

Appendix A:

**Tables of Energy Levels for the $(v_3 = v_4 = 1)$, $(v_5 = v_9 = 1)$,
and $(v_9 = 2)$, $(v_5 = v_7 = 1)$ Vibrational States, and List of Transitions Belonging to
the $\nu_3 + \nu_7$ Band of CH_2D_2 .**

Electronic supplementary materials to:

**High Resolution Fourier Transform Spectroscopy of CH_2D_2 in the Region 2350 -
2650 cm^{-1} : The Bands $\nu_5 + \nu_7$, $2\nu_9$, $\nu_3 + \nu_4$, $\nu_3 + \nu_7$, and $\nu_5 + \nu_9$**

O. N. Ulenikov, E. S. Bekhtereva, S. V. Grebneva

Laboratory of Molecular Spectroscopy, Physics Department,
Tomsk State University, Tomsk, 634050, Russia,
and Institute of Atmospheric Optics SB RAN, Tomsk, 634055, Russia

H. Hollenstein, M. Quack

Physical Chemistry, ETH-Zürich,
CH-8093 Zürich, Switzerland

Table 1A. Experimental Rovibrational Term Values for the $(v_3 = v_4 = 1)$ and $(v_5 = v_9 = 1)$ Vibrational States of the CH_2D_2 Molecule (in cm^{-1}).

Table 2A. Experimental Rovibrational Term Values for the $(v_9 = 2)$ and $(v_5 = v_7 = 1)$ Vibrational States of the CH_2D_2 Molecule (in cm^{-1}).

Table 3A. List of Transitions Belonging to the $\nu_3 + \nu_7$ Band of CH_2D_2 .

Table 1A. Experimental Rovibrational Term Values for the ($v_3 = v_4 = 1$) and ($v_5 = v_9 = 1$)
Vibrational States of the CH₂D₂ Molecule (in cm⁻¹)^a

