Supporting Information: Singlet Fission and Triplet Pair Recombination in Bipentacenes with a Twist

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I. Transient Spectroscopy

A detailed description of transient absorption spectroscopy has previously been reported.[1,2,3] Here, a resonant pump pulse with a pulse width of ~100 fs is generated with a 1 kHz amplified Ti:Sapphire system with an optical parametric amplifier. A femtosecond supercontinuum probe in a thin sapphire plate is generated using the laser with a mechanical delay. A nanosecond supercontinuum probe pulse was generated in a fiber laser (Leukos) with an electronic delay.

Time-resolved photoluminescence data was collected using the upconversion technique. Dilute solution phase samples were excited with 500 nm pump pulses and emission was collected at 680 nm. The emitted light is focused and overlapped with an 800 nm gate pulse in a nonlinear crystal (BBO) optimized for sum frequency generation. The upconverted light is filtered and detected with a photomultiplier tube. The arrival time of the gate pulse is mechanically delayed.

It has been previously reported that BP22 has a 200% triplet yield. A full calculation of the triplet yield was not performed for BP11 and BP12 since it was assumed they were structurally similar to BP22 and with no features that should affect triplet yield. Triplet yields were approximated however for both BP11 and BP12. Triplet yield approximations were done using the bleach of the deconvoluted triplet and singlet spectra from Global Analysis. Since the area of both spectra remain constant as singlet fission occurs and singlet becomes two triplets, we assume that all of the singlets are becoming triplets and therefore we have about 200% yield.

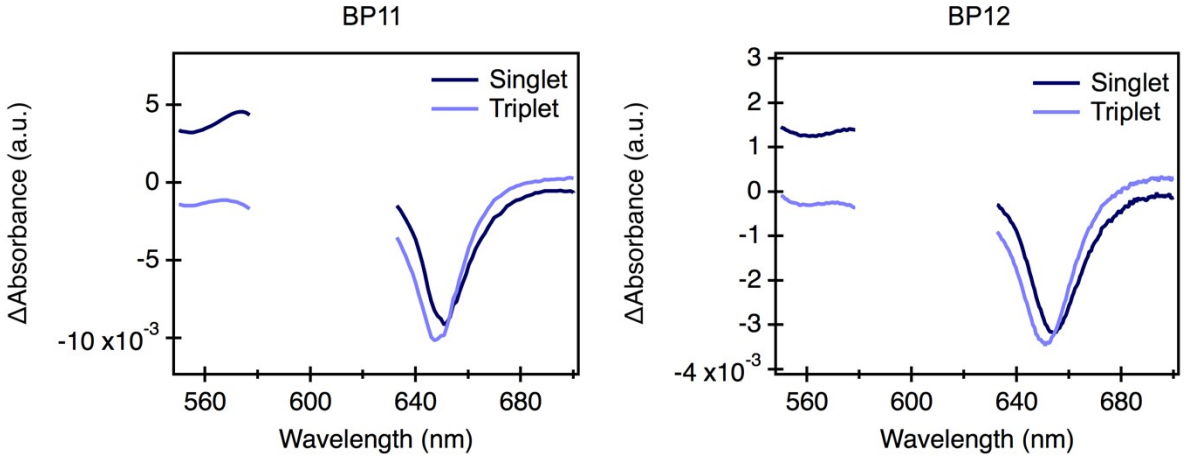


Figure S1: Triplet and Singlet spectra from Global Analysis demonstrating the unchanging bleach signal. The transient absorption spectra were taken in chloroform and excited at 600 nm (~200 μJ/cm^2).

To ensure that only one exciton was excited per dimer, a power dependence study was done. The excited state dynamics at two different laser powers were examined for BP11 and BP12. The kinetic cuts taken from the resulting TA spectra are shown below. The two spectra for BP11 and BP12 are each very similar to each other, indicating that within these power ranges only one exciton is being excited on a dimer and there are two exciton interactions.

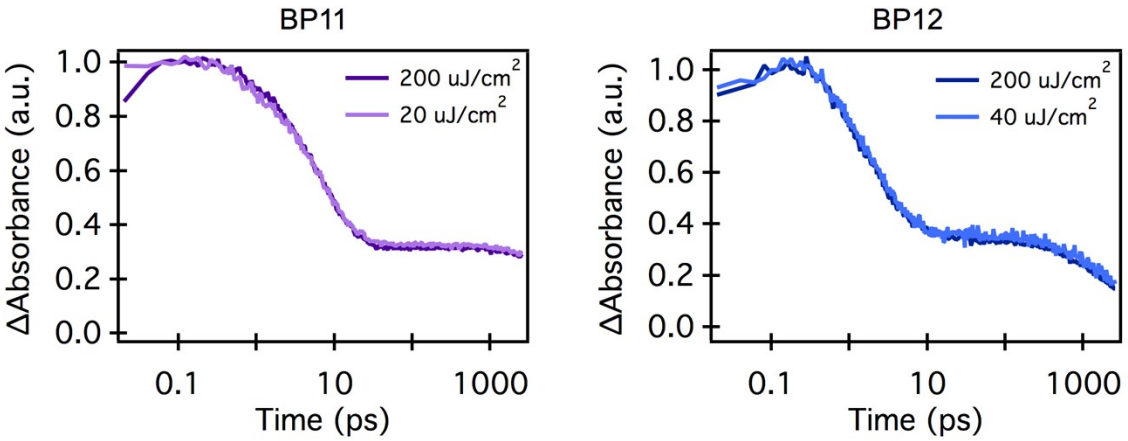


Figure S2: Kinetic traces from the transient absorption spectra taken at different powers in chloroform excited at 600 nm. Left: Kinetic trace taken at 450 nm. Right: Kinetic trace taken at 450 nm.

The sensitization experiments are shown in Figure S3. A solution of the pentacene dimer and anthracene was excited at 360 nm. Anthracene then undergoes intersystem crossing resulting in a free triplet, which is then transferred to the pentacene dimer through collisions since the anthracene triplet is higher in energy than the pentacene triplet. The triplet spectrum is overlaid with the triplet spectrum obtained from intersystem crossing. For BP11, the line shape matches the sensitization spectrum pretty well expect for the shape of the peak around 510 nm. For BP12, the general line shape is very similar with some deviations. We attribute the difference in shape of the spectra to the fact that bound triplet pairs form in the dimers as a result of singlet fission.

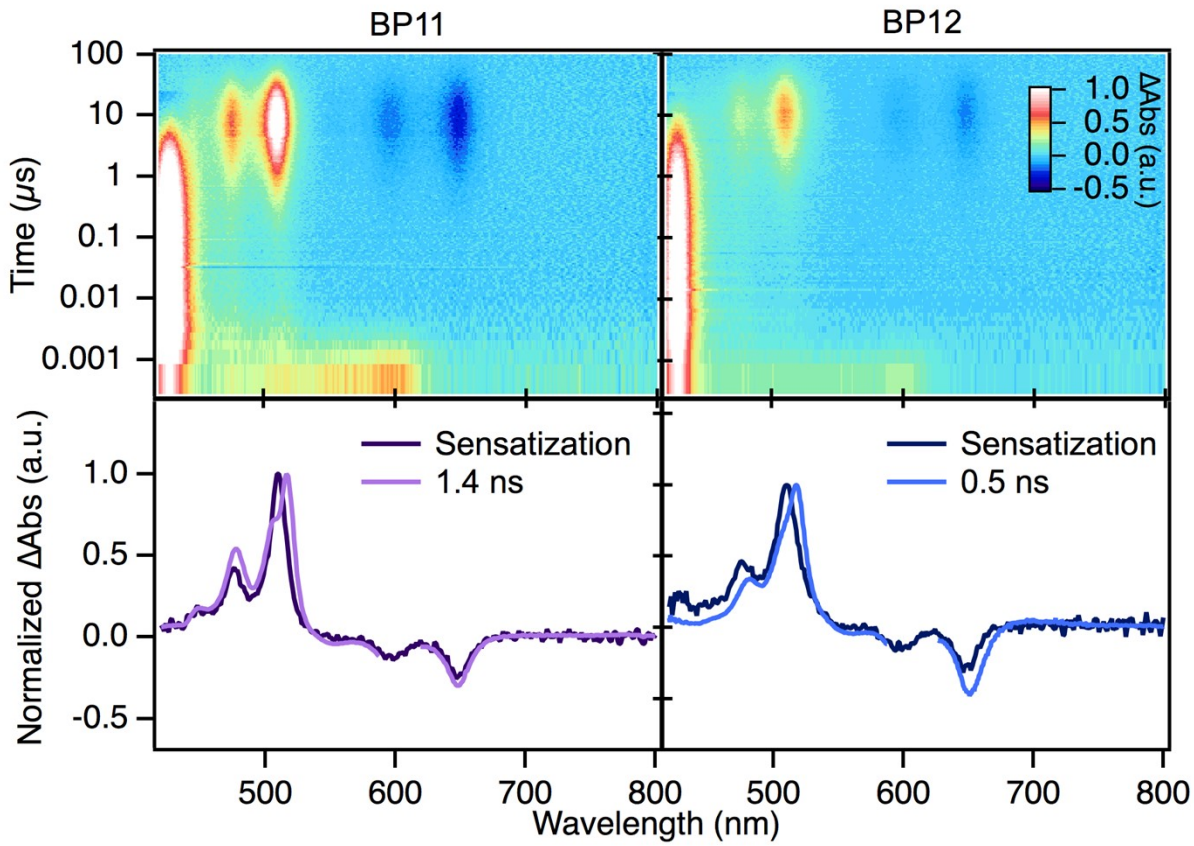


Figure S3: Triplet photosensitization spectra we taken of a solution of dimer (~50 μM) and ~15mM anthracene in chloroform. The sample was excited at 360 nm (~200 μJ/cm^2) in order to excite only the anthracene molecules.

Two exponents were used to fit both data sets: one for the rate of singlet fission and the other for exciton decay. The fit for two kinetic traces, one showing triplet rise and decay and the other showing singlet decay, are shown in Figure #. These traces demonstrate the accuracy of the fit Global Analysis assigned to the data.

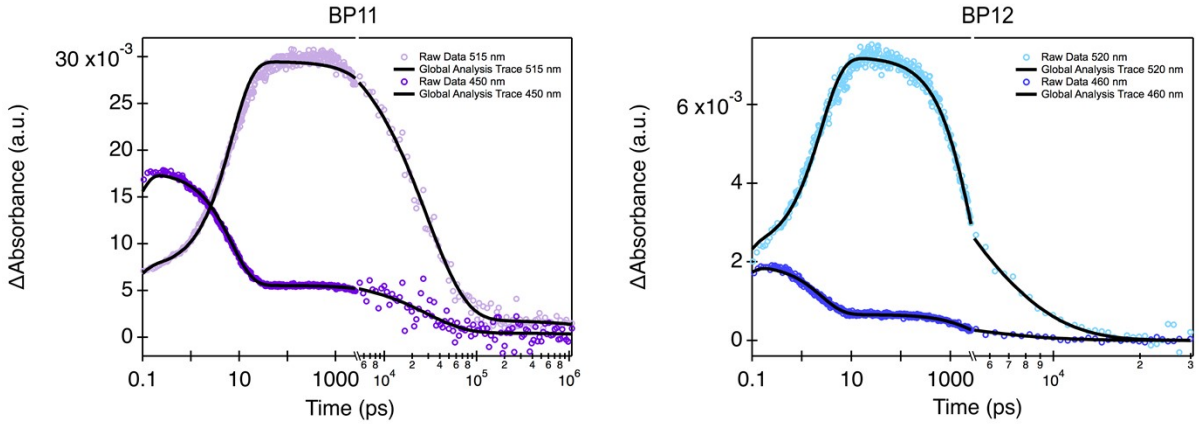


Figure S4: The kinetic raw data and traces from Global Analysis. Left: Singlet decay was taken at 450 nm and triplet rise and decay at 515 nm. Right: Singlet decay was taken at 460 nm and triplet rise and decay at 520 nm.

