

Table 1: Spectrum assignments, rel FCF and signals

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
1	1_0^0	0.000	1	1
2	$1_0^1 1_1^0$	6.900	0.550	0.264
3	$1_0^2 1_2^0$	13.800	0.302	0.070
4	$1_0^3 1_3^0$	20.700	0.166	0.018
5	$1_0^4 1_4^0$	27.600	0.091	0.005
6	$1_0^1 2_1^0$	6.900	0.450	0.216
7	$1_0^2 2_2^0$	13.800	0.202	0.047
8	$1_0^3 2_3^0$	20.700	0.091	0.010
9	$1_0^4 2_4^0$	27.600	0.041	0.002
10	$1_0^1 2_0^1 1_2^0$	15.200	0.495	0.114
11	$1_0^1 2_0^2 1_3^0$	23.500	0.334	0.037
12	$1_0^1 2_0^3 1_4^0$	31.800	0.200	0.011
13	$1_0^1 2_0^4 1_5^0$	40.100	0.112	0.003
14	$1_0^2 2_0^1 1_3^0$	22.100	0.408	0.045
15	$1_0^2 2_0^2 1_4^0$	30.400	0.367	0.019
16	$1_0^2 2_0^3 1_5^0$	38.700	0.275	0.007
17	$1_0^3 2_0^1 1_4^0$	29.000	0.299	0.016
18	$1_0^3 2_0^2 1_5^0$	37.300	0.336	0.009
19	$1_0^4 2_0^1 1_5^0$	35.900	0.205	0.005
20	$1_0^2 2_1^0 1_2^0$	13.800	0.495	0.114
21	$1_0^2 2_1^1 1_3^0$	20.700	0.334	0.037
22	$1_0^2 2_1^2 1_4^0$	27.600	0.200	0.011
23	$1_0^2 2_1^3 1_5^0$	20.700	0.408	0.045
24	$1_0^2 2_2^0 1_4^0$	27.600	0.367	0.020
25	$1_0^2 2_2^1 1_5^0$	34.500	0.275	0.007
26	$1_0^2 2_2^2 1_6^0$	27.600	0.299	0.016
27	$1_0^2 2_2^3 1_7^0$	34.500	0.336	0.009
28	$1_0^2 2_3^0 1_6^0$	41.400	0.302	0.004
29	$1_0^1 2_0^1 1_1^0 2_1^0$	15.200	0.010	0.002
30	$1_0^1 2_0^2 1_1^0 2_2^0$	23.500	0.067	0.007
31	$1_0^1 2_0^3 1_2^0 2_1^0$	23.500	0.190	0.021
32	$1_0^1 2_0^3 1_1^0 2_3^0$	31.800	0.193	0.010
33	$1_0^1 2_0^3 1_3^0 2_1^0$	31.800	0.291	0.015
34	$1_0^1 2_0^4 1_3^0 2_2^0$	40.100	0.125	0.003

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
35	$1^2_0 2^1_1 0^0_2$	22.100	0.190	0.021
36	$1^2_0 2^1_2 0^0_1$	22.100	0.067	0.007
37	$1^2_0 2^2_1 0^0_2$	30.400	0.235	0.012
38	$1^2_0 2^3_1 0^0_3$	38.700	0.182	0.005
39	$1^2_0 2^4_1 0^0_3$	47.000	0.167	0.002
40	$1^3_0 2^1_1 0^0_3$	29.000	0.291	0.015
41	$1^3_0 2^1_3 0^0_1$	29.000	0.193	0.010
42	$1^3_0 2^2_1 0^0_2$	37.300	0.182	0.005
43	$1^4_0 2^1_1 0^0_3$	35.900	0.125	0.003
44	$1^4_0 2^2_1 0^0_3$	44.200	0.167	0.002
45	$1^1_0 2^1_2 0^0_2$	15.200	0.495	0.114
46	$1^1_0 2^2_2 0^0_3$	23.500	0.408	0.045
47	$1^1_0 2^3_2 0^0_4$	31.800	0.299	0.016
48	$1^1_0 2^4_2 0^0_5$	40.100	0.205	0.005
49	$1^2_0 2^1_2 0^0_3$	22.100	0.334	0.037
