Supporting Information for Vibrational Analysis Based on Cavity-enhanced Raman Spectroscopy: Cyclohexane

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Computational Details

Conformational Analysis

Two conformers of hexane (Figure S1) have been considered in this study. After optimization with very tight criteria, populations of the two conformers were calculated using the Boltzmann distribution. The chair conformer takes 99.996% amount, therefore only the chair conformer was used for the simulation. The chair conformer and the labels of the carbon atoms are shown in Figure S2.

Parameters of Resonances Analysis

For Fermi resonances,

Step 1:

$$|\omega_i - (\omega_j + \omega_k)| \leq 200 \text{ cm}^{-1} \tag{1}$$

Step 2:

$$\frac{{F_{ijk}}^4}{64(1+\delta_{jk})^2|\omega_i - (\omega_j + \omega_k)|^3} \geq 1 \text{ cm}^{-1} \tag{2}$$

Step 3:

$$\frac{1}{\sqrt{8(1+\delta_{ij})}} \frac{F_{ijk}}{\omega_i + \omega_j - \omega_k} \geq 0.1 \tag{3}$$

For 1-1 Darling–Dennison resonances,

Step 1:

$$|\omega_i - \omega_j| \leq 100 \text{ cm}^{-1} \tag{4}$$

Step 2:

$$\left|\langle 1_i | \tilde{\mathcal{H}} | 1_j \rangle\right| \geq 10 \text{ cm}^{-1} \tag{5}$$

Step 3:

$$\max(C^{(2)}_{1_i,1_j}, C^{(2)}_{1_j,1_i}) \geq 0.3 \tag{6}$$

For 1-3 Darling–Dennison resonances,

Step 1:

$$|\omega_i - \omega_j - \omega_k - \omega_l| \leq 100 \text{ cm}^{-1} \tag{7}$$

Step 2:

$$\left|\langle 1_i \,|\, \tilde{\mathcal{H}} \,|\, 1_j 1_k 1_l \rangle\right| \geq 10 \text{ cm}^{-1} \tag{8}$$

Step 3:

$$\max(C^{(2)}_{1_i,1_j,1_k,1_l}, C^{(2)}_{1_j,1_k,1_l,1_i}) \geq 0.3 \tag{9}$$

For 2-2 Darling–Dennison resonances,

Step 1:

$$|\omega_i + \omega_j - (\omega_k + \omega_l)| \leq 100 \text{ cm}^{-1} \tag{10}$$

Step 2:

$$\left|\langle 1_i 1_j \,|\, \tilde{\mathcal{H}} \,|\, 1_k 1_l \rangle\right| \geq 10 \text{ cm}^{-1} \tag{11}$$

where i, j, k, l refer to normal modes, ω to the harmonic wavenumbers, F_{ijk} is the third derivative of the potential energy with respect to the dimensionless normal coordinates, q_i, q_j and q_k. $\tilde{\mathcal{H}}$ is the contact-transformed Hamiltonian[1] and δ is the Kronecker symbol. Equation 3, 6 and 9 in FRs and DDRs are coefficients related to intensity-specific terms.[2] In the commercial version, only two steps were used in resonance analysis. Only Equation 1 (step 1) and Equation 2 (step 2) were used in the commercial version for Fermi resonances analysis, Equation 2 (step 1) and Equation 2 (step 2) for 1-1 Darling-Dennison resonances analysis, and then Equation 7 (step 1) and Equation 8 (step 2) for 1-3 Darling-Dennison resonances. The intensity specific terms connect to Equations 3, 6 and 9. The parameters used in this study were testified in reference.[2]

Vibrational Hamiltonian

Molecular modes are first placed into Eckart orientation, to minimize the coupling between vibration and rotation. Then, the rotational contributions are taken into account by Coriolis coupling. The final vibrational Hamiltonian of interest here is presented in Equation 12,

$$\begin{aligned}\mathcal{H}^v =& \frac{1}{2}\sum_i \omega_i({p_i}^2 + {q_i}^2) + \frac{1}{6}\sum_{i,j,k} \mathrm{f}_{ijk}\, q_i\, q_j\, q_k + \frac{1}{24}\sum_{i,j,k,l} \mathrm{f}_{ijkl}\, q_i\, q_j\, q_k\, q_l \\ &+ \sum_\tau B_\tau^{\mathrm{eq}} \sum_{i,j,k,l} \zeta_{ij,\tau}\zeta_{kl,\tau}\sqrt{\frac{\omega_j\omega_l}{\omega_i\omega_k}}\, q_i p_j\, q_k p_l\end{aligned} \tag{12}$$

The first term is the harmonic Hamitonian, the second term is the first-order perturbation, and the third is the second-order perturbation. The last term represents the Coriolis couplings. B_τ^{eq} is the rotational constant. $\zeta_{ij,\tau}$ is the Coriolis constant coupling of modes i and j along the rotational axis I_τ.

Computational Results

The chair conformer of the cyclohexane was studied. 48 normal modes are described in Figure S1 with the increasing order of their energies at the harmonic level. Labels of the carbon atoms are shown in Figure S2. Because the positions of carbon atoms are identical, many vibrational modes are degenerated. The normal modes structure, as well as the displacement vectors, are presented in Figure S4. Duschinsky transformation of these 48 nodes, diagonalized J matrix, and low K vector value in Figure S3 show high consistency of normal modes from B3PW91/jun-cc-pVTZ and revDSD-PBE86-D3/jun-cc-pVTZ.

Supplementary Figures

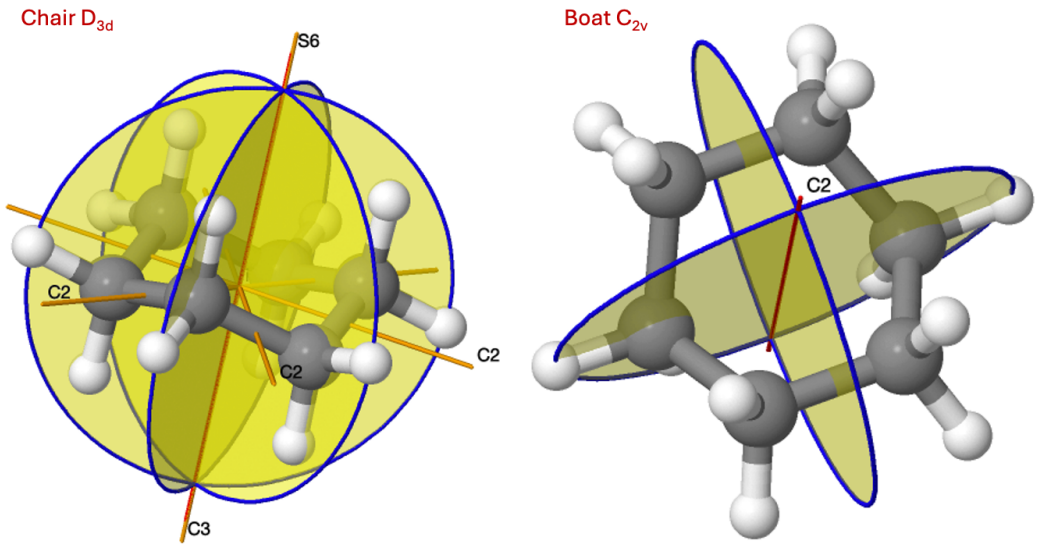

Figure S1: The structure of the two cyclohexane conformers. The left panel is the chair conformer with the D_{3d} point groups, the right panel is the boat conformer with C_{2v} point groups. The structure is plotted by JSmol from 'chemtube3d.com'.

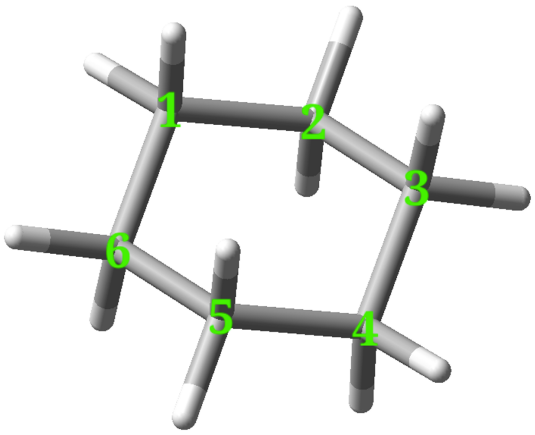

Figure S2: The structure of the chair conformer and the numbering of the carbon atoms for the normal modes analysis.

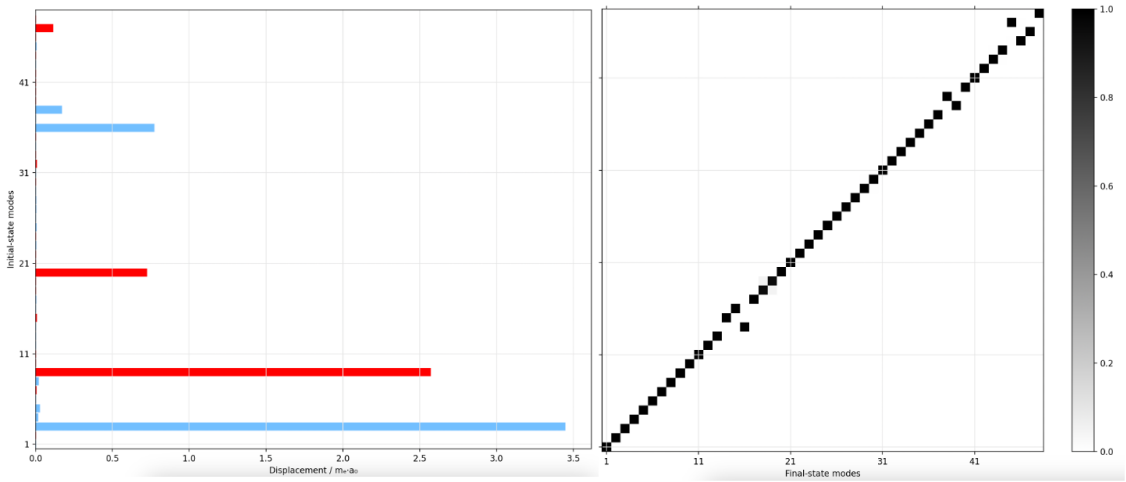

Figure S3: The Duschinsky matrix (J,left panel) and K vector (right panel) in Duschinsky transformation of B3PW91/jun-cc-pVTZ and revDSD-PBE86-D3/jun-cc-pVTZ based on Equation 1 in article.[3–5]

