ELECTRONIC SUPPLEMENTARY INFORMATION:

A Comprehensive Study of the Molecular Vibrations in Solid-State Benzylic Amide [2]Catenane:

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We include here two additional tables (Table S1 and Table S2).

In Table S1 we show a comparison between the main peaks of the experimental IR spectrum and those of the theoretical calculation. For each peak, the most relevant discrete normal modes are selected. The description of normal modes is made in terms of usual internal vibrational coordinates. They are ordered by decreasing contribution to the corresponding normal mode.

In Table S2 we include a description of over 1000 vibrational modes of the catenane crystal. We include the observed peaks in the experimental and theoretical spectra and a brief description of the modes in terms of usual internal vibrational coordinates, ordered by decreasing relevance. The last column is the calculated IR activity expressed with respect to the most active mode. Those modes with a remarkable IR activity are highlighted in red and are the ones included in the discussion of the main text and Table S1). The modes highlighted in green are those relevant in Raman spectroscopy.

These tables contain the following abbreviations and symbols:

Vibrational modes:
ν: stretching
δ: in-plane bending
π: out-of-plane bending
sci: scissoring
τ: torsion
ω: wagging

Other notations:
a: antisymmetric
r: benzene ring
rd: benzene ring deformation
rb: benzene ring breathing
s: symmetric
*: hydrogen bond
**: Peaks not obsereved in the IR spectrum but relevant in Raman

Table S1

Peaks (cm^{-1})		Mode	ν_n	Description
(exp.)	(calc.)		(cm^{-1})	
--	--	1537[1]	113.0	πCCCN
477	478	1230	477.4	s-out-of-plane-rd + δCCN + νCN + δCNC
		1226	479.2	s-out-of-plane-rd + δCCN + δCNC + νCN
502	499	1216	499.2	νCN + δCNC + δCCN + s-out-of-plane-rd
	511	1208	512.0	νCN + δCCN + s-out-of-plane-rd + δCNC
604	599	1181	598.5	δCCN + s-out-of-plane-rd + δCNC + νCN
		1179	599.8	δCCN + s-out-of-plane-rd + δCNC + νCN
609	605	1171	606.7	s-out-of-plane-rd + δCNC + δCCN + νCN
623	629	1165	628.5	a-in-plane-rd + r-νCH + πCCNH
		1163	632.1	a-in-plane-rd + r-νCH + πCCNH
641	635	1151	635.9	a-in-plane-rd + r-νCH
654	646	1135	646.6	a-in-plane-rd + r-νCH + δCNC + δCCN
669	666	1128	665.2	s-out-of-plane-rd + δCNC + δCCN + νCN
		1121	667.8	s-out-of-plane-rd + δCNC + δCCN + νCN
690	682	1111	681.9	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC
		1110	682.8	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC
705	688	1100	688.6	s-in-plane-rd + πCCNH + δCNC + νCC + νCN
		1099	688.6	s-in-plane-rd + πCCNH + δCNC + νCC + νCN
		1098	689.2	s-in-plane-rd + πCCNH + δCCN + νCC + νCN
725	700	1088	699.5	πCCNH + δCCN + νCC + νCN + s-out-of-plane-rd
		1085	700.4	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd
732	705	1078	705.0	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd
		1077	705.1	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd
778	770	1025	769.9	δCCN + δCNC + νCC + a-out-of-plane-rd
		1021	770.6	s-out-of-plane-rd + δCCN + νCC + δCNC
785	783	1015	783.2	s-out-of-plane-rd + δCCN + νCC + δCNC
801	808	995	809.0	s-out-of-plane-rd + δCCN + νCN
813	813	992	813.6	s-in-plane-rd + δCCN + νCC
822	821	979	820.6	s-out-of-plane-rd + δCCN + νCC
		977	822.1	s-out-of-plane-rd + δCCN + νCC + r-νCH
857	861	936	861.2	s-out-of-plane-rd + δCCN + νCN
993	984	823	985.1	s-out-of-plane-rd + δCCN + δCNC
1083	1092	727	1092.3	a-in-plane-rd + δCCC + δCCN
		726	1092.9	a-in-plane-rd + δCCC + δCCN
1220	1224	600	1225.5	τCH2 + δCCN + νCC + δCNC + s-in-plane-rd
1246	1246	584	1246.8	τCH2 + δCCN + δCNC + a-in-plane-rd
1264	1266	575	1266.2	δCCN + δCNC + νCC+ νCN
		574	1266.2	δCCN + νCC+ νCN + δCNC
		571	1267.2	νCN+ νCC + δCCN + a-in-plane-rd
1270	1278	566	1278.1	νCC+ νCN + δCCN + a-in-plane-rd
		563	1280.7	δCCN + νCC+ νCN + δCNC
		561	1282.1	δCCN + νCC+ νCN + a-in-plane-rd
1284	1285	560	1286.4	νCC+ νCN + δCCN + s-in-plane-rd
		556	1287.0	νCC+ δCCN + νCN + a-in-plane-rd
1302	1303	542	1303.5	νCC+ δCCN + νCN + a-in-plane-rd

[1] This mode has been included in the table due to its remarkable activity although it falls outside of the experimental wavenumber range.

Table S1

Peaks (cm^{-1})		Mode	ν_n	Description
(exp.)	(calc.)		(cm^{-1})	
		538	1304.9	δCCN + a-in-plane-rd + νCC + νCN
1323	1317	514	1319.6	δCCN + δCNC + ωCH2
1355	1348	472	1364.5	a-in-plane-rd + δCCN
		469	1364.8	a-in-plane-rd + νCC
1421	1418	435	1414.2	a-in-plane-rd + δCCN + νCN
		423	1418.2	a-in-plane-rd + δCCN
1477	1472	374	1472.7	νCC + a-in-plane-rd + νCN
		372	1473.0	νCC + s-in-plane-rd + νCN
1501	1505	367	1505.0	νCC + s-in-plane-rd
1530	1521	352	1520.3	νCN + δCNH + νCC + νNC
		351	1520.4	νCC + νCN + δCNH + νNC
		350	1521.0	νCN + νCC + δCNH + νNC
		349	1521.0	νCN + νCC + δCNH + νNC
		348	1521.1	νCN + δCNH + νNC + νCC
		347	1521.1	νCN + νCC + δCNH + νNC
		345	1521.5	νCN + νCC + δCNH + νNC
		343	1522.0	νCN + νCC + δCNH + νNC
		342	1522.0	νCN + νCC + νNC + δCNH
1535	1528	336	1527.7	νCN + νCC + νNC + δCNH
		334	1529.0	νCN + νCC + νNC + δCNH
1546	1537	324	1537.2	νCN + νNC+ δCNH
1579	1574	312	1572.8	νCC + a-in-plane-rd + νCO + δCCN
		311	1573.0	νCC + s-in-plane-rd + νCO + δCCN
		308	1573.5	νCC + νCO + δCCN + s-in-plane-rd
		307	1573.6	νCC + νCO + δCCN + s-in-plane-rd
		304	1574.8	νCC + νCO + δCCN + a-in-plane-rd
		302	1575.2	νCC + δCCN + in-plane-rd
1602	1592	284	1592.6	νCO + νCC + δCCN + a-in-plane-rd
		283	1592.6	νCO + νCC + δCCN + a-in-plane-rd
		282	1592.9	νCO + s-in-plane-rd + νCC + δCCN
		281	1593.0	νCC + νCO + s-in-plane-rd + νCN + δCCN
	2598	274	1597.9	νCC + a-in-plane-rd
		273	1598.2	νCO + νCN + νCC + δCCN + a-in-plane-rd
1630	1607	272	1607.7	νCO + νCN + νCC + δCCN + a-in-plane-rd
		271	1608.0	νCO + νCN + νCC + δCCN + a-in-plane-rd
		267	1609.4	s-in-plane-rd + a-in-plane-rd
		262	1610.2	s-in-plane-rd
		256	1612.4	νCO + νCC + νCN+ δCCN + s-in-plane-rd
1642	1616	253	1613.9	s-in-plane-rd + νCC + νCN+ νCO
		248	1616.4	νCO + νCC + νCN+ δCCN + a-in-plane-rd
		245	1617.6	νCO + νCC + νCN+ δCCN + a-in-plane-rd
		241	1621.4	νCO + νCN + νCC + δCCN + s-in-plane-rd
		238	1623.8	νCO + νCN + νCC + δCCN + a-in-plane-rd
		234	1626.0	νCO + νCN + νCC + δCCN + a-in-plane-rd
1661	1640	231	1635.7	νCO + νCN + νCC + δCCN + a-in-plane-rd
		226	1640.0	νCO + νCN + νCC + δCCN + s-in-plane-rd
		225	1640.5	νCO + νCN + νCC + δCCN + s-in-plane-rd
3295	3309	30	3309.2	νNH + δCNC
		27	3310.3	νNH + δCNC + νOH*

Table S1

Peaks (cm^{-1})		Mode	ν_n	Description
(exp.)	(calc.)		(cm^{-1})	
		25	3311.2	νNH + δCNC
3325	3339	22	3340.0	νNH + δCNC + νOH*
		20	3340.3	νNH + νCN + δCNC + νOH*
		19	3340.3	νNH + δCNC + νOH*
3363	3352	16	3350.9	νNH + δCNC + νOH*
		14	3351.2	νNH + δCNC + νOH*
		13	3351.3	νNH + δCNC + νOH*
		9	3353.1	νNH + δCNC
3426	3410	8	3409.7	νNH + δCNC
		5	3410.2	νNH + νCN + δCNC + νOH*

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
--	--	1537[2]	113.00	πCCCN	4.18
477	478	1232	476.15	s-out-of-plane-rd + δCCN + νCN + δCNC	0.00
		1231	476.87	s-out-of-plane-rd + δCCN + νCN + δCNC	0.00
		1230	477.36	s-out-of-plane-rd + δCCN + νCN + δCNC	1.44
		1229	477.53	s-out-of-plane-rd + δCCN + νCN + δCNC	0.03
		1228	477.78	s-out-of-plane-rd + δCCN + νCN + δCNC	0.59
		1227	478.67	s-out-of-plane-rd + δCCN + νCN + δCNC	0.00
		1226	479.24	s-out-of-plane-rd + δCCN + δCNC + νCN	1.84
		1225	480.73	s-out-of-plane-rd + δCCN + νCN + δCNC	0.02
486	487	1224	485.34	s-out-of-plane-rd + δCCN + νCN + δCNC	0.00
		1223	485.68	s-out-of-plane-rd + δCCN + νCN + δCNC	0.01
		1222	486.64	s-out-of-plane-rd + δCCN + δCNC + νCN	0.16
		1221	486.94	s-out-of-plane-rd + δCCN + δCNC + νCN	0.12
		1220	487.63	s-out-of-plane-rd + δCCN + δCNC + νCN	0.27
		1219	487.86	s-out-of-plane-rd + δCCN + δCNC + νCN	0.00
		1218	488.03	s-out-of-plane-rd + δCCN + δCNC + νCN	0.29
		1217	488.35	s-out-of-plane-rd + δCCN + δCNC + νCN	0.23
502	499	1216	499.24	νCN + δCNC + δCCN + s-out-of-plane-rd	4.27
		1215	500.18	δCNC + νCN + δCCN + s-out-of-plane-rd	0.00
		1214	501.48	δCNC + νCN + s-out-of-plane-rd + δCCN	0.17
		1213	501.64	νCN + δCNC + s-out-of-plane-rd + δCCN	0.00
		1212	502.58	νCN + δCNC + s-out-of-plane-rd + δCCN	0.00
		1211	502.95	δCCN + δCNC + νCN + s-out-of-plane-rd	0.12
		1210	503.92	νCN + δCCN + s-out-of-plane-rd + δCNC	0.00
		1209	504.33	δCCN + νCN + s-out-of-plane-rd + δCNC	0.01
	511	1208	512.04	νCN + δCCN + s-out-of-plane-rd + δCNC	1.65
		1207	512.27	δCCN + νCN + s-out-of-plane-rd + δCNC	0.16
		1206	513.11	δCCN + νCN + s-out-of-plane-rd + δCNC	0.00
		1205	513.56	δCCN + νCN + s-out-of-plane-rd + δCNC	0.00
		1204	515.94	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1203	516.73	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1202	517.45	δCCN + s-out-of-plane-rd + δCNC + νCN	0.71
		1201	517.80	δCCN + s-out-of-plane-rd + δCNC + νCN	0.01
569	563	1200	558.63	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1199	559.68	δCCN + s-out-of-plane-rd + δCNC + νCN	0.56
		1198	560.35	s-out-of-plane-rd + δCCN + δCNC + νCN + νCH	0.00
		1197	560.95	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1196	561.21	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1195	561.40	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1194	562.17	δCCN + s-out-of-plane-rd + δCNC + νCN	0.03
		1193	563.46	δCCN + s-out-of-plane-rd + δCNC + νCN	0.35
		1192	564.94	s-out-of-plane-rd + δCCN + δCNC + νCN + νCH	0.15
		1191	565.96	s-out-of-plane-rd + δCCN + δCNC + νCN	0.00
		1190	566.73	δCCN + s-out-of-plane-rd + δCNC + νCN	0.01
		1189	567.19	s-out-of-plane-rd + δCCN + δCNC + νCN	0.00
		1188	568.10	δCCN + s-out-of-plane-rd + δCNC + νCN	0.22
		1187	568.12	s-out-of-plane-rd + δCCN + δCNC + νCN	0.16

[2] This mode has been included in the table due to its remarkable activity although it falls outside of the experimental wavenumber range.