50	$1^2_0 2^2_2 0^0_4$	30.400	0.367	0.019
51	$1^2_0 2^3_2 0^0_5$	38.700	0.336	0.009
52	$1^3_0 2^1_2 0^0_4$	29.000	0.200	0.011
53	$1^3_0 2^2_2 0^0_5$	37.300	0.275	0.007
54	$1^4_0 2^1_2 0^0_5$	35.900	0.112	0.003
55	$1^0_1 2^0_1 2^2_0$	16.600	0.495	0.114
56	$1^0_1 2^0_2 2^3_0$	24.900	0.408	0.045
57	$1^0_1 2^0_3 2^4_0$	33.200	0.299	0.016
58	$1^0_2 2^0_1 2^3_0$	24.900	0.334	0.037
59	$1^0_2 2^0_2 2^4_0$	33.200	0.367	0.019
60	$1^0_2 2^0_3 2^5_0$	41.500	0.336	0.009
61	$1^0_3 2^0_1 2^4_0$	33.200	0.200	0.011
62	$1^0_3 2^0_2 2^5_0$	41.500	0.275	0.007
63	$1^0_3 2^0_3 2^6_0$	49.800	0.302	0.004
64	$1^1_0 2^1_3 1^0_2$	437.000	0.289	0.067
65	$1^1_0 2^1_3 1^0_2$	858.800	0.085	0.020
66	$1^1_0 2^1_3 1^0_2$	1280.600	0.017	0.004
67	$1^1_0 2^2_3 1^0_3$	445.300	0.195	0.022
68	$1^1_0 2^3_3 1^0_3$	867.100	0.057	0.006
69	$1^1_0 2^3_3 1^0_4$	453.600	0.117	0.006

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
70	$1_0^1 2_0^3 3_0^2 1_4^0$	875.400	0.034	0.002
71	$1_0^2 2_0^1 3_0^1 1_3^0$	443.900	0.238	0.026
72	$1_0^2 2_0^1 3_0^2 1_3^0$	865.700	0.070	0.008
73	$1_0^2 2_0^2 3_0^1 1_4^0$	452.200	0.214	0.011
74	$1_0^2 2_0^2 3_0^2 1_4^0$	874.000	0.063	0.003
75	$1_0^2 2_0^3 3_0^1 1_5^0$	460.500	0.161	0.004
76	$1_0^3 2_0^1 3_0^1 1_4^0$	450.800	0.175	0.009
77	$1_0^3 2_0^1 3_0^2 1_4^0$	872.600	0.051	0.003
78	$1_0^3 2_0^2 3_0^1 1_5^0$	459.100	0.196	0.005
79	$1_0^1 2_0^2 3_0^1 1_2^0 2_2^0$	445.300	0.039	0.004
80	$1_0^1 2_0^2 3_0^1 1_2^0 2_1^0$	445.300	0.111	0.012
81	$1_0^1 2_0^2 3_0^2 1_2^0 2_1^0$	867.100	0.033	0.004
82	$1_0^1 2_0^3 3_0^1 1_2^0 2_3^0$	453.600	0.113	0.006
83	$1_0^1 2_0^3 3_0^1 1_3^0 2_1^0$	453.600	0.170	0.009
84	$1_0^1 2_0^3 3_0^2 1_3^0 2_1^0$	875.400	0.050	0.003
85	$1_0^2 2_0^1 3_0^1 1_2^0 2_2^0$	443.900	0.111	0.012
86	$1_0^2 2_0^1 3_0^1 1_2^0 2_1^0$	443.900	0.039	0.004
87	$1_0^2 2_0^1 3_0^2 1_2^0 2_2^0$	865.700	0.033	0.004
88	$1_0^2 2_0^2 3_0^1 1_2^0 2_2^0$	452.200	0.137	0.007
89	$1_0^2 2_0^2 3_0^2 1_2^0 2_2^0$	874.000	0.040	0.002
90	$1_0^2 2_0^3 3_0^1 1_2^0 2_3^0$	460.500	0.106	0.003
91	$1_0^3 2_0^1 3_0^1 1_2^0 2_3^0$	450.800	0.170	0.009
92	$1_0^3 2_0^1 3_0^1 1_3^0 2_1^0$	450.800	0.113	0.006
93	$1_0^3 2_0^1 3_0^2 1_1^0 2_3^0$	872.600	0.050	0.003
94	$1_0^3 2_0^2 3_0^1 1_3^0 2_2^0$	459.100	0.106	0.003
