# Supplemental Information

Polycyclic (Anti)aromatic Hydrocarbons: Interstellar Formation and Spectroscopic Characterization of Biphenylene and Benzopentalene

Athena R. Flint[1], Vincent J. Esposito[2], and Ryan C. Fortenberry[1]

[1]Department of Chemistry and Biochemistry, University of Mississippi, University, MS 38677, USA
[2]NASA Ames Research Center, MS N245-6, Moffett Field, CA 94035, USA

# 1 Excited States of *ortho*-Benzyne

MCSCF excited-state calculations are used to correlate the relative energies of the 1 $^1A_g$ and 2 $^1A_g$ states of the $D_{2h}$-symmetry association of *o*-$C_6H_4$ at the furthest distance from the minimum computed ($r_{C-C}$ = 5.0 Å) with the energies of the low-lying excited states of *o*-$C_6H_4$ in order to determine which electronic states of *o*-$C_6H_4$ would need to be present in order to barrierlessly proceed through the avoided crossing shown in Fig. 1 in the main text. In Fig. 1, the vertical excitation energy at $r_{C-C}$ = 5.0 Å from the 1 $^1A_g$ state to the 2 $^1A_g$ state is 96.9 kcal mol$^{-1}$, or 4.20 eV, determined at the MRCI-F12+Q/cc-pVDZ-F12//MCSCF/aug-cc-pVDZ level of theory with a (6e,6o) active space. The orbitals used to construct this active space are defined in Table S1. Determination of the vertical excitation energy from the MCSCF values only results in a slightly lower value of 3.62 eV.

| | | $a_g$ | $b_{3u}$ | $b_{2u}$ | $b_{1g}$ | $b_{1u}$ | $b_{2g}$ | $b_{3g}$ | $a_u$ |
|---|---|---|---|---|---|---|---|---|---|
| (6e,6o) | Occupied | 10 | 2 | 8 | 2 | 10 | 2 | 8 | 1 |
| | Closed | 9 | 2 | 7 | 1 | 9 | 1 | 7 | 1 |

Table S1: Occupied and closed orbitals used in the MRCI-F12+Q/cc-pVDZ-F12//MCSCF/aug-cc-pVDZ PES for the dimerization of *o*-$C_6H_4$ shown in Fig. 1 in the main text.

| | Active Space | | | | | |
|---|---|---|---|---|---|---|
| State | (6e,7o) | (6e,9o) | (12e,9o) | (12e,11o) | (6e,13o) | (8e,14o) |
| 1 $^1A_1$ | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |
| 2 $^1A_1$ | 8.54 | 6.65 | 7.94 | 6.63 | 6.57 | 6.27 |
| 1 $^1B_1$ | 4.29 | **3.86** | 5.11 | **4.05** | **4.03** | **3.83** |
| 2 $^1B_1$ | 6.99 | 7.42 | 6.63 | 6.66 | 7.13 | 7.29 |
| 1 $^1B_2$ | 8.01 | 7.04 | 7.26 | 7.15 | 6.20 | 6.19 |
| 2 $^1B_2$ | 9.63 | 8.77 | 11.0 | 8.05 | 8.36 | 7.74 |
| 1 $^1A_2$ | **3.54** | 4.11 | **4.33** | 4.61 | 4.63 | 3.94 |
| 2 $^1A_2$ | 6.44 | 8.02 | 6.31 | 8.73 | 7.88 | 6.81 |
| $\lvert\Delta\rvert$ (1 $^1B_1$, 1 $^1A_2$) | 0.75 | 0.25 | 0.78 | 0.56 | 0.60 | 0.11 |

Table S2: MCSCF/aug-cc-pVDZ vertical excitation energies (in eV) for *o*-$C_6H_4$ computed with six different active spaces. Energies are computed for the two lowest-energy states of each symmetry. The lowest-energy excited state located within each calculation is bolded.

As shown in Table S2, there are two excited states of *o*-$C_6H_4$ that can appear when supplied with approximately the same energy as is required to undergo a vertical transition near the dissociation limit in Fig. 1. The order in which these states appear (i.e. which state is lower in energy) is not consistent across the active spaces tested, however. Complete definitions of the active spaces listed in Table S2 are listed in Table S3. The computed HF orbitals for the F12-DZ-optimized *o*-$C_6H_4$ molecule show that the HOMO is of $b_2$ symmetry with a HOMO-1 of $a_2$ symmetry. The energy difference between the HOMO and HOMO-1, both $\pi$ orbitals containing electrons involved in aromaticity, is computed to be 0.0318 eV, indicating that these orbitals are nearly degenerate and could be prone to swapping. The LUMO is of $b_2$ symmetry. A simple excitation of one electron from the HOMO to the LUMO would result in an $A_2$ electronic state, while an excitation of one electron from the HOMO-1 to the LUMO would result in a $B_1$ electronic state. The two active spaces that predict an $A_2$ state to be the first excited state have much larger gaps between the first and second excited states than the other active spaces. The active space with the greatest number of orbitals involved shrinks the gap between the two to 0.11 eV.

Considering that there will still be some interaction energy between the two *o*-$C_6H_4$ monomers at their greatest intermolecular distance in Fig. 1, making a direct numerical comparison to the data in Table S2 would be very challenging. As such, the 2 $^1A_g$ PES in

| | | $a_1$ | $b_1$ | $b_2$ | $a_2$ |
|---|---|---|---|---|---|
| (6e,7o) | Occupied | 12 | 2 | 9 | 1 |
| | Closed | 9 | 1 | 7 | 0 |
| (6e,9o) | Occupied | 12 | 4 | 9 | 1 |
| | Closed | 9 | 1 | 7 | 0 |
| (12e,9o) | Occupied | 12 | 2 | 8 | 1 |
| | Closed | 8 | 1 | 5 | 0 |
| (12e,11o) | Occupied | 12 | 4 | 8 | 1 |
| | Closed | 8 | 1 | 5 | 0 |
| (6e,13o) | Occupied | 13 | 5 | 10 | 2 |
| | Closed | 9 | 1 | 7 | 0 |
| (8e,14o) | Occupied | 13 | 5 | 10 | 2 |
| | Closed | 9 | 0 | 7 | 0 |

Table S3: Sets of occupied and closed orbitals for *o*-$C_6H_4$ that define the active spaces in Table S2.

Fig. 1 is tentatively identified as resulting from the association between $\tilde{X}\ ^1A_1$ *o*-$C_6H_4$ and 1 $^1A_2/^1B_1$ *o*-$C_6H_4$ (note that the $\tilde{A}$ assignment is avoided as neither state can be confirmed as the true first excited state).

## 2 Structures

| | | | |
|---|---|---|---|
| C | 0.0000000000 | 0.6262739089 | 1.1815193381 |
| C | 0.0000000000 | -0.6262739089 | 1.1815193381 |
| C | 0.0000000000 | 1.4703431584 | 0.0853087666 |
| C | 0.0000000000 | -1.4703431584 | 0.0853087666 |
| C | 0.0000000000 | 0.7061089066 | -1.1017852267 |
| C | 0.0000000000 | -0.7061089066 | -1.1017852267 |
| H | 0.0000000000 | 2.5503990468 | 0.0885910802 |
| H | 0.0000000000 | -2.5503990468 | 0.0885910802 |
| H | 0.0000000000 | 1.2215561901 | -2.0553053760 |
| H | 0.0000000000 | -1.2215561901 | -2.0553053760 |
| | T1 Diagnostic | 0.01417630 | |
| | D1 Diagnostic | 0.04284069 | |

| CCSD(T)-F12/cc-pVDZ-F12 Harmonic Frequencies | |
|---|---|
| 390.67 | 1101.73 |
| 438.40 | 1153.02 |
| 465.91 | 1264.23 |
| 596.68 | 1305.20 |
| 612.44 | 1430.11 |
| 739.27 | 1472.25 |
| 854.39 | 1477.66 |
| 860.83 | 1933.96 |
| 911.66 | 3173.88 |
| 948.56 | 3188.49 |
| 984.74 | 3221.03 |
| 1061.44 | 3223.60 |

Table S4: Optimized geometry for *o*-benzyne. Cartesian coordinates in Å.

### 2.1 Unimolecular Products

| | | | |
|---|---|---|---|
| C | 0.0000000000 | -0.7131219361 | 0.7564036549 |
| C | 0.0000000000 | 0.7131219361 | -0.7564036549 |
| C | 0.0000000000 | -0.7131219361 | -0.7564036549 |
| C | 0.0000000000 | 0.7131219361 | 0.7564036549 |
| C | 0.0000000000 | -1.4488851108 | 1.9201809793 |
| C | 0.0000000000 | 1.4488851108 | -1.9201809793 |
| C | 0.0000000000 | -1.4488851108 | -1.9201809793 |
| C | 0.0000000000 | 1.4488851108 | 1.9201809793 |
| C | 0.0000000000 | -0.6965943881 | 3.1281114185 |
| C | 0.0000000000 | 0.6965943881 | -3.1281114185 |
| C | 0.0000000000 | -0.6965943881 | -3.1281114185 |
| C | 0.0000000000 | 0.6965943881 | 3.1281114185 |
| H | 0.0000000000 | -2.5386632299 | 1.9414412863 |
| H | 0.0000000000 | 2.5386632299 | -1.9414412863 |
| H | 0.0000000000 | -2.5386632299 | -1.9414412863 |
| H | 0.0000000000 | 2.5386632299 | 1.9414412863 |
| H | 0.0000000000 | -1.2257870969 | 4.0820322223 |
| H | 0.0000000000 | 1.2257870969 | -4.0820322223 |
| H | 0.0000000000 | -1.2257870969 | -4.0820322223 |
| H | 0.0000000000 | 1.2257870969 | 4.0820322223 |

| | |
|---|---|
| T1 Diagnostic | 0.01200780 |
| D1 Diagnostic | 0.03649517 |

B3LYP/aug-cc-pVDZ Harmonic Frequencies

| | | |
|---|---|---|
| 102.27 | 868.42 | 1308.50 |
| 147.15 | 920.02 | 1419.06 |
| 209.25 | 925.07 | 1444.39 |
| 318.34 | 950.20 | 1461.65 |
| 377.64 | 982.15 | 1463.96 |
| 397.32 | 989.90 | 1506.25 |
| 431.53 | 990.31 | 1623.16 |
| 468.37 | 992.70 | 1626.47 |
| 560.81 | 1009.98 | 1640.03 |
| 594.73 | 1037.34 | 1703.72 |
| 604.39 | 1063.82 | 3168.34 |
| 620.93 | 1103.16 | 3168.48 |
| 729.64 | 1133.78 | 3178.02 |
| 734.21 | 1138.73 | 3178.82 |
| 739.45 | 1171.34 | 3187.03 |
| 750.32 | 1180.60 | 3187.68 |
| 777.28 | 1276.69 | 3194.82 |
| 859.51 | 1293.10 | 3195.43 |

Table S5: Optimized geometry for biphenylene. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -1.0758744851 | 0.0000100595 | -2.8415082874 |
| C | 0.2757983494 | 0.0001639967 | -3.1794238868 |
| C | 1.2657850432 | 0.0000353405 | -2.1719649888 |
| C | 0.8662416349 | -0.0000184565 | -0.8428017852 |
| C | -0.5218049054 | -0.0000791827 | -0.4949120843 |
| C | -1.4877882222 | -0.0000557931 | -1.4892730093 |
| H | -2.5499443654 | -0.0000995315 | -1.2418248088 |
| C | -0.5734815770 | -0.0001640219 | 0.9769357847 |
| C | -1.4021145153 | 0.0000152674 | 2.0571992393 |
| C | -0.5522587364 | 0.0001372814 | 3.2793815682 |
| C | 0.7677472541 | 0.0000809782 | 2.9315228024 |
| C | 0.8142411207 | -0.0000981564 | 1.4653924792 |
| C | 1.6689952411 | -0.0001655955 | 0.4053125704 |
| H | 2.7584543966 | 0.0004930747 | 0.4298797881 |
| H | 1.6188851290 | 0.0002314410 | 3.6072078020 |
| H | -0.9456877347 | 0.0003404312 | 4.2946496730 |
| H | -2.4907666127 | 0.0002476993 | 2.0674134681 |
| H | 2.3233078750 | 0.0001698621 | -2.4403829532 |
| H | 0.5728023176 | 0.0001451435 | -4.2286698805 |
| H | -1.8290820518 | 0.0001197049 | -3.6305824457 |
| | T1 Diagnostic | 0.01259461 | |
| | D1 Diagnostic | 0.04046058 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 111.24 | 852.25 | 1321.46 |
| | 149.52 | 852.38 | 1331.02 |
| | 245.36 | 880.44 | 1405.38 |
| | 280.97 | 900.38 | 1458.61 |
| | 342.36 | 918.25 | 1467.50 |
| | 439.08 | 940.52 | 1528.04 |
| | 459.66 | 954.17 | 1614.17 |
| | 513.21 | 980.58 | 1634.24 |
| | 548.39 | 988.11 | 1637.33 |
| | 571.86 | 1035.79 | 1653.71 |
| | 584.01 | 1080.06 | 3166.25 |
| | 678.35 | 1095.26 | 3171.65 |
| | 682.71 | 1121.21 | 3182.65 |
| | 740.03 | 1163.46 | 3195.13 |
| | 762.72 | 1174.17 | 3198.86 |
| | 769.45 | 1193.53 | 3202.28 |
| | 798.80 | 1249.79 | 3214.20 |
| | 830.66 | 1299.40 | 3236.72 |

Table S6: Optimized geometry for benzopentalene. Cartesian coordinates in Å.

## 2.2 Bimolecular Products

| | | | |
|---|---|---|---|
| H | 0.0000000000 | 0.0000000000 | -1.6662775069 |
| C | 0.0000000000 | 0.0000000000 | -0.6030316726 |
| C | 0.0000000000 | 0.0000000000 | 0.6030316726 |
| H | 0.0000000000 | 0.0000000000 | 1.6662775069 |
| | T1 Diagnostic | 0.01484676 | |
| | D1 Diagnostic | 0.03216889 | |
| CCSD(T)-F12/cc-pVDZ-F12 Harmonic Frequencies | | | |
| | | 607.49 | |
| | | 607.49 | |
| | | 746.16 | |
| | | 746.16 | |
| | | 2007.59 | |
| | | 3412.50 | |
| | | 3505.42 | |

Table S7: Optimized geometry for acetylene. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 1.2120100095 | -0.6997543052 | 0.0000000000 |
| C | 0.0000000000 | -1.3995086105 | 0.0000000000 |
| C | -1.2120100095 | -0.6997543052 | 0.0000000000 |
| C | -1.2120100095 | 0.6997543052 | 0.0000000000 |
| C | 0.0000000000 | 1.3995086105 | 0.0000000000 |
| C | 1.2120100095 | 0.6997543052 | 0.0000000000 |
| H | 2.1569629026 | -1.2453231125 | 0.0000000000 |
| H | 0.0000000000 | -2.4906462249 | 0.0000000000 |
| H | -2.1569629026 | -1.2453231125 | 0.0000000000 |
| H | -2.1569629026 | 1.2453231125 | 0.0000000000 |
| H | 0.0000000000 | 2.4906462249 | 0.0000000000 |
| H | 2.1569629026 | 1.2453231125 | 0.0000000000 |
| | T1 Diagnostic | 0.01139370 | |
| | D1 Diagnostic | 0.03255238 | |
| B3LYP/aug-cc-pVDZ Harmonic Frequencies | | | |
| 411.88 | | 1163.36 | |
| 411.88 | | 1186.67 | |
| 615.52 | | 1186.73 | |
| 615.54 | | 1348.68 | |
| 680.13 | | 1352.98 | |
| 728.39 | | 1491.25 | |
| 855.29 | | 1491.27 | |
| 855.29 | | 1631.46 | |
| 980.99 | | 1631.47 | |
| 980.99 | | 3164.09 | |
| 1004.02 | | 3172.03 | |
| 1012.00 | | 3172.12 | |
| 1014.71 | | 3187.03 | |
| 1054.65 | | 3187.11 | |
| 1054.75 | | 3196.80 | |

Table S8: Optimized geometry for benzene. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.0000000000 | 0.7000622613 | 2.3813440622 |
| C | 0.0000000000 | -0.7000622613 | 2.3813440622 |
| H | 0.0000000000 | 1.2494312642 | 3.3232531827 |
| H | 0.0000000000 | -1.2494312642 | 3.3232531827 |
| C | 0.0000000000 | 1.3962681891 | 1.1738471203 |
| C | 0.0000000000 | -1.3962681891 | 1.1738471203 |
| H | 0.0000000000 | 2.4856043378 | 1.1661563452 |
| H | 0.0000000000 | -2.4856043378 | 1.1661563452 |
| C | 0.0000000000 | 0.7117909839 | -0.0567372306 |
| C | 0.0000000000 | -0.7117909839 | -0.0567372306 |
| C | 0.0000000000 | 1.4494220050 | -1.2815337880 |
| C | 0.0000000000 | -1.4494220050 | -1.2815337880 |
| C | 0.0000000000 | 2.0759976598 | -2.3219288948 |
| C | 0.0000000000 | -2.0759976598 | -2.3219288948 |
| H | 0.0000000000 | 2.6277507568 | -3.2380851767 |
| H | 0.0000000000 | -2.6277507568 | -3.2380851767 |
| | T1 Diagnostic | 0.01289669 | |
| | D1 Diagnostic | 0.03494988 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 103.36 | 651.47 | 1277.50 |
| | 116.52 | 652.12 | 1320.45 |
| | 142.36 | 718.77 | 1448.64 |
| | 177.81 | 767.81 | 1495.28 |
| | 298.50 | 786.06 | 1589.06 |
| | 354.01 | 816.94 | 1629.37 |
| | 419.28 | 895.55 | 2201.34 |
| | 455.65 | 967.64 | 2207.80 |
| | 490.04 | 1006.98 | 3177.12 |
| | 548.06 | 1057.08 | 3188.55 |
| | 559.02 | 1104.57 | 3199.66 |
| | 581.86 | 1173.46 | 3204.64 |
| | 585.69 | 1201.57 | 3478.30 |
| | 591.44 | 1226.16 | 3478.55 |

Table S9: Optimized geometry for *o*-dietheynyl benzene. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| H | 0.0000000000 | 0.0000000000 | -4.2562712219 |
| C | 0.0000000000 | 0.0000000000 | -3.1927122048 |
| C | 0.0000000000 | 0.0000000000 | -1.9796322257 |
| C | 0.0000000000 | 0.0000000000 | -0.6093105969 |
| C | 0.0000000000 | 0.0000000000 | 0.6093105969 |
| C | 0.0000000000 | 0.0000000000 | 1.9796322257 |
| C | 0.0000000000 | 0.0000000000 | 3.1927122048 |
| H | 0.0000000000 | 0.0000000000 | 4.2562712219 |
| | T1 Diagnostic | 0.01538470 | |
| | D1 Diagnostic | 0.03585606 | |
| CCSD(T)-F12/cc-pVDZ-F12 Harmonic Frequencies | | | |
| | | 104.91 | |
| | | 104.95 | |
| | | 234.25 | |
| | | 234.29 | |
| | | 383.27 | |
| | | 383.28 | |
| | | 427.63 | |
| | | 427.63 | |
| | | 615.71 | |
| | | 628.36 | |
| | | 628.40 | |
| | | 628.58 | |
| | | 628.66 | |
| | | 1167.28 | |
| | | 2062.56 | |
| | | 2168.66 | |
| | | 2271.59 | |
| | | 3455.58 | |
| | | 3455.72 | |

Table S10: Optimized geometry for triacetylene. Cartesian coordinates in Å.

## 2.3 Intermediates

| | | | |
|---|---|---|---|
| C | -0.0052274144 | -0.7396921470 | 0.0000000000 |
| C | 0.0052274144 | 0.7396921470 | 0.0000000000 |
| C | 0.0208117967 | -3.5873607555 | 0.0000000000 |
| C | -0.0208117967 | 3.5873607555 | 0.0000000000 |
| H | 0.0272371403 | -4.6786680755 | 0.0000000000 |
| H | -0.0272371403 | 4.6786680755 | 0.0000000000 |
| C | 1.1544775613 | -1.5056341642 | 0.0000000000 |
| C | -1.1544775613 | 1.5056341642 | 0.0000000000 |
| C | -1.2070540771 | -1.4865536041 | 0.0000000000 |
| C | 1.2070540771 | 1.4865536041 | 0.0000000000 |
| H | -2.1583384568 | -0.9516191177 | 0.0000000000 |
| H | 2.1583384568 | 0.9516191177 | 0.0000000000 |
| C | 1.2376246072 | -2.8790308392 | 0.0000000000 |
| C | -1.2376246072 | 2.8790308392 | 0.0000000000 |
| C | -1.1892959698 | -2.8831368134 | 0.0000000000 |
| C | 1.1892959698 | 2.8831368134 | 0.0000000000 |
| H | 2.1943331615 | -3.4031062452 | 0.0000000000 |
| H | -2.1943331615 | 3.4031062452 | 0.0000000000 |
| H | -2.1325305326 | -3.4305006735 | 0.0000000000 |
| H | 2.1325305326 | 3.4305006735 | 0.0000000000 |

| | |
|---|---|
| T1 Diagnostic | 0.01453720 |
| D1 Diagnostic | 0.04569929 |

B3LYP/aug-cc-pVDZ Harmonic Frequencies

| | | |
|---|---|---|
| 42.97 | 848.68 | 1326.59 |
| 96.03 | 865.99 | 1337.59 |
| 131.56 | 943.94 | 1411.22 |
| 242.30 | 951.68 | 1452.59 |
| 312.77 | 975.90 | 1453.65 |
| 416.91 | 986.99 | 1485.90 |
| 417.66 | 994.57 | 1563.74 |
| 428.81 | 996.04 | 1572.20 |
| 462.47 | 1021.68 | 1633.26 |
| 571.73 | 1040.16 | 1634.95 |
| 598.89 | 1061.02 | 3164.55 |
| 616.42 | 1104.44 | 3164.88 |
| 634.81 | 1123.17 | 3170.73 |
| 689.73 | 1161.81 | 3170.77 |
| 718.75 | 1163.65 | 3180.59 |
| 734.76 | 1219.08 | 3180.96 |
| 744.26 | 1250.61 | 3192.81 |
| 775.22 | 1308.10 | 3192.96 |

Table S11: Optimized geometry for I1. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.0000000000 | -0.7447236857 | 0.7165532982 |
| C | 0.0000000000 | 0.7447236857 | -0.7165532982 |
| C | 0.0000000000 | -0.7447236857 | -0.7165532982 |
| C | 0.0000000000 | 0.7447236857 | 0.7165532982 |
| C | 0.0000000000 | -1.4757401096 | 1.9187280190 |
| C | 0.0000000000 | 1.4757401096 | -1.9187280190 |
| C | 0.0000000000 | -1.4757401096 | -1.9187280190 |
| C | 0.0000000000 | 1.4757401096 | 1.9187280190 |
| C | 0.0000000000 | -0.7241165675 | 3.0865080456 |
| C | 0.0000000000 | 0.7241165675 | -3.0865080456 |
| C | 0.0000000000 | -0.7241165675 | -3.0865080456 |
| C | 0.0000000000 | 0.7241165675 | 3.0865080456 |
| H | 0.0000000000 | -2.5656107071 | 1.9516548625 |
| H | 0.0000000000 | 2.5656107071 | -1.9516548625 |
| H | 0.0000000000 | -2.5656107071 | -1.9516548625 |
| H | 0.0000000000 | 2.5656107071 | 1.9516548625 |
| H | 0.0000000000 | -1.2330736445 | 4.0511549613 |
| H | 0.0000000000 | 1.2330736445 | -4.0511549613 |
| H | 0.0000000000 | -1.2330736445 | -4.0511549613 |
| H | 0.0000000000 | 1.2330736445 | 4.0511549613 |
| | T1 Diagnostic | 0.01429784 | |
| | D1 Diagnostic | 0.03987321 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 89.98 | 825.55 | 1317.23 |
| | 133.72 | 858.21 | 1390.61 |
| | 218.32 | 914.06 | 1410.57 |
| | 285.56 | 928.39 | 1420.82 |
| | 364.96 | 929.87 | 1464.92 |
| | 384.56 | 957.44 | 1465.49 |
| | 411.80 | 958.56 | 1519.21 |
| | 417.17 | 959.43 | 1520.99 |
| | 526.80 | 961.07 | 1552.17 |
| | 543.95 | 974.09 | 1657.28 |
| | 582.93 | 1057.83 | 3168.32 |
| | 593.39 | 1110.88 | 3169.45 |
| | 665.09 | 1134.85 | 3173.70 |
| | 710.38 | 1153.37 | 3175.00 |
| | 713.58 | 1167.23 | 3185.79 |
| | 722.43 | 1224.40 | 3186.44 |
| | 758.08 | 1281.64 | 3195.51 |
| | 811.88 | 1314.81 | 3196.31 |

Table S12: Optimized geometry for 1 $^3B_{3g}$ $(C_6H_4)_2$. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.5217079740 | -0.7493564022 | -0.7489810661 |
| C | -0.2944893837 | -0.7316299809 | 0.6966779538 |
| C | -0.3255317360 | 0.6806372928 | 0.6826367133 |
| C | -0.7843114893 | 0.7527512931 | -0.7987637018 |
| C | -0.0420489608 | 1.4720734925 | -1.8671847435 |
| C | 0.6731041935 | 0.7394492486 | -2.7919536461 |
| C | 0.4085930834 | -0.6577122734 | -2.9425905787 |
| C | -0.0718359577 | -1.4272575327 | -1.8644485500 |
| H | 0.0775198601 | -2.5084185253 | -1.8709593238 |
| H | 0.6523273177 | -1.1569687336 | -3.8855242641 |
| H | 1.3103384070 | 1.2361701481 | -3.5289570475 |
| C | 0.0509820156 | 1.4461871581 | 1.7728199064 |
| C | 0.3713045334 | 0.7232237117 | 2.9399586539 |
| C | 0.3586913285 | -0.6835410254 | 2.9744643352 |
| C | 0.0443105056 | -1.4533451250 | 1.8433084221 |
| H | 0.0727488133 | -2.5422063809 | 1.8768675819 |
| H | 0.6156568729 | -1.1866837443 | 3.9077423751 |
| H | 0.6293837180 | 1.2680667706 | 3.8492340541 |
| H | 0.0759726615 | 2.5351687791 | 1.7535025983 |
| H | -1.8497854623 | 1.0264349112 | -0.8619311341 |
| | T1 Diagnostic | 0.03616796 | |
| | D1 Diagnostic | 0.24272911 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 79.50 | 845.75 | 1288.94 |
| | 116.74 | 867.32 | 1330.22 |
| | 201.88 | 889.96 | 1335.00 |
| | 246.29 | 934.25 | 1392.17 |
| | 345.45 | 936.39 | 1445.61 |
| | 389.20 | 948.20 | 1477.00 |
| | 418.93 | 991.43 | 1502.13 |
| | 447.29 | 994.58 | 1561.65 |
| | 485.67 | 1015.37 | 1614.79 |
| | 542.15 | 1044.81 | 1646.47 |
| | 554.85 | 1101.03 | 3018.87 |
| | 621.11 | 1104.12 | 3132.96 |
| | 649.56 | 1128.08 | 3147.03 |
| | 710.96 | 1147.22 | 3170.58 |
| | 729.25 | 1168.73 | 3176.04 |
| | 757.01 | 1184.11 | 3182.44 |
| | 780.10 | 1232.24 | 3193.38 |
| | 796.35 | 1285.03 | 3199.69 |

Table S13: Optimized geometry for I2. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -3.1973961824 | 0.4618133619 | -0.3191537398 |
| H | -4.1675089101 | 0.8433971377 | -0.6367127113 |
| C | -2.9136159658 | -0.8370731499 | -0.0313954886 |
| H | -3.6163780761 | -1.6674813244 | -0.0242530408 |
| C | -1.9920508809 | 1.2910353389 | -0.1782204548 |
| H | -1.9091653081 | 2.3163732609 | -0.5377665292 |
| C | -0.9795671659 | 0.5025359311 | 0.2776930143 |
| C | -1.4860996542 | -0.9179962604 | 0.4363045428 |
| H | -1.4761409644 | -1.1916063546 | 1.5150590418 |
| C | -0.3914105169 | -1.8282176683 | -0.1092609585 |
| C | 0.7763345138 | -0.9687437968 | -0.0326988286 |
| C | 2.7976534276 | 0.9534825555 | 0.0088645697 |
| C | 2.1193246862 | -1.3707289978 | -0.2005118674 |
| C | 0.4614908739 | 0.4226149799 | 0.1646928095 |
| C | 1.4780714992 | 1.3860958304 | 0.1663522517 |
| C | 3.1245048784 | -0.4091971725 | -0.1637913944 |
| H | 2.3439966978 | -2.4257834811 | -0.3604077861 |
| H | 1.2566402720 | 2.4456277376 | 0.2977943814 |
| H | 4.1689088142 | -0.6973723083 | -0.2859733876 |
| H | 3.6024079618 | 1.6912243802 | 0.0133855759 |
| | T1 Diagnostic | 0.01543573 | |
| | D1 Diagnostic | 0.05948058 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 101.49 | 855.94 | 1278.18 |
| | 140.65 | 868.45 | 1300.43 |
| | 244.17 | 883.83 | 1348.55 |
| | 267.47 | 927.02 | 1368.20 |
| | 286.80 | 928.08 | 1439.79 |
| | 424.66 | 970.99 | 1477.13 |
| | 471.36 | 980.50 | 1535.35 |
| | 497.06 | 1004.01 | 1577.43 |
| | 537.02 | 1004.26 | 1621.71 |
| | 546.08 | 1028.21 | 1646.21 |
| | 568.34 | 1031.41 | 2935.40 |
| | 657.55 | 1067.96 | 3167.28 |
| | 688.37 | 1109.48 | 3180.35 |
| | 725.26 | 1130.69 | 3187.15 |
| | 762.13 | 1157.13 | 3190.91 |
| | 765.03 | 1177.62 | 3198.44 |
| | 775.79 | 1210.21 | 3203.11 |
| | 825.11 | 1249.25 | 3227.34 |

