

# Assignment of the methanol OH-stretch overtone spectrum using the pattern recognition method

April 24, 2024

In this document, the reduced energy plots for the A and E components of methanol are presented in Figure 1 and Figure 2 respectively. The list of firmly assigned combination differences multiplets is given in Table 1 while the list of tentative assignments is given in Table 2.

Figures 3 and 4 depict the fitted spectrum and a zoom on a  $1.5 \text{ cm}^{-1}$  region around  $7200.75 \text{ cm}^{-1}$ .

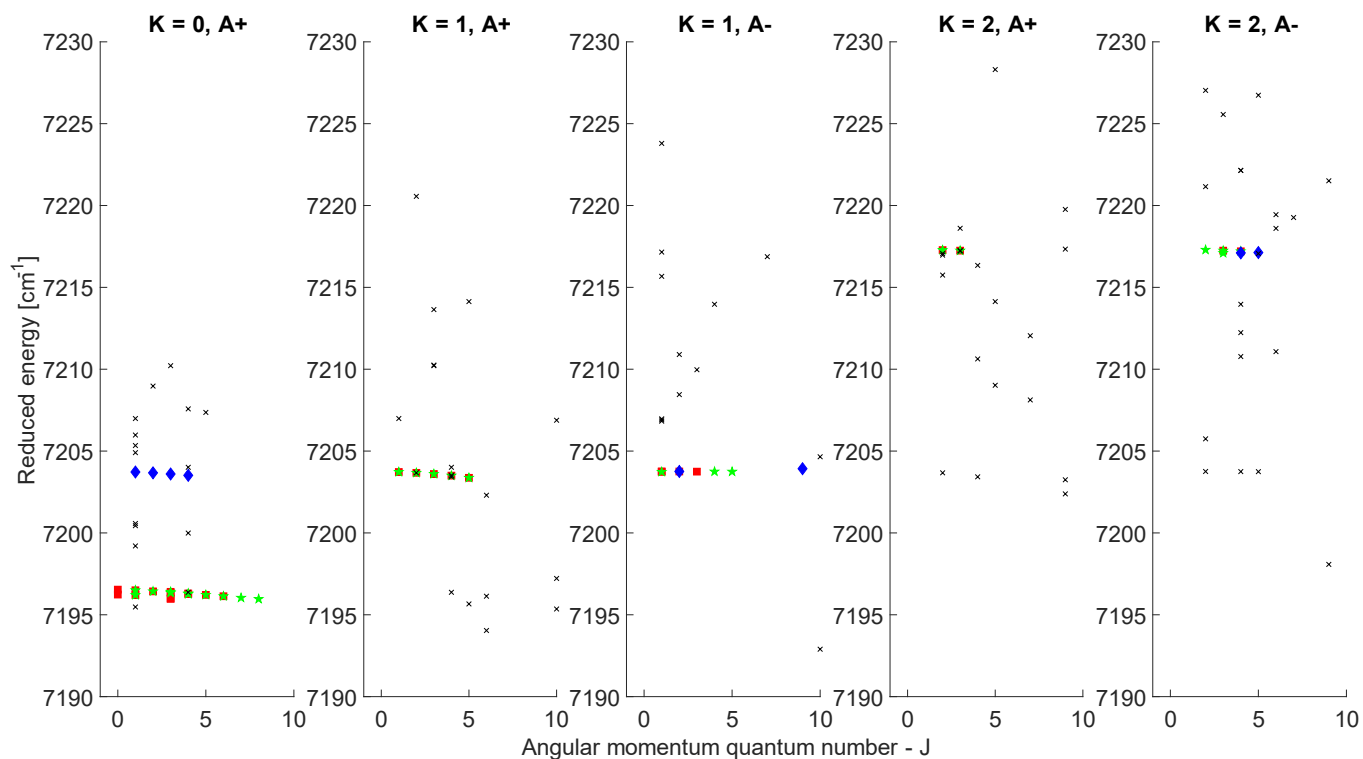


Figure 1: Reduced energy plot for the A component. Green stars are firmly confirmed CDMs, Red squares are CDMs detected by Rakovský *et al.* [Rakovský *et al.*, *Physical Chemistry Chemical physics*, 2021, **23**, 20193-20200]. Blue diamonds are tentative CDMs and black crosses are rejected CDMs.

