

Table 1: Sorted list by frequency of the transitions used to analyse the detected molecules in this work. These transitions were employed in the MADCUBA fitting to derive their physical parameters (Table 3). Frequency shows the rest frequency of the transitions in GHz. Transition lists the upper and lower energy levels involved in each transition. The log  $I$  is the logarithm of the line intensity in nm<sup>2</sup> MHz;  $E_{\text{up}}$  is the energy of higher level in K, and  $\tau$  is the optical depth of the transitions.

Frequency (GHz)	Species	Transition	log $I$ (nm <sup>2</sup> MHz)	$E_{\text{up}}$ (K)	$\tau(\times 10^{-2})$
217.003240	HDCS	$7_{3,5} \rightarrow 6_{3,4}$	-3.1	122	$1.5 \pm 0.8$
217.005500	HDCS	$7_{3,4} \rightarrow 6_{3,3}$	-3.1	122	$1.5 \pm 0.8$
217.022509	CH <sub>3</sub> COCH <sub>3</sub>	$19_{3,16,0} \rightarrow 18_{4,15,1}$	-4.5	115	$11 \pm 3$
217.022509	CH <sub>3</sub> COCH <sub>3</sub>	$19_{4,16,0} \rightarrow 18_{3,15,1}$	-4.5	115	$11 \pm 3$
217.027801	CH <sub>3</sub> <sup>18</sup> OH	$34_{4,30,6} \rightarrow 33_{1,33,6}$	-11.1	1930	$2.5 \cdot 10^{-16}$
217.044616	<sup>13</sup> CH <sub>3</sub> OH	$14_{1,13,0} \rightarrow 13_{2,12,0}$	-4.1	250	$14.4 \pm 1.4$
217.052822	C <sub>2</sub> H <sub>5</sub> OCHO	$40_{3,38,0} \rightarrow 39_{3,37,0}$	-4.0	220	$2 \pm 2$
217.053744	CH <sub>2</sub> (OH)CHO	$33_{10,23,0} \rightarrow 33_{9,24,0}$	-3.6	370	$2.0 \pm 1.2$
217.070504	CH <sub>3</sub> COCH <sub>3</sub>	$19_{3,16,0} \rightarrow 18_{4,15,0}$	-4.7	115	$7 \pm 2$
217.070504	CH <sub>3</sub> COCH <sub>3</sub>	$19_{4,16,0} \rightarrow 18_{3,15,0}$	-5.0	115	$4 \pm 2$
217.082917	CH <sub>3</sub> CHO	$35_{8,27,6} \rightarrow 36_{11,25,3}$	-7.7	1100	$0.0 \pm 0.8$
217.100578	CH <sub>3</sub> COOH	$35_{20,16,0,0} \rightarrow 34_{23,12,0,0}$	-8.9	560	$0 \pm 2$
217.104919	SiO	$5_0 \rightarrow 4_0$	-1.32	31	$6.7 \pm 0.9$
217.132877	CH <sub>3</sub> OD	$9_{1,8,1} \rightarrow 8_{2,6,1}$	-4.3	107	$13 \pm 3$
217.139724	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	$21_{4,17,0} \rightarrow 20_{4,16,1}$	-3.6	124	$4.0 \pm 1.1$
217.150932	CH <sub>3</sub> NCO	$25_{2,23,0} \rightarrow 24_{2,22,0}$	-3.6	159	$8.2 \pm 1.8$
217.164881	CH <sub>3</sub> NCO	$25_{-3,0,1} \rightarrow 24_{-3,0,1}$	-3.6	200	$5.1 \pm 1.6$
217.172867	CH <sub>3</sub> <sup>18</sup> OH	$14_{1,14,1} \rightarrow 13_{2,12,1}$	-4.2	240	$2 \pm 4$
217.177056	CH <sub>3</sub> OCH <sub>3</sub>	$36_{4,32,1} \rightarrow 36_{3,33,1}$	-4.7	640	$2.6 \pm 1.1$
217.189668	CH <sub>3</sub> OCH <sub>3</sub>	$22_{4,19,3} \rightarrow 22_{3,20,3}$	-5.0	250	$3.0 \pm 1.1$
217.189669	CH <sub>3</sub> OCH <sub>3</sub>	$22_{4,19,5} \rightarrow 22_{3,20,5}$	-4.8	250	$4.4 \pm 1.1$
217.191400	CH <sub>3</sub> OCH <sub>3</sub>	$22_{4,19,1} \rightarrow 22_{3,20,1}$	-4.4	250	$11.9 \pm 1.5$
217.193132	CH <sub>3</sub> OCH <sub>3</sub>	$22_{4,19,0} \rightarrow 22_{3,20,0}$	-4.6	250	$7.4 \pm 1.3$
217.238538	DCN	$3_{0,0} \rightarrow 2_{0,0}$	-1.39	21	$29.2 \pm 1.4$
217.261022	C <sub>2</sub> H <sub>5</sub> <sup>13</sup> CN	$24_{3,21} \rightarrow 23_{3,20}$	-2.7	139	$1.7 \pm 0.9$
217.261852	CH <sub>3</sub> COOH	$62_{36,26,0,0} \rightarrow 62_{36,27,0,0}$	-7.4	1750	$0 \pm 2$
217.262302	C <sub>2</sub> H <sub>5</sub> OH	$13_{0,13,1} \rightarrow 12_{1,12,1}$	-4.2	136	$6.8 \pm 1.9$
217.262949	CH <sub>3</sub> <sup>18</sup> OH	$24_{1,24,6} \rightarrow 25_{4,21,6}$	-10.4	1340	$0 \pm 4$
217.263689	HDCS	$7_{2,5} \rightarrow 6_{2,4}$	-3.0	78	$2.3 \pm 0.8$
217.265145	CH <sub>3</sub> COOH	$58_{34,25,0,2} \rightarrow 58_{32,26,0,1}$	-7.0	1530	$0 \pm 2$
217.269794	SO <sub>2</sub>	$94_{21,73} \rightarrow 95_{20,76}$	-10.2	5200	$0.0 \pm 0.5$
217.271611	CH <sub>2</sub> (OH)CHO	$31_{4,27,0} \rightarrow 31_{3,28,0}$	-3.7	290	$2.0 \pm 1.2$
217.272514	CH <sub>3</sub> <sup>18</sup> OH	$32_{6,27,2} \rightarrow 33_{4,29,2}$	-9.1	1350	$0 \pm 4$
217.275916	gGg' - (CH <sub>2</sub> OH) <sub>2</sub>	$21_{6,15,1} \rightarrow 20_{6,14,0}$	-4.2	131	$1.0 \pm 1.3$
217.312626	CH <sub>3</sub> OCHO	$17_{4,13,3} \rightarrow 16_{4,12,3}$	-4.3	290	$6.3 \pm 1.2$
217.325870	<sup>13</sup> CH <sub>3</sub> CHO	$30_{3,28,-2} \rightarrow 29_{4,26,-2}$	-7.9	640	$0.0 \pm 1.1$
217.333395	c - C <sub>2</sub> H <sub>4</sub> O	$53_{35,18} \rightarrow 53_{34,19}$	-6.9	3000	$0.0 \pm 0.6$
217.390186	CH <sub>3</sub> <sup>18</sup> OH	$29_{4,25,0} \rightarrow 30_{1,30,0}$	-8.7	1050	$0 \pm 4$
217.390703	<sup>13</sup> CH <sub>3</sub> CHO	$12_{1,12,1} \rightarrow 11_{1,11,1}$	-3.4	70	$1.8 \pm 1.5$
217.398568	HC <sup>13</sup> CCN	$24 \rightarrow 23$	-1.30	130	$2.0 \pm 0.7$
217.399550	<sup>13</sup> CH <sub>3</sub> OH	$10_{2,8,0} \rightarrow 9_{3,7,0}$	-4.3	162	$12.7 \pm 1.3$

217.400162	$^{13}\text{CH}_3\text{CHO}$	$12_{1,12,0} \rightarrow 11_{1,11,0}$	-3.4	70	$1.8 \pm 1.5$
217.418711	$\text{CH}_3\text{OH}$	$15_{3,12,6} \rightarrow 14_{1,14,6}$	-11.4	940	$0.0 \pm 1.1$
217.419574	$\text{HCC}^{13}\text{CN}$	$24 \rightarrow 23$	-1.30	130	$4.0 \pm 0.6$
217.438703	$\text{CH}_3\text{CONH}_2$	$27_{18,9,0,2} \rightarrow 26_{20,7,0,2}$	-7.0	340	$0 \pm 3$
217.447907	$\text{CH}_2\text{DOH}$	$18_{1,17,2} \rightarrow 18_{2,17,0}$	-4.5	390	$2.0 \pm 1.9$
217.449995	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$24_{1,24,0} \rightarrow 23_{1,23,1}$	-3.6	136	$4.5 \pm 1.1$
217.450270	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$24_{0,24,0} \rightarrow 23_{0,23,1}$	-3.7	136	$3.5 \pm 1.1$
217.469279	$\text{CH}_3\text{CHO}$	$14_{3,11,0} \rightarrow 14_{2,12,0}$	-4.3	118	$3.9 \pm 0.8$
217.473888	$\text{CH}_3\text{COOH}$	$10_{9,2,0,1} \rightarrow 9_{8,1,0,2}$	-4.7	56	$3 \pm 2$
217.474283	$\text{C}_2\text{H}_5\text{CN}$	$62_{2,60} \rightarrow 63_{1,63}$	-7.2	840	$0.0 \pm 1.5$
217.491175	$\text{CHD}_2\text{OH}$	$7_{0,1,2} \rightarrow 6_{1,1,2}$	-4.3	74	$4 \pm 3$
217.496665	$\text{C}_2\text{H}_5\text{OH}$	$13_{1,13,1} \rightarrow 12_{0,12,1}$	-4.2	135	$7.4 \pm 1.9$
217.496667	$\text{c} - \text{C}_2\text{H}_4\text{O}$	$55_{35,20} \rightarrow 55_{34,21}$	-7.1	3300	$0.0 \pm 0.6$
217.499474	$\text{CH}_3^{18}\text{OH}$	$37_{1,36,3} \rightarrow 36_{3,33,3}$	-9.8	1880	$0 \pm 4$
217.516550	$\text{CH}_3^{18}\text{OH}$	$16_{11,6,4} \rightarrow 15_{8,7,7}$	-8.5	1200	$0 \pm 4$
217.539718	$\text{gGg}' - (\text{CH}_2\text{OH})_2$	$22_{2,20,0} \rightarrow 21_{2,19,1}$	-3.9	127	$2.1 \pm 1.3$
217.548152	$\text{C}_2\text{H}_5\text{OH}$	$5_{1,4,1} \rightarrow 4_{0,4,0}$	-4.7	76	$2.4 \pm 1.7$
217.549328	$\text{C}_2\text{H}_5\text{OH}$	$25_{3,22,0} \rightarrow 24_{4,20,1}$	-4.9	340	$0.7 \pm 1.6$
217.550411	$\text{SiS}$	$13_{16} \rightarrow 12_{16}$	-25	$1.63 \cdot 10^4$	$2.0 \cdot 10^{-42}$
217.582747	$\text{CH}_3\text{CONH}_2$	$18_{3,15,0,0} \rightarrow 17_{4,14,0,0}$	-3.8	118	$3 \pm 3$
217.582747	$\text{CH}_3\text{CONH}_2$	$18_{4,15,0,0} \rightarrow 17_{4,14,0,0}$	-5.1	118	$0 \pm 3$
217.582747	$\text{CH}_3\text{CONH}_2$	$18_{4,15,0,0} \rightarrow 17_{3,14,0,0}$	-3.8	118	$3 \pm 3$
217.582747	$\text{CH}_3\text{CONH}_2$	$18_{3,15,0,0} \rightarrow 17_{3,14,0,0}$	-5.1	118	$0 \pm 3$
217.587548	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$21_{2,19,1} \rightarrow 20_{2,18,0}$	-3.7	117	$3.5 \pm 1.1$
217.588868	$\text{C}_2\text{H}_3\text{CN}$	$32_{3,30} \rightarrow 33_{1,33}$	-7.0	260	$0.0 \pm 1.9$
217.595174	$\text{CH}_3\text{NCO}$	$25_{0,0,2} \rightarrow 24_{0,0,2}$	-3.6	188	$6.0 \pm 1.7$
217.595174	$\text{CH}_3\text{NCO}$	$25_{-1,0,2} \rightarrow 24_{-1,0,2}$	-3.6	194	$5.6 \pm 1.6$
217.603747	$\text{CH}_2(\text{OH})\text{CHO}$	$24_{5,19,0} \rightarrow 23_{6,18,0}$	-3.9	187	$1.4 \pm 1.2$
