410	.02292	62	0	62	0	61	0	61	0		-----	
76	792217.189669	792217.235000	.045331	.2310	.02356	62	1	62	0	61	1	61	0		+	
77	797852.414293	797852.105000	-.309293	.2320	.02246	62	1	61	0	61	1	60	0		-----	
78	797845.759723	797845.672000	-.087723	.2310	.02276	62	2	60	0	61	2	59	0		+	
79	795288.837881	795288.628000	-.209881	.2320	.02211	62	2	61	0	61	2	60	0		--	
80	796310.995395	796310.499000	-.496395	.2900	.02128	62	3	59	0	61	3	58	0		-----	
81	796015.586563	796015.581000	-.005563	.2290	.02112	62	3	60	0	61	3	59	0		+	
82	795916.824642	795916.698000	-.126642	.2330	.02064	62	4	59	0	61	4	58	0		+	
83	795928.508377	795928.247000	-.261377	.2450	.02064	62	4	58	0	61	4	57	0		---	
84	795776.656611	795776.950000	.293389	.2430	.02041	62	5	58	0	61	5	57	0		++++	
85	795653.920311	795654.123000	.202689	.2320	.02058	62	6	57	0	61	6	56	0		++	
86	795533.128638	795533.287000	.158362	.2290	.02139	62	7	56	0	61	7	55	0		+	
87	795406.269841	795406.707000	.437159	.2410	.02307	62	8	55	0	61	8	54	0		+++++++	
88	899781.782766	899781.442000	-.340766	.2510	.02988	70	2	68	0	69	2	67	0		-----	
89	899141.425655	899141.411000	-.014655	.2420	.02832	70	1	69	0	69	1	68	0		+	
90	897974.255066	897974.236000	-.019066	.2290	.02696	70	3	67	0	69	3	66	0		+	
91	897449.989565	897450.053000	.063435	.2310	.02631	70	3	68	0	69	3	67	0		+	
92	897394.500438	897394.567000	.066562	.2300	.02549	70	4	66	0	69	4	65	0		+	
93	897367.635446	897367.404000	-.231446	.2420	.02546	70	4	67	0	69	4	66	0		--	
94	897191.719858	897192.540000	.820142	.4540	.02513	70	5	66	0	69	5	65	0		+++++++	
95	897041.012315	897040.918000	-.094315	.2400	.02560	70	6	65	0	69	6	64	0		+	
96	896897.469328	896897.818000	.348672	.2340	.02728	70	7	64	0	69	7	63	0		+++++	
97	896749.734103	896750.051000	.316897	.2290	.03050	70	8	63	0	69	8	62	0		+++++	
98	896592.478502	896592.839000	.360498	.2290	.03539	70	9	62	0	69	9	61	0		+++++	
99	896451.481934	896451.270000	-.211934	.2310	.02779	70	2	69	0	69	2	68	0		--	
100	896422.983640	896423.845000	.861360	.2610	.04191	70	10	60	0	69	10	59	0		*****	
101	893847.762971	893847.591000	-.171971	.2290	.03030	70	0	70	0	69	0	69	0		-	
102	893005.995008	893005.668000	-.327008	.2440	.03111	70	1	70	0	69	1	69	0		-----	
103	887066.278078	887066.191000	-.087078	.2300	.02898	69	2	67	0	68	2	66	0		+	
104	886512.751805	886512.610000	-.141805	.2320	.02765	69	1	68	0	68	1	67	0		-	
105	885286.267079	885286.326000	.058921	.2300	.02627	69	3	66	0	68	3	65	0		+	
106	884796.066301	884795.986000	-.080301	.2300	.02573	69	3	67	0	68	3	66	0		+	
107	884734.676902	884734.844000	.167098	.2340	.02496	69	4	65	0	68	4	64	0		+	
108	884710.328914	884710.283000	-.045914	.2300	.02494	69	4	66	0	68	4	65	0		+	
109	884539.665377	884539.674000	.008623	.2300	.02462	69	5	64	0	68	5	63	0		+	
110	884392.068268	884392.550000	.481732	.2580	.02503	69	6	63	0	68	6	62	0		+++++++	
111	884251.491503	884251.540000	.048497	.2340	.02657	69	7	62	0	68	7	61	0		+	
112	884106.448184	884106.944000	.495816	.2390	.02955	69	8	61	0	68	8	60	0		*****	
113	883951.823969	883952.173000	.349031	.2290	.03410	69	9	60	0	68	9	59	0		+++++	