Table S14: Optimized geometry for I3. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.1989537157 | -0.7355304782 | -0.5762900780 |
| C | 0.1351278206 | -1.2999757714 | 0.5840795534 |
| C | 0.6773148310 | -1.3916293851 | 1.7914937795 |
| C | 0.2671008443 | -0.6249800987 | 2.9768318059 |
| C | -0.2675373364 | 0.6252468763 | 2.9766722509 |
| C | -0.6773462060 | 1.3916108595 | 1.7910063302 |
| C | -0.1344323952 | 1.3001190977 | 0.5838992450 |
| C | 0.1993194944 | 0.7356313794 | -0.5765316966 |
| C | 0.7234359950 | 1.2597723896 | -1.8148326717 |
| C | 0.4009115342 | 0.6027273720 | -2.9702761837 |
| C | -0.4013085273 | -0.6030662740 | -2.9700286433 |
| C | -0.7234858690 | -1.2598918490 | -1.8143772640 |
| H | -1.2690144365 | -2.2035673237 | -1.8253066277 |
| H | -0.7158605964 | -1.0165857064 | -3.9291482814 |
| H | 0.7151545350 | 1.0160750345 | -3.9295682371 |
| H | 1.2690021464 | 2.2034229182 | -1.8261373978 |
| H | -1.5643533812 | 2.0248896659 | 1.9178462785 |
| H | -0.4958308334 | 1.0754365039 | 3.9459052084 |
| H | 0.4950297854 | -1.0750296730 | 3.9462205267 |
| H | 1.5641273881 | -2.0250479828 | 1.9188967459 |
| | T1 Diagnostic | 0.01505980 | |
| | D1 Diagnostic | 0.04806341 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 109.96 | 782.26 | 1360.04 |
| | 128.71 | 802.19 | 1391.22 |
| | 178.55 | 817.82 | 1408.58 |
| | 269.76 | 857.04 | 1463.39 |
| | 286.74 | 876.45 | 1473.87 |
| | 354.67 | 892.51 | 1514.00 |
| | 368.70 | 936.77 | 1593.41 |
| | 436.50 | 963.36 | 1632.79 |
| | 469.40 | 979.51 | 1862.91 |
| | 476.90 | 986.34 | 1932.28 |
| | 500.97 | 1014.74 | 3091.16 |
| | 531.23 | 1098.53 | 3091.37 |
| | 557.93 | 1111.96 | 3147.79 |
| | 609.12 | 1180.47 | 3167.78 |
| | 689.26 | 1196.40 | 3170.32 |
| | 708.15 | 1228.92 | 3178.96 |
| | 716.20 | 1235.72 | 3191.02 |
| | 737.10 | 1236.72 | 3197.87 |

Table S15: Optimized geometry for I4. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.2644989160 | -0.6632532039 | -0.3561460414 |
| C | -0.6482535708 | -1.2183713699 | 0.8677996739 |
| C | -0.7045671269 | -1.2032069120 | 2.1878351900 |
| C | 0.5700023182 | -0.6365962912 | 2.6251356727 |
| C | 1.0073605783 | 0.6443471565 | 2.2149157013 |
| C | 0.1912550905 | 1.5190438883 | 1.5647856185 |
| C | -0.6394542614 | 1.6772608437 | 0.5436010911 |
| C | -0.3789173302 | 0.7560359504 | -0.5883304841 |
| C | -0.1409359793 | 1.2487990737 | -1.8876679210 |
| C | 0.2485899709 | 0.4041594643 | -2.9184079605 |
| C | 0.4411017113 | -0.9761133369 | -2.6759360999 |
| C | 0.1811958081 | -1.5009969509 | -1.4266521521 |
| H | 0.2917563222 | -2.5687790691 | -1.2365225692 |
| H | 0.7697377489 | -1.6294730388 | -3.4848790022 |
| H | 0.4045140732 | 0.8048816870 | -3.9210309030 |
| H | -0.2591630128 | 2.3177634303 | -2.0738329380 |
| H | -1.4081359371 | 2.4529745633 | 0.4850046489 |
| H | 2.0377571058 | 0.9347004458 | 2.4387079908 |
| H | 1.2730834052 | -1.2707307608 | 3.1729188317 |
| H | -1.4755547984 | -1.6503635260 | 2.8210668469 |
| | T1 Diagnostic | 0.02069468 | |
| | D1 Diagnostic | 0.10998526 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 88.46 | 764.64 | 1308.30 |
| | 108.39 | 794.83 | 1335.10 |
| | 143.94 | 822.56 | 1395.26 |
| | 231.77 | 841.87 | 1408.33 |
| | 319.25 | 872.31 | 1447.04 |
| | 335.81 | 913.18 | 1473.09 |
| | 361.73 | 960.65 | 1552.30 |
| | 414.19 | 972.64 | 1625.56 |
| | 430.12 | 986.81 | 1793.89 |
| | 469.99 | 1041.25 | 1818.40 |
| | 524.10 | 1073.40 | 3122.03 |
| | 542.18 | 1108.85 | 3125.05 |
| | 554.35 | 1155.38 | 3133.01 |
| | 616.51 | 1181.12 | 3149.00 |
| | 691.23 | 1190.14 | 3164.14 |
| | 725.09 | 1203.76 | 3175.22 |
| | 736.66 | 1246.99 | 3185.89 |
| | 748.56 | 1287.47 | 3197.03 |

Table S16: Optimized geometry for I5. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.4682358296 | 0.6990340591 | 2.8220658509 |
| C | -0.4682358296 | -0.6990340591 | 2.8220658509 |
| C | -0.0508288517 | 1.3973989500 | 1.6849881688 |
| C | -0.0508288517 | -1.3973989500 | 1.6849881688 |
| C | 0.3704956670 | 0.7137063183 | 0.5372385302 |
| C | 0.3704956670 | -0.7137063183 | 0.5372385302 |
| H | -0.7932673320 | 1.2469390907 | 3.7074992160 |
| H | -0.7932673320 | -1.2469390907 | 3.7074992160 |
| H | -0.0505635690 | 2.4882879632 | 1.6842654990 |
| H | -0.0505635690 | -2.4882879632 | 1.6842654990 |
| C | 0.8295950992 | 1.4159340053 | -0.7134154972 |
| C | 0.8295950992 | -1.4159340053 | -0.7134154972 |
| C | 0.0795048113 | 1.3655799636 | -1.7972500111 |
| C | 0.0795048113 | -1.3655799636 | -1.7972500111 |
| C | -0.7178564336 | 0.7499341832 | -2.6543221192 |
| C | -0.7178564336 | -0.7499341832 | -2.6543221192 |
| H | 1.8434348687 | 1.8287542350 | -0.7434261479 |
| H | 1.8434348687 | -1.8287542350 | -0.7434261479 |
| H | -1.5081292476 | 1.2568972312 | -3.2100896855 |
| H | -1.5081292476 | -1.2568972312 | -3.2100896855 |
| | T1 Diagnostic | 0.01333278 | |
| | D1 Diagnostic | 0.04062285 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 91.70 | 791.04 | 1287.68 |
| | 105.54 | 807.16 | 1299.50 |
| | 196.41 | 842.23 | 1380.82 |
| | 266.89 | 864.77 | 1421.33 |
| | 269.73 | 880.13 | 1462.09 |
| | 320.16 | 898.77 | 1487.68 |
| | 369.84 | 917.04 | 1593.98 |
| | 426.86 | 955.52 | 1631.49 |
| | 445.56 | 994.38 | 1940.34 |
| | 483.02 | 1053.75 | 1966.94 |
| | 534.08 | 1070.56 | 3111.10 |
| | 534.52 | 1106.33 | 3112.68 |
| | 626.82 | 1123.78 | 3166.71 |
| | 634.71 | 1171.71 | 3167.75 |
| | 718.47 | 1181.84 | 3173.98 |
| | 725.96 | 1219.19 | 3179.78 |
| | 740.52 | 1259.61 | 3183.76 |
| | 752.57 | 1264.99 | 3194.29 |

Table S17: Optimized geometry for I6. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.3291746004 | -0.6069447015 | -0.4714651922 |
| C | -0.0727037471 | -0.6707796577 | 1.0029392549 |
| C | -0.2135934559 | 0.6955391233 | 1.4494361178 |
| C | 0.0344293414 | 1.5943406684 | 0.3816522242 |
| C | 0.2031151637 | 0.8656037741 | -0.7942348556 |
| C | 0.1615498709 | 1.2876547719 | -2.1527723051 |
| C | -0.0681262161 | 0.3517811363 | -3.1329630069 |
| C | -0.2804573713 | -1.0449868569 | -2.8194117252 |
| C | -0.1521341303 | -1.5158697665 | -1.5513957150 |
| H | -0.3008588940 | -2.5717634428 | -1.3232555684 |
| H | -0.5555704623 | -1.7228736774 | -3.6286645673 |
| H | -0.1606592183 | 0.6713010468 | -4.1720198354 |
| H | 0.2086051250 | 2.3495838709 | -2.3981324288 |
| H | 0.0650478669 | 2.6804001243 | 0.4589604613 |
| C | -0.2800088503 | 0.7485434376 | 2.9192702039 |
| C | -0.0742309663 | -0.5387975749 | 3.3304091909 |
| C | 0.4036782029 | -1.2758834229 | 2.1422262861 |
| H | -0.1273017547 | -0.9399685136 | 4.3397670641 |
| H | -0.4405638201 | 1.6420591973 | 3.5194282131 |
| H | 1.4222135913 | -0.8003307482 | -0.4149756625 |
| | T1 Diagnostic | 0.02985487 | |
| | D1 Diagnostic | 0.18380480 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 110.00 | 826.12 | 1301.31 |
| | 136.24 | 852.54 | 1342.37 |
| | 216.65 | 863.01 | 1374.49 |
| | 286.78 | 866.40 | 1415.06 |
| | 315.40 | 955.48 | 1435.91 |
| | 413.67 | 960.94 | 1450.39 |
| | 452.71 | 978.94 | 1494.33 |
| | 473.25 | 984.12 | 1525.10 |
| | 496.22 | 1000.11 | 1548.70 |
| | 524.79 | 1036.19 | 1649.26 |
| | 555.74 | 1058.12 | 2937.85 |
| | 610.64 | 1086.28 | 3167.82 |
| | 659.30 | 1112.98 | 3174.96 |
| | 662.87 | 1136.67 | 3188.51 |
| | 702.70 | 1157.55 | 3196.50 |
| | 712.97 | 1176.59 | 3199.25 |
| | 763.84 | 1212.39 | 3202.42 |
| | 800.45 | 1238.61 | 3229.79 |

Table S18: Optimized geometry for I7. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.7091032873 | 0.2431605817 | -3.0032617398 |
| C | 0.7457249364 | 0.2585160278 | -3.0019366818 |
| C | 1.4444677559 | -0.0346614354 | -1.8883467784 |
| C | 0.7456944719 | -0.5147597630 | -0.6292192287 |
| C | -0.7478818481 | -0.1313315907 | -0.5744234868 |
| C | -1.4055246374 | 0.0591780962 | -1.8446300081 |
| H | -2.4935011164 | 0.1467207640 | -1.8504208301 |
| C | -1.4898385882 | -0.0812000134 | 0.6027015876 |
| C | -1.2973891591 | -0.2975668677 | 1.9633230398 |
| C | -0.6216813726 | 0.2285277346 | 3.0832692043 |
| C | 0.7541926936 | 0.3344678938 | 3.1052031689 |
| C | 1.3650935656 | 0.0621038814 | 1.8539013540 |
| C | 1.3510637169 | -0.1495800367 | 0.6526014833 |
| H | 0.7781331086 | -1.6253253564 | -0.6759414417 |
| H | 1.3108042371 | 0.4908591363 | 4.0287353526 |
| H | -1.1890435239 | 0.3390002312 | 4.0138768478 |
| H | -2.5761719544 | -0.0505190203 | 0.4033969724 |
| H | 2.5343270576 | -0.0215043617 | -1.8761364159 |
| H | 1.2703700665 | 0.5349491502 | -3.9179682682 |
| H | -1.2414638708 | 0.4616300184 | -3.9290364443 |
| | T1 Diagnostic | 0.02307370 | |
| | D1 Diagnostic | 0.12831582 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 75.44 | 763.98 | 1302.56 |
| | 95.81 | 796.08 | 1326.66 |
| | 190.77 | 804.68 | 1379.55 |
| | 216.23 | 835.15 | 1416.65 |
| | 239.06 | 878.02 | 1445.58 |
| | 258.70 | 922.84 | 1457.40 |
| | 339.02 | 955.19 | 1508.67 |
| | 397.01 | 971.55 | 1580.36 |
| | 414.41 | 982.01 | 1677.53 |
| | 444.74 | 993.39 | 2268.16 |
| | 497.09 | 1038.31 | 2901.14 |
| | 513.92 | 1140.65 | 3018.22 |
| | 531.26 | 1154.34 | 3122.14 |
| | 598.96 | 1165.53 | 3164.01 |
| | 612.18 | 1187.16 | 3170.43 |
| | 631.84 | 1195.70 | 3190.89 |
| | 684.11 | 1233.07 | 3190.95 |
| | 733.56 | 1263.20 | 3197.83 |

Table S19: Optimized geometry for I8. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.7788034241 | -0.8492843575 | -0.6615243724 |
| C | 0.5102633142 | -1.2742382459 | 0.7191757783 |
| C | -0.2168650921 | 1.3456546039 | 1.6754429503 |
| C | 0.2082404935 | 1.3035529350 | 0.5296649742 |
| C | 0.8176010196 | 0.7689281331 | -0.6999270581 |
| C | 0.2196387679 | 1.3635787433 | -1.9625415920 |
| C | -0.5065204440 | 0.6513353355 | -2.8378580239 |
| C | -0.7883552545 | -0.7706385437 | -2.6272682097 |
| C | -0.2292992501 | -1.4609546346 | -1.6215383626 |
| H | -0.4688088009 | -2.5125666617 | -1.4607812821 |
| H | -1.4865751631 | -1.2679761972 | -3.3025031034 |
| H | -0.9266620800 | 1.1402441982 | -3.7182637817 |
| H | 0.3821237334 | 2.4325495160 | -2.1094476360 |
| H | 1.8852781188 | 1.0394038832 | -0.6768949666 |
| C | -0.5519811021 | 0.7671485929 | 2.9331754080 |
| C | -0.3524816022 | -0.5872957270 | 3.0468155868 |
| C | 0.1378787457 | -1.2481876508 | 1.8833377238 |
| H | -0.5603807293 | -1.1115519108 | 3.9792004854 |
| H | -0.9281080562 | 1.3545152768 | 3.7704524695 |
| H | 1.7823079349 | -1.1890056688 | -0.9737003311 |
| | T1 Diagnostic | 0.01358602 | |
| | D1 Diagnostic | 0.03713162 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 43.30 | 755.52 | 1289.43 |
| | 84.23 | 781.60 | 1296.08 |
| | 185.64 | 865.35 | 1372.90 |
| | 244.10 | 899.03 | 1390.47 |
| | 260.13 | 948.60 | 1430.03 |
| | 345.48 | 955.51 | 1519.21 |
| | 366.75 | 958.93 | 1660.63 |
| | 415.03 | 972.35 | 1712.30 |
| | 438.25 | 978.76 | 2236.36 |
| | 452.99 | 991.57 | 2266.63 |
| | 484.41 | 1059.38 | 2981.14 |
| | 533.00 | 1114.29 | 3015.97 |
| | 570.70 | 1166.01 | 3163.24 |
| | 578.57 | 1187.14 | 3171.44 |
| | 636.28 | 1201.69 | 3184.94 |
| | 654.14 | 1206.41 | 3185.71 |
| | 728.46 | 1238.28 | 3193.31 |
| | 743.98 | 1275.85 | 3201.15 |

Table S20: Optimized geometry for I9. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.6641662935 | 0.7341713144 | 2.5407058366 |
| C | -0.6641662935 | -0.7341713144 | 2.5407058366 |
| H | -1.2713652040 | 1.2469862442 | 3.2888500525 |
| H | -1.2713652040 | -1.2469862442 | 3.2888500525 |
| C | 0.0538459646 | 1.4502721591 | 1.6560258602 |
| C | 0.0538459646 | -1.4502721591 | 1.6560258602 |
| H | 0.0345304271 | 2.5416703024 | 1.6798249933 |
| H | 0.0345304271 | -2.5416703024 | 1.6798249933 |
| C | 0.9065044526 | 0.7925468540 | 0.6054450622 |
| C | 0.9065044526 | -0.7925468540 | 0.6054450622 |
| H | 1.9138332689 | 1.2371733333 | 0.5848343312 |
| H | 1.9138332689 | -1.2371733333 | 0.5848343312 |
| C | 0.2801750618 | 0.6827798313 | -0.7919073691 |
| C | 0.2801750618 | -0.6827798313 | -0.7919073691 |
| C | -0.1264709561 | 1.6684533321 | -1.7151294815 |
| C | -0.1264709561 | -1.6684533321 | -1.7151294815 |
| C | -0.4446207704 | 2.5476353871 | -2.4941362925 |
| C | -0.4446207704 | -2.5476353871 | -2.4941362925 |
| H | -0.7397675563 | 3.3116671109 | -3.1821920673 |
| H | -0.7397675563 | -3.3116671109 | -3.1821920673 |
| | T1 Diagnostic | 0.01340479 | |
| | D1 Diagnostic | 0.03759379 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 59.53 | 646.31 | 1247.03 |
| | 81.30 | 646.71 | 1324.97 |
| | 98.74 | 732.74 | 1325.57 |
| | 122.82 | 763.53 | 1381.47 |
| | 146.90 | 792.28 | 1429.84 |
| | 184.78 | 805.28 | 1634.07 |
| | 240.34 | 928.29 | 1646.89 |
| | 329.28 | 948.61 | 1699.41 |
| | 389.38 | 969.25 | 2179.20 |
| | 431.21 | 977.53 | 2195.64 |
| | 448.80 | 986.22 | 3020.26 |
| | 457.62 | 1051.60 | 3030.16 |
| | 529.87 | 1060.69 | 3156.01 |
| | 556.58 | 1130.54 | 3161.38 |
| | 585.79 | 1171.81 | 3176.24 |
| | 586.99 | 1185.02 | 3185.59 |
| | 597.23 | 1197.08 | 3473.55 |
| | 632.69 | 1214.73 | 3473.64 |

Table S21: Optimized geometry for I10. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.4269479357 | -1.1715853817 | -0.7456352942 |
| C | 1.4624568977 | -0.4081922280 | -1.4305389900 |
| C | 2.3499973458 | 0.3483611008 | -0.7306694536 |
| C | 2.3567749609 | 0.3402228239 | 0.7154107668 |
| H | 3.1222393047 | 0.9115551387 | 1.2416024628 |
| C | 1.4756378028 | -0.4239676139 | 1.4149613647 |
| H | 1.5378450492 | -0.4971525714 | 2.5007037220 |
| C | 0.4331999440 | -1.1793883510 | 0.7312344199 |
| H | -0.0182381632 | -2.0210282339 | 1.2474837638 |
| H | 3.1104502912 | 0.9257195552 | -1.2575543678 |
| H | 1.5145355600 | -0.4691989532 | -2.5175616357 |
| C | -0.7809122465 | -0.3142975674 | 0.0041506363 |
| C | -1.9930922915 | -1.0316994817 | 0.0039991832 |
| C | -3.2044031201 | -0.3798968500 | 0.0105822575 |
| C | -4.3543161254 | 0.0647473956 | 0.0100409284 |
| H | -5.3457085499 | 0.4650744699 | 0.0115757644 |
| C | -0.6818321003 | 1.1167161969 | 0.0115043295 |
| C | -0.6851573572 | 2.3308972032 | 0.0193076697 |
| H | -0.6961642672 | 3.4000047124 | 0.0264073276 |
| H | -0.0302608706 | -2.0068913644 | -1.2670048554 |
| | T1 Diagnostic | 0.01721223 | |
| | D1 Diagnostic | 0.06474417 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 55.41 | 638.93 | 1200.92 |
| | 94.81 | 666.65 | 1343.00 |
| | 122.01 | 696.08 | 1353.37 |
| | 125.55 | 720.38 | 1398.77 |
| | 209.07 | 742.93 | 1427.18 |
| | 212.53 | 796.46 | 1456.27 |
| | 232.44 | 822.71 | 1586.34 |
| | 264.54 | 922.00 | 1666.80 |
| | 315.64 | 968.14 | 2045.86 |
| | 374.09 | 980.26 | 2194.98 |
| | 382.26 | 980.37 | 3174.37 |
| | 421.14 | 983.58 | 3182.74 |
| | 459.96 | 992.18 | 3193.99 |
| | 490.90 | 1009.93 | 3200.46 |
| | 509.92 | 1095.55 | 3215.02 |
| | 582.50 | 1122.34 | 3219.09 |
| | 589.11 | 1176.17 | 3474.49 |
| | 610.18 | 1194.31 | 3477.64 |

Table S22: Optimized geometry for I11. Cartesian coordinates in Å.

## 2.4 Transition States

| | | | |
|---|---|---|---|
| C | 0.0009363646 | 0.0010430485 | -0.0019065142 |
| C | 0.0013465005 | -0.0007387981 | 1.3822491152 |
| C | 1.1107356888 | -0.0022125799 | 2.2017645755 |
| C | 2.3652615643 | -0.0019965158 | 1.5661395714 |
| C | 2.4377146651 | -0.0005867283 | 0.1689140125 |
| C | 1.2745896332 | 0.0004998465 | -0.6084660482 |
| H | 1.3418903261 | -0.0019577955 | -1.697755471 |
| H | 3.4111183608 | -0.0015173632 | -0.3223002347 |
| H | 3.276774886 | -0.0035744275 | 2.16598254 |
| H | 1.0299841516 | -0.0040004813 | 3.2893332556 |
| C | -1.2575707355 | 0.009223229 | -0.8113558586 |
| C | -1.8975325009 | -1.150562948 | -1.2128953541 |
| C | -3.0526956444 | -1.2322207926 | -1.9620834747 |
| C | -3.6370210967 | -0.0152084555 | -2.3561634991 |
| C | -3.042208231 | 1.1952801661 | -1.9841342185 |
| C | -1.8691043423 | 1.2123171949 | -1.2220859481 |
| H | -1.414890641 | 2.1619576043 | -0.9340583904 |
| H | -3.4971042252 | 2.137930932 | -2.2895621233 |
| H | -4.5524274592 | -0.0206995781 | -2.9500251703 |
| H | -3.4990212868 | -2.1877167445 | -2.2398433594 |

| | |
|---|---|
| T1 Diagnostic | 0.01442271 |
| D1 Diagnostic | 0.04289699 |

B3LYP/aug-cc-pVDZ Harmonic Frequencies

| | | |
|---|---|---|
| 58.1463$i$ | 846.7557 | 1325.7918 |
| 91.0380 | 847.1368 | 1326.5011 |
| 91.1515 | 937.9520 | 1425.6950 |
| 292.3186 | 938.2400 | 1426.3236 |
| 293.9068 | 976.0193 | 1452.1951 |
| 298.6726 | 982.0879 | 1483.9235 |
| 409.8485 | 982.2999 | 1566.9811 |
| 413.6263 | 983.1416 | 1571.6606 |
| 541.0649 | 1022.9203 | 1631.9141 |
| 541.3517 | 1040.0840 | 1638.8906 |
| 599.0538 | 1063.9886 | 3166.5028 |
| 621.8843 | 1114.8976 | 3166.5399 |
| 624.9599 | 1116.1950 | 3173.1922 |
| 704.8986 | 1163.9482 | 3173.2588 |
| 705.6357 | 1165.0909 | 3184.2439 |
| 741.3208 | 1229.7712 | 3184.3103 |
| 744.2791 | 1236.3875 | 3195.7889 |
| 744.3565 | 1295.4714 | 3195.9302 |

Table S23: Optimized geometry for TS1. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.0058636309 | -0.0040490812 | 0.0637294643 |
| C | -1.4961658327 | -0.0349705087 | 0.0252531027 |
| C | -1.5048902595 | -1.4544710345 | 0.0018703658 |
| C | 0.0266500381 | -1.4815013096 | 0.0728525523 |
| C | 1.1553176234 | -2.3284068139 | -0.1558929888 |
| C | 2.3559726907 | -1.4726827822 | -0.1632923803 |
| C | 2.3521705584 | -0.0937166101 | -0.1416577305 |
| C | 1.1478178 | 0.7038045499 | -0.0546153043 |
| H | 1.1984094255 | 1.7909050108 | -0.1177106834 |
| H | 3.3052515966 | 0.4369669436 | -0.2106213829 |
| H | 3.3232363994 | -1.9733291988 | -0.2502438472 |
| C | -2.6700976153 | -2.1872688539 | -0.1008481494 |
| C | -3.8654486488 | -1.4324771776 | -0.1590936977 |
| C | -3.8619481173 | -0.0326780695 | -0.129976869 |
| C | -2.6638183854 | 0.7095702176 | -0.0441855681 |
| H | -2.6786262471 | 1.7989890553 | -0.0379198893 |
| H | -4.8135992735 | 0.4974037226 | -0.1806212961 |
| H | -4.8202516965 | -1.9547151999 | -0.2297881732 |
| H | -2.687065546 | -3.2757249666 | -0.1347667923 |
| H | 0.4762181209 | -2.0301838932 | 1.0699672671 |
| | T1 Diagnostic | 0.01392361 | |
| | D1 Diagnostic | 0.04990677 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 787.1590$i$ | 813.7272 | 1296.3433 |
| | 104.7559 | 879.0443 | 1345.2926 |
| | 137.9886 | 909.3610 | 1412.0432 |
| | 212.8622 | 921.9231 | 1429.8840 |
| | 313.7338 | 938.7636 | 1461.2334 |
| | 345.5203 | 954.9092 | 1476.4071 |
| | 398.3373 | 998.9779 | 1514.0937 |
| | 412.7291 | 1007.2944 | 1627.4865 |
| | 460.8540 | 1011.4331 | 1631.3257 |
| | 563.2094 | 1014.5963 | 1699.3553 |
| | 567.0386 | 1037.5345 | 2236.2804 |
| | 602.0299 | 1067.3271 | 3145.2964 |
| | 613.9818 | 1100.2572 | 3162.7587 |
| | 709.5232 | 1129.5139 | 3173.9918 |
| | 739.0471 | 1160.0838 | 3184.3374 |
| | 749.9506 | 1178.4528 | 3185.3645 |
| | 763.9616 | 1216.0131 | 3195.8987 |
| | 783.6320 | 1275.5682 | 3202.2901 |

Table S24: Optimized geometry for TS2. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -3.2189970497 | 0.5025213894 | -0.119913535 |
| H | -4.2046007481 | 0.871100986 | -0.4008987857 |
| C | -2.9578135987 | -0.7642715947 | 0.2785026844 |
| H | -3.6875990621 | -1.5709445683 | 0.3244856931 |
| C | -2.0104147935 | 1.3121384573 | -0.234160077 |
| H | -2.0142230239 | 2.3935807443 | -0.3671840976 |
| C | -0.8766455742 | 0.5716406929 | -0.1705304549 |
| C | -1.5111084187 | -1.0076637655 | 0.5787653652 |
| H | -1.2197232204 | -1.1488492828 | 1.635488202 |
| C | -0.648552152 | -1.1058135753 | -0.5102714484 |
| C | 0.7853893185 | -0.8141058382 | -0.2291607842 |
| C | 2.9337355229 | 0.8997151778 | 0.1976031718 |
| C | 2.057749245 | -1.3647349621 | -0.2048345661 |
| C | 0.5876012711 | 0.578982666 | -0.0435886244 |
| C | 1.6390895881 | 1.4560546877 | 0.182717808 |
| C | 3.1314216187 | -0.4741960049 | 0.0100719778 |
| H | 2.23790845 | -2.4287352245 | -0.3560044713 |
| H | 1.4823549855 | 2.5223066481 | 0.3474515822 |
| H | 4.1491485703 | -0.8669694687 | 0.0256505251 |
| H | 3.7954240711 | 1.5481418356 | 0.3559328353 |
| | T1 Diagnostic | 0.01684149 | |
| | D1 Diagnostic | 0.08582496 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 534.7087$i$ | 835.3875 | 1292.4197 |
| | 113.0865 | 846.8417 | 1367.3486 |
| | 161.6253 | 860.8119 | 1385.0803 |
| | 217.9411 | 892.8741 | 1431.8162 |
| | 333.2438 | 922.3753 | 1455.8447 |
| | 363.2179 | 925.2457 | 1477.6232 |
| | 382.4176 | 954.8583 | 1568.0094 |
| | 436.3473 | 977.4556 | 1612.5626 |
| | 451.3980 | 1004.1735 | 1627.8845 |
| | 515.8435 | 1019.3108 | 1684.4135 |
| | 541.7761 | 1025.5765 | 2999.6742 |
| | 586.9722 | 1074.8777 | 3170.0860 |
| | 597.4258 | 1110.9011 | 3178.1346 |
| | 641.7469 | 1126.2492 | 3188.6039 |
| | 715.7519 | 1145.9453 | 3193.4414 |
| | 740.9605 | 1172.4922 | 3198.2782 |
| | 749.1511 | 1243.0995 | 3202.7501 |
| | 765.6092 | 1260.5459 | 3219.6177 |

