**Electronic supplementary information for:**

# Contrasting the optical properties of the different isomers of oligophenylene

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## Section ESI-1: Variation in optical properties with different conformers

For each oligomer-size of each isomer we perform a conformer search using the OPLS_2005 potential and then select a number of structures for a subsequent DFT(+D) re-optimisation. The latter selection includes for every oligomer-size the lowest energy structure found by OPLS_2005, any ordered structures (e.g. the alter, helix, flat, big and small conformers discussed, below, and in the main paper), any structures previously reported in the literature, and a number of less-ordered structures. As can be seen in tables S1 to S3 the ground state energy differences and variations in optical gap values between the different conformers are typically very small (see also Fig. S1).

***Table S1.*** *(TD-)B3LYP predicted optical gap values and relative ground state energies for selected conformers of p-sexiphenyl.*

| | p-phenylene | |
|---|---|---|
| conformer | relative GS energy (eV) | optical gap (eV) |
| alter | 0 | 3.75 |
| 2 | 0.0024 | 3.76 |
| helix | 0.0032 | 3.75 |
| 27 | 0.2961 | 3.76 |

***Table S2.*** *(TD-)B3LYP+D predicted optical gap values and relative ground state energies for selected conformers of m-sexiphenyl (energies in brackets obtained with plain (TD-)B3LYP).*

| | m-phenylene | |
|---|---|---|
| conformer | relative GS energy (eV) | optical gap (eV) |
| flat | 0 (0) | 4.44 (4.48) |
| big | 0.1357 (0.0153) | 4.51 (4.51) |
| small | 0.1368 (0.0101) | 4.49 (4.48) |
| 64 | 0.1383 (0.0149) | 4.48 (4.47) |
| 81 | 0.1401 (0.02) | 4.46 (4.45) |

***Table S3.*** *(TD-)B3LYP+D predicted optical gap values and relative ground state energies for selected conformers of o-sexiphenyl (energies in brackets obtained with plain (TD-)B3LYP).*

| | o-phenylene | |
|---|---|---|
| conformer | relative GS energy (eV) | optical gap (eV) |
| helix | 0 (0.0087) | 4.35 (4.56) |
| 2 | 0.0294 (0.0019) | 4.32 (4.44) |
| 3 | 0.0839 (0.0036) | 4.44 (4.50) |
| 4 | 0.164 (0) | 4.31 (4.38) |

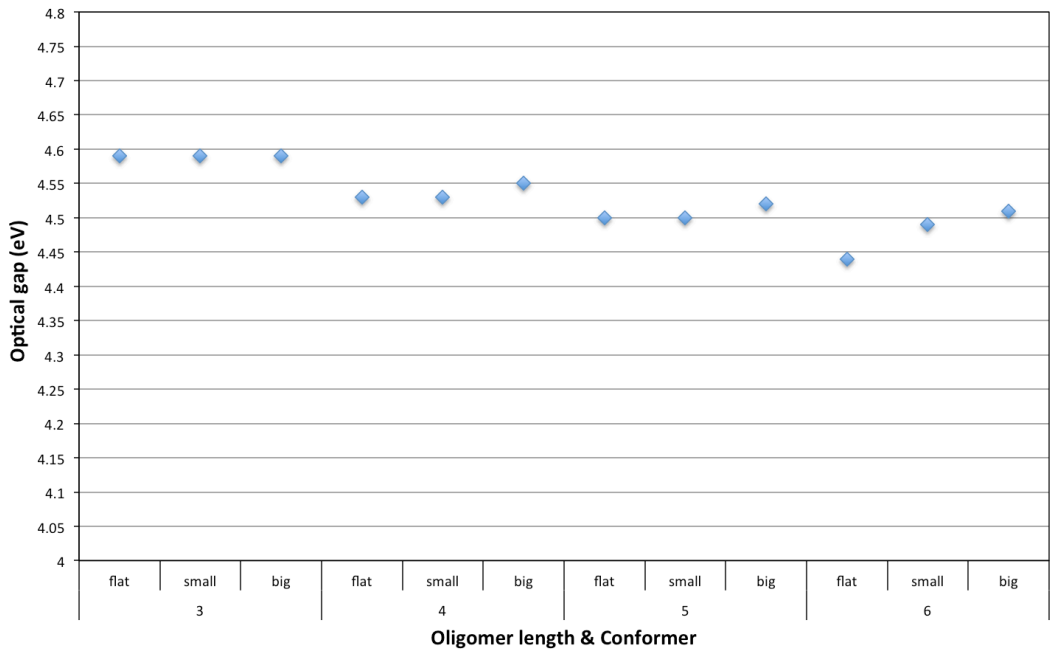


***Figure S1.*** *TD-B3LYP+D predicted optical gap values for three selected m-sexiphenyl conformers.*

**Section ESI-2: Optical gaps and spectra**

As long as the spacing between the first and subsequent vertical excitations is larger than the experimental peak width, one would expect that for molecules in the gas or liquid phase the lowest vertical excitation energy (the optical gap) coincides with the maximum of the first absorption peak and that all experimental absorption intensity at lower-energy/longer wavelength (i.e. between the onset of absorption and the maximum of the first absorption peak) would be due to vibrational broadening. In the case of p-phenylene this condition is fulfilled, only one vertical excitation contributes to first peak in the spectrum below (Fig. S2), while for o-phenylene multiple vertical excitations contribute to the first peak, in line with the featureless absorption spectra of o-phenylene.

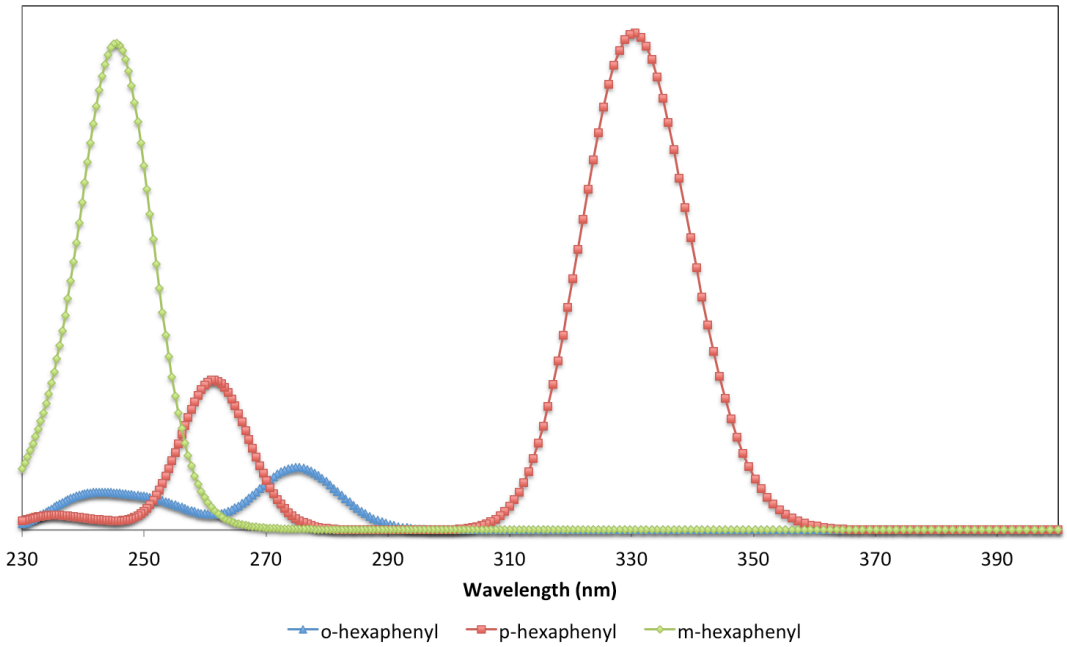


***Figure S2.*** *Optical absorption spectra predicted with TD-B3LYP/DZP.*

**Section ESI-3: Comparison with experimental data**

Below, we compare the TD-B3LYP predicted optical gap values (Table S4) and fluorescence energies (Table S5) for p-phenylene with the experimental data of Banerjee and co-workers for soluble p-phenylene oligomers with alkyl groups on the *para* position of the two terminal phenylene units. Both tables show gasphase data (for the DZP basis set and larger def2-TZVP basis set), solution data for $CH_2Cl_2$ (using the COSMO dielectric screening model with a dielectric permittivity of 8.93), results obtained for structures with isopropyl groups on the *para* position of the terminal phenylene units (to model the experimentally present solubilising alkyl chains) and finally the experimental data (in line with section ESI-2, values obtained from peak maxima).