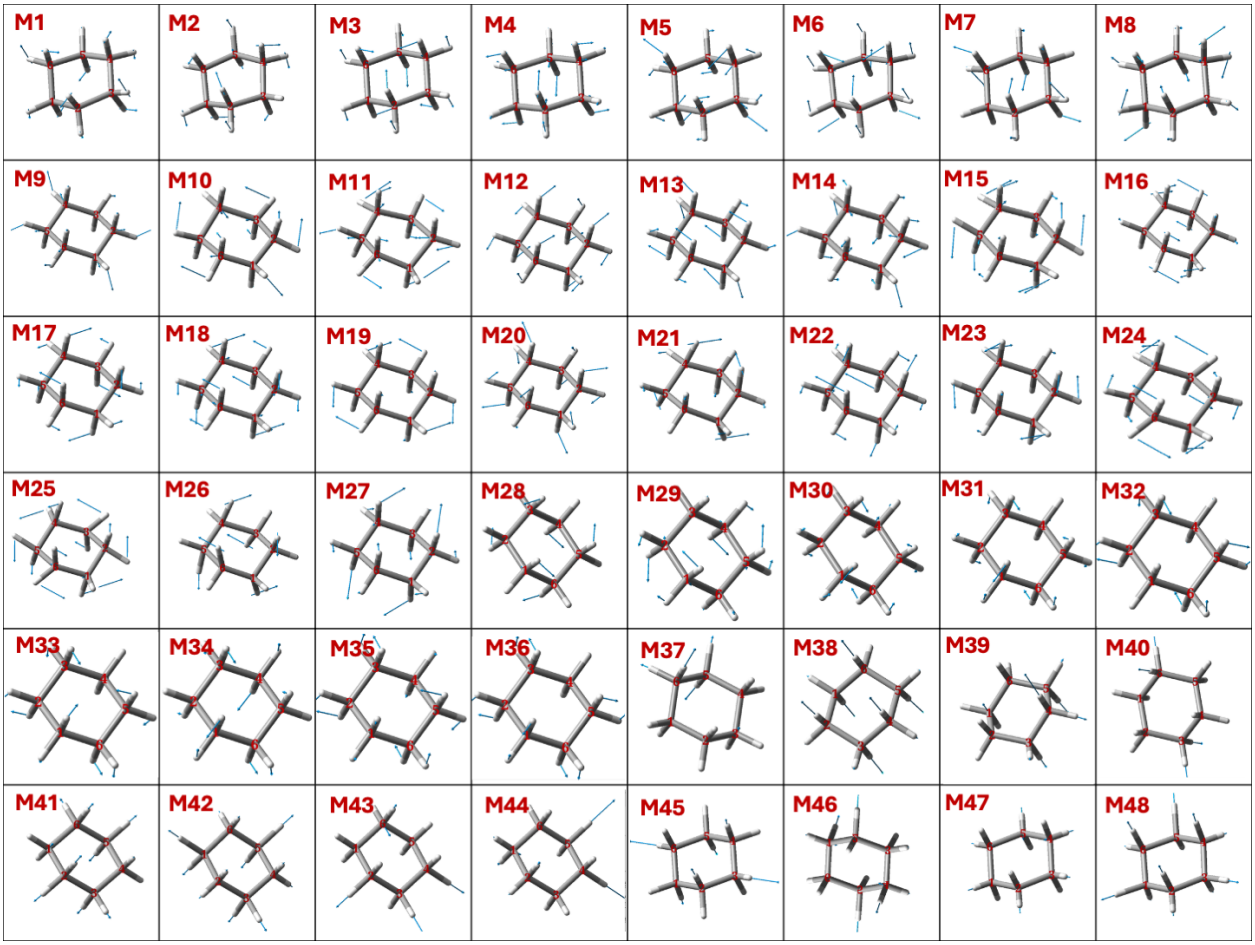

Figure S4: Visualization of 48 normal modes of cyclohexane

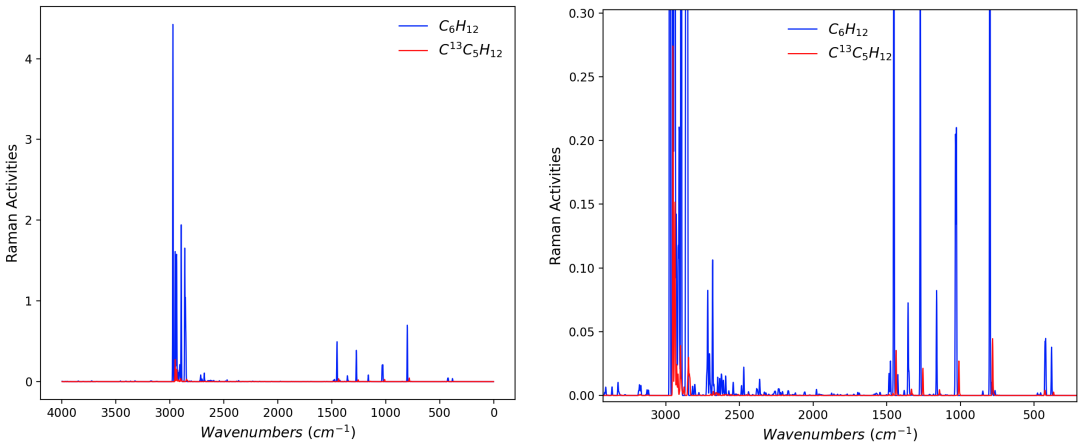

Figure S5: The calculated spectra of $^{12}C_6H_{12}$ and $^{13}C^{12}C_5H_{12}$ with isotopic effects.

Supplementary Tables

Table S1: The 48 normal modes description of cyclohexane: τ is twisting, ρ rocking, ξ scissoring, σ stretching. The displacement vector shown are scaled by 3.3 times.

Modes	energy (cm^{-1})	Band, Symmetry	Normal modes description
1	237.399	ν_{32}, E_U	Ring deform. + τ (C3 and C6)
2	227.958	ν_{32}, E_U	Ring deform. + τ (C2 and C5)
3	382.936	ν_{6}, A_{1G}	Ring breath.+ τ (C1, C2, C4 and C5)
4	423.614	ν_{24}, E_G	Ring deform. + τ (C2, C3, C2 and C6)
5	423.404	ν_{24}, E_G	Ring deform.
6	518.527	ν_{16}, A_{2U}	Ring breath.
7	787.105	ν_{23}, E_G	Ring brearh. (symmetrized)
8	782.613	ν_{23}, E_G	ρ (C1, C3, C4 and C6)
9	799.659	ν_{5}, A_{1G}	ρ (C1, C2, C5 and C4)
10	862.929	ν_{31}, E_U	Ring deformation, τ (C1 and C4)
11	861.259	ν_{31}, E_U	Ring deform.τ (C2 and C6)
12	906.705	ν_{30}, E_U	ρ (C1, C2, C3, C4, C5 and C6)
13	905.855	ν_{30}, E_U	ρ (C1, C2, C3, C4, C5 and C6)
14	1028.762	ν_{15}, A_{2U}	Ring deform. (in plane)
15	1028.079	ν_{22}, E_G	Ring deform. (in plane)+σ (C3-C4, C1-C6)
16	1030.826	ν_{22}, E_G	Ring deform. (in plane)+σ (C2-C3, C5-C6)
17	1059.672	ν_{11}, A_{2G}	ρ (C1, C2, C3, C4, C5 and C6)
18	1092.745	ν_{9}, A_{1U}	Ring deform.
19	1114.795	ν_{8}, A_{1U}	ρ (C1, C2, C3, C4, C5 and C6)
20	1161.392	ν_{4}, A_{1G}	ρ (C1, C2, C3, C4, C5 and C6)
21	1264.250	ν_{29}, E_U	ρ (C1, C2, C3, C4, C5 and C6)

Table S1 continued

Modes	energy (cm-1)	Band, Symmetry	Normal modes descriptions
22	1260.505	ν_{29}, E_U	ρ (C1, C2, C3, C4, C5 and C6)
23	1272.375	ν_{21}, E_G	ρ (C1, C2, C3, C4, C5 and C6)
24	1271.351	ν_{21}, E_G	ρ (C1, C2, C3, C4, C5 and C6)
25	1324.576	ν_{10}, A_{2G}	in plane ρ (C1, C2, C3, C4, C5 and C6)
26	1346.950	ν_{7}, A_{1U}	in plane ρ (C1, C2, C3, C4, C5 and C6)
27	1353.690	ν_{20}, E_G	in plane ρ (C1, C2, C3, C4, C5 and C6)
28	1351.080	ν_{20}, E_G	in plane ρ (C1, C2, C3, C4, C5 and C6)
29	1359.681	ν_{28}, E_U	Ring deform. + τ (C1, C2, C4 and C5)
30	1360.033	ν_{28}, E_U	Ring deform.+ τ (C1, C3, C4 and C6)
31	1450.657	ν_{19}, E_G	ξ (C1, C2, C3, C4, C5 and C6)
32	1449.822	ν_{19}, E_G	ξ (C2, C3, C5 and C6)
33	1458.213	ν_{27}, E_U	ξ (C1, C2, C3, C4, C5 and C6)
34	1456.976	ν_{27}, E_U	ξ (C2, C3, C5 and C6)
35	1459.019	ν_{14}, A_{2U}	ξ (C2, C3, C5 and C6)
36	1475.314	ν_{3}, A_{1G}	ξ (C1, C2, C3, C4, C5 and C6)
37	2888.798	ν_{26}, E_U	C-H σ (C6, C5)
38	2888.209	ν_{26}, E_U	perpendicular C-H σ (C1, C2, C3, C4 C5 and C6)
39	2888.900	ν_{2}, A_{1G}	C-H σ (C1, C3, C4 and C5)
40	2893.868	ν_{18}, E_G	C-H σ (C1, C2, C3, C4 C5 and C6)
41	2894.161	ν_{18}, E_G	C-H σ (C1, C2, C3, C4 C5 and C6)
42	2895.573	ν_{13}, A_{2U}	C-H σ (C1, C2, C3, C4 C5 and C6)
43	2940.890	ν_{25}, E_U	C-H σ (C2, C3, C5 and C6)
44	2940.150	ν_{25}, E_U	C-H σ (C1, C4 and C5)
45	2939.918	ν_{17}, E_G	C-H σ (C3 and C6)

Table S1 continued

Modes	energy (cm-1)	Band, Symmetry	Normal modes descriptions
46	2940.991	ν_{17}, E_G	C-H σ (C1, C2, C4 and C5)
47	2940.709	ν_1, A_{1G}	parallel C-H σ (C1, C2, C3, C4, C5, C6)
48	2945.872	ν_{12}, A_{2U}	all C-H σ (C1, C2, C3, C4, C5, C6)

Table S2: The anharmonic modes after the variational corrections in the range of 200 to 3200 cm^{-1}. The modes number in the combinations are taken from the harmonic normal modes in the increasing order of energy. The Raman is give in Ang^6, IR intensities are given in Km/mol.

Modes	Combinations	Frequencies	Raman Int.	IR Int.
1	+0.900336 x |2(1)>	225.0791	0.00000000	0.00877875
	-0.435196 x |1(1)>			
2	+0.900336 x |1(1)>	240.2775	0.00000000	0.00766034
	+0.435196 x |2(1)>			
3	+0.987511 x |3(1)>	380.8908	0.11404202	0.00000000
	-0.125027 x |2(2)>			
4	+0.711513 x |4(1)>	420.6775	0.12493237	0.00000001
	+0.695440 x |5(1)>			
5	+0.714006 x |5(1)>	425.3316	0.11710163	0.00000000
	-0.691435 x |4(1)>			
6	+0.991256 x |2(2)>	455.1249	0.00632616	0.00000000
	+0.120401 x |3(1)>			
7	+0.992117 x |2(1);1(1)>	466.0999	0.00138392	0.00000000
	-0.125108 x |4(1)>			
8	+0.990861 x |1(2)>	476.1489	0.00580441	0.00000000
	+0.100250 x |3(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
9	+1.000000 x |6(1)>	518.5272	0.00000003	0.79508158
10	+1.000000 x |3(1);2(1)>	609.5732	0.00000000	0.00031412
11	+1.000000 x |3(1);1(1)>	619.5757	0.00000000	0.00039274
12	+1.000000 x |5(1);2(1)>	650.0488	0.00000000	0.00091387
13	+1.000000 x |4(1);2(1)>	651.0048	0.00000000	0.00247452
14	+1.000000 x |4(1);1(1)>	661.0427	0.00000000	0.00087330
15	+1.000000 x |5(1);1(1)>	661.5330	0.00000000	0.00250491
16	+1.000000 x |6(1);2(1)>	748.4675	0.00081300	0.00000000
17	+1.000000 x |6(1);1(1)>	758.5657	0.00086175	0.00000000
18	+1.000000 x |3(2)>	764.4988	0.01180441	0.00000000
19	+0.999794 x |8(1)>	782.6114	0.02989491	0.00000003
20	+0.999794 x |7(1)>	787.1065	0.02821498	0.00000002
21	+1.000000 x |9(1)>	799.6590	2.13317978	0.00000000
22	+1.000000 x |5(1);3(1)>	807.0308	0.00002950	0.00000000
23	+1.000000 x |4(1);3(1)>	807.2666	0.00006147	0.00000000
24	+1.000000 x |5(2)>	847.0485	0.00531442	0.00000000
25	+1.000000 x |5(1);4(1)>	847.6234	0.00006017	0.00000000
26	+1.000000 x |4(2)>	847.6918	0.00537193	0.00000000
27	+0.996069 x |11(1)>	861.2457	0.00000000	2.23726091
28	+0.996069 x |10(1)>	862.9420	0.00000000	2.07858749
29	+1.000000 x |6(1);3(1)>	904.4057	0.00000000	0.02656787
30	+0.868975 x |13(1)> -0.471110 x |12(1)> +0.148465 x |6(1);4(1)>	904.6384	0.00000000	1.71323062