95	$1_2^1 2_1^2 3_1^2$	446.300	0.111	0.004
96	$1_2^1 2_1^2 3_1^3$	868.100	0.063	0.002
97	$1_2^2 1_2^1 3_1^2$	444.900	0.111	0.004
98	$1_2^2 1_2^1 3_1^3$	866.700	0.063	0.002
99	$1_2^2 2_2^2 3_1^2$	453.200	0.137	0.002
100	$1_0^1 2_0^1 3_0^1 1_2^0 3_1^0$	16.200	0.085	0.006
101	$1_0^1 2_0^1 3_0^1 1_2^0 3_1^0$	438.000	0.289	0.020
102	$1_0^1 2_0^1 3_0^3 1_2^0 3_1^0$	859.800	0.165	0.011
103	$1_0^1 2_0^1 3_0^3 1_2^0 3_2^0$	439.000	0.193	0.004
104	$1_0^1 2_0^2 3_0^1 1_3^0 3_1^0$	24.500	0.057	0.002

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
105	$1_0^1 2_0^2 3_0^2 1_3^0 3_1^0$	446.300	0.195	0.006
106	$1_0^1 2_0^2 3_0^3 1_3^0 3_1^0$	868.100	0.111	0.004
107	$1_0^2 2_0^1 3_0^1 1_3^0 3_1^0$	23.100	0.070	0.002
108	$1_0^2 2_0^1 3_0^2 1_3^0 3_1^0$	444.900	0.238	0.008
109	$1_0^2 2_0^1 3_0^3 1_3^0 3_1^0$	866.700	0.136	0.004
110	$1_1^0 2_1^0 3_1^0 1_0^2 3_0^1$	14.800	0.085	0.006
111	$1_1^0 2_1^0 3_1^0 1_0^2 3_0^2$	436.600	0.289	0.020
112	$1_1^0 2_1^0 3_1^0 1_0^2 3_0^3$	858.400	0.165	0.011
113	$1_1^0 2_1^0 3_1^0 1_0^2 3_0^4$	1280.200	0.048	0.003
114	$1_1^0 2_1^0 3_2^0 1_0^2 3_0^3$	437.600	0.193	0.004
115	$1_1^0 2_1^0 3_2^0 1_0^2 3_0^4$	859.400	0.207	0.004
116	$1_1^0 2_2^0 3_1^0 1_0^3 3_0^1$	21.700	0.058	0.002
117	$1_1^0 2_2^0 3_1^0 1_0^3 3_0^2$	443.500	0.195	0.006
118	$1_1^0 2_2^0 3_1^0 1_0^3 3_0^3$	865.300	0.111	0.004
119	$1_2^0 2_1^0 3_1^0 1_0^3 3_0^1$	21.700	0.070	0.002
120	$1_2^0 2_1^0 3_1^0 1_0^3 3_0^2$	443.500	0.238	0.008
121	$1_2^0 2_1^0 3_1^0 1_0^3 3_0^3$	865.300	0.136	0.004
122	$1_2^0 2_2^0 3_1^0 1_0^3 3_0^2$	450.400	0.214	0.003
123	$1_2^0 2_2^0 3_1^0 1_0^3 3_0^3$	872.200	0.122	0.002
124	$1_0^1 2_0^1 3_0^1 2_2^0$	437.000	0.289	0.067
125	$1_0^1 2_0^1 3_0^2 2_2^0$	858.800	0.085	0.020
126	$1_0^1 2_0^1 3_0^3 2_2^0$	1280.600	0.017	0.004
127	$1_0^1 2_0^2 3_0^1 2_3^0$	445.300	0.238	0.026
128	$1_0^1 2_0^2 3_0^2 2_3^0$	867.100	0.070	0.008
129	$1_0^1 2_0^3 3_0^1 2_4^0$	453.600	0.175	0.009
130	$1_0^1 2_0^3 3_0^2 2_4^0$	875.400	0.051	0.003
131	$1_0^2 2_0^1 3_0^1 2_3^0$	443.900	0.195	0.022
132	$1_0^2 2_0^1 3_0^2 2_3^0$	865.700	0.057	0.006
133	$1_0^2 2_0^2 3_0^1 2_4^0$	452.200	0.214	0.011
134	$1_0^2 2_0^2 3_0^2 2_4^0$	874.000	0.063	0.003