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		1186	569.22	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1185	570.09	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
604	599	1184	596.22	s-out-of-plane-rd + δCCN + δCNC + νCN	0.01
		1183	597.12	δCCN + s-out-of-plane-rd + δCNC + νCN	0.00
		1182	597.97	s-out-of-plane-rd + δCCN + δCNC + νCN	0.00
		1181	598.47	δCCN + s-out-of-plane-rd + δCNC + νCN	4.22
		1180	599.13	δCCN + s-out-of-plane-rd + δCNC + νCN	0.11
		1179	599.79	δCCN + s-out-of-plane-rd + δCNC + νCN	3.73
		1178	600.40	δCCN + s-out-of-plane-rd + νCN	0.01
		1177	600.95	δCCN + s-out-of-plane-rd + δCNC + νCN	0.01
609	605	1176	605.05	s-out-of-plane-rd + δCCN + δCNC + νCN	0.31
		1175	605.46	s-out-of-plane-rd + δCCN + δCNC + νCN	0.63
		1174	605.60	δCCN + s-out-of-plane-rd + δCNC + νCN	0.16
		1173	606.29	s-out-of-plane-rd + δCCN + δCNC + νCN	0.42
		1172	606.35	δCCN + νCN + s-out-of-plane-rd	0.65
		1171	606.71	s-out-of-plane-rd + δCNC + δCCN + νCN	1.31
		1170	607.67	s-out-of-plane-rd + δCNC + δCCN + νCN	0.00
		1169	608.09	a-in-plane-rd + r-νCH + δCNC + δCCN	0.00
623	629	1168	627.05	a-in-plane-rd + r-νCH + πCCNH + δCNC	0.05
		1167	627.62	a-in-plane-rd + r-νCH + πCCNH	0.00
		1166	627.74	a-in-plane-rd + r-νCH + πCCNH	0.01
		1165	628.55	a-in-plane-rd + r-νCH + πCCNH	7.40
		1164	631.07	a-in-plane-rd + r-νCH + πCCNH	0.01
		1163	632.06	a-in-plane-rd + r-νCH + πCCNH	1.27
641	635	1162	632.32	a-in-plane-rd + r-νCH	0.02
		1161	632.48	a-in-plane-rd + r-νCH	0.15
		1160	633.56	a-in-plane-rd + r-νCH	0.01
		1159	633.71	a-in-plane-rd + r-νCH	0.01
		1158	633.78	a-in-plane-rd + r-νCH	0.01
		1157	633.92	a-in-plane-rd + r-νCH	0.18
		1156	634.52	a-in-plane-rd + r-νCH	0.02
		1155	634.68	a-in-plane-rd + r-νCH	0.00
		1154	635.04	a-in-plane-rd + r-νCH	0.03
		1153	635.12	a-in-plane-rd + r-νCH + δCNC	0.01
		1152	635.23	a-in-plane-rd + r-νCH + δCNC	0.00
		1151	635.90	a-in-plane-rd + r-νCH	5.23
		1150	636.10	a-in-plane-rd + r-νCH	0.31
		1149	636.39	a-in-plane-rd + r-νCH + νCC + νCN	0.49
		1148	636.52	a-in-plane-rd + r-νCH + νCC + νCN	0.01
		1147	637.26	a-in-plane-rd + r-νCH + νCN	0.00
		1146	637.67	a-in-plane-rd + r-νCH + νCC + νCN	0.00
		1145	637.78	a-in-plane-rd + r-νCH + νCC + νCN	0.00
654	646	1144	643.85	s-in-plane-rd + r-νCH + νCC + νCN	0.47
		1143	644.24	s-in-plane-rd + r-νCH + νCC + νCN	0.00
		1142	644.83	s-in-plane-rd + r-νCH + νCC + νCN	0.01
		1141	645.14	s-in-plane-rd + r-νCH + νCC + νCN	0.01
		1140	645.18	a-in-plane-rd + r-νCH + νCC + νCN	0.00
		1139	645.21	a-in-plane-rd + r-νCH + νCC + νCN	0.00
		1138	645.37	a-in-plane-rd + r-νCH + δCNC	0.04
		1137	645.51	a-in-plane-rd + r-νCH + δCNC	0.02
		1136	646.11	a-in-plane-rd + r-νCH + δCNC	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		1135	646.62	a-in-plane-rd + r-νCH + δCNC + δCCN	1.18
		1134	646.74	a-in-plane-rd + r-νCH + νCC + δCNC	0.03
		1133	647.50	a-in-plane-rd + r-νCH + δCNC + δCCN	0.08
		1132	647.87	a-in-plane-rd + r-νCH	0.36
		1131	648.39	a-in-plane-rd + r-νCH + δCNC + δCCN	0.18
		1130	648.48	a-in-plane-rd + r-νCH + δCNC + δCCN	0.00
		1129	649.05	a-in-plane-rd + r-νCH + δCNC + δCCN	0.00
669	666	1128	665.21	s-out-of-plane-rd + δCNC + δCCN + νCN	4.09
		1127	665.64	s-out-of-plane-rd + δCNC + δCCN + νCN	0.02
		1126	665.90	s-out-of-plane-rd + δCNC + δCCN + νCN	0.00
		1125	666.72	s-out-of-plane-rd + δCNC + δCCN + νCN	0.00
		1124	666.84	s-out-of-plane-rd + δCNC + δCCN + νCN	0.05
		1123	666.86	s-out-of-plane-rd + δCNC + δCCN + νCN	0.19
		1122	667.09	s-out-of-plane-rd + δCNC + δCCN + νCN	0.00
		1121	667.83	s-out-of-plane-rd + δCNC + δCCN + νCN	1.36
		1120	668.28	s-out-of-plane-rd + δCNC + δCCN + νCN	0.07
		1119	669.87	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.00
		1118	670.26	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.00
		1117	670.39	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.07
		1116	670.95	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.00
		1115	671.42	s-out-of-plane-rd + δCNC + δCCN + πCCNH	0.00
		1114	671.74	s-out-of-plane-rd + δCNC + δCCN + πCCNH	0.01
		1113	671.93	s-out-of-plane-rd + δCNC + δCCN + πCCNH	0.30
690	682	1112	681.32	s-out-of-plane-rd + δCNC + δCCN + πCCNH	0.03
		1111	681.85	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	7.34
		1110	682.78	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	4.40
		1109	683.34	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.07
		1108	683.75	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.00
		1107	684.19	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.01
		1106	685.03	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.00
		1105	685.35	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.01
		1104	686.28	s-out-of-plane-rd + δCNC + δCCN + νCN + νCC	0.00
		1103	686.42	s-in-plane-rd + δCNC+ δCCN + νCN + νCC	0.13
705	688	1102	686.78	s-in-plane-rd + δCNC+ δCCN + νCC + νCN	0.00
		1101	687.92	πCCNH + s-out-of-plane-rd + δCNC + νCN	0.00
		1100	688.56	s-in-plane-rd + πCCNH + δCNC + νCC + νCN	2.65
		1099	688.58	s-in-plane-rd + πCCNH + δCNC + νCC + νCN	3.38
		1098	689.23	s-in-plane-rd + πCCNH + δCCN + νCC + νCN	4.56
		1097	690.72	πCCNH + s-in-plane-rd + δCCN + νCC + νCN	0.00
		1096	693.12	s-in-plane-rd + δCNC + δCCN + νCC + νCN	0.25
		1095	693.67	s-out-of-plane-rd + δCCN + δCNC + νCC + νCN	0.98
		1094	693.85	s-in-plane-rd + δCCN + δCNC + νCC + νCN	0.19
		1093	694.63	s-in-plane-rd + δCCN + δCNC + νCC + νCN	0.06
		1092	695.25	s-in-plane-rd + δCCN + δCNC + νCC + νCN	0.66
		1091	695.64	s-in-plane-rd + δCCN + δCNC + νCC + νCN	0.03
		1090	696.90	s-in-plane-rd + δCCN + νCC + νCN + πCCNH	0.00
		1089	697.18	πCCNH + δCCN + νCC + νCN + s-in-plane-rd	0.00
725	700	1088	699.51	πCCNH + δCCN + νCC + νCN + s-out-of-plane-rd	1.20
		1087	699.86	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	0.14
		1086	700.30	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	0.07
		1085	700.42	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	2.95