217.607963	$\text{CH}_3\text{COOH}$	$20_{1,20,1,2} \rightarrow 19_{0,19,1,1}$	-4.6	230	$0.7 \pm 0.6$
217.607963	$\text{CH}_3\text{COOH}$	$20_{0,20,1,2} \rightarrow 19_{1,19,1,1}$	-4.6	230	$0.7 \pm 0.6$
217.607963	$\text{CH}_3\text{COOH}$	$20_{1,20,1,2} \rightarrow 19_{1,19,1,1}$	-4.9	230	$0.4 \pm 0.6$
217.607963	$\text{CH}_3\text{COOH}$	$20_{0,20,1,2} \rightarrow 19_{0,19,1,1}$	-4.9	230	$0.4 \pm 0.6$
217.608054	$\text{CH}_2(\text{OH})\text{CHO}$	$25_{1,24,0} \rightarrow 25_{0,25,0}$	-4.1	171	$1.0 \pm 1.2$
217.611047	$\text{CH}_2(\text{OH})\text{CHO}$	$25_{2,24,0} \rightarrow 25_{1,25,0}$	-4.1	171	$1.0 \pm 1.2$
217.615700	$\text{c} - \text{C}_2\text{H}_4\text{O}$	$15_{4,11} \rightarrow 15_{3,12}$	-3.7	220	$1.1 \pm 0.7$
217.615747	$\text{c} - \text{C}_2\text{H}_4\text{O}$	$15_{5,11} \rightarrow 15_{4,12}$	-3.5	220	$1.8 \pm 0.7$
217.624026	$\text{CH}_3\text{OH}$	$36_{9,27,5} \rightarrow 35_{6,29,8}$	-11.0	2300	$0.0 \pm 1.1$
217.626127	$\text{CH}_2(\text{OH})\text{CHO}$	$9_{5,5,0} \rightarrow 8_{4,4,0}$	-3.7	40	$3.6 \pm 1.3$
217.642677	$\text{CH}_3\text{OH}$	$15_{6,9,3} \rightarrow 16_{5,11,3}$	-4.9	750	$3.8 \pm 1.2$
217.642678	$\text{CH}_3\text{OH}$	$15_{6,10,3} \rightarrow 16_{5,12,3}$	-4.9	750	$3.8 \pm 1.2$
217.648198	$\text{C}_2\text{H}_5\text{CN}$	$62_{3,60} \rightarrow 63_{0,63}$	-7.2	840	$0.0 \pm 1.5$
217.652088	$\text{CH}_3\text{NCO}$	$25_{2,0,1} \rightarrow 24_{2,0,1}$	-3.6	171	$7.1 \pm 1.7$
217.654810	$^{13}\text{CH}_3\text{OH}$	$3_{-2,2,0} \rightarrow 2_{2,0,0}$	-11.5	40	$0.0 \pm 0.9$
217.665067	$\text{HOCH}_2\text{CN}$	$12_{2,10,1} \rightarrow 11_{1,11,1}$	-4.8	46	$2 \pm 2$
217.692541	$\text{H}_2\text{CNH}$	$26_{4,23} \rightarrow 25_{5,20}$	-4.6	1210	$2.7 \pm 1.1$
217.701086	$\text{CH}_3\text{NCO}$	$24_{3,0,1} \rightarrow 23_{3,0,1}$	-3.7	191	$5.0 \pm 1.6$

217.742441	c – C <sub>2</sub> H <sub>4</sub> O	27 <sub>13,15</sub> → 26 <sub>16,10</sub>	–7.8	750	0.0 ± 0.6
217.757265	CH <sub>3</sub> <sup>18</sup> OH	40 <sub>3,38,1</sub> → 40 <sub>3,37,2</sub>	–8.8	1880	0 ± 4
217.776201	CH <sub>3</sub> COOH	16 <sub>4,12,1,0</sub> → 15 <sub>5,11,1,0</sub>	–4.8	210	0.6 ± 0.6
217.776369	CH <sub>3</sub> COOH	16 <sub>5,12,1,0</sub> → 15 <sub>5,11,1,0</sub>	–5.2	210	0.2 ± 0.6
217.776984	CH <sub>3</sub> COOH	16 <sub>4,12,1,0</sub> → 15 <sub>4,11,1,0</sub>	–5.2	210	0.2 ± 0.6
217.777153	CH <sub>3</sub> COOH	16 <sub>5,12,1,0</sub> → 15 <sub>4,11,1,0</sub>	–4.8	210	0.6 ± 0.6
217.791253	CH <sub>3</sub> COOH	32 <sub>24,8,0,1</sub> → 31 <sub>26,5,0,2</sub>	–8.2	500	0 ± 2
217.803743	C <sub>2</sub> H <sub>5</sub> OH	5 <sub>3,3,2</sub> → 4 <sub>2,2,2</sub>	–4.4	24	5.9 ± 1.8
217.817663	SiS	12 <sub>0</sub> → 11 <sub>0</sub>	–1.88	68	3.5 ± 0.5
217.827178	<sup>33</sup> SO	5 <sub>6,5</sub> → 4 <sub>5,4</sub>	–3.1	35	0.9 ± 0.7
217.829834	<sup>33</sup> SO	5 <sub>6,6</sub> → 4 <sub>5,5</sub>	–3.0	35	1.1 ± 0.7
217.830697	CH <sub>2</sub> (OH)CHO	9 <sub>5,4,0</sub> → 8 <sub>4,5,0</sub>	–3.7	40	3.6 ± 1.3
217.831769	<sup>33</sup> SO	5 <sub>6,7</sub> → 4 <sub>5,6</sub>	–2.9	35	1.3 ± 0.7
217.832642	<sup>33</sup> SO	5 <sub>6,8</sub> → 4 <sub>5,7</sub>	–2.8	35	1.5 ± 0.7
217.844009	aGg' – (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>2,20,0</sub> → 21 <sub>3,19,0</sub>	–4.4	127	0.7 ± 0.9
217.848300	aGg' – (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>2,20,1</sub> → 21 <sub>3,19,1</sub>	–4.8	128	0.3 ± 0.9
217.875073	CH <sub>3</sub> COOH	17 <sub>3,14,1,0</sub> → 16 <sub>4,13,1,0</sub>	–4.7	210	0.6 ± 0.6
217.875074	CH <sub>3</sub> COOH	17 <sub>4,14,1,0</sub> → 16 <sub>4,13,1,0</sub>	–5.2	210	0.2 ± 0.6
217.875079	CH <sub>3</sub> COOH	17 <sub>3,14,1,0</sub> → 16 <sub>3,13,1,0</sub>	–5.2	210	0.2 ± 0.6
217.875080	CH <sub>3</sub> COOH	17 <sub>4,14,1,0</sub> → 16 <sub>3,13,1,0</sub>	–4.7	210	0.6 ± 0.6
217.886504	CH <sub>3</sub> OH	20 <sub>1,19,1</sub> → 20 <sub>0,20,1</sub>	–4.1	510	19.8 ± 1.4
217.888414	C <sub>2</sub> H <sub>5</sub> OCHO	33 <sub>1,32,1</sub> → 32 <sub>2,31,1</sub>	–4.4	280	1 ± 2
217.888549	C <sub>2</sub> H <sub>5</sub> OCHO	33 <sub>2,32,1</sub> → 32 <sub>2,31,1</sub>	–4.0	280	1 ± 2
217.888643	C <sub>2</sub> H <sub>5</sub> OCHO	33 <sub>1,32,1</sub> → 32 <sub>1,31,1</sub>	–4.0	280	1 ± 2
217.888778	C <sub>2</sub> H <sub>5</sub> OCHO	33 <sub>2,32,1</sub> → 32 <sub>1,31,1</sub>	–4.4	280	1 ± 2
217.912999	HC <sup>13</sup> CCN	24 <sub>–1</sub> → 23 <sub>1</sub>	–1.76	450	1.4 ± 0.3
217.914798	c – C <sub>2</sub> H <sub>4</sub> O	23 <sub>11,13</sub> → 22 <sub>14,8</sub>	–7.4	550	0.0 ± 0.6
217.969828	CH <sub>3</sub> <sup>18</sup> OH	37 <sub>5,32,5</sub> → 38 <sub>8,31,2</sub>	–9.2	1990	0 ± 4
218.002461	CH <sub>3</sub> NCO	25 <sub>1,0,–3</sub> → 24 <sub>1,0,–3</sub>	–3.7	260	2.8 ± 1.5
218.010022	CH <sub>3</sub> COOH	20 <sub>1,20,0,0</sub> → 19 <sub>0,19,0,0</sub>	–4.5	113	3 ± 2
218.010022	CH <sub>3</sub> COOH	20 <sub>0,20,0,0</sub> → 19 <sub>1,19,0,0</sub>	–4.5	113	3 ± 2
218.010022	CH <sub>3</sub> COOH	20 <sub>1,20,0,0</sub> → 19 <sub>1,19,0,0</sub>	–4.6	113	2 ± 2
218.010022	CH <sub>3</sub> COOH	20 <sub>0,20,0,0</sub> → 19 <sub>0,19,0,0</sub>	–4.6	113	2 ± 2
218.022107	DC(O)NH <sub>2</sub>	11 <sub>0,11</sub> → 10 <sub>0,10</sub>	–2.5	64	9.4 ± 1.8
218.023075	CH <sub>3</sub> CONH <sub>2</sub>	16 <sub>12,4,0,0</sub> → 16 <sub>9,8,0,0</sub>	–8.1	131	0 ± 3
218.036555	C <sub>2</sub> H <sub>5</sub> OCHO	41 <sub>2,40,0</sub> → 40 <sub>2,39,0</sub>	–4.0	230	2 ± 2
218.039428	C <sub>2</sub> H <sub>5</sub> OCHO	70 <sub>6,65,0</sub> → 70 <sub>4,66,0</sub>	–6.6	680	0 ± 2
218.039456	CH <sub>3</sub> NCO	25 <sub>1,0,2</sub> → 24 <sub>1,0,2</sub>	–3.6	194	5.6 ± 1.6
218.044215	CH <sub>3</sub> COOH	20 <sub>1,20,0,1</sub> → 19 <sub>1,19,0,2</sub>	–4.4	112	3 ± 3
218.044215	CH <sub>3</sub> COOH	20 <sub>0,20,0,1</sub> → 19 <sub>0,19,0,2</sub>	–4.4	112	3 ± 3
218.044215	CH <sub>3</sub> COOH	20 <sub>1,20,0,1</sub> → 19 <sub>0,19,0,2</sub>	–4.8	112	1 ± 2
218.044215	CH <sub>3</sub> COOH	20 <sub>0,20,0,1</sub> → 19 <sub>1,19,0,2</sub>	–4.8	112	1 ± 2
218.044534	CH <sub>3</sub> NCO	25 <sub>0,0,3</sub> → 24 <sub>0,0,3</sub>	–3.7	250	3.0 ± 1.5
218.050177	CH <sub>3</sub> COOH	18 <sub>3,16,1,0</sub> → 17 <sub>2,15,1,0</sub>	–4.6	210	0.7 ± 0.6
218.050177	CH <sub>3</sub> COOH	18 <sub>2,16,1,0</sub> → 17 <sub>3,15,1,0</sub>	–4.6	210	0.7 ± 0.6
218.050177	CH <sub>3</sub> COOH	18 <sub>3,16,1,0</sub> → 17 <sub>3,15,1,0</sub>	–5.1	210	0.2 ± 0.6

218.050177	CH <sub>3</sub> COOH	18 <sub>2,16,1,0</sub> → 17 <sub>2,15,1,0</sub>	-5.1	210	0.2 ± 0.6
218.069900	CH <sub>3</sub> NCO	25 <sub>1,0,3</sub> → 24 <sub>1,0,3</sub>	-3.7	260	2.9 ± 1.5
218.073385	CH <sub>2</sub> DOH	32 <sub>3,30,2</sub> → 32 <sub>3,30,1</sub>	-8.9	1190	0.0 ± 1.8
218.073998	HC(O)NH <sub>2</sub>	57 <sub>6,51</sub> → 57 <sub>6,52</sub>	-6.1	1810	0.0 ± 1.5
218.077116	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>20,3,0</sub> → 21 <sub>20,2,1</sub>	-4.6	320	0.3 ± 0.9
218.077116	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>20,2,0</sub> → 21 <sub>20,1,1</sub>	-4.7	320	0.3 ± 0.9
218.091411	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>3,18,1</sub> → 19 <sub>2,17,1</sub>	-4.9	119	4 ± 2
218.091411	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>2,18,1</sub> → 19 <sub>3,17,1</sub>	-5.4	119	1 ± 2
218.091448	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>3,18,1</sub> → 19 <sub>2,17,2</sub>	-5.1	119	3 ± 2
218.091448	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>2,18,1</sub> → 19 <sub>3,17,2</sub>	-5.1	119	3 ± 2
218.108438	CH <sub>3</sub> OCHO	17 <sub>4,13,5</sub> → 16 <sub>4,12,5</sub>	-4.3	290	6.4 ± 1.2
218.109544	CH <sub>2</sub> DOH	18 <sub>0,18,0</sub> → 17 <sub>1,16,2</sub>	-4.8	360	1.2 ± 1.9