***Table S4.*** Optical gap values *(in eV) of p-phenylene oligomers compared to experimental data (*Banerjee et al., *JACS* **2009**, *131*, 1780-1786). **Substituted at both chain ends with isopropyl groups in para position. (Values in brackets obtained with the larger def2-TZVP basis set).*

| Oligomer length | p-phenylene gas phase | p-phenylene $CH_2Cl_2$ | Substituted* p-phenylene $CH_2Cl_2$ | Experiment $CH_2Cl_2$ |
|---|---|---|---|---|
| 3 | 4.48 (4.44) | 4.37 | 4.24 | 4.28 |
| 4 | 4.11 (4.09) | 3.99 | 3.92 | 4.07 |
| 5 | 3.89 (3.87) | 3.78 | 3.73 | 3.95 |
| 6 | 3.75 | 3.63 | | 3.85 |
| 7 | 3.65 | 3.54 | | 3.80 |

***Table S5.*** *Fluorescence energies (in eV) of p-phenylene oligomers compared to experimental data (*Banerjee et al., *JACS* **2009**, *131*, 1780-1786). **Substituted at both chain ends with isopropyl groups in para position. (Values in brackets obtained with the larger def2-TZVP basis set).*

| Oligomer length | p-phenylene gas phase | p-phenylene $CH_2Cl_2$ | Substituted* p-phenylene $CH_2Cl_2$ | Experiment $CH_2Cl_2$ |
|---|---|---|---|---|
| 3 | 3.78 (3.72) | 3.67 | 3.54 | 3.50 |
| 4 | 3.39 (3.36) | 3.29 | | 3.28 |
| 5 | 3.15 | 3.06 | | 3.15 |
| 6 | 2.99 | 2.92 | | 3.08 |
| 7 | 2.89 | | | 3.04 |

As can be seen the calculations and experimental data display the same trend with oligomer size, where the former is red-shifted relative to the latter for the longer oligomers when including a description of implicit solvent effects and short alkyl groups. This underestimation of the optical gap values and fluorescence energies for the longer oligomers is probably related to the fact that the theoretical conjugation length is longer than in than experiment, discussed in the main text. As mentioned there, this is likely (in part) due to the fact that our calculations involve idealised athermal minimum energy structures and ignore thermal vibrations.