135	$1_0^2 2_0^3 3_0^1 2_5^0$	460.500	0.196	0.005
136	$1_0^3 2_0^1 3_0^1 2_4^0$	450.800	0.117	0.006
137	$1_0^3 2_0^1 3_0^2 2_4^0$	872.600	0.034	0.002
138	$1_0^3 2_0^2 3_0^1 2_5^0$	459.100	0.161	0.004
139	$1_0^1 2_0^1 3_0^1 2_2^0 3_1^0$	16.200	0.085	0.006

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
140	$1_0^1 2_0^1 3_0^2 2_2^0 3_1^0$	438.000	0.289	0.020
141	$1_0^1 2_0^1 3_0^2 2_2^0 3_1^0$	859.800	0.165	0.011
142	$1_0^1 2_0^1 3_0^2 2_2^0 3_2^0$	439.000	0.192	0.004
143	$1_0^1 2_0^2 3_0^1 2_3^0 3_1^0$	24.500	0.070	0.002
144	$1_0^1 2_0^2 3_0^2 2_3^0 3_1^0$	446.300	0.238	0.008
145	$1_0^1 2_0^2 3_0^2 2_3^0 3_1^0$	868.100	0.136	0.004
146	$1_0^2 2_0^1 3_0^1 2_3^0 3_1^0$	23.100	0.057	0.002
147	$1_0^2 2_0^1 3_0^2 2_3^0 3_1^0$	444.900	0.195	0.006
148	$1_0^2 2_0^1 3_0^2 2_3^0 3_1^0$	866.700	0.111	0.004
149	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	17.600	0.085	0.006
150	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	439.400	0.289	0.020
151	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	861.200	0.164	0.011
152	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	1283.000	0.048	0.003
153	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	440.400	0.192	0.004
154	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	862.200	0.207	0.004
155	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	25.900	0.070	0.002
156	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	447.700	0.238	0.008
157	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	869.500	0.136	0.004
158	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	25.900	0.057	0.002
159	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	447.700	0.195	0.006
160	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	869.500	0.111	0.004
161	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	456.000	0.214	0.003
162	$1_1^0 2_1^0 3_1^0 2_2^0 3_0^1$	877.800	0.122	0.002
163	$1_0^1 3_0^1 1_1^0$	428.700	0.321	0.154
164	$1_0^1 3_0^2 1_1^0$	850.500	0.094	0.045
165	$1_0^1 3_0^3 1_1^0$	1272.300	0.019	0.009
166	$1_0^2 3_0^1 1_2^0$	435.600	0.177	0.041
167	$1_0^2 3_0^2 1_2^0$	857.400	0.052	0.012
168	$1_0^2 3_0^3 1_2^0$	1279.200	0.010	0.002
169	$1_0^3 3_0^1 1_3^0$	442.500	0.097	0.011