Table S25: Optimized geometry for TS3. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.0078966781 | 0.0175093493 | -0.0236838267 |
| C | -0.0009695122 | -0.019699564 | 1.5515894176 |
| C | 1.4646951222 | -0.0396735343 | 1.5358953157 |
| C | 1.5222044176 | -0.0020537844 | 0.1273091299 |
| C | 2.6997250907 | -0.0751054677 | -0.5840973331 |
| C | 3.8815837816 | -0.1265719059 | 0.1936558858 |
| C | 3.8364039813 | -0.145038629 | 1.594127292 |
| C | 2.6220081725 | -0.1245504838 | 2.3090890125 |
| H | 2.6111001741 | -0.1509687554 | 3.3980328587 |
| H | 4.775780838 | -0.180584379 | 2.1477983587 |
| H | 4.8499047629 | -0.1492566901 | -0.3068355136 |
| H | 2.7412713371 | -0.0755849132 | -1.6731566412 |
| C | -0.9961220886 | -0.5048067616 | 2.463743888 |
| C | -1.7828168588 | -1.5416046482 | 2.0554616531 |
| C | -1.4776359874 | -2.0342671065 | 0.6938400573 |
| C | -0.6677727924 | -1.2537809905 | -0.0069701165 |
| H | -1.9970992013 | -2.8986100085 | 0.2745530864 |
| H | -2.6586901341 | -1.897459175 | 2.6017169482 |
| H | -1.0690303422 | -0.0826446285 | 3.4673951889 |
| H | -0.4758536959 | 0.8042109324 | -0.6298333509 |
| | T1 Diagnostic | 0.01722609 | |
| | D1 Diagnostic | 0.08606647 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 333.5226$i$ | 838.4987 | 1284.6267 |
| | 93.1797 | 847.0832 | 1293.9200 |
| | 136.8523 | 858.9768 | 1373.4720 |
| | 198.3796 | 877.0367 | 1434.9984 |
| | 286.6542 | 917.8191 | 1456.3198 |
| | 384.9497 | 926.0359 | 1474.3241 |
| | 406.2948 | 977.7546 | 1556.4410 |
| | 445.6295 | 980.7528 | 1616.9112 |
| | 475.2738 | 1010.0991 | 1654.8738 |
| | 557.4884 | 1015.3639 | 1734.4492 |
| | 567.5949 | 1071.0733 | 3062.5615 |
| | 598.4565 | 1091.7900 | 3155.1881 |
| | 622.5646 | 1109.4314 | 3166.7327 |
| | 657.5133 | 1137.3512 | 3170.5061 |
| | 713.5345 | 1145.8012 | 3181.4330 |
| | 737.6502 | 1175.7012 | 3185.1965 |
| | 758.0953 | 1234.2171 | 3191.7977 |
| | 768.9657 | 1247.8680 | 3198.7226 |

Table S26: Optimized geometry for TS4. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -3.2678767787 | 0.536103057 | -0.09239488 |
| H | -4.2785640518 | 0.92750483 | -0.1964443554 |
| C | -2.9309661966 | -0.7743548269 | -0.0171432113 |
| H | -3.5934552855 | -1.6348550989 | -0.030577918 |
| C | -2.0472047865 | 1.4001535511 | -0.0425706109 |
| H | -2.0691684921 | 2.4840159156 | -0.146068428 |
| C | -0.9649374071 | 0.5948856012 | 0.083966801 |
| C | -1.4418125888 | -0.8196737804 | 0.0850288395 |
| H | -1.1310090227 | -1.5719027248 | 1.0581091735 |
| C | -0.3916581154 | -1.7749748713 | -0.0715044768 |
| C | 0.8188526017 | -0.8780260432 | -0.0159005854 |
| C | 2.8399182308 | 1.050625862 | 0.0068901724 |
| C | 2.1490393212 | -1.2824390244 | -0.0648718027 |
| C | 0.4942962369 | 0.5152751332 | 0.0444595115 |
| C | 1.5000508117 | 1.4774065636 | 0.0613972082 |
| C | 3.1636925199 | -0.3069981459 | -0.0572075729 |
| H | 2.3916985024 | -2.3437712239 | -0.1178658491 |
| H | 1.2658014586 | 2.5408321094 | 0.1188663608 |
| H | 4.2098448171 | -0.6106749597 | -0.1027220279 |
| H | 3.6384702251 | 1.7936940762 | 0.0145026514 |
| | T1 Diagnostic | 0.01413069 | |
| | D1 Diagnostic | 0.05112215 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 1063.8327$i$ | 812.1656 | 1298.4053 |
| | 115.6702 | 846.0109 | 1315.9075 |
| | 147.0696 | 865.0401 | 1366.3519 |
| | 250.2437 | 890.5825 | 1379.8322 |
| | 261.3357 | 919.4800 | 1451.5532 |
| | 336.4456 | 943.1184 | 1473.3643 |
| | 435.7422 | 956.6608 | 1567.3977 |
| | 460.6478 | 969.1555 | 1609.3851 |
| | 530.0300 | 998.7009 | 1634.9907 |
| | 531.9241 | 1036.5153 | 1670.5844 |
| | 563.6797 | 1059.4034 | 2125.2519 |
| | 583.5288 | 1077.9860 | 3169.3239 |
| | 672.5052 | 1097.5565 | 3179.4521 |
| | 679.0296 | 1140.3128 | 3189.1491 |
| | 744.6631 | 1165.6476 | 3199.1692 |
| | 758.8815 | 1173.1484 | 3200.0329 |
| | 768.0374 | 1218.4874 | 3213.8338 |
| | 796.6799 | 1264.9982 | 3245.5668 |

Table S27: Optimized geometry for TS5. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.121624842072 | -0.363862898201 | 0.435308612141 |
| C | 1.397472120829 | 0.043703999464 | 0.180161997404 |
| C | 1.402320719709 | 1.482814601096 | 0.512674294292 |
| C | 0.118696038280 | 1.889540679910 | 0.298479471904 |
| C | -1.079974084311 | 2.174952405240 | -0.181559741076 |
| H | -1.203741357641 | 2.973639727039 | -0.922800270108 |
| C | 2.622097720666 | 2.082426391609 | 0.931177520527 |
| C | 3.786950688214 | 1.398930463887 | 0.637724383901 |
| C | 3.776824759309 | 0.129156834586 | -0.021127084697 |
| C | 2.603628447626 | -0.555109163422 | -0.277162543272 |
| H | 2.606906843717 | -1.547052313716 | -0.727689263889 |
| H | 4.730362079597 | -0.327402609145 | -0.287819047184 |
| H | 4.748231279777 | 1.856123820260 | 0.873764985252 |
| H | 2.639136864368 | 3.074379144049 | 1.381376302550 |
| C | -1.060890592856 | -0.650055086000 | 0.953433261451 |
| C | -2.279709984274 | 0.126805199619 | 0.638356956568 |
| C | -2.287583395068 | 1.397290274353 | 0.172314786702 |
| H | -3.248920228062 | 1.879862232885 | -0.010481987004 |
| H | -3.234392881684 | -0.356407207599 | 0.851768914611 |
| H | -1.160368880269 | -1.448814495912 | 1.698242449927 |

| | |
|---|---|
| T1 Diagnostic | 0.01534847 |
| D1 Diagnostic | 0.05717683 |

B3LYP/aug-cc-pVDZ Harmonic Frequencies

| | | |
|---|---|---|
| 464.0765$i$ | 759.5834 | 1339.7766 |
| 107.3288 | 811.9144 | 1358.9374 |
| 165.8966 | 817.1932 | 1393.4140 |
| 198.5730 | 838.4193 | 1443.7674 |
| 267.6377 | 874.9598 | 1460.8151 |
| 343.6953 | 903.4864 | 1516.0612 |
| 360.5776 | 924.0747 | 1606.0947 |
| 403.5837 | 961.0780 | 1611.3111 |
| 438.5815 | 965.6039 | 1854.1787 |
| 481.4686 | 1001.7008 | 1879.1572 |
| 507.9430 | 1003.1814 | 3093.5370 |
| 551.4656 | 1099.0766 | 3093.7577 |
| 564.1894 | 1110.9192 | 3168.5356 |
| 609.9067 | 1168.9370 | 3174.9655 |
| 692.7163 | 1186.4319 | 3184.3721 |
| 722.1762 | 1205.3409 | 3188.4488 |
| 736.4117 | 1236.1455 | 3195.6371 |
| 747.2651 | 1279.3794 | 3202.3763 |

Table S28: Optimized geometry for TS6. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.005645937 | -0.0374594699 | 0.2129692331 |
| C | 1.2377462047 | 0.5095689744 | 0.390404741 |
| C | 2.5302056803 | 0.7613469383 | 0.5019190974 |
| C | 3.6903724121 | -0.02133213 | 0.0453286368 |
| C | 3.6821571131 | -1.3998050496 | -0.0985836448 |
| C | 2.4352351753 | -2.040885403 | -0.0221721122 |
| C | 1.1711114091 | -2.097179819 | 0.1555786634 |
| C | -0.096702811 | -1.4994252279 | 0.4059689053 |
| C | -1.3583920779 | -2.1351660761 | 0.4298257739 |
| C | -2.5068475879 | -1.4043587194 | 0.2004320063 |
| C | -2.4069273066 | -0.0249414207 | -0.1542239887 |
| C | -1.2030685034 | 0.6374081962 | -0.1901469379 |
| H | -1.1542057598 | 1.6930911988 | -0.4553865151 |
| H | -3.3171344633 | 0.5233320241 | -0.402341376 |
| H | -3.4840559205 | -1.8824029152 | 0.2516164672 |
| H | -1.4089002163 | -3.2079568591 | 0.6218021562 |
| H | 1.4348934854 | -2.1314494229 | -1.022748682 |
| H | 4.6029011644 | -1.9663326805 | -0.2217918979 |
| H | 4.665074119 | 0.461915783 | 0.1317335675 |
| H | 2.8477239464 | 1.4998610785 | 1.2551799066 |
| | T1 Diagnostic | 0.03396611 | |
| | D1 Diagnostic | 0.21997410 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 1132.2699$i$ | 706.6714 | 1301.4333 |
| | 63.1516 | 724.5292 | 1329.5021 |
| | 135.1268 | 774.3775 | 1384.9141 |
| | 197.7064 | 783.2234 | 1439.2900 |
| | 205.3305 | 807.7514 | 1466.6400 |
| | 254.2246 | 814.0835 | 1474.7966 |
| | 332.7727 | 893.8084 | 1519.2693 |
| | 369.9674 | 921.9989 | 1626.7111 |
| | 392.6085 | 930.6328 | 1843.4392 |
| | 435.3792 | 964.0744 | 2018.4618 |
| | 473.8813 | 1010.8400 | 2408.4685 |
| | 500.6130 | 1017.7445 | 3042.7841 |
| | 523.3037 | 1112.3351 | 3168.7673 |
| | 554.9603 | 1135.6055 | 3173.4345 |
| | 563.0673 | 1172.8611 | 3174.7688 |
| | 613.5958 | 1187.8766 | 3191.0072 |
| | 684.7192 | 1210.6760 | 3202.7173 |
| | 702.0356 | 1269.8177 | 3206.2819 |

Table S29: Optimized geometry for TS7. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.021562677452 | 0.043761621539 | -0.346625906352 |
| C | -1.432865024645 | 0.056638674776 | -0.439635167755 |
| C | -2.598662330670 | 0.717847448057 | -0.379064458821 |
| C | -3.808424071827 | -0.112432114967 | -0.293845092849 |
| C | -3.679746525550 | -1.453832690523 | -0.012611023528 |
| C | -2.392475007529 | -1.952718798403 | 0.376170668298 |
| C | -1.375811852455 | -1.574082049030 | -0.584606265242 |
| C | 0.120912220661 | -1.364031506980 | -0.353954832159 |
| C | 1.341010307474 | -2.015497263885 | -0.260029515744 |
| C | 2.475854128796 | -1.192643753152 | -0.135317753415 |
| C | 2.377719940061 | 0.211394357303 | -0.122936438934 |
| C | 1.145214908217 | 0.869172209957 | -0.233313479237 |
| H | 1.082311998985 | 1.956707925099 | -0.216580032700 |
| H | 3.290064980109 | 0.800576710400 | -0.022864922529 |
| H | 3.461411215709 | -1.650782896941 | -0.044100564430 |
| H | 1.434315876324 | -3.101358038841 | -0.267103294083 |
| H | -1.616188365203 | -1.814794513032 | -1.637337767859 |
| H | -4.569634484813 | -2.065516234902 | 0.152873222789 |
| H | -4.791274711770 | 0.357888040429 | -0.327039301088 |
| H | -2.666537879323 | 1.806561873100 | -0.353771074363 |

| | |
|---|---|
| T1 Diagnostic | 0.01731862 |
| D1 Diagnostic | 0.08041929 |

B3LYP/aug-cc-pVDZ Harmonic Frequencies

| | | |
|---|---|---|
| 441.2088$i$ | 844.9777 | 1291.1056 |
| 106.9438 | 859.5005 | 1329.2591 |
| 159.4315 | 872.9580 | 1376.3014 |
| 216.7841 | 896.5663 | 1386.9773 |
| 316.1337 | 929.5785 | 1455.7004 |
| 357.2293 | 943.5675 | 1463.2612 |
| 393.9398 | 977.6515 | 1482.5705 |
| 428.0872 | 993.6168 | 1610.5251 |
| 472.2384 | 1000.5058 | 1629.5568 |
| 527.4575 | 1005.7807 | 1716.0687 |
| 564.4052 | 1019.9726 | 2973.0807 |
| 585.5106 | 1095.4807 | 3160.6971 |
| 622.8367 | 1126.5382 | 3171.6313 |
| 666.6545 | 1154.6787 | 3171.8809 |
| 700.1991 | 1163.6320 | 3181.7614 |
| 745.7990 | 1174.0722 | 3191.8778 |
| 758.6746 | 1198.9080 | 3194.5392 |
| 763.9492 | 1273.4221 | 3198.9913 |

Table S30: Optimized geometry for TS8. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.00107744 | 0.1556973278 | -0.0311789777 |
| C | -0.0475030143 | 0.1214978049 | 1.3636848788 |
| C | 1.1405759392 | 0.0064594504 | 2.0978947654 |
| C | 2.3757605549 | -0.1199935855 | 1.4599255666 |
| C | 2.4127737185 | -0.0848856541 | 0.0265928788 |
| C | 1.2280959306 | 0.0759124008 | -0.6992268774 |
| H | 1.263978539 | 0.1443386985 | -1.7864769615 |
| C | 3.7843140886 | -0.085007714 | -0.5125403984 |
| C | 4.5771551383 | -1.1415142313 | -0.5735244523 |
| C | 5.3886057536 | -2.065812744 | -0.0421769877 |
| C | 5.2418943778 | -2.0825246805 | 1.4443810219 |
| C | 4.5826248242 | -1.1143981575 | 2.064801248 |
| C | 3.6938563976 | -0.1443401565 | 2.1924256015 |
| H | 3.9564684898 | 0.7709537977 | 2.7344733088 |
| H | 5.5267842619 | -3.0077018058 | 1.9499473793 |
| H | 5.8683151276 | -2.876510564 | -0.5790470635 |
| H | 4.2657309459 | -0.5228917389 | -1.6930701262 |
| H | 1.1085281565 | -0.0014092502 | 3.1884045815 |
| H | -1.0034697199 | 0.193428732 | 1.882252033 |
| H | -0.9182472461 | 0.2618622796 | -0.6079959111 |
| | T1 Diagnostic | 0.01637891 | |
| | D1 Diagnostic | 0.06330282 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 1257.1414$i$ | 743.9126 | 1286.6002 |
| | 76.2503 | 755.8522 | 1302.4215 |
| | 125.5786 | 786.4329 | 1355.8769 |
| | 193.1147 | 812.3166 | 1406.4034 |
| | 245.0623 | 841.3742 | 1465.1629 |
| | 277.8964 | 868.7992 | 1477.0225 |
| | 307.8902 | 887.2648 | 1594.3029 |
| | 381.3329 | 936.9019 | 1628.6197 |
| | 415.5382 | 944.6340 | 1827.3122 |
| | 432.9315 | 984.9497 | 1948.7045 |
| | 463.0596 | 1050.4349 | 2155.0432 |
| | 479.0517 | 1064.0641 | 3105.2252 |
| | 541.0974 | 1108.5338 | 3160.3370 |
| | 581.0506 | 1115.6129 | 3170.3873 |
| | 632.9583 | 1172.6884 | 3176.2183 |
| | 648.0233 | 1189.6592 | 3187.3991 |
| | 694.9476 | 1227.8341 | 3199.2225 |
| | 730.4533 | 1258.7374 | 3252.9632 |

Table S31: Optimized geometry for TS9. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.0012396634 | 0.0256283956 | -0.0117321268 |
| C | -0.0001362271 | 0.005942969 | 1.5296654623 |
| C | 1.4071923807 | -0.0046367856 | 1.8988342388 |
| C | 2.2220325622 | 0.1262824857 | 0.7086026776 |
| C | 1.39660144 | 0.0968400134 | -0.3897036229 |
| C | 1.3899331502 | 0.2270273427 | -1.863918767 |
| C | 0.0804697188 | 0.2854708875 | -2.251082414 |
| C | -0.8312873184 | 0.4319273576 | -1.0722617256 |
| H | -0.2665951351 | 0.3428232925 | -3.2818771816 |
| H | 2.2717774446 | 0.2541606616 | -2.5023661188 |
| H | 3.3002112961 | 0.2742466001 | 0.7205209429 |
| C | 1.7611421 | -0.1961921017 | 3.2400113758 |
| C | 0.7605260798 | -0.4277178677 | 4.1860642822 |
| C | -0.6028522075 | -0.4789393757 | 3.8169470057 |
| C | -1.0001559442 | -0.2833366045 | 2.5024581935 |
| H | -2.0505492087 | -0.3095587924 | 2.2160688984 |
| H | -1.3553464884 | -0.6764999494 | 4.5805446859 |
| H | 1.0343407081 | -0.5888096463 | 5.2289290769 |
| H | 2.8101761965 | -0.1950792667 | 3.537285421 |
| H | -0.2324257441 | 1.0473412849 | 0.9693660119 |
| | T1 Diagnostic | 0.01818231 | |
| | D1 Diagnostic | 0.09428567 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 858.6020$i$ | 823.2218 | 1289.1193 |
| | 112.2446 | 842.0631 | 1322.3138 |
| | 182.4284 | 848.1515 | 1328.1140 |
| | 235.8860 | 878.4323 | 1384.4526 |
| | 272.3390 | 911.5345 | 1445.3701 |
| | 326.9973 | 943.8298 | 1478.2603 |
| | 426.4130 | 964.8481 | 1501.2793 |
| | 461.0129 | 984.0689 | 1560.8954 |
| | 493.6660 | 989.5848 | 1595.0417 |
| | 511.9204 | 1028.0613 | 1625.6053 |
| | 549.9525 | 1043.4851 | 2305.0698 |
| | 576.1180 | 1077.7792 | 3175.2682 |
| | 643.0403 | 1101.3698 | 3184.4846 |
| | 674.0450 | 1130.5144 | 3193.9421 |
| | 714.6338 | 1155.4154 | 3196.5056 |
| | 737.8898 | 1171.9502 | 3205.9246 |
| | 759.7087 | 1220.1294 | 3207.2910 |
| | 772.5201 | 1267.0847 | 3215.7396 |

Table S32: Optimized geometry for TS10. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.0626142975 | -0.0251405793 | -0.0371832271 |
| C | -0.0890161043 | 0.0619850177 | 1.3689351844 |
| C | 1.0793192492 | 0.0835349687 | 2.1018638636 |
| C | 2.3742325454 | 0.0336498445 | 1.4498184379 |
| C | 2.3862778324 | -0.1008257103 | -0.0214083643 |
| C | 1.1674412179 | -0.0771362911 | -0.6999946564 |
| H | 1.1866835389 | -0.1315068502 | -1.7901667997 |
| C | 3.6692209859 | -0.0142980623 | -0.7574372605 |
| C | 4.8412298054 | -0.5076892665 | -0.4016866206 |
| C | 5.9741065626 | -0.8118282916 | 0.2247554025 |
| C | 6.1200624316 | -0.3016009761 | 1.5987968305 |
| C | 4.8937748966 | -0.0639747079 | 2.1322052539 |
| C | 3.6406418879 | -0.2452925491 | 2.196431562 |
| H | 2.9662585241 | 1.0314907238 | 1.691483726 |
| H | 7.073391597 | -0.2584840406 | 2.1194209153 |
| H | 6.6735010134 | -1.5619266793 | -0.1527081509 |
| H | 3.6471811665 | 0.6771434091 | -1.6091092906 |
| H | 1.0570251169 | 0.1612392178 | 3.1880573511 |
| H | -1.0451519652 | 0.1059565085 | 1.8918508034 |
| H | -0.9916467903 | -0.066291071 | -0.6041521795 |
| | T1 Diagnostic | 0.01611278 | |
| | D1 Diagnostic | 0.06095786 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 665.0641$i$ | 727.5453 | 1271.0654 |
| | 111.7187 | 764.3575 | 1305.5014 |
| | 129.0006 | 772.4475 | 1374.5477 |
| | 185.1814 | 816.0192 | 1396.8243 |
| | 249.5289 | 839.6423 | 1442.6118 |
| | 288.8801 | 863.1577 | 1466.4763 |
| | 337.0881 | 940.6974 | 1538.2198 |
| | 363.6066 | 957.6704 | 1625.2924 |
| | 416.9405 | 968.3181 | 1912.3689 |
| | 449.0080 | 979.0527 | 1997.8656 |
| | 469.0715 | 1033.2649 | 2407.2119 |
| | 485.3274 | 1043.6305 | 3094.8694 |
| | 515.0188 | 1067.9105 | 3155.2285 |
| | 527.6651 | 1116.9322 | 3165.1963 |
| | 632.9985 | 1167.4720 | 3176.8646 |
| | 642.0073 | 1191.6618 | 3196.1352 |
| | 676.1129 | 1207.3510 | 3204.2717 |
| | 717.2109 | 1224.5360 | 3220.0916 |

Table S33: Optimized geometry for TS11. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.0632349412 | 0.0539432901 | 0.0192239029 |
| C | -0.1103881651 | 0.207385117 | 1.5406640408 |
| C | 1.3425211567 | 0.1042569784 | 2.0674254043 |
| C | 2.2016479996 | 0.1890360062 | 0.9636433623 |
| C | 1.450043643 | 0.17303647 | -0.2429859563 |
| C | 1.9223536305 | 0.6786737042 | -1.531866682 |
| C | 1.0475919739 | 1.3076991115 | -2.3534554617 |
| C | -0.3583031727 | 1.4818907509 | -1.9951115263 |
| C | -0.8843666579 | 0.9416573861 | -0.8769178054 |
| H | -1.9407100459 | 1.0664809515 | -0.6370215455 |
| H | -0.9904096741 | 2.0679618366 | -2.6634044359 |
| H | 1.4046079767 | 1.7504388093 | -3.2839305541 |
| H | 2.9875215174 | 0.6286079045 | -1.7559626046 |
| H | 2.2086263743 | -0.8487301779 | 0.0624936131 |
| C | 1.3834788675 | -0.3156360479 | 3.4342647366 |
| C | 0.057736737 | -0.5129936632 | 3.8209403473 |
| C | -0.6357665356 | -0.4095848356 | 2.5882010898 |
| H | -0.3542532269 | -0.7107255265 | 4.8047603871 |
| H | 2.284714555 | -0.4254406517 | 4.0344387546 |
| H | -0.3965014521 | -0.9786942002 | -0.1866414255 |
| | T1 Diagnostic | 0.02942740 | |
| | D1 Diagnostic | 0.17596485 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 1271.1145$i$ | 764.2571 | 1279.3266 |
| | 100.3226 | 783.0973 | 1301.9336 |
| | 117.3369 | 822.6978 | 1344.6947 |
| | 223.0549 | 836.6883 | 1392.7090 |
| | 242.4801 | 873.0023 | 1407.9640 |
| | 327.9828 | 959.7013 | 1449.0471 |
| | 403.9302 | 962.4711 | 1491.9702 |
| | 424.6884 | 970.5101 | 1603.1376 |
| | 489.2541 | 983.8129 | 1651.0381 |
| | 497.5168 | 1011.9552 | 1681.9110 |
| | 527.6712 | 1039.6181 | 1989.5668 |
| | 559.9938 | 1046.8258 | 2995.5788 |
| | 598.6980 | 1085.9384 | 3171.1703 |
| | 646.9134 | 1147.3638 | 3181.3314 |
| | 661.7872 | 1158.1096 | 3193.0238 |
| | 665.2151 | 1160.8000 | 3200.8880 |
| | 685.9525 | 1195.6216 | 3210.3107 |
| | 719.6925 | 1242.5876 | 3255.2010 |

Table S34: Optimized geometry for TS12. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.1118614112 | 0.3284039964 | 0.0276891685 |
| C | -0.0865492451 | 0.1042405818 | 1.4610680842 |
| C | 1.0546796149 | -0.1912718105 | 2.1170389845 |
| C | 2.404896208 | -0.1898887802 | 1.4308482515 |
| C | 2.2703215909 | -0.1699064595 | -0.1161478398 |
| C | 1.0237313468 | 0.1947604673 | -0.7199813296 |
| H | 0.9846212235 | 0.2693580021 | -1.8070302167 |
| C | 3.4351400545 | -0.5920392567 | -0.8487327571 |
| C | 4.5537138466 | -1.1778988712 | -0.7756170429 |
| C | 5.6358677694 | -1.927409165 | -0.3345266957 |
| C | 5.6921515361 | -2.1431056655 | 1.041019734 |
| C | 4.5780845545 | -1.6239476061 | 1.7427412611 |
| C | 3.4546185844 | -1.1387708483 | 1.857377506 |
| H | 2.8486888995 | 0.7890770184 | 1.7100462547 |
| H | 6.527958775 | -2.6551396523 | 1.5124331001 |
| H | 6.397616418 | -2.3137973407 | -1.012023355 |
| H | 3.3177123555 | 0.6290946188 | -0.8527105676 |
| H | 1.0619277443 | -0.3582999277 | 3.1939328315 |
| H | -1.0245954128 | 0.1573324271 | 2.0152793101 |
| H | -1.0612194661 | 0.539121539 | -0.4630216166 |
| | T1 Diagnostic | 0.02545600 | |
| | D1 Diagnostic | 0.14808700 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 1161.3886$i$ | 699.3934 | 1246.2502 |
| | 49.2249 | 742.4863 | 1291.1423 |
| | 101.1596 | 782.5726 | 1380.0320 |
| | 171.5404 | 817.5874 | 1405.5889 |
| | 226.8992 | 826.0383 | 1441.1838 |
| | 309.1981 | 879.2268 | 1465.4896 |
| | 335.3656 | 941.5063 | 1569.7501 |
| | 355.6523 | 950.8663 | 1670.6170 |
| | 408.6439 | 969.4775 | 2008.3544 |
| | 425.7230 | 979.0771 | 2161.1457 |
| | 466.2791 | 1001.1728 | 2197.2286 |
| | 490.1007 | 1040.5228 | 2935.4326 |
| | 520.7896 | 1106.6025 | 3172.4268 |
| | 545.5530 | 1120.4271 | 3179.3045 |
| | 553.6347 | 1148.9853 | 3185.8908 |
| | 632.6919 | 1161.5642 | 3195.2121 |
| | 671.4719 | 1205.1617 | 3204.0407 |
| | 687.8554 | 1229.4731 | 3214.1949 |

Table S35: Optimized geometry for TS13. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.7582145536 | -0.1331079919 | 0.7515957517 |
| C | 0.6708238265 | -0.009335173 | 0.5906645816 |
| C | -1.2984588583 | -0.2326419562 | 2.0480204677 |
| C | 1.4696411373 | 0.2583522654 | 1.7402390521 |
| C | -0.4806506544 | -0.0516724127 | 3.1583197639 |
| C | 0.8945656331 | 0.2338914559 | 2.9982994591 |
| C | -1.5426889252 | -0.0324517353 | -0.4209439512 |
| C | 1.1781465453 | -0.300207432 | -0.664100174 |
| C | -2.0606176472 | 0.186126462 | -1.510529977 |
| C | 1.3757600043 | -0.6490279093 | -1.876502897 |
| C | -0.3199555932 | 0.1190604441 | -3.5696414532 |
| C | 0.8877235133 | 0.2060016177 | -3.166227438 |
| H | -2.3712004643 | -0.3819215122 | 2.1673650421 |
| H | -0.9108476135 | -0.0918654642 | 4.1590336526 |
| H | 1.5122680897 | 0.4151896528 | 3.8782983244 |
| H | 2.5382768287 | 0.4297259232 | 1.6156098767 |
| H | 1.8306883544 | -1.5799211002 | -2.2172725569 |
| H | 1.7441034734 | 0.7456132664 | -3.5825349208 |
| H | -1.0514301698 | 0.3331326999 | -4.332245319 |
| H | -2.6864637635 | 0.5523218964 | -2.2955269728 |
| | T1 Diagnostic | 0.02852655 | |
| | D1 Diagnostic | 0.18401851 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 235.3243$i$ | 643.5506 | 1249.5132 |
| | 91.1738 | 664.4064 | 1279.7517 |
| | 120.8255 | 684.1531 | 1328.2509 |
| | 160.4572 | 723.2515 | 1450.5407 |
| | 178.5626 | 743.8275 | 1463.6656 |
| | 202.1400 | 757.8649 | 1548.3611 |
| | 215.1391 | 762.8617 | 1619.4738 |
| | 287.1997 | 779.0098 | 1702.4235 |
| | 361.2491 | 826.2394 | 1959.6456 |
| | 371.3224 | 856.9963 | 2124.3229 |
| | 420.4284 | 946.6735 | 3114.8957 |
| | 450.9157 | 982.6296 | 3168.9644 |
| | 465.6753 | 1037.2248 | 3176.9210 |
| | 506.9590 | 1052.6117 | 3186.5798 |
| | 539.5071 | 1106.0835 | 3197.2553 |
| | 561.7098 | 1144.4631 | 3204.1639 |
| | 574.5861 | 1167.6199 | 3355.6990 |
| | 591.7635 | 1200.4386 | 3473.9086 |