**Section ESI-4: Orbitals involved in electronic excitations**

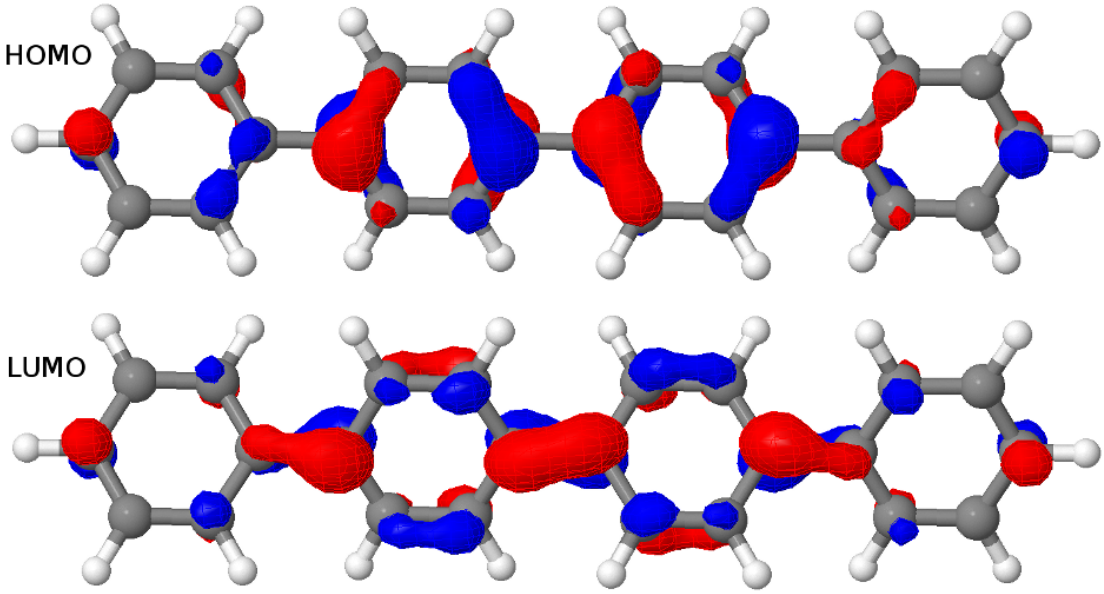


***Figure S3.*** *HOMO and LUMO for the p-quaterphenyl oligomer.*

**Section ESI-5: Changes between ground and excited states**

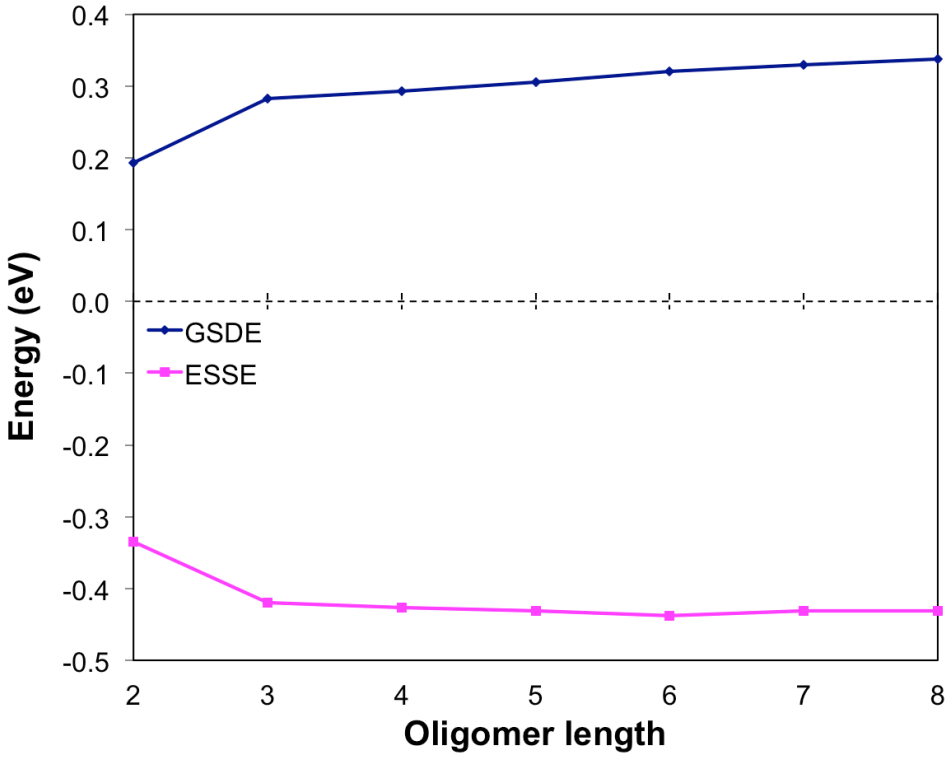


***Figure S4A.*** *Variation in the ESSE and GSDE with oligomer length for p-phenylene.*

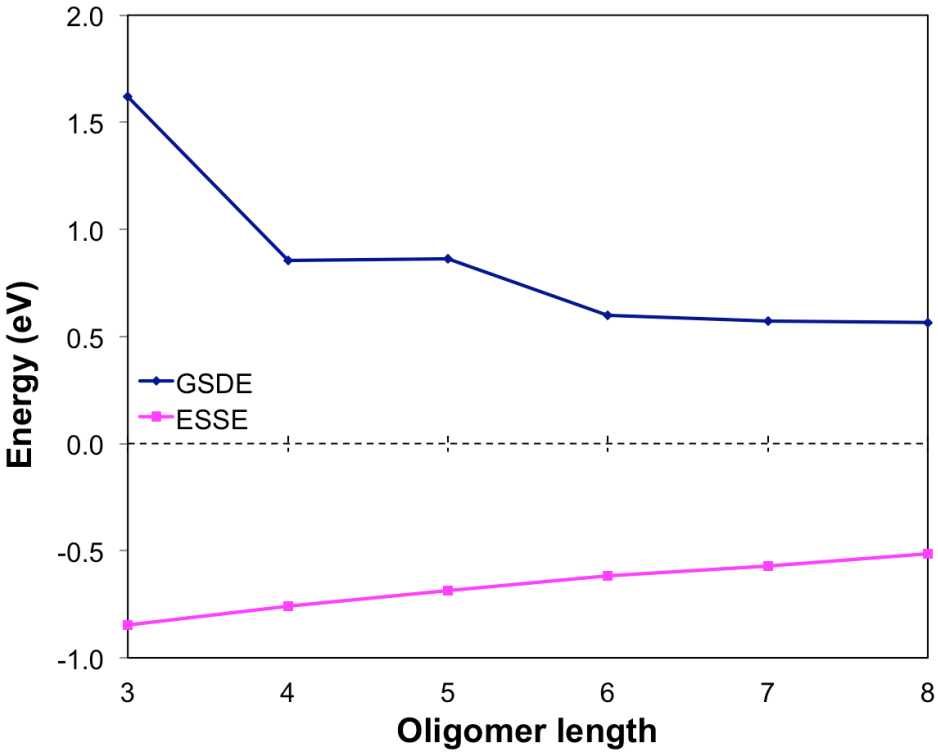


***Figure S4B.*** *Variation in the ESSE and GSDE with oligomer length for o-phenylene.*

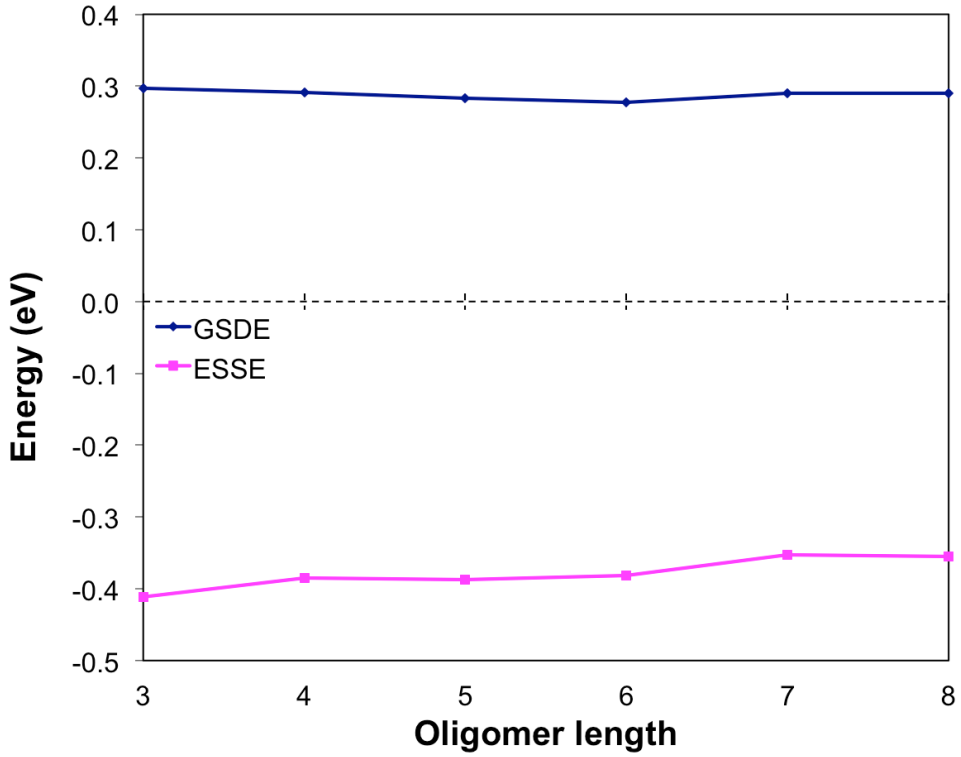


***Figure S4C.*** *Variation in the ESSE and GSDE with oligomer length for m-phenylene.*

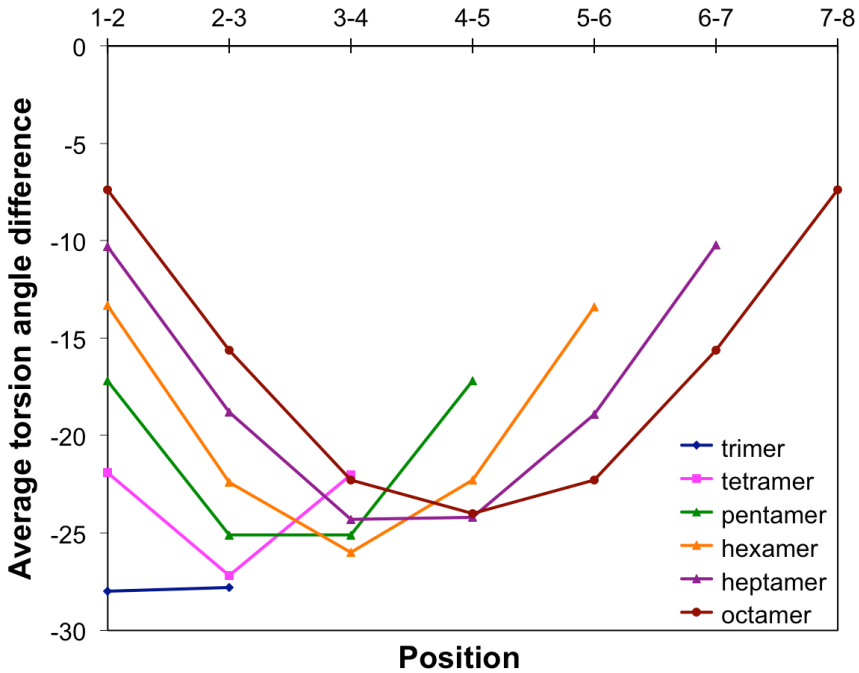


***Figure S5.*** *Variation of the TD-B3LYP calculated ground state - excited state interphenylene torsion angle difference along the oligomer for the different p-phenylene oligomers.*

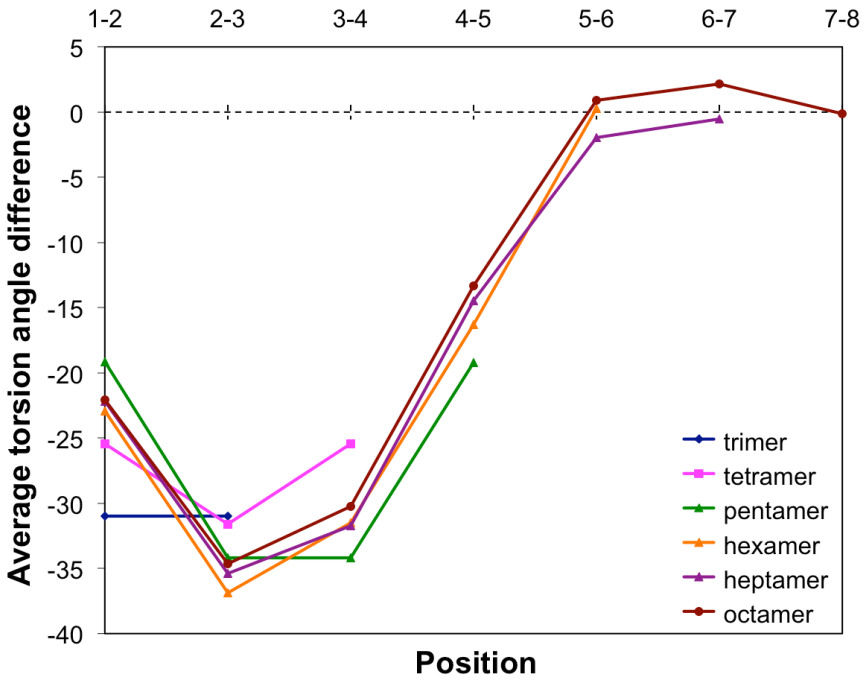


***Figure S6.*** *Variation of the TD-B3LYP calculated ground state - excited state interphenylene torsion angle difference along the oligomer for the different o-phenylene oligomers.*

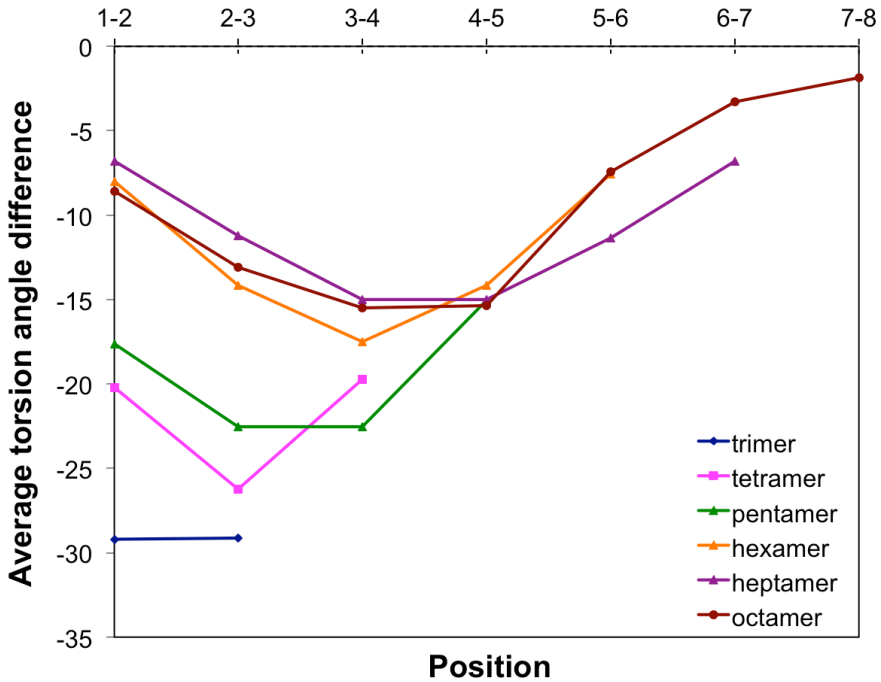


***Figure S7.*** *Variation of the TD-B3LYP+D calculated ground state - excited state interphenylene torsion angle difference along the oligomer for the different o-phenylene oligomers.*