170	$1_0^3 3_0^2 1_3^0$	864.300	0.028	0.003
171	$1_0^4 3_0^1 1_4^0$	449.400	0.053	0.003
172	$1_0^2 3_0^1 1_2^0 2_1^0$	435.600	0.289	0.067
173	$1_0^2 3_0^2 1_2^0 2_1^0$	857.400	0.085	0.020
174	$1_0^2 3_0^3 1_2^0 2_1^0$	1279.200	0.017	0.004

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
175	$1^3_0 3^1_0 1^0_1 2^0_2$	442.500	0.195	0.022
176	$1^3_0 3^1_0 1^0_2 2^0_1$	442.500	0.238	0.026
177	$1^3_0 3^2_0 1^0_1 2^0_2$	864.300	0.057	0.006
178	$1^3_0 3^2_0 1^0_2 2^0_1$	864.300	0.070	0.008
179	$1^4_0 3^1_0 1^0_1 2^0_3$	449.400	0.117	0.006
180	$1^4_0 3^1_0 1^0_2 2^0_2$	449.400	0.214	0.011
181	$1^4_0 3^1_0 1^0_3 2^0_1$	449.400	0.175	0.009
182	$1^4_0 3^2_0 1^0_1 2^0_3$	871.200	0.034	0.002
183	$1^4_0 3^2_0 1^0_2 2^0_2$	871.200	0.063	0.003
184	$1^4_0 3^2_0 1^0_3 2^0_1$	871.200	0.051	0.003
185	$1^5_0 3^1_0 1^0_2 2^0_3$	456.300	0.161	0.004
186	$1^5_0 3^1_0 1^0_3 2^0_2$	456.300	0.196	0.005
187	$1^1_0 3^1_0 1^0_1 3^0_1$	7.900	0.095	0.014
188	$1^1_0 3^2_0 1^0_1 3^0_1$	429.700	0.321	0.046
189	$1^1_0 3^3_0 1^0_1 3^0_1$	851.500	0.183	0.026
190	$1^1_0 3^3_0 1^0_1 3^0_2$	430.700	0.214	0.009
191	$1^1_0 3^4_0 1^0_1 3^0_1$	1273.300	0.054	0.008
192	$1^1_0 3^4_0 1^0_1 3^0_2$	852.500	0.230	0.010
193	$1^1_0 3^5_0 1^0_1 3^0_2$	1274.300	0.097	0.004
194	$1^1_0 3^5_0 1^0_1 3^0_3$	853.500	0.231	0.003
195	$1^2_0 3^1_0 1^0_2 3^0_1$	14.800	0.052	0.004
196	$1^2_0 3^2_0 1^0_2 3^0_1$	436.600	0.177	0.012
197	$1^2_0 3^3_0 1^0_2 3^0_1$	858.400	0.101	0.007
198	$1^2_0 3^3_0 1^0_2 3^0_2$	437.600	0.118	0.002
199	$1^2_0 3^4_0 1^0_2 3^0_1$	1280.200	0.030	0.002
200	$1^2_0 3^4_0 1^0_2 3^0_2$	859.400	0.126	0.003
201	$1^3_0 3^2_0 1^0_3 3^0_1$	443.500	0.097	0.003
202	$1^3_0 3^3_0 1^0_3 3^0_1$	865.300	0.055	0.002
203	$1^1_0 3^1_0 2^0_1$	428.700	0.263	0.126
204	$1^1_0 3^2_0 2^0_1$	850.500	0.077	0.037
205	$1^1_0 3^3_0 2^0_1$	1272.300	0.015	0.007
206	$1^2_0 3^1_0 2^0_2$	435.600	0.118	0.027
207	$1^2_0 3^2_0 2^0_2$	857.400	0.035	0.008
208	$1^3_0 3^1_0 2^0_3$	442.500	0.053	0.006
209	$1^1_0 3^1_0 2^0_1 3^0_1$	7.900	0.078	0.011

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
210	$1_0^1 3_0^2 2_1^0 3_1^0$	429.700	0.263	0.038
211	$1_0^1 3_0^3 2_1^0 3_1^0$	851.500	0.150	0.021