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
31	+0.867115 x |12(1)>	906.0270	0.00000000	1.71700057
	+0.470742 x |13(1)>			
	+0.158849 x |6(1);5(1)>			
32	+0.979062 x |6(1);5(1)>	943.5351	0.00000000	0.03167510
	+0.125155 x |6(1);4(1)>			
	-0.115541 x |13(1)>			
	-0.111467 x |12(1)>			
33	+0.980313 x |6(1);4(1)>	943.8674	0.00000000	0.02928937
	-0.123731 x |6(1);5(1)>			
	+0.117227 x |12(1)>			
34	+0.892492 x |8(1);2(1)>	1006.7106	0.00000000	0.33375163
	-0.377138 x |15(1)>			
	+0.175718 x |7(1);2(1)>			
	+0.133671 x |7(1);1(1)>			
	-0.111712 x |8(1);1(1)>			
35	+0.914188 x |7(1);2(1)>	1014.1419	0.00000000	0.09446657
	-0.300059 x |8(1);2(1)>			
	-0.199975 x |15(1)>			
	-0.141499 x |8(1);1(1)>			
	+0.119220 x |7(1);1(1)>			
36	+0.868556 x |8(1);1(1)>	1018.3901	0.00000000	0.15504643
	+0.286409 x |7(1);2(1)>			
	+0.252945 x |15(1)>			
	-0.247170 x |7(1);1(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.196232 x |8(1);2(1)>			
37	+0.811262 x |7(1);1(1)>	1022.4272	0.00000000	0.24178079
	+0.420680 x |8(1);1(1)>			
	-0.326033 x |15(1)>			
	-0.173365 x |8(1);2(1)>			
	-0.168905 x |7(1);2(1)>			
38	+0.819677 x |14(1)>	1026.7928	0.62632269	0.00000000
	-0.572826 x |16(1)>			
39	+1.000000 x |9(1);2(1)>	1027.4270	0.00000000	0.00005554
40	+0.819677 x |16(1)>	1032.7956	0.61473738	0.00000000
	+0.572826 x |14(1)>			
41	+0.804673 x |15(1)>	1035.5194	0.00000000	1.38562800
	+0.498677 x |7(1);1(1)>			
	+0.211800 x |8(1);2(1)>			
	-0.190100 x |8(1);1(1)>			
	+0.151080 x |7(1);2(1)>			
42	+1.000000 x |9(1);1(1)>	1037.0116	0.00000000	0.00003824
43	+1.000000 x |6(2)>	1038.0170	0.00253145	0.00000000
44	+1.000000 x |17(1)>	1059.6715	0.00047256	0.00000000
45	+1.000000 x |11(1);2(1)>	1088.8904	0.00088886	0.00000000
46	+0.935171 x |18(1)>	1089.0521	0.00000000	0.03520694
	-0.354197 x |19(1)>			
47	+1.000000 x |10(1);2(1)>	1090.9619	0.00072759	0.00000000
48	+1.000000 x |11(1);1(1)>	1098.6097	0.00086824	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
49	+1.000000 x |10(1);1(1)>	1100.5750	0.00095464	0.00000000
50	+0.935171 x |19(1)> +0.354197 x |18(1)>	1118.4873	0.00000000	0.00010692
51	+1.000000 x |13(1);2(1)>	1133.3395	0.00279118	0.00000000
52	+1.000000 x |12(1);2(1)>	1135.9886	0.00113015	0.00000000
53	+1.000000 x |12(1);1(1)>	1143.9739	0.00311081	0.00000000
54	+1.000000 x |13(1);1(1)>	1144.6086	0.00115321	0.00000000
55	+0.992119 x |20(1)> -0.125295 x |9(1);3(1)>	1161.0621	0.24770545	0.00000000
56	+1.000000 x |8(1);3(1)>	1165.2465	0.00019318	0.00000000
57	+1.000000 x |7(1);3(1)>	1169.9215	0.00019333	0.00000000
58	+0.992119 x |9(1);3(1)> +0.125295 x |20(1)>	1182.0783	0.00319492	0.00000000
59	+1.000000 x |8(1);5(1)>	1205.4518	0.00139300	0.00000000
60	+1.000000 x |8(1);4(1)>	1205.8600	0.00078266	0.00000000
61	+1.000000 x |7(1);5(1)>	1210.4139	0.00087950	0.00000000
62	+1.000000 x |7(1);4(1)>	1210.7127	0.00144456	0.00000000
63	+1.000000 x |9(1);5(1)>	1222.2993	0.00002157	0.00000000
64	+1.000000 x |9(1);4(1)>	1222.5156	0.00002382	0.00000000
65	+1.000000 x |11(1);3(1)>	1243.7182	0.00000000	0.00052933
66	+1.000000 x |10(1);3(1)>	1245.5177	0.00000000	0.00038064
67	+1.000000 x |15(1);2(1)>	1254.7188	0.00038513	0.00000000
68	+0.968056 x |14(1);2(1)> +0.242481 x |21(1)>	1256.1021	0.00000000	0.13586005

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
69	+0.781716 x |16(1);2(1)> -0.604979 x |22(1)> +0.120778 x |14(1);1(1)>	1257.2136	0.00000000	0.72376869
70	+0.732478 x |22(1)> +0.619145 x |16(1);2(1)> -0.249369 x |14(1);1(1)>	1260.8498	0.00000000	1.00489520
71	+0.909951 x |21(1)> -0.275425 x |16(1);1(1)> -0.240526 x |14(1);2(1)> +0.136939 x |17(1);2(1)>	1263.4009	0.00000000	1.49611509
72	+1.000000 x |15(1);1(1)>	1264.3033	0.00035623	0.00000000
73	+0.959503 x |14(1);1(1)> +0.268985 x |22(1)>	1266.4975	0.00000000	0.11543997
74	+0.960491 x |16(1);1(1)> +0.267439 x |21(1)>	1268.8509	0.00000000	0.12897794
75	+0.975026 x |24(1)> +0.222093 x |23(1)>	1271.2951	0.61124063	0.00000001
76	+0.975026 x |23(1)> -0.222093 x |24(1)>	1272.4314	0.60457610	0.00000000
77	+0.997439 x |11(1);4(1)>	1284.1893	0.00000000	0.01145025
78	+1.000000 x |11(1);5(1)>	1284.5514	0.00000000	0.01181196
79	+1.000000 x |10(1);5(1)>	1285.5737	0.00000000	0.01699611
80	+0.991289 x |10(1);4(1)> +0.119792 x |17(1);2(1)>	1286.5170	0.00000000	0.00302233
81	+0.967636 x |17(1);2(1)>	1288.4343	0.00000000	0.04678154

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	-0.184089 x |12(1);3(1)>			
	-0.136325 x |21(1)>			
	-0.105016 x |10(1);4(1)>			
82	+0.994891 x |13(1);3(1)>	1289.7739	0.00000000	0.00073030
83	+0.978037 x |12(1);3(1)>	1290.6088	0.00000000	0.00316169
	+0.164250 x |17(1);2(1)>			
	-0.119957 x |21(1)>			
84	+0.996581 x |17(1);1(1)>	1298.6280	0.00000000	0.02201817
85	+1.000000 x |8(1);6(1)>	1301.0335	0.00000000	0.00001891
86	+1.000000 x |7(1);6(1)>	1305.5595	0.00000000	0.00008795
87	+1.000000 x |9(1);6(1)>	1317.6626	0.00000000	0.02041673
88	+0.992324 x |18(1);2(1)>	1320.7395	0.00061974	0.00000000
	+0.122076 x |27(1)>			
89	+1.000000 x |25(1)>	1324.5762	0.00030093	0.00000000
90	+1.000000 x |13(1);5(1)>	1329.0300	0.00000000	0.00133790
91	+1.000000 x |13(1);4(1)>	1329.2165	0.00000000	0.00168358
92	+1.000000 x |12(1);5(1)>	1329.9642	0.00000000	0.00145658
93	+1.000000 x |12(1);4(1)>	1330.1173	0.00000000	0.00119103
94	+0.980971 x |18(1);1(1)>	1330.2508	0.00235869	0.00000000
	+0.191484 x |28(1)>			
95	+0.964259 x |19(1);2(1)>	1341.8479	0.00260323	0.00000000
	-0.258964 x |27(1)>			
96	+1.000000 x |26(1)>	1346.9497	0.00000000	0.04448223
97	+0.731844 x |28(1)>	1348.5607	0.05540155	0.00000000
	-0.655213 x |19(1);1(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	-0.163273 x |18(1);1(1)>			
98	+0.911021 x |27(1)>	1354.5160	0.13318874	0.00000000
	+0.254211 x |19(1);2(1)>			
	+0.226371 x |19(1);1(1)>			
	+0.158264 x |28(1)>			
	-0.120905 x |10(1);6(1)>			
	-0.108501 x |18(1);2(1)>			
99	+0.720002 x |19(1);1(1)>	1355.0523	0.08890667	0.00000000
	+0.621133 x |28(1)>			
	-0.262857 x |27(1)>			
	+0.102359 x |11(1);6(1)>			
	-0.101150 x |18(1);1(1)>			
100	+0.759232 x |29(1)>	1358.7064	0.00000000	0.02328235
	+0.650820 x |30(1)>			
101	+0.759232 x |30(1)>	1361.0075	0.00000000	0.08500039
	-0.650820 x |29(1)>			
102	+0.990627 x |11(1);6(1)>	1380.0960	0.00686290	0.00000000
	-0.115861 x |28(1)>			
103	+0.991328 x |10(1);6(1)>	1381.8501	0.00608912	0.00000000
	+0.116466 x |27(1)>			
104	+1.000000 x |20(1);2(1)>	1388.6916	0.00000000	0.01460859
105	+1.000000 x |20(1);1(1)>	1398.2047	0.00000000	0.01328425
106	+1.000000 x |15(1);3(1)>	1409.5709	0.00000000	0.05385467
107	+1.000000 x |14(1);3(1)>	1412.1412	0.00011519	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
108	+1.000000 x |16(1);3(1)>	1413.9271	0.00010568	0.00000000
109	+0.971672 x |13(1);6(1)> +0.230141 x |32(1)>	1423.9863	0.02735947	0.00000000
110	+0.972450 x |12(1);6(1)> -0.226661 x |31(1)>	1424.8749	0.02398946	0.00000000
111	+1.000000 x |17(1);3(1)>	1444.8702	0.00000011	0.00000000
112	+0.956310 x |15(1);5(1)> +0.290494 x |34(1)>	1450.0334	0.00000000	0.56351562
113	+0.797424 x |32(1)> +0.542589 x |31(1)> -0.194059 x |13(1);6(1)> +0.134218 x |12(1);6(1)> +0.116659 x |17(1);5(1)>	1450.2509	0.81432297	0.00000000
114	+1.000000 x |15(1);4(1)>	1450.6477	0.00000000	0.13413553
115	+1.000000 x |14(1);5(1)>	1451.7752	0.00064109	0.00000000
116	+0.797344 x |31(1)> -0.545808 x |32(1)> +0.183882 x |12(1);6(1)> +0.124760 x |17(1);4(1)> +0.124118 x |13(1);6(1)>	1451.9932	0.82001451	0.00000000
117	+1.000000 x |14(1);4(1)>	1452.0888	0.00135987	0.00000000
118	+1.000000 x |16(1);5(1)>	1453.8928	0.00189483	0.00000000
119	+1.000000 x |16(1);4(1)>	1454.0591	0.00098222	0.00000000
120	+0.775198 x |34(1)> -0.577799 x |33(1)>	1456.9689	0.00000000	6.41096341

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	-0.255375 x |15(1);5(1)>			
121	+0.815515 x |33(1)>	1458.8508	0.00000000	5.95500042
	+0.560965 x |34(1)>			
	-0.142318 x |15(1);5(1)>			
122	+1.000000 x |35(1)>	1459.0186	0.00000000	15.23919921
123	+0.984510 x |36(1)>	1474.4493	0.08333293	0.00000000
	-0.143431 x |22(1);2(1)>			
124	+1.000000 x |18(1);3(1)>	1476.1848	0.00000000	0.00000009
125	+0.814192 x |17(1);5(1)>	1483.8295	0.02313866	0.00000000
	-0.569008 x |17(1);4(1)>			
	-0.111221 x |32(1)>			
126	+0.812402 x |17(1);4(1)>	1483.9975	0.02790226	0.00000000
	+0.567139 x |17(1);5(1)>			
	-0.131580 x |31(1)>			
127	+0.989634 x |22(1);2(1)>	1486.9319	0.00289618	0.00000000
	+0.142076 x |36(1)>			
128	+1.000000 x |21(1);2(1)>	1492.4441	0.00023111	0.00000000
129	+1.000000 x |19(1);3(1)>	1497.8745	0.00000000	0.00000109
130	+1.000000 x |22(1);1(1)>	1497.9855	0.00029092	0.00000000
131	+1.000000 x |24(1);2(1)>	1499.3513	0.00000000	0.11231347
132	+1.000000 x |23(1);2(1)>	1499.7317	0.00000000	0.00494449
133	+0.998304 x |21(1);1(1)>	1501.7213	0.00169053	0.00000000
134	+1.000000 x |24(1);1(1)>	1508.1899	0.00000000	0.00510316
135	+1.000000 x |23(1);1(1)>	1510.2179	0.00000000	0.11838942