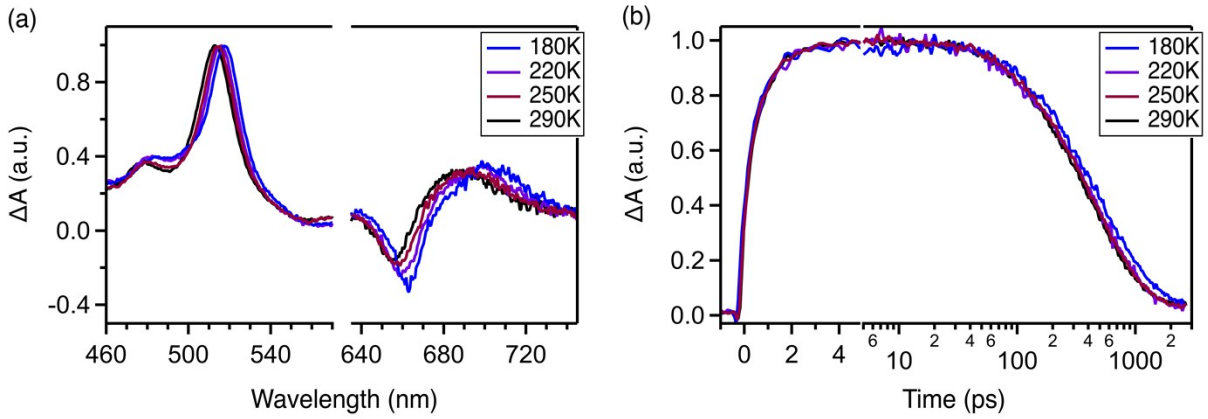


Figure S5: Temperature dependence of the (a) transient spectra (averaged over 10 – 100 ps delay times) and (b) kinetic decay associated with the maximum of the triplet excited state absorption signal (~ 520 nm).

To compare to the temperature dependence of the molecules embedded in an inert polystyrene (PS) matrix, temperature dependence of **BP22** was taken in a mixed toluene/chloroform solution. The solution was kept above the freezing point to facilitate transient studies. Over the range of temperatures measured, 180 – 290 K, the transient spectra show a weak red-shifting of the triplet absorption features and a small narrowing of the GSB, similar to what is observed in PS. The kinetic trace associated with the maximum of the triplet excited state absorption is nearly temperature independent, consistent with the results reported in the main manuscript.

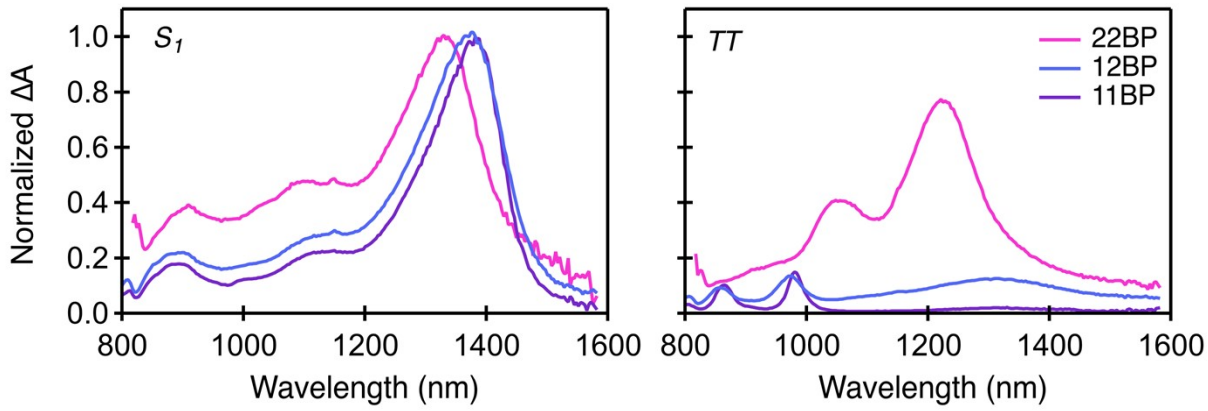


Figure S6: NIR transient absorption spectra of **22BP**, **12BP**, and **11BP** corresponding to the (left) singlet and (right) triplet pair. While all compounds show a strong singlet excited state absorption peak near 1300 nm, only **22BP** shows a strong triplet excited state transition near 1200 nm, which has previously been assigned to $TT \rightarrow S_n$.

NIR transient absorption spectra were used to confirm systematic changes in the chromophore-chromophore coupling strength. While all pentacene based compounds show a strong NIR singlet transition near 1300 nm, only **22BP** shows a corresponding strong triplet excited state absorption spectrum in this region (~ 1200 nm). This peak is significantly diminished and

broadened in **12BP** and nearly completely absent in **11BP**. Ths trend is consistent with the reduction in rate constants for singlet fission.

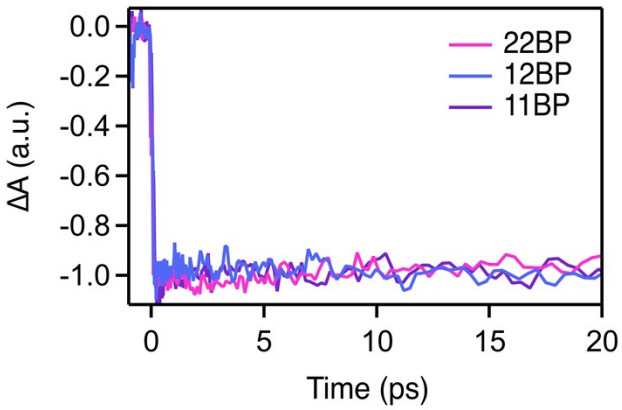


Figure S7: Decay kinetics at the isosbestic point between the singlet and triplet pair for **22BP** (646 nm), **12BP** (655 nm), and **11BP** (657 nm).

Quantitative singlet fission can be inferred from the presence of an isosbestic point between the singlet and triplet transient absorption spectra. This ensures sequential decay of the singlet to the triplet without any additional products. As can be seen in Figure S7, the decay kinetics of all compounds are “flat” during singlet fission and indistinguishable on time scales shorter than ground state repopulation.

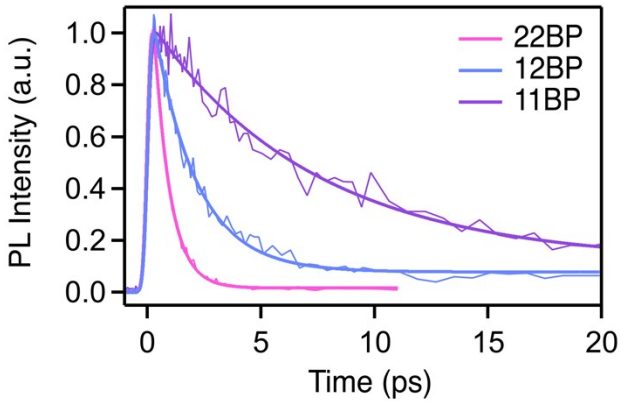


Figure S8: Time-resolved emission kinetics of **22BP**, **12BP**, and **11BP** at 680 nm.

Time-resolved emission data were collected from dilute solutions using the photoluminescence upconversion technique (Figure S6). Here, the samples were excited at 500 nm and emission was collected at 680 nm. The decays show only the prompt fluorescence corresponding to the singlet state. Residual emission after this prompt decay is a result of impurity emission that resembles the monomer and which exists in the samples at a level of 1 – 5%.

II. UV-Vis Spectroscopy

The UV/Vis spectra of the three dimers examined in the main text and TIPS pentacene are shown below. The three spectra show the three absorptions from 550 nm to 650 nm that are characteristic of pentacenes. The three spectra are also very similar to each other, which is expected. The 22BP spectrum has an absorption at around 500 nm that is not seen in the other dimers, which we believe is due to orbital overlap present in 22BP that is not in the other dimers.

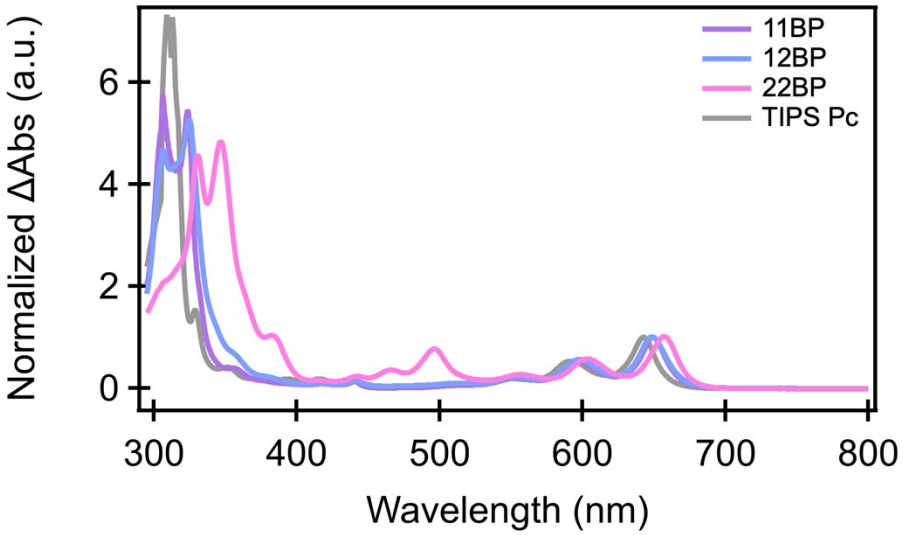


Figure S9: UV/Vis spectra taken of pentacene dimers and TIPS pentacene in chloroform.

III. Electronic structure calculation: The geometries of 22BP, 12BP and 11BP molecules are optimized using the ωB97X-D3 functional and Pople's 6-31G* basis. For computational simplicity, the optimization of the ^{1}(TT) state is performed by optimizing the lowest quintet state of the molecules whose electronic configuration is expected to be similar to that of the diabatic ^{1}(TT) state. In case of 12BP, the geometry optimization is considerably more difficult than 22BP and 11BP due to the lack of symmetry in the molecule. Therefore, we take as the optimized structure the lowest energy structure obtained in 600 optimization steps. For 11BP, the calculated normal modes contain one imaginary frequency in each of the two electronic states at the optimized geometry. These imaginary modes are not included in the subsequent rate calculation, assuming the removal of 1-2 modes does not significantly influence the total rate calculation of molecule as large as bipentacene (> 200 modes).

Following the work by Fuemmeler et al.[33], we calculate the adiabatic energies of S_0S_0 and ^{1}(TT) states by multiconfigurational quasi-degenerate perturbation theory (XMCQDPT) with intruder state avoidance (ISA) shift of 0.02 a.u. The orbitals used in the XMCQDPT calculation were optimized at CASSCF(8o8e)-SA6 level with SBKJC effective core potential valence double-ζ basis plus a d-polarization function taken from Pople's 6-31G*basis for a carbon atom.

The vibronic coupling between S_0S_0 and ^{1}(TT) state is calculated via the NACME subroutine as implemented in GAMESS-US[34] that finds the nonadiabatic coupling matrix element between two state-averaged MC-SCF wavefunctions. Prior to the NACME calculations, the orbitals are optimized using CASSCF(4o4e)-SA2 with SBKJC+d basis as in the XMCQDPT calculation. All electronic structure calculations described above are performed using GAMESS-US[34].