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		1084	700.60	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	0.00
		1083	701.01	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	0.12
732	705	1082	702.31	πCCNH + νCC + νCN + δCCN	0.00
		1081	703.35	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	0.81
		1080	703.85	πCCNH + νCC + νCN + δCCN	0.00
		1079	704.22	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	0.01
		1078	705.04	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	2.00
		1077	705.15	πCCNH + νCC + νCN + δCCN + s-out-of-plane-rd	4.57
769	762	1038	762.20	δCCN + δCNC + νCC + νCN	0.14
		1037	762.63	δCCN + δCNC + νCC + s-out-of-plane-rd	0.33
		1036	763.48	δCCN + δCNC + νCC + s-out-of-plane-rd	0.00
		1035	763.71	δCCN + νCN + s-out-of-plane-rd	0.10
		1034	764.06	δCCN + δCNC + s-out-of-plane-rd	0.00
		1033	764.30	δCCN + δCNC + νCC + s-out-of-plane-rd	0.00
		1032	766.27	δCCN + δCNC + s-out-of-plane-rd	0.15
778	770	1031	767.03	δCCN + δCNC + νCC + s-out-of-plane-rd	0.15
		1030	768.36	δCCN + δCNC + νCC + s-out-of-plane-rd	0.00
		1029	768.44	νCC + δCCN + δCNC + s-out-of-plane-rd	0.00
		1028	768.61	δCCN + δCNC + νCC + s-out-of-plane-rd	0.00
		1027	769.22	νCC + δCCN + δCNC + s-out-of-plane-rd	0.02
		1026	769.58	νCC + δCCN + δCNC + s-out-of-plane-rd	0.00
		1025	769.88	δCCN + δCNC + νCC + a-out-of-plane-rd	1.57
		1024	770.24	δCCN + δCNC + νCC + a-out-of-plane-rd	0.00
		1023	770.43	δCCN + δCNC + νCC + a-out-of-plane-rd	0.14
		1022	770.49	s-out-of-plane-rd + νCC + δCCN + δCNC	0.17
		1021	770.56	s-out-of-plane-rd + δCCN + νCC + δCNC	3.50
		1020	772.25	s-out-of-plane-rd + δCCN + νCC + δCNC	0.62
		1019	772.48	s-out-of-plane-rd + δCCN + νCC	0.01
		1018	772.63	s-out-of-plane-rd + δCCN + νCC + δCNC	0.14
		1017	773.46	s-out-of-plane-rd + δCCN + νCC + δCNC	0.00
785	783	1016	782.90	s-out-of-plane-rd + δCCN + νCC + δCNC	0.02
		1015	783.23	s-out-of-plane-rd + δCCN + νCC + δCNC	3.33
		1014	783.35	s-out-of-plane-rd + δCCN + νCC + δCNC	0.08
		1013	783.52	s-out-of-plane-rd + δCCN + νCC + δCNC	0.11
		1012	783.79	s-out-of-plane-rd + δCCN + νCC + δCNC	0.08
		1011	784.06	s-in-plane-rd + δCCN + νCC + δCNC	0.56
		1010	784.48	s-in-plane-rd + δCCN + νCC + δCNC	0.06
801	808	1000	806.73	s-out-of-plane-rd + δCCN + νCN	0.32
		999	807.21	s-out-of-plane-rd + δCCN + νCN	0.79
		998	807.46	s-out-of-plane-rd + δCCN + νCN	0.01
		997	807.81	s-out-of-plane-rd + δCCN + νCN	0.00
		996	808.38	s-out-of-plane-rd + δCCN + νCN	0.35
		995	808.99	s-out-of-plane-rd + δCCN + νCN	1.18
		994	809.23	a-out-of-plane-rd + δCCN + νCC	0.02
		993	809.73	s-in-plane-rd + δCCN + νCC	0.00
813	813	992	813.57	s-in-plane-rd + δCCN + νCC	1.06
		991	813.73	s-in-plane-rd + δCCN + νCC	0.06
		990	813.89	s-in-plane-rd + δCCN + νCC	0.00
		989	814.38	s-in-plane-rd + δCCN + νCC	0.48
		988	814.46	s-in-plane-rd + δCCN + νCC	0.20
		987	814.66	s-in-plane-rd + δCCN + νCC	0.03

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		986	814.89	s-in-plane-rd + δCCN + νCC	0.02
		985	815.06	s-in-plane-rd + δCCN + νCC	0.00
822	821	984	818.63	s-out-of-plane-rd + δCCN + νCC	0.00
		983	818.76	s-out-of-plane-rd + δCCN + νCC	0.00
		982	819.83	s-out-of-plane-rd + δCCN + νCC	0.06
		981	819.90	s-out-of-plane-rd + δCCN + νCC + r-νCH	0.05
		980	820.41	s-out-of-plane-rd + δCCN + νCC + r-νCH	0.12
		979	820.57	s-out-of-plane-rd + δCCN + νCC	1.28
		978	821.70	s-out-of-plane-rd + νCC	0.51
		977	822.08	s-out-of-plane-rd + δCCN + νCC + r-νCH	1.06
		976	824.93	s-out-of-plane-rd + δCCN + νCC	0.04
		975	825.33	s-out-of-plane-rd + δCCN + νCC	0.64
		974	826.18	s-out-of-plane-rd + δCCN + νCC	0.04
		973	826.57	s-out-of-plane-rd + δCCN + νCC	0.30
		972	828.61	s-out-of-plane-rd + δCCN + νCC	0.00
		971	829.19	s-out-of-plane-rd + δCCN + νCC	0.00
		970	830.26	s-out-of-plane-rd + δCCN + νCC	0.00
		969	830.57	s-out-of-plane-rd + δCCN + νCC	0.00
857	861	944	856.90	s-out-of-plane-rd + δCCN + νCN + νCC	0.11
		943	856.97	s-out-of-plane-rd + δCCN + νCN + νCC	0.05
		942	857.10	s-out-of-plane-rd + δCCN + νCN + νCC	0.09
		941	857.11	s-out-of-plane-rd + δCCN + νCN + νCC	0.11
		940	857.69	s-out-of-plane-rd + δCCN + νCN + νCC	0.13
		939	857.79	s-out-of-plane-rd + δCCN + νCN + νCC	0.17
		938	858.00	s-out-of-plane-rd + δCCN + νCN	0.05
		937	858.13	s-out-of-plane-rd + δCCN + νCN + νCC	0.04
		936	861.22	s-out-of-plane-rd + δCCN + νCN	1.92
		935	861.81	s-out-of-plane-rd + δCCN + νCN	0.01
		934	862.06	s-out-of-plane-rd + δCCN	0.03
		933	862.28	s-out-of-plane-rd + δCCN	0.00
		932	862.38	s-out-of-plane-rd + δCCN	0.97
		931	862.99	s-out-of-plane-rd + δCCN	0.00
		930	863.37	s-out-of-plane-rd + δCCN	0.32
		929	863.79	s-out-of-plane-rd + δCNC	0.00
**	**	921	874.49	s-in-plane-rd + πCNCC + δHCH	0.00
887	882	920	882.02	a-out-of-plane-rd + δCCN	0.01
		919	882.04	a-out-of-plane-rd + δCCN	0.02
		918	882.04	a-out-of-plane-rd + δCCN	0.12
		917	882.13	a-out-of-plane-rd + δCCN	0.02
903	895	916	894.09	a-out-of-plane-rd + δCCN	0.03
		915	894.19	a-out-of-plane-rd + δCCN	0.48
		914	894.22	a-out-of-plane-rd + δCCN	0.18
		913	894.33	a-out-of-plane-rd + δCCN	0.09
		912	895.42	a-out-of-plane-rd + δCCN	0.22
		911	895.55	a-out-of-plane-rd + δCCN	0.38
		910	895.59	a-out-of-plane-rd + δCCN + r-νCH	0.19
		909	895.81	a-out-of-plane-rd	0.01
		908	896.31	a-out-of-plane-rd + δCCN	0.01
		907	896.33	a-out-of-plane-rd + δCCN	0.01
		906	896.46	a-out-of-plane-rd + δCCN	0.61
		905	896.47	a-out-of-plane-rd + δCCN	0.18

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
912	917	904	916.96	s-in-plane-rd + δCCN + νCC	0.01
		903	917.11	a-out-of-plane-rd + δCCN	0.19
		902	917.50	a-out-of-plane-rd + δCCN	0.18
		901	917.67	a-out-of-plane-rd + δCCN	0.08
		900	917.86	s-in-plane-rb + δCNC	0.12
		899	918.12	s-in-plane-rb	0.01
		898	918.34	s-in-plane-rb	0.04
		897	918.71	a-out-of-plane-rd	0.01
923	922	896	920.25	a-out-of-plane-rd + δCCN	0.03
		895	920.78	a-out-of-plane-rd + δCCN	0.00
		894	920.92	a-out-of-plane-rd + δCCN + r-νCH	0.14
		893	921.26	a-out-of-plane-rd + δCCN + r-νCH	0.00
		892	922.11	a-out-of-plane-rd + δCCN	0.05
		891	922.51	a-out-of-plane-rd + δCNC + r-νCH	0.00
		890	922.76	a-out-of-plane-rd + δCNC	0.18
		889	923.08	s-out-of-plane-rd + δCNC	0.00
938	938	888	938.00	s-out-of-plane-rd + δCNC	0.10
		887	938.21	s-out-of-plane-rd + δCNC	0.08
		886	939.39	s-out-of-plane-rd + δCNC	0.03
		885	940.44	s-out-of-plane-rd + δCNC	0.00
		884	942.21	s-out-of-plane-rd + δCNC	0.00
		883	942.35	s-out-of-plane-rd + δCNC	0.00
		882	943.34	s-out-of-plane-rd + δCNC	0.00
		881	943.97	s-out-of-plane-rd + δCNC	0.00
946	945	880	945.86	s-out-of-plane-rd + δCNC	0.07
		879	946.43	s-out-of-plane-rd + δCNC	0.65
		878	947.04	s-out-of-plane-rd + δCNC	0.05
		877	947.24	s-out-of-plane-rd + δCCN + δCNC	0.00
		876	947.44	s-out-of-plane-rd + δCCN + δCNC	0.01
		875	947.60	s-out-of-plane-rd + δCCN + δCNC	0.12
		874	948.25	s-out-of-plane-rd + δCCN + δCNC	0.00
		873	948.99	s-out-of-plane-rd + δCCN + δCNC	0.00
963	954	872	951.94	s-out-of-plane-rd + δCCN + δCNC	0.03
		871	952.27	s-out-of-plane-rd + δCCN + δCNC	0.02
		870	952.38	s-out-of-plane-rd + δCCN + δCNC	0.01
		869	952.97	s-out-of-plane-rd + δCCN + δCNC	0.00
		868	953.04	s-out-of-plane-rd + δCCN + δCNC	0.01
		867	953.58	s-out-of-plane-rd + δCCN + δCNC	0.02
		866	953.69	s-out-of-plane-rd + δCCN + δCNC	0.05
		865	953.82	a-out-of-plane-rd + δCCN + δCNC	0.01
		864	954.40	a-out-of-plane-rd + δCCN + δCNC	0.57
		863	954.51	a-out-of-plane-rd + δCCN + δCNC	0.31
		862	954.89	a-out-of-plane-rd + δCNC	0.02
		861	955.30	a-out-of-plane-rd + δCCN + δCNC	0.00
		860	957.13	a-out-of-plane-rd + δCCN + δCNC	0.00
		859	957.31	a-out-of-plane-rd + δCCN + δCNC	0.00
		858	957.80	a-out-of-plane-rd + δCCN + δCNC	0.00
		857	958.60	a-out-of-plane-rd + δCCN + δCNC	0.00
971	965	856	962.46	a-out-of-plane-rd + δCCN + δCNC	0.00
		855	962.51	a-out-of-plane-rd	0.01
		854	963.70	a-out-of-plane-rd	0.01