218.113149	CH <sub>3</sub> OH	26 <sub>10,16,3</sub> → 25 <sub>13,13,0</sub>	-9.7	1620	0.0 ± 1.1
218.113149	CH <sub>3</sub> OH	26 <sub>10,17,3</sub> → 25 <sub>13,12,0</sub>	-9.7	1620	0.0 ± 1.1
218.125574	C <sub>2</sub> H <sub>5</sub> OCHO	41 <sub>1,40,0</sub> → 40 <sub>1,39,0</sub>	-4.0	230	2 ± 2
218.126928	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>19,4,0</sub> → 21 <sub>19,3,1</sub>	-4.4	300	0.5 ± 0.9
218.126928	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>19,3,0</sub> → 21 <sub>19,2,1</sub>	-4.6	300	0.4 ± 0.9
218.127207	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>3,18,0</sub> → 19 <sub>2,17,1</sub>	-4.8	119	6 ± 2
218.127207	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>2,18,0</sub> → 19 <sub>3,17,1</sub>	-4.8	119	6 ± 2
218.127207	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>2,18,0</sub> → 19 <sub>2,17,1</sub>	-4.8	119	6 ± 2
218.127207	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>3,18,0</sub> → 19 <sub>3,17,1</sub>	-4.8	119	6 ± 2
218.127863	CHD <sub>2</sub> OH	7 <sub>2,1,0</sub> → 7 <sub>1,2,0</sub>	-4.7	69	1.5 ± 1.9
218.138971	CH <sub>2</sub> DOH	35 <sub>4,31,2</sub> → 35 <sub>4,31,0</sub>	-7.4	1430	0.0 ± 1.8
218.143815	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	14 <sub>1,13,0</sub> → 13 <sub>2,12,0</sub>	-4.5	96	0.8 ± 0.8
218.143839	gGg' - (CH <sub>2</sub> OH) <sub>2</sub>	21 <sub>5,16,0</sub> → 20 <sub>5,15,1</sub>	-4.1	126	1.5 ± 1.3
218.144614	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	14 <sub>1,13,2</sub> → 13 <sub>2,12,2</sub>	-4.5	96	0.8 ± 0.8
218.144753	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	14 <sub>1,13,1</sub> → 13 <sub>2,12,1</sub>	-4.5	96	0.8 ± 0.8
218.155689	CH <sub>3</sub> OD	14 <sub>-1,14,0</sub> → 14 <sub>0,14,0</sub>	-3.6	240	25 ± 4
218.162929	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>3,18,0</sub> → 19 <sub>2,17,0</sub>	-4.7	119	7 ± 2
218.162929	CH <sub>3</sub> COCH <sub>3</sub>	20 <sub>2,18,0</sub> → 19 <sub>3,17,0</sub>	-4.9	119	4 ± 2
218.180385	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>18,5,0</sub> → 21 <sub>18,4,1</sub>	-4.3	280	0.7 ± 0.9
218.180385	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>18,4,0</sub> → 21 <sub>18,3,1</sub>	-4.4	280	0.6 ± 0.9
218.181680	HC(O)NH <sub>2</sub>	10 <sub>1,9</sub> → 9 <sub>1,8</sub>	-3.1	480	7.6 ± 0.7
218.189200	H <sup>13</sup> C(O)NH <sub>2</sub>	10 <sub>1,9</sub> → 9 <sub>1,8</sub>	-2.5	61	3.9 ± 0.5
218.198998	O <sup>13</sup> CS	18 → 17	-2.7	99	11.4 ± 0.5
218.208741	CH <sub>3</sub> COOH	42 <sub>18,24,1,0</sub> → 41 <sub>20,21,1,0</sub>	-9.0	860	0.0 ± 0.6
218.208877	CH <sub>3</sub> COOH	42 <sub>19,24,1,0</sub> → 41 <sub>20,21,1,0</sub>	-7.6	860	0.0 ± 0.6
218.209992	CH <sub>3</sub> COOH	19 <sub>2,18,1,0</sub> → 18 <sub>2,17,1,0</sub>	-4.7	220	0.6 ± 0.6
218.209992	CH <sub>3</sub> COOH	19 <sub>1,18,1,0</sub> → 18 <sub>1,17,1,0</sub>	-4.7	220	0.6 ± 0.6
218.209992	CH <sub>3</sub> COOH	19 <sub>2,18,1,0</sub> → 18 <sub>1,17,1,0</sub>	-4.8	220	0.5 ± 0.6
218.209992	CH <sub>3</sub> COOH	19 <sub>1,18,1,0</sub> → 18 <sub>2,17,1,0</sub>	-4.8	220	0.5 ± 0.6
218.218686	CH <sub>3</sub> CHO	12 <sub>2,10,2</sub> → 12 <sub>0,12,2</sub>	-8.5	82	0.0 ± 0.8
218.223563	c - C <sub>2</sub> H <sub>4</sub> O	18 <sub>13,5</sub> → 17 <sub>16,2</sub>	-7.5	370	0.0 ± 0.6
218.238988	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>17,6,0</sub> → 21 <sub>17,5,1</sub>	-4.2	270	1.0 ± 0.9
218.238988	aGg' - (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>17,5,0</sub> → 21 <sub>17,4,1</sub>	-4.3	270	0.7 ± 0.9
218.239435	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>2,38,0</sub> → 39 <sub>2,37,0</sub>	-4.0	220	2 ± 2

218.247359	CH <sub>3</sub> OH	24 <sub>1,24,2</sub> → 23 <sub>3,21,1</sub>	−9.7	700	0.0 ± 1.1
218.250203	CH <sub>3</sub> COOH	57 <sub>11,46,0,0</sub> → 58 <sub>10,49,0,0</sub>	−9.2	1130	0 ± 2
218.250203	CH <sub>3</sub> COOH	57 <sub>12,46,0,0</sub> → 58 <sub>9,49,0,0</sub>	−9.2	1130	0 ± 2
218.260585	CH <sub>2</sub> (OH)CHO	20 <sub>3,17,0</sub> → 19 <sub>4,16,0</sub>	−3.6	126	3.7 ± 1.3
218.273796	CH <sub>3</sub> OH	4 <sub>3,2,5</sub> → 5 <sub>0,5,4</sub>	−11.0	350	0.0 ± 1.1
218.280872	CH <sub>3</sub> <sup>18</sup> OH	31 <sub>6,25,7</sub> → 30 <sub>8,22,7</sub>	−11.7	1960	4.3 · 10 <sup>−17</sup>
218.280900	CH <sub>3</sub> OCHO	17 <sub>3,14,2</sub> → 16 <sub>3,13,2</sub>	−4.0	100	20.3 ± 1.4
218.287868	HOCH <sub>2</sub> CN	8 <sub>3,6,0</sub> → 7 <sub>2,5,0</sub>	−4.6	28	5 ± 2
218.297890	CH <sub>3</sub> OCHO	17 <sub>3,14,0</sub> → 16 <sub>3,13,0</sub>	−4.0	100	20.3 ± 1.4
218.304671	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>16,7,0</sub> → 21 <sub>16,6,1</sub>	−4.1	250	1.2 ± 0.9
218.304671	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>16,6,0</sub> → 21 <sub>16,5,1</sub>	−4.2	250	0.9 ± 0.9
218.316390	CH <sub>2</sub> DOH	5 <sub>2,4,1</sub> → 5 <sub>1,5,1</sub>	−4.8	59	3.8 ± 1.9
218.324250	CH <sub>3</sub> OCH <sub>3</sub>	65 <sub>5,60,1</sub> → 64 <sub>8,57,1</sub>	−8.0	2000	0.0 ± 1.0
218.324353	CH <sub>3</sub> OCH <sub>3</sub>	65 <sub>5,60,0</sub> → 64 <sub>8,57,0</sub>	−8.2	2000	0.0 ± 1.0
218.324723	HC <sub>3</sub> N*	24 → 23	−1.29	131	15.6 ± 1.0
218.326994	CH <sub>3</sub> COOH	37 <sub>28,9,1,0</sub> → 36 <sub>30,6,1,0</sub>	−8.7	780	0.0 ± 0.6
218.335654	c − C <sub>2</sub> H <sub>4</sub> O	14 <sub>3,11</sub> → 14 <sub>2,12</sub>	−3.6	183	1.8 ± 0.7
218.335661	c − C <sub>2</sub> H <sub>4</sub> O	14 <sub>4,11</sub> → 14 <sub>3,12</sub>	−3.8	183	1.1 ± 0.7
218.344100	CH <sub>2</sub> (OH)CHO	37 <sub>10,28,0</sub> → 37 <sub>9,29,0</sub>	−3.6	450	1.5 ± 1.2
218.349044	CH <sub>3</sub> CONH <sub>2</sub>	25 <sub>5,21,0,2</sub> → 25 <sub>3,22,0,2</sub>	−4.5	210	0 ± 3
218.349044	CH <sub>3</sub> CONH <sub>2</sub>	25 <sub>4,21,0,2</sub> → 25 <sub>4,22,0,2</sub>	−4.5	210	0 ± 3
218.349044	CH <sub>3</sub> CONH <sub>2</sub>	25 <sub>5,21,0,2</sub> → 25 <sub>4,22,0,2</sub>	−5.3	210	0 ± 3
218.349044	CH <sub>3</sub> CONH <sub>2</sub>	25 <sub>4,21,0,2</sub> → 25 <sub>3,22,0,2</sub>	−5.3	210	0 ± 3
218.354946	CH <sub>3</sub> NCO	25 <sub>2,0,3</sub> → 24 <sub>2,0,3</sub>	−3.7	270	2.3 ± 1.5
218.356609	CH <sub>3</sub> NCO	25 <sub>2,0,−3</sub> → 24 <sub>2,0,−3</sub>	−3.7	270	2.3 ± 1.5
218.371495	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>4,19,0</sub> → 21 <sub>4,18,1</sub>	−3.7	133	3.1 ± 1.0
218.379983	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>15,8,0</sub> → 21 <sub>15,7,1</sub>	−4.0	230	1.4 ± 1.0
218.379983	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>15,7,0</sub> → 21 <sub>15,6,1</sub>	−4.1	230	1.1 ± 0.9
218.381206	CH <sub>3</sub> COOH	34 <sub>26,8,0,0</sub> → 33 <sub>28,5,0,0</sub>	−8.4	570	0 ± 2
218.389970	C <sub>2</sub> H <sub>3</sub> CN	24 <sub>3,21</sub> → 23 <sub>3,20</sub>	−2.7	140	24 ± 9
218.398555	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>7,17</sub> → 22 <sub>7,16</sub>	−3.0	230	4 ± 2
218.398555	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>7,16</sub> → 22 <sub>7,15</sub>	−3.0	230	4 ± 2
218.402435	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>6,18</sub> → 22 <sub>6,17</sub>	−3.0	200	5 ± 2
218.402451	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>6,17</sub> → 22 <sub>6,16</sub>	−3.0	200	5 ± 2
218.406015	C <sub>2</sub> H <sub>3</sub> CN	22 <sub>3,20</sub> → 23 <sub>1,23</sub>	−6.9	135	0.0 ± 1.9
218.408679	C <sub>2</sub> H <sub>5</sub> <sup>13</sup> CN	24 <sub>2,22</sub> → 23 <sub>2,21</sub>	−2.7	135	1.8 ± 0.9
218.421801	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>8,16</sub> → 22 <sub>8,15</sub>	−3.1	260	3 ± 2