Table S36: Optimized geometry for TS14. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | -0.131237351029 | 0.021509360056 | -0.046086047945 |
| C | -1.573567988433 | -0.040381009211 | -0.464491982104 |
| C | -2.655837678138 | -0.569940988223 | -0.939227336905 |
| C | -3.777824214226 | 0.097888930369 | -1.402248384870 |
| C | -3.778422785718 | 1.526275243972 | -1.400683778945 |
| C | -2.657111863234 | 2.194001376170 | -0.936495931603 |
| C | -1.574348015254 | 1.664514082214 | -0.462964712321 |
| C | -0.131741371834 | 1.603452099802 | -0.045312403250 |
| C | 0.824560668038 | 2.261688079230 | -1.009100862340 |
| C | 1.621897047188 | 1.547742353574 | -1.820867304202 |
| C | 1.622958159363 | 0.079975126888 | -1.820954763191 |
| C | 0.826364265779 | -0.635224965878 | -1.009564761414 |
| H | 0.838430152428 | -1.725851092394 | -1.025780764938 |
| H | 2.299479000156 | -0.433508893629 | -2.505583996288 |
| H | 2.297445335585 | 2.062262078859 | -2.505674457954 |
| H | 0.835048939345 | 3.352335225885 | -1.025187381840 |
| H | 0.002420087118 | 2.013207402148 | 0.967628744994 |
| H | -4.695740765542 | 2.022114736133 | -1.715035076254 |
| H | -4.694553999961 | -0.398391175972 | -1.717404820888 |
| H | 0.002420378370 | -0.388830969995 | 0.966671022260 |
| | T1 Diagnostic | 0.01673429 | |
| | D1 Diagnostic | 0.07944648 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 360.6767$i$ | 785.8322 | 1300.2437 |
| | 52.9182 | 789.2890 | 1316.5012 |
| | 71.5990 | 863.1410 | 1322.4516 |
| | 193.8184 | 907.0478 | 1375.9169 |
| | 210.1330 | 917.4630 | 1403.4102 |
| | 380.1328 | 954.8463 | 1427.5314 |
| | 388.4281 | 956.1574 | 1654.1319 |
| | 431.8998 | 975.8233 | 1708.1356 |
| | 434.2073 | 988.0987 | 1748.4948 |
| | 472.9689 | 1026.8992 | 1855.5436 |
| | 551.6810 | 1067.1620 | 3022.2357 |
| | 555.0184 | 1083.1711 | 3033.3571 |
| | 600.3955 | 1151.1206 | 3166.3822 |
| | 606.4346 | 1188.6550 | 3173.2684 |
| | 647.2528 | 1197.4195 | 3187.0450 |
| | 684.2678 | 1222.2170 | 3194.1794 |
| | 692.0460 | 1237.3343 | 3197.5177 |
| | 723.9311 | 1242.0956 | 3214.3912 |

Table S37: Optimized geometry for TS15. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.002972368584 | -0.023877229844 | 0.081305962043 |
| C | -1.160720795861 | 0.812378129587 | -0.338327176216 |
| C | -1.783947792143 | 0.603840258492 | -1.519865992167 |
| C | -1.397650841889 | -0.498444965505 | -2.378917705647 |
| H | -1.919840646467 | -0.633338216010 | -3.326897011089 |
| C | -0.454197396998 | -1.410068697952 | -1.990367638115 |
| H | -0.236589188981 | -2.281012440561 | -2.607841758686 |
| C | 0.190875521344 | -1.284985703558 | -0.718472501813 |
| H | 0.636998107979 | -2.152200960922 | -0.249632171706 |
| H | -2.601922052577 | 1.251938069346 | -1.834740952893 |
| H | -1.464479443249 | 1.630983003893 | 0.314378394235 |
| C | 1.341417565597 | 0.378028431633 | -0.577437650000 |
| C | 2.343234128473 | -0.583567057762 | -0.425544472118 |
| C | 3.513182135709 | -0.563183654101 | -1.167328793441 |
| C | 4.585521472781 | -0.671244353888 | -1.758975007983 |
| H | 5.517551942218 | -0.752575333925 | -2.275012013911 |
| C | 1.420330517798 | 1.499147730508 | -1.454399538193 |
| C | 1.568843462474 | 2.428508185852 | -2.226953193438 |
| H | 1.710661649671 | 3.256028478218 | -2.889020599297 |
| H | 0.104246285535 | -0.150257673500 | 1.162397820434 |

| | |
|---|---|
| T1 Diagnostic | 0.02065010 |
| D1 Diagnostic | 0.10846305 |

B3LYP/aug-cc-pVDZ Harmonic Frequencies

| | | |
|---|---|---|
| 321.5993*i* | 637.9690 | 1208.7029 |
| 55.7746 | 649.8721 | 1344.7774 |
| 86.5486 | 687.8228 | 1354.1501 |
| 101.6013 | 707.4158 | 1415.5577 |
| 127.8555 | 767.2610 | 1455.8220 |
| 201.2438 | 774.7744 | 1463.3877 |
| 225.5823 | 837.1211 | 1567.5832 |
| 294.6564 | 871.8878 | 1670.0882 |
| 318.7941 | 966.3171 | 2075.2781 |
| 332.6268 | 970.8830 | 2163.7268 |
| 400.8431 | 983.2509 | 3116.4971 |
| 472.7202 | 989.5502 | 3176.4499 |
| 479.2424 | 993.9486 | 3184.5921 |
| 536.0093 | 1035.8453 | 3196.5990 |
| 566.2872 | 1114.6346 | 3202.7939 |
| 572.2522 | 1138.9263 | 3273.2613 |
| 592.3252 | 1177.1676 | 3476.4821 |
| 610.1921 | 1191.2061 | 3479.5597 |

Table S38: Optimized geometry for TS16. Cartesian coordinates in Å.

| | | | |
|---|---|---|---|
| C | 0.007606766904 | 0.046393562039 | -0.035999066862 |
| C | -0.005235089405 | 0.262263445973 | 1.431125885023 |
| H | 0.650712759600 | -0.339574543583 | 2.053646078953 |
| C | -1.222713970933 | 0.789919238345 | 2.032921983841 |
| H | -1.270276731094 | 0.865391493214 | 3.118734024645 |
| C | -2.275249795485 | 1.168453905701 | 1.259380916244 |
| C | -2.262792398413 | 0.958224643343 | -0.170810463892 |
| C | -1.198260557844 | 0.375597166948 | -0.784682845356 |
| H | -1.227224366880 | 0.135554459863 | -1.846981502975 |
| H | -3.150320204227 | 1.217034538827 | -0.748441816594 |
| H | -3.171934483244 | 1.579957370177 | 1.723020118566 |
| H | 0.672338107645 | -0.707804903289 | -0.447536789148 |
| C | 0.926094673185 | 1.302294602019 | 0.536507831509 |
| C | 2.273484545859 | 1.024720157900 | 0.591410856300 |
| C | 3.534637794319 | 0.871405496923 | 0.628534378493 |
| C | 4.795957695276 | 0.495534181175 | 0.698716597652 |
| H | 5.575373657823 | 1.263738515470 | 0.596639512644 |
| C | 0.441757361462 | 2.637953002438 | 0.334388825180 |
| C | 0.074888818417 | 3.781029093698 | 0.160238686628 |
| H | -0.233951582963 | 4.792853572817 | 0.006241789150 |
| | T1 Diagnostic | 0.01835618 | |
| | D1 Diagnostic | 0.06754873 | |
| | B3LYP/aug-cc-pVDZ Harmonic Frequencies | | |
| | 56.8048$i$ | 611.9508 | 1224.8971 |
| | 66.0967 | 645.9197 | 1347.1425 |
| | 123.2744 | 671.0172 | 1350.0174 |
| | 124.0447 | 713.9509 | 1426.4934 |
| | 195.7014 | 755.5365 | 1456.3420 |
| | 229.1394 | 817.1497 | 1531.5353 |
| | 267.0451 | 822.6437 | 1586.5211 |
| | 328.4226 | 916.4756 | 1667.3028 |
| | 361.8186 | 966.9241 | 1956.3958 |
| | 395.4377 | 977.8738 | 2207.6833 |
| | 414.0624 | 980.4606 | 3117.9948 |
| | 435.7259 | 984.1544 | 3178.4936 |
| | 441.0388 | 988.1294 | 3186.9853 |
| | 470.4645 | 1011.4338 | 3196.7288 |
| | 517.5650 | 1103.5710 | 3203.3670 |
| | 575.7751 | 1139.6492 | 3206.2920 |
| | 588.1775 | 1177.2448 | 3212.3418 |
| | 596.1405 | 1195.9549 | 3479.1275 |

Table S39: Optimized geometry for TS17. Cartesian coordinates in Å.

## 3 Frequencies

| 0.005 Å | | | 0.010 Å | | |
|---|---|---|---|---|---|
| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) | Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
| 3260.8 | 3118.8 | 3132.1 | 3261.0 | 3117.8 | 3131.1 |
| 3250.2 | 3108.6 | 3121.3 | 3250.4 | 3108.4 | 3120.8 |
| 3232.4 | 3094.9 | 3094.9 | 3232.6 | 3094.6 | 3094.6 |
| 3218.9 | 3081.2 | 3081.2 | 3219.2 | 3081.6 | 3081.6 |
| 1578.8 | 1540.5 | 1539.5 | 1579.1 | 1540.0 | 1538.8 |
| 1546.8 | 1507.4 | 1510.3 | 1547.2 | 1505.8 | 1508.4 |
| 1274.6 | 1249.5 | 1249.3 | 1273.9 | 1245.6 | 1245.3 |
| 1194.2 | 1174.6 | 1174.6 | 1193.3 | 1173.9 | 1173.9 |
| 1120.3 | 1095.6 | 1094.5 | 1119.8 | 1092.2 | 1090.8 |
| 1052.1 | 1033.8 | 1031.6 | 1051.3 | 1032.6 | 1030.0 |
| 948.8 | 928.2 | 928.0 | 948.6 | 927.3 | 927.1 |
| 873.6 | 859.4 | 859.4 | 873.5 | 853.0 | 853.0 |
| 847.5 | 850.7 | 850.7 | 847.8 | 845.0 | 845.0 |
| 818.6 | 936.1 | 936.1 | 819.1 | 922.0 | 922.0 |
| 727.4 | 715.9 | 715.9 | 727.4 | 713.4 | 713.4 |
| 577.2 | 573.8 | 573.8 | 577.7 | 568.7 | 568.7 |
| 563.3 | 606.1 | 606.1 | 563.9 | 594.8 | 594.8 |
| 521.0 | 538.8 | 538.8 | 521.2 | 524.4 | 524.4 |

Table S40: QFF harmonic, fundamental, and corrected fundamental frequencies for $C_4H_4$ computed at the F12-DZ level of theory with the inclusion of core correlation.

| 0.005 Å | | | 0.010 Å | | |
|---|---|---|---|---|---|
| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) | Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
| 3261.1 | 3117.0 | 3128.8 | 3261.4 | 3119.6 | 3134.3 |
| 3250.5 | 3109.6 | 3121.6 | 3250.8 | 3110.1 | 3123.8 |
| 3232.8 | 3093.0 | 3093.0 | 3233.0 | 3096.5 | 3096.5 |
| 3219.5 | 3080.0 | 3080.0 | 3219.7 | 3082.8 | 3082.8 |
| 1583.6 | 1533.8 | 1535.6 | 1583.9 | 1544.5 | 1543.0 |
| 1553.7 | 1509.6 | 1510.4 | 1554.1 | 1513.6 | 1516.5 |
| 1276.1 | 1232.5 | 1232.2 | 1275.4 | 1245.2 | 1245.0 |
| 1198.0 | 1155.1 | 1155.1 | 1197.1 | 1172.2 | 1172.2 |
| 1121.6 | 1083.3 | 1078.7 | 1121.1 | 1093.2 | 1082.7 |
| 1053.7 | 1012.5 | 1009.5 | 1052.9 | 1032.0 | 1029.1 |
| 952.5 | 912.1 | 911.4 | 952.3 | 930.8 | 930.5 |
| 873.4 | 843.1 | 843.1 | 873.3 | 852.3 | 852.3 |
| 857.3 | 822.1 | 822.1 | 857.6 | 834.3 | 834.3 |
| 844.4 | 816.6 | 816.6 | 844.7 | 840.8 | 840.8 |
| 731.1 | 687.4 | 687.4 | 731.1 | 716.6 | 716.6 |
| 580.3 | 533.7 | 533.7 | 580.8 | 565.4 | 565.4 |
| 576.3 | 583.6 | 583.6 | 576.8 | 579.9 | 579.9 |
| 525.5 | 476.6 | 476.6 | 525.6 | 513.2 | 513.2 |

Table S41: QFF harmonic, fundamental, and corrected fundamental frequencies for $C_4H_4$ computed at the F12-TZ level of theory with the inclusion of core correlation.

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 2963.9 | 2928.3 | 2928.5 |
| 2963.8 | 2927.8 | 2929.7 |
| 2961.6 | 2925.6 | 2936.3 |
| 2961.3 | 2926.1 | 2924.8 |
| 2953.5 | 2918.9 | 2915.5 |
| 2953.5 | 2918.0 | 2919.0 |
| 2946.8 | 2910.7 | 2915.3 |
| 2946.4 | 2910.3 | 2915.8 |
| 1757.4 | 1725.8 | 1721.4 |
| 1692.2 | 1666.9 | 1665.9 |
| 1609.0 | 1586.7 | 1585.5 |
| 1574.2 | 1554.2 | 1559.7 |
| 1425.7 | 1387.1 | 1387.1 |
| 1338.1 | 1327.0 | 1325.0 |
| 1323.9 | 1312.5 | 1312.6 |
| 1295.2 | 1284.6 | 1288.8 |
| 1266.3 | 1255.7 | 1255.2 |
| 1249.8 | 1192.1 | 1190.4 |
| 1129.0 | 1118.6 | 1118.3 |
| 1107.8 | 1098.5 | 1097.3 |
| 1080.9 | 1065.0 | 1064.8 |
| 1059.0 | 1051.5 | 1051.5 |
| 1048.7 | 1042.7 | 1042.7 |
| 1045.0 | 1037.4 | 1037.4 |
| 1026.4 | 1018.7 | 1018.6 |
| 1001.9 | 996.1 | 996.2 |
| 1000.2 | 981.0 | 984.4 |
| 967.4 | 960.9 | 960.9 |
| 963.0 | 956.1 | 955.7 |
| 959.5 | 952.5 | 952.5 |
| 957.1 | 948.4 | 947.5 |
| 946.6 | 941.3 | 941.3 |
| 937.2 | 918.9 | 918.3 |
| 926.5 | 918.8 | 918.7 |
| 875.3 | 868.8 | 868.3 |
| 803.0 | 796.2 | 796.2 |
| 776.0 | 768.5 | 759.0 |
| 740.5 | 737.0 | 736.9 |
| 727.4 | 725.4 | 725.0 |
| 723.7 | 719.7 | 719.7 |
| 635.9 | 629.8 | 629.2 |
| 553.6 | 550.1 | 550.1 |
| 538.8 | 535.0 | 535.0 |
| 514.7 | 511.5 | 511.6 |
| 444.6 | 441.2 | 442.4 |
| 415.0 | 411.4 | 411.4 |
| 391.3 | 390.8 | 390.8 |
| 363.2 | 360.4 | 360.8 |
| 352.4 | 349.5 | 349.5 |
| 294.2 | 294.7 | 294.7 |
| 242.6 | 241.2 | 241.2 |
| 202.1 | 201.4 | 201.4 |
| 113.9 | 115.8 | 115.8 |
| 101.3 | 101.6 | 101.6 |

Table S42: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for biphenylene generated with parameter set (a).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3102.5 | 3070.5 | 3077.4 |
| 3097.5 | 3063.1 | 3066.2 |
| 3084.1 | 3055.8 | 3051.9 |
| 3081.9 | 3053.6 | 3055.7 |
| 3073.9 | 3044.6 | 3057.0 |
| 3072.6 | 3041.7 | 3062.9 |
| 3060.1 | 3031.3 | 3050.4 |
| 3059.9 | 3030.8 | 3050.3 |
| 1658.8 | 1630.0 | 1626.1 |
| 1594.8 | 1561.9 | 1558.5 |
| 1565.9 | 1540.6 | 1542.9 |
| 1560.1 | 1533.0 | 1534.9 |
| 1464.5 | 1446.5 | 1450.3 |
| 1463.4 | 1445.0 | 1447.5 |
| 1443.2 | 1422.3 | 1419.2 |
| 1403.0 | 1387.1 | 1383.3 |
| 1361.8 | 1344.7 | 1342.7 |
| 1346.3 | 1330.1 | 1330.3 |
| 1344.6 | 1330.6 | 1330.7 |
| 1283.9 | 1268.6 | 1268.2 |
| 1248.6 | 1225.6 | 1224.2 |
| 1150.8 | 1117.3 | 1116.8 |
| 1087.5 | 1077.5 | 1083.1 |
| 1068.9 | 1054.4 | 1054.4 |
| 1068.1 | 1053.5 | 1053.5 |
| 1060.7 | 1048.3 | 1050.2 |
| 1025.7 | 1013.3 | 1013.3 |
| 1012.3 | 1000.1 | 999.9 |
| 1007.4 | 996.5 | 996.5 |
| 989.0 | 976.3 | 976.3 |
| 976.2 | 965.0 | 964.8 |
| 974.8 | 963.2 | 961.9 |
| 958.5 | 950.6 | 950.6 |
| 904.3 | 893.1 | 893.2 |
| 868.9 | 858.3 | 858.3 |
| 820.7 | 812.0 | 812.7 |
| 804.1 | 796.5 | 796.5 |
| 789.6 | 780.7 | 780.7 |
| 787.0 | 782.0 | 782.0 |
| 736.4 | 728.3 | 730.4 |
| 679.4 | 671.1 | 671.4 |
| 660.9 | 651.7 | 651.7 |
| 585.5 | 579.1 | 579.1 |
| 576.2 | 569.7 | 569.8 |
| 525.8 | 518.6 | 518.6 |
| 510.6 | 504.3 | 506.9 |
| 425.8 | 420.3 | 420.3 |
| 422.9 | 419.3 | 419.3 |
| 383.0 | 377.4 | 378.0 |
| 361.9 | 357.5 | 357.5 |
| 298.9 | 294.8 | 294.8 |
| 215.4 | 212.7 | 212.7 |
| 135.7 | 134.1 | 134.1 |
| 107.7 | 105.8 | 105.8 |

Table S43: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for biphenylene generated with parameter set (b).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3202.6 | 3149.5 | 3149.3 |
| 3185.6 | 3135.4 | 3137.0 |
| 3143.5 | 3099.2 | 3099.8 |
| 3138.6 | 3090.5 | 3091.2 |
| 3111.6 | 3054.1 | 3052.8 |
| 3110.3 | 3052.8 | 3054.0 |
| 3095.2 | 3040.8 | 3041.1 |
| 3093.1 | 3037.3 | 3038.4 |
| 2114.5 | 2089.6 | 2092.9 |
| 1985.1 | 1954.8 | 1956.2 |
| 1904.3 | 1870.3 | 1881.4 |
| 1780.5 | 1743.7 | 1733.6 |
| 1608.9 | 1580.1 | 1578.8 |
| 1565.8 | 1535.2 | 1536.6 |
| 1563.3 | 1529.1 | 1529.4 |
| 1519.0 | 1485.4 | 1485.2 |
| 1500.8 | 1480.3 | 1479.9 |
| 1453.6 | 1422.1 | 1420.0 |
| 1400.1 | 1371.1 | 1374.2 |
| 1342.9 | 1319.2 | 1319.8 |
| 1301.7 | 1283.2 | 1279.8 |
| 1244.1 | 1225.9 | 1226.7 |
| 1237.7 | 1218.9 | 1221.1 |
| 1156.9 | 1138.6 | 1138.3 |
| 1155.0 | 1136.7 | 1141.2 |
| 1139.9 | 1120.9 | 1121.0 |
| 1135.5 | 1108.6 | 1105.1 |
| 1013.6 | 978.3 | 977.7 |
| 966.1 | 921.1 | 917.0 |
| 966.1 | 944.7 | 943.5 |
| 949.4 | 906.6 | 907.6 |
| 946.7 | 926.4 | 926.3 |
| 911.9 | 888.2 | 888.2 |
| 903.1 | 879.3 | 878.7 |
| 889.2 | 845.4 | 845.4 |
| 879.9 | 860.7 | 860.7 |
| 864.7 | 837.7 | 837.5 |
| 812.5 | 795.1 | 794.3 |
| 758.1 | 751.5 | 749.9 |
| 732.6 | 721.7 | 720.6 |
| 720.6 | 712.5 | 713.1 |
| 717.3 | 709.6 | 710.0 |
| 657.5 | 646.1 | 646.4 |
| 581.4 | 572.7 | 576.5 |
| 539.7 | 533.0 | 533.0 |
| 455.9 | 449.1 | 448.6 |
| 429.6 | 425.6 | 425.6 |
| 322.2 | 317.1 | 317.1 |
| 257.9 | 250.7 | 250.7 |
| 249.1 | 245.8 | 245.4 |
| 249.0 | 242.7 | 242.7 |
| 175.3 | 171.1 | 171.1 |
| 130.3 | 128.6 | 128.6 |
| 80.5 | 76.3 | 76.3 |

Table S44: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for biphenylene generated with parameter set (c).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3096.7 | 3073.9 | 3073.6 |
| 3092.9 | 3068.8 | 3064.5 |
| 3084.0 | 3060.5 | 3063.0 |
| 3081.3 | 3059.1 | 3052.7 |
| 3075.7 | 3053.3 | 3054.4 |
| 3074.1 | 3053.3 | 3050.5 |
| 3062.1 | 3037.5 | 3037.5 |
| 3060.9 | 3036.8 | 3047.9 |
| 1642.6 | 1602.6 | 1596.8 |
| 1604.5 | 1568.5 | 1570.9 |
| 1547.1 | 1514.2 | 1514.5 |
| 1543.8 | 1511.1 | 1511.4 |
| 1392.9 | 1347.8 | 1345.5 |
| 1375.5 | 1361.9 | 1358.4 |
| 1373.9 | 1362.0 | 1364.1 |
| 1332.0 | 1321.9 | 1322.2 |
| 1304.8 | 1292.2 | 1292.7 |
| 1242.4 | 1234.1 | 1232.4 |
| 1235.4 | 1223.5 | 1223.3 |
| 1222.4 | 1196.9 | 1196.7 |
| 1181.3 | 1163.7 | 1163.4 |
| 1136.2 | 1083.4 | 1082.8 |
| 1039.7 | 1036.7 | 1032.3 |
| 1016.3 | 1014.9 | 1015.8 |
| 979.6 | 974.1 | 972.9 |
| 961.4 | 954.4 | 946.5 |
| 945.2 | 939.6 | 943.4 |
| 933.9 | 925.9 | 925.9 |
| 932.7 | 924.7 | 924.7 |
| 906.1 | 899.4 | 901.8 |
| 886.4 | 882.0 | 882.0 |
| 877.9 | 869.8 | 869.8 |
| 849.6 | 833.6 | 832.7 |
| 845.2 | 839.2 | 839.2 |
| 823.2 | 816.2 | 816.3 |
| 787.1 | 772.5 | 771.9 |
| 727.2 | 725.4 | 736.2 |
| 717.5 | 717.8 | 717.8 |
| 704.0 | 704.3 | 704.3 |
| 694.8 | 693.0 | 693.0 |
| 646.0 | 642.2 | 642.4 |
| 584.6 | 582.3 | 582.3 |
| 540.9 | 540.2 | 540.2 |
| 534.1 | 533.8 | 533.8 |
| 468.1 | 468.1 | 471.2 |
| 460.9 | 459.5 | 459.5 |
| 373.3 | 376.1 | 376.1 |
| 362.6 | 364.8 | 365.7 |
| 350.5 | 356.5 | 356.5 |
| 306.4 | 313.1 | 313.1 |
| 262.9 | 269.2 | 269.2 |
| 199.1 | 210.6 | 210.6 |
| 121.5 | 142.2 | 142.2 |
| 95.1 | 123.5 | 123.5 |

Table S45: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for biphenylene generated with parameter set (d).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3147.7 | 3107.1 | 3107.2 |
| 3138.4 | 3097.5 | 3098.0 |
| 3124.0 | 3083.6 | 3082.4 |
| 3120.6 | 3079.5 | 3079.4 |
| 3114.3 | 3073.7 | 3073.7 |
| 3113.0 | 3073.3 | 3081.3 |
| 3108.6 | 3066.8 | 3065.1 |
| 3108.4 | 3065.4 | 3065.5 |
| 1890.2 | 1860.9 | 1859.1 |
| 1842.5 | 1816.5 | 1812.6 |
| 1800.9 | 1772.4 | 1769.3 |
| 1683.7 | 1618.7 | 1618.4 |
| 1536.2 | 1509.1 | 1508.5 |
| 1513.8 | 1489.4 | 1489.6 |
| 1481.4 | 1457.2 | 1456.9 |
| 1443.6 | 1365.4 | 1365.2 |
| 1364.2 | 1337.7 | 1337.7 |
| 1358.0 | 1334.6 | 1334.4 |
| 1341.6 | 1321.0 | 1323.3 |
| 1301.5 | 1278.1 | 1274.3 |
| 1266.4 | 1248.3 | 1248.2 |
| 1215.7 | 1195.2 | 1195.2 |
| 1194.5 | 1179.9 | 1179.6 |
| 1179.9 | 1162.9 | 1163.0 |
| 1162.9 | 1147.9 | 1144.1 |
| 1136.2 | 1123.3 | 1123.3 |
| 1111.9 | 1097.0 | 1096.8 |
| 1110.3 | 1095.8 | 1095.8 |
| 1104.6 | 1088.8 | 1088.8 |
| 1085.2 | 1063.6 | 1063.7 |
| 1084.1 | 1069.2 | 1069.2 |
| 1076.9 | 1059.6 | 1057.3 |
| 1075.9 | 1060.8 | 1060.8 |
| 1036.3 | 1023.4 | 1024.1 |
| 1008.9 | 996.6 | 998.0 |
| 960.1 | 950.4 | 950.0 |
| 847.2 | 840.1 | 840.0 |
| 827.5 | 812.5 | 815.0 |
| 825.7 | 819.3 | 818.8 |
| 810.1 | 804.5 | 804.0 |
| 748.3 | 739.2 | 740.1 |
| 664.4 | 655.9 | 655.8 |
| 617.3 | 609.3 | 610.3 |
| 599.6 | 594.3 | 594.3 |
| 559.8 | 553.9 | 552.7 |
| 491.3 | 485.6 | 485.4 |
| 427.9 | 422.5 | 420.6 |
| 406.5 | 402.5 | 402.5 |
| 338.9 | 349.7 | 349.7 |
| 334.1 | 329.8 | 329.8 |
| 236.5 | 234.5 | 234.4 |
| 232.3 | 230.4 | 230.4 |
| 125.1 | 124.7 | 124.7 |
| 101.7 | 101.8 | 101.8 |

Table S46: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for biphenylene generated with parameter set (e).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3120.0 | 3096.0 | 3096.0 |
| 3117.4 | 3093.2 | 3091.9 |
| 3110.4 | 3083.8 | 3085.0 |
| 3108.2 | 3082.2 | 3081.0 |
| 3101.2 | 3078.4 | 3084.7 |
| 3100.4 | 3076.1 | 3080.6 |
| 3088.9 | 3063.4 | 3063.4 |
| 3087.2 | 3062.4 | 3078.2 |
| 1685.2 | 1648.4 | 1656.6 |
| 1633.7 | 1601.6 | 1613.2 |
| 1593.1 | 1563.7 | 1564.7 |
| 1574.7 | 1539.9 | 1538.5 |
| 1411.5 | 1397.1 | 1396.5 |
| 1409.2 | 1394.2 | 1398.8 |
| 1407.0 | 1373.7 | 1372.0 |
| 1377.3 | 1364.3 | 1361.9 |
| 1336.0 | 1320.0 | 1321.0 |
| 1273.5 | 1261.5 | 1261.5 |
| 1272.3 | 1260.6 | 1260.5 |
| 1229.9 | 1212.6 | 1212.7 |
| 1214.4 | 1195.8 | 1195.8 |
| 1160.7 | 1113.6 | 1114.6 |
| 1088.2 | 1080.8 | 1075.2 |
| 1058.5 | 1051.6 | 1052.5 |
| 1018.7 | 1008.6 | 1007.9 |
| 1000.7 | 989.2 | 989.2 |
| 999.0 | 987.3 | 987.3 |
| 997.9 | 987.1 | 985.0 |
| 990.9 | 982.2 | 984.8 |
| 964.3 | 954.0 | 954.3 |
| 944.6 | 935.5 | 935.5 |
| 938.3 | 926.0 | 926.0 |
| 899.0 | 888.9 | 888.9 |
| 887.0 | 876.9 | 873.3 |
| 885.1 | 875.0 | 875.0 |
| 823.1 | 813.6 | 813.3 |
| 762.8 | 760.5 | 760.5 |
| 753.4 | 746.2 | 738.3 |
| 746.9 | 743.0 | 743.0 |
| 746.1 | 739.5 | 739.5 |
| 678.1 | 670.7 | 670.9 |
| 637.4 | 629.9 | 629.9 |
| 574.4 | 568.7 | 568.7 |
| 561.7 | 556.3 | 556.3 |
| 500.2 | 493.3 | 493.3 |
| 489.5 | 484.4 | 485.8 |
| 403.5 | 399.1 | 399.1 |
| 383.9 | 382.1 | 382.1 |
| 377.7 | 373.1 | 373.7 |
| 330.5 | 328.0 | 328.0 |
| 280.9 | 277.7 | 277.7 |
| 208.7 | 207.6 | 207.6 |
| 129.5 | 128.6 | 128.6 |
| 102.4 | 103.0 | 103.0 |

Table S47: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for biphenylene generated with parameter set (f).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 2981.0 | 2945.9 | 2945.9 |
| 2975.3 | 2940.7 | 2942.7 |
| 2975.0 | 2940.3 | 2938.3 |
| 2970.3 | 2939.6 | 2940.0 |
| 2961.3 | 2926.7 | 2927.3 |
| 2956.9 | 2920.5 | 2924.1 |
| 2952.3 | 2921.1 | 2920.9 |
| 2947.6 | 2911.1 | 2920.7 |
| 1674.7 | 1659.1 | 1658.5 |
| 1634.5 | 1607.9 | 1607.8 |
| 1585.6 | 1559.2 | 1559.0 |
| 1555.6 | 1529.3 | 1528.2 |
| 1484.2 | 1459.4 | 1460.6 |
| 1367.0 | 1352.2 | 1351.9 |
| 1364.3 | 1351.4 | 1350.2 |
| 1290.3 | 1341.9 | 1340.7 |
| 1251.9 | 1227.1 | 1227.0 |
| 1229.6 | 1209.3 | 1209.3 |
| 1148.4 | 1136.9 | 1136.8 |
| 1111.6 | 1096.3 | 1096.3 |
| 1085.5 | 1070.5 | 1071.6 |
| 1062.8 | 1055.0 | 1055.0 |
| 1055.2 | 1047.8 | 1047.8 |
| 1041.5 | 1032.9 | 1035.0 |
| 1030.5 | 1023.0 | 1023.0 |
| 1005.3 | 1000.1 | 1000.3 |
| 989.5 | 971.1 | 971.1 |
| 986.9 | 979.6 | 979.6 |
| 980.6 | 974.3 | 974.3 |
| 974.3 | 970.5 | 970.6 |
| 940.2 | 919.9 | 919.6 |
| 939.7 | 935.4 | 935.4 |
| 937.9 | 931.5 | 931.5 |
| 904.5 | 898.4 | 898.1 |
| 870.6 | 862.9 | 862.9 |
| 796.9 | 792.6 | 792.3 |
| 760.6 | 758.1 | 758.1 |
| 737.4 | 733.5 | 733.5 |
| 723.8 | 718.0 | 718.0 |
| 694.0 | 690.8 | 690.8 |
| 630.0 | 624.3 | 624.4 |
| 602.7 | 597.9 | 597.9 |
| 566.5 | 562.1 | 562.2 |
| 506.7 | 503.4 | 503.4 |
| 436.7 | 433.8 | 433.3 |
| 423.6 | 420.7 | 420.7 |
| 408.5 | 404.2 | 404.2 |
| 399.0 | 395.7 | 395.7 |
| 355.3 | 355.1 | 355.1 |
| 252.4 | 250.1 | 250.1 |
| 234.3 | 233.3 | 233.3 |
| 223.6 | 222.1 | 222.1 |
| 116.8 | 118.0 | 118.0 |
| 99.4 | 98.8 | 98.8 |