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		853	964.31	a-out-of-plane-rd + δCCN + δCNC	0.00
		852	965.13	a-out-of-plane-rd + δCCN + δCNC	0.06
		851	965.29	a-out-of-plane-rd + δCCN + δCNC	0.02
		850	965.37	a-out-of-plane-rd + δCCN	0.09
		849	965.62	a-out-of-plane-rd + δCNC	0.12
		848	965.87	a-out-of-plane-rd + δCNC	0.15
		847	966.09	a-out-of-plane-rd	0.01
		846	966.20	a-out-of-plane-rd	0.02
		845	966.48	a-out-of-plane-rd	0.01
		844	967.07	a-out-of-plane-rd	0.00
		843	967.15	a-out-of-plane-rd	0.00
		842	967.36	a-out-of-plane-rd	0.03
		841	968.09	a-out-of-plane-rd	0.00
978	974	840	972.67	a-out-of-plane-rd	0.01
		839	973.03	a-out-of-plane-rd	0.21
		838	973.81	a-out-of-plane-rd	0.00
		837	973.86	a-out-of-plane-rd	0.00
		836	974.97	a-out-of-plane-rd	0.09
		835	975.18	a-out-of-plane-rd	0.00
		834	975.60	a-out-of-plane-rd	0.00
		833	975.81	a-out-of-plane-rd	0.00
		832	978.75	a-out-of-plane-rd	0.00
		831	979.06	a-out-of-plane-rd	0.04
		830	979.20	a-out-of-plane-rd	0.00
		829	979.45	a-out-of-plane-rd	0.04
		828	980.30	a-out-of-plane-rd + r-νCH	0.00
		827	980.61	a-out-of-plane-rd + r-νCH	0.07
		826	980.85	a-out-of-plane-rd + δCCN + δCNC	0.00
		825	981.08	a-out-of-plane-rd + δCCN + δCNC	0.08
993	984	824	984.18	a-out-of-plane-rd + δCCN + δCNC	0.00
		823	985.07	s-out-of-plane-rd + δCCN + δCNC	2.28
		822	985.57	a-out-of-plane-rd + δCCN + δCNC	0.03
		821	985.70	a-out-of-plane-rd + δCCN + δCNC	0.02
		820	986.19	a-out-of-plane-rd + δCCN + δCNC	0.00
		819	986.39	a-out-of-plane-rd + δCCN + δCNC	0.00
		818	986.92	a-out-of-plane-rd + δCCN + δCNC	0.01
		817	987.43	a-out-of-plane-rd + δCCN + δCNC	0.00
1000	990	816	989.83	a-out-of-plane-rd + δCCN + δCNC	0.00
		815	990.24	a-out-of-plane-rd + δCCN + δCNC	0.00
		814	990.56	a-out-of-plane-rd + δCCN + δCNC	0.00
		813	990.65	a-out-of-plane-rd + δCCN + δCNC	0.01
		812	991.12	a-out-of-plane-rd + δCCN + δCNC	0.17
		811	991.29	a-out-of-plane-rd + δCCN + δCNC	0.12
		810	991.67	a-out-of-plane-rd + δCCN + δCNC	0.01
		809	992.21	s-in-plane-rd	0.47
**	**	792	1000.04	s-in-plane-rd + s-r-νCH	0.01
		789	1000.75	s-in-plane-rd + s-r-νCH	0.00
		788	1003.76	s-in-plane-rd + s-r-νCH	0.03
		786	1004.00	s-in-plane-rd + s-r-νCH	0.01
		785	1004.01	s-in-plane-rd + s-r-νCH	0.01
1021	1022	784	1019.41	s-in-plane-rd + r-νCH + νCC + δCNC	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		783	1019.49	s-in-plane-rd + vCC + δCNC	0.00
		782	1019.70	s-in-plane-rd + r-vCH + vCC	0.01
		781	1019.76	s-in-plane-rd + r-vCH + vCC + δCNC	0.01
		780	1020.18	s-in-plane-rd + r-vCH + vCC + δCNC	0.04
		779	1020.19	s-in-plane-rd + r-vCH + vCC + δCNC	0.00
		778	1020.66	s-in-plane-rd + r-vCH + vCC + δCNC	0.06
		777	1020.74	s-in-plane-rd + r-vCH + vCC	0.01
		776	1021.14	s-in-plane-rd + r-vCH + vCC	0.60
		775	1021.30	s-in-plane-rd + r-vCH + vCC + δCNC	0.02
		774	1021.61	s-in-plane-rd + r-vCH + vCC	0.01
		773	1021.89	s-in-plane-rd + vCC	0.57
		772	1024.04	s-in-plane-rd	0.02
		771	1024.24	s-in-plane-rd + r-vCH	0.35
		770	1024.32	s-in-plane-rd + vCC	0.09
		769	1024.49	s-in-plane-rd + vCC	0.49
1025	1028	768	1027.04	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.01
		767	1027.13	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.11
		766	1027.83	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.01
		765	1028.02	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.03
		764	1028.64	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.13
		763	1029.08	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.75
		762	1029.22	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.17
		761	1029.61	vCN + δCNC + δCCN + vNC + a-in-plane-rd	0.19
1042	1046	760	1044.11	δCNC + vCN + δCCN + vNC + s-out-of-plane-rd	0.09
		759	1044.45	δCNC + vCN + δCCN + vNC	0.06
		758	1044.55	δCNC + vCN + δCCN + s-in-plane-rd	0.00
		757	1044.88	δCNC + vCN + δCCN + s-in-plane-rd	0.01
		756	1045.21	δCNC + vCN + s-in-plane-rd	0.00
		755	1045.43	vNC + δCNC + vCN + δCCN + δCCC	0.05
		754	1045.59	vNC + δCNC + δCCN + δCCC	0.01
		753	1045.71	vNC + δCNC + vCC+ a-in-plane-rd	0.21
		752	1045.86	vNC + δCNC + δCCN + a-in-plane-rd	0.05
		751	1046.28	vNC + δCNC + δCCN + a-in-plane-rd	0.09
		750	1046.42	vNC + δCNC + δCCN + a-in-plane-rd	0.06
		749	1046.68	vNC + δCNC + δCCN + a-in-plane-rd	0.07
		748	1046.80	vNC + δCNC + vCC + a-in-plane-rd	0.01
		747	1047.05	vNC + vCC + δCNC + a-in-plane-rd	0.01
		746	1047.25	vNC + vCN + δCNC + a-in-plane-rd	0.04
		745	1047.56	vNC + vCN + δCNC + a-in-plane-rd	0.01
1055	1060	744	1059.73	vNC + vCN + δCNC + δCCN	0.02
		743	1059.80	vCN + vNC + δCCN + a-in-plane-rd	0.32
		742	1059.93	vCN + δCCN + δCNC + vNC	0.46
		741	1060.12	vCN + a-in-plane-rd + δCCN	0.02
		740	1061.66	vCN + s-in-plane-rd + δCCC	0.00
		739	1061.76	a-in-plane-rd + δCCC + vCN	0.00
		738	1061.81	a-in-plane-rd + δCCC + δCCN	0.00
		737	1062.30	a-in-plane-rd + δCCN + δCCC	0.02
1083	1092	736	1089.14	a-in-plane-rd + δCCC	0.01
		735	1089.43	a-in-plane-rd + δCCC + δCCN	0.00
		734	1089.65	a-in-plane-rd + δCCC + δCCN	0.01
		733	1089.79	a-in-plane-rd + δCCC + δCCN	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		732	1090.21	a-in-plane-rd + δCCC + δCCN	0.09
		731	1090.43	a-in-plane-rd + δCCC + δCCN	0.00
		730	1090.55	a-in-plane-rd + δCCC + δCCN	0.06
		729	1090.79	a-in-plane-rd + δCCC + δCCN	0.00
		728	1091.39	a-in-plane-rd + δCCC + δCCN	0.64
		727	1092.29	a-in-plane-rd + δCCC + δCCN	1.29
		726	1092.88	a-in-plane-rd + δCCC + δCCN	1.98
		725	1093.76	a-in-plane-rd + δCCC + δCCN	0.14
		724	1094.46	a-in-plane-rd + δCCC + νCN	0.00
		723	1095.00	a-in-plane-rd + δCCC + δCCN	0.00
		722	1095.47	a-in-plane-rd + δCCC + νCN	0.00
		721	1096.09	a-in-plane-rd + δCCC + νCN	0.00
1109	1118	720	1118.27	a-in-plane-rd + δCCC + δCCN	0.34
		719	1118.69	a-in-plane-rd + δCCC + δCCN	0.48
		718	1118.85	a-in-plane-rd + δCCC + δCCN	0.01
		717	1119.33	a-in-plane-rd + δCCC + δCCN	0.01
1114	1123	716	1121.98	a-in-plane-rd + δCCC + δCCN	0.08
		715	1122.11	a-in-plane-rd + δCCC + δCCN	0.00
		714	1122.63	a-in-plane-rd + δCCC + νCN	0.01
		713	1122.65	a-in-plane-rd + δCCC + νCN	0.00
		712	1123.81	a-in-plane-rd + δCCC + νCN	0.16
		711	1124.33	a-in-plane-rd + δCCC + νCN	0.21
		710	1124.48	a-in-plane-rd + δCCC + δCCN	0.03
		709	1124.87	a-in-plane-rd + δCCC	0.00
		708	1124.95	a-in-plane-rd + δCCC	0.04
		707	1125.34	a-in-plane-rd + δCCC + νCN	0.00
		706	1125.41	νCN+ νCC + a-in-plane-rd + δCCC	0.04
		705	1125.72	νCN+ νCC + a-in-plane-rd + δCCC	0.00
1127	1139	692	1139.38	s-in-plane-rd + νCC + νCN + δCCN	0.00
		691	1139.43	νCC+ νCN + s-in-plane-rd + δCCN	0.07
		690	1139.99	s-in-plane-rd + νCC + νCN + δCCN	0.17
		689	1140.18	s-in-plane-rd + νCC + νCN + δCCN	0.07
1167	1173	688	1168.98	s-in-plane-rd + νCC + νCN + δCCN	0.01
		687	1169.01	s-in-plane-rd + νCN + νCC + δCCN	0.01
		686	1169.61	s-in-plane-rd + νCN + νCC + δCCN	0.00
		685	1169.63	s-in-plane-rd + νCN + νCC + δCCN	0.00
		684	1170.25	s-in-plane-rd + νCN + νCC + δCCN	0.00
		683	1170.42	s-in-plane-rd + νCN + νCC + δCCN	0.05
		682	1170.81	νCN+ νCC + s-in-plane-rd + δCCN	0.00
		681	1171.24	νCN+ νCC + s-in-plane-rd + δCCN	0.00
		680	1171.81	νCN+ νCC + s-in-plane-rd + δCCN	0.52
		679	1172.09	s-in-plane-rd + νCN + νCC + δCCN	0.70
		678	1172.23	νCC+ νCN + s-in-plane-rd + δCCN	0.04
		677	1172.78	νCC+ νCN + s-in-plane-rd + δCCN	0.00
		676	1172.93	νCC+ νCN + s-in-plane-rd + δCCN	0.00
		675	1173.19	s-in-plane-rd + νCC+ νCN + δCCN	0.05
		674	1173.32	s-in-plane-rd + νCC+ νCN + δCCN	0.07
		673	1173.38	s-in-plane-rd + νCC+ νCN + δCCN	0.01
		672	1173.76	s-in-plane-rd + νCC+ νCN + δCCN	0.14
		671	1174.28	s-in-plane-rd + νCC+ νCN + δCCN	0.19
		670	1174.57	s-in-plane-rd + νCC+ νCN + δCCN	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		669	1174.84	s-in-plane-rd + vCC+ vCN + δCCN	0.00
		668	1175.06	s-in-plane-rd + vCC+ vCN + δCCN	0.25
		667	1175.40	s-in-plane-rd + vCC+ vCN + δCCN	0.00
		666	1175.79	vCN + vCC + s-in-plane-rd+ δCNC	0.66
		665	1176.02	s-in-plane-rd + vCC+ vCN + δCCN	0.13
1176	1181	664	1180.88	s-in-plane-rd + vCC + vCN + δCNC	0.00
		663	1181.08	s-in-plane-rd + vCC + vCN + δCNC	0.00
		662	1181.46	s-in-plane-rd + vCC + vCN + δCNC	0.04
		661	1181.57	s-in-plane-rd + vCC + vCN + δCNC	0.05
		660	1181.80	s-in-plane-rd + vCC + vCN + δCNC	0.00
		659	1182.24	s-in-plane-rd + vCC + vCN + δCNC	0.00
		658	1182.80	s-in-plane-rd + vCC + vCN + δCNC	0.00
		657	1183.21	s-in-plane-rd + vCC + vCN + δCNC	0.00
		656	1183.31	s-in-plane-rd + vCC + vCN + δCNC	0.05
		655	1183.49	s-in-plane-rd + vCC + vCN + δCNC	0.02
		654	1183.59	s-in-plane-rd + vCC + vCN + δCNC	0.02
		653	1183.97	s-in-plane-rd + vCC + vCN + δCNC	0.13
1182	1190	652	1188.95	s-in-plane-rd + vCC + vCN + δCNC	0.07
		651	1189.39	s-in-plane-rd + vCC + vCN + δCNC	0.00
		650	1189.81	s-in-plane-rd + vCC + vCN + δCNC	0.08
		649	1190.26	s-in-plane-rd + vCC + vCN + δCNC	0.01
		648	1190.50	s-in-plane-rd + vCC + vCN + δCNC	0.01
		647	1190.70	s-in-plane-rd + vCC + vCN + δCNC	0.00
		646	1191.25	s-in-plane-rd + vCC + vCN + δCNC	0.03
		645	1191.50	s-in-plane-rd + vCC + vCN	0.00
		644	1195.99	s-in-plane-rd + vCC + vCN	0.00
		643	1196.01	s-in-plane-rd + vCC + vCN	0.00
		642	1197.67	s-in-plane-rd + vCC + vCN	0.00
		641	1197.91	s-in-plane-rd + vCC + vCN + δCCN	0.00
1198	1206	640	1203.16	vCC + s-in-plane-rd + vCN + δCCN	0.04
		639	1203.51	vCC + s-in-plane-rd + vCN + δCCN	0.00
		638	1203.69	vCC + s-in-plane-rd + vCN + δCCN	0.00
		637	1203.80	vCC + s-in-plane-rd + vCN + δCCN	0.00
		636	1204.56	vCC + s-in-plane-rd + vCN + δCCN	0.07
		635	1204.80	vCC + s-in-plane-rd + vCN + δCCN	0.00
		634	1205.04	s-in-plane-rd + vCC+ δCCN + vCN	0.47
		633	1205.11	vCC + s-in-plane-rd + δCCN + vCN	0.21
		632	1206.12	vCC + s-in-plane-rd + δCCN + vCN	0.29
		631	1206.28	vCC + s-in-plane-rd + δCCN + vCN	0.55
		630	1206.37	vCC + s-in-plane-rd + δCCN + vCN	0.00
		629	1206.66	vCC + s-in-plane-rd + δCCN + vCN	0.00
		628	1206.84	vCC + s-in-plane-rd + δCCN + vCN	0.01
		627	1206.86	s-in-plane-rd + vCC+ δCCN + vCN	0.01
		626	1207.12	s-in-plane-rd + vCC + vCN+ δCCN	0.26
		625	1207.19	vCC + s-in-plane-rd + vCN + δCCN	0.02
		624	1207.42	vCC + s-in-plane-rd + vCN + δCCN	0.74
		623	1207.78	vCC + s-in-plane-rd + vCN + δCCN	0.47
		622	1207.87	s-in-plane-rd + vCC + vCN+ δCCN	0.03
		621	1208.31	vCC + s-in-plane-rd + vCN + δCCN	0.00
1211	1213	620	1211.09	vCC + s-in-plane-rd + vCN + δCCN	0.01
		619	1211.33	vCC + s-in-plane-rd + vCN + δCNC	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		618	1211.41	s-in-plane-rd + νCC + νCN + δCNC	0.00
		617	1211.72	s-in-plane-rd + νCC + νCN	0.00
		616	1214.02	s-in-plane-rd + νCC + τCH2	0.01
		615	1214.25	s-in-plane-rd + νCC + νCN + τCH2	0.00
		614	1214.31	s-in-plane-rd + νCC + νCN	0.21
		613	1214.63	s-in-plane-rd + νCC	0.18
		612	1215.20	s-in-plane-rd + νCC + τCH2	0.02
		611	1215.59	s-in-plane-rd + νCC + τCH2 + δCNC	0.02
		610	1215.70	τCH2 + δCNC + s-in-plane-rd + νCC	0.00
		609	1215.84	s-in-plane-rd + νCC+ νCN	0.01
1220	1224	608	1222.02	δCNC + τCH2 + s-in-plane-rd + δCCN	0.01
		607	1222.15	δCNC + τCH2 + s-in-plane-rd + δCCN	0.02
		606	1222.25	δCNC + τCH2 + s-in-plane-rd + δCCN	0.12
		605	1222.26	τCH2 + δCNC + s-in-plane-rd + δCCN	0.13
		604	1222.28	τCH2 + δCCN + δCNC + s-in-plane-rd	0.07
		603	1222.40	τCH2 + νCC + νCN + δCCN	0.33
		602	1222.47	τCH2 + νCC + δCCN + s-in-plane-rd	0.04
		601	1222.71	τCH2 + δCCN + δCNC + s-in-plane-rd	0.10
		600	1225.55	τCH2 + δCCN + νCC + δCNC + s-in-plane-rd	1.09
		599	1225.79	τCH2 + δCCN + νCC + νCO + s-in-plane-rd	0.00
		598	1226.00	τCH2 + δCCN + νCC + νCN + s-in-plane-rd	0.00
		597	1226.03	τCH2 + νCC+ νCN + δCCN + a-in-plane-rd	0.00
1234	1240	596	1236.56	τCH2 + δCNC + δCCN + a-in-plane-rd	0.00
		595	1236.73	τCH2 + δCNC + δCCN + a-in-plane-rd	0.00
		594	1237.11	τCH2 + δCNC + δCCN + a-in-plane-rd	0.00
		593	1237.16	τCH2 + δCNC + δCCN + a-in-plane-rd	0.01
		592	1240.12	τCH2 + δCNC + δCCC + a-in-plane-rd	0.16
		591	1240.18	τCH2 + δCCN + νCC + νCN + s-in-plane-rd	0.01
		590	1241.26	τCH2 + δCNC + δCCC + a-in-plane-rd	0.00
		589	1241.61	τCH2 + δCCN + δCNC + a-in-plane-rd	0.01
		588	1242.08	τCH2 + δCCN + δCNC + a-in-plane-rd	0.23
		587	1242.23	τCH2 + δCCN + δCNC + a-in-plane-rd	0.01
		586	1243.25	τCH2 + δCCN + δCNC + a-in-plane-rd	0.06
		585	1243.39	τCH2 + δCCN + δCNC + a-in-plane-rd	0.01
1246	1246	584	1246.77	τCH2 + δCCN + δCNC + a-in-plane-rd	1.24
		583	1246.84	τCH2 + δCCN + δCNC + a-in-plane-rd	0.33
		582	1246.96	τCH2 + δCCN + δCNC + a-in-plane-rd	0.00
		581	1247.37	τCH2 + δCCN + δCNC + a-in-plane-rd	0.02
		580	1248.13	τCH2 + νCC + νCN + a-in-plane-rd	0.00
		579	1248.29	τCH2 + νCC + νCN + a-in-plane-rd	0.01
		578	1248.50	τCH2 + νCC + νCN + a-in-plane-rd	0.00
		577	1248.77	τCH2 + νCC + νCN + a-in-plane-rd	0.00
1264	1266	576	1265.86	νCC + νCN + δCCN + a-in-plane-rd	0.20
		575	1266.18	δCCN + δCNC + νCC + νCN	3.86
		574	1266.24	δCCN + νCC + νCN + δCNC	5.20
		573	1266.66	νCC + νCN + δCCN + a-in-plane-rd	0.16
		572	1266.85	νCN + νCC + δCCN + a-in-plane-rd	0.31
		571	1267.24	νCN + νCC + δCCN + a-in-plane-rd	1.61
		570	1267.48	νCN + νCC + δCCN + a-in-plane-rd	0.04
		569	1267.60	νCN + νCC + δCCN + a-in-plane-rd	0.04
1270	1278	568	1277.68	νCN + νCC + δCCN + a-in-plane-rd	0.01