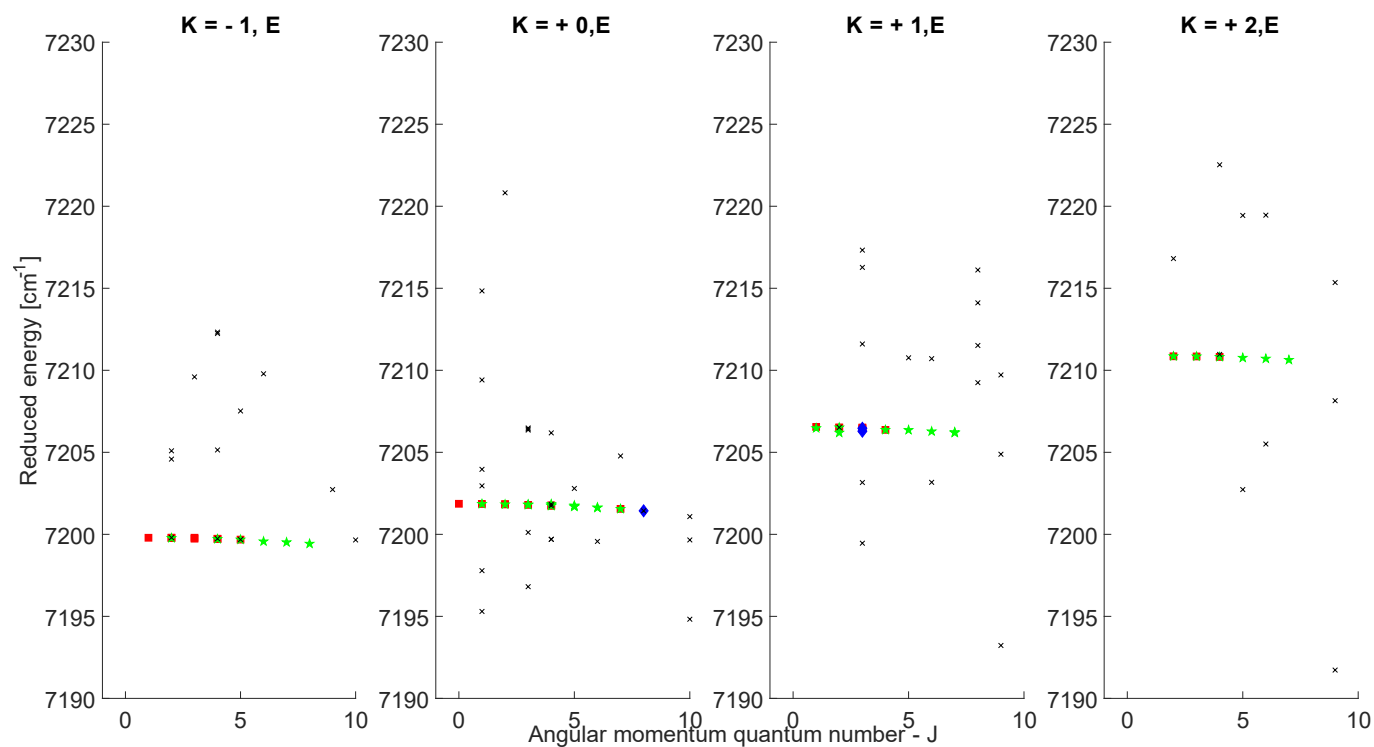


Figure 2: Reduced energy plot for the E component. Green stars are firmly confirmed assignments, Red squares are CDMs detected by Rakovský *et al.* Blue diamonds are tentative assignments and black crosses are rejected CDMs.