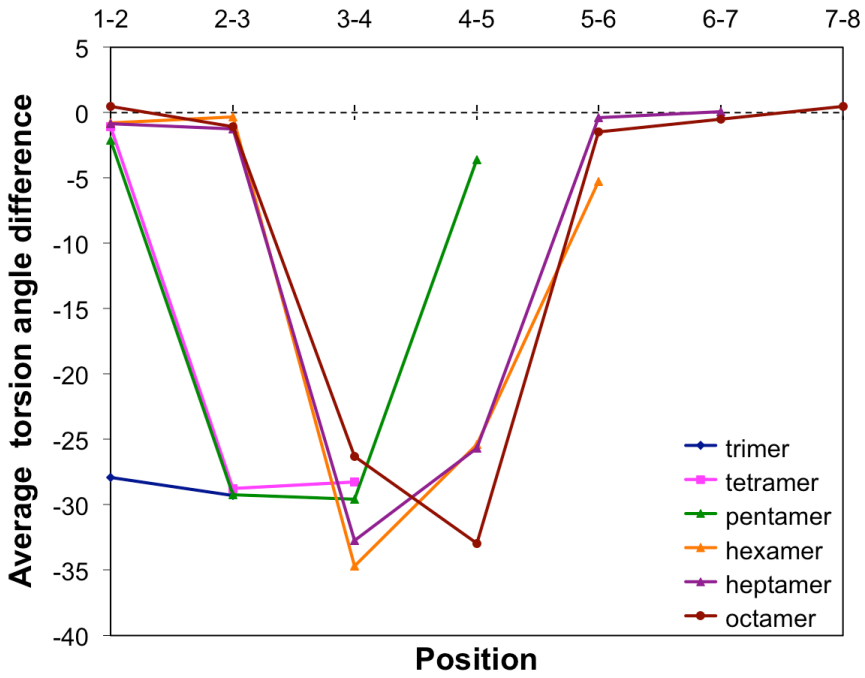


***Figure S8.*** *Variation of the TD-B3LYP calculated ground state - excited state interphenylene torsion angle difference along the oligomer for the different m-phenylene oligomers.*

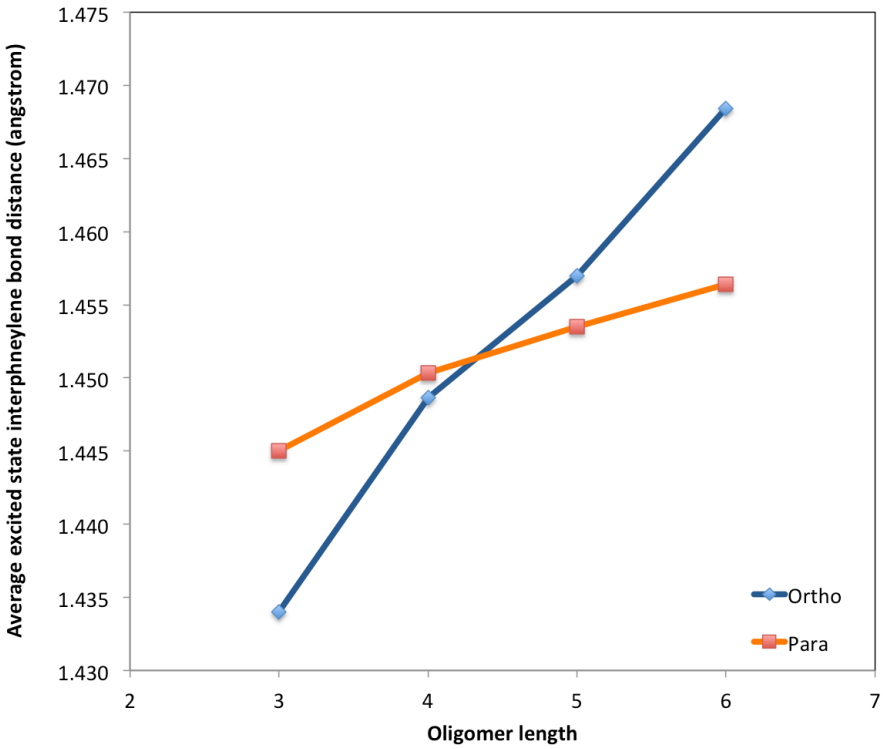


***Figure S9.*** *Variation in average excited state interphenylene bond length with oligomer length.*

**Section ESI-6: Cartesian coordinates of selected oligomers.**

All p-phenylene structures are optimised with (TD-)B3LYP. The m-phenylene and o-phenylene oligomers are optimised with (TD-)B3LYP+D.

Ground state Cartesian coordinates of p-terphenyl.

| | | | |
|---|---|---|---|
| C | -4.8807509 | 1.6966321 | -0.2310490 |
| C | -3.4943229 | 1.5502940 | -0.2428697 |
| C | -5.7022880 | 0.6018206 | 0.0434414 |
| C | -5.1229107 | -0.6409867 | 0.3053510 |
| C | -3.7365075 | -0.7872655 | 0.2938720 |
| C | -2.8949543 | 0.3055618 | 0.0197881 |
| C | -1.4184829 | 0.1500481 | 0.0092316 |
| C | -0.5746229 | 1.1532963 | 0.5159603 |
| C | 0.8092704 | 1.0068821 | 0.5072187 |
| C | 1.4184551 | -0.1499017 | -0.0088190 |
| C | 0.5745308 | -1.1531107 | -0.5156087 |
| C | -0.8093605 | -1.0067632 | -0.5067230 |
| H | -2.8657010 | 2.4089801 | -0.4846143 |
| H | -3.2968799 | -1.7586706 | 0.5260439 |
| H | -5.7548281 | -1.5027148 | 0.5289236 |
| H | -5.3225042 | 2.6715436 | -0.4462305 |
| H | -6.7877263 | 0.7165391 | 0.0530286 |
| H | -1.4293171 | -1.7929484 | -0.9407627 |
| H | 1.4291364 | 1.7930608 | 0.9414036 |
| H | -1.0108261 | 2.0511486 | 0.9568096 |
| H | 1.0106404 | -2.0509262 | -0.9566192 |
| C | 2.8949341 | -0.3054657 | -0.0195193 |
| C | 3.7367241 | 0.7881338 | -0.2899149 |
| C | 5.1231071 | 0.6417338 | -0.3017118 |
| C | 5.7023279 | -0.6020181 | -0.0440296 |
| C | 3.4942204 | -1.5511039 | 0.2391403 |
| C | 4.8806152 | -1.6976089 | 0.2267636 |
| H | 3.2973507 | 1.7603885 | -0.5189901 |
| H | 5.3222039 | -2.6733166 | 0.4386333 |
| H | 2.8656003 | -2.4105554 | 0.4781425 |
| H | 6.7877432 | -0.7168639 | -0.0539999 |
| H | 5.7551234 | 1.5041572 | -0.5222907 |

Excited state Cartesian coordinates of p-terphenyl.

| | | | |
|---|---|---|---|
| C | 1.1981225 | -0.1705275 | -5.0380995 |
| C | 1.2062468 | -0.1686299 | -3.6537288 |
| C | 0.0000133 | -0.0000684 | -5.7512031 |
| C | -1.1981011 | 0.1704369 | -5.0381172 |
| C | -1.2062484 | 0.1685199 | -3.6537448 |
| C | -0.0000055 | -0.0000570 | -2.8976151 |
| C | -0.0000086 | -0.0000293 | -1.4521998 |
| C | 1.2135812 | 0.0455179 | -0.6873899 |
| C | 1.2135809 | 0.0456453 | 0.6873734 |
| C | -0.0000070 | 0.0001645 | 1.4521955 |
| C | -1.2135992 | -0.0453761 | 0.6873821 |
| C | -1.2136010 | -0.0454361 | -0.6873839 |
| H | 2.1518446 | -0.3258893 | -3.1365832 |
| H | -2.1518544 | 0.3257910 | -3.1366128 |
| H | -2.1361131 | 0.3110607 | -5.5792323 |
| H | 2.1361524 | -0.3110746 | -5.5792007 |
| H | 0.0000120 | -0.0001324 | -6.8424430 |
| H | -2.1710873 | -0.1155694 | -1.2012163 |
| H | 2.1710619 | 0.1158686 | 1.2011964 |
| H | 2.1710594 | 0.1156495 | -1.2012328 |
| H | -2.1710808 | -0.1155485 | 1.2012147 |
| C | 0.0000014 | 0.0001290 | 2.8976133 |
| C | 1.2062949 | -0.1681784 | 3.6537243 |
| C | 1.1981614 | -0.1702182 | 5.0380946 |
| C | 0.0000030 | -0.0001548 | 5.7512085 |
| C | -1.2062871 | 0.1683285 | 3.6537581 |
| C | -1.1981571 | 0.1700540 | 5.0381302 |
| H | 2.1519468 | -0.3251080 | 3.1365787 |
| H | -2.1362263 | 0.3102631 | 5.5792530 |
| H | -2.1519335 | 0.3254102 | 3.1366452 |
| H | 0.0000057 | -0.0002478 | 6.8424482 |
| H | 2.1362222 | -0.3105933 | 5.5791871 |