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		567	1277.78	vCC + vCN + δCCN + a-in-plane-rd	0.01
		566	1278.09	vCC + vCN + δCCN + a-in-plane-rd	2.38
		565	1278.20	vCN + vCC + δCCN + a-in-plane-rd	0.10
		564	1280.62	vCC+ vCN + δCCN + a-in-plane-rd	0.18
		563	1280.71	δCCN + vCC + vCN + δCNC	11.70
		562	1281.80	δCCN + vCC + vCN + δCNC	0.03
		561	1282.10	δCCN + vCC+ vCN + a-in-plane-rd	2.24
1284	1285	560	1286.35	vCC+ vCN + δCCN + s-in-plane-rd	3.17
		559	1286.55	δCCN + vCC + vCN + s-in-plane-rd	0.62
		558	1286.68	δCCN + vCC + vCN + a-in-plane-rd	0.01
		557	1286.86	vCC + vCN + δCCN + a-in-plane-rd	0.83
		556	1286.99	vCC + δCCN + vCN + a-in-plane-rd	3.58
		555	1287.10	vCC + δCCN + vCN + s-in-plane-rd	0.11
		554	1287.28	vCC + δCCN + vCN + s-in-plane-rd	0.01
		553	1287.69	δCCN + vCC+ vCN + a-in-plane-rd	0.01
		552	1293.16	δCCN + vCC + vCN + a-in-plane-rd	0.01
		551	1293.36	vCC + δCCN + vCN + a-in-plane-rd	0.08
		550	1293.40	vCC + δCCN + vCN + a-in-plane-rd	0.53
		549	1293.78	δCCN + vCC + vCN + a-in-plane-rd	0.01
		548	1298.25	vCC + δCCN + vCN + a-in-plane-rd	0.00
		547	1298.41	vCC + δCCN + δCNC + a-in-plane-rd	0.82
		546	1298.44	vCC + δCCN + vNC + a-in-plane-rd	0.09
		545	1298.59	vCC + δCCN + vCN + a-in-plane-rd	0.00
1302	1303	544	1303.13	vCC+ δCCN + vCN + a-in-plane-rd	0.29
		543	1303.34	vCC+ δCCN + vCN + a-in-plane-rd	0.01
		542	1303.48	vCC+ δCCN + vCN + a-in-plane-rd	4.60
		541	1303.69	vCC+ δCCN + vCN + a-in-plane-rd	0.48
		540	1304.20	vCC+ δCCN + vCN + s-in-plane-rd	0.01
		539	1304.82	δCCN + vCC+vCN + s-in-plane-rd	0.14
		538	1304.93	δCCN + a-in-plane-rd + vCC + vCN	1.06
		537	1305.12	δCCN + a-in-plane-rd + vCC + vCN	0.19
		536	1305.23	δCCN + vCC + vCN + a-in-plane-rd	0.63
		535	1305.38	δCCN + vCC + a-in-plane-rd + δCNC	0.00
		534	1305.54	δCCN + vCC + a-in-plane-rd + δCNC	0.15
		533	1305.70	δCCN + vCC + a-in-plane-rd + δCNC	0.01
		532	1306.36	δCCN + vCC + δCNC + a-in-plane-rd	0.00
		531	1307.24	δCCN + vCC + δCNC + a-in-plane-rd	0.00
		530	1307.60	δCCN + vCC + δCNC + a-in-plane-rd	0.01
		529	1307.98	δCCN + vCC + δCNC	0.01
		528	1308.48	δCCN + vCC + δCNC + a-in-plane-rd	0.00
		527	1308.83	δCCN + vCC + δCNC + τCH2	0.03
		526	1309.18	δCCN + vCC + δCNC + τCH2	0.06
		525	1309.48	δCCN + vCC + δCNC	0.00
		524	1309.78	δCCN + vCC + δCNC	0.01
		523	1309.87	vCC + δCNC + τCH2 + a-in-plane-rd	0.66
		522	1310.41	vCC + δCNC + τCH2 + a-in-plane-rd	0.00
		521	1311.16	δCCN + δCNC + τCH2+ a-in-plane-rd	0.00
1323	1317	520	1317.23	δCCN + δCNC + τCH2	0.00
		519	1317.34	δCCN + δCNC + τCH2	0.00
		518	1318.27	δCCN + δCNC + τCH2	0.07
		517	1318.53	vCC+ δCNC + τCH2	0.42