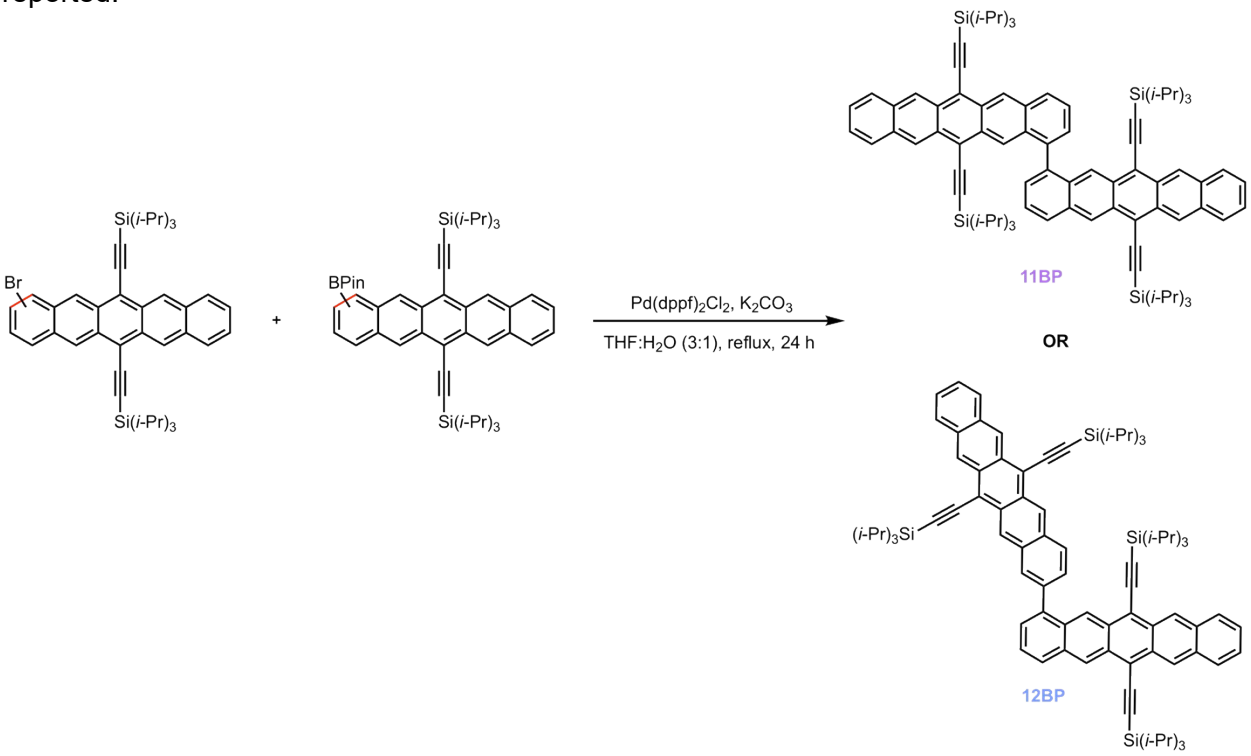
IV. Synthetic Information

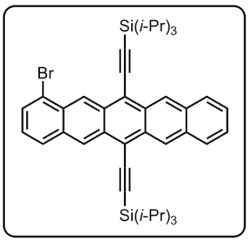
A. General Methods

General Methods: Reagents and solvents were purchased from Alfa Aesar®, Sigma-Aldrich®, Acros organics®, TCI America®, Mallinckrodt®, and Oakwood® Products and were used without further purification. Reactions were done under an argon atmosphere in oven dried glassware. Bruker 400 MHz (100 MHz for ^{13}C) and 500 MHz (125 MHz for ^{13}C) were used to take ^{1}H-NMR and ^{13}C-NMR spectra. ^{1}H-NMR and ^{13}C-NMR spectral data is reported in chemical shift (δ ppm). coupling constants (J) are reported in hertz (Hz), and multiplicity is reported using standard abbreviations: s (singlet), b (broad), d (doublet), t (triplet), q (quartet), m (multiplet) and virt (virtual). XEVO G2-XS Waters® equipped with a QTOF detector with multiple inlet and ionization abilities was used to obtain mass spectral data. The $[M]^+$ or $[M+H]^+$ ions peaks are reported. A Schlenk manifold with purification columns packed with activated alumina and supported copper catalyst (Glass Contour, Irvine, CA) was used for anhydrous solvents.

B. General Synthetic protocol for the synthesis of Bispentacenes:

Synthesis of Br/Bpin derivative of TIPS pentacenes and bipentacenes has been previously reported.[1]



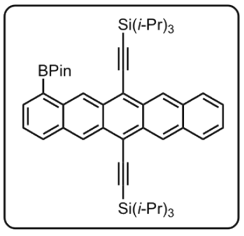


Yield: 16%

^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.72 (s, 1H), 9.41-9.33 (m, 3H), 8.04-7.96 (m, 3H), 7.77-7.75 (m, 1H), 7.48-7.45 (2H), 7.29-7.25 (m, 1H) and 1.48-1.38 (m, 42H).

^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 132.8, 132.5, 132.4, 130.94, 130.9, 130.8, 132.75, 130.72, 129.8, 128.9, 128.7, 128.66, 127.3, 126.9, 126.6, 126.3, 126.3, 126.2, 125.8, 123.4, 119.3, 118.3, 108.0, 107.5, 104.5, 104.3, 19.1, 19.0 and 11.7.

MS (ASAP): Calculated: 717.2947; Observed: 717.2939

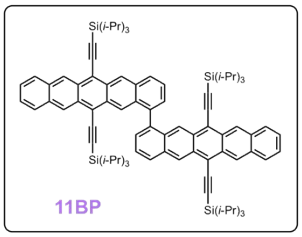


Yield: 80%

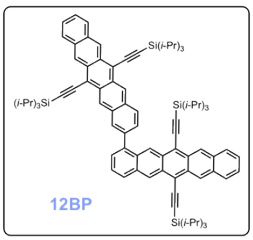
^{1}H-NMR (400 MHz, $CDCl_3$, δ ppm): 9.93 (s, 1H), 9.52 (s, 1H), 9.37 (s, 2H), 8.12-8.08 (m, 2H), 8.04-8.00 (m, 2H), 7.47-7.44 (m, 3H), 1.54 (s, 12H) and 1.44-1.40 (m, 42H).

^{13}C-NMR (100 MHz, $CDCl_3$, δ ppm): 137.4, 134.5, 132.6, 132.4, 132.3, 132.2, 131.6, 130.7, 130.6, 130.4, 128.6, 127.3, 126.8, 126.7, 126.2, 125.96, 125.1, 118.9, 118.3, 107.6, 107.0, 105.5, 104.9, 83.9, 24.9, 19.2, 19.0, 12.0 and 11.7.

MS (ASAP): Calculated: 765.4694; Observed: 765.4688



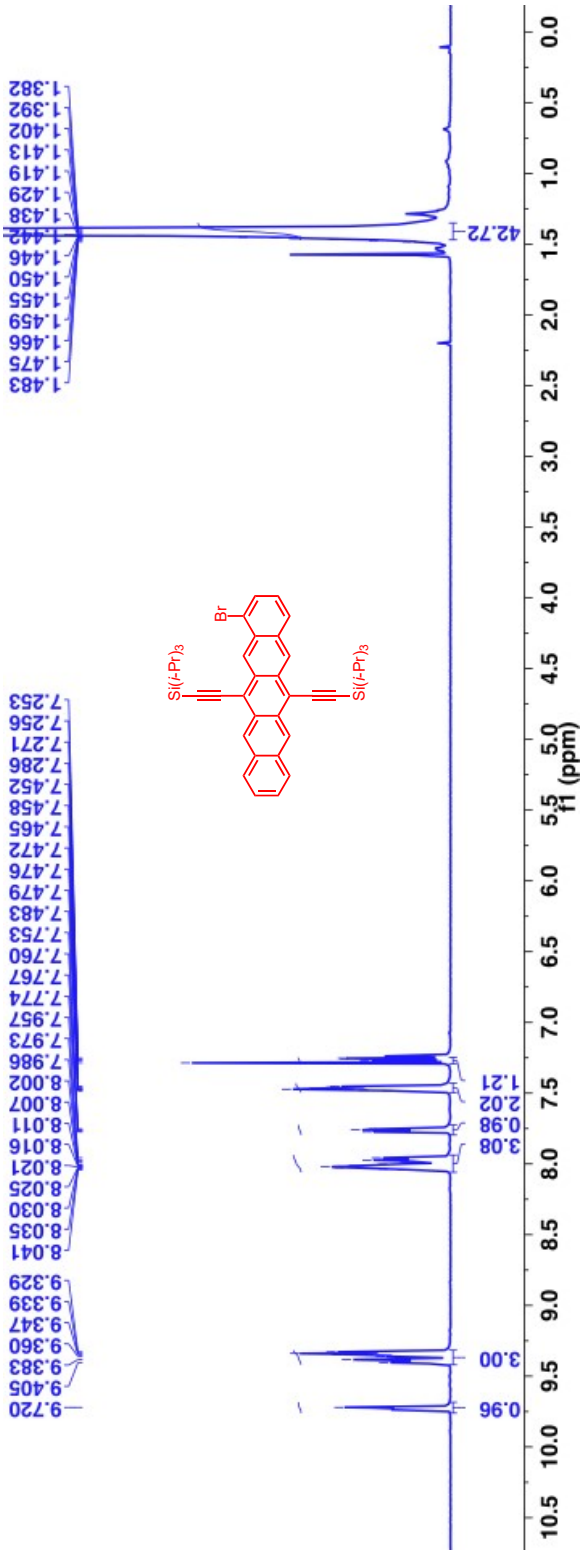
Yield: 84% (Pale blue solid)
^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.51 (s, 1H), 9.31 (s, 1H), 9.15 (s, 1H), 9.07 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.61-7.58 (m, 1H), 7.52-7.51 (m, 1H), 7.41-7.34 (m, 2H), 1.496-1.44 (m, 21H), 0.87-0.86 (m, 9H) and 0.76-0.68 (m, 12H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 139.3, 132.7, 132.3, 132.2, 132.1, 130.8, 130.6, 129.1, 128.7, 128.6, 128.2, 126.9, 126.5, 126.1, 125.9, 125.9, 125.8, 125.7, 118.9, 117.9, 107.4, 106.8, 104.9, 103.8, 19.1, 18.6, 18.5, 11.8 and 11.2.
MS (ASAP): Calculated: 1275.7450; Observed: 1275.7440



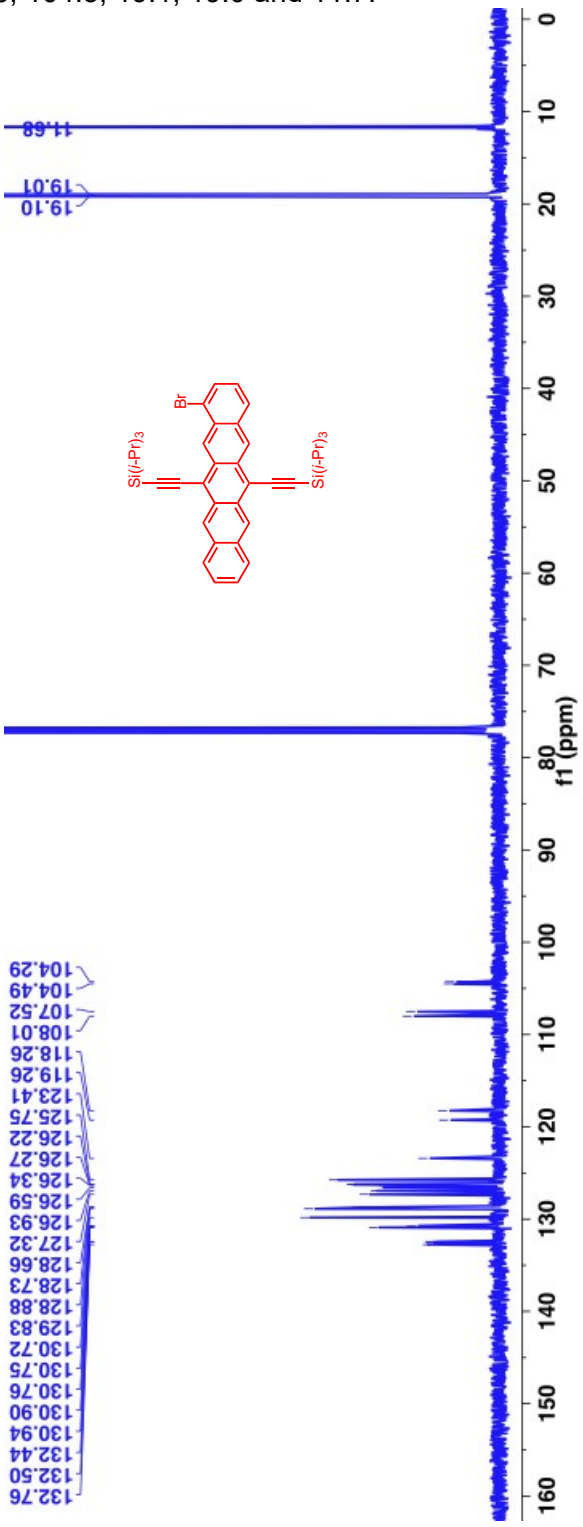
Yield: 65% (Deep blue solid)
^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.47 (s, 1H), 9.45 (s, 1H), 9.42 (s, 1H), 9.40-9.38 (m, 3H), 9.34 (s, 1H), 9.28 (s, 1H), 8.21 (s, 1H), 8.15-8.09 (m, 2H), 8.05-7.996 (m, 3H), 7.94-7.92 (m, 1H), 7.71-7.69 (m, 1H), 7.60-7.55 (m, 2H), 7.49-7.39 (m, 4H), 1.51-1.40 (m, 42H), 1.39-1.34 (m, 20H) and 0.86-0.73 (m, 22H).
^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 140.6, 138.7, 132.7, 132.6, 132.33, 132.31, 132.2, 131.9, 131.3, 130.9, 130.87, 130.8, 130.7, 130.66, 130.6, 130.55, 129.1, 128.8, 128.7, 128.68, 128.6, 128.55, 126.9, 126.8, 126.6, 126.5, 126.4, 126.38, 126.3, 126.2, 126.1, 125.98, 125.7, 125.6, 119.0, 118.4, 118.0, 107.7, 107.4, 107.2, 107.1, 104.7, 104.67, 103.95, 19.06, 19.05, 18.99, 18.5, 11.8, 11.7, 11.65 and 11.4.
MS (ASAP): Calculated: 1275.7450; Observed: 1275.7386