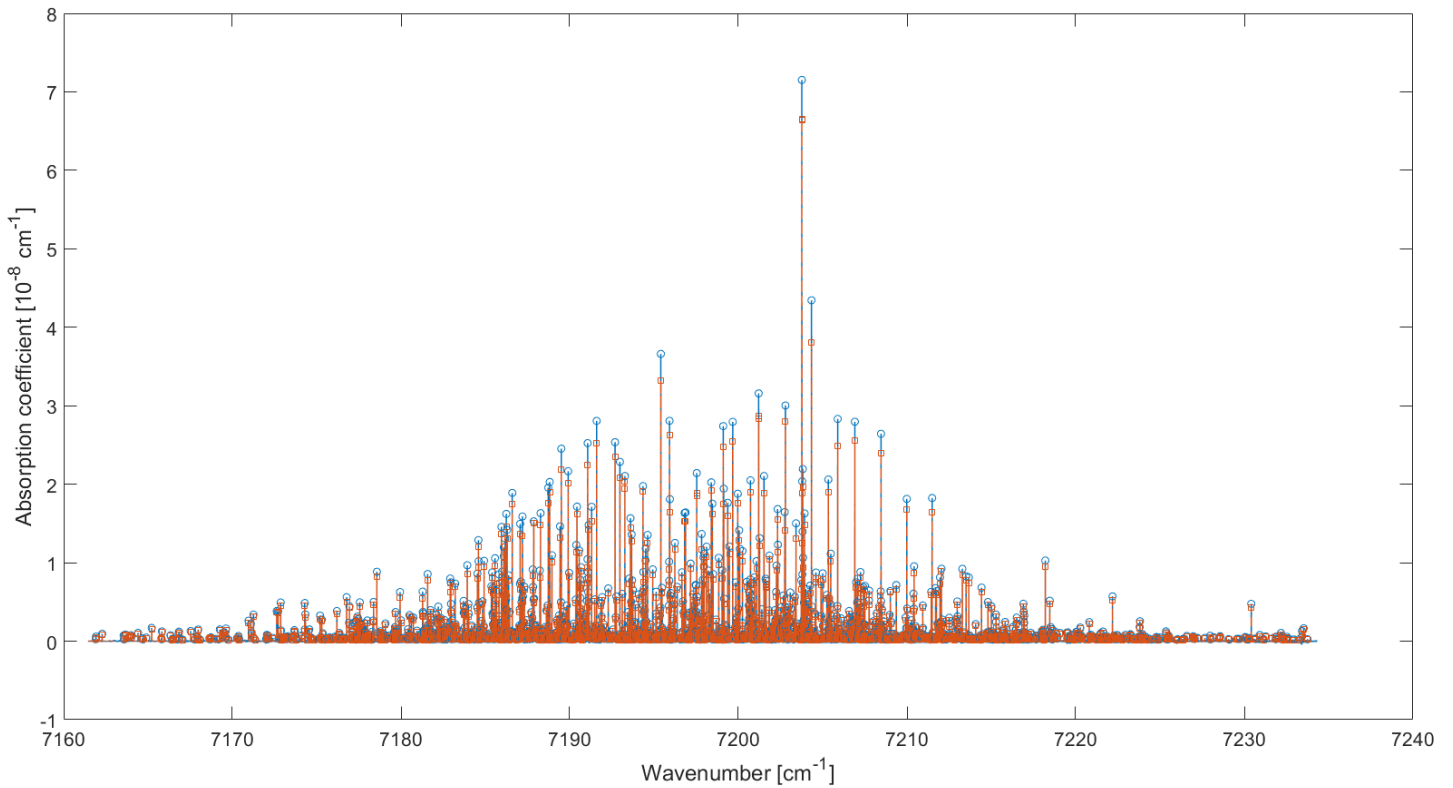


Figure 3: Absorption coefficient plotted against wavenumber. The blue line represents experimental data, with blue dots indicating the peaks of detected transitions. The red line represents data fitted using a sum of Gaussian functions, with red squares denoting the peaks of the Gaussian fits