218.421801	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>8,15</sub> → 22 <sub>8,14</sub>	−3.1	260	3 ± 2
218.440063	CH <sub>3</sub> OH	4 <sub>2,3,1</sub> → 3 <sub>1,2,1</sub>	−4.0	45	28.0 ± 1.5
218.443493	CH <sub>3</sub> <sup>18</sup> OH	20 <sub>6,14,6</sub> → 21 <sub>8,13,6</sub>	−11.3	1420	0 ± 4
218.443493	CH <sub>3</sub> <sup>18</sup> OH	20 <sub>6,15,6</sub> → 21 <sub>8,13,6</sub>	−11.3	1420	0 ± 4
218.451297	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>5,19</sub> → 22 <sub>5,18</sub>	−2.9	180	6 ± 2
218.452357	C <sub>2</sub> H <sub>3</sub> CN	23 <sub>5,18</sub> → 22 <sub>5,17</sub>	−2.9	180	6 ± 2
218.454831	CH <sub>3</sub> CONH <sub>2</sub>	10 <sub>9,2,0,1</sub> → 9 <sub>8,1,0,1</sub>	−4.0	56	4 ± 3
218.459213	HC(O)NH <sub>2</sub>	10 <sub>1,9</sub> → 9 <sub>1,8</sub>	−2.5	61	20.4 ± 1.9
218.461796	NH <sub>2</sub> CN	11 <sub>1,11,0</sub> → 10 <sub>1,10,0</sub>	−2.1	77	8.9 ± 1.1

218.463739	$\text{C}_2\text{H}_3\text{CN}$	$23_{9,15} \rightarrow 22_{9,14}$	-3.2	300	$2 \pm 2$
218.463739	$\text{C}_2\text{H}_3\text{CN}$	$23_{9,14} \rightarrow 22_{9,13}$	-3.2	300	$2 \pm 2$
218.468381	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{14,9,0} \rightarrow 21_{14,8,1}$	-4.0	220	$1.7 \pm 1.0$
218.468381	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{14,8,0} \rightarrow 21_{14,7,1}$	-4.1	220	$1.3 \pm 1.0$
218.475632	$\text{H}_2\text{CO}$	$3_{2,2} \rightarrow 2_{2,1}$	-3.1	68	$34 \pm 14$
218.482385	$\text{CHD}_2\text{OH}$	$11_{2,1,2} \rightarrow 11_{1,2,2}$	-4.4	163	$2 \pm 2$
218.489438	$\text{CH}_3\text{OCH}_3$	$23_{3,21,3} \rightarrow 23_{2,22,3}$	-5.1	260	$2.3 \pm 1.1$
218.489438	$\text{CH}_3\text{OCH}_3$	$23_{3,21,5} \rightarrow 23_{2,22,5}$	-5.4	260	$1.1 \pm 1.1$
218.491914	$\text{CH}_3\text{OCH}_3$	$23_{3,21,1} \rightarrow 23_{2,22,1}$	-4.5	260	$9.0 \pm 1.3$
218.494390	$\text{CH}_3\text{OCH}_3$	$23_{3,21,0} \rightarrow 23_{2,22,0}$	-4.9	260	$3.4 \pm 1.1$
218.518802	$^{13}\text{CH}_3\text{CHO}$	$12_{1,12,-2} \rightarrow 11_{1,11,-2}$	-3.7	270	$0.6 \pm 1.2$
218.519997	$\text{C}_2\text{H}_3\text{CN}$	$23_{10,14} \rightarrow 22_{10,13}$	-3.2	340	$2 \pm 2$
218.519997	$\text{C}_2\text{H}_3\text{CN}$	$23_{10,13} \rightarrow 22_{10,12}$	-3.2	340	$2 \pm 2$
218.530526	$\text{C}_2\text{H}_3\text{CN}$	$24_{3,21} \rightarrow 23_{3,20}$	-3.5	680	$1.7 \pm 0.7$
218.536793	$\text{C}_2\text{H}_5\text{OCHO}$	$39_{3,36,0} \rightarrow 38_{3,35,0}$	-4.0	220	$2 \pm 2$
218.541803	$\text{CH}_3\text{NCO}$	$25_{1,24,0} \rightarrow 24_{1,23,0}$	-3.5	142	$9.9 \pm 1.9$
218.554507	$\text{C}_2\text{H}_5\text{OH}$	$21_{5,16,2} \rightarrow 21_{4,17,2}$	-4.1	230	$6.7 \pm 1.9$
218.573646	$\text{C}_2\text{H}_3\text{CN}$	$23_{4,20} \rightarrow 22_{4,19}$	-2.9	160	$7 \pm 2$
218.574680	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{13,10,0} \rightarrow 21_{13,9,1}$	-3.9	210	$2.0 \pm 1.0$
218.574680	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{13,9,0} \rightarrow 21_{13,8,1}$	-4.0	210	$1.5 \pm 1.0$
218.576877	$\text{CH}_3\text{OD}$	$10_{-5,6,1} \rightarrow 11_{-4,8,1}$	-4.6	230	$3 \pm 3$
218.576909	$\text{CH}_3\text{OD}$	$24_{2,22,0} \rightarrow 23_{4,19,0}$	-7.4	680	$0 \pm 3$
218.585072	$\text{C}_2\text{H}_3\text{CN}$	$23_{3,21} \rightarrow 22_{3,20}$	-2.9	145	$8 \pm 2$
218.597232	$\text{CH}_3\text{CONH}_2$	$10_{9,1,0,2} \rightarrow 9_{8,2,0,2}$	-4.0	56	$4 \pm 3$
218.615092	$\text{C}_2\text{H}_3\text{CN}$	$23_{4,19} \rightarrow 22_{4,18}$	-2.9	160	$7 \pm 2$
218.633851	$\text{CH}_3\text{COCH}_3$	$12_{9,4,0} \rightarrow 11_{8,3,1}$	-5.0	66	$6 \pm 2$
218.654089	$\text{C}_2\text{H}_5\text{OH}$	$7_{2,5,2} \rightarrow 6_{1,6,2}$	-4.7	29	$3.3 \pm 1.7$
218.655977	$\text{C}_2\text{H}_5\text{OH}$	$60_{8,53,1} \rightarrow 61_{6,55,2}$	-7.6	1670	$0.0 \pm 1.6$
218.663526	$\text{HOCH}_2\text{CN}$	$11_{2,9,1} \rightarrow 11_{1,11,0}$	-4.6	40	$4 \pm 2$
218.663615	$\text{NH}_2\text{CN}$	$76_{2,74,0} \rightarrow 76_{2,75,0}$	-8.0	2900	$0.0 \pm 0.9$
218.666470	$\text{C}_2\text{H}_3\text{CN}$	$23_{12,11} \rightarrow 22_{12,10}$	-3.4	440	$1 \pm 2$
218.666470	$\text{C}_2\text{H}_3\text{CN}$	$23_{12,12} \rightarrow 22_{12,11}$	-3.4	440	$1 \pm 2$
218.682561	$\text{HC}_3\text{N}^*$	$24_{-1} \rightarrow 23_1$	-2.3	850	$2.2 \pm 0.8$
218.693940	$\text{HOCH}_2\text{CN}$	$67_{6,61,1} \rightarrow 67_{5,62,1}$	-4.9	1070	$0 \pm 2$
218.704503	$\text{CH}_3\text{OD}$	$46_{4,42,0} \rightarrow 46_{-4,43,0}$	-8.5	2400	$0 \pm 3$
218.704976	$\text{SiS}$	$13_{15} \rightarrow 12_{15}$	-24	$1.54 \cdot 10^4$	$6.4 \cdot 10^{-40}$
218.705810	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{12,11,0} \rightarrow 21_{12,10,1}$	-3.8	195	$2.2 \pm 1.0$
218.705810	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{12,10,0} \rightarrow 21_{12,9,1}$	-4.0	195	$1.7 \pm 1.0$
218.709071	$\text{CHD}_2\text{OH}$	$7_{0,2,1} \rightarrow 6_{1,2,1}$	-4.8	65	$1.4 \pm 1.8$
218.712336	$\text{gGg}' - (\text{CH}_2\text{OH})_2$	$22_{3,20,1} \rightarrow 21_{3,19,0}$	-3.9	127	$2.1 \pm 1.3$
218.742654	$\text{C}_2\text{H}_5\text{OCHO}$	$42_{1,42,0} \rightarrow 41_{1,41,0}$	-3.9	230	$2 \pm 2$
218.744718	$\text{C}_2\text{H}_5\text{OCHO}$	$42_{0,42,0} \rightarrow 41_{0,41,0}$	-3.9	230	$2 \pm 2$
218.747442	$\text{CH}_3\text{COCH}_3$	$43_{39,5,1} \rightarrow 43_{38,6,2}$	-6.5	870	$0 \pm 2$
218.754755	$\text{CH}_3\text{CHO}$	$27_{5,22,2} \rightarrow 28_{3,26,1}$	-8.0	410	$0.0 \pm 0.8$
218.760066	$\text{H}_2\text{CO}$	$3_{2,1} \rightarrow 2_{2,0}$	-3.1	68	$34 \pm 14$
218.760084	$\text{CH}_3\text{OD}$	$26_{2,24,1} \rightarrow 26_{-2,25,1}$	-8.0	790	$0 \pm 3$

218.760153	CH <sub>3</sub> COCH <sub>3</sub>	68 <sub>47,21,1</sub> → 68 <sub>46,22,2</sub>	−7.4	1950	0 ± 2
218.774291	CH <sub>3</sub> CONH <sub>2</sub>	19 <sub>15,4,0,0</sub> → 18 <sub>16,2,0,0</sub>	−7.7	181	0 ± 3
218.774838	CH <sub>3</sub> COCH <sub>3</sub>	12 <sub>9,4,1</sub> → 11 <sub>8,3,1</sub>	−5.3	66	3 ± 2
218.777238	CH <sub>3</sub> COCH <sub>3</sub>	66 <sub>37,29,0</sub> → 66 <sub>36,30,1</sub>	−6.5	1770	0 ± 2
218.805956	CH <sub>3</sub> COCH <sub>3</sub>	63 <sub>45,18,1</sub> → 63 <sub>44,19,1</sub>	−6.9	1690	0 ± 2
218.807292	H <sub>2</sub> CS	20 <sub>1,19</sub> → 20 <sub>1,20</sub>	−4.9	360	1.03 ± 0.17
218.830592	CH <sub>3</sub> OCHO	18 <sub>13,5,5</sub> → 17 <sub>13,4,5</sub>	−4.7	400	1.7 ± 1.1
218.854392	HC <sub>3</sub> N*	24 <sub>1</sub> → 23 <sub>−1</sub>	−2.3	850	2.2 ± 0.8
219.075881	HOCH <sub>2</sub> CN	24 <sub>2,23,0</sub> → 23 <sub>2,22,0</sub>	−3.4	138	14 ± 3
219.089720	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>10,13,0</sub> → 21 <sub>10,12,1</sub>	−3.8	174	2.8 ± 1.0
219.089728	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>10,12,0</sub> → 21 <sub>10,11,1</sub>	−3.9	174	2.2 ± 1.0
219.094939	CH <sub>2</sub> (OH)CHO	27 <sub>3,25,0</sub> → 27 <sub>2,26,0</sub>	−3.8	210	1.7 ± 1.2
219.122919	CH <sub>2</sub> (OH)CHO	29 <sub>3,26,0</sub> → 29 <sub>2,27,0</sub>	−3.7	250	2.0 ± 1.2
219.123664	CH <sub>2</sub> (OH)CHO	35 <sub>9,26,0</sub> → 36 <sub>6,31,0</sub>	−6.2	400	0.0 ± 1.2
219.144216	HOCH <sub>2</sub> CN	14 <sub>4,10,0</sub> → 13 <sub>3,10,1</sub>	−4.5	69	3 ± 2
219.154534	CH <sub>3</sub> OCHO	18 <sub>11,7,5</sub> → 17 <sub>11,6,5</sub>	−4.5	370	2.8 ± 1.1
219.173757	HC <sub>3</sub> N*	24 <sub>1</sub> → 23 <sub>−1</sub>	−1.76	450	6.5 ± 0.8
219.186535	CH <sub>3</sub> OD	3 <sub>−3,1,0</sub> → 4 <sub>−2,3,0</sub>	−5.3	54	2 ± 3
219.194666	CH <sub>3</sub> OCHO	18 <sub>16,3,4</sub> → 17 <sub>16,2,4</sub>	−5.1	460	0.5 ± 1.1
219.219931	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>1,20,1</sub> → 20 <sub>2,19,1</sub>	−4.9	122	5 ± 2