Ground state Cartesian coordinates of p-sexiphenyl.

| | | | |
|---|---|---|---|
| C | -2.7494957 | 1.3102033 | -0.6170785 |
| C | -1.3642284 | 1.2189222 | -0.5254262 |
| C | -3.5790237 | 0.2368996 | -0.2476043 |
| C | -2.9522096 | -0.9322708 | 0.2181676 |
| C | -1.5669715 | -1.0235030 | 0.3099912 |
| C | -0.7373660 | 0.0498337 | -0.0593777 |
| C | 0.7389084 | -0.0469524 | 0.0400775 |
| C | 1.5206940 | 1.0593706 | 0.4163528 |
| C | 2.9056543 | 0.9679393 | 0.5118646 |
| C | 3.5799724 | -0.2345066 | 0.2360378 |
| C | 2.7983066 | -1.3406925 | -0.1407146 |
| C | 1.4133935 | -1.2492074 | -0.2364701 |
| H | -0.7544989 | 2.0614964 | -0.8556081 |
| H | -1.1212168 | -1.9354608 | 0.7103209 |
| H | -3.5620866 | -1.7748058 | 0.5481975 |
| H | -3.1954494 | 2.2222249 | -1.0170791 |
| H | 0.8463833 | -2.1211271 | -0.5667431 |
| H | 3.4728736 | 1.8398304 | 0.8419000 |
| H | 1.0325757 | 2.0007996 | 0.6735032 |
| H | 3.2866134 | -2.2821505 | -0.3974487 |
| C | 5.0560863 | -0.3322049 | 0.3381798 |
| C | 5.8874871 | 0.7378049 | -0.0362985 |
| C | 7.2725869 | 0.6455460 | 0.0596517 |
| C | 7.8964145 | -0.5210020 | 0.5349307 |
| C | 5.6802180 | -1.4989890 | 0.8132050 |
| C | 7.0652947 | -1.5910092 | 0.9091088 |
| H | 5.4434773 | 1.6476764 | -0.4433547 |
| H | 7.5097813 | -2.5007761 | 1.3158822 |
| H | 5.0685306 | -2.3386783 | 1.1471588 |
| H | 7.8847189 | 1.4852075 | -0.2736157 |
| C | 9.3740322 | -0.6188373 | 0.6392461 |
| C | 10.1466327 | 0.4851437 | 1.0417558 |
| C | 10.0437521 | -1.8187507 | 0.3401127 |
| C | 11.4311669 | -1.9113595 | 0.4407105 |

| | | | |
|---|---|---|---|
| C | 11.5340940 | 0.3926057 | 1.1418476 |
| C | 12.1836458 | -0.8061883 | 0.8422051 |
| H | 9.4714286 | -2.6833490 | -0.0003795 |
| H | 11.9285195 | -2.8518031 | 0.1953935 |
| H | 13.2698412 | -0.8788061 | 0.9212620 |
| H | 12.1110818 | 1.2613733 | 1.4647011 |
| H | 9.6505676 | 1.4209855 | 1.3044672 |
| C | -5.0554697 | 0.3337659 | -0.3457816 |
| C | -5.8368637 | -0.7709626 | -0.7271062 |
| C | -5.7299956 | 1.5341409 | -0.0618625 |
| C | -7.1153397 | 1.6250726 | -0.1546747 |
| C | -7.2222079 | -0.6798341 | -0.8197773 |
| C | -7.8964384 | 0.5203771 | -0.5357511 |
| H | -5.1628097 | 2.4046009 | 0.2720232 |
| H | -7.6043014 | 2.5646948 | 0.1075992 |
| H | -7.7899642 | -1.5501889 | -1.1530098 |
| H | -5.3483908 | -1.7106734 | -0.9899082 |
| C | -9.3746054 | 0.6171909 | -0.6330286 |
| C | -10.1982654 | -0.4511427 | -0.2355999 |
| C | -9.9938903 | 1.7804275 | -1.1241537 |
| C | -11.3821869 | 1.8719878 | -1.2137991 |
| C | -12.1857440 | 0.8024107 | -0.8149280 |
| C | -11.5865117 | -0.3596178 | -0.3255177 |
| H | -9.7452203 | -1.3556580 | 0.1736423 |
| H | -12.2049004 | -1.1993935 | -0.0026047 |
| H | -13.2726263 | 0.8740206 | -0.8847725 |
| H | -11.8387742 | 2.7827960 | -1.6060967 |
| H | -9.3776804 | 2.6145529 | -1.4639251 |

Excited state Cartesian coordinates of p-sexiphenyl.

| | | | |
|---|---|---|---|
| C | -2.8621558 | 1.2022933 | -0.1077806 |
| C | -1.4856233 | 1.2033134 | -0.1094706 |
| C | -3.6216092 | -0.0000755 | -0.0016486 |
| C | -2.8620955 | -1.2024502 | 0.1039609 |
| C | -1.4855605 | -1.2034508 | 0.1050437 |
| C | -0.7229849 | -0.0000561 | -0.0022929 |
| C | 0.7229834 | -0.0000250 | -0.0023117 |
| C | 1.4855573 | 1.2033780 | 0.1049425 |
| C | 2.8620915 | 1.2023803 | 0.1038528 |
| C | 3.6216093 | 0.0000026 | -0.0017001 |
| C | 2.8621574 | -1.2023748 | -0.1077506 |
| C | 1.4856243 | -1.2033981 | -0.1094301 |
| H | -0.9748292 | 2.1577543 | -0.2284380 |
| H | -0.9747037 | -2.1578918 | 0.2237403 |
| H | -3.3757501 | -2.1556271 | 0.2240899 |
| H | -3.3758812 | 2.1554537 | -0.2277392 |
| H | 0.9748307 | -2.1578472 | -0.2283364 |
| H | 3.3757419 | 2.1555667 | 0.2239206 |
| H | 0.9747005 | 2.1578263 | 0.2235787 |
| H | 3.3758830 | -2.1555418 | -0.2276557 |
| C | 5.0724141 | -0.0000034 | -0.0011218 |
| C | 5.8300027 | 1.1911066 | -0.1928103 |
| C | 7.2107505 | 1.1885515 | -0.1908734 |
| C | 7.9595100 | 0.0000085 | 0.0003696 |
| C | 5.8298148 | -1.1911169 | 0.1912814 |
| C | 7.2105632 | -1.1885485 | 0.1907853 |
| H | 5.3172749 | 2.1325926 | -0.3864095 |
| H | 7.7313424 | -2.1268329 | 0.3840088 |
| H | 5.3168957 | -2.1326097 | 0.3843393 |
| H | 7.7317272 | 2.1268385 | -0.3835545 |
| C | 9.4268381 | 0.0000206 | 0.0012159 |
| C | 10.1644756 | 1.1649696 | 0.3207443 |
| C | 10.1648646 | -1.1649229 | -0.3174320 |
| C | 11.5554328 | -1.1625426 | -0.3174527 |

| | | | |
|---|---|---|---|
| C | 11.5550430 | 1.1625891 | 0.3224660 |
| C | 12.2635720 | 0.0000212 | 0.0029466 |
| H | 9.6382714 | -2.0765460 | -0.6009276 |
| H | 12.0945317 | -2.0753128 | -0.5788103 |
| H | 13.3548578 | 0.0000175 | 0.0036237 |
| H | 12.0938205 | 2.0753609 | 0.5844789 |
| H | 9.6375356 | 2.0765929 | 0.6035958 |
| C | -5.0724135 | -0.0000534 | -0.0010306 |
| C | -5.8300254 | -1.1911510 | -0.1926996 |
| C | -5.8297887 | 1.1910725 | 0.1913937 |
| C | -7.2105365 | 1.1885326 | 0.1909023 |
| C | -7.2107739 | -1.1885649 | -0.1907743 |
| C | -7.9595091 | -0.0000046 | 0.0004603 |
| H | -5.3168480 | 2.1325501 | 0.3844680 |
| H | -7.7312953 | 2.1268237 | 0.3841469 |
| H | -7.7317690 | -2.1268404 | -0.3834615 |
| H | -5.3173150 | -2.1326512 | -0.3862780 |
| C | -9.4268376 | 0.0000265 | 0.0012515 |
| C | -10.1645282 | -1.1649154 | 0.3206841 |
| C | -10.1648130 | 1.1650096 | -0.3173724 |
| C | -11.5553809 | 1.1626706 | -0.3174742 |
| C | -12.2635727 | 0.0001098 | 0.0028189 |
| C | -11.5550959 | -1.1624941 | 0.3223234 |
| H | -9.6376326 | -2.0765681 | 0.6035232 |
| H | -12.0939160 | -2.0752643 | 0.5842545 |
| H | -13.3548585 | 0.0001434 | 0.0034250 |
| H | -12.0944369 | 2.0754713 | -0.5788133 |
| H | -9.6381778 | 2.0766336 | -0.6007864 |

Ground state Cartesian coordinates of m-terphenyl.