J	$(v_3 = v_4 = 1)$					$(v_5 = v_9 = 1)$		
	K_a	K_c	$E/hc, \text{cm}^{-1}$	Δ	δ	$E/hc, \text{cm}^{-1}$	Δ	δ
	1		2	3	4	5	6	7
0	0	0	2469.2023		-3	2560.5489		35
1	0	1	2475.8352	1	1	2567.0382	1	15
1	1	1	2476.1267	5	7	2567.8357	2	14
1	1	0	2476.6836	4	11	2568.3656	1	20
2	0	2	2488.7681	1	1	2579.8289	9	-6
2	1	2	2488.8475	9	13	2580.2875	3	1
2	1	1	2490.4958	1	4	2581.8759	5	14
2	2	1	2491.4568	5	10	2584.2688	4	17
2	2	0	2491.8091	6	8	2584.4586	4	19
3	0	3	2507.7939	2	-2	2598.6636	10	-15
3	1	3	2507.8036	2	8	2598.8629	8	-18
3	1	2	2510.8843	3	-6	2601.9901	5	2
3	2	2	2511.3183	5	10	2603.7394	5	10
3	2	1	2512.6148	2	16	2604.5683	4	21
3	3	1	2514.7732	2	-1	2609.1517	5	8
3	3	0	2514.9353	2	1	2609.1981	3	13
4	0	4	2532.9832	7	0	2623.4187	12	-38
4	1	4	2532.9593	5	44	2623.4908	15	-38
4	1	3	2537.4502	6	-17	2628.4777	7	-14
4	2	3	2537.5544	7	-18	2629.5464	4	2
4	2	2	2540.2957	5	12	2631.5749	15	26
4	3	2	2541.6075	8	17	2635.3929	3	25
4	3	1	2542.4437	6	19	2635.6869	9	29
4	4	1	2546.4599	3	-13	2642.5882	8	-1
4	4	0	2546.5153	16	-18	2642.5969	6	-6
5	0	5	2564.4137	15	69	2654.1042	11	-40
5	1	5	2564.4137	15	26	2654.1285	5	-31
5	1	4	2570.0678	6	-51	2661.0451	6	-34
5	2	4	2570.0707	9	-34	2661.5770	9	-15
5	2	3	2574.4465	6	5	2665.3070	4	0
5	3	3	2574.9962	7	9	2668.1550	5	26
5	3	2	2577.1398	9	12	2669.1416	4	42
5	4	2	2580.0635	3	13	2675.4562	6	30
5	4	1	2580.4720	11	15	2675.5344	4	37
5	5	1	2586.8993	10	-12	2684.6091	2	-36
5	5	0	2586.9154	7	-11	2684.6113	2	-30
6	0	6	2602.1337	20	52	2690.7470	3	-25
6	1	6	2602.1337	20	49	2690.7544	8	-31
6	1	5	2608.8479	4	4	2699.5066	12	-48
6	2	5	2608.8466	9	-35	2699.7293	5	-27
6	2	4	2614.6708	5	10	2705.4969	4	-30
6	3	4	2614.7877	4	-3	2707.3402	6	13
6	3	3	2618.6385	7	-67	2709.6109	5	30
6	4	3	2620.3922	4	27	2714.9539	4	52
6	4	2	2621.7892	7	21	2715.3003	5	62
6	5	2	2627.1050	7	-2	2724.0515	7	22
6	5	1	2627.2575	8	3	2724.0687	4	21
6	6	1	2636.2365	9	-2	2735.2175	18	-62
6	6	0	2636.2365	9	-42	2735.2175	18	-65
7	0	7	2646.1435	15	67	2733.3650	4	-4
7	1	7	2646.1435	15	66	2733.3650	4	-8
7	1	6	2653.9064	5	-44	2743.8491	6	-40
7	2	6	2653.9070	15	-32	2743.9304	8	-22
7	2	5	2660.8759	5	8	2751.8250	3	-45
7	3	5	2660.8900	2	-7	2752.8272	4	-6
7	3	4	2666.4959	7	-43	2756.9301	4	7
7	4	4	2667.2879	14	27	2761.0340	11	39
7	4	3	2670.3385	20	13	2762.0810	3	71

Table 1A (cont.)