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
136	+1.000000 x |18(1);5(1)>	1515.3749	0.00000000	0.00008843
137	+1.000000 x |18(1);4(1)>	1515.6074	0.00000000	0.00010381
138	+1.000000 x |19(1);5(1)>	1538.5129	0.00000000	0.07242704
139	+1.000000 x |19(1);4(1)>	1538.7327	0.00000000	0.07166439
140	+1.000000 x |20(1);3(1)>	1543.1100	0.00424835	0.00000000
141	+0.996349 x |15(1);6(1)>	1546.3250	0.00568801	0.00000000
142	+1.000000 x |14(1);6(1)>	1547.1860	0.00000000	0.00232688
143	+1.000000 x |16(1);6(1)>	1549.1964	0.00000000	0.00199991
144	+1.000000 x |25(1);2(1)>	1552.4108	0.00000000	0.00003912
145	+1.000000 x |25(1);1(1)>	1561.9810	0.00000000	0.00015620
146	+1.000000 x |8(2)>	1565.0285	0.00356578	0.00000000
147	+1.000000 x |8(1);7(1)>	1569.9520	0.00482360	0.00000000
148	+1.000000 x |26(1);2(1)>	1573.8630	0.00049683	0.00000000
149	+1.000000 x |7(2)>	1574.3298	0.00330342	0.00000000
150	+1.000000 x |28(1);2(1)>	1578.5394	0.00000000	0.01411218
151	+1.000000 x |17(1);6(1)>	1579.4746	0.00000000	0.00000134
152	+1.000000 x |27(1);2(1)>	1581.3432	0.00000000	0.00635447
153	+1.000000 x |9(1);8(1)>	1581.7708	0.00041604	0.00000000
154	+1.000000 x |20(1);5(1)>	1583.9139	0.00111757	0.00000000
155	+1.000000 x |26(1);1(1)>	1583.9636	0.00043666	0.00000000
156	+1.000000 x |20(1);4(1)>	1584.1836	0.00113884	0.00000000
157	+1.000000 x |9(1);7(1)>	1586.3682	0.00036743	0.00000000
158	+1.000000 x |29(1);2(1)>	1587.2956	0.00021901	0.00000000
159	+1.000000 x |30(1);2(1)>	1587.7350	0.00038142	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
160	+1.000000 x |28(1);1(1)>	1588.0403	0.00000000	0.00624788
161	+1.000000 x |27(1);1(1)>	1591.5115	0.00000000	0.01397523
162	+1.000000 x |29(1);1(1)>	1596.8983	0.00036383	0.00000000
163	+1.000000 x |30(1);1(1)>	1597.1865	0.00020825	0.00000000
164	+1.000000 x |9(2)>	1598.2413	0.00022994	0.00000000
165	+1.000000 x |18(1);6(1)>	1610.7797	0.00000002	0.00000000
166	+1.000000 x |19(1);6(1)>	1633.5357	0.00000000	0.00000000
167	+1.000000 x |22(1);3(1)>	1643.4835	0.00000000	0.04105519
168	+1.000000 x |11(1);8(1)>	1643.6791	0.00000000	0.00807993
169	+1.000000 x |10(1);8(1)>	1645.1771	0.00000000	0.00845840
170	+1.000000 x |21(1);3(1)>	1647.2048	0.00000000	0.04308794
171	+1.000000 x |11(1);7(1)>	1648.0833	0.00000000	0.00832496
172	+1.000000 x |10(1);7(1)>	1649.9991	0.00000000	0.00822535
173	+1.000000 x |24(1);3(1)>	1653.9815	0.00037875	0.00000000
174	+1.000000 x |23(1);3(1)>	1655.0310	0.00037692	0.00000000
175	+1.000000 x |11(1);9(1)>	1659.5032	0.00000000	0.00826840
176	+1.000000 x |10(1);9(1)>	1661.1982	0.00000000	0.00798789
177	+1.000000 x |32(1);2(1)>	1677.3875	0.00000000	0.03357915
178	+1.000000 x |31(1);2(1)>	1678.7051	0.00000000	0.00646589
179	+1.000000 x |20(1);6(1)>	1679.1514	0.00000000	0.00075566
180	+1.000000 x |22(1);5(1)>	1683.0572	0.00000000	0.00602285
181	+1.000000 x |22(1);4(1)>	1683.0688	0.00000000	0.00745933
182	+1.000000 x |34(1);2(1)>	1684.7214	0.00269903	0.00000000
183	+1.000000 x |33(1);2(1)>	1686.2504	0.00042409	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
184	+1.000000 x |35(1);2(1)>	1686.4572	0.00307222	0.00000000
185	+1.000000 x |21(1);5(1)>	1687.0989	0.00000000	0.00786527
186	+1.000000 x |32(1);1(1)>	1687.4431	0.00000000	0.00655818
187	+1.000000 x |21(1);4(1)>	1687.6213	0.00000000	0.00655820
188	+1.000000 x |31(1);1(1)>	1688.1900	0.00000000	0.03320927
189	+1.000000 x |13(1);8(1)>	1688.6197	0.00000000	0.02561634
190	+1.000000 x |12(1);8(1)>	1689.5457	0.00000000	0.00927367
191	+1.000000 x |13(1);7(1)>	1693.2921	0.00000000	0.00957972
192	+1.000000 x |24(1);5(1)>	1694.0276	0.00021179	0.00000000
193	+1.000000 x |12(1);7(1)>	1694.2524	0.00000000	0.02721993
194	+1.000000 x |34(1);1(1)>	1694.4351	0.00043787	0.00000000
195	+1.000000 x |24(1);4(1)>	1694.6907	0.00043520	0.00000000
196	+1.000000 x |23(1);4(1)>	1695.3705	0.00022272	0.00000000
197	+1.000000 x |23(1);5(1)>	1695.6784	0.00043219	0.00000000
198	+1.000000 x |33(1);1(1)>	1696.0151	0.00276953	0.00000000
199	+1.000000 x |35(1);1(1)>	1696.1913	0.00306781	0.00000000
200	+1.000000 x |36(1);2(1)>	1703.1652	0.00000000	0.00101594
201	+1.000000 x |13(1);9(1)>	1704.7832	0.00000000	0.00208231
202	+1.000000 x |12(1);9(1)>	1705.6245	0.00000000	0.00200861
203	+1.000000 x |25(1);3(1)>	1707.2302	0.00000002	0.00000000
204	+1.000000 x |36(1);1(1)>	1713.0280	0.00000000	0.00125872
205	+1.000000 x |11(2)>	1720.7716	0.00174140	0.00000000
206	+1.000000 x |11(1);10(1)>	1724.2444	0.00064708	0.00000000
207	+1.000000 x |10(2)>	1724.2493	0.00174009	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
208	+1.000000 x |26(1);3(1)>	1728.7531	0.00000000	0.00000149
209	+1.000000 x |28(1);3(1)>	1733.7016	0.00017597	0.00000000
210	+1.000000 x |27(1);3(1)>	1736.5121	0.00017993	0.00000000
211	+1.000000 x |29(1);3(1)>	1742.3576	0.00000000	0.01307827
212	+1.000000 x |30(1);3(1)>	1742.7424	0.00000000	0.01329730
213	+1.000000 x |25(1);5(1)>	1747.6086	0.00032394	0.00000000
214	+1.000000 x |25(1);4(1)>	1747.8179	0.00032180	0.00000000
215	+1.000000 x |13(1);11(1)>	1766.8913	0.00077776	0.00000000
216	+1.000000 x |12(1);11(1)>	1767.5551	0.00104693	0.00000000
217	+1.000000 x |13(1);10(1)>	1768.4360	0.00105296	0.00000000
218	+1.000000 x |12(1);10(1)>	1769.5100	0.00077499	0.00000000
219	+1.000000 x |26(1);5(1)>	1769.7202	0.00000000	0.00278068
220	+1.000000 x |26(1);4(1)>	1769.8563	0.00000000	0.00316891
221	+1.000000 x |28(1);5(1)>	1773.5431	0.00010082	0.00000000
222	+1.000000 x |28(1);4(1)>	1773.7776	0.00010536	0.00000000
223	+1.000000 x |27(1);4(1)>	1776.5550	0.00010417	0.00000000
224	+1.000000 x |27(1);5(1)>	1776.5796	0.00010023	0.00000000
225	+1.000000 x |22(1);6(1)>	1778.5733	0.00066911	0.00000000
226	+1.000000 x |21(1);6(1)>	1782.3524	0.00067292	0.00000000
227	+1.000000 x |29(1);5(1)>	1782.4852	0.00000000	0.03045619
228	+1.000000 x |29(1);4(1)>	1782.7701	0.00000000	0.03018408
229	+1.000000 x |30(1);5(1)>	1782.9500	0.00000000	0.03013792
230	+1.000000 x |30(1);4(1)>	1783.1367	0.00000000	0.03029676
231	+1.000000 x |24(1);6(1)>	1789.4443	0.00000000	0.01904212

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
232	+1.000000 x |23(1);6(1)>	1790.5085	0.00000000	0.01948312
233	+1.000000 x |15(1);8(1)>	1809.1335	0.00000000	0.01739634
234	+1.000000 x |14(1);8(1)>	1811.4709	0.00052696	0.00000000
235	+1.000000 x |13(2)>	1811.7765	0.00052207	0.00000000
236	+1.000000 x |13(1);12(1)>	1813.1093	0.00000893	0.00000000
237	+1.000000 x |16(1);8(1)>	1813.5776	0.00045361	0.00000000
238	+1.000000 x |12(2)>	1813.6085	0.00053123	0.00000000
239	+1.000000 x |15(1);7(1)>	1813.7105	0.00000000	0.01812259
240	+1.000000 x |14(1);7(1)>	1816.1357	0.00045564	0.00000000
241	+1.000000 x |16(1);7(1)>	1818.0803	0.00052114	0.00000000
242	+1.000000 x |15(1);9(1)>	1826.5970	0.00000000	0.02265184
243	+1.000000 x |14(1);9(1)>	1826.8254	0.00008601	0.00000000
244	+1.000000 x |16(1);9(1)>	1828.8548	0.00008613	0.00000000
245	+1.000000 x |32(1);3(1)>	1832.8988	0.00144682	0.00000000
246	+1.000000 x |31(1);3(1)>	1833.5009	0.00145574	0.00000000
247	+1.000000 x |34(1);3(1)>	1840.1877	0.00000000	0.00547653
248	+1.000000 x |33(1);3(1)>	1841.4173	0.00000000	0.00574630
249	+1.000000 x |35(1);3(1)>	1841.7438	0.00000000	0.09162842
250	+1.000000 x |25(1);6(1)>	1843.1924	0.00000000	0.00000117
251	+1.000000 x |17(1);8(1)>	1843.5907	0.00061532	0.00000000
252	+1.000000 x |17(1);7(1)>	1848.5396	0.00059376	0.00000000
253	+1.000000 x |36(1);3(1)>	1858.2638	0.00340482	0.00000000
254	+1.000000 x |17(1);9(1)>	1859.2753	0.00000008	0.00000000
255	+1.000000 x |26(1);6(1)>	1865.0409	0.00000008	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
256	+1.000000 x |28(1);6(1)>	1869.1716	0.00000000	0.06075261
257	+1.000000 x |27(1);6(1)>	1871.9858	0.00000000	0.06055517
258	+1.000000 x |32(1);5(1)>	1872.8258	0.00146722	0.00000000
259	+1.000000 x |32(1);4(1)>	1873.1946	0.00133121	0.00000000
260	+1.000000 x |31(1);5(1)>	1873.8679	0.00135882	0.00000000
261	+1.000000 x |31(1);4(1)>	1874.0135	0.00149042	0.00000000
262	+1.000000 x |18(1);8(1)>	1875.6441	0.00000000	0.00315442
263	+1.000000 x |29(1);6(1)>	1878.1588	0.00036552	0.00000000
264	+1.000000 x |30(1);6(1)>	1878.5359	0.00036331	0.00000000
265	+1.000000 x |34(1);5(1)>	1880.1290	0.00000000	0.02475780
266	+1.000000 x |18(1);7(1)>	1880.4254	0.00000000	0.00299899
267	+1.000000 x |34(1);4(1)>	1880.7037	0.00000000	0.02217994
268	+1.000000 x |33(1);5(1)>	1881.7194	0.00000000	0.02207001
269	+1.000000 x |33(1);4(1)>	1881.8966	0.00000000	0.02476194
270	+1.000000 x |35(1);5(1)>	1882.2849	0.00000000	0.00107205
271	+1.000000 x |35(1);4(1)>	1882.5329	0.00000000	0.00105645
272	+1.000000 x |14(1);11(1)>	1888.0559	0.00000000	0.00463883
273	+1.000000 x |15(1);11(1)>	1888.3868	0.00046576	0.00000000
274	+1.000000 x |14(1);10(1)>	1889.9498	0.00000000	0.00468533
275	+1.000000 x |15(1);10(1)>	1890.1026	0.00046662	0.00000000
276	+1.000000 x |16(1);11(1)>	1890.2786	0.00000000	0.00455582
277	+1.000000 x |18(1);9(1)>	1890.7011	0.00000000	0.00000029
278	+1.000000 x |16(1);10(1)>	1892.0564	0.00000000	0.00440488
279	+1.000000 x |19(1);8(1)>	1897.5301	0.00000000	0.00936168