Table S48: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for benzopentalene generated with parameter set (a).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3113.5 | 3089.2 | 3089.2 |
| 3099.7 | 3068.8 | 3068.8 |
| 3093.5 | 3066.5 | 3065.8 |
| 3091.1 | 3068.2 | 3069.4 |
| 3081.9 | 3051.8 | 3055.5 |
| 3078.8 | 3047.8 | 3047.1 |
| 3068.6 | 3038.9 | 3046.5 |
| 3060.1 | 3030.4 | 3047.8 |
| 1619.5 | 1592.2 | 1592.0 |
| 1607.4 | 1578.7 | 1578.6 |
| 1548.5 | 1522.0 | 1520.8 |
| 1541.3 | 1514.7 | 1511.5 |
| 1498.6 | 1472.2 | 1472.3 |
| 1477.5 | 1458.3 | 1456.6 |
| 1423.6 | 1406.4 | 1405.2 |
| 1397.5 | 1275.9 | 1275.6 |
| 1351.1 | 1337.2 | 1337.5 |
| 1318.8 | 1306.4 | 1307.1 |
| 1313.5 | 1294.5 | 1294.5 |
| 1281.3 | 1266.5 | 1266.5 |
| 1216.8 | 1213.3 | 1213.4 |
| 1186.2 | 1163.1 | 1161.3 |
| 1130.6 | 1118.3 | 1119.4 |
| 1072.8 | 1058.7 | 1058.7 |
| 1056.8 | 1043.7 | 1043.9 |
| 1055.5 | 1039.7 | 1039.7 |
| 1030.1 | 1016.3 | 1016.3 |
| 1025.4 | 1013.4 | 1013.2 |
| 1012.2 | 999.1 | 996.6 |
| 1004.1 | 992.0 | 992.0 |
| 982.7 | 972.3 | 972.3 |
| 949.7 | 938.6 | 938.5 |
| 921.9 | 911.7 | 912.5 |
| 901.0 | 890.8 | 890.9 |
| 871.2 | 867.4 | 867.5 |
| 805.0 | 799.6 | 799.6 |
| 802.0 | 796.0 | 796.0 |
| 778.5 | 771.3 | 771.4 |
| 759.9 | 753.5 | 755.0 |
| 748.2 | 739.2 | 739.2 |
| 687.4 | 679.9 | 679.9 |
| 658.6 | 651.4 | 651.4 |
| 616.7 | 609.4 | 609.4 |
| 558.2 | 551.7 | 551.8 |
| 511.6 | 505.0 | 505.0 |
| 490.1 | 485.1 | 485.1 |
| 475.6 | 471.4 | 471.2 |
| 421.8 | 417.5 | 417.5 |
| 414.8 | 410.2 | 410.2 |
| 305.3 | 301.3 | 301.3 |
| 265.5 | 262.8 | 262.8 |
| 241.1 | 237.3 | 237.3 |
| 133.6 | 132.4 | 132.4 |
| 109.7 | 109.3 | 109.3 |

Table S49: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for benzopentalene generated with parameter set (b).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3231.1 | 3178.4 | 3177.6 |
| 3182.4 | 3139.8 | 3139.3 |
| 3160.4 | 3109.6 | 3117.9 |
| 3139.1 | 3091.1 | 3087.5 |
| 3127.2 | 3077.3 | 3086.1 |
| 3100.7 | 3042.8 | 3042.6 |
| 3084.9 | 3028.4 | 3027.0 |
| 3066.4 | 3007.7 | 3009.3 |
| 2009.3 | 1968.9 | 1968.2 |
| 1926.1 | 1894.1 | 1892.7 |
| 1828.6 | 1794.4 | 1792.6 |
| 1701.7 | 1663.4 | 1667.0 |
| 1643.7 | 1612.6 | 1613.8 |
| 1616.2 | 1584.7 | 1584.1 |
| 1523.5 | 1491.7 | 1489.8 |
| 1485.9 | 1456.5 | 1456.4 |
| 1431.4 | 1389.0 | 1389.0 |
| 1403.2 | 1378.6 | 1376.7 |
| 1384.0 | 1356.6 | 1356.3 |
| 1327.7 | 1299.8 | 1299.6 |
| 1250.9 | 1222.3 | 1221.8 |
| 1249.4 | 1227.3 | 1226.8 |
| 1187.1 | 1162.1 | 1162.6 |
| 1171.7 | 1150.9 | 1143.6 |
| 1159.5 | 1142.1 | 1134.3 |
| 1121.8 | 1100.0 | 1098.1 |
| 1069.1 | 1047.8 | 1049.1 |
| 1054.7 | 1043.2 | 1043.2 |
| 1009.6 | 989.3 | 988.1 |
| 986.3 | 963.0 | 963.0 |
| 960.1 | 921.0 | 921.0 |
| 913.3 | 889.9 | 889.9 |
| 901.2 | 862.9 | 862.9 |
| 892.0 | 868.1 | 868.1 |
| 887.1 | 871.2 | 871.2 |
| 853.9 | 824.7 | 824.8 |
| 853.0 | 835.9 | 836.0 |
| 769.6 | 746.4 | 750.6 |
| 758.3 | 752.2 | 751.7 |
| 727.4 | 719.7 | 719.5 |
| 693.4 | 684.0 | 683.9 |
| 646.0 | 635.3 | 635.5 |
| 594.9 | 587.9 | 587.9 |
| 571.0 | 557.7 | 557.8 |
| 546.5 | 544.9 | 549.1 |
| 460.6 | 455.7 | 454.2 |
| 448.9 | 443.7 | 443.7 |
| 375.3 | 369.6 | 369.6 |
| 284.9 | 281.2 | 281.1 |
| 272.2 | 268.8 | 266.8 |
| 259.4 | 254.4 | 254.4 |
| 171.8 | 171.0 | 171.0 |
| 110.0 | 110.7 | 110.7 |
| 96.9 | 96.9 | 96.9 |

Table S50: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for benzopentalene generated with parameter set (c).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3103.5 | 3077.8 | 3077.8 |
| 3094.8 | 3070.8 | 3068.5 |
| 3086.1 | 3064.3 | 3069.1 |
| 3078.5 | 3053.2 | 3052.8 |
| 3076.4 | 3056.7 | 3056.6 |
| 3075.5 | 3054.7 | 3055.7 |
| 3069.4 | 3046.3 | 3049.3 |
| 3061.6 | 3033.7 | 3048.0 |
| 1613.1 | 1585.1 | 1583.5 |
| 1609.8 | 1578.8 | 1579.1 |
| 1535.6 | 1501.0 | 1500.5 |
| 1528.5 | 1487.3 | 1486.7 |
| 1496.9 | 1468.2 | 1469.3 |
| 1391.8 | 1378.6 | 1379.6 |
| 1351.4 | 1340.5 | 1339.2 |
| 1313.7 | 1298.0 | 1298.2 |
| 1259.7 | 1241.7 | 1241.6 |
| 1244.5 | 1227.3 | 1227.2 |
| 1227.6 | 1214.5 | 1214.7 |
| 1208.3 | 1196.4 | 1196.6 |
| 1163.2 | 1074.1 | 1073.6 |
| 1128.8 | 1119.7 | 1119.8 |
| 1092.5 | 1081.6 | 1080.0 |
| 1051.2 | 1036.8 | 1036.7 |
| 1011.3 | 998.9 | 999.1 |
| 985.7 | 974.7 | 973.4 |
| 938.0 | 928.0 | 928.0 |
| 934.0 | 924.1 | 924.1 |
| 927.9 | 924.0 | 924.2 |
| 914.5 | 906.4 | 906.3 |
| 897.4 | 888.2 | 888.2 |
| 890.2 | 875.6 | 875.8 |
| 877.9 | 869.9 | 869.9 |
| 848.2 | 838.5 | 838.3 |
| 807.2 | 783.8 | 783.6 |
| 736.4 | 731.2 | 731.4 |
| 725.4 | 726.0 | 726.0 |
| 716.3 | 712.0 | 712.0 |
| 694.1 | 692.0 | 692.0 |
| 661.3 | 656.2 | 656.2 |
| 642.7 | 636.2 | 636.2 |
| 581.6 | 575.2 | 575.1 |
| 580.7 | 576.8 | 576.8 |
| 518.2 | 513.4 | 513.4 |
| 448.8 | 443.3 | 443.3 |
| 441.8 | 437.7 | 437.3 |
| 432.8 | 429.0 | 429.0 |
| 397.5 | 393.9 | 393.8 |
| 361.3 | 359.7 | 359.7 |
| 271.3 | 269.3 | 269.3 |
| 226.7 | 225.4 | 225.4 |
| 222.6 | 221.1 | 221.1 |
| 120.5 | 120.7 | 120.7 |
| 96.0 | 95.7 | 95.7 |

Table S51: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for benzopentalene generated with parameter set (d).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3161.6 | 3122.6 | 3122.1 |
| 3139.1 | 3098.9 | 3098.8 |
| 3133.4 | 3094.2 | 3094.3 |
| 3125.5 | 3073.5 | 3077.1 |
| 3112.6 | 3081.9 | 3081.9 |
| 3109.0 | 3066.7 | 3067.3 |
| 3104.2 | 3061.9 | 3065.6 |
| 3103.4 | 3061.5 | 3061.6 |
| 1791.4 | 1764.7 | 1763.1 |
| 1759.3 | 1730.2 | 1729.6 |
| 1709.0 | 1683.3 | 1682.2 |
| 1613.5 | 1587.7 | 1587.0 |
| 1556.1 | 1530.7 | 1531.4 |
| 1480.5 | 1453.8 | 1453.6 |
| 1441.2 | 1419.7 | 1419.6 |
| 1406.7 | 1384.6 | 1382.9 |
| 1366.6 | 1343.9 | 1344.0 |
| 1339.6 | 1314.1 | 1314.5 |
| 1291.0 | 1270.0 | 1270.0 |
| 1262.3 | 1244.7 | 1243.8 |
| 1257.0 | 1237.3 | 1237.6 |
| 1201.7 | 1187.5 | 1187.7 |
| 1181.0 | 1161.8 | 1160.7 |
| 1161.2 | 1141.4 | 1141.4 |
| 1151.4 | 1137.0 | 1137.0 |
| 1136.6 | 1114.4 | 1113.7 |
| 1118.0 | 1100.2 | 1100.2 |
| 1115.5 | 1100.9 | 1100.8 |
| 1066.7 | 1054.1 | 1054.1 |
| 1058.4 | 1043.6 | 1043.6 |
| 1050.4 | 1037.3 | 1037.3 |
| 1035.0 | 1017.4 | 1017.4 |
| 1031.1 | 1017.9 | 1017.9 |
| 974.6 | 961.2 | 961.2 |
| 928.7 | 920.1 | 920.1 |
| 885.5 | 872.9 | 871.6 |
| 866.7 | 859.4 | 859.4 |
| 843.1 | 832.1 | 831.9 |
| 816.9 | 810.6 | 810.4 |
| 776.9 | 768.5 | 768.5 |
| 739.6 | 725.0 | 724.4 |
| 655.2 | 649.8 | 649.8 |
| 629.1 | 621.3 | 624.3 |
| 584.3 | 577.7 | 577.7 |
| 513.1 | 504.8 | 508.4 |
| 481.9 | 475.9 | 475.9 |
| 470.3 | 464.1 | 462.6 |
| 412.2 | 407.8 | 407.8 |
| 382.1 | 377.9 | 377.9 |
| 259.6 | 256.9 | 256.7 |
| 258.2 | 256.0 | 256.0 |
| 239.5 | 237.9 | 237.9 |
| 123.9 | 123.2 | 123.2 |
| 103.9 | 101.6 | 101.6 |

Table S52: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for benzopentalene generated with parameter set (e).

| Harm. ($cm^{-1}$) | Fund. ($cm^{-1}$) | Corr. ($cm^{-1}$) |
|---|---|---|
| 3128.9 | 3104.0 | 3107.9 |
| 3117.9 | 3093.4 | 3093.2 |
| 3115.0 | 3098.7 | 3098.4 |
| 3112.2 | 3085.5 | 3086.5 |
| 3104.5 | 3083.7 | 3085.4 |
| 3104.4 | 3078.0 | 3078.6 |
| 3096.8 | 3074.4 | 3088.9 |
| 3089.0 | 3061.2 | 3079.6 |
| 1650.0 | 1623.5 | 1622.4 |
| 1638.3 | 1612.1 | 1610.8 |
| 1566.8 | 1537.0 | 1536.9 |
| 1557.1 | 1526.9 | 1525.9 |
| 1525.1 | 1493.1 | 1493.4 |
| 1428.3 | 1411.6 | 1415.3 |
| 1393.3 | 1380.6 | 1382.9 |
| 1346.8 | 1333.2 | 1333.5 |
| 1285.9 | 1272.6 | 1272.6 |
| 1285.2 | 1272.8 | 1272.9 |
| 1261.6 | 1248.5 | 1248.8 |
| 1227.5 | 1210.8 | 1211.2 |
| 1194.7 | 1171.7 | 1169.8 |
| 1161.6 | 1153.5 | 1153.5 |
| 1141.1 | 1130.5 | 1130.3 |
| 1089.0 | 1080.5 | 1080.4 |
| 1047.8 | 1036.1 | 1035.7 |
| 1021.5 | 1601.8 | 1601.9 |
| 1002.6 | 992.0 | 992.0 |
| 994.4 | 983.1 | 983.1 |
| 971.6 | 961.7 | 961.7 |
| 955.5 | 950.0 | 950.3 |
| 952.4 | 941.5 | 941.5 |
| 931.6 | 924.5 | 924.5 |
| 922.9 | 914.2 | 914.6 |
| 895.7 | 884.6 | 884.6 |
| 851.9 | 852.7 | 852.3 |
| 774.0 | 758.1 | 758.5 |
| 769.3 | 768.0 | 767.9 |
| 759.5 | 754.2 | 754.2 |
| 751.4 | 746.5 | 746.5 |
| 715.0 | 708.4 | 708.4 |
| 674.5 | 665.7 | 665.7 |
| 629.8 | 624.4 | 624.4 |
| 607.4 | 602.0 | 601.9 |
| 543.7 | 539.3 | 539.3 |
| 485.6 | 479.2 | 479.2 |
| 463.9 | 459.5 | 459.5 |
| 462.4 | 458.7 | 458.4 |
| 414.0 | 408.8 | 408.8 |
| 386.7 | 384.3 | 384.3 |
| 289.1 | 285.7 | 285.7 |
| 247.1 | 245.3 | 245.3 |
| 232.7 | 242.9 | 242.9 |
| 128.6 | 128.9 | 128.9 |
| 103.8 | 106.7 | 106.7 |

Table S53: Harmonic, fundamental, and corrected fundamental PM6-QFF frequencies for benzopentalene generated with parameter set (f).

## 4 Parameters

| | Parameter Set | | | | | |
|---|---|---|---|---|---|---|
| Parameter | (a) | (b) | (c) | (d) | (e) | (f) |
| $U_{ss}$ [H] (eV) | −10.62417845 | −12.29020873 | −7.481284187 | −13.10412803 | −10.54740849 | −13.07499687 |
| $\xi_s$ [H] (bohr$^{-1}$) | 0.9343456413 | 0.988528116 | 1.233229717 | 1.004165987 | 1.156914908 | 0.9601081811 |
| $\beta_s$ [H] (eV) | −9.13449619 | −14.87978102 | −12.85983021 | −14.79240561 | −10.15652675 | −14.74259751 |
| Gss [H] (eV) | 14.87388987 | 10.40573841 | 21.49924844 | 9.852551171 | 14.30014613 | 10.27401911 |
| $U_{ss}$ [C] (eV) | −50.80835869 | −49.08000601 | −53.45777372 | −50.81362974 | −51.22193781 | −50.55218045 |
| $U_{pp}$ [C] (eV) | −40.02817535 | −37.41883835 | −34.94132153 | −36.26937902 | −39.03473656 | −36.21926573 |
| $\xi_s$ [C] (bohr$^{-1}$) | 1.286277777 | 1.132441093 | 2.040303158 | 1.170333749 | 1.363058869 | 1.103663522 |
| $\xi_p$ [C] (bohr$^{-1}$) | 1.683540171 | 1.566990739 | 1.544949905 | 1.710583289 | 1.696330363 | 1.698493108 |
| $\beta_s$ [C] (eV) | −15.61978375 | −14.67759231 | −20.619989 | −14.51058256 | −15.14946218 | −14.67161171 |
| $\beta_p$ [C] (eV) | −7.780154413 | −8.956318028 | −8.411633354 | −8.659170187 | −8.78069328 | −9.86607095 |
| Gss [C] (eV) | 14.55486162 | 11.74851741 | 15.9546568 | 13.9570122 | 14.78882229 | 13.00772185 |
| Gpp [C] (eV) | 10.1755911 | 17.64251981 | 10.13999083 | 16.34933065 | 10.4034427 | 15.89067939 |
| Gpp [C] (eV) | 11.81135762 | 10.78814306 | 6.561874699 | 9.953932612 | 9.388305095 | 9.847830034 |
| Gp2 [C] (eV) | 10.88197111 | 11.65287048 | 9.365156701 | 10.03842449 | 9.567303279 | 10.25068184 |
| Hsp [C] (eV) | 2.370417524 | 2.316089752 | 0.7124654175 | 0.1887688752 | 3.689747683 | 1.276514355 |
| FN11 [C] | 0.07575873211 | 0.1012986548 | 0.08268633774 | 0.03232578889 | 0.09254031567 | 0.05624142398 |

Table S54: Semiempirical parameters generated from each reparameterization detailed in Table 3 of the main text. The FN11 parameter is equivalent to the PM6 Gaussian multiplier parameter $a$.

## 5 Rotational Constants

| | Parameter Set | | | | | |
|---|---|---|---|---|---|---|
| Constant | (a) | (b) | (c) | (d) | (e) | (f) |
| $A_e$ (MHz) | 2376.8 | 2549.7 | 2781.8 | 2627.6 | 2508.7 | 2580.5 |
| $B_e$ (MHz) | 585.6 | 612.7 | 685.3 | 639.2 | 627.1 | 626.8 |
| $C_e$ (MHz) | 469.8 | 494.0 | 549.8 | 514.1 | 501.7 | 504.3 |
| $A_0$ (MHz) | 2371.8 | 2536.3 | 2767.4 | 2616.3 | 2496.8 | 2569.1 |
| $B_0$ (MHz) | 584.3 | 610.0 | 682.9 | 636.8 | 624.9 | 624.6 |
| $C_0$ (MHz) | 469.0 | 491.8 | 548.1 | 512.3 | 500.0 | 502.6 |
| $\Delta_J$ (Hz) | 3.837 | 4.407 | 3.957 | 5.366 | 3.598 | 4.707 |
| $\Delta_K$ (Hz) | 117.549 | 129.271 | 136.525 | 160.239 | 107.206 | 137.035 |
| $\Delta_{JK}$ (Hz) | −0.839 | 0.929 | −3.208 | −0.450 | 0.060 | 0.060 |
| $\delta_J$ (Hz) | 0.959 | 1.019 | 0.989 | 1.289 | 0.869 | 1.109 |
| $\delta_K$ (Hz) | 16.968 | 16.489 | 15.619 | 21.105 | 13.880 | 18.317 |
| $\Phi_J$ ($\mu$Hz) | 0.086 | 0.054 | 0.038 | 0.115 | 0.046 | 0.084 |
| $\Phi_K$ ($\mu$Hz) | 17.845 | 14.555 | 1.855 | 23.359 | 14.457 | 17.888 |
| $\Phi_{JK}$ ($\mu$Hz) | 0.449 | 0.618 | 0.994 | 0.689 | 0.484 | 0.599 |
| $\Phi_{KJ}$ ($\mu$Hz) | −3.133 | −3.773 | −10.592 | −5.498 | −3.621 | −4.650 |
| $\phi_J$ ($\mu$Hz) | 0.037 | 0.025 | 0.018 | 0.050 | 0.021 | 0.036 |
| $\phi_K$ ($\mu$Hz) | 18.236 | 16.192 | 13.363 | 25.978 | 11.151 | 19.925 |
| $\phi_{JK}$ ($\mu$Hz) | 0.705 | 0.542 | 0.533 | 0.935 | 0.454 | 0.694 |

Table S55: PM6-QFF-computed rotational constants for $(C_6H_4)_2$ with each parameter set (see Table 3 of the main text).

| | Parameter Set | | | | | |
|---|---|---|---|---|---|---|
| Constant | (a) | (b) | (c) | (d) | (e) | (f) |
| $A_e$ (MHz) | 2301.5 | 2453.6 | 2587.3 | 2539.9 | 2391.0 | 2491.1 |
| $B_e$ (MHz) | 619.6 | 643.9 | 727.3 | 672.6 | 658.9 | 660.1 |
| $C_e$ (MHz) | 488.2 | 510.0 | 567.7 | 531.8 | 516.6 | 521.8 |
| $A_0$ (MHz) | 2296.5 | 2441.7 | 2570.8 | 2529.8 | 2380.0 | 2480.8 |
| $B_0$ (MHz) | 618.3 | 641.2 | 725.1 | 670.3 | 656.7 | 657.9 |
| $C_0$ (MHz) | 487.3 | 507.9 | 565.9 | 530.1 | 514.9 | 520.1 |
| $\Delta_J$ (Hz) | 4.527 | 4.887 | 5.007 | 6.146 | 4.317 | 5.366 |
| $\Delta_K$ (Hz) | 119.257 | 124.594 | 140.663 | 157.991 | 113.322 | 134.877 |
| $\Delta_{JK}$ (Hz) | −3.837 | 0.540 | −0.150 | −1.679 | −1.709 | −1.289 |
| $\delta_J$ (Hz) | 1.229 | 1.199 | 1.379 | 1.559 | 1.139 | 1.349 |
| $\delta_K$ (Hz) | 17.478 | 17.238 | 20.656 | 22.245 | 15.919 | 19.247 |
| $\Phi_J$ ($\mu$Hz) | 0.127 | 0.078 | 0.149 | 0.159 | 0.096 | 0.118 |
| $\Phi_K$ ($\mu$Hz) | 19.971 | 16.232 | 18.507 | 27.734 | 13.005 | 20.235 |
| $\Phi_{JK}$ ($\mu$Hz) | 0.451 | 0.488 | 0.276 | 0.734 | 0.244 | 0.552 |
| $\Phi_{KJ}$ ($\mu$Hz) | −4.821 | −4.370 | −3.424 | −7.158 | −2.687 | −5.197 |
| $\phi_J$ ($\mu$Hz) | 0.055 | 0.036 | 0.067 | 0.070 | 0.043 | 0.052 |
| $\phi_K$ ($\mu$Hz) | 20.174 | 17.439 | 24.760 | 28.920 | 16.003 | 21.850 |
| $\phi_{JK}$ ($\mu$Hz) | 0.892 | 0.587 | 1.003 | 1.134 | 0.639 | 0.837 |

Table S56: PM6-QFF-computed rotational constants for $C_{12}H_8$ with each parameter set (see Table 3 of the main text).

| | F12-DZ + core | | F12-TZ + core | |
|---|---|---|---|---|
| Constant | 0.005 Å | 0.010 Å | 0.005 Å | 0.010 Å |
| $A_e$ (GHz) | 16.911 | 16.911 | 16.947 | 16.947 |
| $B_e$ (GHz) | 12.943 | 12.943 | 12.966 | 12.966 |
| $C_e$ (GHz) | 7.332 | 7.332 | 7.346 | 7.346 |
| $A_0$ (GHz) | 16.790 | 16.790 | 16.827 | 16.826 |
| $B_0$ (GHz) | 12.864 | 12.864 | 12.885 | 12.885 |
| $C_0$ (GHz) | 7.278 | 7.278 | 7.292 | 7.292 |
| $\Delta_J$ (kHz) | 5.567 | 5.566 | 5.546 | 5.545 |
| $\Delta_K$ (kHz) | 2.479 | 2.476 | 2.274 | 2.271 |
| $\Delta_{JK}$ (kHz) | 3.564 | 3.567 | 3.776 | 3.779 |
| $\delta_J$ (kHz) | 2.171 | 2.171 | 2.161 | 2.160 |
| $\delta_K$ (kHz) | 8.165 | 8.166 | 8.229 | 8.230 |
| $\Phi_J$ (mHz) | 2.631 | 2.638 | 2.554 | 2.554 |
| $\Phi_K$ (mHz) | 61.208 | 61.208 | 61.916 | 62.121 |
| $\Phi_{JK}$ (mHz) | 47.334 | 47.291 | 48.270 | 48.286 |
| $\Phi_{KJ}$ (mHz) | −101.053 | −100.989 | −102.342 | −102.582 |
| $\phi_J$ (mHz) | 1.350 | 1.353 | 1.310 | 1.311 |
| $\phi_K$ (mHz) | 51.801 | 51.819 | 51.710 | 51.657 |
| $\phi_{JK}$ (mHz) | 22.842 | 22.834 | 23.218 | 23.239 |

Table S57: Rotational constants for four QFFs computed for $C_4H_4$.

| | F12-DZ | | F12-DZ + core | |
|---|---|---|---|---|
| Constant | 0.010 Å | 0.015 Å | 0.010 Å | 0.015 Å |
| $A_e$ (GHz) | 7.084 | 7.108 | 7.084 | 7.108 |
| $B_e$ (GHz) | 5.654 | 5.675 | 5.654 | 5.675 |
| $C_e$ (GHz) | 3.144 | 3.155 | 3.144 | 3.155 |
| $A_0$ (GHz) | 7.041 | 7.065 | 7.041 | 7.065 |
| $B_0$ (GHz) | 5.615 | 5.636 | 5.615 | 5.636 |
| $C_0$ (GHz) | 3.122 | 3.133 | 3.122 | 3.133 |
| $\Delta_J$ (kHz) | 0.660 | 0.663 | 0.660 | 0.663 |
| $\Delta_K$ (kHz) | 1.419 | 1.443 | 1.416 | 1.440 |
| $\Delta_{JK}$ (kHz) | 0.487 | 0.465 | 0.491 | 0.469 |
| $\delta_J$ (kHz) | 0.267 | 0.268 | 0.267 | 0.268 |
| $\delta_K$ (kHz) | 1.030 | 1.022 | 1.033 | 1.024 |
| $\Phi_J$ (mHz) | 0.285 | 0.286 | 0.286 | 0.287 |
| $\Phi_K$ (mHz) | 11.965 | 11.783 | 11.999 | 11.813 |
| $\Phi_{JK}$ (mHz) | 3.986 | 3.880 | 4.001 | 3.894 |
| $\Phi_{KJ}$ (mHz) | −14.197 | −13.917 | −14.244 | −13.958 |
| $\phi_J$ (mHz) | 0.142 | 0.143 | 0.142 | 0.143 |
| $\phi_K$ (mHz) | 1.216 | 1.224 | 1.213 | 1.222 |
| $\phi_{JK}$ (mHz) | 2.342 | 2.291 | 2.351 | 2.299 |

Table S58: Rotational constants for four QFFs computed for $C_6H_4$.