V. NMR Spectra

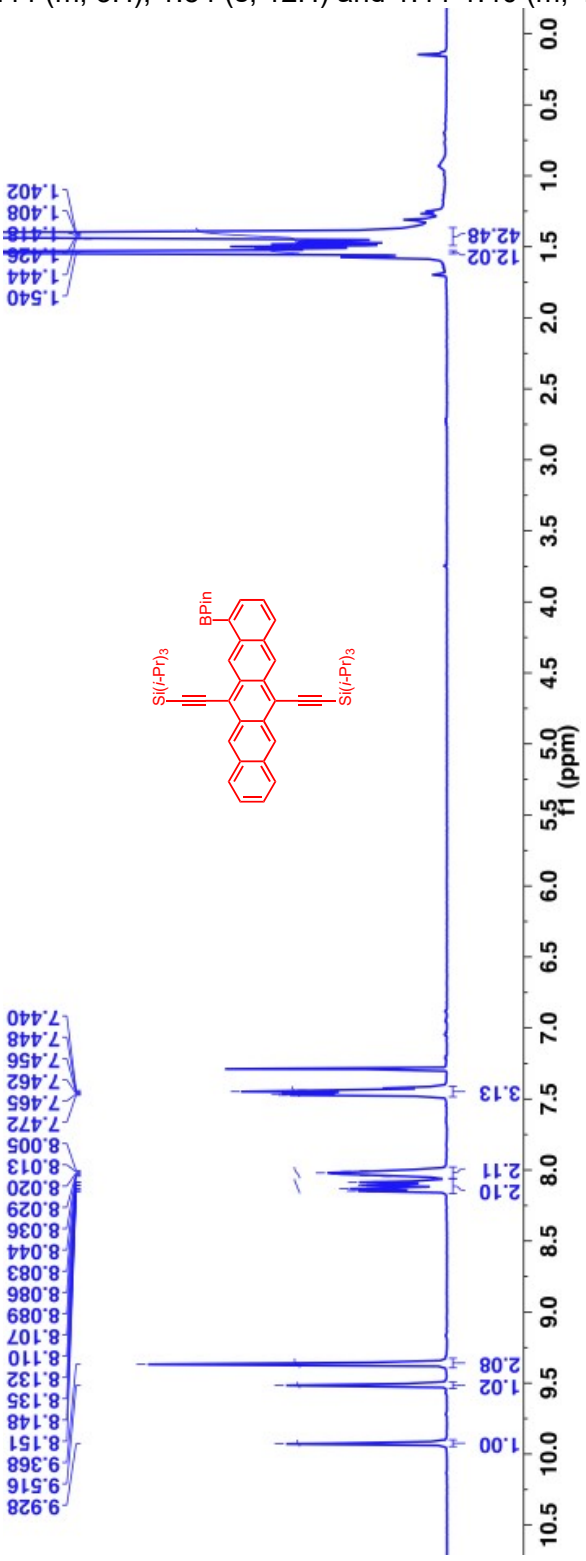
^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.72 (s, 1H), 9.41-9.33 (m, 3H), 8.04-7.96 (m, 3H), 7.77-7.75 (m, 1H), 7.48-7.45 (2H), 7.29-7.25 (m, 1H) and 1.48-1.38 (m, 42H).



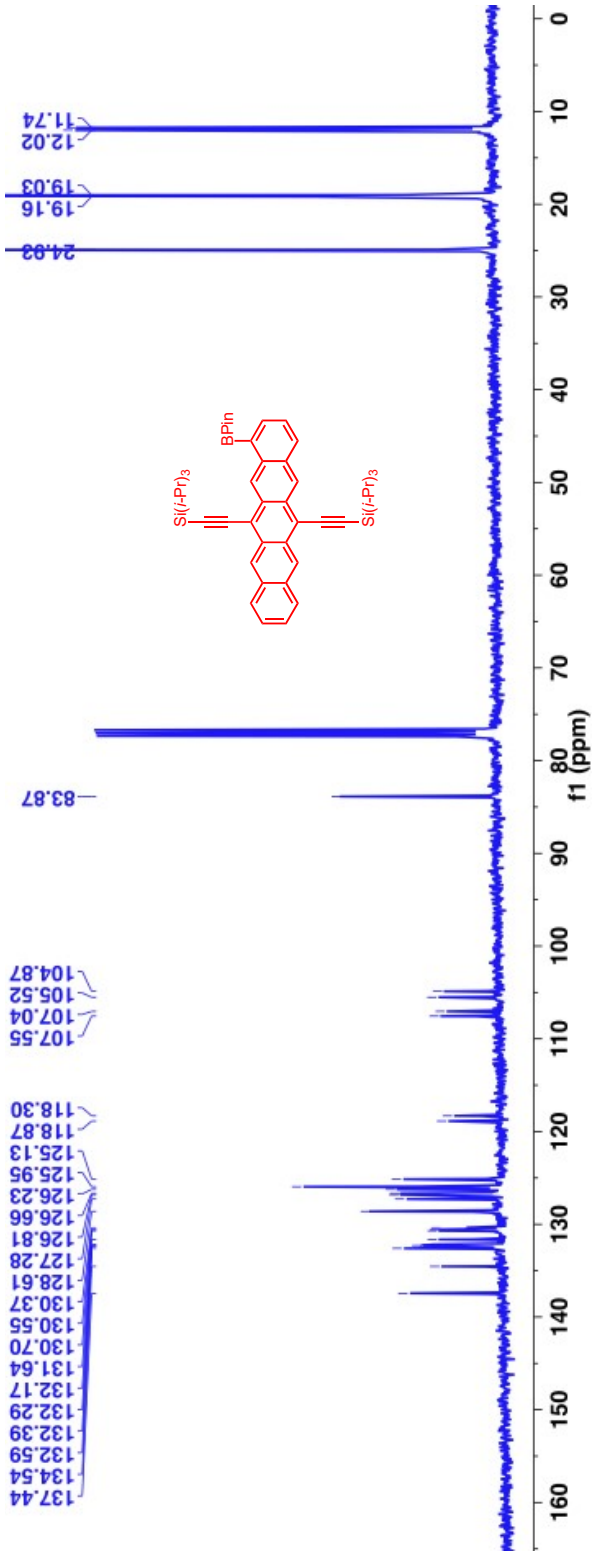
^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 132.8, 132.5, 132.4, 130.94, 130.9, 130.8, 132.75, 130.72, 129.8, 128.9, 128.7, 128.66, 127.3, 126.9, 126.6, 126.3, 126.3, 126.2, 125.8, 123.4, 119.3, 118.3, 108.0, 107.5, 104.5, 104.3, 19.1, 19.0 and 11.7.



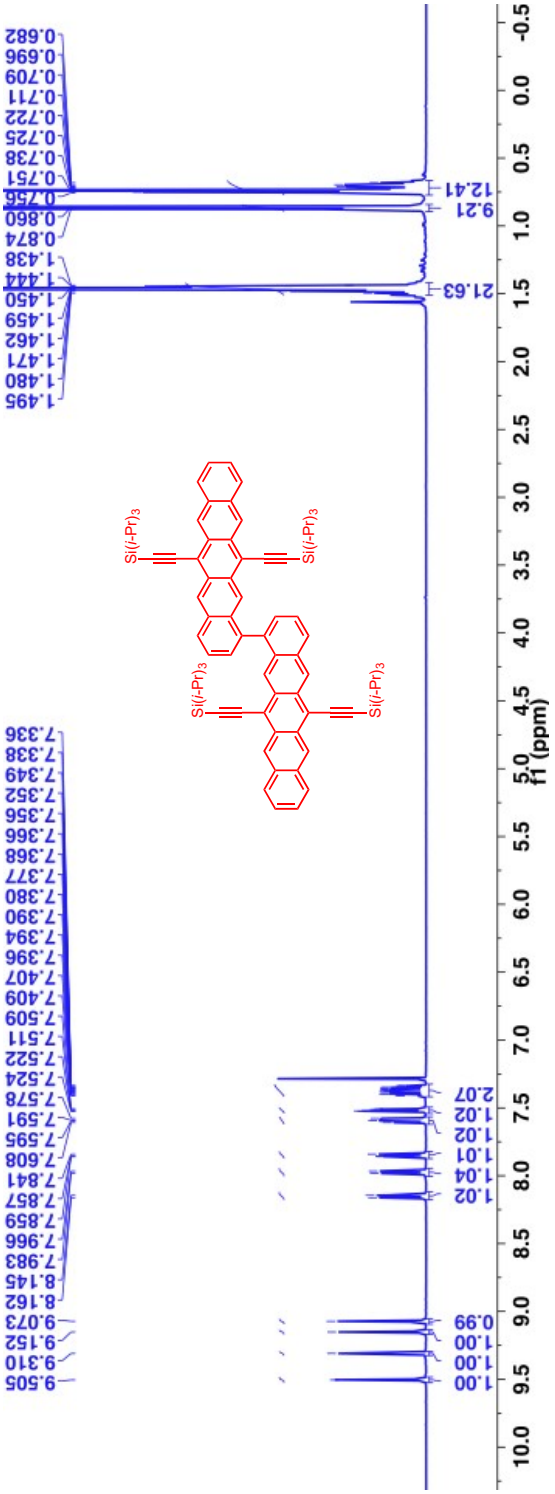
^{1}H-NMR (400 MHz, $CDCl_3$, δ ppm): 9.93 (s, 1H), 9.52 (s, 1H), 9.37 (s, 2H), 8.12-8.08 (m, 2H), 8.04-8.00 (m, 2H), 7.47-7.44 (m, 3H), 1.54 (s, 12H) and 1.44-1.40 (m, 42H).



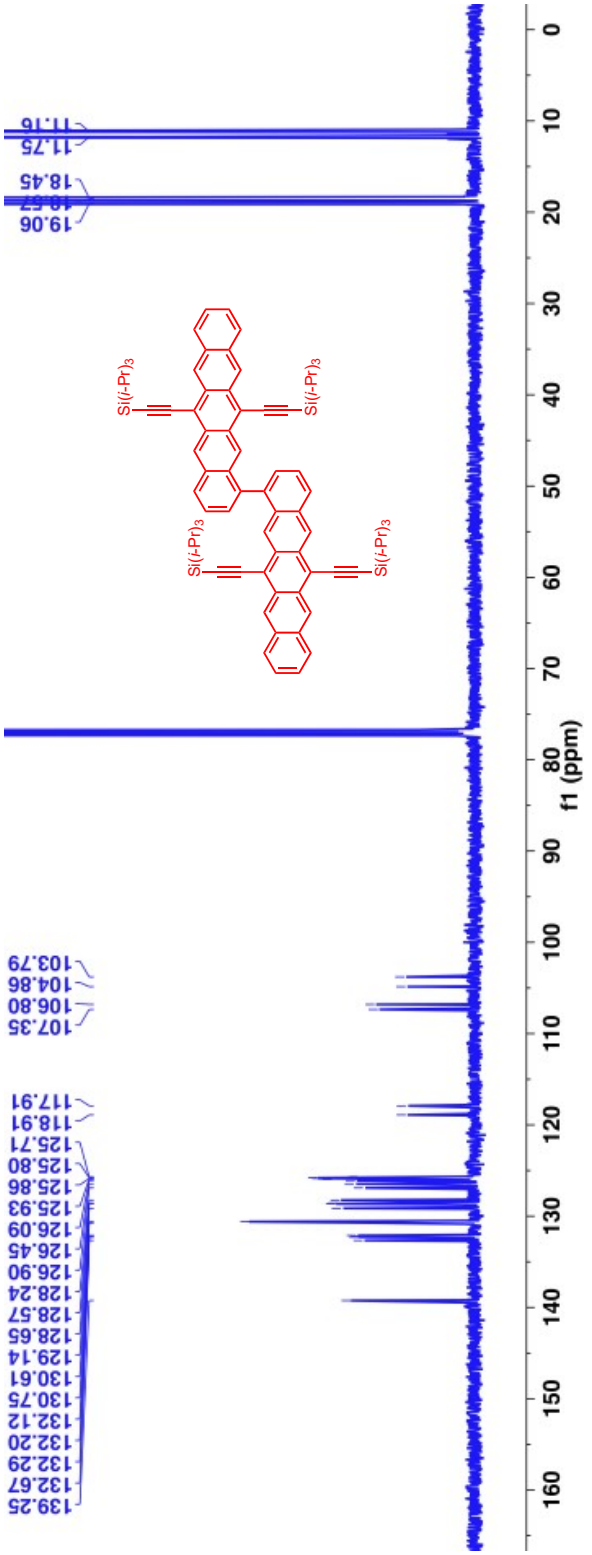
^{13}C-NMR (100 MHz, $CDCl_3$, δ ppm): 137.4, 134.5, 132.6, 132.4, 132.3, 132.2, 131.6, 130.7, 130.6, 130.4, 128.6, 127.3, 126.8, 126.7, 126.2, 125.96, 125.1, 118.9, 118.3, 107.6, 107.0, 105.5, 104.9, 83.9, 24.9, 19.2, 19.0, 12.0 and 11.7.



