

Supporting Information for:
Vibrational States and Nitrile Lifetimes of Cyanophenylalanine
Isotopomers in Solution

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Vibrational frequencies of isotopomers (units cm⁻¹)

Mode	Molecule 1 (¹² C ¹⁴ N)	Molecule 2 (¹² C ¹⁵ N)	Molecule 3 (¹³ C ¹⁴ N)	Molecule 4 (¹³ C ¹⁵ N)
1	3444	3444.15	3443.95	3444.08
2	3382.13	3382.28	3382.09	3382.2
3	2811.96	2810.53	2812.42	2811.89
4	3082.77	3082.95	3082.81	3082.76
5	3095.82	3095.82	3095.82	3095.77
6	3052.27	3052.83	3052.54	3052.26
7	3069.05	3069.1	3069.11	3069.07
8	2979.02	2979.01	2979.79	2979.02
9	2942.62	2942.67	2942.55	2942.57
10	2947.9	2948.12	2947.66	2947.9
11	2283.97	2257.26	2232.24	2202.56
12	1741.84	1741.51	1742.88	1743.49
13	1610.44	1611.12	1610.98	1610.43
14	1669.71	1670.43	1669.71	1669.47
15	1569.79	1572.61	1571.56	1570.83
16	1507.97	1509.43	1507.76	1507.25
17	1506.61	1506.99	1506.26	1506.61
18	1433.11	1432.79	1432.47	1432.17
19	1337.55	1337.12	1336.75	1336.33
20	1370.99	1370.59	1370.19	1369.6

21	1357.51	1356.74	1356.21	1355.7
22	1343.9	1343.94	1343.92	1343.54
23	1309.12	1308.09	1306.77	1306.13
24	1292.46	1293.36	1292.21	1293.14
25	1220.93	1220.39	1219.53	1219.71
26	1203.8	1201.86	1202.93	1201.24
27	1185.26	1181.73	1182.66	1180.61
28	1216.47	1220.16	1215.63	1218.92
29	1183.78	1181.96	1183.81	1180.25
30	1168.11	1167.92	1167.63	1167.42
31	1137.98	1137.5	1138.01	1139.04
32	1060.58	1060.27	1060.22	1059.96
33	1020.38	1021.83	1019.79	1020.86
34	983.32	983.13	982.69	982.43
35	972.95	972.96	972.83	972.96
36	967.86	967.42	967.08	967.61
37	960.33	962.35	961.68	961.27
38	842.18	842.44	841.48	841.21
39	827.17	826.95	827.05	826.78
40	836.55	836.47	836.49	835.98
41	832	831.93	831.86	831.99
42	835.38	835.27	835.1	835.11
43	796.96	796.57	796.64	796.28
44	744.95	742.71	743.35	741.57
45	724.19	723.76	723.84	723.94
46	709.83	708.86	713.35	715.67
47	653.01	652.71	649.75	649.88
48	638.59	637.88	639.05	639.23
49	567.19	566.39	559.57	560.1
50	561.26	561.31	549.44	548.67
51	525.87	524.71	525.26	524.03
52	487.92	487.25	483.15	482.04
53	457.49	456.02	455.5	453.26
54	407.05	406.44	406.58	406.52

55	387.54	387.55	386.73	386.73
56	381.52	380.15	377.43	375.66
57	322.89	321.96	322.95	323.79
58	280.43	278.15	278.11	275.79
59	264.8	265.08	265.15	265.39
60	229.19	229.15	228.92	228.96
61	185.86	185.14	185.66	184.66
62	151.2	149.44	150.32	148.48
63	181.32	178.31	180.87	178.05
64	19.43	19	19.5	19.09
65	75.69	76.17	75.73	76.28
66	62.76	62.98	62.49	62.78