J	$(v_3 = v_4 = 1)$					$(v_5 = v_9 = 1)$		
	K_a	K_c	$E/hc, \text{cm}^{-1}$	Δ	δ	$E/hc, \text{cm}^{-1}$	Δ	δ
	1		2	3	4	5	6	7
7	5	3	2674.1448	15	14	2770.1627	6	46
7	5	2	2674.8466	3	-8	2770.2583	5	55
7	6	2	2682.9809	7	17	2781.2208	2	-3
7	6	1	2683.0275	15	11	2781.2243	2	-2
7	7	1	2694.3782	5	21	2794.4057	13	-37
7	7	0	2694.3782	5	11	2794.4057	13	-37
8	0	8	2696.4289	22	70	2781.9796		21
8	1	8	2696.4289	22	72	2781.9717	2	22
8	1	7	2705.2622	4	-64	2794.1238	6	-22
8	2	7	2705.2664	8	-49	2794.1396	3	-18
8	2	6	2713.3013	3	20	2804.1050	8	-49
8	3	6	2713.2917	8	-1	2804.4978	4	-24
8	3	5	2720.4117	7	12	2810.8028	3	-27
8	4	5	2720.5991	4	7	2813.6079	3	-18
8	4	4	2725.6865	6	20	2815.9640	3	53
8	5	4	2727.9076	2	11	2822.9547	2	39
8	5	3	2729.9046	7	-33	2823.3135	2	65
8	6	3	2736.5845	9	0	2833.8654	3	27
8	6	2	2736.8587	7	-12	2833.8876	3	25
8	7	2	2747.6545	7	11	2846.9683	6	-23
8	7	1	2747.6667	10	0	2846.9683	6	-30
8	8	1	2761.1831	4	5	2862.1563	7	5
8	8	0	2761.1831	4	3	2862.1563	7	5
9	0	9	2752.9677	20	70	2836.5714	12	47
9	1	9	2752.9677	20	84	2836.5869	17	23
9	1	8	2762.9131	14	-39	2850.6342	4	-19
9	2	8	2762.9202	9	-39	2850.3510	5	7
9	2	7	2772.0150	10	26	2861.9561	4	-67
9	3	7	2772.0127	7	18	2862.2616	8	-39
9	3	6	2780.2591	7	38	2870.8736	5	-55
9	4	6	2780.2520	15	-13	2872.5549	4	-26
9	4	5	2787.2690	24	62	2876.8140	11	15
9	5	5	2788.2286	4	11	2882.4071	6	-1
9	5	4	2792.2283	22	-11	2883.4131	5	65
9	6	4	2797.0130	12	-6	2893.1763	4	26
9	6	3	2798.0330	13	-61	2893.2782	3	41
9	7	3	2807.7697	3	-2	2906.1717	9	-11
9	7	2	2807.8604	6	-7	2906.1767	12	-9
9	8	2	2820.9917	10	78	2921.2838	10	-31
9	8	1	2820.9917	10	41	2921.2838	10	-32
9	9	1	2836.5517	29	-62	2938.4588	6	64
9	9	0	2836.5517	29	-63	2938.4588	6	64
10	0	10	2815.7285	21	-35	2897.2466	3	18
10	1	10	2815.7285	21	52	2897.2745		-20
10	1	9	2826.8277	9	-20	2912.5026	9	45
10	2	9	2826.8369	7	-48	2912.5866	11	27
10	2	8	2837.0418	19	24	2925.8890	2	-19
10	3	8	2837.0474	5	13	2926.0788	22	-12
10	3	7	2846.3007	7	51	2936.8355	6	-70
10	4	7	2846.2247	14	-69	2937.7637	6	-58
10	4	6	2854.7211	8	-16	2944.3326	4	-4
10	5	6	2854.9713	7	-24	2948.4855	6	-48
10	5	5	2861.2917	5	122	2950.6676	6	56
10	6	5	2864.1349	9	18	2959.1535	7	-9
10	6	4	2866.7482	20	-83	2959.5048	16	47
10	7	4	2874.7427	10	9	2972.0379	6	-15
10	7	3	2875.1571	13	-19	2972.0641	10	0

Table 1A (cont.)

