Electronic Supplementary Material (ESI) for RSC Advances.

Excited-State deactivation mechanisms of protonated and neutral phenylalanine: a theoretical study

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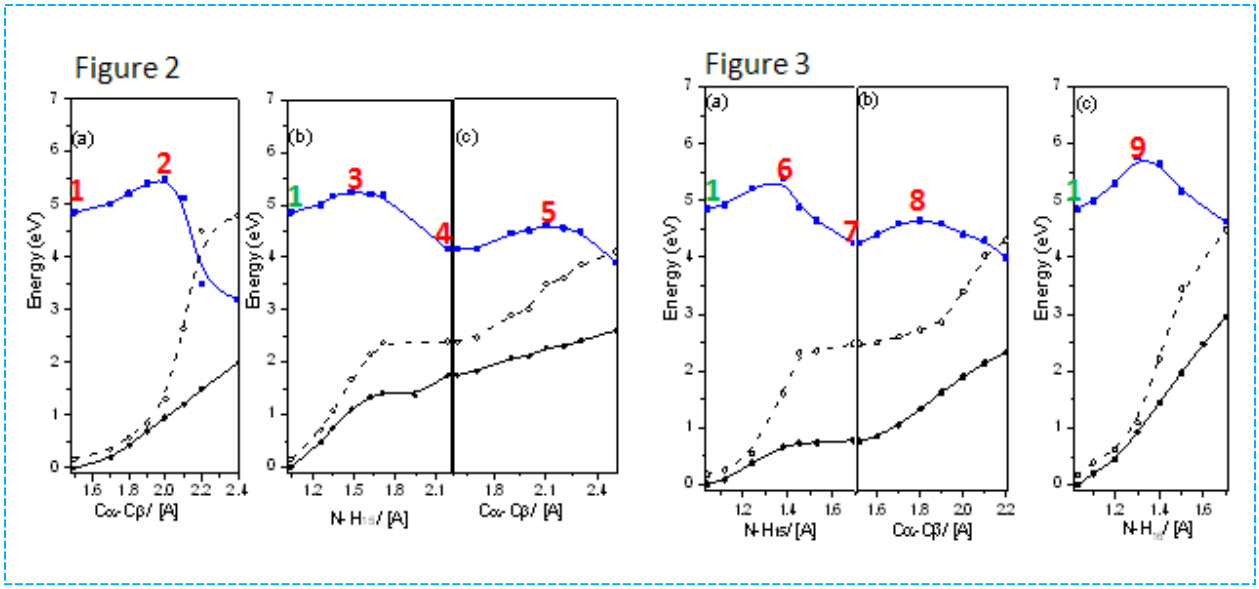
This supplementary file contains one figure and one Table.

Figure SM1: Selected points on the potential energy profiles for which the vibrational frequencies have been calculated; (based on Figure 2 and Figure 3, main text).

Table SM1: The S_1 state vibrational frequencies (in cm^{-1}) of selected points, calculated at the CC2/def2-SVP level of theory.

Figure SM1



Vibrational normal Modes	Point 1.0	Point 2.0	Point 3.0	Point 4.0	Point 5.0	Point 6.0	Point 7.0	Point 8.0	Point 9.0
1.0	0.0	-496.2	-1198.6	0.0	-516.9	-1183.0	0.0	-111.5	-5773.6
2.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-899.9
3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-503.0
4.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	-456.8
5.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
6.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
7.0	40.8	0.0	0.0	56.0	0.0	0.0	25.4	0.0	0.0
8.0	57.0	26.2	55.6	79.1	48.9	60.6	51.2	61.8	0.0
9.0	95.8	59.7	66.5	157.7	89.7	63.7	72.2	73.2	0.0
10.0	103.5	77.3	104.3	181.8	117.7	91.7	113.9	108.5	0.0
11.0	182.2	99.9	149.8	241.5	140.7	152.0	188.1	122.6	49.8
12.0	216.3	136.8	201.9	298.8	165.0	186.3	202.2	185.1	86.2
13.0	236.4	161.1	250.8	327.2	237.9	210.8	289.4	229.5	139.8
14.0	256.5	232.1	292.9	358.6	264.2	254.5	318.7	269.0	198.7
15.0	292.6	284.3	320.0	392.2	273.0	280.8	335.6	320.2	271.1
16.0	324.5	287.0	390.5	418.3	290.2	358.7	339.1	324.4	313.3
17.0	368.5	302.0	407.2	442.6	372.8	375.6	346.7	334.8	335.0
18.0	402.4	326.5	415.0	490.6	377.8	424.0	393.1	341.2	343.9
19.0	432.0	356.9	483.3	514.8	384.0	466.1	446.8	397.5	359.0
20.0	497.3	430.0	511.3	557.7	416.7	531.8	470.9	405.1	407.7
21.0	533.6	489.4	521.4	596.8	494.6	542.6	483.7	461.0	490.3