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
280	+1.000000 x |36(1);5(1)>	1898.4851	0.00025019	0.00000000
281	+1.000000 x |36(1);4(1)>	1898.7502	0.00023956	0.00000000
282	+1.000000 x |19(1);7(1)>	1902.0574	0.00000000	0.00915604
283	+1.000000 x |19(1);9(1)>	1913.7429	0.00000000	0.00000022
284	+1.000000 x |17(1);11(1)>	1920.5724	0.00000000	0.01313814
285	+1.000000 x |17(1);10(1)>	1922.2965	0.00000000	0.01317216
286	+1.000000 x |15(1);13(1)>	1933.0131	0.00060728	0.00000000
287	+1.000000 x |15(1);12(1)>	1933.8925	0.00060111	0.00000000
288	+1.000000 x |14(1);13(1)>	1934.4402	0.00000000	0.01648026
289	+1.000000 x |14(1);12(1)>	1935.5447	0.00000000	0.01614093
290	+1.000000 x |16(1);13(1)>	1936.7419	0.00000000	0.01614879
291	+1.000000 x |16(1);12(1)>	1937.3566	0.00000000	0.01634856
292	+1.000000 x |20(1);8(1)>	1941.9370	0.00167515	0.00000000
293	+1.000000 x |20(1);7(1)>	1946.4511	0.00165641	0.00000000
294	+1.000000 x |18(1);11(1)>	1951.4976	0.00133093	0.00000000
295	+1.000000 x |18(1);10(1)>	1953.3060	0.00133645	0.00000000
296	+1.000000 x |20(1);9(1)>	1959.7462	0.00336180	0.00000000
297	+1.000000 x |17(1);13(1)>	1966.8811	0.00000000	0.00676794
298	+1.000000 x |17(1);12(1)>	1967.7877	0.00000000	0.00709398
299	+1.000000 x |32(1);6(1)>	1967.8020	0.00000000	0.00009158
300	+1.000000 x |31(1);6(1)>	1968.5844	0.00000000	0.00012522
301	+1.000000 x |34(1);6(1)>	1975.2564	0.00297393	0.00000000
302	+1.000000 x |19(1);11(1)>	1975.7696	0.00034809	0.00000000
303	+1.000000 x |33(1);6(1)>	1976.4331	0.00298431	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
304	+1.000000 x |35(1);6(1)>	1976.7263	0.00851303	0.00000000
305	+1.000000 x |19(1);10(1)>	1977.5046	0.00034806	0.00000000
306	+1.000000 x |36(1);6(1)>	1993.1030	0.00000000	0.29619120
307	+1.000000 x |18(1);13(1)>	1998.6087	0.00017362	0.00000000
308	+1.000000 x |18(1);12(1)>	1999.4847	0.00017118	0.00000000
309	+1.000000 x |19(1);13(1)>	2020.8289	0.00069387	0.00000000
310	+1.000000 x |20(1);11(1)>	2021.5843	0.00000000	0.02412109
311	+1.000000 x |19(1);12(1)>	2021.6515	0.00069509	0.00000000
312	+1.000000 x |20(1);10(1)>	2023.3114	0.00000000	0.02379335
313	+1.000000 x |22(1);8(1)>	2042.4443	0.00000000	0.01119349
314	+1.000000 x |21(1);8(1)>	2046.8100	0.00000000	0.00269719
315	+1.000000 x |22(1);7(1)>	2047.6168	0.00000000	0.00266983
316	+1.000000 x |21(1);7(1)>	2051.2379	0.00000000	0.01167773
317	+1.000000 x |24(1);8(1)>	2053.7573	0.00199041	0.00000000
318	+1.000000 x |23(1);8(1)>	2054.8466	0.00186409	0.00000000
319	+1.000000 x |15(2)>	2055.1782	0.00235753	0.00000000
320	+1.000000 x |14(2)>	2055.5165	0.00144023	0.00000000
321	+1.000000 x |15(1);14(1)>	2056.1647	0.00000000	0.02268329
322	+1.000000 x |16(1);15(1)>	2058.2000	0.00000000	0.02276379
323	+1.000000 x |24(1);7(1)>	2058.3818	0.00187238	0.00000000
324	+1.000000 x |16(1);14(1)>	2058.8947	0.00107687	0.00000000
325	+1.000000 x |23(1);7(1)>	2059.3674	0.00197800	0.00000000
326	+1.000000 x |22(1);9(1)>	2059.4456	0.00000000	0.00074497
327	+1.000000 x |16(2)>	2059.7233	0.00143974	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
328	+1.000000 x |21(1);9(1)>	2063.1914	0.00000000	0.00077545
329	+1.000000 x |20(1);13(1)>	2065.4183	0.00000000	0.06917256
330	+1.000000 x |20(1);12(1)>	2066.2642	0.00000000	0.06964091
331	+1.000000 x |24(1);9(1)>	2069.9838	0.00009387	0.00000000
332	+1.000000 x |23(1);9(1)>	2071.0156	0.00009539	0.00000000
333	+1.000000 x |17(1);14(1)>	2087.7863	0.00044893	0.00000000
334	+1.000000 x |17(1);15(1)>	2088.0761	0.00000000	0.00000128
335	+1.000000 x |17(1);16(1)>	2089.9283	0.00046372	0.00000000
336	+1.000000 x |25(1);8(1)>	2107.2902	0.00000070	0.00000000
337	+1.000000 x |25(1);7(1)>	2111.8719	0.00000049	0.00000000
338	+1.000000 x |18(1);14(1)>	2117.3157	0.00000000	0.00907944
339	+1.000000 x |17(2)>	2119.1831	0.00516157	0.00000000
340	+1.000000 x |18(1);16(1)>	2119.5220	0.00000000	0.00899289
341	+1.000000 x |18(1);15(1)>	2119.8201	0.00000001	0.00000000
342	+1.000000 x |22(1);11(1)>	2120.9183	0.00087846	0.00000000
343	+1.000000 x |22(1);10(1)>	2122.4406	0.00101755	0.00000000
344	+1.000000 x |25(1);9(1)>	2123.3401	0.00000006	0.00000000
345	+1.000000 x |21(1);11(1)>	2124.4751	0.00102854	0.00000000
346	+1.000000 x |21(1);10(1)>	2126.4371	0.00088942	0.00000000
347	+1.000000 x |26(1);8(1)>	2129.2899	0.00000000	0.03664442
348	+1.000000 x |24(1);11(1)>	2131.2342	0.00000000	0.01341810
349	+1.000000 x |23(1);11(1)>	2132.5228	0.00000000	0.00965092
350	+1.000000 x |24(1);10(1)>	2133.1678	0.00000000	0.00958473
351	+1.000000 x |28(1);8(1)>	2133.1768	0.00119673	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
352	+1.000000 x |26(1);7(1)>	2134.0702	0.00000000	0.03634574
353	+1.000000 x |23(1);10(1)>	2134.0963	0.00000000	0.01366230
354	+1.000000 x |27(1);8(1)>	2135.9895	0.00095737	0.00000000
355	+1.000000 x |28(1);7(1)>	2137.8899	0.00095510	0.00000000
356	+1.000000 x |27(1);7(1)>	2140.5021	0.00120761	0.00000000
357	+1.000000 x |29(1);8(1)>	2141.9570	0.00000000	0.00874990
358	+1.000000 x |19(1);15(1)>	2142.0409	0.00000000	0.00000000
359	+1.000000 x |30(1);8(1)>	2142.4399	0.00000000	0.00907465
360	+1.000000 x |19(1);14(1)>	2144.3517	0.00000000	0.11999847
361	+1.000000 x |26(1);9(1)>	2145.0490	0.00000000	0.00000634
362	+1.000000 x |19(1);16(1)>	2146.4152	0.00000000	0.11942300
363	+1.000000 x |29(1);7(1)>	2146.5775	0.00000000	0.00904677
364	+1.000000 x |30(1);7(1)>	2146.9120	0.00000000	0.00864626
365	+1.000000 x |28(1);9(1)>	2149.1383	0.00089504	0.00000000
366	+1.000000 x |18(1);17(1)>	2151.2722	0.00000000	0.00160009
367	+1.000000 x |27(1);9(1)>	2151.7704	0.00089212	0.00000000
368	+1.000000 x |29(1);9(1)>	2157.9394	0.00000000	0.04057238
369	+1.000000 x |30(1);9(1)>	2158.3124	0.00000000	0.04056311
370	+1.000000 x |22(1);13(1)>	2165.4619	0.00767343	0.00000000
371	+1.000000 x |22(1);12(1)>	2166.6245	0.00213984	0.00000000
372	+1.000000 x |21(1);13(1)>	2169.5606	0.00213376	0.00000000
373	+1.000000 x |21(1);12(1)>	2170.1706	0.00759028	0.00000000
374	+1.000000 x |19(1);17(1)>	2173.6501	0.00000000	0.00006811
375	+1.000000 x |24(1);13(1)>	2176.6195	0.00000000	0.03812021

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
376	+1.000000 x |24(1);12(1)>	2177.7391	0.00000000	0.03784938
377	+1.000000 x |23(1);13(1)>	2177.9327	0.00000000	0.03779944
378	+1.000000 x |23(1);12(1)>	2178.4936	0.00000000	0.03817214
379	+1.000000 x |18(2)>	2182.5242	0.00173515	0.00000000
380	+1.000000 x |25(1);11(1)>	2184.7211	0.00000000	0.14917272
381	+1.000000 x |25(1);10(1)>	2186.4318	0.00000000	0.15083213
382	+1.000000 x |20(1);15(1)>	2188.1870	0.00000000	0.03149879
383	+1.000000 x |20(1);14(1)>	2189.5307	0.00033840	0.00000000
384	+1.000000 x |20(1);16(1)>	2191.5375	0.00034151	0.00000000
385	+1.000000 x |19(1);18(1)>	2206.3764	0.00331701	0.00000000
386	+1.000000 x |26(1);11(1)>	2206.4807	0.00339311	0.00000000
387	+1.000000 x |26(1);10(1)>	2208.2354	0.00336727	0.00000000
388	+1.000000 x |28(1);11(1)>	2210.6962	0.00000000	0.05843370
389	+1.000000 x |28(1);10(1)>	2212.1461	0.00000000	0.04360049
390	+1.000000 x |27(1);11(1)>	2213.0758	0.00000000	0.04454060
391	+1.000000 x |27(1);10(1)>	2215.2242	0.00000000	0.05816670
392	+1.000000 x |30(1);11(1)>	2219.6636	0.00302836	0.00000000
393	+1.000000 x |29(1);11(1)>	2219.6938	0.00090527	0.00000000
394	+1.000000 x |20(1);17(1)>	2220.8451	0.00000001	0.00000000
395	+1.000000 x |29(1);10(1)>	2221.0387	0.00304044	0.00000000
396	+1.000000 x |30(1);10(1)>	2221.7660	0.00091986	0.00000000
397	+1.000000 x |19(2)>	2229.3807	0.00100098	0.00000000
398	+1.000000 x |32(1);8(1)>	2229.4302	0.01368820	0.00000000
399	+1.000000 x |25(1);13(1)>	2230.2947	0.00000000	0.00773608

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
400	+1.000000 x |25(1);12(1)>	2231.1314	0.00000000	0.00803442
401	+1.000000 x |31(1);8(1)>	2231.9473	0.00140053	0.00000000
402	+1.000000 x |31(1);7(1)>	2235.2474	0.01382703	0.00000000
403	+1.000000 x |32(1);7(1)>	2235.6629	0.00143260	0.00000000
404	+1.000000 x |34(1);8(1)>	2237.3267	0.00000000	0.09673351
405	+1.000000 x |35(1);8(1)>	2239.3197	0.00000000	0.00626434
406	+1.000000 x |33(1);8(1)>	2239.6108	0.00000000	0.00378694
407	+1.000000 x |34(1);7(1)>	2242.8716	0.00000000	0.00393165
408	+1.000000 x |33(1);7(1)>	2243.3351	0.00000000	0.09555085
409	+1.000000 x |35(1);7(1)>	2244.0715	0.00000000	0.00646906
410	+1.000000 x |32(1);9(1)>	2248.7231	0.00021766	0.00000000
411	+1.000000 x |31(1);9(1)>	2249.5710	0.00020825	0.00000000
412	+1.000000 x |26(1);13(1)>	2251.9225	0.00038668	0.00000000
413	+1.000000 x |26(1);12(1)>	2252.8300	0.00036540	0.00000000
414	+1.000000 x |20(1);18(1)>	2253.1978	0.00000000	0.00000002
415	+1.000000 x |28(1);13(1)>	2255.3475	0.00000000	0.07384582
416	+1.000000 x |36(1);8(1)>	2255.6574	0.00917062	0.00000000
417	+1.000000 x |34(1);9(1)>	2255.9001	0.00000000	0.04295604
418	+1.000000 x |33(1);9(1)>	2257.1567	0.00000000	0.04340121
419	+1.000000 x |28(1);12(1)>	2257.2656	0.00000000	0.07317984
420	+1.000000 x |35(1);9(1)>	2257.9320	0.00000000	0.00368432
421	+1.000000 x |27(1);12(1)>	2258.9809	0.00000000	0.07462395
422	+1.000000 x |27(1);13(1)>	2259.0414	0.00000000	0.07277709
423	+1.000000 x |36(1);7(1)>	2260.2937	0.00909871	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
424	+1.000000 x |29(1);13(1)>	2265.1276	0.00096236	0.00000000
425	+1.000000 x |30(1);13(1)>	2265.3165	0.00157531	0.00000000
426	+1.000000 x |29(1);12(1)>	2265.7976	0.00156717	0.00000000
427	+1.000000 x |30(1);12(1)>	2266.3782	0.00095992	0.00000000
428	+1.000000 x |36(1);9(1)>	2274.1715	0.00265298	0.00000000
429	+1.000000 x |20(1);19(1)>	2275.6006	0.00000000	0.00000011
430	+1.000000 x |22(1);14(1)>	2288.0293	0.00000000	0.03845471
431	+1.000000 x |22(1);15(1)>	2288.3998	0.00020776	0.00000000
432	+1.000000 x |22(1);16(1)>	2290.4079	0.00000000	0.01218852
433	+1.000000 x |21(1);14(1)>	2292.1034	0.00000000	0.01231543
434	+1.000000 x |21(1);15(1)>	2292.1274	0.00021071	0.00000000
435	+1.000000 x |21(1);16(1)>	2293.9671	0.00000000	0.03915177
436	+1.000000 x |24(1);14(1)>	2298.6648	0.00187912	0.00000000
437	+1.000000 x |24(1);15(1)>	2298.8540	0.00000000	0.01195707
438	+1.000000 x |23(1);15(1)>	2299.9030	0.00000000	0.01197402
439	+1.000000 x |23(1);14(1)>	2300.3328	0.00008769	0.00000000
440	+1.000000 x |24(1);16(1)>	2301.3370	0.00008445	0.00000000
441	+1.000000 x |23(1);16(1)>	2301.8176	0.00189984	0.00000000
442	+1.000000 x |32(1);11(1)>	2310.5931	0.00000000	0.04422052
443	+1.000000 x |31(1);11(1)>	2311.1847	0.00000000	0.04544038
444	+1.000000 x |32(1);10(1)>	2312.0924	0.00000000	0.04504047
445	+1.000000 x |31(1);10(1)>	2313.1135	0.00000000	0.04420587
446	+1.000000 x |34(1);11(1)>	2317.7523	0.00076176	0.00000000
447	+1.000000 x |22(1);17(1)>	2318.1339	0.00000000	0.02977985