| | | | |
|---|---|---|---|
| C | -4.6204175 | 1.2414269 | -0.9107846 |
| C | -3.4686864 | 0.5157690 | -1.2127842 |
| C | -4.8110146 | 1.7577045 | 0.3724655 |
| C | -3.8387047 | 1.5411685 | 1.3507906 |
| C | -2.6870376 | 0.8152363 | 1.0490273 |
| C | -2.4810285 | 0.2897904 | -0.2383592 |
| C | -1.3165726 | -1.6351046 | -1.3629883 |
| C | -1.2546277 | -0.4831069 | -0.5613251 |
| C | -0.0048989 | -0.0840493 | -0.0640661 |
| C | 1.1685443 | -0.8004071 | -0.3433013 |
| C | 1.0738928 | -1.9488977 | -1.1467699 |
| C | -0.1598948 | -2.3576558 | -1.6497852 |
| H | -3.3195246 | 0.1383385 | -2.2259510 |
| H | -1.9464960 | 0.6300023 | 1.8290486 |
| H | -3.9811748 | 1.9328468 | 2.3598243 |
| H | -5.3704798 | 1.4117672 | -1.6855979 |
| H | -5.7126793 | 2.3254901 | 0.6089390 |
| H | -0.2206952 | -3.2515679 | -2.2734319 |
| H | 0.0565829 | 0.8099437 | 0.5582588 |
| H | 1.9759369 | -2.5088846 | -1.3984229 |
| C | 2.4779217 | -0.3488335 | 0.1930443 |
| C | 2.8174903 | 1.0148241 | 0.2204050 |
| C | 4.0462952 | 1.4368510 | 0.7268139 |
| C | 4.9634580 | 0.5051129 | 1.2170639 |
| C | 3.4114875 | -1.2751594 | 0.6891782 |
| C | 4.6402275 | -0.8530426 | 1.1955093 |
| H | 2.1192223 | 1.7500571 | -0.1831293 |
| H | 5.3464700 | -1.5896417 | 1.5834120 |
| H | 3.1593908 | -2.3369665 | 0.7000518 |
| H | 5.9250652 | 0.8358910 | 1.6136218 |
| H | 4.2921964 | 2.5005167 | 0.7306348 |
| H | -2.2802488 | -1.9794193 | -1.7413918 |

Excited state Cartesian coordinates of m-terphenyl.

| | | | |
|---|---|---|---|
| C | -4.7996940 | 0.8948204 | -0.8253991 |
| C | -3.6838376 | 0.1041893 | -1.0352538 |
| C | -4.7658054 | 1.9541651 | 0.1000937 |
| C | -3.5816791 | 2.2001031 | 0.8090860 |
| C | -2.4552049 | 1.4201027 | 0.6011931 |
| C | -2.4606311 | 0.3341586 | -0.3328106 |
| C | -1.3535172 | -1.7169381 | -1.2643644 |
| C | -1.2878360 | -0.4806420 | -0.5508314 |
| C | -0.0053182 | -0.0784032 | -0.0586627 |
| C | 1.1789125 | -0.8607475 | -0.2441725 |
| C | 1.0422463 | -2.0861199 | -0.9664960 |
| C | -0.2045769 | -2.4933083 | -1.4553397 |
| H | -3.7398849 | -0.6895519 | -1.7787430 |
| H | -1.5639768 | 1.6204279 | 1.1932886 |
| H | -3.5443357 | 3.0120877 | 1.5379617 |
| H | -5.7126039 | 0.6963089 | -1.3899374 |
| H | -5.6479409 | 2.5748331 | 0.2626750 |
| H | -0.2858884 | -3.4464803 | -1.9797806 |
| H | 0.0902607 | 0.9065460 | 0.3860586 |
| H | 1.9000447 | -2.7397091 | -1.1097517 |
| C | 2.4531423 | -0.4241240 | 0.2780094 |
| C | 2.5494676 | 0.6558993 | 1.2139761 |
| C | 3.7731201 | 1.0720727 | 1.7141488 |
| C | 4.9628279 | 0.4502047 | 1.3103413 |
| C | 3.6823400 | -1.0416722 | -0.1099589 |
| C | 4.8988179 | -0.6125836 | 0.3903543 |
| H | 1.6450421 | 1.1423479 | 1.5750622 |
| H | 5.8174695 | -1.1019407 | 0.0615094 |
| H | 3.6752626 | -1.8503084 | -0.8391709 |
| H | 5.9239234 | 0.7850085 | 1.7027094 |
| H | 3.8066935 | 1.8914206 | 2.4348864 |
| H | -2.3068399 | -2.0921672 | -1.6306813 |

Ground state Cartesian coordinates of m-sexiphenyl.

| | | | |
|---|---|---|---|
| C | -6.1227358 | 1.4518272 | -2.6374351 |
| C | -5.6091189 | 1.2828276 | -1.3522697 |
| C | -5.7406725 | 2.5508791 | -3.4090368 |
| C | -4.8395865 | 3.4787499 | -2.8832384 |
| C | -4.3259714 | 3.3099741 | -1.5979898 |
| C | -4.7018953 | 2.2089750 | -0.8092872 |
| C | -4.9786628 | 1.5853918 | 1.6112624 |
| C | -4.1575782 | 2.0279110 | 0.5605077 |
| C | -2.8104273 | 2.3037959 | 0.8389448 |
| C | -2.2727119 | 2.1505183 | 2.1254040 |
| C | -3.1189307 | 1.7073821 | 3.1554180 |
| C | -4.4591460 | 1.4281480 | 2.8948137 |
| H | -5.8954362 | 0.4063496 | -0.7680838 |
| H | -3.6418804 | 4.0555144 | -1.1889050 |
| H | -4.5400397 | 4.3459631 | -3.4749891 |
| H | -6.8199505 | 0.7153586 | -3.0416765 |
| H | -6.1430546 | 2.6836587 | -4.4149644 |
| H | -5.1075918 | 1.0837433 | 3.7025507 |
| H | -2.1618117 | 2.6477861 | 0.0320297 |
| H | -2.7170252 | 1.5572837 | 4.1585017 |
| C | -0.8399604 | 2.4416174 | 2.3895316 |
| C | -0.4445403 | 3.1113862 | 3.5594489 |
| C | 0.9013335 | 3.3880767 | 3.7925775 |
| C | 1.8733470 | 3.0045447 | 2.8702923 |
| C | 0.1501935 | 2.0613027 | 1.4713341 |
| C | 1.5088623 | 2.3321703 | 1.6919113 |
| H | -1.1992406 | 3.4380345 | 4.2763990 |
| H | -0.1451261 | 1.5397391 | 0.5598336 |
| H | 2.9262583 | 3.2042625 | 3.0750688 |
| H | 1.1967646 | 3.9094922 | 4.7048966 |
| H | -6.0356300 | 1.3887321 | 1.4250655 |
| C | 2.5368600 | 1.9103250 | 0.7055867 |
| C | 2.4508749 | 0.6627765 | 0.0695834 |
| C | 3.4016227 | 0.2442230 | -0.8731758 |

| | | | |
|---|---|---|---|
| C | 4.4644683 | 1.1103632 | -1.1799355 |
| C | 3.6121940 | 2.7535030 | 0.3799999 |
| C | 4.5643572 | 2.3523706 | -0.5555024 |
| H | 1.6205465 | -0.0009755 | 0.3144500 |
| H | 5.3948805 | 3.0167126 | -0.8011889 |
| H | 3.6863368 | 3.7379907 | 0.8442760 |
| C | 3.2896810 | -1.0861487 | -1.5247775 |
| C | 3.5598922 | -1.2424302 | -2.8942728 |
| C | 2.9011848 | -2.2149282 | -0.7880971 |
| C | 3.4391129 | -2.4926475 | -3.4979200 |
| C | 2.7759418 | -3.4802107 | -1.3807051 |
| C | 3.0505254 | -3.6044604 | -2.7528908 |
| H | 2.6897459 | -2.1056716 | 0.2767067 |
| H | 2.9831260 | -4.5828276 | -3.2313164 |
| H | 5.2287201 | 0.7971049 | -1.8927467 |
| H | 3.8407162 | -0.3744530 | -3.4928330 |
| C | 2.8760345 | -4.8547120 | 0.7238407 |
| C | 2.3710258 | -4.6586263 | -0.5729965 |
| C | 2.4945190 | -5.9616745 | 1.4808996 |
| C | 1.5990666 | -6.8969878 | 0.9586647 |
| C | 1.0889087 | -6.7150273 | -0.3282162 |
| C | 1.4708725 | -5.6085303 | -1.0856595 |
| H | 1.3003759 | -7.7633652 | 1.5516596 |
| H | 2.9061726 | -6.0987078 | 2.4827254 |
| H | 1.0466350 | -5.4633077 | -2.0808330 |
| H | 0.3814237 | -7.4357325 | -0.7429191 |
| H | 3.6506343 | -2.6021032 | -4.5632594 |
| H | 3.5955099 | -4.1432374 | 1.1329372 |