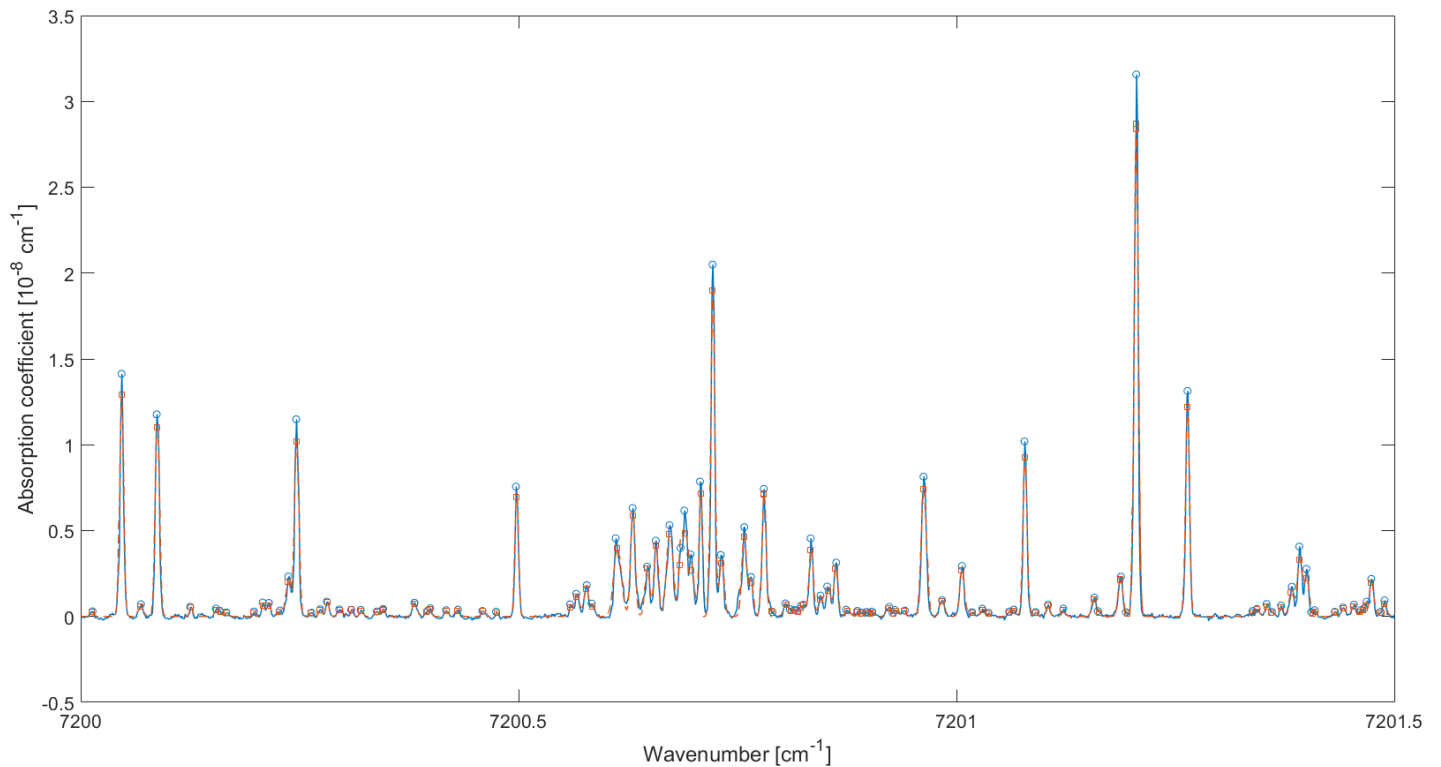


Figure 4: Zoom on a  $1.5 \text{ cm}^{-1}$  wide region around  $7200.75 \text{ cm}^{-1}$  of the absorption coefficient plotted against wavenumber. The blue line represents experimental data, with blue dots indicating the peaks of detected transitions. The red line represents data fitted using a sum of Gaussian functions, with red squares denoting the peaks of the Gaussian fits

Table 1: List of firmly assigned CDMs. The energy of the transitions are the experimental ones. Energies of non-observed transitions are labeled by a dash symbol.