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
448	+1.000000 x |33(1);11(1)>	2318.7549	0.00177080	0.00000000
449	+1.000000 x |34(1);10(1)>	2319.2732	0.00177135	0.00000000
450	+1.000000 x |35(1);11(1)>	2319.6383	0.00003828	0.00000000
451	+1.000000 x |33(1);10(1)>	2320.6999	0.00075427	0.00000000
452	+1.000000 x |35(1);10(1)>	2321.3111	0.00003697	0.00000000
453	+1.000000 x |20(2)>	2321.4013	0.00224306	0.00000000
454	+1.000000 x |21(1);17(1)>	2322.6081	0.00000000	0.02930050
455	+1.000000 x |24(1);17(1)>	2329.4770	0.00418597	0.00000000
456	+1.000000 x |23(1);17(1)>	2330.6494	0.00419111	0.00000000
457	+1.000000 x |36(1);11(1)>	2335.9827	0.00000000	0.00300591
458	+1.000000 x |36(1);10(1)>	2337.6854	0.00000000	0.00323312
459	+1.000000 x |25(1);14(1)>	2351.4734	0.00135274	0.00000000
460	+1.000000 x |22(1);18(1)>	2351.6119	0.00013774	0.00000000
461	+1.000000 x |25(1);15(1)>	2352.3882	0.00000000	0.00000041
462	+1.000000 x |32(1);13(1)>	2353.4595	0.00000000	0.06314079
463	+1.000000 x |25(1);16(1)>	2353.5481	0.00133431	0.00000000
464	+1.000000 x |31(1);12(1)>	2355.2407	0.00000000	0.06207266
465	+1.000000 x |31(1);13(1)>	2355.3011	0.00000000	0.00100026
466	+1.000000 x |32(1);12(1)>	2355.3327	0.00000000	0.00092032
467	+1.000000 x |21(1);18(1)>	2355.6079	0.00013585	0.00000000
468	+1.000000 x |34(1);13(1)>	2360.5927	0.01380040	0.00000000
469	+1.000000 x |24(1);18(1)>	2361.6408	0.00000000	0.00271759
470	+1.000000 x |34(1);12(1)>	2362.6717	0.00410388	0.00000000
471	+1.000000 x |23(1);18(1)>	2362.7001	0.00000000	0.00273708

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
472	+1.000000 x |33(1);12(1)>	2362.7702	0.01414082	0.00000000
473	+1.000000 x |35(1);13(1)>	2362.8378	0.00463783	0.00000000
474	+1.000000 x |33(1);13(1)>	2363.0855	0.00389503	0.00000000
475	+1.000000 x |35(1);12(1)>	2363.8151	0.00421631	0.00000000
476	+1.000000 x |26(1);14(1)>	2374.0159	0.00000000	0.08216812
477	+1.000000 x |22(1);19(1)>	2374.3469	0.00366226	0.00000000
478	+1.000000 x |26(1);15(1)>	2374.3940	0.00000004	0.00000000
479	+1.000000 x |26(1);16(1)>	2376.2035	0.00000000	0.08400356
480	+1.000000 x |28(1);14(1)>	2377.4925	0.00858078	0.00000000
481	+1.000000 x |21(1);19(1)>	2378.0974	0.00364216	0.00000000
482	+1.000000 x |28(1);15(1)>	2378.2150	0.00000000	0.01222416
483	+1.000000 x |36(1);13(1)>	2379.0486	0.00000000	0.01402869
484	+1.000000 x |36(1);12(1)>	2379.9523	0.00000000	0.01357958
485	+1.000000 x |27(1);15(1)>	2380.8796	0.00000000	0.01217397
486	+1.000000 x |28(1);16(1)>	2381.0856	0.00085546	0.00000000
487	+1.000000 x |27(1);14(1)>	2381.6588	0.00083904	0.00000000
488	+1.000000 x |27(1);16(1)>	2382.3249	0.00860924	0.00000000
489	+1.000000 x |25(1);17(1)>	2382.9291	0.00558163	0.00000000
490	+1.000000 x |24(1);19(1)>	2383.3110	0.00000000	0.00242236
491	+1.000000 x |23(1);19(1)>	2384.4081	0.00000000	0.00243190
492	+1.000000 x |30(1);14(1)>	2386.4642	0.00000000	0.08372180
493	+1.000000 x |29(1);15(1)>	2387.1301	0.00000736	0.00000000
494	+1.000000 x |29(1);14(1)>	2387.4460	0.00000000	0.05222745
495	+1.000000 x |30(1);15(1)>	2387.4999	0.00000732	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
496	+1.000000 x |29(1);16(1)>	2388.2450	0.00000000	0.08255043
497	+1.000000 x |30(1);16(1)>	2389.9021	0.00000000	0.05050746
498	+1.000000 x |26(1);17(1)>	2403.0672	0.00000000	0.06377324
499	+1.000000 x |28(1);17(1)>	2407.6216	0.00143008	0.00000000
500	+1.000000 x |27(1);17(1)>	2410.5893	0.00143471	0.00000000
501	+1.000000 x |25(1);18(1)>	2415.2278	0.00000000	0.01614918
502	+1.000000 x |29(1);17(1)>	2417.7496	0.00000000	0.01794875
503	+1.000000 x |30(1);17(1)>	2418.0910	0.00000000	0.01836517
504	+1.000000 x |22(1);20(1)>	2421.1035	0.00000000	0.11525692
505	+1.000000 x |21(1);20(1)>	2424.8330	0.00000000	0.11603613
506	+1.000000 x |24(1);20(1)>	2432.1925	0.00093020	0.00000000
507	+1.000000 x |23(1);20(1)>	2433.2279	0.00093644	0.00000000
508	+1.000000 x |25(1);19(1)>	2435.2464	0.00000000	0.01062046
509	+1.000000 x |26(1);18(1)>	2437.8241	0.00886478	0.00000000
510	+1.000000 x |28(1);18(1)>	2441.9480	0.00000000	0.05195966
511	+1.000000 x |27(1);18(1)>	2444.7202	0.00000000	0.05177206
512	+1.000000 x |29(1);18(1)>	2450.3238	0.00087337	0.00000000
513	+1.000000 x |30(1);18(1)>	2450.6886	0.00086626	0.00000000
514	+1.000000 x |26(1);19(1)>	2460.6860	0.00134489	0.00000000
515	+1.000000 x |28(1);19(1)>	2463.6499	0.00000000	0.00177866
516	+1.000000 x |27(1);19(1)>	2466.3229	0.00000000	0.00172345
517	+1.000000 x |29(1);19(1)>	2469.6423	0.03367466	0.00000000
518	+1.000000 x |30(1);19(1)>	2470.0224	0.03359546	0.00000000
519	+1.000000 x |32(1);15(1)>	2476.3561	0.00000000	0.00186115

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
520	+1.000000 x |31(1);15(1)>	2477.1979	0.00000000	0.00200056
521	+1.000000 x |32(1);14(1)>	2478.2386	0.00021282	0.00000000
522	+1.000000 x |31(1);14(1)>	2479.0768	0.00008932	0.00000000
523	+1.000000 x |32(1);16(1)>	2480.3047	0.00008995	0.00000000
524	+1.000000 x |31(1);16(1)>	2481.0597	0.00021440	0.00000000
525	+1.000000 x |34(1);15(1)>	2483.4958	0.00370729	0.00000000
526	+1.000000 x |33(1);15(1)>	2484.9057	0.00369473	0.00000000
527	+1.000000 x |34(1);14(1)>	2485.3679	0.00000000	0.01532441
528	+1.000000 x |35(1);15(1)>	2485.4469	0.01716417	0.00000000
529	+1.000000 x |25(1);20(1)>	2485.7590	0.00000003	0.00000000
530	+1.000000 x |33(1);14(1)>	2486.6112	0.00000000	0.01460018
531	+1.000000 x |34(1);16(1)>	2487.4484	0.00000000	0.01489829
532	+1.000000 x |35(1);14(1)>	2487.5409	0.00000000	0.13097292
533	+1.000000 x |33(1);16(1)>	2488.6265	0.00000000	0.01491501
534	+1.000000 x |35(1);16(1)>	2489.5847	0.00000000	0.13037384
535	+1.000000 x |36(1);15(1)>	2501.7140	0.00000000	0.00000079
536	+1.000000 x |36(1);14(1)>	2503.6975	0.00011309	0.00000000
537	+1.000000 x |36(1);16(1)>	2505.7199	0.00011191	0.00000000
538	+1.000000 x |26(1);20(1)>	2507.7571	0.00000000	0.00000022
539	+1.000000 x |32(1);17(1)>	2508.8674	0.00013972	0.00000000
540	+1.000000 x |31(1);17(1)>	2509.8556	0.00013419	0.00000000
541	+1.000000 x |28(1);20(1)>	2511.6535	0.00116917	0.00000000
542	+1.000000 x |27(1);20(1)>	2514.3103	0.00116488	0.00000000
543	+1.000000 x |34(1);17(1)>	2516.2410	0.00000000	0.04386599