219.219931	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>2,20,1</sub> → 20 <sub>1,19,1</sub>	−5.3	122	2 ± 2
219.219970	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>1,20,1</sub> → 20 <sub>1,19,2</sub>	−5.0	122	3 ± 2
219.219970	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>2,20,1</sub> → 20 <sub>2,19,2</sub>	−5.0	122	3 ± 2
219.230234	CH <sub>2</sub> (OH)CHO	13 <sub>4,10,0</sub> → 12 <sub>3,9,0</sub>	−3.8	61	2.8 ± 1.3
219.242141	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>1,20,0</sub> → 20 <sub>1,19,1</sub>	−4.5	122	12 ± 3
219.242141	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>2,20,0</sub> → 20 <sub>2,19,1</sub>	−4.5	122	12 ± 3
219.242141	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>2,20,0</sub> → 20 <sub>1,19,1</sub>	−5.5	122	1 ± 2
219.242141	CH <sub>3</sub> COCH <sub>3</sub>	21 <sub>1,20,0</sub> → 20 <sub>2,19,1</sub>	−5.5	122	1 ± 2
219.270291	C <sub>2</sub> H <sub>5</sub> OH	9 <sub>3,7,1</sub> → 9 <sub>2,7,0</sub>	−4.6	110	2.8 ± 1.7
219.275978	SO <sub>2</sub>	22 <sub>7,15</sub> → 23 <sub>6,18</sub>	−3.9	350	2.9 ± 0.5
219.301992	CH <sub>3</sub> OCH <sub>3</sub>	31 <sub>6,26,1</sub> → 30 <sub>7,23,1</sub>	−5.1	500	1.1 ± 1.1
219.303216	CH <sub>2</sub> (OH)CHO	29 <sub>4,26,0</sub> → 29 <sub>3,27,0</sub>	−3.7	250	2.0 ± 1.2
219.310905	CH <sub>3</sub> COCH <sub>3</sub>	12 <sub>9,4,0</sub> → 11 <sub>8,3,0</sub>	−5.1	66	4 ± 2
219.340620	CH <sub>3</sub> CONH <sub>2</sub>	21 <sub>16,6,0,0</sub> → 21 <sub>12,9,0,0</sub>	−7.6	220	0 ± 3
219.341872	t-H <sup>13</sup> COOH	10 <sub>0,10</sub> → 9 <sub>0,9</sub>	−3.2	58	3.6 ± 1.6
219.355009	<sup>34</sup> SO <sub>2</sub>	11 <sub>1,11</sub> → 10 <sub>0,10</sub>	−3.0	60	3.4 ± 1.0
219.385178	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>9,14,0</sub> → 21 <sub>9,13,1</sub>	−3.7	164	3.0 ± 1.0
219.385426	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>9,13,0</sub> → 21 <sub>9,12,1</sub>	−3.8	164	2.4 ± 1.0
219.392056	C <sub>2</sub> H <sub>5</sub> OH	14 <sub>2,12,0</sub> → 13 <sub>1,12,1</sub>	−4.5	151	3.1 ± 1.7
219.392412	HNCO	10 <sub>5,5</sub> → 9 <sub>5,4</sub>	−4.3	1050	0.6 ± 0.8
219.392412	HNCO	10 <sub>5,6</sub> → 9 <sub>5,5</sub>	−4.3	1050	0.6 ± 0.8
219.402428	C <sub>2</sub> H <sub>5</sub> OCHO	39 <sub>4,35,0</sub> → 38 <sub>4,34,0</sub>	−4.0	220	2 ± 2
219.407809	CH <sub>3</sub> <sup>18</sup> OH	4 <sub>2,2,2</sub> → 3 <sub>1,2,2</sub>	−4.0	45	30 ± 8
219.411703	CH <sub>3</sub> OCHO	18 <sub>10,8,5</sub> → 17 <sub>10,7,5</sub>	−4.5	350	3.3 ± 1.2
219.417270	CH <sub>3</sub> OCHO	30 <sub>5,26,1</sub> → 30 <sub>4,27,1</sub>	−5.2	290	0.8 ± 1.1
219.429287	CH <sub>3</sub> <sup>18</sup> OH	15 <sub>0,15,4</sub> → 14 <sub>3,11,4</sub>	−8.6	570	0 ± 4

219.432516	$^{13}\text{CH}_3\text{OCH}_3$	$23_{4,20,4} \rightarrow 23_{3,21,4}$	-4.6	270	$0.3 \pm 0.8$
219.432517	$^{13}\text{CH}_3\text{OCH}_3$	$23_{4,20,3} \rightarrow 23_{3,21,3}$	-4.6	270	$0.3 \pm 0.8$
219.434060	$^{13}\text{CH}_3\text{OCH}_3$	$23_{4,20,1} \rightarrow 23_{3,21,1}$	-4.3	270	$0.5 \pm 0.8$
219.434239	$^{13}\text{CH}_3\text{OCH}_3$	$23_{4,20,2} \rightarrow 23_{3,21,2}$	-4.3	270	$0.5 \pm 0.8$
219.435783	$^{13}\text{CH}_3\text{OCH}_3$	$23_{4,20,0} \rightarrow 23_{3,21,0}$	-4.3	270	$0.5 \pm 0.8$
219.441599	$\text{NH}_2\text{CN}$	$11_{2,10,1} \rightarrow 10_{2,9,1}$	-2.3	191	$4.7 \pm 1.0$
219.445494	$\text{NH}_2\text{CN}$	$11_{6,5,1} \rightarrow 10_{6,4,1}$	-3.0	640	$0.4 \pm 0.9$
219.445494	$\text{NH}_2\text{CN}$	$11_{6,6,1} \rightarrow 10_{6,5,1}$	-3.0	640	$0.4 \pm 0.9$
219.451522	$\text{HOCH}_2\text{CN}$	$14_{4,11,0} \rightarrow 13_{3,11,1}$	-4.5	69	$3 \pm 2$
219.457026	$\text{CH}_3\text{OH}$	$8_{4,4,5} \rightarrow 7_{1,6,5}$	-8.6	490	$0.0 \pm 1.1$
219.463640	$\text{C}_2\text{H}_5\text{CN}$	$22_{2,21} \rightarrow 21_{1,20}$	-4.0	112	$1.4 \pm 1.6$
219.465445	$\text{CH}_3\text{OCH}_3$	$28_{5,24,0} \rightarrow 27_{6,21,0}$	-5.3	410	$1.1 \pm 1.1$
219.465610	$\text{CH}_3\text{OCH}_3$	$28_{5,24,1} \rightarrow 27_{6,21,1}$	-5.0	410	$1.8 \pm 1.1$
219.473986	$\text{NH}_2\text{CN}$	$11_{2,9,1} \rightarrow 10_{2,8,1}$	-2.3	191	$4.7 \pm 1.0$
219.479116	$\text{CH}_3\text{OCHO}$	$18_{14,5,4} \rightarrow 17_{14,4,4}$	-4.8	420	$1.3 \pm 1.1$
219.483539	$\text{CH}_3\text{OCHO}$	$30_{5,26,0} \rightarrow 30_{4,27,0}$	-5.2	290	$0.8 \pm 1.1$
219.496001	$^{34}\text{SO}_2$	$85_{10,76} \rightarrow 86_{7,79}$	-8.8	3600	$0.0 \pm 1.0$
219.505590	$\text{C}_2\text{H}_5\text{CN}$	$24_{2,22} \rightarrow 23_{2,21}$	-2.7	136	$25 \pm 10$
219.513267	$\text{c} - \text{C}_2\text{H}_4\text{O}$	$6_{3,4} \rightarrow 5_{2,3}$	-3.6	40	$3.2 \pm 0.7$
219.521587	$\text{CH}_3\text{COOH}$	$35_{20,15,0,0} \rightarrow 34_{24,10,0,0}$	-8.4	560	$0 \pm 2$
219.540443	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{2,21,1} \rightarrow 21_{2,20,0}$	-3.7	122	$3.3 \pm 1.1$
219.547082	$\text{HNCO}$	$10_{4,6} \rightarrow 9_{4,5}$	-3.7	710	$1.9 \pm 0.8$
219.547082	$\text{HNCO}$	$10_{4,7} \rightarrow 9_{4,6}$	-3.7	710	$1.9 \pm 0.8$
219.551485	$\text{CH}_2\text{DOH}$	$5_{1,5,1} \rightarrow 4_{1,4,1}$	-4.9	48	$3.1 \pm 1.9$
219.552819	$\text{CH}_2\text{DOH}$	$34_{1,33,1} \rightarrow 33_{4,29,2}$	-6.6	1290	$0.0 \pm 1.8$
219.560357	$\text{C}^{18}\text{O}$	$2 \rightarrow 1$	-4.2	15.8	$15.0 \pm 1.4$
219.568480	$\text{CH}_3\text{OCHO}$	$18_{14,5,3} \rightarrow 17_{14,4,3}$	-4.8	420	$1.3 \pm 1.1$
219.568480	$\text{CH}_3\text{OCHO}$	$18_{14,4,3} \rightarrow 17_{14,3,3}$	-4.8	420	$1.3 \pm 1.1$
219.569003	$\text{C}_2\text{H}_5\text{OCHO}$	$31_{15,17,1} \rightarrow 30_{15,16,1}$	-4.3	330	$1 \pm 2$
219.569003	$\text{C}_2\text{H}_5\text{OCHO}$	$31_{15,16,1} \rightarrow 30_{15,15,1}$	-4.3	330	$1 \pm 2$
219.580672	$\text{aGg}' - (\text{CH}_2\text{OH})_2$	$22_{1,21,1} \rightarrow 21_{1,20,0}$	-3.6	122	$4.3 \pm 1.1$
219.584383	$\text{CH}_3\text{OCHO}$	$18_{13,6,3} \rightarrow 17_{13,5,3}$	-4.7	400	$1.8 \pm 1.1$
219.584383	$\text{CH}_3\text{OCHO}$	$18_{13,5,3} \rightarrow 17_{13,4,3}$	-4.7	400	$1.8 \pm 1.1$
219.592845	$\text{C}_2\text{H}_5^{13}\text{CN}$	$25_{2,24} \rightarrow 24_{2,23}$	-2.7	142	$1.8 \pm 0.9$
219.601550	$\text{CH}_3\text{CONH}_2$	$19_{2,17,0,0} \rightarrow 18_{3,16,0,0}$	-3.8	121	$3 \pm 3$
219.601550	$\text{CH}_3\text{CONH}_2$	$19_{3,17,0,0} \rightarrow 18_{2,16,0,0}$	-3.8	121	$3 \pm 3$
219.601550	$\text{CH}_3\text{CONH}_2$	$19_{3,17,0,0} \rightarrow 18_{3,16,0,0}$	-4.5	121	$1 \pm 3$
219.601550	$\text{CH}_3\text{CONH}_2$	$19_{2,17,0,0} \rightarrow 18_{2,16,0,0}$	-4.5	121	$1 \pm 3$
219.602121	$\text{NH}_2\text{CN}$	$11_{4,8,1} \rightarrow 10_{4,7,1}$	-2.5	360	$1.9 \pm 1.0$
219.602121	$\text{NH}_2\text{CN}$	$11_{4,7,1} \rightarrow 10_{4,6,1}$	-2.5	360	$1.9 \pm 1.0$
219.604328	$\text{H}_2^{13}\text{CO}$	$46_{5,41} \rightarrow 46_{5,42}$	-8.6	4000	$0.0 \pm 0.6$
219.609218	$\text{C}_2\text{H}_5\text{OCHO}$	$40_{13,28,0} \rightarrow 39_{13,27,0}$	-4.2	340	$1 \pm 2$
219.609218	$\text{C}_2\text{H}_5\text{OCHO}$	$40_{13,27,0} \rightarrow 39_{13,26,0}$	-4.2	340	$1 \pm 2$
219.622694	$\text{CH}_3\text{OCHO}$	$18_{12,6,3} \rightarrow 17_{12,5,3}$	-4.6	380	$2.3 \pm 1.1$
219.622694	$\text{CH}_3\text{OCHO}$	$18_{12,7,3} \rightarrow 17_{12,6,3}$	-4.6	380	$2.3 \pm 1.1$
219.629396	$\text{HC(O)NH}_2$	$55_{12,44} \rightarrow 56_{11,45}$	-6.6	2000	$0.0 \pm 1.5$

219.630507	HC(O)NH <sub>2</sub>	55 <sub>12,43</sub> → 56 <sub>11,46</sub>	−6.6	2000	0.0 ± 1.5
219.632483	C <sub>2</sub> H <sub>5</sub> CN	24 <sub>2,22</sub> → 23 <sub>2,21</sub>	−3.5	670	1.8 ± 0.7
219.642403	CH <sub>3</sub> OCHO	18 <sub>13,6,4</sub> → 17 <sub>13,5,4</sub>	−4.7	400	1.8 ± 1.1