114	883833.668603	883833.731000	.062397	.2360	.02714	69	2	68	0	68	2	67	0		+	
115	883785.013907	883785.245000	.231093	.2410	.04021	69	10	59	0	68	10	58	0		++	
116	881300.447990	881300.378000	-.069990	.2330	.02935	69	0	69	0	68	0	68	0		+	
117	880433.682820	880433.459000	-.223820	.2350	.03015	69	1	69	0	68	1	68	0		--	
118	1039073.077188	1039073.060000	-.017188	.2310	.03995	81	2	79	0	80	2	78	0		+	
119	1031347.842988	1031347.857000	.014012	.2390	.04152	81	0	81	0	80	0	80	0		+	
120	1030765.312682	1030765.439000	.126318	.2380	.04220	81	1	81	0	80	1	80	0		+	

121	1024872.285664	1024871.754000	-.531664	.2370	.03356	80	1	79	0	79	1	78	0	*****	
122	1024512.439673	1024512.568000	.128327	.2330	.03389	80	3	77	0	79	3	76	0		
123	1047193.967031	1047193.879000	-.088031	.2300	.03417	82	2	81	0	81	2	80	0		
124	1023592.902674	1023593.027000	.124326	.2310	.02952	80	4	76	0	79	4	75	0		
125	1023549.033146	1023549.006000	-.027146	.2290	.03090	80	3	78	0	79	3	77	0		
126	1023526.350417	1023526.747000	.396583	.2600	.02933	80	4	77	0	79	4	76	0		
127	1023305.023115	1023305.263000	.239885	.2340	.02890	80	5	75	0	79	5	74	0		
128	1023302.760508	1023302.740000	-.020508	.2320	.02889	80	5	76	0	79	5	75	0		
129	1022160.321027	1022160.098000	-.223027	.2300	.03322	80	2	79	0	79	2	78	0		
130	1254096.215659	1254096.244000	.028341	.2380	.07910	99	0	99	0	98	0	98	0		
131	1253817.504233	1253817.344000	-.160233	.2300	.07897	99	1	99	0	98	1	98	0		
132	1260666.968062	1260666.440000	-.528062	.2330	.05740	99	1	98	0	98	1	97	0		
133	1258356.725183	1258355.897000	-.828183	.3280	.05869	99	2	98	0	98	2	97	0		
134	1264281.536502	1264281.148000	-.388502	.2520	.07186	99	2	97	0	98	2	96	0		
135	1260584.967325	1260585.244000	.276675	.2580	.05585	99	3	97	0	98	3	96	0		
136	1262905.976284	1262905.946000	-.030284	.3210	.07331	99	3	96	0	98	3	95	0		
137	1260836.538554	1260836.394000	-.144554	.2360	.05455	99	4	96	0	98	4	95	0		
138	1261110.237966	1261109.994000	-.243966	.2420	.05690	99	4	95	0	98	4	94	0		
139	1260534.813410	1260534.943000	.129590	.2300	.05509	99	5	95	0	98	5	94	0		
140	1260549.358062	1260549.739000	.380938	.2400	.05519	99	5	94	0	98	5	93	0		
141	1270681.296649	1270681.038000	-.258649	.2520	.06225	100	2	99	0	99	2	98	0		
142	1271893.317239	1271893.994000	.676761	.3850	.11133	100	9	92	0	99	9	91	0		
143	1272378.730800	1272379.299000	.568200	.2290	.07457	100	7	94	0	99	7	93	0		
144	1272631.495351	1272632.038000	.542649	.2380	.06404	100	6	95	0	99	6	94	0		
145	1272923.428654	1272923.191000	-.237654	.2670	.05900	100	5	96	0	99	5	95	0		
146	1272939.292654	1272938.888000	-.404654	.3160	.05911	100	5	95	0	99	5	94	0		
147	1272955.359663	1272955.594000	.234337	.2510	.05949	100	3	98	0	99	3	97	0		
148	1273520.046154	1273520.394000	.347846	.2560	.06089	100	4	96	0	99	4	95	0		
149	1276679.720036	1276679.397000	-.323036	.2710	.07538	100	2	98	0	99	2	97	0		
150	1278399.133626	1278398.845000	-.288626	.2370	.08702	101	1	101	0	100	1	100	0		
151	1278654.066434	1278654.034000	-.032434	.2330	.08721	101	0	101	0	100	0	100	0		

Table S5. Observed rotational transitions of CHD2I in the v3=1 state.