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
544	+1.000000 x |33(1);17(1)>	2517.6490	0.00000000	0.04398147
545	+1.000000 x |35(1);17(1)>	2518.2285	0.00000000	0.00005071
546	+1.000000 x |22(2)>	2519.2393	0.00319269	0.00000000
547	+1.000000 x |29(1);20(1)>	2520.3930	0.00000000	0.00481667
548	+1.000000 x |30(1);20(1)>	2520.7615	0.00000000	0.00480931
549	+1.000000 x |22(1);21(1)>	2524.0376	0.00051939	0.00000000
550	+1.000000 x |21(2)>	2527.2427	0.00318253	0.00000000
551	+1.000000 x |24(1);22(1)>	2529.8520	0.00000000	0.00292897
552	+1.000000 x |23(1);22(1)>	2531.7617	0.00000000	0.00109600
553	+1.000000 x |24(1);21(1)>	2534.4937	0.00000000	0.00105546
554	+1.000000 x |36(1);17(1)>	2534.5704	0.00000003	0.00000000
555	+1.000000 x |23(1);21(1)>	2534.8386	0.00000000	0.00293102
556	+1.000000 x |24(2)>	2540.1505	0.00966885	0.00000000
557	+1.000000 x |24(1);23(1)>	2541.8194	0.01508708	0.00000000
558	+1.000000 x |32(1);18(1)>	2542.1682	0.00000000	0.07658686
559	+1.000000 x |23(2)>	2542.2687	0.00967695	0.00000000
560	+1.000000 x |31(1);18(1)>	2542.9921	0.00000000	0.07621161
561	+1.000000 x |34(1);18(1)>	2549.3451	0.00018933	0.00000000
562	+1.000000 x |33(1);18(1)>	2550.5776	0.00019155	0.00000000
563	+1.000000 x |35(1);18(1)>	2551.5225	0.00000019	0.00000000
564	+1.000000 x |32(1);19(1)>	2564.1288	0.00000000	0.09524045
565	+1.000000 x |31(1);19(1)>	2564.9066	0.00000000	0.09518536
566	+1.000000 x |36(1);18(1)>	2567.7059	0.00000000	0.00000704
567	+1.000000 x |34(1);19(1)>	2570.7731	0.00580217	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
568	+1.000000 x |33(1);19(1)>	2571.9543	0.00584250	0.00000000
569	+1.000000 x |35(1);19(1)>	2573.0211	0.00000728	0.00000000
570	+1.000000 x |25(1);22(1)>	2583.7569	0.00000000	0.02297643
571	+1.000000 x |25(1);21(1)>	2587.5686	0.00000000	0.02290854
572	+1.000000 x |36(1);19(1)>	2588.9974	0.00000000	0.00000755
573	+1.000000 x |25(1);24(1)>	2592.2349	0.02382960	0.00000000
574	+1.000000 x |25(1);23(1)>	2593.2973	0.02413839	0.00000000
575	+1.000000 x |26(1);22(1)>	2602.6008	0.00433082	0.00000000
576	+1.000000 x |28(1);22(1)>	2606.8251	0.00000000	0.18514442
577	+1.000000 x |26(1);21(1)>	2606.8513	0.00429754	0.00000000
578	+1.000000 x |32(1);20(1)>	2608.4546	0.01704398	0.00000000
579	+1.000000 x |31(1);20(1)>	2609.2528	0.01703197	0.00000000
580	+1.000000 x |27(1);22(1)>	2611.3409	0.00000000	0.02019661
581	+1.000000 x |28(1);21(1)>	2612.5187	0.00000000	0.01992130
582	+1.000000 x |27(1);21(1)>	2613.6694	0.00000000	0.18281307
583	+1.000000 x |34(1);20(1)>	2615.3415	0.00000000	0.07817860
584	+1.000000 x |26(1);24(1)>	2616.3955	0.00000000	0.00294187
585	+1.000000 x |33(1);20(1)>	2616.5408	0.00000000	0.07705920
586	+1.000000 x |26(1);23(1)>	2617.4638	0.00000000	0.00383005
587	+1.000000 x |35(1);20(1)>	2617.5870	0.00000000	0.00476321
588	+1.000000 x |30(1);22(1)>	2618.3814	0.01382106	0.00000000
589	+1.000000 x |28(1);24(1)>	2618.8206	0.01272601	0.00000000
590	+1.000000 x |29(1);22(1)>	2618.8535	0.00490669	0.00000000
591	+1.000000 x |29(1);21(1)>	2621.8446	0.01370288	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
592	+1.000000 x |28(1);23(1)>	2621.8904	0.00730844	0.00000000
593	+1.000000 x |27(1);23(1)>	2622.6503	0.01255032	0.00000000
594	+1.000000 x |30(1);21(1)>	2622.9910	0.00492708	0.00000000
595	+1.000000 x |27(1);24(1)>	2623.4788	0.00738695	0.00000000
596	+1.000000 x |30(1);24(1)>	2624.7644	0.00000000	0.21614520
597	+1.000000 x |29(1);23(1)>	2625.5237	0.00000000	0.21567907
598	+1.000000 x |29(1);24(1)>	2628.5161	0.00000000	0.14631265
599	+1.000000 x |30(1);23(1)>	2629.9786	0.00000000	0.14574396
600	+1.000000 x |36(1);20(1)>	2633.3332	0.04061167	0.00000000
601	+1.000000 x |25(2)>	2646.6532	0.04373047	0.00000000
602	+1.000000 x |26(1);25(1)>	2668.7320	0.00000000	0.44514314
603	+1.000000 x |28(1);25(1)>	2671.7440	0.01620143	0.00000000
604	+1.000000 x |27(1);25(1)>	2674.3595	0.01654023	0.00000000
605	+1.000000 x |29(1);25(1)>	2678.0179	0.00000000	0.90996171
606	+1.000000 x |30(1);25(1)>	2678.4336	0.00000000	0.90484756
607	+0.851882 x |26(2)> +0.431196 x |28(2)> +0.297267 x |27(2)>	2681.2532	0.32237880	0.00000000
608	+1.000000 x |28(1);26(1)>	2686.0096	0.00000000	0.08005653
609	+1.000000 x |27(1);26(1)>	2688.7562	0.00000000	0.08377021
610	+0.841700 x |28(2)> -0.472605 x |27(2)> -0.261124 x |26(2)>	2695.8689	0.02227157	0.00000000
611	+1.000000 x |28(1);27(1)>	2700.3442	0.02373449	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
612	+1.000000 x |29(1);26(1)>	2702.7316	0.01343232	0.00000000
613	+0.829624 x |27(2)> -0.453995 x |26(2)> +0.324980 x |28(2)>	2702.8176	0.06295965	0.00000000
614	+1.000000 x |30(1);26(1)>	2703.1487	0.01262614	0.00000000
615	+1.000000 x |30(1);28(1)>	2703.7744	0.00000000	0.57525237
616	+1.000000 x |29(1);27(1)>	2706.2573	0.00000000	0.56658793
617	+1.000000 x |29(1);28(1)>	2707.4757	0.00000000	0.15119810
618	+1.000000 x |32(1);22(1)>	2708.5422	0.00000000	0.20835858
619	+1.000000 x |31(1);22(1)>	2710.2726	0.00000000	0.08427897
620	+1.000000 x |30(1);27(1)>	2710.5423	0.00000000	0.15170348
621	+1.000000 x |32(1);21(1)>	2713.2059	0.00000000	0.08414203
622	+1.000000 x |31(1);21(1)>	2713.3791	0.00000000	0.20727254
623	+1.000000 x |29(2)>	2713.7864	0.10276168	0.00000000
624	+1.000000 x |30(2)>	2714.4445	0.10327241	0.00000000
625	+1.000000 x |30(1);29(1)>	2715.5708	0.03680927	0.00000000
626	+1.000000 x |34(1);22(1)>	2715.6833	0.02344975	0.00000000
627	+1.000000 x |33(1);22(1)>	2717.8419	0.00371151	0.00000000
628	+1.000000 x |35(1);22(1)>	2718.4290	0.01071926	0.00000000
629	+1.000000 x |34(1);21(1)>	2720.3613	0.00391941	0.00000000
630	+1.000000 x |32(1);24(1)>	2720.6245	0.00360580	0.00000000
631	+1.000000 x |33(1);21(1)>	2720.8545	0.02373193	0.00000000
632	+1.000000 x |31(1);24(1)>	2721.2601	0.00098423	0.00000000
633	+1.000000 x |32(1);23(1)>	2721.4847	0.00096475	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
634	+1.000000 x |35(1);21(1)>	2722.2041	0.01019866	0.00000000
635	+1.000000 x |31(1);23(1)>	2722.4758	0.00356311	0.00000000
636	+1.000000 x |34(1);24(1)>	2727.6232	0.00000000	0.06003044
637	+1.000000 x |34(1);23(1)>	2728.4866	0.00000000	0.05734402
638	+1.000000 x |33(1);24(1)>	2728.6663	0.00000000	0.05743738
639	+1.000000 x |35(1);24(1)>	2729.4461	0.00000000	0.00453757
640	+1.000000 x |33(1);23(1)>	2729.8525	0.00000000	0.06105827
641	+1.000000 x |35(1);23(1)>	2730.4815	0.00000000	0.00481185
642	+1.000000 x |36(1);22(1)>	2734.5224	0.00000000	0.01234136
643	+1.000000 x |36(1);21(1)>	2738.2567	0.00000000	0.01051024
644	+1.000000 x |36(1);24(1)>	2745.9851	0.00088105	0.00000000
645	+1.000000 x |36(1);23(1)>	2747.0247	0.00089042	0.00000000
646	+1.000000 x |32(1);25(1)>	2774.1545	0.00350844	0.00000000
647	+1.000000 x |31(1);25(1)>	2774.9599	0.00348378	0.00000000
648	+1.000000 x |34(1);25(1)>	2781.1360	0.00000000	0.02594889
649	+1.000000 x |33(1);25(1)>	2782.3710	0.00000000	0.02553251
650	+1.000000 x |35(1);25(1)>	2783.3784	0.00000000	0.00003761
651	+1.000000 x |32(1);26(1)>	2795.8096	0.00000000	0.02100258
652	+1.000000 x |31(1);26(1)>	2796.7276	0.00000000	0.02075965
653	+1.000000 x |36(1);25(1)>	2799.5466	0.00000020	0.00000000
654	+1.000000 x |32(1);28(1)>	2799.5693	0.00718450	0.00000000
655	+1.000000 x |31(1);28(1)>	2800.3819	0.00484024	0.00000000
656	+1.000000 x |32(1);27(1)>	2802.2035	0.00484215	0.00000000
657	+1.000000 x |34(1);26(1)>	2803.0770	0.00595051	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
658	+1.000000 x |31(1);27(1)>	2803.1242	0.00716835	0.00000000
659	+1.000000 x |33(1);26(1)>	2804.3920	0.00591680	0.00000000
660	+1.000000 x |35(1);26(1)>	2805.4722	0.00001016	0.00000000
661	+1.000000 x |34(1);28(1)>	2806.5156	0.00000000	0.54630746
662	+1.000000 x |33(1);28(1)>	2807.7045	0.00000000	0.31157212
663	+1.000000 x |32(1);29(1)>	2808.8903	0.00000000	0.16734005
664	+1.000000 x |35(1);28(1)>	2809.0499	0.00000000	0.04554433
665	+1.000000 x |34(1);27(1)>	2809.1395	0.00000000	0.30951279
666	+1.000000 x |32(1);30(1)>	2809.2575	0.00000000	0.21401809
667	+1.000000 x |31(1);29(1)>	2809.6906	0.00000000	0.21227753
668	+1.000000 x |31(1);30(1)>	2810.0700	0.00000000	0.16830930
669	+1.000000 x |33(1);27(1)>	2810.4503	0.00000000	0.55050815
670	+1.000000 x |35(1);27(1)>	2811.7553	0.00000000	0.04697955
671	+1.000000 x |34(1);29(1)>	2815.9239	0.00355023	0.00000000
672	+1.000000 x |34(1);30(1)>	2816.3103	0.00575942	0.00000000
673	+1.000000 x |33(1);29(1)>	2817.1470	0.00565969	0.00000000
674	+1.000000 x |33(1);30(1)>	2817.5061	0.00365321	0.00000000
675	+1.000000 x |35(1);29(1)>	2818.2629	0.00259174	0.00000000
676	+1.000000 x |35(1);30(1)>	2818.6217	0.00257870	0.00000000
677	+1.000000 x |36(1);26(1)>	2821.3544	0.00000000	0.00002099
678	+1.000000 x |36(1);28(1)>	2824.6639	0.00164207	0.00000000
679	+1.000000 x |36(1);27(1)>	2827.3763	0.00162368	0.00000000
680	+1.000000 x |36(1);29(1)>	2834.2568	0.00000000	0.23796399
681	+1.000000 x |36(1);30(1)>	2834.6123	0.00000000	0.23957551

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
682	+0.626926 x |41(1)>	2851.7497	1.57834668	0.00000000
	-0.350387 x |31(2)>			
	-0.317797 x |35(1);34(1)>			
	-0.312094 x |33(2)>			
	+0.263775 x |36(1);32(1)>			
	+0.253074 x |40(1)>			
	+0.226209 x |32(2)>			
	-0.169735 x |36(1);31(1)>			
	-0.168287 x |35(1);33(1)>			
	+0.152944 x |34(2)>			
683	+0.507565 x |39(1)>	2856.4026	2.98418738	0.00000000
	-0.471254 x |40(1)>			
	-0.350702 x |32(2)>			
	-0.301084 x |34(2)>			
	-0.243715 x |35(2)>			
	-0.216690 x |31(2)>			
	+0.198214 x |36(1);31(1)>			
	+0.186802 x |35(1);33(1)>			
	-0.174895 x |33(2)>			
	-0.168975 x |32(1);31(1)>			
	+0.148766 x |34(1);33(1)>			
	+0.100417 x |41(1)>			
684	+0.584056 x |42(1)>	2859.8330	0.00000000	22.58549282
	-0.451674 x |38(1)>			
	-0.395788 x |34(1);32(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	-0.294638 x |37(1)>			
	+0.235856 x |33(1);31(1)>			
	+0.199106 x |36(1);35(1)>			
	+0.147834 x |34(1);31(1)>			
	+0.143585 x |35(1);32(1)>			
	-0.143252 x |33(1);32(1)>			
	-0.127030 x |36(1);34(1)>			
	+0.125502 x |44(1)>			
	+0.118989 x |35(1);31(1)>			
685	+0.486390 x |42(1)>	2860.4904	0.00000000	32.90553280
	+0.454831 x |38(1)>			
	+0.450085 x |37(1)>			
	+0.316297 x |33(1);31(1)>			
	-0.227082 x |34(1);32(1)>			
	-0.194576 x |34(1);31(1)>			
	+0.187785 x |33(1);32(1)>			
	-0.173066 x |35(1);31(1)>			
	+0.156789 x |36(1);35(1)>			
	-0.154494 x |44(1)>			
	-0.138606 x |35(1);32(1)>			
	+0.129594 x |36(1);34(1)>			
	-0.121543 x |36(1);33(1)>			
686	+0.545855 x |40(1)>	2862.0643	4.91825281	0.00000001
	+0.392741 x |39(1)>			
	-0.324444 x |41(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.262794 x |32(1);31(1)>			
	-0.231014 x |32(2)>			
	-0.223867 x |34(1);33(1)>			
	-0.210034 x |35(1);33(1)>			
	-0.202759 x |35(2)>			
	-0.195282 x |31(2)>			
	-0.178678 x |34(2)>			
	-0.171000 x |36(1);31(1)>			
	-0.167041 x |33(2)>			
	+0.162181 x |35(1);34(1)>			
	-0.106958 x |36(1);32(1)>			
687	+0.626454 x |37(1)>	2862.1945	0.00000000	10.23292200
	-0.525346 x |38(1)>			
	-0.288436 x |33(1);31(1)>			
	+0.227880 x |35(1);32(1)>			
	+0.200879 x |43(1)>			
	-0.193478 x |34(1);32(1)>			
	-0.190387 x |35(1);31(1)>			
	-0.179892 x |36(1);33(1)>			
	-0.149512 x |36(1);34(1)>			
	-0.104648 x |34(1);31(1)>			
688	+0.667462 x |39(1)>	2894.6888	5.91375207	0.00000000
	+0.501146 x |46(1)>			
	+0.378859 x |32(2)>			
	+0.262088 x |31(2)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.201205 x |35(2)>			
	+0.149680 x |34(2)>			
689	+0.924854 x |32(1);31(1)>	2901.9495	0.05393821	0.00000000
	+0.203922 x |34(1);33(1)>			
	+0.185247 x |35(1);33(1)>			
	-0.142888 x |35(1);34(1)>			
	+0.116595 x |36(1);31(1)>			
	-0.114664 x |40(1)>			
690	+0.780225 x |35(1);32(1)>	2902.9778	0.00000000	9.13340890
	-0.347334 x |44(1)>			
	+0.334218 x |34(1);32(1)>			
	+0.323753 x |33(1);31(1)>			
	+0.136024 x |35(1);31(1)>			
	-0.102989 x |34(1);31(1)>			
	-0.100013 x |36(1);34(1)>			
691	+0.796561 x |35(1);31(1)>	2903.9307	0.00000000	7.76424858
	-0.354449 x |34(1);31(1)>			
	+0.332337 x |43(1)>			
	+0.270062 x |33(1);32(1)>			
	-0.134942 x |35(1);32(1)>			
	-0.112725 x |34(1);32(1)>			
	-0.106532 x |33(1);31(1)>			
	+0.105633 x |36(1);33(1)>			
692	+0.720421 x |33(1);32(1)>	2906.0676	0.00000000	0.05397983