<i>J</i>	$(v_3 = v_4 = 1)$					$(v_5 = v_9 = 1)$		
	<i>K_a</i>	<i>K_c</i>	<i>E/hc, cm⁻¹</i>	Δ	δ	<i>E/hc, cm⁻¹</i>	Δ	δ
	1		2	3	4	5	6	7
10	8	3	2887.5985	2	9	2987.0397	6	-38
10	8	2	2887.6253	7	-6	2987.0397	6	-47
10	9	2	2902.8835	13	-14	3004.1558	5	-16
10	9	1	2902.8835	13	-19	3004.1558	5	-16
10	10	1	2920.4268	5	-12	3023.2983	6	46
10	10	0	2920.4268	5	-13	3023.2983	6	46
11	0	11	2884.6817		117	2963.6819	7	19
11	1	11	2884.6817		-63	2963.7089	6	37
11	1	10	2896.9771	4	18	2980.8083	31	91
11	2	10	2896.9873	8	-44	2981.0467	5	-34
11	2	9	2908.3575	5	53	2995.7452	3	13
11	3	9	2908.3678	11	7	2995.9818	8	-1
11	3	8	2918.6633	12	48	3008.5757	9	-50
11	4	8	2918.8676	12	38	3009.1777	6	-59
11	4	7	2928.1104	21	-70	3018.1453	7	-14
11	5	7	2928.1099	2	-91	3021.2120	8	-68
11	5	6	2936.5713	5	-47	3024.9882	15	41
11	6	6	2937.7950	5	81	3031.7632	3	-41
11	6	5	2942.7494	8	9	3032.7213	7	34
11	7	5	2948.5159	9	110	3044.5844	8	-18
11	7	4	2949.8624	5	-37	3044.6850	11	-1
11	8	4				3059.4429	27	-25
11	8	3	2961.2140	4	96	3059.4429	27	-80
11	9	3	2975.9792	19	-92	3076.4694	11	-26
11	9	2	2975.9792	19	-93	3076.4694	11	-28
11	10	2	2993.2589	13	41	3095.5738	6	11
11	10	1	2993.2589	13	39	3095.5738	6	11
11	11	1	3012.7540	10	18	3116.6614	16	-73
11	11	0	3012.7540	10	18	3116.6614	16	-73
12	0	12	2959.8212		18	3036.5178	7	9
12	1	12	2959.8212		-79	3036.5178	7	-16
12	1	11	2973.3284		51	3054.3470	4	78
12	2	11	2973.3376	6	-52	3054.6034	5	47
12	2	10	2985.9167	11	61	3071.6435	25	109
12	3	10	2985.9338	25	5	3072.5186	3	83
12	3	9	2997.3418	25	30	3086.1502	10	-9
12	4	9	2997.4197	7	-66	3086.9708	8	8
12	4	8	3007.7367	44	-13	3097.9029	6	-31
12	5	8	3007.6822	6	-137	3100.7590	2	2
12	5	7	3017.4974	2	-11	3106.1032	16	49
12	6	7	3017.8261	2	55	3110.9257	7	-60
12	6	6	3025.4263		76	3113.0537	8	39
12	7	6				3123.8103	5	-13
12	7	5	3032.1551	11	40	3124.1340	4	11
12	8	5	3041.3480	9	23	3138.5110	10	3
12	8	4				3138.5359	3	4
12	9	4	3055.8567	9	-13	3155.4137	7	4
12	9	3	3055.9079	8	-32	3155.4137	7	-8
12	10	3	3072.8091	2	17	3174.4558	6	30
12	10	2	3072.8091	2	17	3174.4558	6	29
12	11	2	3092.0703	3	-9	3195.5317	20	45
12	11	1	3092.0703	3	-9	3195.5317	20	45
12	12	1	3113.8883	18	18	3218.5465	13	8
12	12	0	3113.8883	18	19	3218.5465	13	8

Table 1A (cont.)