Excited state Cartesian coordinates of m-sexiphenyl.

| | | | |
|---|---|---|---|
| C | -5.0116060 | -2.1406980 | -0.0068637 |
| C | -4.8313433 | -0.9250081 | 0.6514135 |
| C | -4.0617676 | -2.5915109 | -0.9261555 |
| C | -2.9319890 | -1.8135244 | -1.1901330 |
| C | -2.7551940 | -0.5972329 | -0.5370222 |
| C | -3.6955708 | -0.1328515 | 0.4029112 |
| C | -4.5529818 | 1.9838059 | 1.4856779 |
| C | -3.4744042 | 1.1431377 | 1.1218263 |
| C | -2.1825656 | 1.5459961 | 1.4540659 |
| C | -1.9063354 | 2.7675598 | 2.1300898 |
| C | -3.0263852 | 3.5768010 | 2.4921599 |
| C | -4.3152353 | 3.1860953 | 2.1692525 |
| H | -5.5644539 | -0.6033490 | 1.3932225 |
| H | -1.8820967 | 0.0124196 | -0.7744218 |
| H | -2.1849889 | -2.1586378 | -1.9048590 |
| H | -5.8940548 | -2.7458190 | 0.2096205 |
| H | -4.1943068 | -3.5472691 | -1.4353833 |
| H | -5.1563443 | 3.8286695 | 2.4338370 |
| H | -1.3627331 | 0.8658618 | 1.2390538 |
| H | -2.8689593 | 4.5307190 | 2.9924653 |
| C | -0.5431843 | 3.1628198 | 2.4199309 |
| C | -0.2403070 | 4.2030695 | 3.3432136 |
| C | 1.0965982 | 4.5328542 | 3.6003917 |
| C | 2.1507700 | 3.8720111 | 2.9588056 |
| C | 0.5419217 | 2.5038292 | 1.7704360 |
| C | 1.9118814 | 2.8297014 | 2.0123144 |
| H | -1.0314112 | 4.7142077 | 3.8879799 |
| H | 0.3115155 | 1.7465814 | 1.0323861 |
| H | 3.1692044 | 4.1825267 | 3.1839966 |
| H | 1.3246059 | 5.3214612 | 4.3188889 |
| H | -5.5718031 | 1.7118173 | 1.2082270 |
| C | 2.9795918 | 2.1343535 | 1.3290155 |
| C | 2.7035439 | 1.1921710 | 0.2899499 |
| C | 3.7084441 | 0.5014682 | -0.3862808 |

| | | | |
|---|---|---|---|
| C | 5.0556182 | 0.7353072 | -0.0328869 |
| C | 4.3556984 | 2.3440332 | 1.6483835 |
| C | 5.3569152 | 1.6574674 | 0.9833489 |
| H | 1.6790258 | 1.0395341 | -0.0411475 |
| H | 6.3987658 | 1.8278467 | 1.2611552 |
| H | 4.6360451 | 3.0390217 | 2.4384445 |
| C | 3.3655502 | -0.4557658 | -1.4690638 |
| C | 4.1547361 | -0.5384149 | -2.6297814 |
| C | 2.2452624 | -1.2978431 | -1.3671756 |
| C | 3.8259159 | -1.4318682 | -3.6467057 |
| C | 1.9031268 | -2.2072325 | -2.3801032 |
| C | 2.7130270 | -2.2623339 | -3.5280565 |
| H | 1.6298098 | -1.2457823 | -0.4677905 |
| H | 2.4882298 | -2.9822886 | -4.3159947 |
| H | 5.8554049 | 0.1782211 | -0.5210517 |
| H | 5.0166128 | 0.1205348 | -2.7426629 |
| C | 0.4187165 | -3.7027746 | -0.9982605 |
| C | 0.7369328 | -3.1180833 | -2.2370296 |
| C | -0.6478861 | -4.5922250 | -0.8767357 |
| C | -1.4210791 | -4.9230068 | -1.9909691 |
| C | -1.1267770 | -4.3419228 | -3.2261363 |
| C | -0.0637307 | -3.4465654 | -3.3462932 |
| H | -2.2513664 | -5.6249999 | -1.8956941 |
| H | -0.8720455 | -5.0358113 | 0.0948555 |
| H | 0.1414030 | -2.9833415 | -4.3127933 |
| H | -1.7337055 | -4.5801533 | -4.1018029 |
| H | 4.4473068 | -1.4854593 | -4.5425376 |
| H | 1.0344321 | -3.4801308 | -0.1255276 |

Ground state Cartesian coordinates of o-terphenyl.

| | | | |
|---|---|---|---|
| C | -3.3958000 | -0.4946823 | -1.3413088 |
| C | -2.6936025 | -0.1555208 | -0.1839940 |
| C | -1.3850478 | -0.6186283 | 0.0258520 |
| C | -2.8034020 | -1.3093476 | -2.3072750 |
| C | -1.5043664 | -1.7824883 | -2.1063445 |
| C | -0.8017666 | -1.4394306 | -0.9532203 |
| C | -0.6550614 | -0.2702212 | 1.2766692 |
| C | -1.2839239 | -0.5175883 | 2.5083539 |
| C | 0.6550474 | 0.2702737 | 1.2766713 |
| C | -0.6478500 | -0.2581976 | 3.7203141 |
| C | 0.6478723 | 0.2581360 | 3.7203165 |
| C | 1.2839247 | 0.5175922 | 2.5083589 |
| C | 1.3850380 | 0.6186774 | 0.0258556 |
| C | 0.8017546 | 1.4394415 | -0.9532482 |
| C | 2.6935998 | 0.1555779 | -0.1839677 |
| C | 1.5043546 | 1.7824579 | -2.1063849 |
| C | 2.8034002 | 1.3093328 | -2.3072868 |
| C | 3.3958069 | 0.4947196 | -1.3412823 |
| H | -3.3511606 | -1.5747872 | -3.2134463 |
| H | -4.4091157 | -0.1164656 | -1.4902972 |
| H | 0.2132179 | -1.8093381 | -0.8043999 |
| H | -1.0342575 | -2.4240725 | -2.8540244 |
| H | -3.1564245 | 0.4927894 | 0.5627381 |
| H | -2.2853731 | -0.9514522 | 2.5053754 |
| H | -1.1602692 | -0.4677733 | 4.6609692 |
| H | 1.1603109 | 0.4676552 | 4.6609739 |
| H | 2.2853775 | 0.9514482 | 2.5053859 |
| H | 3.1564177 | -0.4927170 | 0.5627806 |
| H | 4.4091331 | 0.1165203 | -1.4902439 |
| H | 3.3511616 | 1.5747465 | -3.2134639 |
| H | 1.0342392 | 2.4240003 | -2.8540964 |
| H | -0.2132352 | 1.8093419 | -0.8044487 |

Excited state Cartesian coordinates of o-terphenyl.

| | | | |
|---|---|---|---|
| C | -3.4038576 | -0.6007990 | -1.2786398 |
| C | -2.8003232 | -0.4004227 | -0.0537218 |
| C | -1.3927901 | -0.5211950 | 0.1141379 |
| C | -2.6417125 | -0.9741180 | -2.4208342 |
| C | -1.2838921 | -1.1699368 | -2.2936253 |
| C | -0.6261375 | -0.9413781 | -1.0595325 |
| C | -0.7153108 | -0.1667206 | 1.3267773 |
| C | -1.3807818 | -0.2229633 | 2.5844117 |
| C | 0.7158171 | 0.1680704 | 1.3263596 |
| C | -0.7031416 | -0.0989140 | 3.7758295 |
| C | 0.7044321 | 0.1030384 | 3.7754899 |
| C | 1.3817026 | 0.2256880 | 2.5837168 |
| C | 1.3928748 | 0.5213103 | 0.1131207 |
| C | 0.6257932 | 0.9403648 | -1.0606806 |
| C | 2.8003302 | 0.4002613 | -0.0551612 |
| C | 1.2830851 | 1.1676194 | -2.2952561 |
| C | 2.6408304 | 0.9714965 | -2.4228085 |
| C | 3.4033920 | 0.5992877 | -1.2805321 |
| H | -3.1394032 | -1.1321562 | -3.3790154 |
| H | -4.4812881 | -0.4559047 | -1.3765620 |
| H | 0.3276296 | -1.4441025 | -0.8937966 |
| H | -0.6913754 | -1.5103224 | -3.1452104 |
| H | -3.4121258 | -0.0728191 | 0.7868702 |
| H | -2.4469213 | -0.4503626 | 2.6083519 |
| H | -1.2414668 | -0.1831837 | 4.7211635 |
| H | 1.2430464 | 0.1884221 | 4.7205592 |
| H | 2.4478563 | 0.4530891 | 2.6070546 |
| H | 3.4124327 | 0.0734697 | 0.7855287 |
| H | 4.4807683 | 0.4541918 | -1.3787371 |
| H | 3.1381526 | 1.1284766 | -3.3813554 |
| H | 0.6902673 | 1.5072092 | -3.1469504 |
| H | -0.3278830 | 1.4433037 | -0.8950707 |