upper state	E (cm <sup>-1</sup> )	lower state E (cm <sup>-1</sup> ), lines E (cm <sup>-1</sup> )							
		(0,0,+A) 0	(2,0,+A) 4.8405	(1,1,-A) 11.7328	(2,1,+A) 14.9043				
(1,0,+A)	7197.8218	7197.8218	7192.9803	7186.0879	7182.9178				
	7198.1151	7198.1151	7193.2733	7186.3817	7183.2108				
(2,0,+A)		(1,0,+A) 1.6135	(3,0,+A) 9.6806	(1,1,+A) 11.7049	(2,1,-A) 14.9878	(3,1,+A) 19.7031			
	7201.2812	7199.6677	7191.5997	7189.5761	7186.2931	7181.5781			
(3,0,+A)		(2,0,+A) 4.8405	(2,1,+A) 14.9043	(4,0,+A) 16.1335	(3,1,-A) 19.8701	(4,1,+A) 26.1012			
	7206.0457	7201.2052	7191.1404	7189.9113	7186.1753	7179.9445			
	7206.1043	7201.2638	7191.1989	7189.9698	7186.2337	7180.003			
(4,0,+A)		(3,0,+A) 9.6806	(3,1,+A) 19.7031	(5,0,+A) 24.1988	(4,1,-A) 26.3795	(5,1,+A) 34.0983			
	7212.4348	7202.7542	7192.7307	7188.2348	7186.0545	7178.3369			
	7212.4732	7202.7926	7192.769	7188.2735	7186.0927	7178.3752			
(5,0,+A)		(4,0,+A) 16.1335	(4,1,+A) 26.1012	(6,0,+A) 33.8759	(5,1,-A) 34.5156	(6,1,+A) 43.694			
	7220.4706	7204.3371	7194.3699	7186.5946	7185.9547	7176.7775			
(6,0,+A)		(5,0,+A) 24.1988	(5,1,+A) 34.0983	(6,1,-A) 44.2782	(7,0,+A) 45.164	(7,1,+A) 54.8878			
	7230.0906	7205.8918	7195.9926	7185.8121	7184.9264	7175.2039			
(7,0,+A)		(6,0,+A) 33.8759	(6,1,+A) 43.694	(7,1,-A) 55.6666	(8,0,+A) 58.0623	(8,1,+A) 67.6792			
	7241.3148	7207.4389	7197.6211	7185.6484	7183.2526	7173.6368			
(8,0,+A)		(7,0,+A) 45.164	(7,1,+A) 54.8878	(8,1,-A) 68.6803	(9,0,+A) 72.5699	(9,1,+A) 82.0677			
	7254.1772	7209.0132	7199.2894	7185.4964	7181.607	7172.1106			
(1,1,+A)		(0,0,+A) 0	(2,0,+A) 4.8405	(1,1,-A) 11.7328	(2,1,+A) 14.9043	(2,2,+A) 31.049			
	7205.3378	7205.3378	7200.4978	7193.6059	7190.433	7174.29			
(1,1,-A)		(1,0,+A) 1.6135	(1,1,+A) 11.7049	(2,1,-A) 14.9878	(2,2,-A) 31.0489				
	7205.3465	7203.733	7193.6411	7190.3575	7174.2975				
(2,1,+A)		(1,0,+A) 1.6135	(3,0,+A) 9.6806	(1,1,+A) 11.7049	(2,1,-A) 14.9878	(3,1,+A) 19.7031	(2,2,-A) 31.0489	(3,2,+A) 35.8902	
	7208.5211	7206.9076	7198.841	7196.8169	7193.5341	7188.8176	7177.4732	-	
(3,1,+A)		(2,0,+A) 4.8405	(2,1,+A) 14.9043	(4,0,+A) 16.1335	(3,1,-A) 19.8701	(4,1,+A) 26.1012	(2,2,+A) 31.049	(3,2,-A) 35.8898	(4,2,+A) 42.345
	7213.3014	7208.4609	7198.3973	7197.168	7193.4312	7187.1994	7182.2522	7177.4121	-
(4,1,+A)		(3,0,+A) 9.6806	(3,1,+A) 19.7031	(5,0,+A) 24.1988	(4,1,-A) 26.3795	(5,1,+A) 34.0983	(3,2,+A) 35.8902	(4,2,-A) 42.3438	(5,2,+A) 50.4135
	7219.6703	7209.9897	7199.9673	-	7193.2897	7185.572	7183.7797	7177.3271	-
(4,1,-A)		(4,0,+A) 16.1335	(3,1,-A) 19.8701	(4,1,+A) 26.1012	(5,1,-A) 34.5156	(3,2,-A) 35.8898	(4,2,+A) 42.345	(5,2,-A) 50.4108	
	7219.9171	7203.7835	7200.0467	7193.8154	7185.401	7184.0276	7177.5725	7169.507	
(5,1,+A)		(4,0,+A) 16.1335	(4,1,+A) 26.1012	(6,0,+A) 33.8759	(5,1,-A) 34.5156	(4,2,+A) 42.345	(6,1,+A) 43.694	(5,2,-A) 50.4108	(6,2,+A) 60.0956
	7227.6228	-	7201.5216	7193.7459	-	7185.2771	7183.9281	7177.2118	7167.5284
(5,1,-A)		(5,0,+A) 24.1988	(4,1,-A) 26.3795	(5,1,+A) 34.0983	(4,2,-A) 42.3438	(6,1,-A) 44.2782	(5,2,+A) 50.4135	(6,2,-A) 60.0903	
	7227.9972	7203.7984	7201.6171	7193.8989	7185.654	7183.7185	7177.5848	7167.9077	
(2,2,-A)		(1,1,-A) 11.7328	(2,1,+A) 14.9043	(3,1,-A) 19.8701	(2,2,+A) 31.049	(3,2,-A) 35.8898	(3,3,-A) 44.2928		
	7222.1465	7210.4137	7207.2421	7202.2755	-	7186.2566	7177.8538		
(2,2,+A)		(1,1,+A) 11.7049	(2,1,-A) 14.9878	(3,1,+A) 19.7031	(2,2,-A) 31.0489	(3,2,+A) 35.8902	(3,3,+A) 44.2928		
	7222.1286	7210.4237	7207.1402	7202.4259	7191.0785	-	7177.8362		
(3,2,-A)		(2,1,-A) 14.9878	(3,1,+A) 19.7031	(4,1,-A) 26.3795	(2,2,-A) 31.0489	(3,2,+A) 35.8902	(4,2,-A) 42.3438	(3,3,+A) 44.2928	(4,3,-A) 50.7463
	7226.7977	-	7207.0946	7200.4178	7195.75	7190.9075	7184.4531	7182.5047	7176.0521
	7226.9452	-	7207.2421	7200.5668	7195.8972	7191.0554	7184.6015	7182.6535	-
(3,2,+A)		(2,1,+A) 14.9043	(3,1,-A) 19.8701	(4,1,+A) 26.1012	(2,2,+A) 31.049	(3,2,-A) 35.8898	(4,2,+A) 42.345	(3,3,-A) 44.2928	(4,3,+A) 50.7463