<i>J</i>	$(v_3 = v_4 = 1)$					$(v_5 = v_9 = 1)$		
	<i>K_a</i>	<i>K_c</i>	<i>E/hc</i> , cm ⁻¹	Δ	δ	<i>E/hc</i> , cm ⁻¹	Δ	δ
	1		2	3	4	5	6	7
13	0	13				3115.3795	8	-46
13	1	13				3115.3795	8	-48
13	1	12	3055.8494		47	3135.0328	19	61
13	2	12	3055.8610	11	-53	3135.0530	12	64
13	2	11	3069.6849	13	82	3154.1291	12	-115
13	3	11	3069.7008	14	-33	3152.7998	4	-38
13	3	10	3082.2834	10	68	3169.6952	12	98
13	4	10	3082.3413	10	-16	3168.4473	6	59
13	4	9	3093.7194	10	114	3183.4347	8	41
13	5	9	3093.6645	2	-54	3183.0466	6	4
13	5	8				3193.6424	4	0
13	6	8	3104.3133	8	-32	3196.5306	9	-44
13	6	7				3200.4162	14	23
13	7	7				3209.6836	11	1
13	7	6				3210.5567	3	40
13	8	6	3128.3316	5	4	3224.2563	15	30
13	8	5	3130.0742	7	-67	3224.3485	5	38
13	9	5				3241.0022	19	12
13	9	4				3241.0070	31	2
13	10	4	3159.1166	4	27	3259.9556	8	5
13	10	3	3159.1273	2	17	3259.9556	8	3
13	11	3	3178.0563	4	26	3281.0047	4	-28
13	11	2	3178.0563	4	22	3281.0047	4	-28
13	12	2				3304.0466	7	-4
13	12	1				3304.0466	7	-4
13	13	1				3328.9794	7	-8
13	13	0				3328.9794	7	-8
14	0	14				3200.4129		-4
14	1	14				3200.4129		-7
14	1	13	3144.5133	2	23	3221.5077	5	49
14	2	13	3144.5286	2	-82	3221.5077	5	14
14	2	12	3159.6201	7	31	3240.7164	6	-40
14	3	12	3159.6401	2	-23			
14	4	11				3258.2753	4	-72
14	4	10	3185.9591	3	-48	3274.8077	6	129
14	5	10				3274.0293	5	17
14	5	9				3287.2518	18	-86
14	6	9	3197.3752	7	58	3288.4552	15	7
14	7	8				3302.1380	18	-14
14	7	7	3217.8427	1	22			
14	8	7				3316.6831	2	26
14	8	6				3316.9638	4	-25
14	9	6				3333.2535	13	-21
14	11	4	3270.7539	2	39			
14	11	3	3270.7539	2	11			
15	0	15				3291.6903	6	-38
15	1	15				3291.6903	6	-44
15	1	14	3239.2888	8	41	3314.1653	6	-52
15	2	14	3239.2339		-33	3314.1653	6	-70
15	2	13	3255.6955	5	-43			
15	4	13	3255.7187	10	69			
16	0	16				3389.3422		-24
16	1	16				3389.3422		10
16	2	14	3357.8714	10	-34			

^{a)} In Table 1A, $\Delta = \{\sum_{i=1}^n (E_i - E)^2 / (n - 1)\}^{1/2} / hc$ is the experimental uncertainty of the term value, equal to one standard deviation in units of 10^{-4} cm⁻¹; δ is the difference $(E^{exp.} - E^{calc.}) / hc$, also in units of 10^{-4} cm⁻¹; Δ is not quoted when the energy value was obtained from only one transition.

Table 2A. Experimental Rovibrational Term Values for the ($v_9 = 2$) and ($v_5 = v_7 = 1$)
Vibrational States of the CH₂D₂ Molecule (in cm⁻¹)^a