Ground state Cartesian coordinates of o-sexiphenyl.

| | | | |
|---|---|---|---|
| C | -2.9690255 | 0.3946100 | 0.1667970 |
| C | -1.5737717 | 0.5000585 | 0.0203537 |
| C | -0.7458364 | -0.0277140 | 1.0386275 |
| C | -3.5524535 | -0.1925354 | 1.2861236 |
| C | -2.7354982 | -0.6980042 | 2.2958468 |
| C | -1.3540781 | -0.6134386 | 2.1624262 |
| C | 0.7452401 | 0.0278989 | 1.0389039 |
| C | 1.3530569 | 0.6136812 | 2.1629019 |
| C | 1.5735603 | -0.4998895 | 0.0209537 |
| C | 2.7344262 | 0.6983286 | 2.2967965 |
| C | 3.5517599 | 0.1928961 | 1.2873616 |
| C | 2.9687548 | -0.3943299 | 0.1678573 |
| C | 1.0750182 | -1.1668509 | -1.2181370 |
| C | 0.2165432 | -2.2930968 | -1.2220529 |
| C | 1.5265961 | -0.6578174 | -2.4469775 |
| C | -0.1740997 | -2.8346279 | -2.4597760 |
| C | 0.2788629 | -2.3118446 | -3.6678881 |
| C | 1.1431699 | -1.2182630 | -3.6607251 |
| H | -4.6394885 | -0.2488355 | 1.3685144 |
| H | -3.6054510 | 0.8170709 | -0.6126332 |
| H | -0.7139272 | -1.0517396 | 2.9280191 |
| H | -3.1685569 | -1.1743441 | 3.1767846 |
| H | 0.7126174 | 1.0519501 | 2.9282724 |
| H | 3.1671554 | 1.1747174 | 3.1778699 |
| H | 4.6387622 | 0.2492808 | 1.3701218 |
| H | 3.6054735 | -0.8167794 | -0.6113386 |
| H | 1.5031026 | -0.7878250 | -4.5965137 |
| H | -0.0350954 | -2.7654309 | -4.6098354 |
| H | -0.8180108 | -3.7157163 | -2.4635815 |
| C | 0.6268814 | -3.3058034 | 1.0525335 |
| C | -0.2588713 | -2.9668978 | 0.0165193 |
| C | -1.6112285 | -3.3183083 | 0.1549134 |
| C | -2.0664920 | -3.9822884 | 1.2926383 |
| C | -1.1772761 | -4.3097478 | 2.3173099 |

| | | | |
|---|---|---|---|
| C | 0.1713967 | -3.9685290 | 2.1912815 |
| H | 0.8774212 | -4.2250939 | 2.9835336 |
| H | -1.5328937 | -4.8266347 | 3.2106778 |
| H | -3.1254205 | -4.2304294 | 1.3855568 |
| H | -2.3198051 | -3.0332562 | -0.6241257 |
| H | 2.1604932 | 0.2291552 | -2.4406478 |
| H | 1.6820843 | -3.0491255 | 0.9609334 |
| C | -1.0747699 | 1.1667794 | -1.2186855 |
| C | -0.2161171 | 2.2928866 | -1.2225534 |
| C | 0.1749907 | 2.8341285 | -2.4602541 |
| C | -1.5260392 | 0.6575833 | -2.4475767 |
| C | -1.1421721 | 1.2177596 | -3.6613095 |
| C | -0.2776987 | 2.3112101 | -3.6684088 |
| C | 0.2590367 | 2.9668472 | 0.0160282 |
| H | 0.0365986 | 2.7645902 | -4.6103417 |
| H | 0.8190625 | 3.7150980 | -2.4640195 |
| H | -2.1600449 | -0.2293149 | -2.4412857 |
| H | -1.5018918 | 0.7872081 | -4.5971288 |
| C | -0.6269861 | 3.3061726 | 1.0516718 |
| C | 1.6114215 | 3.3179987 | 0.1547827 |
| C | -0.1717359 | 3.9690686 | 2.1904157 |
| C | 2.0664543 | 3.9821315 | 1.2925094 |
| C | 1.1769716 | 4.3100167 | 2.3168134 |
| H | 2.3201887 | 3.0326248 | -0.6239640 |
| H | 3.1254059 | 4.2300648 | 1.3857182 |
| H | 1.5324101 | 4.8270194 | 3.2101861 |
| H | -1.6822137 | 3.0496937 | 0.9597788 |
| H | -0.8779674 | 4.2259830 | 2.9823712 |

Excited state Cartesian coordinates of o-sexiphenyl.

| | | | |
|---|---|---|---|
| C | -2.9928463 | 0.0457708 | 0.2107391 |
| C | -1.6024827 | 0.2905937 | 0.0712934 |
| C | -0.7365014 | -0.0316891 | 1.1895385 |
| C | -3.5650219 | -0.4221082 | 1.3803336 |
| C | -2.7324704 | -0.6767844 | 2.4889308 |
| C | -1.3667866 | -0.4895086 | 2.3723265 |
| C | 0.7373885 | 0.0325172 | 1.1890335 |
| C | 1.3684080 | 0.4913302 | 2.3710542 |
| C | 1.6026507 | -0.2906403 | 0.0705002 |
| C | 2.7341534 | 0.6787853 | 2.4866350 |
| C | 3.5659962 | 0.4232446 | 1.3777079 |
| C | 2.9930884 | -0.0456503 | 0.2088738 |
| C | 1.1701790 | -0.9231450 | -1.1834892 |
| C | 0.2009318 | -1.9961292 | -1.2624225 |
| C | 1.7299739 | -0.4734465 | -2.4027483 |
| C | -0.2043475 | -2.4592935 | -2.5319984 |
| C | 0.3414996 | -1.9639846 | -3.7030040 |
| C | 1.3368378 | -0.9680633 | -3.6315785 |
| H | -4.6442424 | -0.5689720 | 1.4439421 |
| H | -3.6482469 | 0.3050520 | -0.6225486 |
| H | -0.7343388 | -0.7735652 | 3.2128481 |
| H | -3.1514907 | -1.0501366 | 3.4248790 |
| H | 0.7364831 | 0.7760406 | 3.2117498 |
| H | 3.1537527 | 1.0529377 | 3.4220048 |
| H | 4.6452497 | 0.5702238 | 1.4404891 |
| H | 3.6479727 | -0.3055932 | -0.6246134 |
| H | 1.7755608 | -0.5632550 | -4.5446661 |
| H | 0.0232139 | -2.3597592 | -4.6685053 |
| H | -0.9267973 | -3.2749519 | -2.5850569 |
| C | 0.5250538 | -2.9826745 | 1.0275005 |
| C | -0.3140030 | -2.6837803 | -0.0773143 |
| C | -1.6649316 | -3.1016259 | -0.0158893 |
| C | -2.1624725 | -3.7469474 | 1.1041656 |
| C | -1.3209764 | -4.0198300 | 2.1923684 |

| | | | |
|---|---|---|---|
| C | 0.0260667 | -3.6492561 | 2.1382070 |
| H | 0.6892025 | -3.8731200 | 2.9753679 |
| H | -1.7170505 | -4.5216375 | 3.0769643 |
| H | -3.2182927 | -4.0166796 | 1.1496205 |
| H | -2.3384637 | -2.8502168 | -0.8341414 |
| H | 2.4430394 | 0.3493386 | -2.3708560 |
| H | 1.5742957 | -2.6980423 | 0.9895634 |
| C | -1.1707679 | 0.9221073 | -1.1834334 |
| C | -0.2015710 | 1.9950512 | -1.2637230 |
| C | 0.2030578 | 2.4571867 | -2.5338766 |
| C | -1.7312691 | 0.4714783 | -2.4020307 |
| C | -1.3387680 | 0.9651144 | -3.6314517 |
| C | -0.3434202 | 1.9609387 | -3.7041905 |
| C | 0.3138733 | 2.6837017 | -0.0794215 |
| H | -0.0256245 | 2.3559199 | -4.6701774 |
| H | 0.9254937 | 3.2727876 | -2.5879803 |
| H | -2.4443493 | -0.3512516 | -2.3690951 |
| H | -1.7779775 | 0.5595998 | -4.5439896 |
| C | -0.5246886 | 2.9833738 | 1.0255580 |
| C | 1.6647769 | 3.1017738 | -0.0189895 |
| C | -0.0252596 | 3.6509258 | 2.1354840 |
| C | 2.1627585 | 3.7480866 | 1.1002975 |
| C | 1.3217478 | 4.0217534 | 2.1886792 |
| H | 2.3379613 | 2.8497769 | -0.8373470 |
| H | 3.2185625 | 4.0180016 | 1.1450293 |
| H | 1.7181698 | 4.5243628 | 3.0726635 |
| H | -1.5739146 | 2.6985885 | 0.9883542 |
| H | -0.6880259 | 3.8753747 | 2.9727809 |