	7226.9471	7212.0428	7207.076	7200.8449	7195.8972	-	7184.6015	7182.6535	7176.2009	
(4,2,-A)		(3,1,-A)	(4,1,+A)	(5,1,-A)	(3,2,-A)	(4,2,+A)	(3,3,-A)	(5,2,-A)	(4,3,+A)	(5,3,-A)
		19.8701	26.1012	34.5156	35.8898	42.345	44.2928	50.4108	50.7463	58.813
	7233.3726	-	7207.2713	7198.8569	7197.4835	7191.0269	-	-	7182.6262	7174.5608
(1,+0,E)		(1,-1,E)	(2,-1,E)	(0,+0,E)	(2,+0,E)	(1,+1,E)	(2,+1,E)			
		5.4897	8.7166	9.122	13.9628	16.2412	19.4686			
	7203.4676	7197.9778	-	7194.3465	7189.5046	7187.2255	7183.9993			
(2,+0,E)		(1,-1,E)	(2,-1,E)	(1,+0,E)	(3,-1,E)	(1,+1,E)	(3,+0,E)	(2,+1,E)	(3,+1,E)	
		5.4897	8.7166	10.7357	13.5565	16.2412	18.8026	19.4686	24.3097	
	7206.6771	7201.1873	7197.9613	7195.9415	7193.1195	-	7187.8737	7187.2084	7182.367	
(3,+0,E)		(2,-1,E)	(3,-1,E)	(2,+0,E)	(2,+1,E)	(4,-1,E)	(3,+1,E)	(4,+0,E)	(4,+1,E)	
		8.7166	13.5565	13.9628	19.4686	20.0091	24.3097	25.2542	30.7644	
	7211.4971	7202.7805	7197.9405	7197.5346	7192.0288	7191.4875	7187.1868	7186.2423	7180.7334	
	7211.5221	7202.8055	-	7197.5588	7192.0525	7191.5118	-	7186.2669	7180.7583	
(4,+0,E)		(3,-1,E)	(3,+0,E)	(4,-1,E)	(3,+1,E)	(5,-1,E)	(4,+1,E)	(5,+0,E)	(5,+1,E)	
		13.5565	18.8026	20.0091	24.3097	28.0735	30.7644	33.3165	38.8326	
	7217.9081	-	7199.1056	7197.8989	7193.5973	-	7187.1425	7184.5908	7179.0755	
	7217.9401	7204.3836	-	7197.9316	7193.6304	7189.8654	7187.1768	7184.6233	7179.1083	
	7218.01	-	7199.2074	7198.0016	7193.6998	7189.9357	7187.2452	7184.693	-	
(5,+0,E)		(4,-1,E)	(4,+0,E)	(5,-1,E)	(4,+1,E)	(6,-1,E)	(5,+1,E)	(6,+0,E)	(6,+1,E)	
		20.0091	25.2542	28.0735	30.7644	37.7492	38.8326	42.9878	48.5142	
	7225.9442	-	7200.69	7197.8708	7195.1802	7188.1942	7187.1114	-	7177.4304	
	7225.9622	7205.9532	7200.708	7197.8886	7195.1979	-	7187.1284	7182.9744	7177.4482	
	7226.0118	7206.0027	7200.7576	-	7195.2481	7188.2623	-	7183.0245	7177.4972	
(6,+0,E)		(5,-1,E)	(5,+0,E)	(6,-1,E)	(5,+1,E)	(6,+1,E)	(7,-1,E)	(7,+0,E)	(7,+1,E)	
		28.0735	33.3165	37.7492	38.8326	48.5142	49.0352	54.2664	59.8092	
	7235.5791	7207.5055	7202.2624	7197.8301	7196.7464	-	7186.5436	7181.313	7175.7699	
	7235.5916	7207.518	7202.2755	7197.8423	7196.7584	7187.0764	7186.5565	7181.3258	-	
(7,+0,E)		(6,-1,E)	(6,+0,E)	(6,+1,E)	(7,-1,E)	(7,+1,E)	(8,-1,E)	(8,+0,E)	(8,+1,E)	
		37.7492	42.9878	48.5142	49.0352	59.8092	61.9303	67.1503	72.7174	
	7246.8271	7209.0779	7203.839	-	7197.7926	7187.0172	7184.8961	7179.6772	7174.1102	
(1,+1,E)		(0,+0,E)	(1,+0,E)	(2,+0,E)	(2,+1,E)	(2,+2,E)				
		9.122	10.7357	13.9628	19.4686	20.3003				
	7208.0876	7198.9655	7197.3513	7194.1245	7188.6182	7187.7868				
(2,-1,E)		(1,-1,E)	(1,+0,E)	(3,-1,E)	(2,+0,E)	(3,+0,E)	(2,-2,E)	(3,-2,E)		
		5.4897	10.7357	13.5565	13.9628	18.8026	22.841	27.6819		
	7204.6243	-	7193.8885	7191.0666	7190.6607	7185.8212	7181.7831	7176.9429		
(2,+1,E)		(1,+0,E)	(2,+0,E)	(1,+1,E)	(3,+0,E)	(2,+2,E)	(3,+1,E)	(3,+2,E)		
		10.7357	13.9628	16.2412	18.8026	20.3003	24.3097	25.1412		
	7211.0455	7200.3098	7197.0817	7194.8052	-	7190.7444	7186.7357	7185.9042		
	7211.366	-	7197.4032	7195.1252	7192.5622	7191.0666	7187.0559	7186.224		
(4,-1,E)		(3,-1,E)	(3,+0,E)	(4,+0,E)	(3,-2,E)	(5,-1,E)	(5,+0,E)	(4,-2,E)	(5,-2,E)	
		13.5565	18.8026	25.2542	27.6819	28.0735	33.3165	34.1368	42.2058	
	7215.8833	7202.3268	7197.0817	7190.6283	7188.2005	7187.8093	7182.5674	7181.7472	7173.6787	
(4,+1,E)		(3,+0,E)	(3,+1,E)	(3,+2,E)	(4,+0,E)	(4,+2,E)	(5,+0,E)	(5,+1,E)	(5,+2,E)	
		18.8026	24.3097	25.1412	25.2542	31.5961	33.3165	38.8326	39.6651	
	7222.5387	-	7198.229	-	7197.2851	7190.942	7189.2211	7183.7059	7182.8744	
(5,-1,E)		(4,-1,E)	(4,+0,E)	(5,+0,E)	(4,-2,E)	(6,-1,E)	(5,-2,E)	(6,+0,E)	(6,-2,E)	
		20.0091	25.2542	33.3165	34.1368	37.7492	42.2058	42.9878	51.8894	
	7223.9346	7203.9255	7198.6811	7190.6179	7189.7969	7186.1857	7181.7298	7180.9476	-	
(5,+1,E)		(4,+0,E)	(4,+1,E)	(4,+2,E)	(5,+0,E)	(5,+2,E)	(6,+0,E)	(6,+1,E)	(6,+2,E)	
		25.2542	30.7644	31.5961	33.3165	39.6651	42.9878	48.5142	49.3488	
	7230.6139	7205.3597	7199.8495	7199.0184	7197.2978	7190.9483	7187.6255	7182.0996	7181.2656	
(6,-1,E)		(5,-1,E)	(5,+0,E)	(5,-2,E)	(6,+0,E)	(7,-1,E)	(6,-2,E)	(7,+0,E)	(7,-2,E)	
		28.0735	33.3165	42.2058	42.9878	49.0352	51.8894	54.2664	63.188	
	7233.5255	7205.4519	7200.208	-	-	7184.4895	7181.6354	7179.2584	7170.3386	
(6,+1,E)		(5,+0,E)	(5,+1,E)	(5,+2,E)	(6,+0,E)	(6,+2,E)	(7,+0,E)	(7,+1,E)	(7,+2,E)	
		33.3165	38.8326	39.6651	42.9878	49.3488	54.2664	59.8092	60.6473	
	7240.2327	-	7201.4001	7200.5668	7197.2447	7190.8838	7185.9656	7180.4239	7179.5857	
(7,-1,E)		(6,-1,E)	(6,+0,E)	(6,-2,E)	(7,+0,E)	(8,-1,E)	(7,-2,E)	(8,+0,E)	(8,-2,E)	
		37.7492	42.9878	51.8894	54.2664	61.9303	63.188	67.1503	76.1021	
	7244.792	7207.0428	7201.8037	-	7190.5253	7182.8625	-	7177.6428	7168.6908	
(7,+1,E)		(6,+0,E)	(6,+1,E)	(6,+2,E)	(7,+0,E)	(7,+2,E)	(8,+0,E)	(8,+1,E)	(8,+2,E)	
		42.9878	48.5142	49.3488	54.2664	60.6473	67.1503	72.7174	73.5611	
	7251.466	7208.4782	7202.9515	7202.1166	7197.1994	-	-	7178.7485	7177.9054	
	7251.504	-	7202.9898	-	7197.237	7190.8556	7184.3535	7178.7866	7177.9427	
(8,-1,E)		(7,-1,E)	(7,+0,E)	(7,-2,E)	(8,+0,E)	(8,-2,E)	(9,-1,E)	(9,+0,E)	(9,-2,E)	