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.690991 x |34(1);31(1)>			
693	+0.659408 x |31(2)>	2908.5094	0.63699162	0.00000000
	-0.568578 x |32(2)>			
	+0.332209 x |41(1)>			
	+0.197614 x |36(1);32(1)>			
	+0.187777 x |40(1)>			
	-0.156845 x |36(1);31(1)>			
	-0.129644 x |45(1)>			
694	+0.650475 x |35(1);33(1)>	2913.4867	0.14237460	0.00000000
	+0.464910 x |34(2)>			
	-0.386120 x |33(2)>			
	-0.346571 x |36(1);31(1)>			
	+0.183574 x |35(1);34(1)>			
	-0.143862 x |34(1);33(1)>			
	-0.136012 x |41(1)>			
695	+0.541197 x |34(1);32(1)>	2913.6516	0.00000000	7.55550984
	+0.429558 x |33(1);31(1)>			
	-0.330139 x |38(1)>			
	+0.320581 x |44(1)>			
	-0.307830 x |35(1);32(1)>			
	+0.273496 x |33(1);32(1)>			
	-0.254643 x |34(1);31(1)>			
	-0.192278 x |36(1);34(1)>			
	-0.156597 x |35(1);31(1)>			
696	+0.484036 x |35(1);34(1)>	2914.1688	0.08874025	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.471522 x |34(1);33(1)>			
	+0.378015 x |34(2)>			
	-0.324484 x |32(2)>			
	-0.311755 x |31(2)>			
	+0.243942 x |35(2)>			
	-0.236927 x |35(1);33(1)>			
	+0.189096 x |33(2)>			
	+0.172323 x |36(1);32(1)>			
697	+0.496930 x |33(1);32(1)>	2914.7151	0.00000000	9.47638942
	-0.486820 x |34(1);31(1)>			
	-0.335765 x |37(1)>			
	-0.325263 x |43(1)>			
	-0.294121 x |35(1);31(1)>			
	-0.262715 x |34(1);32(1)>			
	-0.225878 x |33(1);31(1)>			
	+0.197027 x |36(1);33(1)>			
	+0.195312 x |35(1);32(1)>			
	+0.111003 x |44(1)>			
698	+0.682269 x |34(1);33(1)>	2915.7912	0.16968185	0.00000000
	-0.347383 x |35(2)>			
	-0.313658 x |36(1);31(1)>			
	+0.295018 x |31(2)>			
	-0.281649 x |33(2)>			
	+0.237494 x |32(2)>			
	-0.154341 x |36(1);32(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	-0.132178 x |46(1)>			
	-0.127848 x |34(2)>			
	+0.123224 x |35(1);34(1)>			
699	+0.595045 x |35(1);34(1)>	2921.0471	0.06075379	0.00000000
	+0.594196 x |36(1);32(1)>			
	+0.326731 x |32(2)>			
	-0.258186 x |34(2)>			
	-0.222335 x |34(1);33(1)>			
	-0.134270 x |35(2)>			
	+0.123241 x |36(1);31(1)>			
	+0.121361 x |31(2)>			
700	+0.649453 x |36(1);35(1)>	2921.7965	0.00000000	8.96496642
	-0.545886 x |33(1);31(1)>			
	+0.417436 x |34(1);32(1)>			
	+0.311122 x |42(1)>			
701	+0.753119 x |36(1);34(1)>	2925.6403	0.00000000	25.39036611
	+0.474058 x |44(1)>			
	-0.324484 x |36(1);33(1)>			
	+0.256279 x |35(1);32(1)>			
	+0.102404 x |35(1);31(1)>			
702	+0.775309 x |35(2)>	2926.5868	0.24474416	0.00000000
	-0.438198 x |34(2)>			
	-0.308960 x |33(2)>			
	-0.147776 x |36(1);31(1)>			
	+0.135720 x |34(1);33(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.129707 x |45(1)>			
	+0.127458 x |36(1);32(1)>			
	-0.122735 x |41(1)>			
703	+0.748230 x |36(1);33(1)>	2926.7797	0.00000000	26.24680169
	+0.490446 x |43(1)>			
	+0.331181 x |36(1);34(1)>			
	-0.259784 x |35(1);31(1)>			
704	+0.586398 x |33(2)>	2929.3474	0.29708362	0.00000000
	+0.441191 x |35(1);33(1)>			
	-0.410395 x |36(1);31(1)>			
	-0.351003 x |34(2)>			
	-0.216143 x |31(2)>			
	+0.171859 x |40(1)>			
	-0.162545 x |45(1)>			
	+0.150106 x |41(1)>			
	-0.140109 x |47(1)>			
	+0.107763 x |34(1);33(1)>			
705	+0.694316 x |45(1)>	2936.7268	2.61321523	0.00000000
	-0.428672 x |47(1)>			
	+0.399521 x |36(1);32(1)>			
	-0.236256 x |35(1);34(1)>			
	-0.151614 x |41(1)>			
	-0.146832 x |35(2)>			
	+0.136511 x |33(2)>			
	+0.114757 x |34(1);33(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.103781 x |46(1)>			
706	+0.700628 x |47(1)>	2938.3890	2.02131348	0.00000000
	-0.454146 x |36(1);31(1)>			
	+0.250355 x |45(1)>			
	+0.237932 x |36(1);32(1)>			
	-0.213611 x |35(1);33(1)>			
	-0.174858 x |40(1)>			
	-0.161732 x |35(1);34(1)>			
	+0.139833 x |33(2)>			
	-0.127870 x |41(1)>			
	+0.120883 x |36(2)>			
	+0.103239 x |46(1)>			
707	+0.781424 x |36(2)>	2941.6859	3.42697691	0.00000000
	+0.464906 x |46(1)>			
	-0.229606 x |33(2)>			
	-0.190664 x |45(1)>			
	-0.137225 x |34(2)>			
	-0.109294 x |31(2)>			
708	+1.000000 x |48(1)>	2945.8723	0.00000000	142.6119061
709	+0.555091 x |45(1)>	2950.6522	3.39042098	0.00000000
	+0.456428 x |41(1)>			
	-0.386153 x |36(1);32(1)>			
	+0.297602 x |47(1)>			
	+0.290446 x |35(1);34(1)>			
	+0.210949 x |36(1);31(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.204838 x |40(1)>			
	+0.184376 x |35(1);33(1)>			
	+0.157344 x |36(2)>			
	-0.118296 x |34(2)>			
710	+0.496085 x |40(1)>	2952.2846	1.85311528	0.00000000
	+0.440508 x |47(1)>			
	+0.417155 x |36(1);31(1)>			
	+0.297869 x |35(1);33(1)>			
	+0.266061 x |34(1);33(1)>			
	+0.244249 x |36(1);32(1)>			
	-0.221701 x |41(1)>			
	-0.185592 x |35(1);34(1)>			
	-0.164656 x |45(1)>			
	-0.160950 x |32(1);31(1)>			
	-0.157760 x |36(2)>			
711	+0.711983 x |36(1);35(1)>	2952.7349	0.00000000	28.92283635
	-0.562632 x |42(1)>			
	+0.303828 x |33(1);31(1)>			
	-0.289908 x |34(1);32(1)>			
712	+0.556861 x |44(1)>	2967.7396	0.00000000	94.04745597
	-0.407011 x |43(1)>			
	+0.385173 x |37(1)>			
	+0.355859 x |36(1);33(1)>			
	-0.327735 x |36(1);34(1)>			
	+0.208293 x |38(1)>			

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
	+0.206040 x |35(1);31(1)>			
	+0.188173 x |35(1);32(1)>			
	+0.102394 x |34(1);31(1)>			
	-0.100251 x |33(1);32(1)>			
713	+0.566489 x |43(1)>	2970.2895	0.00000000	102.7210791
	+0.428813 x |44(1)>			
	+0.383441 x |38(1)>			
	-0.327663 x |36(1);34(1)>			
	-0.322515 x |36(1);33(1)>			
	-0.211544 x |37(1)>			
	+0.205765 x |35(1);32(1)>			
	-0.179975 x |35(1);31(1)>			
	-0.101122 x |33(1);31(1)>			
714	+0.672006 x |46(1)>	2971.7255	13.43825944	0.00000000
	-0.549533 x |36(2)>			
	-0.338368 x |39(1)>			
	-0.185703 x |33(2)>			
	-0.175959 x |34(2)>			
	-0.138341 x |31(2)>			
	-0.132775 x |32(2)>			
	-0.122275 x |35(2)>			
715	+1.000000 x |38(1);2(1)>	3116.4079	0.00665697	0.00000000
716	+1.000000 x |39(1);2(1)>	3117.1829	0.00000000	0.01270278
717	+1.000000 x |37(1);2(1)>	3117.1949	0.00620364	0.00000000

Table S2 continued

Modes	Combinations	Frequencies	Raman Int.	IR Int.
718	+1.000000 x |40(1);2(1)>	3121.8671	0.00000000	0.09702212
719	+1.000000 x |41(1);2(1)>	3122.0147	0.00000000	0.13033586
720	+1.000000 x |42(1);2(1)>	3123.4663	0.00239287	0.00000000
721	+1.000000 x |38(1);1(1)>	3126.3978	0.00608217	0.00000000
722	+1.000000 x |37(1);1(1)>	3126.7810	0.00677027	0.00000000
723	+1.000000 x |39(1);1(1)>	3126.8275	0.00000000	0.01332677
724	+1.000000 x |40(1);1(1)>	3131.3238	0.00000000	0.13164637
725	+1.000000 x |41(1);1(1)>	3131.9977	0.00000000	0.09641537
726	+1.000000 x |42(1);1(1)>	3133.0593	0.00244648	0.00000000
727	+1.000000 x |45(1);2(1)>	3167.9014	0.00000000	0.25746250
728	+1.000000 x |44(1);2(1)>	3167.9702	0.01573155	0.00000000
729	+1.000000 x |47(1);2(1)>	3168.6621	0.00000000	0.13296164
730	+1.000000 x |43(1);2(1)>	3168.6649	0.00806356	0.00000000
731	+1.000000 x |46(1);2(1)>	3168.8171	0.00000000	0.02127249
732	+1.000000 x |48(1);2(1)>	3174.0788	0.01087690	0.00000000
733	+1.000000 x |44(1);1(1)>	3177.4054	0.00809533	0.00000000
734	+1.000000 x |45(1);1(1)>	3177.4614	0.00000000	0.13745740
735	+1.000000 x |43(1);1(1)>	3178.2940	0.01589010	0.00000000
736	+1.000000 x |47(1);1(1)>	3178.3036	0.00000000	0.26262188
737	+1.000000 x |46(1);1(1)>	3178.3270	0.00000000	0.01375916
738	+1.000000 x |48(1);1(1)>	3183.6586	0.01080607	0.00000000

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