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		516	1319.08	νCC + τCH2 + δCNC	0.44
		515	1319.33	νCC + ωCH2 + δCNC	0.02
		514	1319.64	δCCN + δCNC + ωCH2	2.11
		513	1320.25	νCC + ωCH2+ δCNC	0.01
		496	1347.01	ωCH2 + δCNC + νCC+ a-in-plane-rd	0.35
		495	1347.42	ωCH2 + δCNC + νCC+ a-in-plane-rd	0.07
		494	1347.47	ωCH2 + δCNC + νCC+ a-in-plane-rd	0.00
		493	1347.72	ωCH2 + δCNC + νCC	0.61
		492	1348.13	ωCH2 + δCNC + νCC	0.07
		491	1348.24	δCNC + νCC + ωCH2	0.01
		490	1348.43	ωCH2 + νCC + δCNC + a-in-plane-rd	0.02
		489	1348.97	νCC + ωCH2 + δCNC + a-in-plane-rd	0.00
	1348	488	1351.27	ωCH2 + νCC + δCNC + a-in-plane-rd	0.00
		487	1351.57	ωCH2 + νCC + δCNC + a-in-plane-rd	0.00
		486	1351.72	ωCH2 + νCC + δCNC + a-in-plane-rd	0.00
		485	1351.81	ωCH2 + νCC + δCNC + a-in-plane-rd	0.01
		484	1352.75	ωCH2 + νCC + δCNC + a-in-plane-rd	0.09
		483	1353.00	ωCH2 + νCC + νCN + a-in-plane-rd	0.01
		482	1353.35	ωCH2 + νCC + νCN + a-in-plane-rd	0.22
		481	1353.52	ωCH2 + a-in-plane-rd+ νCC + νCN	0.03
		480	1363.81	a-in-plane-rd + δCCN	0.00
		479	1363.88	a-in-plane-rd + δCCN	0.09
		478	1363.90	a-in-plane-rd + δCCN	0.71
		477	1364.00	a-in-plane-rd + δCCN	0.46
		476	1364.09	a-in-plane-rd + νCC + νCN	0.94
		475	1364.28	a-in-plane-rd + δCCN	0.19
		474	1364.31	a-in-plane-rd + νCC + δCCN	0.39
1355		473	1364.35	a-in-plane-rd + δCCN	0.25
		472	1364.52	a-in-plane-rd + δCCN	1.15
		471	1364.63	a-in-plane-rd + νCC + νCN	0.11
		470	1364.70	a-in-plane-rd + νCC	0.18
		469	1364.82	a-in-plane-rd + νCC	1.52
		468	1364.87	a-in-plane-rd + νCC + νCN	0.11
		467	1364.89	a-in-plane-rd + νCC + δCCN	0.07
		466	1364.94	a-in-plane-rd + νCC + δCCN	0.41
	1365	465	1364.96	a-in-plane-rd + δCCN	0.34
		464	1365.11	a-in-plane-rd + νCC + δCCN	0.01
		463	1365.28	a-in-plane-rd + δCCN	0.02
		462	1365.36	a-in-plane-rd + δCCN	0.21
		461	1365.39	a-in-plane-rd + δCCN	0.03
		460	1366.42	a-in-plane-rd + δCCN	0.65
		459	1366.61	a-in-plane-rd + δCCN	0.00
		458	1366.62	a-in-plane-rd + νCC + νCN	0.01
		457	1366.70	a-in-plane-rd + νCC + νCN	0.01
		456	1367.20	a-in-plane-rd + νCC + νCN	0.28
		455	1367.37	a-in-plane-rd + νCC + νCN	0.09
		454	1367.55	a-in-plane-rd + νCC + νCN	0.00
		453	1367.66	a-in-plane-rd + νCC + νCN	0.00
		452	1368.56	a-in-plane-rd + νCC + δCCN	0.00
		451	1368.70	a-in-plane-rd + νCC + δCCN	0.00
		450	1368.88	a-in-plane-rd + νCC + δCCN	0.02

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		449	1368.99	a-in-plane-rd + vCC + δCCN	0.06
1421	1418	448	1410.86	a-in-plane-rd + δCCN	0.77
		447	1411.30	a-in-plane-rd + δCCN	0.03
		446	1411.55	a-in-plane-rd + δCCN	0.08
		445	1411.70	δCCN + a-in-plane-rd	0.05
		444	1411.89	a-in-plane-rd + δCCN	0.00
		443	1412.12	a-in-plane-rd + δCCN	0.00
		442	1412.46	δCCN + a-in-plane-rd + vCO	0.00
		441	1412.53	a-in-plane-rd + δCCN	0.00
		440	1413.06	a-in-plane-rd + δCCN + sci-CH2	0.00
		439	1413.50	a-in-plane-rd + δCCN + sci-CH2	0.22
		438	1413.66	a-in-plane-rd + δCCN + sci-CH2	0.00
		437	1414.08	a-in-plane-rd + δCCN + sci-CH2	0.49
		436	1414.19	a-in-plane-rd + δCCN + vCO	0.02
		435	1414.23	a-in-plane-rd + δCCN + vCN	1.72
		434	1414.93	a-in-plane-rd + δCCN + vCO	0.02
		433	1415.14	a-in-plane-rd + δCCN + vCO	0.00
		432	1415.15	a-in-plane-rd + δCCN + vCO	0.00
		431	1415.80	a-in-plane-rd + δCCN	0.18
		430	1415.83	a-in-plane-rd + δCCN	0.04
		429	1416.15	a-in-plane-rd + δCCN	0.00
		428	1417.08	a-in-plane-rd + δCCN	0.00
		427	1417.49	a-in-plane-rd + δCCN	0.02
		426	1417.64	a-in-plane-rd + δCCN	0.00
		425	1417.68	a-in-plane-rd + δCCN	0.00
		424	1417.74	a-in-plane-rd + δCCN	0.00
		423	1418.21	a-in-plane-rd + δCCN	4.44
		422	1418.33	a-in-plane-rd + δCCN	0.06
		421	1418.40	a-in-plane-rd + δCCN	0.03
		420	1418.42	δCCN + a-in-plane-rd	0.01
		419	1418.44	δCCN + a-in-plane-rd	0.01
		418	1419.31	δCCN + a-in-plane-rd	0.05
		417	1419.38	sci-CH2 + δCCN + a-in-plane-rd	0.01
		416	1422.10	sci-CH2 + δCCN + a-in-plane-rd	0.01
		415	1422.21	sci-CH2 + δCCN + a-in-plane-rd	0.00
		414	1422.95	sci-CH2 + δCCN + a-in-plane-rd	0.08
		413	1422.99	sci-CH2 + δCCN + a-in-plane-rd	0.10
		412	1423.11	sci-CH2 + δCCN + a-in-plane-rd	0.29
		411	1423.31	sci-CH2 + δCCN + a-in-plane-rd	0.41
		410	1423.63	sci-CH2 + δCCN + a-in-plane-rd	0.42
		409	1423.72	sci-CH2 + δCCN + a-in-plane-rd	0.00
		408	1426.90	sci-CH2 + δCCN + a-in-plane-rd	0.07
		407	1426.98	sci-CH2 + δCCN + a-in-plane-rd	0.04
		406	1427.20	sci-CH2 + δCCN + a-in-plane-rd	0.05
		405	1427.56	sci-CH2 + δCCN + a-in-plane-rd	0.03
		404	1427.75	sci-CH2 + δCCN + a-in-plane-rd	0.04
		403	1427.85	sci-CH2 + δCCN + a-in-plane-rd	0.05
		402	1427.93	sci-CH2 + δCCN + a-in-plane-rd	0.02
		401	1428.30	sci-CH2 + δCCN + a-in-plane-rd	0.02
1434	1436	400	1436.24	sci-CH2 + δCCN + a-in-plane-rd	0.48
		399	1436.47	sci-CH2 + δCCN + a-in-plane-rd	0.96

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		398	1437.67	sci-CH2 + δCCN + a-in-plane-rd	0.03
		397	1437.78	sci-CH2 + δCCN + a-in-plane-rd	0.08
1477	1472	396	1462.51	sci-CH2 + δCCN	0.00
		395	1462.63	sci-CH2 + δCCN + a-in-plane-rd	0.00
		394	1463.19	sci-CH2 + δCCN + a-in-plane-rd	0.00
		393	1463.39	sci-CH2 + δCCN + a-in-plane-rd	0.00
		392	1468.86	sci-CH2 + δCCN + a-in-plane-rd	0.11
		391	1469.22	sci-CH2 + δCCN + a-in-plane-rd	0.13
		390	1469.41	sci-CH2 + δCCN + a-in-plane-rd	0.29
		389	1469.52	sci-CH2 + δCCN + a-in-plane-rd	0.13
		388	1469.81	sci-CH2 + δCCN + a-in-plane-rd	0.01
		387	1469.84	sci-CH2 + δCCN + a-in-plane-rd	0.11
		386	1470.12	sci-CH2 + δCCN	0.00
		385	1470.33	a-in-plane-rd + vCC + vCN	0.00
		384	1470.40	a-in-plane-rd + vCC + vCN	0.00
		383	1470.44	a-in-plane-rd + vCC + vCN	0.01
		382	1470.54	a-in-plane-rd + vCC + vCN	0.06
		381	1470.68	a-in-plane-rd + vCC + vCN	0.00
		380	1471.90	a-in-plane-rd + vCC + vCN	0.03
		379	1472.18	a-in-plane-rd + vCC + vCN	0.26
		378	1472.42	a-in-plane-rd + vCC + vCN	0.05
		377	1472.44	vCC + a-in-plane-rd + vCN	0.04
		376	1472.47	a-in-plane-rd + vCC + vCN	0.04
		375	1472.53	vCC + a-in-plane-rd + vCN	0.12
		374	1472.67	vCC + a-in-plane-rd + vCN	1.17
		373	1472.79	vCC + a-in-plane-rd + vCN	0.01
		372	1472.98	vCC + s-in-plane-rd + vCN	1.55
		371	1473.04	vCC + a-in-plane-rd + vCN	0.04
		370	1473.17	vCC + s-in-plane-rd + vCN	0.01
		369	1473.35	vCC + s-in-plane-rd + vCN	0.01
1501	1505	368	1505.02	vCC + s-in-plane-rd + vCN	0.36
		367	1505.03	vCC + s-in-plane-rd	1.07
		366	1505.16	vCC + s-in-plane-rd	0.45
		365	1505.21	vCC + s-in-plane-rd	0.37
		364	1505.28	vCC + s-in-plane-rd	0.02
		363	1505.33	vCC + s-in-plane-rd	0.05
		362	1505.57	vCC + s-in-plane-rd	0.00
		361	1505.62	vCC + a-in-plane-rd	0.00
1512	1510	360	1509.06	vCC + a-in-plane-rd + vCN	0.00
		359	1509.11	vCC + a-in-plane-rd	0.00
		358	1509.34	a-in-plane-rd + vCC	0.00
		357	1509.42	vCC + a-in-plane-rd	0.28
1523		356	1510.90	vCC + a-in-plane-rd	0.00
		355	1510.99	a-in-plane-rd + vCC	0.00
		354	1511.16	a-in-plane-rd + vCC	0.30
		353	1511.27	a-in-plane-rd + vCC	0.09
1530	1521	352	1520.34	vCN + δCNH + vCC + vNC	4.25
		351	1520.40	vCC + vCN + δCNH + vNC	1.92
		350	1520.95	vCN + vCC + δCNH + vNC	18.50
		349	1520.99	vCN + vCC + δCNH + vNC	24.62
		348	1521.05	vCN + δCNH + vNC + vCC	6.25