# 6 Resonances

| Coriolis Resonances | | |
|---|---|---|
| 11 | 10 | C |
| 12 | 10 | A |
| 15 | 14 | A |
| **Type 1 Fermi Resonances** | | |
| 4 | 0 | |
| 5 | 0 | |
| 11 | 5* | |
| 12 | 5 | |
| 13 | 5 | |
| 14 | 5 | |
| 15 | 8 | |
| 16 | 8 | |
| 17 | 8 | |
| 17 | 10 | |
| **Type 2 Fermi Resonances** | | |
| 5 | 4 | 1 |
| 13 | 12 | 4 |
| 14 | 11 | 4 |
| 15 | 12 | 6 |
| 16 | 13 | 6 |
| 16 | 15 | 9 |
| 17 | 13 | 5** |

*Resonance not present in the $r = 0.005$ Å F12-DZ + core QFF
**Resonance not present in either F12-DZ + core QFF

Table S59: Coriolis and Type 1 and 2 Fermi resonances computed across the $r = 0.005$, 0.010 Å core-correlated F12-DZ and F12-TZ QFFs for $C_4H_4$. Resonances not present across all QFFs are indicated.

| Coriolis Resonances | | |
|---|---|---|
| 6 | 5 | C |
| 12 | 11 | C |
| 13 | 11 | C |
| 14 | 11 | A |
| 20 | 19 | B |
| 21 | 19 | C |
| 21 | 20 | A |
| 22 | 21 | A |
| **Type 1 Fermi Resonances** | | |
| 12 | 4 | |
| 18 | 8 | |
| 20 | 8 | |
| 20 | 12 | |
| 21 | 12 | |
| 21 | 13 | |
| 22 | 12 | |
| 22 | 13 | |
| 23 | 19 | |
| **Type 2 Fermi Resonances** | | |
| 7 | 4 | 3 |
| 8 | 4 | 2 |
| 10 | 4 | 2 |
| 11 | 4 | 3 |
| 13 | 10 | 4 |
| 13 | 12 | 4 |
| 16 | 14 | 4 |
| 17 | 9 | 4 |
| 17 | 11 | 4 |
| 18 | 16 | 5 |
| 19 | 13 | 6 |
| 20 | 14 | 6 |
| 20 | 18 | 5 |
| 21 | 5 | 4 |
| 21 | 7 | 4 |
| 21 | 13 | 9 |
| 21 | 17 | 8 |
| 21 | 19 | 9 |
| 22 | 14 | 6 |
| 22 | 15 | 7 |
| 22 | 15 | 9 |
| 22 | 16 | 8 |
| 22 | 18 | 9 |
| 22 | 18 | 11 |
| 22 | 20 | 10 |
| 22 | 20 | 12 |
| 22 | 20 | 13 |
| 23 | 14 | 5 |
| 23 | 14 | 7 |
| 23 | 15 | 6 |
| 23 | 15 | 8 |
| 23 | 16 | 7 |
| 23 | 18 | 8 |
| 23 | 18 | 10 |
| 23 | 18 | 12 |
| 23 | 20 | 11 |

Table S60: Coriolis and Type 1 and 2 Fermi resonances computed across the $r = 0.010$, 0.015 Å F12-DZ and core-correlated F12-DZ QFFs for $o$-$C_6H_4$. All resonances are present across all QFFs.

| Coriolis Resonances | | |
|---|---|---|
| 11 | 9 | C |
| 12 | 10 | C |
| 14 | 12 | C |
| 15 | 13 | C |
| 16 | 14 | C |
| 22 | 21 | A |
| 23 | 20 | A |
| 24 | 21 | B |
| 25 | 23 | B |
| 26 | 23 | A |
| 27 | 26 | B |
| 29 | 27 | B |
| 30 | 28 | C |
| 31 | 18 | A |
| 31 | 22 | B |
| 32 | 18 | C |
| 32 | 31 | B |
| 33 | 22 | A |
| 33 | 24 | B |
| 33 | 32 | A |
| 34 | 25 | B |
| 34 | 26 | A |
| 35 | 26 | C |
| 35 | 27 | A |
| 42 | 41 | B |
| 43 | 40 | C |
| 45 | 43 | A |
| 46 | 42 | A |
| 47 | 44 | C |
| 52 | 51 | B |
| 53 | 51 | A |
| Type 1 Fermi Resonances | | |
| 11 | 0 | |
| 11 | 5 | |
| 12 | 0 | |
| 12 | 5 | |
| 28 | 8 | |
| 29 | 8 | |
| 30 | 8 | |
| 31 | 8 | |
| 32 | 8 | |
| 37 | 12 | |
| 38 | 12 | |
| 40 | 12 | |
| 41 | 16 | |
| 45 | 26 | |
| 45 | 29 | |
| 45 | 36 | |
| 46 | 36 | |
| 48 | 36 | |
| 49 | 36 | |
| 50 | 47 | |
| 53 | 47 | |
| Type 2 Fermi Resonances | | |
| 12 | 11 | 1 |
| 12 | 11 | 4 |
| 13 | 8 | 6 |

| | | |
|---|---|---|
| 13 | 9 | 0 |
| 13 | 10 | 1 |
| 13 | 11 | 7 |
| 13 | 12 | 6 |
| 14 | 8 | 7 |
| 14 | 10 | 0 |
| 14 | 11 | 6 |
| 14 | 12 | 7 |
| 15 | 8 | 1 |
| 15 | 9 | 3 |
| 15 | 10 | 2 |
| 15 | 11 | 0 |
| 16 | 8 | 0 |
| 16 | 9 | 2 |
| 16 | 10 | 3 |
| 16 | 11 | 1 |
| 17 | 10 | 2 |
| 17 | 11 | 5 |
| 18 | 8 | 2 |
| 18 | 8 | 6 |
| 18 | 9 | 0 |
| 18 | 9 | 5 |
| 19 | 8 | 3 |
| 19 | 8 | 7 |
| 19 | 9 | 1 |
| 19 | 9 | 4 |
| 20 | 8 | 5 |
| 22 | 8 | 4 |
| 24 | 8 | 2 |
| 25 | 8 | 7 |
| 26 | 8 | 5 |
| 32 | 30 | 8 |
| 35 | 25 | 8 |
| 35 | 28 | 11 |
| 35 | 29 | 10 |
| 35 | 30 | 9 |
| 36 | 26 | 8 |
| 36 | 30 | 11 |
| 40 | 18 | 8 |
| 40 | 25 | 11 |
| 40 | 28 | 12 |
| 40 | 35 | 11 |
| 41 | 27 | 10 |
| 41 | 33 | 15 |
| 41 | 39 | 15 |
| 41 | 39 | 17 |
| 42 | 20 | 10 |
| 42 | 26 | 10 |
| 42 | 29 | 14 |
| 42 | 30 | 13 |
| 42 | 32 | 13 |
| 42 | 35 | 16 |
| 43 | 14 | 9 |
| 43 | 28 | 10 |
| 43 | 28 | 14 |
| 43 | 29 | 11 |
| 43 | 29 | 15 |
| 43 | 32 | 16 |
| 43 | 36 | 15 |
| 44 | 15 | 9 |
| 44 | 17 | 9 |
| 45 | 21 | 12 |

| | | |
|---|---|---|
| 45 | 34 | 17 |
| 45 | 37 | 28 |
| 45 | 39 | 26 |
| 45 | 41 | 30 |
| 46 | 39 | 18 |
| 46 | 39 | 24 |
| 46 | 39 | 28 |
| 46 | 41 | 19 |
| 46 | 45 | 28 |
| 47 | 12 | 8 |
| 47 | 13 | 9 |
| 47 | 14 | 10 |
| 47 | 17 | 11 |
| 47 | 32 | 15 |
| 48 | 21 | 11 |
| 48 | 21 | 15 |
| 48 | 23 | 12 |
| 48 | 23 | 16 |
| 48 | 31 | 18 |
| 48 | 33 | 15 |
| 48 | 33 | 17 |
| 48 | 34 | 12 |
| 48 | 38 | 28 |
| 48 | 39 | 32 |
| 48 | 41 | 29 |
| 48 | 41 | 36 |
| 48 | 42 | 37 |
| 48 | 45 | 30 |
| 49 | 21 | 14 |
| 49 | 23 | 13 |
| 49 | 33 | 19 |
| 49 | 35 | 33 |
| 49 | 37 | 30 |
| 49 | 37 | 32 |
| 49 | 38 | 26 |
| 49 | 39 | 19 |
| 49 | 40 | 34 |
| 49 | 41 | 24 |
| 49 | 41 | 28 |
| 49 | 46 | 43 |
| 50 | 21 | 13 |
| 50 | 23 | 14 |
| 50 | 33 | 18 |
| 50 | 34 | 19 |
| 50 | 35 | 34 |
| 50 | 37 | 26 |
| 50 | 38 | 22 |
| 50 | 38 | 30 |
| 50 | 43 | 38 |
| 50 | 45 | 40 |
| 51 | 9 | 8 |
| 51 | 11 | 10 |
| 51 | 15 | 10 |
| 51 | 26 | 13 |
| 51 | 26 | 24 |
| 51 | 28 | 20 |
| 51 | 30 | 14 |
| 51 | 36 | 18 |
| 51 | 36 | 24 |
| 51 | 36 | 28 |
| 52 | 37 | 28 |
| 52 | 38 | 25 |

| | | |
|---|---|---|
| 52 | 49 | 44 |
| 53 | 21 | 14 |
| 53 | 23 | 13 |
| 53 | 34 | 18 |
| 53 | 48 | 40 |
| 53 | 50 | 43 |

Table S61: PM6-QFF Coriolis and Fermi resonances for biphenylene generated using parameter set (a).

| Coriolis Resonances | | |
|---|---|---|
| 13 | 11 | C |
| 15 | 9 | C |
| 27 | 22 | C |
| 30 | 21 | C |
| 30 | 27 | C |
| 31 | 25 | C |
| 33 | 26 | A |
| 34 | 33 | C |
| 35 | 28 | B |
| 35 | 30 | C |
| 37 | 30 | B |
| 37 | 35 | A |
| 40 | 37 | B |
| 41 | 39 | A |
| 42 | 39 | C |
| 42 | 41 | B |
| 43 | 40 | C |
| 44 | 40 | B |
| 44 | 43 | A |
| 47 | 42 | A |
| 48 | 45 | C |
| 52 | 51 | B |
| 53 | 51 | A |
| **Type 1 Fermi Resonances** | | |
| 9 | 0 | |
| 9 | 4 | |
| 10 | 0 | |
| 10 | 4 | |
| 11 | 0 | |
| 11 | 4 | |
| 12 | 0 | |
| 12 | 1 | |
| 12 | 4 | |
| 12 | 5 | |
| 13 | 0 | |
| 13 | 1 | |
| 13 | 4 | |
| 35 | 8 | |
| 35 | 14 | |
| 39 | 8 | |
| 39 | 14 | |
| 40 | 14 | |
| 40 | 20 | |
| 42 | 31 | |
| 43 | 31 | |
| 44 | 20 | |
| 44 | 31 | |

| | | |
|---|---|---|
| 45 | 31 | |
| 46 | 31 | |
| 46 | 34 | |
| 46 | 39 | |
| 47 | 39 | |
| 48 | 39 | |
| 49 | 39 | |
| 50 | 39 | |
| 53 | 48 | |
| Type 2 Fermi Resonances | | |
| 9 | 8 | 2 |
| 10 | 8 | 3 |
| 10 | 9 | 1 |
| 10 | 9 | 5 |
| 11 | 8 | 1 |
| 11 | 9 | 3 |
| 11 | 10 | 2 |
| 12 | 8 | 7 |
| 12 | 9 | 5 |
| 12 | 10 | 4 |
| 12 | 11 | 2 |
| 12 | 11 | 6 |
| 13 | 8 | 6 |
| 13 | 9 | 4 |
| 13 | 10 | 5 |
| 13 | 11 | 3 |
| 13 | 11 | 7 |
| 13 | 12 | 1 |
| 13 | 12 | 5 |
| 14 | 8 | 0 |
| 14 | 9 | 2 |
| 14 | 10 | 3 |
| 14 | 11 | 1 |
| 14 | 12 | 3 |
| 14 | 12 | 7 |
| 14 | 13 | 2 |
| 14 | 13 | 6 |
| 15 | 8 | 1 |
| 15 | 8 | 5 |
| 15 | 9 | 3 |
| 15 | 9 | 7 |
| 15 | 10 | 2 |
| 15 | 10 | 6 |
| 15 | 11 | 0 |
| 15 | 11 | 4 |
| 15 | 12 | 6 |
| 15 | 13 | 7 |
| 16 | 8 | 4 |
| 16 | 9 | 2 |
| 16 | 9 | 6 |
| 16 | 10 | 3 |
| 16 | 10 | 7 |
| 16 | 11 | 1 |
| 16 | 11 | 5 |
| 17 | 8 | 3 |
| 17 | 9 | 1 |
| 17 | 9 | 5 |
| 17 | 10 | 0 |
| 17 | 10 | 4 |
| 17 | 11 | 2 |
| 18 | 8 | 2 |

| | | |
|---|---|---|
| 18 | 9 | 0 |
| 18 | 9 | 4 |
| 18 | 10 | 1 |
| 18 | 10 | 5 |
| 18 | 11 | 3 |
| 19 | 8 | 1 |
| 19 | 8 | 5 |
| 19 | 9 | 7 |
| 20 | 8 | 0 |
| 34 | 31 | 8 |
| 35 | 27 | 8 |
| 39 | 27 | 11 |
| 39 | 30 | 9 |
| 39 | 31 | 8 |
| 39 | 34 | 14 |
| 39 | 35 | 15 |
| 40 | 22 | 8 |
| 40 | 31 | 9 |
| 40 | 34 | 9 |
| 42 | 31 | 12 |
| 42 | 34 | 10 |
| 42 | 34 | 12 |
| 42 | 35 | 13 |
| 43 | 21 | 8 |
| 43 | 25 | 9 |
| 43 | 30 | 10 |
| 43 | 34 | 15 |
| 43 | 34 | 19 |
| 43 | 35 | 16 |
| 43 | 35 | 20 |
| 43 | 39 | 19 |
| 44 | 28 | 17 |
| 44 | 29 | 16 |
| 44 | 32 | 15 |
| 44 | 38 | 12 |
| 44 | 41 | 21 |
| 44 | 41 | 27 |
| 45 | 17 | 8 |
| 45 | 19 | 9 |
| 45 | 21 | 9 |
| 45 | 25 | 8 |
| 45 | 34 | 10 |
| 45 | 40 | 19 |
| 46 | 23 | 11 |
| 46 | 24 | 14 |
| 46 | 26 | 10 |
| 46 | 26 | 17 |
| 46 | 28 | 9 |
| 46 | 28 | 18 |
| 46 | 29 | 15 |
| 46 | 32 | 16 |
| 46 | 38 | 18 |
| 46 | 41 | 31 |
| 46 | 44 | 21 |
| 46 | 44 | 27 |
| 46 | 44 | 35 |
| 47 | 26 | 14 |
| 47 | 37 | 18 |
| 47 | 44 | 30 |
| 48 | 14 | 8 |
| 48 | 16 | 8 |
| 48 | 17 | 10 |

| | | |
|---|---|---|
| 48 | 18 | 9 |
| 48 | 20 | 8 |
| 48 | 21 | 11 |
| 48 | 22 | 9 |
| 48 | 22 | 18 |
| 48 | 34 | 20 |
| 48 | 35 | 21 |
| 48 | 40 | 22 |
| 48 | 40 | 30 |
| 49 | 23 | 12 |
| 49 | 24 | 13 |
| 49 | 35 | 26 |
| 49 | 36 | 19 |
| 49 | 36 | 21 |
| 49 | 37 | 17 |
| 49 | 41 | 30 |
| 49 | 44 | 25 |
| 49 | 47 | 35 |
| 50 | 23 | 13 |
| 50 | 24 | 12 |
| 50 | 28 | 15 |
| 50 | 29 | 18 |
| 50 | 32 | 17 |
| 50 | 38 | 19 |
| 50 | 38 | 21 |
| 50 | 41 | 25 |
| 50 | 46 | 33 |
| 50 | 49 | 35 |
| 51 | 9 | 8 |
| 51 | 14 | 9 |
| 51 | 34 | 22 |
| 51 | 35 | 25 |
| 51 | 39 | 22 |
| 51 | 39 | 30 |
| 51 | 40 | 34 |
| 51 | 40 | 39 |
| 51 | 45 | 35 |
| 52 | 23 | 16 |
| 52 | 32 | 21 |
| 52 | 49 | 45 |
| 53 | 35 | 26 |
| 53 | 46 | 40 |
| 53 | 50 | 43 |

Table S62: PM6-QFF Coriolis and Fermi resonances for biphenylene generated using parameter set (b).

| Coriolis Resonances | | |
|---|---|---|
| 12 | 11 | C |
| 15 | 14 | C |
| 17 | 13 | C |
| 18 | 14 | C |
| 19 | 17 | C |
| 21 | 18 | C |
| 21 | 20 | C |
| 22 | 19 | C |
| 29 | 28 | A |
| 29 | 28 | B |
| 30 | 25 | A |

| | | |
|---|---|---|
| 31 | 27 | B |
| 31 | 30 | B |
| 32 | 28 | A |
| 34 | 29 | A |
| 34 | 32 | A |
| 34 | 32 | B |
| 35 | 30 | A |
| 35 | 30 | B |
| 35 | 33 | A |
| 36 | 35 | A |
| 36 | 35 | B |
| 39 | 33 | B |
| 40 | 34 | B |
| 42 | 37 | C |
| 44 | 41 | B |
| 44 | 43 | B |
| 45 | 43 | C |
| 52 | 49 | A |
| 52 | 49 | B |
| 53 | 49 | A |

Type 1 Fermi Resonances

| | |
|---|---|
| 12 | 0 |
| 12 | 2 |
| 12 | 3 |
| 12 | 7 |
| 13 | 0 |
| 13 | 4 |
| 13 | 7 |
| 14 | 0 |
| 14 | 7 |
| 15 | 0 |
| 15 | 3 |
| 15 | 4 |
| 15 | 7 |
| 16 | 3 |
| 16 | 7 |
| 17 | 7 |
| 26 | 8 |
| 27 | 8 |
| 30 | 10 |
| 34 | 10 |
| 36 | 10 |
| 37 | 15 |
| 39 | 15 |
| 39 | 18 |
| 44 | 27 |
| 44 | 30 |
| 44 | 33 |
| 45 | 36 |
| 46 | 27 |
| 46 | 30 |
| 46 | 33 |
| 46 | 41 |
| 47 | 43 |
| 48 | 45 |
| 49 | 45 |
| 50 | 43 |
| 50 | 45 |
| 51 | 45 |

Type 2 Fermi Resonances

| | | |
|---|---|---|
| 13 | 12 | 0 |
| 13 | 12 | 3 |
| 14 | 12 | 1 |
| 14 | 12 | 2 |
| 14 | 12 | 6 |
| 14 | 13 | 2 |
| 15 | 11 | 1 |
| 15 | 11 | 2 |
| 15 | 11 | 5 |
| 15 | 12 | 1 |
| 15 | 12 | 6 |
| 15 | 13 | 2 |
| 15 | 13 | 6 |
| 15 | 14 | 0 |
| 15 | 14 | 3 |
| 15 | 14 | 7 |
| 17 | 11 | 0 |
| 17 | 11 | 3 |
| 17 | 12 | 0 |
| 17 | 12 | 7 |
| 17 | 13 | 3 |
| 17 | 14 | 1 |
| 17 | 14 | 2 |
| 17 | 14 | 3 |
| 17 | 14 | 6 |
| 17 | 15 | 2 |
| 17 | 15 | 5 |
| 18 | 9 | 1 |
| 18 | 10 | 0 |
| 18 | 11 | 1 |
| 18 | 12 | 1 |
| 18 | 12 | 2 |
| 18 | 12 | 3 |
| 18 | 12 | 5 |
| 18 | 12 | 6 |
| 18 | 13 | 5 |
| 18 | 14 | 2 |
| 18 | 14 | 3 |
| 18 | 14 | 7 |
| 19 | 10 | 1 |
| 19 | 11 | 0 |
| 19 | 11 | 3 |
| 19 | 11 | 7 |
| 19 | 12 | 2 |
| 19 | 12 | 3 |
| 19 | 12 | 7 |
| 20 | 9 | 2 |
| 20 | 11 | 1 |
| 20 | 11 | 2 |
| 20 | 11 | 3 |
| 21 | 9 | 1 |
| 21 | 9 | 2 |
| 21 | 11 | 1 |
| 21 | 11 | 2 |
| 21 | 11 | 3 |
| 21 | 11 | 5 |
| 22 | 9 | 3 |
| 22 | 11 | 0 |
| 22 | 11 | 2 |
| 22 | 11 | 3 |
| 23 | 8 | 0 |
| 23 | 8 | 1 |

| | | |
|---|---|---|
| 23 | 9 | 0 |
| 23 | 9 | 1 |
| 23 | 10 | 3 |
| 24 | 8 | 0 |
| 24 | 8 | 1 |
| 24 | 9 | 0 |
| 24 | 9 | 1 |
| 26 | 8 | 1 |
| 26 | 8 | 2 |
| 26 | 8 | 5 |
| 26 | 9 | 0 |
| 26 | 9 | 3 |
| 26 | 10 | 1 |
| 26 | 10 | 5 |
| 27 | 8 | 4 |
| 27 | 10 | 4 |
| 27 | 10 | 7 |
| 28 | 8 | 5 |
| 30 | 8 | 7 |
| 30 | 26 | 9 |
| 30 | 27 | 8 |
| 30 | 28 | 9 |
| 30 | 28 | 11 |
| 33 | 8 | 4 |
| 33 | 18 | 8 |
| 33 | 30 | 10 |
| 34 | 8 | 2 |
| 34 | 8 | 5 |
| 34 | 8 | 6 |
| 34 | 23 | 10 |
| 34 | 26 | 8 |
| 34 | 26 | 10 |
| 34 | 27 | 11 |
| 34 | 30 | 11 |
| 34 | 33 | 11 |
| 35 | 29 | 11 |
| 35 | 32 | 12 |
| 36 | 8 | 7 |
| 36 | 18 | 8 |
| 36 | 26 | 9 |
| 36 | 27 | 10 |
| 36 | 28 | 9 |
| 36 | 30 | 10 |
| 36 | 34 | 11 |
| 36 | 34 | 12 |
| 36 | 34 | 13 |
| 37 | 17 | 8 |
| 37 | 22 | 10 |
| 37 | 27 | 9 |
| 37 | 30 | 12 |
| 37 | 36 | 11 |
| 37 | 36 | 12 |
| 41 | 15 | 8 |
| 41 | 17 | 9 |
| 41 | 18 | 8 |
| 41 | 20 | 10 |
| 41 | 21 | 8 |
| 41 | 27 | 10 |
| 41 | 34 | 13 |
| 41 | 37 | 13 |
| 42 | 22 | 10 |
| 42 | 27 | 11 |

| | | |
|---|---|---|
| 42 | 33 | 13 |
| 42 | 36 | 12 |
| 42 | 36 | 13 |
| 43 | 13 | 9 |
| 43 | 19 | 9 |
| 43 | 30 | 14 |
| 43 | 37 | 13 |
| 44 | 16 | 9 |
| 44 | 26 | 16 |
| 44 | 38 | 17 |
| 44 | 38 | 26 |
| 44 | 39 | 21 |
| 44 | 40 | 19 |
| 45 | 12 | 9 |
| 45 | 15 | 8 |
| 45 | 15 | 10 |
| 45 | 19 | 12 |
| 45 | 22 | 11 |
| 45 | 26 | 11 |
| 45 | 30 | 15 |
| 45 | 36 | 15 |
| 45 | 36 | 18 |
| 45 | 36 | 20 |
| 46 | 32 | 17 |
| 46 | 32 | 22 |
| 46 | 34 | 16 |
| 46 | 35 | 21 |
| 46 | 39 | 21 |
| 46 | 40 | 19 |
| 46 | 43 | 25 |
| 47 | 21 | 16 |
| 47 | 25 | 17 |
| 47 | 29 | 18 |
| 47 | 29 | 21 |
| 47 | 29 | 23 |
| 47 | 29 | 24 |
| 47 | 31 | 26 |
| 47 | 32 | 21 |
| 47 | 35 | 19 |
| 47 | 35 | 23 |
| 47 | 35 | 26 |
| 47 | 38 | 21 |
| 47 | 39 | 22 |
| 47 | 45 | 38 |
| 47 | 46 | 37 |
| 47 | 46 | 42 |
| 48 | 18 | 16 |
| 48 | 25 | 13 |
| 48 | 25 | 19 |
| 48 | 25 | 22 |
| 48 | 29 | 18 |
| 48 | 29 | 23 |
| 48 | 31 | 22 |
| 48 | 32 | 20 |
| 48 | 32 | 21 |
| 48 | 32 | 23 |
| 48 | 32 | 24 |
| 48 | 35 | 23 |
| 48 | 35 | 24 |
| 48 | 37 | 31 |
| 48 | 38 | 27 |
| 48 | 39 | 28 |

| | | |
|---|---|---|
| 48 | 39 | 37 |
| 48 | 40 | 27 |
| 48 | 40 | 33 |
| 48 | 42 | 39 |
| 48 | 43 | 38 |
| 48 | 43 | 40 |
| 48 | 44 | 42 |
| 48 | 45 | 40 |
| 48 | 47 | 43 |
| 49 | 9 | 8 |
| 49 | 10 | 9 |
| 49 | 11 | 10 |
| 49 | 12 | 10 |
| 49 | 14 | 11 |
| 49 | 18 | 13 |
| 49 | 20 | 12 |
| 49 | 22 | 14 |
| 49 | 30 | 19 |
| 49 | 37 | 30 |
| 49 | 37 | 36 |
| 49 | 41 | 26 |
| 49 | 43 | 42 |
| 49 | 45 | 37 |
| 50 | 16 | 12 |
| 50 | 25 | 14 |
| 50 | 25 | 15 |
| 50 | 25 | 18 |
| 50 | 26 | 16 |
| 50 | 29 | 22 |
| 50 | 29 | 23 |
| 50 | 29 | 24 |
| 50 | 31 | 20 |
| 50 | 31 | 21 |
| 50 | 32 | 23 |
| 50 | 32 | 24 |
| 50 | 35 | 20 |
| 50 | 35 | 21 |
| 50 | 35 | 23 |
| 50 | 35 | 24 |
| 50 | 38 | 26 |
| 50 | 38 | 37 |
| 50 | 40 | 26 |
| 50 | 42 | 38 |
| 50 | 43 | 39 |
| 50 | 44 | 36 |
| 50 | 46 | 41 |
| 50 | 47 | 42 |
| 50 | 48 | 42 |
| 51 | 16 | 13 |
| 51 | 25 | 18 |
| 51 | 29 | 22 |
| 51 | 29 | 26 |
| 51 | 31 | 20 |
| 51 | 31 | 21 |
| 51 | 31 | 27 |
| 51 | 32 | 22 |
| 51 | 35 | 21 |
| 51 | 37 | 29 |
| 51 | 38 | 28 |
| 51 | 39 | 27 |
| 51 | 39 | 30 |
| 51 | 40 | 28 |

| | | |
|---|---|---|
| 51 | 40 | 37 |
| 51 | 42 | 40 |
| 51 | 43 | 39 |
| 51 | 45 | 39 |
| 51 | 46 | 45 |
| 51 | 47 | 42 |
| 52 | 35 | 23 |
| 52 | 51 | 49 |
| 53 | 16 | 14 |
| 53 | 29 | 21 |
| 53 | 31 | 26 |
| 53 | 35 | 26 |
| 53 | 38 | 27 |
| 53 | 39 | 28 |
| 53 | 41 | 38 |
| 53 | 44 | 37 |
| 53 | 46 | 42 |
| 53 | 47 | 45 |

Table S63: PM6-QFF Coriolis and Fermi resonances for biphenylene generated using parameter set (c).

| Coriolis Resonances | | |
|---|---|---|
| 14 | 11 | C |
| 22 | 21 | C |
| 24 | 22 | C |
| 25 | 23 | C |
| 26 | 21 | C |
| 26 | 24 | C |
| 34 | 29 | A |
| 34 | 32 | C |
| 35 | 26 | C |
| 39 | 35 | A |
| 40 | 39 | B |
| 42 | 36 | C |
| 42 | 41 | B |
| 43 | 40 | C |
| 45 | 40 | B |
| 45 | 43 | A |
| 47 | 44 | C |
| 48 | 42 | A |
| 52 | 51 | B |
| 53 | 51 | A |
| **Type 1 Fermi Resonances** | | |
| 8 | 0 | |
| 9 | 0 | |
| 9 | 4 | |
| 10 | 0 | |
| 10 | 4 | |
| 10 | 5 | |
| 11 | 0 | |
| 11 | 4 | |
| 29 | 8 | |
| 31 | 8 | |
| 32 | 8 | |
| 35 | 8 | |
| 35 | 12 | |
| 36 | 8 | |

| | | |
|---|---|---|
| 36 | 12 | |
| 36 | 16 | |
| 37 | 12 | |
| 38 | 12 | |
| 40 | 12 | |
| 40 | 20 | |
| 41 | 16 | |
| 45 | 25 | |
| 45 | 32 | |
| 45 | 36 | |
| 46 | 32 | |
| 46 | 36 | |
| 47 | 36 | |
| 48 | 32 | |
| 48 | 36 | |
| 49 | 36 | |
| 50 | 47 | |
| 53 | 47 | |
| Type 2 Fermi Resonances | | |
| 9 | 8 | 2 |
| 10 | 8 | 3 |
| 10 | 9 | 1 |
| 10 | 9 | 4 |
| 10 | 9 | 5 |
| 11 | 8 | 1 |
| 11 | 9 | 3 |
| 11 | 10 | 2 |
| 12 | 8 | 0 |
| 12 | 8 | 4 |
| 12 | 11 | 1 |
| 12 | 11 | 4 |
| 12 | 11 | 5 |
| 13 | 8 | 6 |
| 13 | 8 | 7 |
| 13 | 9 | 5 |
| 13 | 10 | 0 |
| 13 | 10 | 4 |
| 13 | 11 | 2 |
| 13 | 11 | 6 |
| 13 | 11 | 7 |
| 14 | 8 | 6 |
| 14 | 8 | 7 |
| 14 | 9 | 4 |
| 14 | 10 | 5 |
| 14 | 11 | 3 |
| 14 | 11 | 6 |
| 14 | 11 | 7 |
| 15 | 8 | 1 |
| 15 | 8 | 4 |
| 15 | 8 | 5 |
| 15 | 9 | 3 |
| 15 | 9 | 6 |
| 15 | 9 | 7 |
| 15 | 10 | 6 |
| 15 | 10 | 7 |
| 15 | 11 | 4 |
| 15 | 11 | 5 |
| 16 | 8 | 0 |
| 16 | 8 | 4 |
| 16 | 8 | 5 |
| 16 | 9 | 2 |

| | | |
|---|---|---|
| 16 | 9 | 3 |
| 16 | 9 | 6 |
| 16 | 9 | 7 |
| 17 | 8 | 2 |
| 17 | 8 | 3 |
| 32 | 25 | 8 |
| 34 | 23 | 8 |
| 34 | 24 | 9 |
| 35 | 23 | 9 |
| 35 | 24 | 8 |
| 35 | 26 | 10 |
| 35 | 32 | 11 |
| 36 | 26 | 9 |
| 36 | 32 | 8 |
| 36 | 35 | 11 |
| 36 | 35 | 15 |
| 39 | 31 | 12 |
| 40 | 22 | 8 |
| 40 | 23 | 11 |
| 40 | 34 | 11 |
| 40 | 35 | 13 |
| 41 | 39 | 19 |
| 41 | 39 | 21 |
| 42 | 24 | 9 |
| 42 | 24 | 14 |
| 42 | 25 | 10 |
| 42 | 25 | 13 |
| 42 | 32 | 10 |
| 42 | 32 | 13 |
| 42 | 35 | 14 |
| 43 | 21 | 8 |
| 43 | 23 | 9 |
| 43 | 25 | 11 |
| 43 | 25 | 15 |
| 43 | 26 | 10 |
| 43 | 32 | 15 |
| 43 | 35 | 16 |
| 43 | 35 | 20 |
| 43 | 36 | 15 |
| 43 | 36 | 19 |
| 44 | 19 | 9 |
| 44 | 21 | 9 |
| 44 | 26 | 11 |
| 45 | 28 | 12 |
| 45 | 29 | 17 |
| 45 | 30 | 18 |
| 45 | 31 | 16 |
| 45 | 33 | 15 |
| 45 | 39 | 25 |
| 45 | 41 | 19 |
| 45 | 41 | 21 |
| 45 | 41 | 24 |
| 46 | 27 | 12 |
| 46 | 28 | 12 |
| 46 | 29 | 18 |
| 46 | 30 | 17 |
| 46 | 31 | 15 |
| 46 | 31 | 21 |
| 46 | 33 | 16 |
| 46 | 38 | 26 |
| 46 | 39 | 24 |
| 46 | 41 | 25 |

| | | |
|---|---|---|
| 46 | 45 | 24 |
| 46 | 45 | 35 |
| 47 | 12 | 8 |
| 47 | 17 | 9 |
| 47 | 18 | 10 |
| 47 | 19 | 11 |
| 47 | 21 | 11 |
| 47 | 22 | 17 |
| 47 | 23 | 18 |
| 47 | 32 | 16 |
| 47 | 35 | 15 |
| 47 | 35 | 21 |
| 47 | 36 | 25 |
| 47 | 40 | 26 |
| 48 | 29 | 12 |
| 48 | 30 | 21 |
| 48 | 33 | 18 |
| 48 | 39 | 22 |
| 48 | 39 | 26 |
| 48 | 45 | 26 |
| 49 | 27 | 13 |
| 49 | 27 | 14 |
| 49 | 28 | 13 |
| 49 | 28 | 14 |
| 49 | 35 | 29 |
| 49 | 37 | 19 |
| 49 | 37 | 21 |
| 49 | 38 | 20 |
| 49 | 38 | 32 |
| 49 | 41 | 26 |
| 49 | 48 | 35 |
| 49 | 48 | 43 |
| 50 | 27 | 13 |
| 50 | 27 | 14 |
| 50 | 28 | 13 |
| 50 | 28 | 14 |
| 50 | 29 | 16 |
| 50 | 30 | 15 |
| 50 | 31 | 17 |
| 50 | 33 | 18 |
| 50 | 37 | 32 |
| 50 | 38 | 35 |
| 50 | 41 | 23 |
| 50 | 45 | 40 |
| 50 | 46 | 34 |
| 51 | 9 | 8 |
| 51 | 11 | 10 |
| 51 | 19 | 10 |
| 51 | 26 | 25 |
| 51 | 32 | 22 |
| 51 | 34 | 21 |
| 51 | 35 | 23 |
| 51 | 36 | 22 |
| 51 | 36 | 26 |
| 51 | 40 | 32 |
| 51 | 44 | 35 |
| 52 | 27 | 19 |
| 52 | 49 | 44 |
| 53 | 35 | 29 |
| 53 | 46 | 40 |
| 53 | 50 | 43 |