212	$1_0^1 3_0^3 2_1^0 3_2^0$	430.700	0.175	0.007
213	$1_0^1 3_0^4 2_1^0 3_1^0$	1273.300	0.044	0.006
214	$1_0^1 3_0^4 2_1^0 3_2^0$	852.500	0.188	0.008
215	$1_0^1 3_0^5 2_1^0 3_2^0$	1274.300	0.079	0.003
216	$1_0^1 3_0^5 2_1^0 3_3^0$	853.500	0.189	0.002
217	$1_0^2 3_0^1 2_2^0 3_1^0$	14.800	0.035	0.002
218	$1_0^2 3_0^2 2_2^0 3_1^0$	436.600	0.118	0.008
219	$1_0^2 3_0^3 2_2^0 3_1^0$	858.400	0.067	0.005
220	$2_0^1 1_1^0$	8.300	0.450	0.216
221	$2_0^2 1_2^0$	16.600	0.202	0.047
222	$2_0^3 1_3^0$	24.900	0.091	0.010
223	$2_0^4 1_4^0$	33.200	0.041	0.002
224	$2_0^1 2_1^0$	8.300	0.550	0.264
225	$2_0^2 2_2^0$	16.600	0.302	0.070
226	$2_0^3 2_3^0$	24.900	0.166	0.018
227	$2_0^4 2_4^0$	33.200	0.091	0.005
228	$2_0^1 3_0^1 1_1^0$	430.100	0.263	0.126
229	$2_0^1 3_0^2 1_1^0$	851.900	0.077	0.037
230	$2_0^1 3_0^3 1_1^0$	1273.700	0.015	0.007
231	$2_0^2 3_0^1 1_2^0$	438.400	0.118	0.027
232	$2_0^2 3_0^2 1_2^0$	860.200	0.035	0.008
233	$2_0^3 3_0^1 1_3^0$	446.700	0.053	0.006
234	$2_0^2 3_0^1 1_2^0 1_1^0$	438.400	0.289	0.067
235	$2_0^2 3_0^2 1_2^0 1_1^0$	860.200	0.085	0.020
236	$2_0^2 3_0^3 1_2^0 1_1^0$	1282.000	0.017	0.004
237	$2_0^3 3_0^1 1_2^0 1_2^0$	446.700	0.238	0.026
238	$2_0^3 3_0^1 1_2^0 2_1^0$	446.700	0.195	0.022
239	$2_0^3 3_0^2 1_2^0 1_2^0$	868.500	0.070	0.008
240	$2_0^3 3_0^2 1_2^0 2_1^0$	868.500	0.057	0.006
241	$2_0^4 3_0^1 1_2^0 1_3^0$	455.000	0.175	0.009
242	$2_0^4 3_0^1 1_2^0 2_2^0$	455.000	0.214	0.011
243	$2_0^4 3_0^1 1_3^0 2_1^0$	455.000	0.117	0.006
244	$2_0^4 3_0^2 1_2^0 1_3^0$	876.800	0.051	0.003

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
245	$2_0^4 3_0^2 1_2^0 2_2^0$	876.800	0.063	0.003
246	$2_0^4 3_0^2 1_3^0 2_1^0$	876.800	0.034	0.002
247	$2_0^5 3_0^1 1_2^0 2_3^0$	463.300	0.196	0.005
248	$2_0^5 3_0^1 1_3^0 2_2^0$	463.300	0.160	0.004
249	$2_0^1 3_0^1 1_1^0 3_1^0$	9.300	0.078	0.011
250	$2_0^1 3_0^2 1_1^0 3_1^0$	431.100	0.263	0.038
251	$2_0^1 3_0^3 1_1^0 3_1^0$	852.900	0.150	0.021
252	$2_0^1 3_0^3 1_1^0 3_2^0$	432.100	0.175	0.007
253	$2_0^1 3_0^4 1_1^0 3_1^0$	1274.700	0.044	0.006
254	$2_0^1 3_0^4 1_1^0 3_2^0$	853.900	0.188	0.008
255	$2_0^1 3_0^5 1_1^0 3_2^0$	1275.700	0.079	0.003
256	$2_0^1 3_0^5 1_1^0 3_3^0$	854.900	0.189	0.002
257	$2_0^2 3_0^1 1_2^0 3_1^0$	17.600	0.035	0.002