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		347	1521.11	vCN + vCC + δCNH + vNC	10.98
		346	1521.32	vCN + vCC + δCNH + vNC	0.85
		345	1521.47	vCN + vCC + δCNH + vNC	5.67
		344	1521.77	vCC + vCN + δCNH + vNC	0.38
		343	1521.95	vCN + vCC + δCNH + vNC	3.71
		342	1521.98	vCN + vCC + vNC + δCNH	3.80
		341	1522.42	vCN + vCC + vNC + δCNH	0.19
		340	1522.74	vCN + δCCN + δCNH	0.12
		339	1523.41	vCN + vCC + vNC + δCNH	0.00
		338	1523.71	vCN + vCC + vNC + δCNH	0.08
		337	1525.57	vCN + vCC + vNC + δCNH	0.92
1535	1528	336	1527.66	vCN + vCC + vNC + δCNH	9.91
		335	1527.91	vCN + vCC + vNC + δCNH	0.25
		334	1528.95	vCN + vCC + vNC + δCNH	16.62
		333	1529.21	vCN + vCC	0.05
		332	1529.71	vCN + vCC + vNC + δCNH	0.01
		331	1529.84	vCC + vCN + vNC + δCNH	0.43
		330	1529.93	vCC + vCN + vNC + δCNH	0.12
		329	1530.76	vCN + vCC + vNC + δCNH	0.02
		328	1532.71	vCN + vCC + vNC + δCNH	0.00
		327	1533.11	vCN + vNC + δCNH	0.00
		326	1533.43	vCN + vNC+ δCNH	0.02
		325	1533.88	vCN + vNC+ δCNH	0.11
1546	1537	324	1537.19	vCN + vNC+ δCNH	12.91
		323	1537.69	vCN + vNC+ δCNH	0.19
		322	1538.05	vCN + vNC+ δCNH	0.02
		321	1540.77	vCN + vNC+ δCNH	0.04
1579	1574	320	1569.41	vCC + a-in-plane-rd + δCCN	0.00
		319	1569.77	vCC + a-in-plane-rd + δCCN	0.02
		318	1569.86	vCC + s-in-plane-rd + δCCN	0.12
		317	1569.96	vCC + s-in-plane-rd + δCCN	0.01
		316	1570.11	vCC + s-in-plane-rd + vCO + δCCN	0.00
		315	1570.20	vCC + a-in-plane-rd + vCO + δCCN	0.00
		314	1570.27	vCC + a-in-plane-rd + vCO + δCCN	0.00
		313	1570.32	vCC + a-in-plane-rd + vCO + δCCN	0.02
		312	1572.84	vCC + a-in-plane-rd + vCO + δCCN	2.11
		311	1573.04	vCC + s-in-plane-rd + vCO + δCCN	1.11
		310	1573.23	vCC + s-in-plane-rd + vCO + δCCN	0.01
		309	1573.40	vCC + vCO + δCCN + a-in-plane-rd	0.03
		308	1573.50	vCC + vCO + δCCN + s-in-plane-rd	1.17
		307	1573.57	vCC + vCO + δCCN + s-in-plane-rd	5.53
		306	1573.69	vCC + vCO + δCCN + s-in-plane-rd	0.17
		305	1574.00	vCC + vCO + δCCN + s-in-plane-rd	0.37
		304	1574.76	vCC + vCO + δCCN + a-in-plane-rd	4.43
		303	1575.05	vCC + s-in-plane-rd + vCO	0.03
		302	1575.16	vCC + δCCN + in-plane-rd	3.86
		301	1575.43	vCC + δCCN + in-plane-rd	0.01
		300	1575.66	vCC+ vCO + δCCN + s-in-plane-rd	0.92
		299	1575.86	vCC+ vCO + δCCN + a-in-plane-rd	0.00
		298	1576.02	vCC+ a-in-plane-rd + vCO + δCCN	0.53
		297	1576.27	vCC + δCNC + a-in-plane-rd	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		296	1578.92	a-in-plane-rd	0.01
		295	1579.11	a-in-plane-rd + s-in-plane-rd	0.01
		294	1579.21	a-in-plane-rd + s-in-plane-rd	0.02
		293	1579.35	a-in-plane-rd	0.04
		292	1579.47	a-in-plane-rd	0.00
		291	1579.66	a-in-plane-rd	0.00
		290	1579.77	a-in-plane-rd	0.00
		289	1579.89	a-in-plane-rd	0.00
1602	1592	288	1591.64	vCC + vCO + δCNC + a-in-plane-rd	0.00
		287	1592.01	vCC + vCO + δCNC + a-in-plane-rd	0.00
		286	1592.17	vCC + vCO + δCNC + a-in-plane-rd	0.02
		285	1592.25	vCO + vCC + δCCN + a-in-plane-rd	0.02
		284	1592.61	vCO + vCC + δCCN + a-in-plane-rd	2.24
		283	1592.64	vCO + vCC + δCCN + a-in-plane-rd	1.74
		282	1592.95	vCO + s-in-plane-rd + vCC + δCCN	1.36
		281	1593.04	vCC +vCO + s-in-plane-rd+ vCN + δCCN	2.99
	1598	280	1596.90	a-in-plane-rd+ vCO	0.00
		279	1597.08	vCC + s-in-plane-rd + vCO + δCNC	0.18
		278	1597.16	a-in-plane-rd + vCC + vCO + δCNC	0.01
		277	1597.24	a-in-plane-rd	0.13
		276	1597.49	vCC + vCO + δCNC + a-in-plane-rd	0.00
		275	1597.75	vCC + vCO + a-in-plane-rd	0.12
		274	1597.93	vCC + a-in-plane-rd	5.21
		273	1598.19	vCO + vCN + vCC +δCCN + a-in-plane-rd	1.30
1630	1607	272	1607.73	vCO + vCN + vCC +δCCN + a-in-plane-rd	6.37
		271	1608.04	vCO + vCN + vCC +δCCN + a-in-plane-rd	100.00
		270	1609.20	vCO + vCN + vCC +δCCN + s-in-plane-rd	0.12
		269	1609.26	vCO + vCN + vCC + δCCN + s-in-plane-rd	0.01
		268	1609.36	s-in-plane-rd + a-in-plane-rd + vCO + δCCN	0.03
		267	1609.42	s-in-plane-rd + a-in-plane-rd	6.51
		266	1609.46	s-in-plane-rd + a-in-plane-rd	0.08
		265	1609.88	s-in-plane-rd + a-in-plane-rd	0.02
		264	1609.96	s-in-plane-rd	0.14
		263	1610.10	s-in-plane-rd	0.02
		262	1610.25	s-in-plane-rd	3.90
		261	1610.40	vCC + vCN + δCCN + s-in-plane-rd	0.01
		260	1610.72	vCO + vCN + vCC + δCCN + s-in-plane-rd	0.01
		259	1611.44	vCO + vCC + vCN + δCCN + a-in-plane-rd	0.00
		258	1611.45	vCO + vCC + vCN + δCCN + a-in-plane-rd	0.02
		257	1612.20	vCO + vCC + vCN + δCCN + a-in-plane-rd	0.25
		256	1612.37	vCO + vCC + vCN + δCCN + s-in-plane-rd	16.72
		255	1612.78	vCO + vCC + vCN + δCCN + a-in-plane-rd	0.00
1642	1616	254	1613.85	s-in-plane-rd + vCC + vCN+ vCO	0.01
		253	1613.94	s-in-plane-rd + vCC + vCN+ vCO	5.96
		252	1614.05	s-in-plane-rd + vCO + vCC + vCN+ δCCN	0.02
		251	1615.03	s-in-plane-rd + vCO + vCC + vCN+ δCCN	0.00
		250	1615.48	s-in-plane-rd + vCO + vCC + vCN+ δCCN	0.02
		249	1615.88	s-in-plane-rd	0.36
		248	1616.42	vCO + vCC + vCN + δCCN + a-in-plane-rd	40.10
		247	1617.00	vCO + vCC + vCN + δCCN + s-in-plane-rd	0.01
		246	1617.06	vCO + vCC + vCN + δCCN + a-in-plane-rd	0.05

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		245	1617.62	vCO + vCC + vCN + δCCN + a-in-plane-rd	41.26
		244	1618.86	vCO + vCC + vCN + δCCN + a-in-plane-rd	0.00
		243	1619.57	vCO + vCC + vCN + δCCN + s-in-plane-rd	0.01
		242	1619.78	vCO + vCC + vCN + δCCN + s-in-plane-rd	0.00
		241	1621.39	vCO + vCN + vCC + δCCN + s-in-plane-rd	16.18
		240	1623.46	vCO + vCN + vCC + δCCN + s-in-plane-rd	0.02
		239	1623.61	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.04
		238	1623.78	vCO + vCN + vCC + δCCN + a-in-plane-rd	1.13
		237	1624.00	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.00
		236	1625.29	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.03
		235	1625.45	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.00
		234	1626.05	vCO + vCN + vCC + δCCN + a-in-plane-rd	5.54
		233	1626.54	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.00
1661	1640	232	1634.36	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.00
		231	1635.70	vCO + vCN + vCC + δCCN + a-in-plane-rd	2.59
		230	1635.84	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.05
		229	1638.14	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.02
		228	1638.63	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.12
		227	1638.72	vCO + vCN + vCC + δCCN + a-in-plane-rd	0.00
		226	1639.99	vCO + vCN + vCC + δCCN + a-in-plane-rd	47.70
		225	1640.53	vCO + vCN + vCC + δCCN + a-in-plane-rd	5.66
		224	2961.96	s-vCH2 + δCCN + vCC + vCN	0.09
		223	2962.06	s-vCH2 + δCCN + vCC + vCN	0.11
		222	2963.48	s-vCH2 + δCCN + vCC + vCN	0.03
		221	2964.28	s-vCH2	0.09
		220	2964.80	s-vCH2	0.21
		219	2965.72	s-vCH2 + δCCN	0.13
		218	2967.88	s-vCH2 + δCCN + vCC + vCN	0.01
2793	2964	217	2968.13	s-vCH2 + δCCN + vCC + vCN	0.14
		216	2968.29	s-vCH2 + δCCN + vCC + vCN	0.01
		215	2969.91	s-vCH2 + δCCN + vCC + vCN	0.01
		214	2970.10	s-vCH2 + δCCN + vCC + vCN	0.04
		213	2970.45	s-vCH2 + δCCN + vCC + vCN	0.10
		212	2970.71	s-vCH2 + δCCN + vCC + vCN	0.00
		211	2970.90	s-vCH2 + δCCN + vCC + vCN	0.01
		210	2970.94	s-vCH2 + δCCN + vCC + vCN	0.01
		209	2971.23	s-vCH2 + δCCN + vCC + vCN	0.01
		208	2989.47	s-vCH2 + δCCN + vCC + vCN	0.18
		207	2990.10	s-vCH2 + δCCN + vCC + vCN	0.12
		206	2991.22	s-vCH2 + δCCN + vCC + vCN	0.11
		205	2991.37	s-vCH2 + δCCN + vCC + vCN	0.19
2850	2991	204	2992.56	s-vCH2 + δCCN + vCC + vCN	0.11
		203	2992.86	s-vCH2 + δCCN + vCC + vCN	0.06
		202	2995.23	s-vCH2 + δCCN + vCC + vCN	0.08
		201	2996.63	s-vCH2 + δCCN + vCN + vCC	0.08
		200	3007.71	a-vCH2 + δCCN + vCN + vCC	0.12
		199	3007.85	a-vCH2 + δCCN + vCN + vCC	0.00
		198	3008.01	a-vCH2 + δCCN + vCN + vCC	0.25
2872	3008	197	3008.55	a-vCH2 + δCCN + vCN + vCC	0.03
		196	3008.69	a-vCH2 + δCCN + vCN + vCC	0.19
		195	3008.74	a-vCH2 + δCCN + vCN + vCC	0.03