	49.0352	54.2664	63.188	67.1503	76.1021	76.4335	81.637	90.6322
7257.6401	7208.605	7203.3725	-	7190.4889	7181.538	-	7176.0024	7167.0086
(2,+2,E)	(1,+1,E)	(2,+1,E)	(3,+1,E)	(3,+2,E)	(3,+3,E)			
	16.2412	19.4686	24.3097	25.1412	42.8417			
7215.7063	7199.4651	7196.2377	7191.3958	7190.5642	7172.8655			
(3,+2,E)	(2,+1,E)	(2,+2,E)	(3,+1,E)	(4,+1,E)	(4,+2,E)	(3,+3,E)	(4,+3,E)	
	19.4686	20.3003	24.3097	30.7644	31.5961	42.8417	49.2953	
7220.5469	7201.0783	7200.2465	7196.2377	7189.7819	7188.95	7177.7055	-	
(4,+2,E)	(3,+1,E)	(3,+2,E)	(4,+1,E)	(5,+1,E)	(5,+2,E)	(3,+3,E)	(4,+3,E)	(5,+3,E)
	24.3097	25.1412	30.7644	38.8326	39.6651	42.8417	49.2953	57.3624
7226.9858	7202.6761	7201.8446	7196.2214	7188.152	7187.32	-	7177.6894	7169.6245
(5,+2,E)	(4,+1,E)	(4,+2,E)	(5,+1,E)	(6,+1,E)	(4,+3,E)	(6,+2,E)	(5,+3,E)	(6,+3,E)
	30.7644	31.5961	38.8326	48.5142	49.2953	49.3488	57.3624	67.0428
7235.0165	7204.2522	7203.42	7196.1836	7186.5021	7185.7206	7185.667	7177.6549	7167.9743
(6,+2,E)	(5,+1,E)	(5,+2,E)	(6,+1,E)	(5,+3,E)	(7,+1,E)	(7,+2,E)	(6,+3,E)	(7,+3,E)
	38.8326	39.6651	48.5142	57.3624	59.8092	60.6473	67.0428	78.3367
7244.6666	7205.8341	7205.0014	7196.1531	-	7184.857	7184.0189	7177.6246	-
(7,+2,E)	(6,+1,E)	(6,+2,E)	(7,+1,E)	(6,+3,E)	(8,+1,E)	(8,+2,E)	(7,+3,E)	(8,+3,E)
	48.5142	49.3488	59.8092	67.0428	72.7174	73.5611	78.3367	91.2441
7255.9099	7207.3956	7206.5612	7196.1017	7188.8663	7183.1922	7182.3486	7177.5725	-