<i>J</i>	$(v_3 = v_4 = 1)$					$(v_5 = v_9 = 1)$		
	<i>K_a</i>	<i>K_c</i>	<i>E/hc</i> , cm ⁻¹	Δ	δ	<i>E/hc</i> , cm ⁻¹	Δ	δ
	1		2	3	4	5	6	7
0	0	0	2458.7952		-4	2422.0270		-6
1	0	1	2465.3685	1	-8	2428.4689	2	-6
1	1	1	2465.9160	1	-1	2429.8372		-17
1	1	0	2466.5905	1	-8	2430.1678	1	0
2	0	2	2478.1499	3	-1	2441.2997		-4
2	1	2	2478.3770	7	7	2442.3925		-6
2	1	1	2480.4175	3	-13	2443.3790	20	-16
2	2	1	2482.0287	7	-2	2447.4537	2	8
2	2	0	2482.3738	6	17	2447.5064	6	3
3	0	3	2496.7646	7	3	2460.4211	2	0
3	1	3	2496.8298	15	0	2461.1904	3	-15
3	1	2	2500.8337	3	-8	2463.1638	14	8
3	2	2	2501.7764	2	5	2466.7765	7	0
3	2	1	2503.1371	3	-11	2467.0345	9	1
3	3	1	2506.1880	5	4	2474.3161	11	27
3	3	0	2506.3121	2	-4	2474.3208		18
4	0	4	2521.1064	8	16	2485.7201	1	-4
4	1	4	2521.1217	6	13	2486.2012	2	-15
4	1	3	2527.3731	8	0	2489.4653	12	27
4	2	3	2527.7741	3	7	2492.4961	1	-3
4	2	2	2530.8573	2	0	2493.2214	8	-5
4	3	2	2533.0485	4	-31	2500.1685	3	3
4	3	1	2533.7331	6	7	2500.2076	10	3
4	4	1	2538.2735	4	16	2510.4102	35	19
4	4	0	2538.3054	8	-3	2510.4102	35	13
5	0	5	2551.1428	4	15	2517.1179	7	-11
5	1	5	2551.1462	8	15	2517.3898		-26
5	1	4	2559.6630	8	8	2522.1981	7	19
5	2	4	2559.7928	9	10	2524.5743	13	-4
5	2	3	2565.1312	16	-66	2526.1066	9	2
5	3	3	2566.3722	4	-3	2532.4978	18	-29
5	3	2	2568.3847	6	22	2532.6511	6	-16
5	4	2	2572.0811	6	30	2542.7260	3	10
5	4	1				2542.7307	7	11
5	5	1	2578.1103	5	-3	2555.6318	13	45
5	5	0	2578.1204	4	-9	2555.6318	13	46
6	0	6	2586.8489	9	3	2554.5839	11	-27
6	1	6	2586.8496	9	2	2554.7287	7	-24
6	1	5	2597.6035	5	6	2561.2522	5	41
6	2	5	2597.6385	6	-2	2562.9623		-37
6	2	4	2605.4362	11	-25	2565.6608	4	-1
6	3	4	2605.9812	6	-7	2571.2974	9	-22
6	3	3	2610.0259	18	-68	2571.7292	4	-32
6	4	3	2612.5889	17	19	2581.5243		-115
6	4	2	2613.6278	2	20	2581.5584	19	-3
6	5	2	2618.8253	10	21	2594.3918	9	17
6	5	1	2618.9504	7	81	2594.3918	9	17
6	6	1	2625.7017	10	-22	2609.8489	20	65
6	6	0	2625.7017	10	-48	2609.8489	20	-75
7	0	7	2628.2191	7	6	2598.1197	17	-21
7	1	7	2628.2191	7	-5	2598.1911	4	-38
7	1	6	2641.1820	7	1	2606.4898	10	41
7	2	6	2641.1907	15	-31	2607.6208	4	3
7	2	5	2651.4062	12	-35	2611.8098	4	11
7	3	5	2651.5958	17	-3	2616.5354	7	-32
7	3	4	2658.1376	3	-11	2617.5269	10	-30
7	4	4	2659.6136	12	33	2626.8474		-21
7	4	3	2662.2059	3	45	2626.9300	11	-7

Table 2A (cont.)