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		194	3008.93	a-νCH2 + δCCN + νCN + νCC	0.00
		193	3009.58	a-νCH2 + δCCN + νCN + νCC	0.10
		192	3009.92	s-νCH2 + δCCN + νCN + νCC	0.04
		191	3009.99	s-νCH2 + δCCN + νCN + νCC	0.03
		190	3010.75	s-νCH2 + δCCN + νCN + νCC	0.06
		189	3010.79	s-νCH2 + δCCN + νCN + νCC	0.06
		188	3012.12	s-νCH2 + δCCN + νCN + νCC	0.03
		187	3012.62	s-νCH2 + δCCN + νCN + νCC	0.05
		186	3012.86	s-νCH2 + δCCN + νCN + νCC	0.04
		185	3013.66	s-νCH2 + δCCN + νCN + νCC	0.04
2919	3042	184	3041.27	a-νCH2 + δCCN + νCN + νCC	0.00
		183	3041.44	a-νCH2 + δCCN + νCN	0.01
		182	3041.69	a-νCH2 + δCCN + νCN + νNH	0.01
		181	3042.17	a-νCH2 + δCCN + νCN + νNH	0.01
		180	3042.21	a-νCH2 + δCCN + νCN + νCC	0.01
		179	3042.38	a-νCH2 + δCCN	0.01
		178	3042.47	a-νCH2 + δCCN + νCN	0.00
		177	3042.54	a-νCH2 + δCCN + νCN + νCC	0.01
2931	3051	176	3050.43	a-νCH2 + δCCN + νCN + νCC	0.05
		175	3050.71	a-νCH2 + δCCN + νCN + νCC	0.05
		174	3050.98	a-νCH2 + δCCN + νCN + νCC	0.05
		173	3050.98	a-νCH2 + δCCN + νCN + νCC	0.02
		172	3051.08	a-νCH2 + δCCN + νCN + νCC	0.07
		171	3051.11	a-νCH2 + δCCN + νCN + νCC	0.04
		170	3051.79	a-νCH2 + δCCN + νCN + νCC	0.05
		169	3052.50	a-νCH2 + δCCN + νCN + νCC	0.05
2954	3065	168	3064.58	a-νCH2 + δCCN + νCN + νCC	0.03
		167	3064.74	a-νCH2 + δCCN + νCN + νCC	0.03
		166	3065.07	a-νCH2 + δCCN + νCN + νCC	0.03
		165	3065.17	a-νCH2 + δCCN + νCN + νCC	0.02
		164	3065.29	a-νCH2 + δCCN + νCN + νCC	0.02
		163	3065.42	a-νCH2 + δCCN + νCN	0.04
		162	3065.54	a-νCH2 + δCCN + νCN	0.02
		161	3065.68	a-νCH2 + νCN	0.02
3009	3098	160	3095.54	a-r-νCH + a-in-plane-rd	0.01
		159	3095.77	a-r-νCH + a-in-plane-rd	0.00
		158	3095.88	a-r-νCH + a-in-plane-rd	0.00
		157	3095.99	a-r-νCH + a-in-plane-rd	0.04
		156	3096.52	a-r-νCH + a-in-plane-rd	0.11
		155	3096.59	a-r-νCH + a-in-plane-rd	0.05
		154	3096.65	a-r-νCH + a-in-plane-rd	0.01
		153	3096.73	a-r-νCH + a-in-plane-rd	0.00
		152	3097.60	a-r-νCH + a-in-plane-rd	0.17
		151	3097.64	a-r-νCH + a-in-plane-rd	0.00
		150	3097.67	a-r-νCH + a-in-plane-rd	0.02
		149	3097.70	a-r-νCH + a-in-plane-rd	0.10
		148	3097.73	a-r-νCH + a-in-plane-rd	0.15
		147	3097.79	a-r-νCH + a-in-plane-rd	0.05
		146	3097.80	a-r-νCH + a-in-plane-rd	0.37
		145	3097.84	a-r-νCH + a-in-plane-rd	0.11
		144	3097.85	a-r-νCH + a-in-plane-rd	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		143	3097.95	s-r-vCH + s-in-plane-rd	0.01
		142	3098.22	a-r-vCH + a-in-plane-rd	0.06
		141	3098.24	a-r-vCH + a-in-plane-rd	0.02
		140	3098.57	a-r-vCH + a-in-plane-rd	0.06
		139	3098.73	a-r-vCH + a-in-plane-rd	0.22
		138	3098.78	a-r-vCH + a-in-plane-rd	0.00
		137	3098.89	a-r-vCH + a-in-plane-rd	0.00
		136	3104.21	a-r-vCH + a-in-plane-rd	0.06
		135	3104.38	a-r-vCH + a-in-plane-rd	0.02
		134	3104.81	a-r-vCH + a-in-plane-rd	0.02
		133	3104.89	r-vCH + in-plane-rd	0.18
		132	3105.07	r-vCH + in-plane-rd	0.42
		131	3105.21	r-vCH + in-plane-rd	0.03
		130	3105.45	r-vCH + in-plane-rd	0.00
3014	3104	129	3105.56	r-vCH + in-plane-rd	0.08
		128	3108.16	r-vCH + in-plane-rd	0.01
		127	3108.31	r-vCH + in-plane-rd	0.00
		126	3108.56	r-vCH + in-plane-rd	0.02
		125	3108.62	r-vCH + in-plane-rd	0.01
		124	3108.75	r-vCH + in-plane-rd	0.01
		123	3108.76	r-vCH + in-plane-rd	0.00
		122	3108.93	r-vCH + in-plane-rd	0.01
		121	3109.16	r-vCH + in-plane-rd	0.01
		120	3113.46	r-vCH + in-plane-rd	0.01
		119	3113.90	r-vCH + in-plane-rd	0.00
		118	3114.06	r-vCH + in-plane-rd	0.02
		117	3114.31	r-vCH	0.00
		116	3114.60	r-vCH	0.01
		115	3114.88	r-vCH + in-plane-rd	0.00
		114	3115.01	r-vCH + in-plane-rd	0.02
3026	3119	113	3115.32	r-vCH + in-plane-rd	0.00
		112	3118.16	r-vCH + in-plane-rd	0.02
		111	3118.24	r-vCH + in-plane-rd	0.04
		110	3118.49	r-vCH + in-plane-rd	0.01
		109	3118.59	r-vCH + in-plane-rd	0.07
		108	3118.61	r-vCH + in-plane-rd	0.00
		107	3118.64	r-vCH + in-plane-rd	0.20
		106	3118.97	r-vCH + in-plane-rd	0.02
		105	3119.07	r-vCH + in-plane-rd	0.07
		104	3122.32	r-vCH + in-plane-rd	0.02
		103	3122.62	r-vCH + in-plane-rd	0.01
		102	3122.80	r-vCH + in-plane-rd	0.04
		101	3123.16	r-vCH + in-plane-rd	0.01
		100	3123.19	r-vCH + in-plane-rd	0.00
3036	3122	99	3123.29	r-vCH + in-plane-rd	0.05
		98	3123.36	r-vCH + in-plane-rd	0.00
		97	3123.52	r-vCH + in-plane-rd	0.00
		96	3123.67	r-vCH + in-plane-rd	0.10
		95	3123.70	r-vCH + in-plane-rd	0.00
		94	3123.78	r-vCH + in-plane-rd	0.00
		93	3123.89	r-vCH + in-plane-rd	0.02

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		92	3123.96	r-vCH + in-plane-rd	0.00
		91	3124.25	r-vCH + in-plane-rd	0.01
		90	3124.30	r-vCH + in-plane-rd	0.03
		89	3124.39	r-vCH + in-plane-rd	0.00
3049	3130	88	3129.45	r-vCH + in-plane-rd	0.03
		87	3129.72	r-vCH + in-plane-rd	0.01
		86	3130.37	r-vCH + in-plane-rd	0.01
		85	3130.50	r-vCH + in-plane-rd	0.05
		84	3130.67	r-vCH + in-plane-rd	0.02
		83	3130.77	s-r-vCH + in-plane-rd	0.01
		82	3131.43	r-vCH + in-plane-rd	0.02
		81	3131.58	r-vCH + in-plane-rd	0.10
3057	3139	80	3137.35	r-vCH + in-plane-rd	0.02
		79	3137.53	s-r-vCH + in-plane-rd	0.00
		78	3137.78	r-vCH + in-plane-rd	0.00
		77	3137.86	r-vCH + in-plane-rd	0.04
		76	3138.03	r-vCH + in-plane-rd	0.00
		75	3138.14	s-r-vCH + in-plane-rd	0.01
		74	3138.34	r-vCH + in-plane-rd	0.02
		73	3138.73	r-vCH + in-plane-rd	0.01
		72	3139.62	r-vCH + in-plane-rd	0.03
		71	3139.75	r-vCH + in-plane-rd	0.00
		70	3139.83	r-vCH + in-plane-rd	0.03
		69	3139.89	r-vCH + in-plane-rd	0.00
		68	3140.48	r-vCH + in-plane-rd	0.02
		67	3140.67	r-vCH + in-plane-rd	0.02
		66	3140.68	r-vCH + in-plane-rd	0.01
		65	3140.86	r-vCH + in-plane-rd	0.00
3069	3146	64	3145.98	s-r-vCH + in-plane-rd	0.06
		63	3146.05	s-r-vCH + in-plane-rd	0.00
		62	3146.09	a-r-vCH + in-plane-rd	0.01
		61	3146.13	s-r-vCH + in-plane-rd	0.00
		60	3146.26	s-r-vCH + s-in-plane-rd	0.00
		59	3146.35	s-r-vCH + s-in-plane-rd	0.00
		58	3146.38	r-vCH + in-plane-rd	0.00
		57	3146.50	r-vCH + in-plane-rd	0.03
		56	3146.56	r-vCH + in-plane-rd	0.03
		55	3146.59	r-vCH + in-plane-rd	0.03
		54	3146.71	r-vCH + in-plane-rd	0.01
		53	3146.72	r-vCH + in-plane-rd	0.02
		52	3146.80	r-vCH + in-plane-rd	0.01
		51	3146.89	r-vCH + in-plane-rd	0.01
		50	3147.07	r-vCH + in-plane-rd	0.01
		49	3147.15	r-vCH + in-plane-rd	0.01
		48	3149.77	r-vCH + in-plane-rd	0.01
		47	3149.81	r-vCH + in-plane-rd	0.03
		46	3149.94	r-vCH + in-plane-rd	0.02
		45	3149.99	r-vCH + in-plane-rd	0.01
		44	3150.63	r-vCH + in-plane-rd	0.01
		43	3150.65	r-vCH + in-plane-rd	0.01
		42	3150.81	r-vCH + in-plane-rd	0.00

Table S2

Peaks (cm^{-1})		Mode	ν_n	Description	IR activity
(exp.)	(calc.)		(cm^{-1})		(%)
		41	3150.86	r-νCH + in-plane-rd	0.00
		40	3169.45	r-νCH + in-plane-rd	0.04
		39	3169.52	r-νCH + in-plane-rd	0.00
		38	3169.94	r-νCH + in-plane-rd	0.00
		37	3169.98	r-νCH + in-plane-rd	0.00
3082	3170	36	3170.48	r-νCH + in-plane-rd	0.00
		35	3170.52	r-νCH + in-plane-rd	0.04
		34	3170.69	r-νCH + in-plane-rd	0.02
		33	3170.77	r-νCH + in-plane-rd	0.01
3295	3309	32	3309.01	νNH + νCN + δCNC	0.92
		31	3309.10	νNH + νCN + δCNC	0.34
		30	3309.18	νNH + δCNC	21.74
		29	3309.25	νNH + δCNC + νOH*	0.45
		28	3309.82	νNH + δCNC	0.01
		27	3310.30	νNH + δCNC + νOH*	1.12
		26	3310.71	νNH + δCNC + νOH*	0.02
		25	3311.25	νNH + δCNC	8.03
3325	3339	24	3339.38	νNH + δCNC	0.13
		23	3339.49	νNH + δCNC + νOH*	0.12
		22	3339.98	νNH + δCNC + νOH*	1.40
		21	3340.20	νNH + δCNC	0.01
		20	3340.28	νNH + νCN + δCNC + νOH*	4.00
		19	3340.32	νNH + δCNC + νOH*	12.24
		18	3340.40	νNH + δCNC	0.95
		17	3341.20	νNH + δCNC + νOH*	0.42
3363	3352	16	3350.90	νNH + δCNC + νOH*	1.79
		15	3351.11	νNH + δCNC + νOH*	0.74
		14	3351.24	νNH + δCNC + νOH*	2.24
		13	3351.32	νNH + δCNC + νOH*	4.99
		12	3351.42	νNH + δCNC	0.08
		11	3351.50	νNH + δCNC + νOH*	0.14
		10	3351.66	νNH + δCNC + νOH*	0.43
		9	3353.11	νNH + δCNC	8.13
3426	3410	8	3409.74	νNH + δCNC	5.27
		7	3409.77	νNH + δCNC	0.65
		6	3409.85	νNH + δCNC + νOH*	0.14
		5	3410.17	νNH + νCN + δCNC + νOH*	5.22
		4	3410.33	νNH + δCNC	0.02
		3	3410.50	νNH + δCNC	0.39
		2	3410.74	νNH + νCN + δCNC + νOH*	0.42
		1	3411.53	νNH + νCN + δCNC + νOH*	0.81