22.0	546.5	534.1	572.6	642.4	504.2	547.9	510.2	491.0	546.9
23.0	582.3	552.9	582.1	665.9	511.3	587.4	554.6	504.3	573.3
24.0	604.4	622.6	630.0	706.4	550.8	595.7	585.4	532.4	589.3
25.0	609.6	638.3	669.6	734.7	570.2	599.0	662.3	566.8	626.9
26.0	664.9	656.2	698.6	755.2	636.1	636.9	748.9	668.7	672.0
27.0	687.3	705.9	720.9	757.7	665.8	655.1	776.7	721.7	702.7
28.0	695.3	720.3	745.6	782.0	697.0	688.1	789.0	750.1	736.5
29.0	728.5	733.5	776.1	845.7	716.9	699.9	808.0	786.2	745.3
30.0	739.1	773.7	846.5	872.8	738.6	714.7	859.3	796.1	787.7
31.0	758.4	784.0	850.0	906.1	779.3	737.5	873.2	805.3	827.2
32.0	848.9	836.5	856.8	920.1	785.9	768.4	902.7	901.5	909.8
33.0	908.2	843.4	910.5	941.5	811.8	842.1	931.5	932.0	932.2
34.0	953.3	894.9	924.4	955.7	862.4	920.2	953.7	953.8	958.9
35.0	958.5	930.8	955.4	977.5	882.9	957.7	971.9	955.3	966.6
36.0	973.7	974.3	985.6	1018.5	912.5	969.5	985.7	973.5	977.5
37.0	1011.5	983.5	996.6	1041.5	954.8	975.3	999.9	993.3	998.1
38.0	1060.7	997.5	1010.5	1052.8	981.4	1036.9	1022.6	1003.6	1008.4
39.0	1119.0	1057.5	1060.1	1101.3	998.0	1089.1	1063.5	1025.5	1052.5
40.0	1141.7	1074.3	1099.5	1135.4	1021.1	1142.3	1089.6	1082.8	1104.9
41.0	1173.5	1096.9	1103.8	1181.6	1040.1	1155.6	1104.8	1095.8	1124.6
42.0	1175.1	1137.9	1131.4	1186.5	1060.7	1173.9	1154.5	1104.5	1138.2
43.0	1187.8	1145.4	1159.9	1192.4	1097.8	1175.0	1161.7	1153.0	1154.4
44.0	1213.9	1172.6	1173.5	1206.8	1122.2	1188.0	1205.5	1169.8	1171.3
45.0	1228.6	1177.4	1179.5	1233.3	1150.2	1218.9	1210.1	1202.9	1213.3
46.0	1301.0	1189.8	1219.4	1275.3	1170.9	1229.1	1235.2	1212.7	1240.5
47.0	1325.2	1301.2	1231.5	1313.9	1190.4	1283.5	1258.9	1248.9	1279.6
48.0	1352.0	1323.9	1243.2	1347.1	1242.8	1322.9	1276.3	1258.8	1318.9
49.0	1374.1	1327.0	1269.6	1369.8	1288.3	1353.4	1330.4	1320.1	1343.8
50.0	1403.4	1402.3	1321.8	1385.0	1324.0	1379.7	1346.4	1343.7	1379.1
51.0	1437.1	1446.3	1333.1	1425.5	1347.4	1405.4	1381.5	1348.7	1387.3
52.0	1456.6	1470.5	1359.8	1436.7	1362.7	1439.3	1398.4	1383.3	1422.3
53.0	1493.2	1477.6	1377.3	1452.9	1380.9	1469.9	1427.3	1399.1	1457.1
54.0	1521.0	1497.1	1404.1	1483.0	1419.2	1495.5	1469.4	1408.5	1485.8
55.0	1550.7	1503.8	1430.4	1520.6	1469.8	1550.5	1490.9	1468.4	1490.0
56.0	1572.9	1596.2	1451.5	1567.7	1479.1	1554.1	1502.5	1492.0	1509.6
57.0	1630.8	1627.5	1462.7	1633.2	1528.7	1575.1	1540.3	1500.6	1546.7
58.0	1679.9	1633.2	1487.8	1811.2	1531.7	1625.1	1570.6	1570.6	1638.6
59.0	1683.3	1683.1	1502.5	2872.6	1645.3	1692.6	1660.7	1660.8	1701.1
60.0	1798.6	1719.9	1627.4	2975.4	1661.6	1701.4	1671.0	1671.2	1852.2
61.0	3023.6	3109.7	1807.0	3008.8	2949.9	1782.1	3033.2	3042.3	3012.1
62.0	3054.1	3117.4	3034.8	3126.4	3115.2	3057.7	3046.0	3099.8	3077.7

63.0	3093.9	3173.4	3077.9	3167.0	3185.9	3091.1	3137.0	3124.0	3135.5
64.0	3130.4	3197.7	3106.8	3181.7	3194.6	3125.0	3203.7	3204.4	3210.5
65.0	3154.8	3200.2	3158.4	3197.5	3199.1	3174.7	3206.5	3209.7	3213.7
66.0	3201.6	3208.2	3169.0	3207.6	3210.2	3194.4	3208.9	3217.8	3217.8
67.0	3213.2	3210.3	3189.9	3224.0	3216.1	3214.3	3220.0	3221.4	3226.7
68.0	3221.6	3215.3	3194.4	3423.3	3224.2	3220.5	3221.7	3228.6	3229.9
69.0	3222.5	3235.6	3234.6	3504.8	3491.6	3230.5	3229.7	3301.0	3375.7
70.0	3232.1	3239.1	3399.9	3890.4	3532.8	3286.0	3470.5	3484.1	3478.8
71.0	3436.3	3419.1	3522.8	3925.2	3619.9	3487.1	3570.9	3523.0	3512.3
72.0	3521.1	3547.2	3526.8	4194.8	4176.7	3508.3	3590.8	3581.4	23810.6