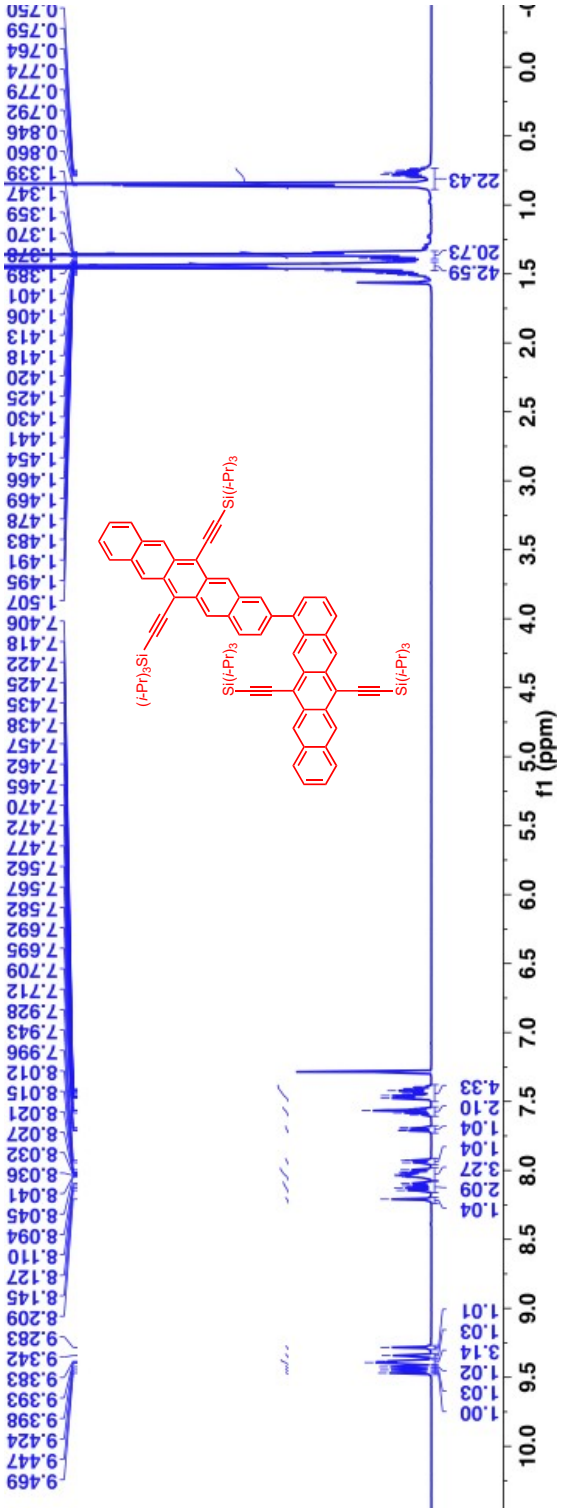
^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.51 (s, 1H), 9.31 (s, 1H), 9.15 (s, 1H), 9.07 (s, 1H), 8.15 (d, *J* = 8.5 Hz, 1H), 7.97 (d, *J* = 8.5 Hz, 1H), 7.85 (d, *J* = 8.5 Hz, 1H), 7.61-7.58 (m, 1H), 7.52-7.51 (m, 1H), 7.41-7.34 (m, 2H), 1.496-1.44 (m, 21H), 0.87-0.86 (m, 9H) and 0.76-0.68 (m, 12H).



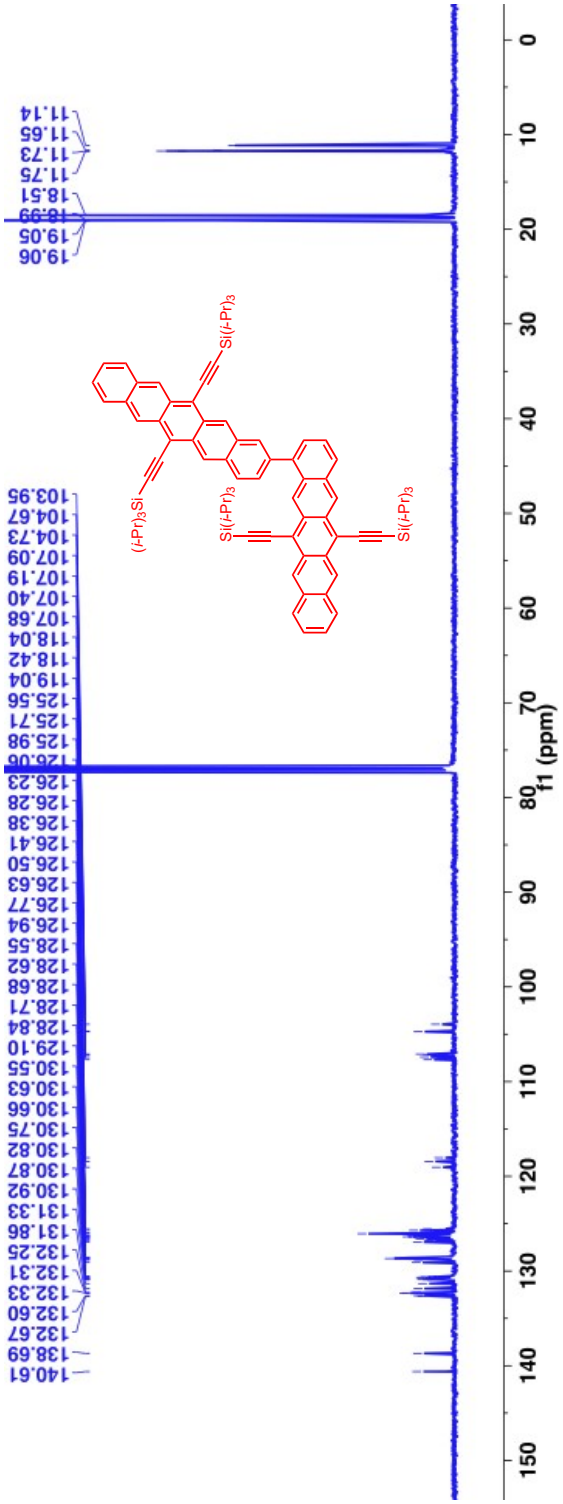
^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 139.3, 132.7, 132.3, 132.2, 132.1, 130.8, 130.6, 129.1, 128.7, 128.6, 128.2, 126.9, 126.5, 126.1, 125.9, 125.9, 125.8, 125.7, 118.9, 117.9, 107.4, 106.8, 104.9, 103.8, 19.1, 18.6, 18.5, 11.8 and 11.2.



^{1}H-NMR (500 MHz, $CDCl_3$, δ ppm): 9.47 (s, 1H), 9.45 (s, 1H), 9.42 (s, 1H), 9.40-9.38 (m, 3H), 9.34 (s, 1H), 9.28 (s, 1H), 8.21 (s, 1H), 8.15-8.09 (m, 2H), 8.05-7.996 (m, 3H), 7.94-7.92 (m, 1H), 7.71-7.69 (m, 1H), 7.60-7.55 (m, 2H), 7.49-7.39 (m, 4H), 1.51-1.40 (m, 42H), 1.39-1.34 (m, 20H) and 0.86-0.73 (m, 22H).



^{13}C-NMR (125 MHz, $CDCl_3$, δ ppm): 140.6, 138.7, 132.7, 132.6, 132.33, 132.31, 132.2, 131.9, 131.3, 130.9, 130.87, 130.8, 130.7, 130.66, 130.6, 130.55, 129.1, 128.8, 128.7, 128.68, 128.6, 128.55, 126.9, 126.8, 126.6, 126.5, 126.4, 126.38, 126.3, 126.2, 126.1, 125.98, 125.7, 125.6, 119.0, 118.4, 118.0, 107.7, 107.4, 107.2, 107.1, 104.7, 104.67, 103.95, 19.06, 19.05, 18.99, 18.5, 11.8, 11.7, 11.65 and 11.4.



VI. Single Crystal X-Ray Diffraction
VII. References

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Appendix A. Minimized Geometry

Minimized geometries were calculated with DFT using ωB97X-D3 functional and a 6-31G* basis using GAMESS (US) software.[4,5] The ^{1}(TT) state geometry was obtained by minimizing the quintet ground state, whose electronic configuration resembles that of diabatic ^{1}(TT) state. Coordinates of the two electronic states, S_0S_0 and ^{1}(TT), of each dimer are shown.

11BP/S_0S_0

ATOM	CHARGE	X	Y	Z
C	6.0	-6.0508227684	4.0473904725	-0.0322481717
C	6.0	6.0508227684	-4.0473904725	-0.0322481717
C	6.0	-1.5822916117	3.2110314590	-3.2792209186
C	6.0	1.5822916117	-3.2110314590	-3.2792209186
C	6.0	-3.0955796542	-2.1901423589	0.0295388528
C	6.0	3.0955796542	2.1901423589	0.0295388528
C	6.0	-2.0255869835	-0.1004898061	-1.5981897195
C	6.0	2.0255869835	0.1004898061	-1.5981897195
C	6.0	-0.3381072869	0.6643387874	-3.2477088708
C	6.0	0.3381072869	-0.6643387874	-3.2477088708
C	6.0	-2.5693123810	-3.2773507431	0.0364547585
C	6.0	2.5693123810	3.2773507431	0.0364547585
C	6.0	-5.4202002246	-1.6738114812	1.6225060337
C	6.0	5.4202002246	1.6738114812	1.6225060337
C	6.0	-6.5357632900	-1.4431202276	2.4056271248
C	6.0	6.5357632900	1.4431202276	2.4056271248
C	6.0	-3.2354492601	2.4220368632	-1.6391338565
C	6.0	3.2354492601	-2.4220368632	-1.6391338565