Table S64: PM6-QFF Coriolis and Fermi resonances for biphenylene generated using parameter set (d).

| Coriolis Resonances | | |
|---|---|---|
| 11 | 9 | C |
| 12 | 11 | C |
| 14 | 12 | C |
| 15 | 13 | C |
| 16 | 12 | B |
| 17 | 12 | C |
| 18 | 13 | C |
| 19 | 17 | C |
| 22 | 17 | C |
| 23 | 21 | A |
| 28 | 23 | B |
| 30 | 24 | A |
| 31 | 23 | C |
| 31 | 28 | A |
| 32 | 22 | A |
| 32 | 24 | B |
| 33 | 30 | B |
| 33 | 32 | B |
| 35 | 27 | A |
| 37 | 35 | A |
| 42 | 40 | C |
| 43 | 41 | B |
| 44 | 43 | B |
| 45 | 41 | A |
| 46 | 44 | C |
| 52 | 50 | B |
| 53 | 50 | A |
| Type 1 Fermi Resonances | | |
| 12 | 0 | |
| 12 | 3 | |
| 13 | 0 | |
| 13 | 4 | |
| 13 | 6 | |
| 14 | 0 | |
| 14 | 3 | |
| 14 | 4 | |
| 14 | 6 | |
| 33 | 8 | |
| 34 | 8 | |
| 40 | 15 | |
| 42 | 31 | |
| 43 | 31 | |
| 45 | 23 | |
| 45 | 34 | |
| 45 | 37 | |
| 47 | 34 | |
| 47 | 37 | |
| 48 | 37 | |
| 49 | 37 | |
| 50 | 46 | |
| 51 | 46 | |
| Type 2 Fermi Resonances | | |

| | | |
|---|---|---|
| 12 | 10 | 1 |
| 12 | 11 | 0 |
| 12 | 11 | 6 |
| 13 | 11 | 1 |
| 13 | 11 | 2 |
| 13 | 11 | 5 |
| 13 | 11 | 7 |
| 13 | 12 | 1 |
| 13 | 12 | 7 |
| 14 | 10 | 2 |
| 14 | 10 | 7 |
| 14 | 11 | 6 |
| 14 | 12 | 0 |
| 14 | 12 | 3 |
| 14 | 12 | 4 |
| 14 | 12 | 6 |
| 14 | 13 | 2 |
| 14 | 13 | 7 |
| 15 | 10 | 6 |
| 15 | 11 | 1 |
| 15 | 11 | 5 |
| 15 | 11 | 7 |
| 15 | 12 | 7 |
| 15 | 13 | 6 |
| 15 | 14 | 7 |
| 17 | 8 | 1 |
| 17 | 11 | 0 |
| 17 | 11 | 4 |
| 18 | 8 | 0 |
| 18 | 8 | 3 |
| 18 | 9 | 1 |
| 18 | 9 | 2 |
| 18 | 10 | 3 |
| 18 | 10 | 6 |
| 19 | 8 | 2 |
| 19 | 8 | 5 |
| 19 | 8 | 7 |
| 19 | 9 | 0 |
| 19 | 9 | 4 |
| 19 | 10 | 1 |
| 19 | 10 | 5 |
| 19 | 11 | 0 |
| 19 | 11 | 3 |
| 19 | 11 | 4 |
| 19 | 11 | 6 |
| 20 | 8 | 3 |
| 20 | 8 | 4 |
| 20 | 9 | 1 |
| 20 | 9 | 2 |
| 20 | 9 | 5 |
| 20 | 10 | 0 |
| 20 | 10 | 4 |
| 20 | 11 | 1 |
| 20 | 11 | 2 |
| 20 | 11 | 5 |
| 20 | 11 | 7 |
| 22 | 8 | 2 |
| 22 | 8 | 5 |
| 22 | 9 | 0 |
| 22 | 9 | 4 |
| 22 | 10 | 1 |
| 22 | 10 | 5 |

| | | |
|---|---|---|
| 23 | 8 | 4 |
| 23 | 9 | 2 |
| 23 | 10 | 3 |
| 23 | 10 | 4 |
| 24 | 8 | 1 |
| 24 | 9 | 0 |
| 24 | 9 | 4 |
| 24 | 10 | 2 |
| 24 | 10 | 5 |
| 25 | 8 | 0 |
| 25 | 8 | 6 |
| 25 | 9 | 1 |
| 25 | 9 | 5 |
| 25 | 10 | 4 |
| 26 | 8 | 7 |
| 26 | 9 | 0 |
| 27 | 8 | 4 |
| 27 | 8 | 6 |
| 33 | 8 | 2 |
| 34 | 31 | 8 |
| 37 | 23 | 8 |
| 37 | 34 | 8 |
| 40 | 23 | 9 |
| 40 | 25 | 9 |
| 40 | 27 | 9 |
| 40 | 29 | 10 |
| 40 | 31 | 11 |
| 40 | 34 | 9 |
| 41 | 17 | 9 |
| 41 | 18 | 8 |
| 41 | 25 | 10 |
| 41 | 27 | 10 |
| 41 | 34 | 13 |
| 42 | 23 | 11 |
| 42 | 27 | 11 |
| 42 | 29 | 8 |
| 42 | 34 | 14 |
| 43 | 36 | 17 |
| 44 | 13 | 8 |
| 44 | 14 | 9 |
| 44 | 17 | 9 |
| 44 | 18 | 10 |
| 44 | 34 | 13 |
| 45 | 36 | 19 |
| 45 | 36 | 22 |
| 45 | 43 | 31 |
| 46 | 12 | 9 |
| 46 | 15 | 8 |
| 46 | 15 | 10 |
| 46 | 29 | 11 |
| 47 | 36 | 18 |
| 47 | 38 | 26 |
| 47 | 39 | 31 |
| 47 | 42 | 35 |
| 47 | 43 | 33 |
| 47 | 44 | 39 |
| 48 | 28 | 20 |
| 48 | 35 | 18 |
| 48 | 36 | 33 |
| 48 | 38 | 31 |
| 48 | 39 | 26 |
| 48 | 41 | 38 |

| | | |
|---|---|---|
| 48 | 43 | 34 |
| 48 | 44 | 38 |
| 48 | 45 | 41 |
| 49 | 16 | 10 |
| 49 | 16 | 13 |
| 49 | 35 | 19 |
| 49 | 36 | 31 |
| 49 | 38 | 17 |
| 49 | 38 | 24 |
| 49 | 40 | 35 |
| 49 | 42 | 38 |
| 49 | 43 | 26 |
| 49 | 46 | 39 |
| 49 | 47 | 44 |
| 50 | 9 | 8 |
| 50 | 10 | 9 |
| 50 | 11 | 10 |
| 50 | 15 | 9 |
| 50 | 18 | 12 |
| 50 | 25 | 12 |
| 50 | 27 | 12 |
| 50 | 29 | 13 |
| 50 | 34 | 19 |
| 50 | 41 | 29 |
| 51 | 16 | 12 |
| 51 | 21 | 13 |
| 51 | 30 | 19 |
| 51 | 35 | 20 |
| 51 | 35 | 31 |
| 51 | 38 | 23 |
| 51 | 39 | 24 |
| 51 | 40 | 36 |
| 51 | 42 | 39 |
| 51 | 46 | 45 |
| 51 | 47 | 40 |
| 51 | 48 | 44 |
| 51 | 49 | 42 |
| 52 | 21 | 14 |
| 52 | 38 | 26 |
| 52 | 49 | 44 |
| 52 | 51 | 50 |
| 53 | 30 | 18 |
| 53 | 32 | 18 |
| 53 | 36 | 31 |
| 53 | 43 | 40 |
| 53 | 45 | 42 |
| 53 | 49 | 46 |

Table S65: PM6-QFF Coriolis and Fermi resonances for biphenylene generated using parameter set (e).

| Coriolis Resonances | | |
|---|---|---|
| 11 | 9 | C |
| 13 | 11 | C |
| 22 | 21 | C |
| 24 | 22 | C |
| 27 | 23 | C |
| 28 | 21 | C |
| 28 | 24 | C |

| | | |
|---|---|---|
| 30 | 24 | B |
| 34 | 29 | A |
| 34 | 33 | C |
| 35 | 28 | C |
| 35 | 30 | B |
| 39 | 35 | A |
| 40 | 39 | B |
| 42 | 37 | C |
| 42 | 41 | B |
| 43 | 40 | C |
| 44 | 40 | B |
| 44 | 43 | A |
| 47 | 42 | A |
| 48 | 45 | C |
| 52 | 51 | B |
| 53 | 51 | A |

Type 1 Fermi Resonances

| | |
|---|---|
| 9 | 0 |
| 9 | 4 |
| 9 | 5 |
| 10 | 0 |
| 10 | 4 |
| 10 | 5 |
| 11 | 0 |
| 11 | 4 |
| 31 | 8 |
| 33 | 8 |
| 35 | 8 |
| 37 | 8 |
| 37 | 16 |
| 40 | 14 |
| 40 | 20 |
| 41 | 14 |
| 41 | 16 |
| 44 | 27 |
| 44 | 33 |
| 46 | 27 |
| 46 | 33 |
| 46 | 37 |
| 47 | 33 |
| 47 | 37 |
| 48 | 37 |
| 49 | 37 |
| 50 | 37 |
| 50 | 48 |
| 53 | 48 |

Type 2 Fermi Resonances

| | | |
|---|---|---|
| 10 | 8 | 2 |
| 10 | 8 | 3 |
| 10 | 9 | 1 |
| 10 | 9 | 5 |
| 11 | 8 | 1 |
| 11 | 9 | 2 |
| 11 | 9 | 3 |
| 11 | 10 | 2 |
| 11 | 10 | 3 |
| 12 | 8 | 6 |
| 12 | 8 | 7 |
| 12 | 9 | 5 |
| 12 | 10 | 0 |

| | | |
|---|---|---|
| 12 | 10 | 4 |
| 12 | 11 | 6 |
| 12 | 11 | 7 |
| 13 | 8 | 6 |
| 13 | 8 | 7 |
| 13 | 9 | 4 |
| 13 | 9 | 5 |
| 13 | 10 | 5 |
| 13 | 11 | 3 |
| 13 | 11 | 6 |
| 13 | 11 | 7 |
| 14 | 8 | 0 |
| 14 | 8 | 4 |
| 14 | 9 | 2 |
| 14 | 10 | 3 |
| 14 | 11 | 1 |
| 14 | 11 | 4 |
| 14 | 11 | 5 |
| 15 | 8 | 1 |
| 15 | 8 | 5 |
| 15 | 9 | 2 |
| 15 | 9 | 3 |
| 15 | 9 | 6 |
| 15 | 9 | 7 |
| 15 | 10 | 2 |
| 15 | 10 | 3 |
| 15 | 10 | 6 |
| 15 | 10 | 7 |
| 15 | 11 | 0 |
| 15 | 11 | 4 |
| 15 | 11 | 5 |
| 16 | 8 | 0 |
| 16 | 8 | 4 |
| 16 | 8 | 5 |
| 16 | 9 | 2 |
| 16 | 9 | 3 |
| 16 | 9 | 6 |
| 16 | 9 | 7 |
| 16 | 10 | 2 |
| 16 | 10 | 3 |
| 16 | 10 | 6 |
| 16 | 10 | 7 |
| 16 | 11 | 4 |
| 16 | 11 | 5 |
| 17 | 8 | 3 |
| 17 | 9 | 5 |
| 18 | 8 | 2 |
| 18 | 9 | 4 |
| 19 | 8 | 4 |
| 19 | 8 | 5 |
| 33 | 27 | 8 |
| 35 | 24 | 8 |
| 35 | 33 | 11 |
| 37 | 24 | 11 |
| 37 | 33 | 8 |
| 37 | 35 | 11 |
| 37 | 35 | 15 |
| 40 | 22 | 8 |
| 40 | 23 | 11 |
| 40 | 34 | 11 |
| 40 | 35 | 12 |
| 42 | 27 | 10 |

| | | |
|---|---|---|
| 42 | 27 | 12 |
| 42 | 33 | 10 |
| 42 | 33 | 12 |
| 42 | 35 | 13 |
| 43 | 21 | 8 |
| 43 | 23 | 9 |
| 43 | 27 | 15 |
| 43 | 28 | 10 |
| 43 | 33 | 15 |
| 43 | 34 | 9 |
| 43 | 35 | 16 |
| 43 | 37 | 15 |
| 44 | 25 | 14 |
| 44 | 26 | 11 |
| 44 | 29 | 18 |
| 44 | 31 | 16 |
| 44 | 32 | 15 |
| 44 | 41 | 21 |
| 44 | 41 | 24 |
| 45 | 19 | 9 |
| 45 | 21 | 9 |
| 46 | 25 | 11 |
| 46 | 25 | 15 |
| 46 | 26 | 14 |
| 46 | 29 | 17 |
| 46 | 30 | 18 |
| 46 | 31 | 15 |
| 46 | 31 | 21 |
| 46 | 32 | 16 |
| 46 | 38 | 28 |
| 46 | 39 | 24 |
| 46 | 41 | 27 |
| 46 | 44 | 24 |
| 46 | 44 | 35 |
| 47 | 29 | 14 |
| 47 | 30 | 21 |
| 47 | 39 | 22 |
| 47 | 39 | 28 |
| 47 | 44 | 28 |
| 48 | 14 | 8 |
| 48 | 17 | 10 |
| 48 | 18 | 9 |
| 48 | 21 | 11 |
| 48 | 22 | 18 |
| 48 | 33 | 16 |
| 48 | 35 | 15 |
| 48 | 35 | 21 |
| 48 | 37 | 27 |
| 48 | 40 | 28 |
| 49 | 25 | 12 |
| 49 | 26 | 13 |
| 49 | 35 | 29 |
| 49 | 36 | 19 |
| 49 | 36 | 21 |
| 49 | 38 | 20 |
| 49 | 38 | 33 |
| 49 | 39 | 17 |
| 49 | 41 | 28 |
| 49 | 47 | 35 |
| 49 | 47 | 43 |
| 50 | 25 | 12 |
| 50 | 25 | 13 |

| | | |
|---|---|---|
| 50 | 26 | 12 |
| 50 | 26 | 13 |
| 50 | 30 | 15 |
| 50 | 31 | 18 |
| 50 | 32 | 17 |
| 50 | 36 | 20 |
| 50 | 36 | 33 |
| 50 | 38 | 21 |
| 50 | 41 | 23 |
| 50 | 44 | 40 |
| 51 | 9 | 8 |
| 51 | 11 | 10 |
| 51 | 33 | 22 |
| 51 | 35 | 23 |
| 51 | 37 | 22 |
| 51 | 37 | 28 |
| 51 | 40 | 33 |
| 51 | 45 | 35 |
| 52 | 26 | 19 |
| 52 | 32 | 21 |
| 52 | 49 | 45 |
| 53 | 35 | 29 |
| 53 | 46 | 40 |
| 53 | 50 | 43 |

Table S66: PM6-QFF Coriolis and Fermi resonances for biphenylene generated using parameter set (f).

| Coriolis Resonances | | |
|---|---|---|
| 11 | 8 | C |
| 11 | 10 | C |
| 13 | 11 | C |
| 14 | 13 | C |
| 15 | 13 | C |
| 22 | 21 | A |
| 24 | 17 | B |
| 27 | 24 | A |
| 28 | 23 | B |
| 28 | 26 | B |
| 28 | 27 | B |
| 30 | 28 | B |
| 32 | 19 | B |
| 32 | 20 | B |
| 32 | 26 | B |
| 33 | 31 | B |
| 34 | 30 | A |
| 42 | 40 | C |
| 43 | 40 | C |
| 45 | 43 | A |
| 46 | 42 | A |
| 47 | 43 | C |
| 47 | 44 | C |
| 49 | 44 | A |
| 52 | 51 | A |
| 52 | 51 | B |
| 53 | 51 | A |
| 53 | 51 | B |
| Type 1 Fermi Resonances | | |

| | |
|---|---|
| 11 | 4 |
| 11 | 6 |
| 12 | 0 |
| 12 | 1 |
| 35 | 10 |
| 35 | 11 |
| 36 | 12 |
| 37 | 15 |
| 38 | 9 |
| 38 | 16 |
| 41 | 18 |
| 41 | 23 |
| 45 | 23 |
| 45 | 27 |
| 45 | 29 |
| 45 | 35 |
| 45 | 38 |
| 46 | 26 |
| 46 | 29 |
| 46 | 35 |
| 48 | 35 |
| 48 | 40 |
| 48 | 42 |
| 49 | 47 |
| 50 | 40 |
| 50 | 42 |
| 52 | 47 |

Type 2 Fermi Resonances

| | | |
|---|---|---|
| 11 | 10 | 6 |
| 13 | 10 | 5 |
| 13 | 11 | 4 |
| 13 | 11 | 7 |
| 14 | 10 | 5 |
| 14 | 10 | 7 |
| 14 | 11 | 5 |
| 14 | 11 | 7 |
| 15 | 9 | 2 |
| 15 | 10 | 5 |
| 15 | 10 | 7 |
| 15 | 11 | 4 |
| 16 | 9 | 2 |
| 16 | 10 | 5 |
| 16 | 11 | 4 |
| 16 | 11 | 6 |
| 16 | 11 | 7 |
| 17 | 8 | 0 |
| 17 | 8 | 1 |
| 17 | 8 | 3 |
| 17 | 9 | 1 |
| 17 | 11 | 1 |
| 17 | 11 | 3 |
| 18 | 8 | 1 |
| 18 | 9 | 2 |
| 19 | 8 | 1 |
| 19 | 8 | 2 |
| 33 | 30 | 8 |
| 35 | 30 | 11 |
| 35 | 33 | 11 |
| 38 | 25 | 11 |
| 38 | 29 | 10 |
| 40 | 30 | 12 |

| | | |
|---|---|---|
| 41 | 36 | 12 |
| 42 | 29 | 11 |
| 42 | 29 | 14 |
| 42 | 35 | 15 |
| 43 | 15 | 9 |
| 43 | 29 | 13 |
| 43 | 30 | 13 |
| 44 | 14 | 8 |
| 44 | 18 | 11 |
| 44 | 30 | 11 |
| 45 | 24 | 12 |
| 45 | 39 | 18 |
| 45 | 39 | 20 |
| 45 | 41 | 23 |
| 46 | 39 | 30 |
| 46 | 39 | 33 |
| 46 | 45 | 26 |
| 46 | 45 | 29 |
| 47 | 13 | 10 |
| 47 | 35 | 13 |
| 48 | 24 | 12 |
| 48 | 37 | 30 |
| 48 | 39 | 18 |
| 48 | 39 | 19 |
| 48 | 39 | 20 |
| 48 | 41 | 18 |
| 48 | 41 | 20 |
| 48 | 46 | 35 |
| 49 | 22 | 13 |
| 49 | 22 | 14 |
| 49 | 32 | 18 |
| 49 | 37 | 29 |
| 49 | 37 | 30 |
| 49 | 37 | 33 |
| 49 | 41 | 25 |
| 50 | 34 | 30 |
| 50 | 45 | 35 |
| 50 | 48 | 43 |
| 50 | 49 | 40 |
| 51 | 18 | 14 |
| 51 | 29 | 13 |
| 51 | 35 | 18 |
| 52 | 28 | 15 |
| 52 | 36 | 23 |
| 52 | 46 | 38 |
| 52 | 48 | 44 |
| 52 | 50 | 43 |
| 53 | 34 | 18 |
| 53 | 37 | 25 |
| 53 | 52 | 47 |

Table S67: PM6-QFF Coriolis and Fermi resonances for benzopentalene generated using parameter set (a).

| Coriolis Resonances | | |
|---|---|---|
| 14 | 11 | C |
| 24 | 22 | C |
| 25 | 20 | A |
| 27 | 21 | C |

| | | |
|---|---|---|
| 28 | 21 | C |
| 28 | 27 | C |
| 34 | 27 | C |
| 34 | 28 | C |
| 34 | 33 | C |
| 37 | 32 | C |
| 37 | 33 | C |
| 39 | 34 | A |
| 40 | 38 | C |
| 42 | 37 | C |
| 42 | 38 | C |
| 42 | 40 | C |
| 43 | 40 | C |
| 44 | 42 | A |
| 47 | 43 | C |
| 47 | 46 | C |
| 49 | 46 | A |
| 52 | 51 | A |
| 52 | 51 | B |
| 53 | 51 | A |

Type 1 Fermi Resonances

| | |
|---|---|
| 8 | 0 |
| 8 | 2 |
| 8 | 3 |
| 9 | 0 |
| 9 | 1 |
| 9 | 3 |
| 10 | 0 |
| 10 | 1 |
| 10 | 3 |
| 10 | 5 |
| 10 | 7 |
| 11 | 0 |
| 11 | 1 |
| 11 | 5 |
| 11 | 6 |
| 11 | 7 |
| 12 | 0 |
| 12 | 1 |
| 12 | 2 |
| 12 | 4 |
| 13 | 0 |
| 13 | 1 |
| 13 | 2 |
| 13 | 3 |
| 13 | 6 |
| 13 | 7 |
| 33 | 8 |
| 33 | 9 |
| 34 | 8 |
| 34 | 10 |
| 37 | 9 |
| 38 | 14 |
| 44 | 21 |
| 44 | 24 |
| 44 | 27 |
| 44 | 28 |
| 45 | 32 |
| 46 | 24 |
| 47 | 38 |
| 48 | 33 |

| | | |
|---|---|---|
| 48 | 34 | |
| 48 | 38 | |
| 49 | 38 | |
| 49 | 47 | |
| 50 | 40 | |
| 50 | 42 | |
| 50 | 46 | |
| 50 | 47 | |
| 52 | 47 | |
| Type 2 Fermi Resonances | | |
| 9 | 8 | 2 |
| 9 | 8 | 3 |
| 10 | 8 | 0 |
| 10 | 8 | 1 |
| 10 | 8 | 2 |
| 10 | 9 | 1 |
| 10 | 9 | 3 |
| 11 | 8 | 0 |
| 11 | 8 | 5 |
| 11 | 9 | 5 |
| 11 | 10 | 5 |
| 11 | 10 | 6 |
| 11 | 10 | 7 |
| 12 | 8 | 0 |
| 12 | 8 | 4 |
| 12 | 9 | 0 |
| 12 | 9 | 2 |
| 12 | 9 | 4 |
| 12 | 10 | 0 |
| 12 | 10 | 1 |
| 12 | 10 | 6 |
| 12 | 10 | 7 |
| 12 | 11 | 0 |
| 12 | 11 | 1 |
| 12 | 11 | 6 |
| 12 | 11 | 7 |
| 13 | 8 | 5 |
| 13 | 8 | 7 |
| 13 | 9 | 7 |
| 13 | 10 | 5 |
| 13 | 10 | 7 |
| 13 | 11 | 1 |
| 13 | 11 | 7 |
| 13 | 12 | 1 |
| 13 | 12 | 5 |
| 13 | 12 | 7 |
| 14 | 8 | 3 |
| 14 | 8 | 4 |
| 14 | 8 | 6 |
| 14 | 9 | 1 |
| 14 | 9 | 3 |
| 14 | 9 | 4 |
| 14 | 9 | 6 |
| 14 | 10 | 1 |
| 14 | 10 | 4 |
| 14 | 10 | 5 |
| 14 | 10 | 6 |
| 14 | 11 | 4 |
| 14 | 11 | 5 |
| 14 | 11 | 7 |
| 14 | 12 | 2 |

| | | |
|---|---|---|
| 14 | 12 | 4 |
| 14 | 12 | 5 |
| 14 | 12 | 6 |
| 14 | 12 | 7 |
| 14 | 13 | 5 |
| 14 | 13 | 7 |
| 15 | 8 | 0 |
| 15 | 8 | 2 |
| 15 | 8 | 3 |
| 15 | 8 | 4 |
| 15 | 9 | 0 |
| 15 | 9 | 3 |
| 15 | 9 | 4 |
| 15 | 10 | 4 |
| 15 | 10 | 6 |
| 15 | 11 | 4 |
| 15 | 11 | 5 |
| 15 | 11 | 7 |
| 15 | 12 | 2 |
| 15 | 12 | 4 |
| 15 | 12 | 5 |
| 15 | 13 | 7 |
| 16 | 8 | 2 |
| 16 | 8 | 3 |
| 16 | 8 | 4 |
| 16 | 8 | 5 |
| 16 | 8 | 6 |
| 16 | 9 | 3 |
| 16 | 10 | 2 |
| 16 | 10 | 3 |
| 16 | 10 | 4 |
| 16 | 10 | 5 |
| 16 | 10 | 6 |
| 16 | 10 | 7 |
| 16 | 11 | 3 |
| 16 | 11 | 5 |
| 16 | 11 | 6 |
| 16 | 11 | 7 |
| 17 | 8 | 0 |
| 17 | 8 | 1 |
| 17 | 8 | 2 |
| 17 | 8 | 3 |
| 17 | 8 | 4 |
| 17 | 9 | 1 |
| 17 | 9 | 2 |
| 17 | 9 | 3 |
| 17 | 10 | 7 |
| 18 | 8 | 0 |
| 18 | 8 | 2 |
| 18 | 8 | 3 |
| 18 | 9 | 2 |
| 18 | 9 | 3 |
| 19 | 8 | 1 |
| 19 | 8 | 3 |
| 19 | 8 | 6 |
| 37 | 33 | 8 |
| 38 | 37 | 14 |
| 40 | 34 | 14 |
| 42 | 24 | 10 |
| 42 | 28 | 10 |
| 42 | 33 | 9 |
| 42 | 34 | 14 |

| | | |
|---|---|---|
| 43 | 24 | 9 |
| 43 | 34 | 13 |
| 44 | 23 | 10 |
| 44 | 26 | 11 |
| 44 | 26 | 16 |
| 44 | 31 | 14 |
| 44 | 36 | 13 |
| 46 | 21 | 11 |
| 46 | 24 | 11 |
| 46 | 27 | 10 |
| 46 | 33 | 11 |
| 46 | 34 | 11 |
| 46 | 34 | 21 |
| 47 | 17 | 8 |
| 47 | 17 | 11 |
| 47 | 19 | 10 |
| 47 | 21 | 8 |
| 47 | 21 | 10 |
| 47 | 37 | 22 |
| 47 | 37 | 27 |
| 47 | 38 | 21 |
| 47 | 42 | 34 |
| 48 | 23 | 13 |
| 48 | 36 | 19 |
| 48 | 36 | 21 |
| 48 | 39 | 16 |
| 48 | 39 | 27 |
| 48 | 39 | 28 |
| 48 | 44 | 27 |
| 48 | 45 | 32 |
| 49 | 23 | 13 |
| 49 | 25 | 15 |
| 49 | 26 | 14 |
| 49 | 29 | 16 |
| 49 | 30 | 17 |
| 49 | 31 | 16 |
| 49 | 35 | 20 |
| 49 | 36 | 19 |
| 49 | 36 | 21 |
| 49 | 39 | 22 |
| 49 | 45 | 32 |
| 49 | 45 | 33 |
| 50 | 25 | 12 |
| 50 | 30 | 17 |
| 50 | 34 | 31 |
| 50 | 39 | 21 |
| 50 | 41 | 24 |
| 50 | 44 | 34 |
| 50 | 45 | 38 |
| 50 | 48 | 43 |
| 51 | 22 | 21 |
| 51 | 27 | 21 |
| 51 | 32 | 22 |
| 51 | 33 | 22 |
| 51 | 33 | 27 |
| 51 | 34 | 22 |
| 51 | 37 | 21 |
| 51 | 37 | 33 |
| 51 | 46 | 34 |
| 52 | 44 | 37 |
| 52 | 48 | 46 |
| 52 | 50 | 43 |

| | | |
|---|---|---|
| 53 | 52 | 47 |

Table S68: PM6-QFF Coriolis and Fermi resonances for benzopentalene generated using parameter set (b).