J	$(v_3 = v_4 = 1)$					$(v_5 = v_9 = 1)$		
	K_a	K_c	$E/hc, \text{cm}^{-1}$	Δ	δ	$E/hc, \text{cm}^{-1}$	Δ	δ
	1		2	3	4	5	6	7
7	5	3	2666.3556	11	66	2639.6453	4	10
7	5	2	2666.8526	6	84	2639.6483	6	40
7	6	2				2655.0564	10	10
7	6	1				2655.0564	10	-34
7	7	1	2681.2269		-38	2672.8211		-99
7	7	0	2681.2269		-45	2672.8211		6
8	0	8	2675.2591	23	-4	2647.7259	3	-35
8	1	8	2675.2591	23	5	2647.7597	10	-56
8	1	7	2690.3914	5	-23	2657.8026	18	32
8	2	7	2690.3932	8	68	2658.4893	5	8
8	2	6	2702.9400	5	-69	2664.4397	10	15
8	3	6	2702.9953	8	-17	2668.1758	15	-15
8	3	5	2712.2154	5	-25	2670.0920	18	-24
8	4	5	2712.8844	5	7	2678.6667	11	-2
8	4	4	2717.7031	1	39	2678.9012	20	-32
8	5	4				2691.4043	5	23
8	5	3				2691.4185	20	-73
9	0	9	2727.9897	18	0	2703.4070	16	-38
9	1	9	2727.9897	18	22	2703.4239	19	-42
9	1	8	2745.2447	8	-27	2715.1380	6	46
9	2	8	2745.2442	2	5	2715.5253	6	11
9	2	7	2760.0389	28	90	2723.4099	10	24
9	3	7	2760.0544	6	5	2726.1581	4	-43
9	3	6				2729.4045	24	-4
9	4	6	2772.1141	16	1	2736.9752	5	-7
9	4	5	2779.6594	5	2	2737.5510	5	-21
9	5	5				2749.6786	21	48
9	5	4				2749.7235	12	2
9	6	4				2764.9414	10	25
9	6	3				2764.9340	12	-84
10	0	10	2786.4175	16	-33	2765.1614	3	-10
10	1	10	2786.4175	16	-24	2765.1717		10
10	1	9	2805.7603	13	-31	2778.4799	28	18
10	2	9	2805.7586	12	-4	2778.6909	10	15
10	2	8	2822.7242	26	-76	2788.5687	8	61
10	3	8	2822.7242	26	-37	2790.4426	5	3
10	3	7	2836.9794	7	-63	2795.3694	7	-36
10	4	7	2837.0557	2	6	2801.7486	8	3
10	4	6	2847.2287	10	-34	2802.9576	18	-81
10	5	6				2814.4697	3	96
10	5	5				2814.6018	10	21
10	6	5				2829.6412	18	5
10	6	4				2829.6383	15	-41
10	7	3				2847.4012	3	45
11	0	11	2850.5846	6	21	2832.9816	11	58
11	1	11	2850.5846	6	24	2832.9816	11	17
11	1	10				2847.8459	10	31
11	2	10	2871.9597	5	16	2847.9549	10	13
11	2	9	2891.0265	12	-39	2859.7608	2	30
11	3	9	2891.0265	12	13	2860.9442	3	-19
11	3	8	2907.5618	6	-41	2867.8557	4	-62
11	4	8	2907.5827	3	24	2872.9677	8	95
11	4	7				2875.1981	15	-9
11	5	7				2885.8043	14	2
11	6	6				2900.8630	7	4
11	6	5				2900.8714	11	-2
11	7	4				2918.2480	3	-1

Table 2A (cont.)

J	K_a	K_c	$(v_3 = v_4 = 1)$			$(v_5 = v_9 = 1)$		
			$E/hc, \text{cm}^{-1}$	Δ	δ	$E/hc, \text{cm}^{-1}$	Δ	δ
	1		2	3	4	5	6	7
12	0	12	2920.4933	13	16			
12	1	12	2920.4933	13	18			
12	1	11	2943.8534	14	-53	2923.2361	3	-2
12	2	11	2943.8534	14	-49	2923.2922	15	-13
12	2	10	2964.9859	39	62	2936.9155	16	-17
12	3	10	2964.9859	39	114	2937.6174	17	-36
12	3	9	2983.6740	15	5	2946.7096	5	45
12	4	9	2983.6783	11	26	2950.5083	7	35
12	4	8				2954.2306	8	-52
12	5	8				2963.6109	9	-44
12	5	7				2964.3308	3	49
12	6	7				2978.6102	5	-21
13	1	12	3021.4846	9	-11	3004.6578	4	-30
13	2	12	3021.4846	9	-14	3004.6844	8	31
13	2	11	3044.6153	18	69	3020.0148	5	-32
13	3	11	3044.6153	18	63	3020.4086	21	-71
13	3	10				3031.7078	1	-17
13	4	10	3065.3729	6	-70	3034.3560	17	8
13	4	9				3039.9584	3	-48
13	5	9				3047.9218	18	93
13	5	8				3049.3447	9	21
13	6	8				3062.8849	5	-36
14	1	13	3104.8567	8	-2	3092.1092		-65
14	2	13	3104.8567	8	27			
14	2	12	3129.9885	8	9	3109.0651	5	-37
14	3	12	3129.9885	8	-12	3109.2792		-105
14	3	11				3122.7113	9	7
14	4	11				3124.4305	9	36
15	1	14	3193.9942	15	29			
15	2	14	3193.9942	15	-55			
15	2	13				3204.0847	16	41
15	3	13				3204.1980	10	22
15	3	12				3219.6101	13	139
15	4	12				3220.6380	10	-76
15	4	11				3230.8887	5	-39