219.648628	NH <sub>2</sub> CN	11 <sub>3,8,1</sub> → 10 <sub>3,7,1</sub>	−2.8	260	1.1 ± 1.0
219.648628	NH <sub>2</sub> CN	11 <sub>3,9,1</sub> → 10 <sub>3,8,1</sub>	−2.8	260	1.1 ± 1.0
219.656769	HNCO	10 <sub>3,8</sub> → 9 <sub>3,7</sub>	−3.2	430	5.0 ± 0.8
219.656771	HNCO	10 <sub>3,7</sub> → 9 <sub>3,6</sub>	−3.2	430	5.0 ± 0.8
219.661381	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>12,29,0</sub> → 39 <sub>12,28,0</sub>	−4.1	320	1 ± 2
219.661381	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>12,28,0</sub> → 39 <sub>12,27,0</sub>	−4.1	320	1 ± 2
219.663624	HN <sup>13</sup> CO	10 <sub>3,8,11</sub> → 9 <sub>3,7,10</sub>	−3.6	450	0 ± 2
219.663625	HN <sup>13</sup> CO	10 <sub>3,7,11</sub> → 9 <sub>3,6,10</sub>	−3.6	450	0 ± 2
219.663626	HN <sup>13</sup> CO	10 <sub>3,8,9</sub> → 9 <sub>3,7,8</sub>	−3.7	450	0 ± 2
219.663627	HN <sup>13</sup> CO	10 <sub>3,7,9</sub> → 9 <sub>3,6,8</sub>	−3.7	450	0 ± 2
219.663666	HN <sup>13</sup> CO	10 <sub>3,8,10</sub> → 9 <sub>3,7,9</sub>	−3.6	450	0 ± 2
219.663667	HN <sup>13</sup> CO	10 <sub>3,7,10</sub> → 9 <sub>3,6,9</sub>	−3.6	450	0 ± 2
219.675114	HC <sub>3</sub> N*	24 <sub>0</sub> → 23 <sub>0</sub>	−2.2	770	2.7 ± 0.8
219.695831	CH <sub>3</sub> OCHO	18 <sub>11,8,3</sub> → 17 <sub>11,7,3</sub>	−4.5	370	2.8 ± 1.1
219.695831	CH <sub>3</sub> OCHO	18 <sub>11,7,3</sub> → 17 <sub>11,6,3</sub>	−4.5	370	2.8 ± 1.1
219.705128	CH <sub>3</sub> OCHO	18 <sub>4,15,3</sub> → 17 <sub>4,14,3</sub>	−4.3	300	6.4 ± 1.2
219.707349	HC <sub>3</sub> N*	24 <sub>−2</sub> → 23 <sub>2</sub>	−2.2	780	2.7 ± 0.8
219.719651	NH <sub>2</sub> CN	11 <sub>0,11,1</sub> → 10 <sub>0,10,1</sub>	−2.2	135	6.6 ± 1.1
219.723226	HC(O)NH <sub>2</sub>	59 <sub>5,54</sub> → 58 <sub>7,51</sub>	−7.2	1910	0.0 ± 1.5
219.730737	NH <sub>2</sub> CN	11 <sub>5,6,0</sub> → 10 <sub>5,5,0</sub>	−2.7	420	1.3 ± 1.0
219.730737	NH <sub>2</sub> CN	11 <sub>5,7,0</sub> → 10 <sub>5,6,0</sub>	−2.7	420	1.3 ± 1.0
219.733850	HNCO	10 <sub>2,9</sub> → 9 <sub>2,8</sub>	−2.9	230	9.9 ± 0.9
219.737193	HNCO	10 <sub>2,8</sub> → 9 <sub>2,7</sub>	−2.9	230	9.9 ± 0.9
219.740451	HN <sup>13</sup> CO	10 <sub>2,9,11</sub> → 9 <sub>2,8,10</sub>	−3.3	230	1 ± 2
219.740456	HN <sup>13</sup> CO	10 <sub>2,9,9</sub> → 9 <sub>2,8,8</sub>	−3.3	230	0 ± 2
219.740471	HN <sup>13</sup> CO	10 <sub>2,9,10</sub> → 9 <sub>2,8,9</sub>	−3.3	230	0 ± 2
219.741866	HC <sub>3</sub> N*	24 <sub>2</sub> → 23 <sub>−2</sub>	−2.2	780	2.7 ± 0.8
219.743742	HN <sup>13</sup> CO	10 <sub>2,8,11</sub> → 9 <sub>2,7,10</sub>	−3.3	230	1 ± 2
219.743747	HN <sup>13</sup> CO	10 <sub>2,8,9</sub> → 9 <sub>2,7,8</sub>	−3.3	230	0 ± 2
219.743762	HN <sup>13</sup> CO	10 <sub>2,8,10</sub> → 9 <sub>2,7,9</sub>	−3.3	230	0 ± 2
219.752078	CH <sub>3</sub> OH	5 <sub>5,1,3</sub> → 6 <sub>3,3,3</sub>	−11.3	460	0.0 ± 1.1
219.752103	CH <sub>3</sub> OH	5 <sub>5,0,3</sub> → 6 <sub>3,4,3</sub>	−11.3	460	0.0 ± 1.1
219.756528	CH <sub>3</sub> CHO	13 <sub>3,11,3</sub> → 13 <sub>2,12,3</sub>	−4.7	310	0.6 ± 0.8
219.763947	CH <sub>3</sub> OCHO	18 <sub>9,9,5</sub> → 17 <sub>9,8,5</sub>	−4.4	340	3.9 ± 1.2
219.764926	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	20 <sub>4,16,1</sub> → 19 <sub>4,15,0</sub>	−3.6	114	3.9 ± 1.1
219.775870	H <sup>15</sup> NCO	29 <sub>1,29</sub> → 30 <sub>0,30</sub>	−3.2	490	2.6 ± 0.5
219.780002	CH <sub>3</sub> CHO	11 <sub>1,10,6</sub> → 10 <sub>1,9,6</sub>	−3.9	440	1.7 ± 0.8
219.781348	C <sub>2</sub> H <sub>5</sub> OCHO	32 <sub>4,29,1</sub> → 31 <sub>4,28,1</sub>	−4.1	280	1 ± 2
219.785766	C <sub>2</sub> H <sub>5</sub> CN	33 <sub>3,31</sub> → 34 <sub>1,34</sub>	−7.0	280	0.0 ± 1.9
219.787929	C <sub>2</sub> H <sub>5</sub> OCHO	31 <sub>13,19,1</sub> → 30 <sub>13,18,1</sub>	−4.2	310	1 ± 2
219.787930	C <sub>2</sub> H <sub>5</sub> OCHO	31 <sub>13,18,1</sub> → 30 <sub>13,17,1</sub>	−4.2	310	1 ± 2
219.798274	HNCO	10 <sub>0,10</sub> → 9 <sub>0,9</sub>	−2.6	58	17.6 ± 1.1
219.804439	HN <sup>13</sup> CO	10 <sub>0,10,11</sub> → 9 <sub>0,9,10</sub>	−3.0	58	2 ± 2

219.804442	HN <sup>13</sup> CO	10 <sub>0,10,10</sub> → 9 <sub>0,9,9</sub>	−3.0	58	1 ± 2
219.804446	HN <sup>13</sup> CO	10 <sub>0,10,9</sub> → 9 <sub>0,9,8</sub>	−3.1	58	1 ± 2
219.809406	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>8,14,0</sub> → 21 <sub>8,13,1</sub>	−3.8	156	2.5 ± 1.0
219.822126	CH <sub>3</sub> OCHO	18 <sub>10,9,3</sub> → 17 <sub>10,8,3</sub>	−4.5	350	3.3 ± 1.2
219.822126	CH <sub>3</sub> OCHO	18 <sub>10,8,3</sub> → 17 <sub>10,7,3</sub>	−4.5	350	3.3 ± 1.2
219.824788	NH <sub>2</sub> CN	11 <sub>4,8,0</sub> → 10 <sub>4,7,0</sub>	−2.9	290	0.9 ± 0.9
219.824788	NH <sub>2</sub> CN	11 <sub>4,7,0</sub> → 10 <sub>4,6,0</sub>	−2.9	290	0.9 ± 0.9
219.826091	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>10,30,0</sub> → 39 <sub>10,29,0</sub>	−4.1	290	1 ± 2
219.826091	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>10,31,0</sub> → 39 <sub>10,30,0</sub>	−4.1	290	1 ± 2
219.827149	CH <sub>3</sub> OCHO	18 <sub>12,7,4</sub> → 17 <sub>12,6,4</sub>	−4.6	380	2.3 ± 1.1
219.844305	CH <sub>3</sub> OD	28 <sub>−2,27,0</sub> → 27 <sub>−4,24,0</sub>	−7.5	900	0 ± 3
219.852423	CH <sub>3</sub> OH	11 <sub>3,9,1</sub> → 10 <sub>3,7,2</sub>	−12.8	200	0.0 ± 1.1
219.858799	SiS	13 <sub>14</sub> → 12 <sub>14</sub>	−23	1.44 · 10 <sup>4</sup>	2.1 · 10 <sup>−37</sup>
219.859984	C <sub>2</sub> H <sub>5</sub> OCHO	32 <sub>3,29,1</sub> → 31 <sub>3,28,1</sub>	−4.1	280	1 ± 2
219.875828	NH <sub>2</sub> CN	11 <sub>2,10,0</sub> → 10 <sub>2,9,0</sub>	−2.6	121	2.3 ± 1.0
219.883448	CH <sub>3</sub> COOH	30 <sub>15,16,1,0</sub> → 29 <sub>17,13,1,0</sub>	−8.2	510	0.0 ± 0.6
219.893773	NH <sub>2</sub> CN	11 <sub>0,11,0</sub> → 10 <sub>0,10,0</sub>	−2.5	63	3.2 ± 1.0
219.902495	C <sub>2</sub> H <sub>5</sub> CN	12 <sub>3,10</sub> → 11 <sub>2,9</sub>	−4.3	44	1.0 ± 1.5
219.908525	H <sub>2</sub> <sup>13</sup> CO	3 <sub>1,2</sub> → 2 <sub>1,1</sub>	−2.4	33	24.3 ± 0.7
219.914176	NH <sub>2</sub> CN	11 <sub>2,9,0</sub> → 10 <sub>2,8,0</sub>	−2.6	121	2.3 ± 1.0
219.914866	H <sub>2</sub> C <sup>17</sup> O	3 <sub>1,2</sub> → 2 <sub>1,1</sub>	−2.4	33	4.6 ± 1.1
219.927519	H <sub>2</sub> CNH	29 <sub>4,25</sub> → 29 <sub>4,26</sub>	−5.7	1480	0.2 ± 0.7
219.949442	SO	5 <sub>6</sub> → 4 <sub>5</sub>	−2.3	35	37 ± 4
219.957465	CH <sub>3</sub> CONH <sub>2</sub>	24 <sub>15,9,0,2</sub> → 23 <sub>17,6,0,2</sub>	−7.4	270	0 ± 3
219.958236	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>9,32,0</sub> → 39 <sub>9,31,0</sub>	−4.1	270	1 ± 2
219.958265	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>9,31,0</sub> → 39 <sub>9,30,0</sub>	−4.1	270	1 ± 2
219.968030	CH <sub>3</sub> OH	38 <sub>6,32,8</sub> → 37 <sub>9,29,8</sub>	−11.6	2600	0.0 ± 1.1
219.971821	C <sub>2</sub> H <sub>5</sub> OCHO	31 <sub>12,20,1</sub> → 30 <sub>12,19,1</sub>	−4.2	310	1 ± 2
219.971837	C <sub>2</sub> H <sub>5</sub> OCHO	31 <sub>12,19,1</sub> → 30 <sub>12,18,1</sub>	−4.2	310	1 ± 2
219.979312	<sup>13</sup> CH <sub>3</sub> CHO	12 <sub>0,12,−3</sub> → 11 <sub>0,11,−3</sub>	−3.7	280	0.6 ± 1.2
219.983675	CH <sub>3</sub> OH	25 <sub>3,23,1</sub> → 24 <sub>4,20,1</sub>	−4.7	800	5.5 ± 1.2
219.993471	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>4,37,0</sub> → 39 <sub>4,36,0</sub>	−4.0	230	2 ± 2
219.993658	CH <sub>3</sub> OH	23 <sub>5,18,1</sub> → 22 <sub>6,17,1</sub>	−4.8	780	4.7 ± 1.2
220.030339	CH <sub>3</sub> OCHO	18 <sub>9,10,3</sub> → 17 <sub>9,9,3</sub>	−4.4	340	3.9 ± 1.2
220.030339	CH <sub>3</sub> OCHO	18 <sub>9,9,3</sub> → 17 <sub>9,8,3</sub>	−4.4	340	3.9 ± 1.2
220.037967	t-HCOOH	10 <sub>0,10</sub> → 9 <sub>0,9</sub>	−3.2	59	11.0 ± 0.8
220.043336	CH <sub>3</sub> OCHO	18 <sub>11,8,4</sub> → 17 <sub>11,7,4</sub>	−4.5	370	2.8 ± 1.1