C	6.0	-2.1261364420	2.1883424332	-2.4295052959
C	6.0	2.1261364420	-2.1883424332	-2.4295052959
C	6.0	-7.1494097593	-0.1368774033	2.3966558145
C	6.0	7.1494097593	0.1368774033	2.3966558145
C	6.0	-6.6112662806	0.8603739537	1.6054884626
C	6.0	6.6112662806	-0.8603739537	1.6054884626
C	6.0	-7.1091952248	-2.4651464543	3.2385956075
C	6.0	7.1091952248	2.4651464543	3.2385956075
C	6.0	-3.7872815700	1.4213931435	-0.8108456466
C	6.0	3.7872815700	-1.4213931435	-0.8108456466
C	6.0	-8.3087026218	0.0842982196	3.2172622661
C	6.0	8.3087026218	-0.0842982196	3.2172622661
C	6.0	-5.4719668323	0.6404393624	0.8009312111
C	6.0	5.4719668323	-0.6404393624	0.8009312111
C	6.0	-4.9269465508	1.6628199688	-0.0098606930
C	6.0	4.9269465508	-1.6628199688	-0.0098606930
C	6.0	-1.4988998906	0.8875735946	-2.4097022293
C	6.0	1.4988998906	-0.8875735946	-2.4097022293
C	6.0	-3.7109518657	-0.9015558455	0.0162479846
C	6.0	3.7109518657	0.9015558455	0.0162479846
C	6.0	-4.8568841620	-0.6641082950	0.8109455434
C	6.0	4.8568841620	0.6641082950	0.8109455434
C	6.0	-0.4950991856	2.9617800313	-4.0522610365
C	6.0	0.4950991856	-2.9617800313	-4.0522610365
C	6.0	-8.8162347099	-0.9121200761	3.9883519572
C	6.0	8.8162347099	0.9121200761	3.9883519572
C	6.0	-8.2046285036	-2.2094539271	4.0002720626
C	6.0	8.2046285036	2.2094539271	4.0002720626
C	6.0	0.1321176591	1.6750132007	-4.0313580720
C	6.0	-0.1321176591	-1.6750132007	-4.0313580720
C	6.0	-3.1658564732	0.1215792718	-0.7942822960
C	6.0	3.1658564732	-0.1215792718	-0.7942822960
C	6.0	-5.5361270539	2.9543824959	-0.0220474338
C	6.0	5.5361270539	-2.9543824959	-0.0220474338
H	1.0	-6.5057719031	5.0120867971	-0.0413731492
H	1.0	6.5057719031	-5.0120867971	-0.0413731492
H	1.0	-2.0955766724	-4.2330254786	0.0420425742
H	1.0	2.0955766724	4.2330254786	0.0420425742
H	1.0	-8.7686342094	1.0688372770	3.2056882795
H	1.0	8.7686342094	-1.0688372770	3.2056882795
H	1.0	-9.6924965844	-0.7338004940	4.6044160153
H	1.0	9.6924965844	0.7338004940	4.6044160153
H	1.0	-8.6276342588	-2.9878819038	4.6281662187
H	1.0	8.6276342588	2.9878819038	4.6281662187
H	1.0	-2.0648324510	4.1846204853	-3.2893056406
H	1.0	2.0648324510	-4.1846204853	-3.2893056406
H	1.0	-6.6433750871	-3.4469411004	3.2453759254
H	1.0	6.6433750871	3.4469411004	3.2453759254
H	1.0	-0.0892445484	3.7349971416	-4.6974161151
H	1.0	0.0892445484	-3.7349971416	-4.6974161151
H	1.0	-7.0720841360	1.8434876497	1.5975621065

H	1.0	7.0720841360	-1.8434876497	1.5975621065
H	1.0	-4.9574888465	-2.6561427233	1.6263464663
H	1.0	4.9574888465	2.6561427233	1.6263464663
H	1.0	-3.7045484442	3.4011378086	-1.6550436211
H	1.0	3.7045484442	-3.4011378086	-1.6550436211
H	1.0	-1.5618008110	-1.0804121532	-1.5778593735
H	1.0	1.5618008110	1.0804121532	-1.5778593735
H	1.0	1.0055678060	1.5011173417	-4.6532931256
H	1.0	-1.0055678060	-1.5011173417	-4.6532931256

11BP/^{1}(TT)

ATOM	CHARGE	X	Y	Z
C	6.0	-6.0548628000	4.0460288323	-0.0249633257
C	6.0	6.0548628000	-4.0460288323	-0.0249633257
C	6.0	-1.5588075378	3.1995386470	-3.2818419889
C	6.0	1.5588075378	-3.1995386470	-3.2818419889
C	6.0	-3.1124075155	-2.1930369709	0.0150052082
C	6.0	3.1124075155	2.1930369709	0.0150052082
C	6.0	-2.0450276263	-0.1047566150	-1.6075566886
C	6.0	2.0450276263	0.1047566150	-1.6075566886
C	6.0	-0.3330896730	0.6673905203	-3.2436801743
C	6.0	0.3330896730	-0.6673905203	-3.2436801743
C	6.0	-2.5871839207	-3.2851819951	0.0178754483
C	6.0	2.5871839207	3.2851819951	0.0178754483
C	6.0	-5.4241408363	-1.6676646336	1.6169359588
C	6.0	5.4241408363	1.6676646336	1.6169359588
C	6.0	-6.5680855657	-1.4457042961	2.4305950888
C	6.0	6.5680855657	1.4457042961	2.4305950888
C	6.0	-3.2474414450	2.4064141332	-1.6556473800
C	6.0	3.2474414450	-2.4064141332	-1.6556473800
C	6.0	-2.1008762876	2.1817371215	-2.4658361841
C	6.0	2.1008762876	-2.1817371215	-2.4658361841
C	6.0	-7.1711363348	-0.1599402131	2.4240174958
C	6.0	7.1711363348	0.1599402131	2.4240174958
C	6.0	-6.6085096821	0.8545308753	1.6024616380
C	6.0	6.6085096821	-0.8545308753	1.6024616380
C	6.0	-7.1210363295	-2.4613452409	3.2433392822
C	6.0	7.1210363295	2.4613452409	3.2433392822
C	6.0	-3.7826971501	1.4250663547	-0.8480719823
C	6.0	3.7826971501	-1.4250663547	-0.8480719823
C	6.0	-8.3093972609	0.0707120667	3.2293746216
C	6.0	8.3093972609	-0.0707120667	3.2293746216
C	6.0	-5.4994593373	0.6304896510	0.8132898539
C	6.0	5.4994593373	-0.6304896510	0.8132898539
C	6.0	-4.9426324877	1.6709486768	-0.0215570337
C	6.0	4.9426324877	-1.6709486768	-0.0215570337
C	6.0	-1.4860314214	0.9007283967	-2.4432611402
C	6.0	1.4860314214	-0.9007283967	-2.4432611402

C	6.0	-3.7177271813	-0.9192728919	0.0044604191
C	6.0	3.7177271813	0.9192728919	0.0044604191
C	6.0	-4.8836657154	-0.6776771016	0.8227465652
C	6.0	4.8836657154	0.6776771016	0.8227465652
C	6.0	-0.4394455947	2.9581940540	-4.0441561840
C	6.0	0.4394455947	-2.9581940540	-4.0441561840
C	6.0	-8.8302449007	-0.9355051469	4.0113928464
C	6.0	8.8302449007	0.9355051469	4.0113928464
C	6.0	-8.2309010906	-2.2115875673	4.0186162194
C	6.0	8.2309010906	2.2115875673	4.0186162194
C	6.0	0.1730451619	1.6912091955	-4.0208500821
C	6.0	-0.1730451619	-1.6912091955	-4.0208500821
C	6.0	-3.1605443191	0.1216088352	-0.8286730016
C	6.0	3.1605443191	-0.1216088352	-0.8286730016
C	6.0	-5.5398250227	2.9487711811	-0.0259080857
C	6.0	5.5398250227	-2.9487711811	-0.0259080857
H	1.0	-6.5084772285	5.0113240700	-0.0217848411
H	1.0	6.5084772285	-5.0113240700	-0.0217848411
H	1.0	-2.1157497859	-4.2418455489	0.0197355339
H	1.0	2.1157497859	4.2418455489	0.0197355339
H	1.0	-8.7682242254	1.0559801479	3.2216964719
H	1.0	8.7682242254	-1.0559801479	3.2216964719
H	1.0	-9.7058925772	-0.7482287449	4.6255225573
H	1.0	9.7058925772	0.7482287449	4.6255225573
H	1.0	-8.6483284623	-2.9984683517	4.6396188859
H	1.0	8.6483284623	2.9984683517	4.6396188859
H	1.0	-2.0380357593	4.1748932651	-3.2957212434
H	1.0	2.0380357593	-4.1748932651	-3.2957212434
H	1.0	-6.6559863484	-3.4437048839	3.2464756422
H	1.0	6.6559863484	3.4437048839	3.2464756422
H	1.0	-0.0232314341	3.7424409672	-4.6690445881
H	1.0	0.0232314341	-3.7424409672	-4.6690445881
H	1.0	-7.0718301071	1.8369246747	1.5989408263
H	1.0	7.0718301071	-1.8369246747	1.5989408263
H	1.0	-4.9630357565	-2.6510766182	1.6234392017
H	1.0	4.9630357565	2.6510766182	1.6234392017
H	1.0	-3.7116941947	3.3882640080	-1.6750490436
H	1.0	3.7116941947	-3.3882640080	-1.6750490436
H	1.0	-1.5765287300	-1.0824955287	-1.5832802294
H	1.0	1.5765287300	1.0824955287	-1.5832802294
H	1.0	1.0598957895	1.5086365987	-4.6208365677
H	1.0	-1.0598957895	-1.5086365987	-4.6208365677

12BP/S_0S_0

ATOM	CHARGE	X	Y	Z
C	6.0	-0.0973918903	-1.4346483878	0.1214688455
C	6.0	-0.0756070509	1.4008549341	0.0344979223
C	6.0	-1.3226621973	-0.7288296176	0.0714512602

C	6.0	1.1373823873	-0.7468159285	0.1208192385
C	6.0	-1.3112154211	0.7129969412	0.0339919618
C	6.0	1.1485000623	0.6946585646	0.0673920182
C	6.0	-0.1083227246	-2.8623388581	0.1623181482
C	6.0	-0.0646167560	2.8282959039	-0.0087041110
C	6.0	-0.1152550094	-4.0696249219	0.1955873609
C	6.0	-0.0558847657	4.0357827490	-0.0422376023
H	1.0	-0.1245048559	-5.1359584817	0.2267151251
H	1.0	-0.0442764992	5.1020394114	-0.0682619909
C	6.0	2.3912764699	1.3644608326	0.0381997471
C	6.0	-2.5433869283	1.4009407932	-0.0025026367
C	6.0	2.3719172571	-1.4336037721	0.1617064172
C	6.0	-2.5657379080	-1.3980165981	0.0577925724
C	6.0	3.5793260644	-0.7638345293	0.1315284678
C	6.0	-3.7644847169	-0.7103544601	0.0205301993
C	6.0	3.5893073276	0.6766939174	0.0605445543
C	6.0	-3.7532679573	0.7327544366	-0.0062920244
H	1.0	-2.5726974708	-2.4835045742	0.0814358258
H	1.0	2.3624796117	-2.5183463690	0.2110572467
H	1.0	-2.5328971346	2.4865862926	-0.0255514599
H	1.0	2.3983741050	2.4488486151	-0.0129235026
C	6.0	4.8528129878	1.3539764218	-0.0002071410
C	6.0	-5.0095966792	1.4302899238	-0.0310310188
C	6.0	4.8413298481	-1.4515370487	0.1647168278
C	6.0	-5.0326308907	-1.3867181635	0.0151383700
C	6.0	6.0121843513	-0.7684998998	0.1068795086
C	6.0	-6.1959877868	-0.6857209588	-0.0071090454
C	6.0	6.0321968153	0.6712393119	0.0086219753
C	6.0	-6.1845183457	0.7483773075	-0.0281588697
H	1.0	-7.1276774752	1.2862483800	-0.0441116951
H	1.0	6.9580778802	-1.3004706680	0.1417931932
H	1.0	-7.1490308962	-1.2060540151	-0.0093377479
H	1.0	4.8550552247	2.4380242634	-0.0812478390
H	1.0	-4.9959429309	2.5168974757	-0.0461318938
H	1.0	4.8380657475	-2.5355041516	0.2422643343
H	1.0	-5.0378101041	-2.4733458833	0.0307656691
C	6.0	8.7200172596	-0.9869498175	-4.1600534152
C	6.0	11.1447795924	0.4886239357	-4.1962635491
C	6.0	8.9691753033	-0.0236813982	-3.1549895066
C	6.0	9.6681922423	-1.2288707650	-5.1810924877
C	6.0	10.2028231249	0.7182399764	-3.1679653357
C	6.0	10.8979113072	-0.4757651818	-5.2014092494
C	6.0	7.4976643477	-1.7251795670	-4.1360268089
C	6.0	12.3575343757	1.2421216306	-4.2231603743
C	6.0	6.4617558427	-2.3446517248	-4.1014967921
C	6.0	13.3817141949	1.8822417904	-4.2512761047
H	1.0	5.5429958623	-2.8859047436	-4.0686011562
H	1.0	14.2868054028	2.4463382313	-4.2721602736
C	6.0	11.8268581919	-0.7218783332	-6.2351750308
C	6.0	10.4291976740	1.6671792703	-2.1479475046
C	6.0	9.4424637394	-2.1907257799	-6.1903481572