^{a)} See footnote to Table 1A.

Table 3A. List of Transitions Belonging to the $\nu_3 + \nu_7$ Band of CH₂D₂.

Upper			Lower			Line position, Intensity,		$E^{exp.}$,	Mean value E,	$E^{calc.}$,	δ ,
J'	K'_a	K'_c	J	K_a	K_c	in cm^{-1}	$\ln(I_0/I)$	in cm^{-1}	in cm^{-1}	in cm^{-1}	in 10^{-4}cm^{-1}
1			2			3	4	5	6	7	8
8	6	2	7	1	6	2617.9793	0.30	2803.3497			
8	6	2	8	3	6	2557.5415	0.51	2803.3497			
8	6	2	9	3	6	2491.8575	0.42	2803.3491	2803.3496	2803.3466	30
8	6	2	8	5	4	2540.2340	0.10	2803.3497	0.0003 ^{a)}		
8	6	2	9	1	8	2509.8482	0.15	2803.3497			
9	5	4	8	0	8	2624.4592	0.40	2849.8796			
9	5	4	9	2	8	2556.3625	1.54	2849.8802			
9	5	4	10	2	8	2481.1579	0.55	2849.8805	2849.8802	2849.8809	-7
9	5	4	10	0	10	2507.2635	0.14	2849.8800	0.0004 ^{a)}		
9	5	4	9	4	6	2536.2793	0.13	2849.8804			
9	5	4	10	4	6	2465.3790	0.09	2849.8807			
12	8	5	11	5	7	2655.3377	0.50	3117.2972			
12	8	5	12	5	7	2571.1678	0.26	3117.2983	3117.2980	3117.2982	-2
12	8	5	13	7	7	2466.4631	0.87	3117.2972	0.0010 ^{a)}		
12	8	5	13	5	9	2490.6276	0.08	3117.2994			
12	3	9	11	0	11	2646.4176	0.10	3056.7246			
12	3	9	12	2	11	2555.6827	1.08	3056.7310			
12	3	9	13	2	11	2457.7470	0.15	3056.7250	3056.7247	3056.7213	34
12	3	9	11	2	9	2617.2602	0.67	3056.7239	0.0004 ^{a)}		
12	3	9	13	4	9	2431.1007	0.29	3056.7248			
12	3	9	13	0	13	2492.8899	0.11	3056.7247			
12	7	6	11	4	8	2646.6162	0.39	3097.9843			
12	7	6	12	4	8	2558.7507	0.37	3097.9843			
12	7	6	13	4	10	2484.2324	0.27	3097.9833	3097.9845	3097.9912	-67
12	7	6	12	6	6	2544.3400	0.19	3097.9848	0.0007 ^{a)}		
12	7	6	13	8	6	2433.0552	0.32	3097.9855			
12	5	8	11	2	10	2643.9367	0.22	3069.7587			
12	5	8	12	2	10	2553.5457	1.95	3069.7587			
12	5	8	13	4	10	2456.0080	0.29	3069.7589	3069.7588	3069.7667	-79
12	5	8	13	2	12	2487.4479	0.13	3069.7597	0.0008 ^{a)}		
12	5	8	11	4	8	2618.3892	0.27	3069.7573			

^{a)} $\Delta = \{\sum_{i=1}^n (E_i - E)^2 / (n - 1)\}^{1/2} / hc$ in units of cm^{-1} .