| | | |
|---|---|---|
| Coriolis Resonances | | |
| 10 | 9 | C |
| 14 | 13 | C |
| 15 | 12 | C |
| 15 | 14 | C |
| 18 | 16 | C |
| 19 | 18 | C |
| 26 | 25 | C |
| 27 | 20 | A |
| 29 | 28 | B |
| 31 | 30 | A |
| 32 | 31 | A |
| 32 | 31 | B |
| 34 | 32 | B |
| 36 | 33 | A |
| 36 | 35 | A |
| 36 | 35 | B |
| 37 | 36 | A |
| 41 | 37 | C |
| 45 | 41 | C |
| 45 | 44 | C |
| 46 | 43 | A |
| 52 | 49 | A |
| 52 | 49 | B |
| 53 | 49 | A |
| 53 | 49 | B |
| Type 1 Fermi Resonances | | |
| 11 | 0 | |
| 12 | 0 | |
| 13 | 0 | |
| 13 | 1 | |
| 13 | 4 | |
| 13 | 5 | |
| 13 | 6 | |
| 14 | 0 | |
| 14 | 2 | |
| 14 | 3 | |
| 14 | 4 | |
| 15 | 2 | |
| 15 | 6 | |
| 28 | 9 | |
| 31 | 11 | |
| 32 | 9 | |
| 32 | 12 | |
| 33 | 13 | |
| 35 | 10 | |
| 35 | 11 | |
| 36 | 13 | |
| 37 | 11 | |
| 37 | 12 | |
| 37 | 13 | |
| 37 | 16 | |
| 37 | 18 | |

| | |
|---|---|
| 40 | 15 |
| 40 | 18 |
| 40 | 19 |
| 42 | 19 |
| 42 | 26 |
| 43 | 21 |
| 43 | 26 |
| 46 | 26 |
| 46 | 33 |
| 46 | 37 |
| 47 | 33 |
| 47 | 35 |
| 47 | 37 |
| 48 | 37 |
| 50 | 41 |
| 50 | 43 |
| 50 | 44 |
| 51 | 45 |

| Type 2 Fermi Resonances | | |
|---|---|---|
| 13 | 11 | 0 |
| 13 | 11 | 1 |
| 13 | 11 | 4 |
| 13 | 12 | 3 |
| 13 | 12 | 4 |
| 14 | 11 | 0 |
| 14 | 11 | 1 |
| 14 | 11 | 2 |
| 14 | 11 | 6 |
| 14 | 12 | 0 |
| 14 | 12 | 2 |
| 14 | 13 | 0 |
| 14 | 13 | 2 |
| 14 | 13 | 4 |
| 15 | 11 | 0 |
| 15 | 11 | 1 |
| 15 | 11 | 5 |
| 15 | 12 | 3 |
| 15 | 12 | 4 |
| 15 | 13 | 0 |
| 15 | 13 | 1 |
| 15 | 13 | 2 |
| 15 | 13 | 3 |
| 15 | 13 | 5 |
| 15 | 13 | 6 |
| 15 | 14 | 1 |
| 15 | 14 | 2 |
| 15 | 14 | 3 |
| 15 | 14 | 4 |
| 15 | 14 | 6 |
| 16 | 10 | 1 |
| 16 | 11 | 4 |
| 16 | 11 | 6 |
| 16 | 12 | 1 |
| 16 | 12 | 3 |
| 16 | 12 | 7 |
| 16 | 13 | 1 |
| 16 | 13 | 3 |
| 16 | 13 | 4 |
| 16 | 14 | 3 |
| 16 | 14 | 4 |
| 16 | 14 | 5 |

| | | |
|---|---|---|
| 16 | 15 | 5 |
| 16 | 15 | 7 |
| 18 | 11 | 5 |
| 18 | 11 | 6 |
| 18 | 12 | 2 |
| 18 | 13 | 3 |
| 19 | 8 | 3 |
| 19 | 9 | 0 |
| 19 | 9 | 4 |
| 19 | 10 | 1 |
| 19 | 10 | 3 |
| 19 | 11 | 1 |
| 19 | 12 | 2 |
| 19 | 12 | 6 |
| 19 | 13 | 4 |
| 19 | 13 | 6 |
| 20 | 8 | 2 |
| 20 | 8 | 4 |
| 20 | 9 | 0 |
| 20 | 9 | 1 |
| 20 | 9 | 2 |
| 20 | 9 | 3 |
| 20 | 11 | 4 |
| 20 | 12 | 7 |
| 21 | 8 | 2 |
| 21 | 8 | 3 |
| 21 | 10 | 0 |
| 21 | 10 | 1 |
| 21 | 10 | 2 |
| 21 | 10 | 3 |
| 22 | 8 | 4 |
| 22 | 9 | 2 |
| 22 | 9 | 3 |
| 22 | 9 | 4 |
| 22 | 10 | 2 |
| 23 | 8 | 0 |
| 23 | 8 | 2 |
| 23 | 8 | 3 |
| 23 | 8 | 4 |
| 23 | 9 | 0 |
| 23 | 9 | 1 |
| 23 | 9 | 2 |
| 23 | 10 | 1 |
| 24 | 8 | 0 |
| 24 | 8 | 1 |
| 24 | 8 | 4 |
| 24 | 9 | 1 |
| 24 | 9 | 2 |
| 24 | 10 | 1 |
| 24 | 10 | 4 |
| 25 | 8 | 1 |
| 25 | 8 | 4 |
| 25 | 9 | 0 |
| 25 | 10 | 3 |
| 25 | 10 | 4 |
| 26 | 8 | 1 |
| 26 | 9 | 2 |
| 26 | 25 | 8 |
| 28 | 8 | 4 |
| 32 | 8 | 6 |
| 32 | 22 | 9 |
| 32 | 24 | 9 |

| | | |
|---|---|---|
| 32 | 25 | 9 |
| 32 | 25 | 10 |
| 32 | 28 | 10 |
| 32 | 30 | 10 |
| 35 | 19 | 8 |
| 35 | 20 | 8 |
| 35 | 20 | 9 |
| 35 | 22 | 8 |
| 35 | 32 | 11 |
| 35 | 33 | 13 |
| 37 | 18 | 8 |
| 37 | 19 | 8 |
| 37 | 20 | 8 |
| 37 | 20 | 9 |
| 37 | 20 | 10 |
| 37 | 22 | 9 |
| 37 | 22 | 10 |
| 37 | 24 | 8 |
| 37 | 24 | 10 |
| 37 | 25 | 10 |
| 37 | 26 | 8 |
| 41 | 16 | 9 |
| 41 | 25 | 9 |
| 41 | 26 | 13 |
| 41 | 28 | 11 |
| 41 | 32 | 11 |
| 41 | 33 | 14 |
| 42 | 38 | 23 |
| 43 | 16 | 10 |
| 43 | 18 | 8 |
| 43 | 19 | 10 |
| 43 | 20 | 8 |
| 43 | 20 | 10 |
| 43 | 20 | 12 |
| 43 | 22 | 9 |
| 43 | 22 | 10 |
| 43 | 23 | 9 |
| 43 | 24 | 10 |
| 43 | 24 | 12 |
| 43 | 25 | 11 |
| 43 | 25 | 12 |
| 43 | 26 | 12 |
| 43 | 28 | 11 |
| 43 | 32 | 12 |
| 43 | 33 | 14 |
| 43 | 37 | 15 |
| 43 | 37 | 21 |
| 43 | 37 | 22 |
| 43 | 37 | 23 |
| 44 | 15 | 9 |
| 44 | 16 | 9 |
| 44 | 20 | 13 |
| 44 | 21 | 11 |
| 45 | 12 | 8 |
| 45 | 25 | 11 |
| 45 | 26 | 13 |
| 45 | 33 | 20 |
| 45 | 43 | 26 |
| 46 | 36 | 25 |
| 46 | 38 | 23 |
| 46 | 40 | 21 |
| 46 | 42 | 23 |

| | | |
|---|---|---|
| 46 | 42 | 25 |
| 46 | 42 | 26 |
| 47 | 27 | 16 |
| 47 | 27 | 18 |
| 47 | 29 | 20 |
| 47 | 31 | 23 |
| 47 | 36 | 25 |
| 47 | 36 | 26 |
| 47 | 38 | 23 |
| 47 | 39 | 28 |
| 47 | 46 | 37 |
| 48 | 17 | 11 |
| 48 | 20 | 17 |
| 48 | 27 | 15 |
| 48 | 27 | 21 |
| 48 | 29 | 21 |
| 48 | 31 | 22 |
| 48 | 31 | 24 |
| 48 | 31 | 25 |
| 48 | 34 | 23 |
| 48 | 36 | 25 |
| 48 | 38 | 23 |
| 48 | 38 | 28 |
| 48 | 39 | 23 |
| 48 | 39 | 28 |
| 48 | 40 | 26 |
| 48 | 41 | 38 |
| 48 | 42 | 35 |
| 48 | 43 | 38 |
| 48 | 44 | 40 |
| 48 | 47 | 41 |
| 48 | 47 | 44 |
| 49 | 13 | 11 |
| 49 | 14 | 12 |
| 49 | 16 | 11 |
| 49 | 20 | 18 |
| 49 | 22 | 18 |
| 49 | 26 | 15 |
| 49 | 26 | 18 |
| 50 | 17 | 13 |
| 50 | 17 | 15 |
| 50 | 27 | 15 |
| 50 | 27 | 19 |
| 50 | 27 | 24 |
| 50 | 29 | 19 |
| 50 | 29 | 24 |
| 50 | 31 | 21 |
| 50 | 31 | 22 |
| 50 | 31 | 24 |
| 50 | 34 | 21 |
| 50 | 38 | 23 |
| 50 | 38 | 24 |
| 50 | 38 | 28 |
| 50 | 39 | 24 |
| 50 | 39 | 28 |
| 50 | 43 | 38 |
| 50 | 46 | 44 |
| 51 | 17 | 11 |
| 51 | 17 | 14 |
| 51 | 20 | 17 |
| 51 | 27 | 19 |
| 51 | 27 | 23 |

| | | |
|---|---|---|
| 51 | 29 | 20 |
| 51 | 29 | 21 |
| 51 | 29 | 25 |
| 51 | 31 | 22 |
| 51 | 34 | 21 |
| 51 | 38 | 28 |
| 51 | 39 | 28 |
| 51 | 40 | 28 |
| 51 | 41 | 39 |
| 51 | 42 | 35 |
| 51 | 46 | 37 |
| 51 | 46 | 45 |
| 51 | 47 | 41 |
| 51 | 47 | 44 |
| 51 | 48 | 44 |
| 51 | 49 | 48 |
| 52 | 47 | 44 |
| 52 | 51 | 49 |
| 53 | 17 | 12 |
| 53 | 36 | 26 |
| 53 | 38 | 28 |
| 53 | 43 | 36 |
| 53 | 46 | 41 |
| 53 | 47 | 45 |
| 53 | 48 | 43 |
| 53 | 50 | 49 |

Table S69: PM6-QFF Coriolis and Fermi resonances for benzopentalene generated using parameter set (c).

| Coriolis Resonances | | |
|---|---|---|
| 13 | 11 | C |
| 14 | 10 | C |
| 25 | 24 | C |
| 34 | 25 | C |
| 34 | 31 | C |
| 35 | 28 | C |
| 35 | 31 | C |
| 36 | 34 | C |
| 39 | 34 | A |
| 41 | 36 | C |
| 41 | 40 | C |
| 43 | 40 | C |
| 44 | 41 | A |
| 47 | 43 | C |
| 47 | 45 | C |
| 49 | 45 | A |
| 52 | 51 | A |
| 52 | 51 | B |
| 53 | 51 | A |
| 53 | 51 | B |
| **Type 1 Fermi Resonances** | | |
| 8 | 0 | |
| 8 | 2 | |
| 8 | 4 | |
| 9 | 4 | |
| 9 | 5 | |
| 10 | 0 | |

| | |
|---|---|
| 10 | 1 |
| 10 | 6 |
| 10 | 7 |
| 11 | 0 |
| 11 | 1 |
| 12 | 0 |
| 12 | 2 |
| 31 | 8 |
| 31 | 9 |
| 32 | 8 |
| 34 | 8 |
| 34 | 11 |
| 35 | 12 |
| 36 | 9 |
| 36 | 14 |
| 37 | 11 |
| 38 | 12 |
| 44 | 23 |
| 44 | 24 |
| 44 | 25 |
| 44 | 36 |
| 46 | 28 |
| 46 | 35 |
| 48 | 31 |
| 48 | 34 |
| 48 | 35 |
| 48 | 36 |
| 48 | 41 |
| 49 | 35 |
| 49 | 36 |
| 49 | 47 |
| 50 | 40 |
| 50 | 41 |
| 50 | 45 |
| 50 | 47 |
| 52 | 47 |

Type 2 Fermi Resonances

| | | |
|---|---|---|
| 9 | 8 | 5 |
| 10 | 8 | 0 |
| 10 | 8 | 3 |
| 11 | 8 | 0 |
| 11 | 8 | 1 |
| 11 | 10 | 0 |
| 11 | 10 | 1 |
| 11 | 10 | 3 |
| 11 | 10 | 7 |
| 12 | 8 | 0 |
| 12 | 8 | 2 |
| 12 | 9 | 0 |
| 12 | 9 | 5 |
| 12 | 10 | 0 |
| 12 | 10 | 2 |
| 12 | 10 | 6 |
| 12 | 11 | 0 |
| 12 | 11 | 1 |
| 12 | 11 | 2 |
| 12 | 11 | 7 |
| 13 | 8 | 7 |
| 13 | 10 | 1 |
| 13 | 10 | 6 |
| 13 | 10 | 7 |

| | | |
|---|---|---|
| 13 | 11 | 3 |
| 13 | 11 | 6 |
| 13 | 11 | 7 |
| 13 | 12 | 3 |
| 13 | 12 | 6 |
| 13 | 12 | 7 |
| 14 | 8 | 2 |
| 14 | 8 | 3 |
| 14 | 8 | 4 |
| 14 | 8 | 6 |
| 14 | 9 | 5 |
| 14 | 10 | 3 |
| 14 | 10 | 6 |
| 14 | 10 | 7 |
| 14 | 11 | 3 |
| 14 | 11 | 4 |
| 14 | 11 | 6 |
| 15 | 8 | 2 |
| 15 | 8 | 4 |
| 15 | 8 | 5 |
| 15 | 9 | 5 |
| 16 | 8 | 6 |
| 16 | 9 | 6 |
| 30 | 29 | 8 |
| 34 | 31 | 8 |
| 34 | 31 | 11 |
| 35 | 28 | 8 |
| 35 | 31 | 8 |
| 36 | 23 | 9 |
| 36 | 25 | 10 |
| 36 | 25 | 11 |
| 36 | 34 | 8 |
| 36 | 35 | 14 |
| 40 | 23 | 11 |
| 40 | 34 | 10 |
| 40 | 34 | 16 |
| 40 | 36 | 14 |
| 41 | 25 | 11 |
| 41 | 34 | 14 |
| 41 | 34 | 19 |
| 41 | 36 | 14 |
| 43 | 16 | 9 |
| 43 | 20 | 10 |
| 43 | 23 | 9 |
| 43 | 24 | 13 |
| 43 | 24 | 14 |
| 43 | 34 | 13 |
| 43 | 34 | 20 |
| 44 | 26 | 11 |
| 44 | 26 | 14 |
| 44 | 29 | 17 |
| 44 | 33 | 14 |
| 44 | 37 | 24 |
| 44 | 39 | 25 |
| 44 | 42 | 25 |
| 45 | 24 | 11 |
| 45 | 31 | 17 |
| 45 | 34 | 17 |
| 45 | 34 | 20 |
| 45 | 34 | 22 |
| 46 | 42 | 23 |
| 46 | 42 | 31 |

| | | |
|---|---|---|
| 47 | 16 | 10 |
| 47 | 18 | 8 |
| 47 | 19 | 11 |
| 47 | 20 | 11 |
| 47 | 34 | 23 |
| 47 | 36 | 20 |
| 47 | 41 | 34 |
| 48 | 26 | 13 |
| 48 | 36 | 29 |
| 48 | 37 | 16 |
| 48 | 37 | 19 |
| 48 | 39 | 22 |
| 48 | 39 | 24 |
| 48 | 39 | 25 |
| 48 | 42 | 24 |
| 48 | 46 | 28 |
| 49 | 26 | 13 |
| 49 | 27 | 13 |
| 49 | 29 | 15 |
| 49 | 33 | 16 |
| 49 | 33 | 17 |
| 49 | 37 | 34 |
| 49 | 38 | 21 |
| 49 | 39 | 23 |
| 49 | 46 | 31 |
| 50 | 32 | 18 |
| 50 | 33 | 19 |
| 50 | 34 | 33 |
| 50 | 42 | 25 |
| 50 | 42 | 31 |
| 50 | 44 | 34 |
| 50 | 46 | 35 |
| 50 | 48 | 43 |
| 51 | 31 | 22 |
| 51 | 34 | 22 |
| 52 | 44 | 36 |
| 52 | 48 | 45 |
| 52 | 50 | 43 |
| 53 | 52 | 47 |

Table S70: PM6-QFF Coriolis and Fermi resonances for benzopentalene generated using parameter set (d).

| Coriolis Resonances | | |
|---|---|---|
| 10 | 9 | C |
| 11 | 9 | C |
| 14 | 13 | C |
| 15 | 12 | C |
| 15 | 13 | C |
| 16 | 12 | C |
| 18 | 13 | A |
| 22 | 16 | C |
| 22 | 19 | C |
| 23 | 19 | A |
| 26 | 21 | B |
| 26 | 22 | B |
| 26 | 24 | B |
| 29 | 24 | A |
| 29 | 25 | A |

| | | |
|---|---|---|
| 32 | 21 | B |
| 33 | 32 | B |
| 42 | 40 | C |
| 43 | 40 | C |
| 45 | 43 | A |
| 46 | 43 | C |
| 46 | 44 | C |
| 47 | 43 | B |
| 52 | 49 | A |
| 52 | 49 | B |
| 53 | 49 | A |

Type 1 Fermi Resonances

| | |
|---|---|
| 11 | 0 |
| 11 | 2 |
| 11 | 7 |
| 12 | 0 |
| 12 | 1 |
| 12 | 2 |
| 12 | 3 |
| 13 | 5 |
| 13 | 6 |
| 33 | 8 |
| 33 | 9 |
| 35 | 9 |
| 35 | 10 |
| 41 | 13 |
| 45 | 33 |
| 45 | 37 |
| 47 | 35 |
| 47 | 37 |
| 47 | 40 |
| 48 | 37 |
| 48 | 40 |
| 50 | 43 |
| 50 | 44 |
| 50 | 46 |
| 51 | 46 |

Type 2 Fermi Resonances

| | | |
|---|---|---|
| 11 | 10 | 1 |
| 12 | 9 | 2 |
| 12 | 9 | 3 |
| 12 | 10 | 3 |
| 12 | 10 | 4 |
| 12 | 10 | 7 |
| 12 | 11 | 4 |
| 12 | 11 | 7 |
| 13 | 8 | 4 |
| 13 | 8 | 6 |
| 13 | 9 | 1 |
| 13 | 9 | 4 |
| 13 | 9 | 7 |
| 13 | 10 | 5 |
| 13 | 11 | 4 |
| 13 | 11 | 5 |
| 13 | 12 | 2 |
| 13 | 12 | 4 |
| 13 | 12 | 7 |
| 14 | 8 | 0 |
| 14 | 8 | 1 |
| 14 | 8 | 3 |

| | | |
|---|---|---|
| 14 | 9 | 4 |
| 14 | 9 | 7 |
| 14 | 10 | 0 |
| 14 | 10 | 3 |
| 14 | 11 | 7 |
| 14 | 12 | 0 |
| 14 | 12 | 2 |
| 14 | 12 | 4 |
| 14 | 12 | 7 |
| 14 | 13 | 6 |
| 15 | 8 | 0 |
| 15 | 9 | 4 |
| 15 | 9 | 7 |
| 15 | 10 | 2 |
| 15 | 10 | 3 |
| 15 | 11 | 2 |
| 15 | 12 | 1 |
| 15 | 12 | 2 |
| 15 | 12 | 7 |
| 16 | 9 | 6 |
| 16 | 10 | 4 |
| 16 | 10 | 6 |
| 16 | 11 | 4 |
| 16 | 11 | 6 |
| 16 | 11 | 7 |
| 16 | 12 | 6 |
| 16 | 12 | 7 |
| 17 | 8 | 0 |
| 17 | 9 | 4 |
| 17 | 9 | 6 |
| 17 | 10 | 1 |
| 17 | 10 | 4 |
| 17 | 10 | 7 |
| 17 | 11 | 7 |
| 19 | 8 | 2 |
| 19 | 8 | 4 |
| 19 | 8 | 6 |
| 19 | 9 | 4 |
| 19 | 9 | 6 |
| 19 | 10 | 0 |
| 19 | 10 | 2 |
| 19 | 10 | 3 |
| 19 | 10 | 5 |
| 19 | 10 | 7 |
| 20 | 8 | 3 |
| 20 | 9 | 3 |
| 20 | 9 | 6 |
| 20 | 10 | 0 |
| 20 | 10 | 1 |
| 20 | 10 | 3 |
| 20 | 10 | 4 |
| 20 | 10 | 6 |
| 21 | 8 | 1 |
| 21 | 8 | 2 |
| 21 | 8 | 3 |
| 21 | 8 | 6 |
| 21 | 9 | 6 |
| 21 | 10 | 7 |
| 22 | 8 | 0 |
| 22 | 8 | 2 |
| 22 | 8 | 4 |
| 22 | 8 | 6 |

| | | |
|---|---|---|
| 22 | 9 | 1 |
| 22 | 9 | 4 |
| 22 | 9 | 6 |
| 24 | 8 | 1 |
| 24 | 8 | 4 |
| 24 | 8 | 6 |
| 27 | 8 | 6 |
| 37 | 31 | 8 |
| 37 | 33 | 8 |
| 40 | 30 | 10 |
| 40 | 31 | 10 |
| 40 | 33 | 9 |
| 40 | 33 | 10 |
| 40 | 33 | 11 |
| 42 | 19 | 8 |
| 42 | 21 | 8 |
| 42 | 30 | 13 |
| 42 | 31 | 11 |
| 42 | 33 | 8 |
| 42 | 33 | 13 |
| 43 | 19 | 9 |
| 43 | 30 | 12 |
| 43 | 31 | 14 |
| 43 | 33 | 12 |
| 43 | 33 | 14 |
| 43 | 33 | 15 |
| 44 | 16 | 9 |
| 44 | 17 | 8 |
| 44 | 17 | 9 |
| 44 | 22 | 10 |
| 44 | 22 | 11 |
| 44 | 25 | 10 |
| 45 | 39 | 21 |
| 45 | 39 | 22 |
| 45 | 41 | 19 |
| 45 | 41 | 20 |
| 45 | 41 | 21 |
| 45 | 41 | 33 |
| 46 | 19 | 8 |
| 46 | 19 | 10 |
| 47 | 38 | 27 |
| 47 | 39 | 16 |
| 47 | 39 | 20 |
| 47 | 43 | 38 |
| 47 | 45 | 35 |
| 48 | 39 | 17 |
| 48 | 41 | 22 |
| 48 | 47 | 40 |
| 49 | 10 | 8 |
| 49 | 11 | 8 |
| 49 | 14 | 12 |
| 49 | 17 | 12 |
| 49 | 19 | 12 |
| 49 | 19 | 15 |
| 49 | 22 | 17 |
| 49 | 31 | 17 |
| 50 | 23 | 15 |
| 50 | 32 | 13 |
| 50 | 32 | 19 |
| 50 | 34 | 22 |
| 50 | 39 | 21 |
| 50 | 41 | 33 |

| | | |
|---|---|---|
| 50 | 45 | 37 |
| 50 | 47 | 37 |
| 50 | 47 | 40 |
| 51 | 18 | 12 |
| 51 | 34 | 25 |
| 51 | 36 | 19 |
| 51 | 48 | 42 |
| 51 | 50 | 42 |
| 52 | 18 | 12 |
| 52 | 29 | 16 |
| 52 | 32 | 17 |
| 52 | 38 | 27 |
| 52 | 45 | 42 |
| 52 | 48 | 44 |
| 52 | 50 | 49 |
| 53 | 34 | 21 |

Table S71: PM6-QFF Coriolis and Fermi resonances for benzopentalene generated using parameter set (e).

| Coriolis Resonances | | |
|---|---|---|
| 11 | 10 | C |
| 13 | 11 | C |
| 14 | 10 | C |
| 24 | 20 | C |
| 25 | 23 | C |
| 27 | 21 | A |
| 34 | 24 | C |
| 34 | 25 | C |
| 34 | 32 | C |
| 35 | 29 | C |
| 35 | 32 | C |
| 35 | 34 | C |
| 36 | 34 | C |
| 39 | 34 | A |
| 42 | 36 | C |
| 42 | 40 | C |
| 43 | 40 | C |
| 44 | 42 | A |
| 47 | 43 | C |
| 47 | 46 | C |
| 49 | 46 | A |
| 52 | 51 | A |
| 52 | 51 | B |
| 53 | 51 | A |
| 53 | 51 | B |
| **Type 1 Fermi Resonances** | | |
| 8 | 0 | |
| 8 | 2 | |
| 9 | 3 | |
| 10 | 1 | |
| 10 | 6 | |
| 11 | 0 | |
| 11 | 1 | |
| 11 | 6 | |
| 12 | 0 | |
| 12 | 2 | |
| 32 | 8 | |

| | | |
|---|---|---|
| 34 | 8 | |
| 34 | 9 | |
| 34 | 11 | |
| 35 | 9 | |
| 36 | 11 | |
| 36 | 14 | |
| 44 | 23 | |
| 44 | 24 | |
| 44 | 25 | |
| 44 | 34 | |
| 45 | 29 | |
| 45 | 35 | |
| 45 | 36 | |
| 48 | 32 | |
| 48 | 34 | |
| 48 | 35 | |
| 48 | 36 | |
| 48 | 42 | |
| 49 | 36 | |
| 49 | 47 | |
| 50 | 40 | |
| 50 | 42 | |
| 50 | 46 | |
| 50 | 47 | |
| 52 | 47 | |
| Type 2 Fermi Resonances | | |
| 9 | 8 | 3 |
| 11 | 8 | 0 |
| 11 | 8 | 1 |
| 11 | 10 | 5 |
| 11 | 10 | 7 |
| 12 | 8 | 0 |
| 12 | 8 | 2 |
| 12 | 8 | 4 |
| 12 | 9 | 0 |
| 12 | 10 | 0 |
| 12 | 10 | 1 |
| 12 | 10 | 6 |
| 12 | 11 | 0 |
| 12 | 11 | 1 |
| 12 | 11 | 2 |
| 12 | 11 | 6 |
| 13 | 8 | 7 |
| 13 | 10 | 1 |
| 13 | 10 | 6 |
| 13 | 11 | 5 |
| 13 | 11 | 7 |
| 13 | 12 | 5 |
| 13 | 12 | 7 |
| 14 | 8 | 2 |
| 14 | 9 | 3 |
| 14 | 10 | 4 |
| 14 | 10 | 5 |
| 14 | 10 | 7 |
| 14 | 11 | 1 |
| 14 | 11 | 6 |
| 14 | 12 | 4 |
| 14 | 12 | 5 |
| 15 | 8 | 2 |
| 15 | 8 | 4 |
| 15 | 9 | 0 |

| | | |
|---|---|---|
| 15 | 9 | 3 |
| 15 | 9 | 4 |
| 15 | 10 | 4 |
| 15 | 10 | 5 |
| 15 | 11 | 6 |
| 16 | 8 | 2 |
| 16 | 8 | 3 |
| 16 | 8 | 4 |
| 16 | 9 | 3 |
| 17 | 8 | 0 |
| 17 | 8 | 2 |
| 17 | 8 | 5 |
| 18 | 8 | 4 |
| 35 | 29 | 8 |
| 35 | 32 | 8 |
| 37 | 26 | 10 |
| 40 | 34 | 10 |
| 40 | 34 | 14 |
| 40 | 36 | 14 |
| 42 | 25 | 11 |
| 42 | 34 | 14 |
| 42 | 34 | 18 |
| 42 | 36 | 14 |
| 43 | 16 | 9 |
| 43 | 20 | 10 |
| 43 | 23 | 9 |
| 43 | 25 | 11 |
| 43 | 34 | 13 |
| 44 | 26 | 11 |
| 44 | 26 | 14 |
| 44 | 28 | 17 |
| 44 | 33 | 14 |
| 44 | 37 | 13 |
| 44 | 37 | 24 |
| 44 | 39 | 25 |
| 45 | 27 | 12 |
| 45 | 41 | 32 |
| 46 | 24 | 11 |
| 46 | 32 | 10 |
| 46 | 34 | 20 |
| 46 | 34 | 22 |
| 47 | 17 | 10 |
| 47 | 18 | 8 |
| 47 | 19 | 11 |
| 47 | 20 | 11 |
| 47 | 34 | 20 |
| 47 | 34 | 23 |
| 47 | 36 | 20 |
| 48 | 26 | 13 |
| 48 | 37 | 16 |
| 48 | 37 | 19 |
| 48 | 39 | 17 |
| 48 | 39 | 22 |
| 48 | 39 | 24 |
| 48 | 41 | 24 |
| 48 | 44 | 24 |
| 48 | 45 | 29 |
| 49 | 26 | 13 |
| 49 | 27 | 15 |
| 49 | 33 | 17 |
| 49 | 37 | 19 |
| 49 | 37 | 34 |

| | | |
|---|---|---|
| 49 | 39 | 22 |
| 49 | 45 | 32 |
| 50 | 31 | 18 |
| 50 | 39 | 34 |
| 50 | 41 | 24 |
| 50 | 41 | 32 |
| 50 | 44 | 34 |
| 50 | 45 | 35 |
| 50 | 48 | 36 |
| 50 | 48 | 43 |
| 51 | 25 | 13 |
| 51 | 32 | 22 |
| 51 | 34 | 22 |
| 51 | 35 | 20 |
| 52 | 48 | 46 |
| 52 | 50 | 43 |
| 53 | 52 | 47 |

Table S72: PM6-QFF Coriolis and Fermi resonances for benzopentalene generated using parameter set (f).