220.046402	NH <sub>2</sub> CN	80 <sub>4,77,1</sub> → 79 <sub>5,75,0</sub>	−7.9	3400	0.0 ± 0.9
220.055226	CH <sub>2</sub> (OH)CHO	35 <sub>10,26,0</sub> → 35 <sub>9,27,0</sub>	−3.6	410	1.8 ± 1.2
220.056553	CH <sub>3</sub> CONH <sub>2</sub>	11 <sub>10,1,0,0</sub> → 10 <sub>9,1,0,0</sub>	−4.1	72	2 ± 3
220.071805	CH <sub>2</sub> DOH	5 <sub>1,5,0</sub> → 4 <sub>1,4,0</sub>	−4.3	36	16 ± 2
220.078561	CH <sub>3</sub> OH	8 <sub>0,8,1</sub> → 7 <sub>1,6,1</sub>	−4.1	97	23.6 ± 1.5
220.091149	C <sub>2</sub> H <sub>5</sub> <sup>13</sup> CN	83 <sub>11,73</sub> → 82 <sub>12,70</sub>	−6.1	1620	0.0 ± 0.9
220.108160	CH <sub>3</sub> OH	7 <sub>3,5,7</sub> → 8 <sub>6,2,4</sub>	−11.0	690	0.0 ± 1.1
220.116744	CH <sub>3</sub> <sup>18</sup> OH	31 <sub>7,24,5</sub> → 32 <sub>10,23,2</sub>	−10.4	1680	0 ± 4
220.126644	NH <sub>2</sub> CN	11 <sub>3,9,0</sub> → 10 <sub>3,8,0</sub>	−2.3	194	4.8 ± 1.0

220.127920	NH <sub>2</sub> CN	11 <sub>3,8,0</sub> → 10 <sub>3,7,0</sub>	−2.3	194	4.8 ± 1.0
220.145910	CH <sub>3</sub> <sup>18</sup> OH	15 <sub>3,12,6</sub> → 14 <sub>1,13,6</sub>	−11.3	920	0 ± 4
220.146486	CHD <sub>2</sub> OH	24 <sub>1,1,1</sub> → 23 <sub>3,1,2</sub>	−8.6	610	0.0 ± 1.7
220.148562	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>8,33,0</sub> → 39 <sub>8,32,0</sub>	−4.0	260	1 ± 2
220.149350	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>8,32,0</sub> → 39 <sub>8,31,0</sub>	−4.0	260	1 ± 2
220.166888	CH <sub>3</sub> OCHO	17 <sub>4,13,2</sub> → 16 <sub>4,12,2</sub>	−4.0	103	19.7 ± 1.4
220.177569	H <sub>2</sub> CCO	11 <sub>1,11</sub> → 10 <sub>1,10</sub>	−2.8	76	18.1 ± 1.3
220.182163	CH <sub>3</sub> <sup>18</sup> OH	39 <sub>11,29,4</sub> → 40 <sub>9,32,4</sub>	−10.4	2600	2.5 · 10 <sup>−19</sup>
220.190285	CH <sub>3</sub> OCHO	17 <sub>4,13,0</sub> → 16 <sub>4,12,0</sub>	−4.0	103	19.7 ± 1.4
220.195139	CH <sub>3</sub> <sup>18</sup> OH	8 <sub>1,8,1</sub> → 7 <sub>0,7,1</sub>	−3.9	86	23 ± 7
220.195311	C <sub>2</sub> H <sub>5</sub> <sup>13</sup> CN	72 <sub>9,63</sub> → 71 <sub>10,62</sub>	−5.6	1220	0.0 ± 0.9
220.196658	CH <sub>2</sub> (OH)CHO	7 <sub>6,2,0</sub> → 6 <sub>5,1,0</sub>	−3.6	37	4.4 ± 1.3
220.196853	CH <sub>2</sub> (OH)CHO	7 <sub>6,1,0</sub> → 6 <sub>5,2,0</sub>	−3.6	37	4.4 ± 1.3
220.204057	CH <sub>2</sub> (OH)CHO	11 <sub>4,7,0</sub> → 10 <sub>3,8,0</sub>	−3.8	47	2.6 ± 1.3
220.205386	C <sub>2</sub> H <sub>5</sub> OCHO	34 <sub>0,34,1</sub> → 33 <sub>0,33,1</sub>	−4.0	280	1 ± 2
220.205386	C <sub>2</sub> H <sub>5</sub> OCHO	34 <sub>1,34,1</sub> → 33 <sub>1,33,1</sub>	−4.0	280	1 ± 2
220.205400	C <sub>2</sub> H <sub>5</sub> OCHO	34 <sub>0,34,1</sub> → 33 <sub>1,33,1</sub>	−4.3	280	1 ± 2
220.205402	C <sub>2</sub> H <sub>5</sub> OCHO	34 <sub>1,34,1</sub> → 33 <sub>0,33,1</sub>	−4.3	280	1 ± 2
220.225477	CH <sub>3</sub> CONH <sub>2</sub>	14 <sub>12,2,0,1</sub> → 13 <sub>12,1,0,1</sub>	−5.6	104	0 ± 3
220.228330	CH <sub>3</sub> CONH <sub>2</sub>	22 <sub>1,21,0,2</sub> → 22 <sub>1,22,0,2</sub>	−4.9	141	0 ± 3
220.228330	CH <sub>3</sub> CONH <sub>2</sub>	22 <sub>2,21,0,2</sub> → 22 <sub>0,22,0,2</sub>	−4.9	141	0 ± 3
220.228330	CH <sub>3</sub> CONH <sub>2</sub>	22 <sub>1,21,0,2</sub> → 22 <sub>0,22,0,2</sub>	−6.2	141	0 ± 3
220.228330	CH <sub>3</sub> CONH <sub>2</sub>	22 <sub>2,21,0,2</sub> → 22 <sub>1,22,0,2</sub>	−6.2	141	0 ± 3
220.228563	CH <sub>3</sub> OD	27 <sub>0,27,1</sub> → 26 <sub>3,23,1</sub>	−6.4	810	0 ± 3
220.232895	CH <sub>3</sub> CONH <sub>2</sub>	11 <sub>8,4,0,0</sub> → 10 <sub>7,4,0,0</sub>	−4.3	65	2 ± 3
220.249787	gGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>2,20,1</sub> → 21 <sub>2,19,0</sub>	−3.8	127	2.7 ± 1.3
220.250951	CH <sub>3</sub> <sup>18</sup> OH	34 <sub>0,34,7</sub> → 33 <sub>1,32,8</sub>	−9.2	2000	4.5 · 10 <sup>−15</sup>
220.258096	CH <sub>3</sub> OCHO	18 <sub>8,10,5</sub> → 17 <sub>8,9,5</sub>	−4.4	330	4.5 ± 1.2
220.261457	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	8 <sub>2,7,1</sub> → 7 <sub>1,6,1</sub>	−4.6	38	0.7 ± 0.8
220.261544	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	8 <sub>2,7,2</sub> → 7 <sub>1,6,2</sub>	−4.6	38	0.7 ± 0.8
220.263646	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	8 <sub>2,7,0</sub> → 7 <sub>1,6,0</sub>	−4.6	38	0.7 ± 0.8
220.273430	CH <sub>3</sub> CONH <sub>2</sub>	23 <sub>11,12,0,0</sub> → 24 <sub>7,17,0,0</sub>	−8.2	230	0 ± 3
220.276728	CH <sub>3</sub> OH	38 <sub>3,36,7</sub> → 37 <sub>6,32,7</sub>	−11.1	2300	0.0 ± 1.1
220.278636	<sup>13</sup> CH <sub>3</sub> CHO	12 <sub>0,12,1</sub> → 11 <sub>0,11,1</sub>	−3.4	69	1.9 ± 1.5
220.300815	H <sup>13</sup> C(O)NH <sub>2</sub>	51 <sub>7,45</sub> → 50 <sub>8,42</sub>	−5.9	1500	0.0 ± 0.5
220.307380	CH <sub>3</sub> OCHO	18 <sub>10,9,4</sub> → 17 <sub>10,8,4</sub>	−4.5	350	3.4 ± 1.2
220.316088	CH <sub>3</sub> OD	40 <sub>2,38,1</sub> → 39 <sub>5,34,1</sub>	−7.8	1810	0 ± 3
220.317314	<sup>13</sup> CH <sub>3</sub> CHO	12 <sub>0,12,0</sub> → 11 <sub>0,11,0</sub>	−3.4	69	1.9 ± 1.5
220.318507	CH <sub>3</sub> CONH <sub>2</sub>	23 <sub>12,12,0,0</sub> → 24 <sub>8,17,0,0</sub>	−8.2	230	0 ± 3
220.321806	<sup>13</sup> CH <sub>3</sub> OH	17 <sub>7,11,0</sub> → 18 <sub>6,12,0</sub>	−4.8	590	0.9 ± 0.9
220.321807	<sup>13</sup> CH <sub>3</sub> OH	17 <sub>7,10,0</sub> → 18 <sub>6,13,0</sub>	−4.8	590	0.9 ± 0.9
220.355335	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>0,22,1</sub> → 21 <sub>0,21,1</sub>	−4.8	124	5 ± 2
220.355335	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>1,22,1</sub> → 21 <sub>1,21,1</sub>	−5.3	124	2 ± 2
220.355383	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>0,22,1</sub> → 21 <sub>0,21,2</sub>	−5.0	124	4 ± 2
220.355383	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>1,22,1</sub> → 21 <sub>1,21,2</sub>	−5.0	124	4 ± 2
220.361881	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>0,22,0</sub> → 21 <sub>0,21,1</sub>	−4.5	124	11 ± 3

220.361881	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>1,22,0</sub> → 21 <sub>1,21,1</sub>	−4.5	124	11 ± 3
220.361881	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>1,22,0</sub> → 21 <sub>0,21,1</sub>	−5.0	124	3 ± 2
220.361881	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>0,22,0</sub> → 21 <sub>1,21,1</sub>	−5.0	124	3 ± 2
220.367637	CH <sub>3</sub> COCH <sub>3</sub>	11 <sub>11,1,1</sub> → 10 <sub>10,1,2</sub>	−5.2	63	3 ± 2
220.368323	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>0,22,0</sub> → 21 <sub>0,21,0</sub>	−4.6	124	9 ± 3
220.368323	CH <sub>3</sub> COCH <sub>3</sub>	22 <sub>1,22,0</sub> → 21 <sub>1,21,0</sub>	−4.8	124	5 ± 2
220.368333	CH <sub>3</sub> OCHO	18 <sub>8,11,3</sub> → 17 <sub>8,10,3</sub>	−4.4	330	4.5 ± 1.2
220.369877	CH <sub>3</sub> OCHO	18 <sub>8,10,3</sub> → 17 <sub>8,9,3</sub>	−4.4	330	4.5 ± 1.2
220.373415	H <sub>2</sub> CNH	30 <sub>5,25</sub> → 29 <sub>6,24</sub>	−5.2	1630	0.6 ± 0.7
220.390196	H <sup>13</sup> CCCN	25 → 24	−1.29	138	8 ± 4
220.398684	<sup>13</sup> CO	2 → 1	−4.2	15.9	35 ± 5
220.431537	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>7,34,0</sub> → 39 <sub>7,33,0</sub>	−4.0	250	2 ± 2
220.432931	CH <sub>3</sub> COOH	71 <sub>28,44,0,0</sub> → 70 <sub>30,41,0,0</sub>	−9.4	2100	0 ± 2
220.432931	CH <sub>3</sub> COOH	71 <sub>27,44,0,0</sub> → 70 <sub>29,41,0,0</sub>	−9.4	2100	0 ± 2
220.446494	CH <sub>3</sub> CHO	13 <sub>3,10,2</sub> → 13 <sub>2,11,2</sub>	−4.4	105	3.4 ± 0.8
220.446964	C <sub>2</sub> H <sub>5</sub> OCHO	40 <sub>7,33,0</sub> → 39 <sub>7,32,0</sub>	−4.0	250	2 ± 2
220.448427	gGg' − (CH <sub>2</sub> OH) <sub>2</sub>	21 <sub>5,16,1</sub> → 20 <sub>5,15,0</sub>	−4.2	126	1.2 ± 1.3
