

Table 1S. Computed vibrational frequencies of porphycene. Column A: frequencies f_i corresponding to normal mode eigenvectors e_i obtained from BLYP/PW calculations; Column B: effective frequencies $\nu_i = \mu_i / 2\pi$, where μ_i is the median of the Lorentz function fit to the dominant peak in the Fourier transform of the PNM (see text for details); Column C: harmonic frequencies computed using B3LYP/6-31G(d,p) level.

	A	B	C
1	85.5	57.4	61.3
2	99.3	68.1	71.8
3	97.2	82.2	88.5
4	128.8	112.9	119.4
5	143.3	146.7	150.0
6	147.6	127.5	136.8
7	182.3	178.2	186.8
8	199.4	188.5	198.4
9	209.5	193.0	206.4
10	212.3	198.8	209.2
11	237.0	231.5	236.9
12	303.9	298.0	310.6
13	309.8	312.0	323.4
14	314.7	305.6	319.5
15	335.3	332.8	347.1
16	355.4	353.3	370.1
17	377.2	372.5	390.9
18	391.9	382.9	398.6
19	455.5	449.1	472.4
20	474.3	470.7	491.3
21	479.6	471.6	492.8
22	500.9	492.8	511.9
23	597.3	585.3	609.7
24	610.4	600.1	626.2
25	621.3	615.5	639.7
26	627.0	620.7	644.3
27	653.2	646.0	673.3
28	651.1	644.8	674.2
29	653.5	643.5	674.3
30	653.0	643.1	673.4
31	686.5	681.8	713.5
32	688.4	683.5	713.2
33	696.5	687.4	718.1
34	704.1	696.9	725.8
35	733.9	728.2	765.3
36	750.8	745.1	775.4
37	761.8	752.2	788.7
38	768.5	763.2	796.1
39	806.9	798.2	832.8
40	806.5	795.8	832.2
41	806.4	797.2	833.9

42	811.9	803.8	835.6
43	848.7	843.9	877.2
44	866.1	862.6	896.1
45	870.1	864.3	895.1
46	871.9	866.0	896.5
47	876.0	869.8	903.5
48	876.5	871.0	904.9
49	899.0	892.6	947.4
50	917.2	910.6	965.1
51	931.1	923.3	957.2
52	931.9	923.9	957.9
53	941.3	934.5	993.9
54	937.2	932.6	988.6
55	942.6	909.3	933.4
56	957.6	949.8	1016.4
57	972.3	965.7	1028.3
58	975.1	942.5	999.3
59	1027.0	1023.5	1074.9
60	1035.3	1032.3	1082.9
61	1040.5	1037.1	1087.2
62	1043.1	1040.5	1091.6
63	1061.0	1055.3	1121.6
64	1083.2	1077.7	1142.4
65	1124.5	1115.9	1192.7
66	1134.8	1125.5	1210.0
67	1162.6	1151.5	1226.9
68	1167.9	1158.9	1240.1
69	1181.4	1169.8	1270.0
70	1199.7	1188.4	1311.5
71	1215.6	1204.3	1284.9
72	1214.9	1204.1	1291.9
73	1243.3	1233.9	1329.4
74	1258.3	1246.4	1336.4
75	1289.7	1277.9	1370.1
76	1287.4	1276.2	1386.7
77	1317.2	1306.5	1413.1
78	1321.1	1310.3	1402.0
79	1341.1	1330.0	1411.4
80	1355.6	1344.7	1441.6
81	1361.9	1350.3	1448.1
82	1365.2	1351.8	1459.6
83	1390.8	1377.3	1489.2
84	1410.7	1396.9	1508.8
85	1416.1	1405.3	1515.8
86	1447.9	1435.1	1532.2
87	1448.6	1435.3	1531.3
88	1463.3	1447.3	1563.1
89	1473.7	1458.9	1571.0

90	1489.8	1474.2	1592.1
91	1500.6	1482.5	1612.6
92	1511.3	1494.9	1617.4
93	1536.3	1514.4	1631.3
94	1557.9	1535.3	1662.5
95	2748.7	2723.9	2894.7
96	2752.9	2729.6	2895.0
97	3104.7	3091.2	3164.9
98	3104.7	3092.4	3164.8
99	3122.0	3107.6	3183.7
100	3122.2	3106.0	3183.5
101	3165.9	3152.7	3235.6
102	3166.0	3153.2	3235.6
103	3180.9	3169.6	3249.8
104	3180.9	3167.6	3249.8
105	3184.7	3172.6	3256.4
106	3184.6	3173.4	3256.3
107	3197.4	3184.5	3268.1
108	3197.6	3185.4	3268.0