258	$2_0^2 3_0^2 1_2^0 3_1^0$	439.400	0.118	0.008
259	$2_0^2 3_0^3 1_2^0 3_1^0$	861.200	0.067	0.005
260	$2_0^1 3_0^1 2_1^0$	430.100	0.321	0.154
261	$2_0^1 3_0^2 2_1^0$	851.900	0.094	0.045
262	$2_0^1 3_0^3 2_1^0$	1273.700	0.018	0.009
263	$2_0^2 3_0^1 2_2^0$	438.400	0.177	0.041
264	$2_0^2 3_0^2 2_2^0$	860.200	0.052	0.012
265	$2_0^2 3_0^3 2_2^0$	1282.000	0.010	0.002
266	$2_0^3 3_0^1 2_3^0$	446.700	0.097	0.011
267	$2_0^3 3_0^2 2_3^0$	868.500	0.028	0.003
268	$2_0^4 3_0^1 2_4^0$	455.000	0.053	0.003
269	$2_0^1 3_0^1 2_1^0 3_1^0$	9.300	0.095	0.014
270	$2_0^1 3_0^2 2_1^0 3_1^0$	431.100	0.321	0.046
271	$2_0^1 3_0^3 2_1^0 3_1^0$	852.900	0.183	0.026
272	$2_0^1 3_0^3 2_1^0 3_2^0$	432.100	0.214	0.009
273	$2_0^1 3_0^4 2_1^0 3_1^0$	1274.700	0.054	0.008
274	$2_0^1 3_0^4 2_1^0 3_2^0$	853.900	0.230	0.010
275	$2_0^1 3_0^5 2_1^0 3_2^0$	1275.700	0.097	0.004
276	$2_0^1 3_0^5 2_1^0 3_3^0$	854.900	0.231	0.003
277	$2_0^2 3_0^1 2_2^0 3_1^0$	17.600	0.052	0.004
278	$2_0^2 3_0^2 2_2^0 3_1^0$	439.400	0.177	0.012
279	$2_0^2 3_0^3 2_2^0 3_1^0$	861.200	0.101	0.007

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Table 1 – *Continued from previous page*

Peak	Assignment	Position (cm ⁻¹)	Rel. FC factor	Signal
280	$2_0^2 3_0^3 2_2^0 3_2^0$	440.400	0.118	0.002
281	$2_0^2 3_0^4 2_2^0 3_1^0$	1283.000	0.030	0.002
282	$2_0^2 3_0^4 2_2^0 3_2^0$	862.200	0.126	0.003
283	$2_0^3 3_0^2 2_3^0 3_1^0$	447.700	0.097	0.003
284	$2_0^3 3_0^3 2_3^0 3_1^0$	869.500	0.055	0.002
285	3_0^1	421.800	0.584	0.584
286	3_0^2	843.600	0.171	0.171
287	3_0^3	1265.400	0.034	0.034
288	3_0^4	1687.200	0.005	0.005
289	$3_0^1 3_1^0$	1.000	0.172	0.051
290	$3_0^2 3_1^0$	422.800	0.584	0.174
291	$3_0^3 3_1^0$	844.600	0.332	0.099
292	$3_0^3 3_2^0$	423.800	0.389	0.035
293	$3_0^3 3_3^0$	3.000	0.076	0.002
294	$3_0^4 3_1^0$	1266.400	0.098	0.029
295	$3_0^4 3_2^0$	845.600	0.417	0.037
296	$3_0^4 3_3^0$	424.800	0.189	0.005
297	$3_0^5 3_1^0$	1688.200	0.019	0.006
298	$3_0^5 3_2^0$	1267.400	0.176	0.016
299	$3_0^5 3_3^0$	846.600	0.421	0.011
300	$3_0^6 3_2^0$	1689.200	0.045	0.004
301	$3_0^6 3_3^0$	1268.400	0.249	0.007
302	$3_0^6 3_4^0$	847.600	0.364	0.003
303	$3_0^7 3_3^0$	1690.200	0.080	0.002
304	$3_0^7 3_4^0$	1269.400	0.305	0.002