Table 2: List of tentatively assigned CDMs. The energy of the transitions are the experimental ones. Energies of non-observed transitions are labeled by a dash symbol.

upper state	E (cm <sup>-1</sup> )	lower state E (cm <sup>-1</sup> ), lines E (cm <sup>-1</sup> )								
(1,0,+A)		(0,0,+A)	(2,0,+A)	(1,1,-A)	(2,1,+A)					
		0	4.8405	11.7328	14.9043					
	7205.3378	7205.3378	7200.4978	7193.6059	7190.433					
(2,0,+A)		(1,0,+A)	(3,0,+A)	(1,1,+A)	(2,1,-A)	(3,1,+A)				
		1.6135	9.6806	11.7049	14.9878	19.7031				
	7208.5211	7206.9076	7198.841	7196.8169	7193.5341	7188.8176				
(2,1,-A)		(2,0,+A)	(1,1,-A)	(2,1,+A)	(3,1,-A)	(2,2,+A)	(3,2,-A)			
		4.8405	11.7328	14.9043	19.8701	31.049	35.8898			
	7208.6052	7203.7647	7196.8717	7193.6998	-	7177.556	7172.7151			
(3,0,+A)		(2,0,+A)	(2,1,+A)	(4,0,+A)	(3,1,-A)	(4,1,+A)				
		4.8405	14.9043	16.1335	19.8701	26.1012				
	7213.3014	7208.4609	7198.3973	7197.168	7193.4312	7187.1994				
(3,+1,E)		(2,+0,E)	(3,+0,E)	(2,+1,E)	(2,+2,E)	(3,+2,E)	(4,+0,E)	(4,+1,E)	(4,+2,E)	
		13.9628	18.8026	19.4686	20.3003	25.1412	25.2542	30.7644	31.5961	
	7215.9894	7202.0266	-	7196.5219	7195.6888	7190.8479	7190.7354	7185.2255	-	
	7216.1683	-	7197.3657	7196.6991	7195.867	7191.0269	7190.9153	-	7184.5713	
(4,0,+A)		(3,0,+A)	(3,1,+A)	(5,0,+A)	(4,1,-A)	(5,1,+A)				
		9.6806	19.7031	24.1988	26.3795	34.0983				
	7219.686	7210.0054	7199.9833	7195.4871	7193.3057	7185.5878				
(4,2,-A)		(3,1,-A)	(4,1,+A)	(5,1,-A)	(3,2,-A)	(4,2,+A)	(3,3,-A)	(5,2,-A)	(4,3,+A)	(5,3,-A)
		19.8701	26.1012	34.5156	35.8898	42.345	44.2928	50.4108	50.7463	58.813
	7233.2743	-	7207.1731	7198.7576	7197.3855	7190.9297	-	7182.8625	7182.5279	7174.4626
(5,2,-A)		(4,1,-A)	(5,1,+A)	(4,2,-A)	(6,1,-A)	(5,2,+A)	(4,3,-A)	(5,3,+A)	(6,2,-A)	(6,3,-A)
		26.3795	34.0983	42.3438	44.2782	50.4135	50.7463	58.813	60.0903	68.4927
	7241.3805	-	7207.2821	7199.0374	7197.1012	7190.9659	7190.6343	7182.5674	7181.29	-
(8,+0,E)		(7,-1,E)	(7,+0,E)	(7,+1,E)	(8,-1,E)	(8,+1,E)	(9,-1,E)	(9,+0,E)	(9,+1,E)	
		49.0352	54.2664	59.8092	61.9303	72.7174	76.4335	81.637	87.2386	
	7259.6455	-	7205.3791	7199.836	7197.7149	7186.927	7183.2108	7178.0081	7172.4079	
(9,1,-A)		(8,1,-A)	(9,0,+A)	(9,1,+A)	(8,2,-A)	(9,2,+A)	(10,1,-A)			
		68.6803	72.5699	82.0677	84.285	98.8239	99.581			
	7276.6885	7208.0082	7204.1195	7194.6216	-	7177.8638	7177.1084			