C	6.0	8.0326168024	0.2273469635	-2.1277982527
C	6.0	10.3636545983	-2.4235096042	-7.1945258945
C	6.0	8.2753724502	1.1414200955	-1.1186288314
C	6.0	11.5903885147	-1.6640629109	-7.2187282088
C	6.0	9.5117178073	1.8897714652	-1.1386165839
H	1.0	7.0965854790	-0.3182784487	-2.1516499630
H	1.0	8.5151416744	-2.7554274148	-6.1735553421
H	1.0	11.3529765164	2.2372338344	-2.1619674623
H	1.0	12.7487143430	-0.1489460438	-6.2526543182
C	6.0	12.5356341721	-1.9173224273	-8.2711897312
C	6.0	9.7526277108	2.8698429677	-0.1163219095
C	6.0	10.1414555219	-3.4025863077	-8.2234500691
C	6.0	7.3214167251	1.4048533429	-0.0568498335
C	6.0	11.0649009298	-3.6095867938	-9.1983810330
C	6.0	7.6077443291	2.3559071662	0.8790865546
C	6.0	12.2840366638	-2.8546166147	-9.2217013361
C	6.0	8.8301872368	3.0982011463	0.8522220777
H	1.0	13.0099536060	-3.0445775041	-10.0068679574
H	1.0	9.0126394064	3.8414500595	1.6222255343
H	1.0	10.8878673873	-4.3534106333	-9.9692124228
H	1.0	6.8944938804	2.5417850637	1.6770908844
H	1.0	13.4571672400	-1.3420610556	-8.2846143518
H	1.0	10.6874098273	3.4232697390	-0.1411734836
H	1.0	9.2177588838	-3.9748282436	-8.2003074658

12BP/^{1}(TT)

ATOM	CHARGE	X	Y	Z
C	6.0	-0.1141730427	-1.4497468141	0.1529747087
C	6.0	-0.0844123842	1.4132730803	0.0467135373
C	6.0	-1.3649384053	-0.7282206022	0.0940113496
C	6.0	1.1521615361	-0.7546755249	0.1321336102
C	6.0	-1.3501991239	0.7172120842	0.0504141306
C	6.0	1.1666340852	0.6900457742	0.0701164072
C	6.0	-0.1287689283	-2.8585193924	0.2246387702
C	6.0	-0.0681051768	2.8233504102	0.0117815052
C	6.0	-0.1385726735	-4.0689255375	0.2881695432
C	6.0	-0.0509925644	4.0350593784	-0.0171444667
H	1.0	-0.1453135895	-5.1341595597	0.3415498272
H	1.0	-0.0395582560	5.1012336647	-0.0439795129
C	6.0	2.3782974637	1.3473590810	0.0337894581
C	6.0	-2.5484546450	1.3991211984	0.0104871529
C	6.0	2.3516385427	-1.4366000997	0.1644137911
C	6.0	-2.5769730086	-1.3864118975	0.0775600197
C	6.0	3.6028666070	-0.7662529421	0.1218260501
C	6.0	-3.8157817476	-0.6915110602	0.0281918403
C	6.0	3.6165482826	0.6509879797	0.0514219392
C	6.0	-3.8014003728	0.7285939296	0.0026698342
H	1.0	-2.5899283225	-2.4721943199	0.1057345978

H	1.0	2.3433567061	-2.5215034556	0.2171960090
H	1.0	-2.5395660960	2.4849869218	-0.0176776074
H	1.0	2.3920287897	2.4322032122	-0.0162516861
C	6.0	4.8532657085	1.3269866235	-0.0171000972
C	6.0	-5.0282625402	1.4292492134	-0.0231060618
C	6.0	4.8351150767	-1.4585043875	0.1357440034
C	6.0	-5.0566558013	-1.3675253606	0.0139655121
C	6.0	6.0264540477	-0.7763723242	0.0683679615
C	6.0	-6.2386082176	-0.6621083806	-0.0102618972
C	6.0	6.0509878066	0.6379776937	-0.0195024821
C	6.0	-6.2243161508	0.7477187982	-0.0250110599
H	1.0	-7.1618273018	1.2953699938	-0.0294637399
H	1.0	6.9664668899	-1.3203850856	0.0876103509
H	1.0	-7.1870111350	-1.1906172816	-0.0080476135
H	1.0	4.8578938368	2.4114846496	-0.0942041859
H	1.0	-5.0132522633	2.5160143801	-0.0330021469
H	1.0	4.8309525875	-2.5432325671	0.2018473378
H	1.0	-5.0637482532	-2.4543298438	0.0294014475
C	6.0	8.7568819262	-1.0054408059	-4.1978681348
C	6.0	11.1947238852	0.5009668832	-4.2163238182
C	6.0	8.9969531733	-0.0265481345	-3.1615271575
C	6.0	9.7286316182	-1.2430483200	-5.2402933446
C	6.0	10.2277544974	0.7272441952	-3.1669649377
C	6.0	10.9572601031	-0.4804631129	-5.2505595203
C	6.0	7.5571676904	-1.7468673579	-4.1796331840
C	6.0	12.3869036266	1.2547647271	-4.2344487014
C	6.0	6.5238786332	-2.3799655937	-4.1500278429
C	6.0	13.4103243990	1.9036383126	-4.2509657227
H	1.0	5.6070689019	-2.9242750762	-4.1261677422
H	1.0	14.3084842778	2.4790064498	-4.2633571294
C	6.0	11.8775516349	-0.7063323585	-6.2523877413
C	6.0	10.4414427531	1.6565882212	-2.1713339349
C	6.0	9.5125430204	-2.1808145820	-6.2292847588
C	6.0	8.0697890397	0.2031308167	-2.1661290406
C	6.0	10.4588156263	-2.4234748750	-7.2620132006
C	6.0	8.2885568828	1.1430174717	-1.1206888083
C	6.0	11.6616989397	-1.6689130691	-7.2754711637
C	6.0	9.4969516916	1.8924920904	-1.1355399779
H	1.0	7.1374682580	-0.3486449441	-2.1921191950
H	1.0	8.5890845292	-2.7527348696	-6.2244373241
H	1.0	11.3602748084	2.2356965456	-2.1747999467
H	1.0	12.7992663030	-0.1320337971	-6.2637081753
C	6.0	12.6064215515	-1.8956600296	-8.3013540810
C	6.0	9.7317137060	2.8648569662	-0.1379410226
C	6.0	10.2394092365	-3.3856490199	-8.2741592175
C	6.0	7.3350540772	1.3835045477	-0.0876619858
C	6.0	11.1783045798	-3.5923827196	-9.2597778826
C	6.0	7.6009651050	2.3515521176	0.8641972745
C	6.0	12.3704985208	-2.8398552352	-9.2750086249
C	6.0	8.7958371531	3.0928415137	0.8431468359
H	1.0	13.1059432543	-3.0114476364	-10.0550341965

H	1.0	8.9751140563	3.8416595261	1.6085100448
H	1.0	11.0034322740	-4.3384067509	-10.0291039726
H	1.0	6.8729059961	2.5281783964	1.6506261263
H	1.0	13.5256634385	-1.3159696199	-8.3060382868
H	1.0	10.6578639648	3.4328233424	-0.1631248516
H	1.0	9.3146780199	-3.9568471241	-8.2660747239

22BP/S_0S_0

ATOM	CHARGE	X	Y	Z
C	6.0	6.5793220975	1.1827457114	0.4324573708
C	6.0	-6.5793220975	-1.1827457114	0.4324573708
C	6.0	7.0781148473	-1.5027262665	-0.4310805626
C	6.0	-7.0781148473	1.5027262665	-0.4310805626
C	6.0	5.4719116009	0.3567577410	0.0069132462
C	6.0	-5.4719116009	-0.3567577410	0.0069132462
C	6.0	7.9330011017	0.6766098625	0.4353881962
C	6.0	-7.9330011017	-0.6766098625	0.4353881962
C	6.0	5.7243183481	-0.9980960612	-0.4306311868
C	6.0	-5.7243183481	0.9980960612	-0.4306311868
C	6.0	8.1847446290	-0.6782942611	-0.0008925598
C	6.0	-8.1847446290	0.6782942611	-0.0008925598
C	6.0	6.3351207538	2.5077036369	0.8499789716
C	6.0	-6.3351207538	-2.5077036369	0.8499789716
C	6.0	7.3262889149	-2.8234842574	-0.8599060093
C	6.0	-7.3262889149	2.8234842574	-0.8599060093
C	6.0	6.1282364031	3.6472269192	1.2073750722
C	6.0	-6.1282364031	-3.6472269192	1.2073750722
C	6.0	7.5436589117	-3.9575660933	-1.2281864314
C	6.0	-7.5436589117	3.9575660933	-1.2281864314
H	1.0	5.9463102013	4.6499416274	1.5221597875
H	1.0	-5.9463102013	-4.6499416274	1.5221597875
H	1.0	7.7363008141	-4.9555684245	-1.5515108349
H	1.0	-7.7363008141	4.9555684245	-1.5515108349
C	6.0	9.4799076537	-1.1534277486	0.0019471811
C	6.0	-9.4799076537	1.1534277486	0.0019471811
C	6.0	4.6621729018	-1.7788988303	-0.8392835206
C	6.0	-4.6621729018	1.7788988303	-0.8392835206
C	6.0	8.9944104748	1.4578309237	0.8434348931
C	6.0	-8.9944104748	-1.4578309237	0.8434348931
C	6.0	4.1768923511	0.8322095423	0.0066153576
C	6.0	-4.1768923511	-0.8322095423	0.0066153576
C	6.0	10.3318679082	0.9767001357	0.8468484696
C	6.0	-10.3318679082	-0.9767001357	0.8468484696
C	6.0	3.0777416467	0.0340946243	-0.4140563025
C	6.0	-3.0777416467	-0.0340946243	-0.4140563025
C	6.0	10.5792365353	-0.3540938996	0.4176548131
C	6.0	-10.5792365353	0.3540938996	0.4176548131
C	6.0	3.3267973785	-1.2952727576	-0.8439251233

C	6.0	-3.3267973785	1.2952727576	-0.8439251233
H	1.0	3.9862881446	1.8499695706	0.3343934067
H	1.0	-3.9862881446	-1.8499695706	0.3343934067
H	1.0	8.8077558697	2.4764566785	1.1708687652
H	1.0	-8.8077558697	-2.4764566785	1.1708687652
H	1.0	4.8481767941	-2.7971750246	-1.1682534337
H	1.0	-4.8481767941	2.7971750246	-1.1682534337
H	1.0	9.6712744848	-2.1710640174	-0.3258678933
H	1.0	-9.6712744848	2.1710640174	-0.3258678933
C	6.0	11.9063571160	-0.8405691630	0.4131267784
C	6.0	-11.9063571160	0.8405691630	0.4131267784
C	6.0	2.2358876361	-2.0889097645	-1.2644916169
C	6.0	-2.2358876361	2.0889097645	-1.2644916169
C	6.0	11.4190666890	1.7809818420	1.2580009277
C	6.0	-11.4190666890	-1.7809818420	1.2580009277
C	6.0	1.7543368747	0.5240474699	-0.4141017839
C	6.0	-1.7543368747	-0.5240474699	-0.4141017839
C	6.0	12.7032901139	1.2852865560	1.2407779631
C	6.0	-12.7032901139	-1.2852865560	1.2407779631
C	6.0	0.6935627883	-0.2625090559	-0.8271440346
C	6.0	-0.6935627883	0.2625090559	-0.8271440346
C	6.0	12.9486846427	-0.0361722279	0.8151582220
C	6.0	-12.9486846427	0.0361722279	0.8151582220
C	6.0	0.9565943472	-1.5868066263	-1.2573599138
C	6.0	-0.9565943472	1.5868066263	-1.2573599138
H	1.0	13.9651583498	-0.4178635098	0.8049798946
H	1.0	-13.9651583498	0.4178635098	0.8049798946
H	1.0	0.1325594902	-2.2000689277	-1.6102536844
H	1.0	-0.1325594902	2.2000689277	-1.6102536844
H	1.0	13.5323515602	1.9123938117	1.5544334998
H	1.0	-13.5323515602	-1.9123938117	1.5544334998
H	1.0	12.0912690192	-1.8601292634	0.0852929991
H	1.0	-12.0912690192	1.8601292634	0.0852929991
H	1.0	2.4226427984	-3.1031375430	-1.6073782741
H	1.0	-2.4226427984	3.1031375430	-1.6073782741
H	1.0	11.2257397493	2.7989889227	1.5860668009
H	1.0	-11.2257397493	-2.7989889227	1.5860668009
H	1.0	1.5736346776	1.5352553731	-0.0576012129
H	1.0	-1.5736346776	-1.5352553731	-0.0576012129