```

*****
*
*   CALC.DATA   OBS.DATA   OBS-CALC  OBS.ERROR  CALC.ERROR  IDENTIFICATION
*
*****
3985  12822.345532  12822.350000  .004468   .0050     .00097     1  0  1  1  0  0  0  1 | |+++++++|
3986  268981.955661 268981.961000  .005339   .1000     .01451     21 0 21  1 20  0 20  1 | |      + |
3987  268052.671622 268052.684000  .012378   .1000     .01940     21 1 21  1 20  1 20  1 | |      + |
3988  270091.420312 270091.387000  -.033312   .1000     .01935     21 1 20  1 20  1 19  1 | |     - |
3989  269075.006470 269075.055000  .048530   .1000     .01363     21 2 20  1 20  2 19  1 | |    |++ |
3990  269198.115081 269198.090000  -.025081   .1000     .01411     21 2 19  1 20  2 18  1 | |      + |
3991  269098.846873 269098.863000  .016127   .1000     .01290     21 3 18  1 20  3 17  1 | |      + |
3992  269097.461091 269097.531000  .069909   .1000     .01290     21 3 19  1 20  3 18  1 | |    |+++++|
3993  269073.048625 269073.034000  -.014625   .1000     .01213     21 4 17  1 20  4 16  1 | |      + |
3994  269046.976574 269047.023000  .046426   .1000     .01160     21 5 17  1 20  5 16  1 | |    |++ |
3995  269017.289034 269017.291000  .001966   .1000     .01152     21 6 15  1 20  6 14  1 | |      + |
3996  268983.175237 268983.090000  -.085237   .1000     .01196     21 7 15  1 20  7 14  1 | |-----|
3997  268944.320864 268944.353000  .032136   .1000     .01280     21 8 13  1 20  8 12  1 | |      |+ |
3998  268900.584805 268900.614000  .029195   .1000     .01379     21 9 13  1 20  9 12  1 | |      |+ |
3999  268851.898444 268851.917000  .018556   .1000     .01479     21 10 11  1 20 10 10  1 | |      + |
4000  268798.227615 268798.233000  .005385   .1000     .01577     21 11 11  1 20 11 10  1 | |      + |
4001  268739.556245 268739.553000  -.003245   .1000     .01723     21 12  9  1 20 12  8  1 | |      + |
4002  268675.878611 268675.845000  -.033611   .1000     .02021     21 13  9  1 20 13  8  1 | |     - |
4003  268607.195377 268607.071000  -.124377   .1000     .02601     21 14  7  1 20 14  6  1 | |*****|
4004  268533.511449 268533.349000  -.162449   .1000     .03563     21 15  7  1 20 15  6  1 | |*****|
4005  268454.834739 268454.558000  -.276739   1.0000     .04984     21 16  5  1 20 16  4  1 | |      + |
4006  345594.045562 345594.019000  -.026562   .1000     .01534     27  0 27  1 26  0 26  1 | |      + |
4007  344478.686497 344478.646000  -.040497   .1000     .02071     27  1 27  1 26  1 26  1 | |     - |
4008  346058.344471 346058.379000  .034529   .1000     .01493     27  2 25  1 26  2 24  1 | |      |+ |
4009  345798.424276 345798.470000  .045724   .1000     .01365     27  2 26  1 26  2 25  1 | |    |++ |
4010  345855.887625 345855.876000  -.011625   .1000     .01256     27  3 25  1 26  3 24  1 | |      + |
4011  345860.762431 345860.718000  -.044431   .1000     .01259     27  3 24  1 26  3 23  1 | |     -- |
4012  345820.006031 345820.031000  .024969   .1000     .01159     27  4 23  1 26  4 22  1 | |      + |
4013  345783.891457 345783.896000  .004543   .1000     .01098     27  5 23  1 26  5 22  1 | |      + |
4014  345744.380859 345744.361000  -.019859   .1000     .01104     27  6 21  1 26  6 20  1 | |      + |
4015  345699.737932 345699.755000  .017068   .1000     .01181     27  7 21  1 26  7 20  1 | |      + |
4016  345649.291046 345649.298000  .006954   .1000     .01298     27  8 19  1 26  8 18  1 | |      + |
4017  345592.735324 345592.738000  .002676   .1000     .01418     27  9 19  1 26  9 18  1 | |      + |
4018  345529.918958 345529.929000  .010042   .1000     .01518     27 10 17  1 26 10 16  1 | |      + |
4019  345460.762486 345460.763000  .000514   .1000     .01620     27 11 17  1 26 11 16  1 | |      + |
4020  345385.224093 345385.228000  .003907   .1000     .01808     27 12 15  1 26 12 14  1 | |      + |
4021  345303.283185 345303.271000  -.012185   .1000     .02255     27 13 15  1 26 13 14  1 | |      + |
4022  345214.931982 345214.814000  -.117982   .1000     .03122     27 14 13  1 26 14 12  1 | |*****|

```