220.463898	CH <sub>2</sub> (OH)CHO	20 <sub>2,18,0</sub> → 19 <sub>3,17,0</sub>	−3.4	120	5.9 ± 1.4
220.466335	CH <sub>3</sub> COCH <sub>3</sub>	11 <sub>11,0,1</sub> → 10 <sub>10,1,1</sub>	−5.0	63	5 ± 2
220.475808	CH <sub>3</sub> CN	12 <sub>8,0</sub> → 11 <sub>8,0</sub>	−3.1	530	4.5 ± 1.2
220.485859	CH <sub>3</sub> <sup>13</sup> CN	12 <sub>6</sub> → 11 <sub>6</sub>	−2.2	330	5 ± 5
220.489355	NH <sub>2</sub> CN	42 <sub>1,41,1</sub> → 42 <sub>1,42,1</sub>	−6.7	960	0.0 ± 0.9
220.496592	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>7,15,0</sub> → 21 <sub>7,14,1</sub>	−3.8	149	2.7 ± 1.0
220.532327	CH <sub>3</sub> <sup>13</sup> CN	12 <sub>5</sub> → 11 <sub>5</sub>	−2.4	250	5 ± 5
220.539324	CH <sub>3</sub> CN	12 <sub>7,0</sub> → 11 <sub>7,0</sub>	−2.9	420	6.8 ± 1.3
220.552586	CH <sub>2</sub> DOH	17 <sub>1,16,0</sub> → 17 <sub>0,17,0</sub>	−4.1	340	6 ± 2
220.561394	C <sub>2</sub> H <sub>3</sub> CN	24 <sub>1,24</sub> → 23 <sub>1,23</sub>	−2.8	135	9 ± 2
220.570373	CH <sub>3</sub> <sup>13</sup> CN	12 <sub>4</sub> → 11 <sub>4</sub>	−2.2	183	9 ± 5
220.584751	HNCO	10 <sub>1,9</sub> → 9 <sub>1,8</sub>	−2.7	102	15.2 ± 1.0
220.592555	HN <sup>13</sup> CO	10 <sub>1,9,9</sub> → 9 <sub>1,8,10</sub>	−7.7	101	0 ± 2
220.592606	HN <sup>13</sup> CO	10 <sub>1,9,11</sub> → 9 <sub>1,8,10</sub>	−3.1	101	1 ± 2
220.592611	HN <sup>13</sup> CO	10 <sub>1,9,9</sub> → 9 <sub>1,8,8</sub>	−3.1	101	1 ± 2
220.592613	HN <sup>13</sup> CO	10 <sub>1,9,10</sub> → 9 <sub>1,8,9</sub>	−3.1	101	1 ± 2
220.594424	CH <sub>3</sub> CN	12 <sub>−6,0</sub> → 11 <sub>6,0</sub>	−2.7	330	9.6 ± 1.4
220.594424	CH <sub>3</sub> CN	12 <sub>6,0</sub> → 11 <sub>−6,0</sub>	−2.7	330	9.6 ± 1.4
220.599980	CH <sub>3</sub> <sup>13</sup> CN	12 <sub>3</sub> → 11 <sub>3</sub>	−1.84	133	29 ± 8
220.601928	C <sub>2</sub> H <sub>5</sub> OH	13 <sub>1,13,2</sub> → 12 <sub>0,12,2</sub>	−3.9	74	16 ± 3
220.621136	CH <sub>3</sub> <sup>13</sup> CN	12 <sub>2</sub> → 11 <sub>2</sub>	−2.1	97	20 ± 6
220.633834	CH <sub>3</sub> <sup>13</sup> CN	12 <sub>1</sub> → 11 <sub>1</sub>	−2.0	76	24 ± 7
220.641084	CH <sub>3</sub> CN	12 <sub>5,0</sub> → 11 <sub>5,0</sub>	−2.5	250	12.7 ± 1.7
220.646819	CH <sub>3</sub> OCHO	18 <sub>9,10,4</sub> → 17 <sub>9,9,4</sub>	−4.4	340	4.0 ± 1.2
220.660916	C <sub>2</sub> H <sub>5</sub> CN	25 <sub>2,24</sub> → 24 <sub>2,23</sub>	−2.7	143	25 ± 10
220.660927	CH <sub>3</sub> COOH	32 <sub>24,9,0,0</sub> → 31 <sub>26,6,0,0</sub>	−8.2	500	0 ± 2
220.664887	CH <sub>3</sub> COCH <sub>3</sub>	11 <sub>11,1,0</sub> → 10 <sub>10,1,1</sub>	−4.6	63	14 ± 3
220.667095	C <sub>2</sub> H <sub>5</sub> CN	64 <sub>10,54</sub> → 65 <sub>8,57</sub>	−7.2	1010	0.0 ± 1.5
220.668255	CH <sub>3</sub> COOH	44 <sub>8,37,0,2</sub> → 45 <sub>6,40,0,1</sub>	−9.0	650	0 ± 2

220.668255	CH <sub>3</sub> COOH	44 <sub>7,37,0,2</sub> → 45 <sub>5,40,0,1</sub>	−9.0	650	0 ± 2
220.668255	CH <sub>3</sub> COOH	44 <sub>7,37,0,2</sub> → 45 <sub>6,40,0,1</sub>	−9.2	650	0 ± 2
220.668255	CH <sub>3</sub> COOH	44 <sub>8,37,0,2</sub> → 45 <sub>5,40,0,1</sub>	−9.2	650	0 ± 2
220.677966	CH <sub>3</sub> <sup>18</sup> OH	16 <sub>11,6,4</sub> → 17 <sub>13,4,1</sub>	−10.5	1200	0 ± 4
220.679287	CH <sub>3</sub> CN	12 <sub>4,0</sub> → 11 <sub>4,0</sub>	−2.4	183	15.8 ± 1.9
220.684674	gGg' − (CH <sub>2</sub> OH) <sub>2</sub>	23 <sub>1,22,0</sub> → 22 <sub>2,21,0</sub>	−4.0	132	1.6 ± 1.3
220.718048	CH <sub>3</sub> <sup>18</sup> OH	17 <sub>3,15,0</sub> → 18 <sub>0,18,0</sub>	−12.7	390	0 ± 4
220.719482	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>3,20,1</sub> → 21 <sub>2,19,1</sub>	−4.4	128	0.7 ± 0.9
220.763618	CH <sub>3</sub> COCH <sub>3</sub>	11 <sub>11,0,0</sub> → 10 <sub>10,0,1</sub>	−4.6	63	14 ± 3
220.766662	gGg' − (CH <sub>2</sub> OH) <sub>2</sub>	23 <sub>2,22,0</sub> → 22 <sub>1,21,0</sub>	−4.2	132	1.1 ± 1.3
220.779684	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	44 <sub>12,33,1</sub> → 44 <sub>11,34,1</sub>	−4.9	560	0.1 ± 0.9
220.780689	aGg' − (CH <sub>2</sub> OH) <sub>2</sub>	22 <sub>3,20,0</sub> → 21 <sub>2,19,0</sub>	−4.8	127	0.2 ± 0.9
220.791948	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	12 <sub>1,12,4</sub> → 11 <sub>0,11,4</sub>	−4.5	68	0.8 ± 0.8
220.791948	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	12 <sub>1,12,3</sub> → 11 <sub>0,11,3</sub>	−4.5	68	0.8 ± 0.8
220.792294	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	12 <sub>1,12,1</sub> → 11 <sub>0,11,1</sub>	−4.2	68	1.6 ± 0.8
220.792318	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	12 <sub>1,12,2</sub> → 11 <sub>0,11,2</sub>	−4.2	68	1.6 ± 0.8
220.792664	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	12 <sub>1,12,0</sub> → 11 <sub>0,11,0</sub>	−4.2	68	1.6 ± 0.8
220.794911	NH <sub>2</sub> CN	80 <sub>4,76,1</sub> → 79 <sub>5,74,0</sub>	−7.9	3400	0.0 ± 0.9
220.805654	HCCC <sup>15</sup> N	25 → 24	−1.29	138	2.3 ± 1.6
220.811845	CH <sub>3</sub> OCHO	18 <sub>3,16,1</sub> → 17 <sub>2,15,2</sub>	−5.0	106	2.0 ± 1.1
220.814090	CH <sub>3</sub> OCHO	28 <sub>3,25,2</sub> → 28 <sub>2,26,2</sub>	−5.2	250	0.8 ± 1.1
220.815236	CH <sub>3</sub> OCHO	18 <sub>3,16,0</sub> → 17 <sub>2,15,0</sub>	−5.0	106	2.0 ± 1.1
220.839109	CH <sub>3</sub> OH	40 <sub>5,35,5</sub> → 39 <sub>5,35,8</sub>	−10.6	2400	0.0 ± 1.1
220.846542	CH <sub>3</sub> OCH <sub>3</sub>	24 <sub>4,20,0</sub> → 23 <sub>5,19,0</sub>	−5.4	300	1.1 ± 1.1
220.847646	CH <sub>3</sub> OCH <sub>3</sub>	24 <sub>4,20,1</sub> → 23 <sub>5,19,1</sub>	−4.9	300	2.9 ± 1.1
220.848752	CH <sub>3</sub> OCH <sub>3</sub>	24 <sub>4,20,3</sub> → 23 <sub>5,19,3</sub>	−5.5	300	0.7 ± 1.1
220.852810	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	4 <sub>3,1,1</sub> → 3 <sub>2,2,1</sub>	−4.8	22	0.4 ± 0.8
220.852837	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	4 <sub>3,1,2</sub> → 3 <sub>2,2,2</sub>	−4.8	22	0.4 ± 0.8
220.852932	<sup>13</sup> CH <sub>3</sub> OCH <sub>3</sub>	4 <sub>3,1,0</sub> → 3 <sub>2,2,0</sub>	−4.7	22	0.7 ± 0.8
220.880958	C <sub>2</sub> H <sub>3</sub> CN	63 <sub>3,60</sub> → 64 <sub>2,63</sub>	−6.8	950	0.0 ± 1.9
220.886604	gGg' − (CH <sub>2</sub> OH) <sub>2</sub>	21 <sub>4,17,0</sub> → 20 <sub>4,16,1</sub>	−4.0	123	1.6 ± 1.3
220.886784	CH <sub>3</sub> OH	31 <sub>2,29,2</sub> → 31 <sub>1,30,1</sub>	−4.6	1180	7.0 ± 1.2
220.891840	CH <sub>3</sub> OCH <sub>3</sub>	23 <sub>4,20,3</sub> → 23 <sub>3,21,3</sub>	−5.0	270	2.8 ± 1.1
220.891840	CH <sub>3</sub> OCH <sub>3</sub>	23 <sub>4,20,5</sub> → 23 <sub>3,21,5</sub>	−5.3	270	1.4 ± 1.1
220.892562	CH <sub>3</sub> OH	27 <sub>7,21,5</sub> → 27 <sub>10,17,2</sub>	−8.2	1400	0.0 ± 1.1
220.893407	CH <sub>3</sub> OCH <sub>3</sub>	23 <sub>4,20,1</sub> → 23 <sub>3,21,1</sub>	−4.4	270	11.2 ± 1.5
220.894974	CH <sub>3</sub> OCH <sub>3</sub>	23 <sub>4,20,0</sub> → 23 <sub>3,21,0</sub>	−4.8	270	4.2 ± 1.1
220.912662	CH <sub>3</sub> CONH <sub>2</sub>	20 <sub>2,19,0,0</sub> → 19 <sub>2,18,0,0</sub>	−3.9	124	2 ± 3
220.912662	CH <sub>3</sub> CONH <sub>2</sub>	20 <sub>1,19,0,0</sub> → 19 <sub>1,18,0,0</sub>	−3.9	124	2 ± 3
220.912662	CH <sub>3</sub> CONH <sub>2</sub>	20 <sub>2,19,0,0</sub> → 19 <sub>1,18,0,0</sub>	−4.3	124	1 ± 3
220.912662	CH <sub>3</sub> CONH <sub>2</sub>	20 <sub>1,19,0,0</sub> → 19 <sub>2,18,0,0</sub>	−4.3	124	1 ± 3
220.913955	CH <sub>3</sub> OCHO	18 <sub>7,12,3</sub> → 17 <sub>7,11,3</sub>	−4.3	320	5.1 ± 1.2
220.920857	CH <sub>3</sub> OH	25 <sub>6,19,4</sub> → 25 <sub>7,18,4</sub>	−8.6	1340	0.0 ± 1.1
220.926361	CH <sub>3</sub> OCHO	18 <sub>16,2,0</sub> → 17 <sub>16,1,0</sub>	−4.9	270	1.7 ± 1.1
220.926361	CH <sub>3</sub> OCHO	18 <sub>16,3,0</sub> → 17 <sub>16,2,0</sub>	−4.9	270	1.7 ± 1.1