22BP/^{1}(TT)

ATOM	CHARGE	X	Y	Z
C	6.0	6.5626958126	1.1739976220	0.4173391686
C	6.0	-6.5626958126	-1.1739976220	0.4173391686
C	6.0	7.0566259457	-1.4869870918	-0.4348209288
C	6.0	-7.0566259457	1.4869870918	-0.4348209288
C	6.0	5.4818732549	0.3637075069	-0.0016002493
C	6.0	-5.4818732549	-0.3637075069	-0.0016002493
C	6.0	7.8862699651	0.6745771193	0.4209173564

C	6.0	-7.8862699651	-0.6745771193	0.4209173564
C	6.0	5.7335774449	-0.9888051431	-0.4343892700
C	6.0	-5.7335774449	0.9888051431	-0.4343892700
C	6.0	8.1376282856	-0.6771828610	-0.0136700130
C	6.0	-8.1376282856	0.6771828610	-0.0136700130
C	6.0	6.3150400921	2.5150509629	0.8411783272
C	6.0	-6.3150400921	-2.5150509629	0.8411783272
C	6.0	7.3043719368	-2.8271105920	-0.8620859462
C	6.0	-7.3043719368	2.8271105920	-0.8620859462
C	6.0	6.1068878907	3.6505875272	1.1972179142
C	6.0	-6.1068878907	-3.6505875272	1.1972179142
C	6.0	7.5114654567	-3.9616066821	-1.2219972492
C	6.0	-7.5114654567	3.9616066821	-1.2219972492
H	1.0	5.9230003297	4.6532686455	1.5113083496
H	1.0	-5.9230003297	-4.6532686455	1.5113083496
H	1.0	7.6941439511	-4.9637433318	-1.5385848193
H	1.0	-7.6941439511	4.9637433318	-1.5385848193
C	6.0	9.4658129290	-1.1568891869	-0.0064200226
C	6.0	-9.4658129290	1.1568891869	-0.0064200226
C	6.0	4.6398701740	-1.7844800604	-0.8440209968
C	6.0	-4.6398701740	1.7844800604	-0.8440209968
C	6.0	8.9777130483	1.4672780766	0.8390880252
C	6.0	-8.9777130483	-1.4672780766	0.8390880252
C	6.0	4.1531656690	0.8435162749	-0.0072437790
C	6.0	-4.1531656690	-0.8435162749	-0.0072437790
C	6.0	10.2729988165	0.9845100879	0.8384414089
C	6.0	-10.2729988165	-0.9845100879	0.8384414089
C	6.0	3.0932362078	0.0519229906	-0.4097534869
C	6.0	-3.0932362078	-0.0519229906	-0.4097534869
C	6.0	10.5247516489	-0.3676606755	0.4021934568
C	6.0	-10.5247516489	0.3676606755	0.4021934568
C	6.0	3.3458953226	-1.3023251660	-0.8353764248
C	6.0	-3.3458953226	1.3023251660	-0.8353764248
H	1.0	3.9676276327	1.8630830945	0.3167176813
H	1.0	-3.9676276327	-1.8630830945	0.3167176813
H	1.0	8.7870064607	2.4844178872	1.1675972485
H	1.0	-8.7870064607	-2.4844178872	1.1675972485
H	1.0	4.8291653325	-2.8028963644	-1.1693672841
H	1.0	-4.8291653325	2.8028963644	-1.1693672841
H	1.0	9.6528260198	-2.1752306874	-0.3335738879
H	1.0	-9.6528260198	2.1752306874	-0.3335738879
C	6.0	11.8791504782	-0.8496469145	0.4057142187
C	6.0	-11.8791504782	0.8496469145	0.4057142187
C	6.0	2.2249551000	-2.1058536804	-1.2390243425
C	6.0	-2.2249551000	2.1058536804	-1.2390243425
C	6.0	11.3872694672	1.7908283610	1.2567633319
C	6.0	-11.3872694672	-1.7908283610	1.2567633319
C	6.0	1.7420734238	0.5359938396	-0.4143246462
C	6.0	-1.7420734238	-0.5359938396	-0.4143246462
C	6.0	12.6513817633	1.2937100500	1.2404697770
C	6.0	-12.6513817633	-1.2937100500	1.2404697770

C	6.0	0.6967355064	-0.2532288545	-0.8004034480
C	6.0	-0.6967355064	0.2532288545	-0.8004034480
C	6.0	12.9015432986	-0.0504893607	0.8075764249
C	6.0	-12.9015432986	0.0504893607	0.8075764249
C	6.0	0.9639286688	-1.6077414026	-1.2187692338
C	6.0	-0.9639286688	1.6077414026	-1.2187692338
H	1.0	13.9211985027	-0.4239485501	0.8040512254
H	1.0	-13.9211985027	0.4239485501	0.8040512254
H	1.0	0.1318718951	-2.2218536415	-1.5501862410
H	1.0	-0.1318718951	2.2218536415	-1.5501862410
H	1.0	13.4862888093	1.9125236159	1.5553896457
H	1.0	-13.4862888093	-1.9125236159	1.5553896457
H	1.0	12.0648166680	-1.8688295156	0.0775914957
H	1.0	-12.0648166680	1.8688295156	0.0775914957
H	1.0	2.4107869727	-3.1233048192	-1.5723461618
H	1.0	-2.4107869727	3.1233048192	-1.5723461618
H	1.0	11.1936031830	2.8088477713	1.5840764038
H	1.0	-11.1936031830	-2.8088477713	1.5840764038
H	1.0	1.5666134323	1.5534555938	-0.0737030292
H	1.0	-1.5666134323	-1.5534555938	-0.0737030292

Appendix B. Normal mode coordinate and frequency

Normal mode analysis were performed subsequent to the optimization of geometry. The frequencies (cm^{-1}) for the two electronic states, S_0S_0 and ^{1}(TT), of each dimer are shown. Imaginary frequencies are shown in parentheses. The normal mode coordinates are not listed here but we are happy to provide them to anyone interested.

	S_0S_0			^{1}(TT)		
	11BP	12BP	22BP	11BP	12BP	22BP
1	3.0	4.2	2.3	3.8	4.9	3.5
2	1.8	2.4	0.9	2.3	2.2	2.3
3	0.2	1.7	0.4	0.5	2.0	1.1
4	0.2	0.6	0.3	0.2	1.0	0.3
5	0.1	0.3	0.1	0.2	0.9	0.2
6	1.9	1.3	1.5	0.3	0.7	0.1
7	(8.2)	12.2	6.6	(8.3)	14.1	5.7
8	6.3	18.2	12.5	6.3	18.4	11.2
9	14.5	21.9	12.6	14.5	20.6	13.1
10	25.5	29.4	27.2	20.0	26.1	22.8
11	26.9	34.8	36.5	21.2	29.2	29.5
12	52.2	59.9	58.4	50.0	56.2	53.9
13	54.8	67.8	70.1	52.5	63.6	64.5
14	72.2	75.3	70.6	64.6	70.5	65.9
15	72.6	78.1	73.8	65.0	71.5	67.3
16	73.3	82.3	78.4	66.0	72.3	68.4
17	74.4	82.7	79.5	66.4	79.8	76.0

18	98.0	98.2	92.6	97.7	93.3	90.0
19	100.8	107.2	101.3	99.9	106.8	94.0
20	102.0	109.8	102.7	101.4	108.4	101.3
21	122.5	121.9	121.1	121.2	120.2	120.5
22	126.7	127.5	124.6	125.6	128.3	124.2
23	129.4	129.4	128.2	127.6	128.5	127.4
24	135.5	134.3	132.5	133.8	134.1	131.2
25	136.5	137.4	138.2	135.2	137.2	137.0
26	158.7	154.9	148.5	155.4	153.1	147.3
27	174.5	181.4	171.5	171.2	177.8	168.1
28	195.0	199.3	198.0	187.0	191.3	194.1
29	196.1	202.9	201.0	188.3	200.9	195.9
30	211.1	206.5	206.9	208.9	204.2	200.7
31	218.8	226.9	224.4	218.1	226.8	223.5
32	246.9	231.5	227.6	251.7	230.6	230.0
33	247.8	250.2	253.0	252.4	254.8	257.7
34	258.6	259.5	258.5	255.4	257.8	258.3
35	259.3	261.3	265.2	255.6	262.2	259.6
36	262.7	280.1	280.1	262.8	287.1	288.6
37	282.3	291.9	297.6	288.2	296.3	304.9
38	288.2	309.0	315.0	299.8	315.4	320.4
39	321.3	324.0	320.9	321.9	323.4	320.6
40	331.6	331.0	333.3	322.8	325.8	326.9
41	336.3	340.2	343.6	328.5	331.5	334.5
42	338.5	350.6	349.1	334.5	344.1	342.9
43	356.4	357.1	356.9	354.3	356.1	354.6
44	358.0	361.0	360.2	357.3	361.9	361.1
45	388.8	392.8	399.8	384.9	387.1	386.9
46	392.6	398.5	400.1	385.4	387.6	389.7
47	400.0	399.8	401.3	391.6	394.7	402.5
48	401.5	404.4	404.4	396.3	404.2	404.2
49	416.5	416.1	420.2	412.4	414.3	415.9
50	428.4	429.1	439.6	420.7	422.2	420.8
51	440.3	441.4	440.1	425.1	427.7	427.1
52	441.1	446.7	441.5	430.2	431.1	436.3
53	447.5	454.6	449.0	439.2	439.9	440.8
54	451.0	464.8	469.4	440.7	447.4	442.6
55	476.8	479.8	477.7	450.3	456.6	451.0
56	476.9	483.1	477.8	455.4	470.4	471.6
57	485.4	484.0	480.2	483.9	486.4	484.7
58	485.7	489.7	480.6	483.9	488.8	484.8
59	524.3	490.4	487.7	521.9	490.3	486.3
60	525.2	528.4	487.8	522.6	525.2	487.5
61	527.1	528.5	525.0	525.2	525.5	520.1
62	527.2	530.9	527.3	525.3	529.6	527.5
63	529.3	531.5	527.4	544.5	534.2	531.0
64	529.9	535.0	535.0	546.1	549.3	533.8
65	567.3	566.2	567.4	559.7	566.9	563.7
66	568.3	572.7	569.9	560.0	569.3	564.1
67	583.7	580.9	574.6	567.1	569.7	566.1
68	586.8	585.6	581.4	567.6	574.0	566.3

69	587.0	588.6	588.3	568.3	575.2	570.4
70	587.4	598.2	602.5	569.4	577.6	571.5
71	607.0	607.0	608.8	582.4	579.2	576.6
72	607.0	614.5	612.9	582.8	584.6	577.8
73	608.9	614.8	612.9	598.2	601.2	599.5
74	610.6	618.6	613.0	599.1	605.2	604.2
75	616.3	621.2	613.2	607.2	609.0	612.0
76	616.5	623.6	615.4	608.9	613.3	613.3
77	623.2	626.3	622.4	620.7	619.2	620.4
78	624.1	628.0	628.4	623.3	627.4	626.9
79	625.6	631.1	633.6	625.8	628.6	633.0
80	634.7	637.8	636.1	635.0	637.9	635.9
81	638.8	640.2	650.3	637.7	642.5	642.6
82	646.6	655.9	652.5	640.2	643.9	643.9
83	651.8	661.5	664.4	644.8	647.9	650.9
84	670.6	672.3	676.9	650.2	656.2	652.8
85	670.7	676.8	677.0	654.1	665.5	668.5
86	672.4	679.3	677.1	665.0	668.8	671.6
87	672.5	684.6	677.1	665.1	671.6	671.8
88	704.1	703.4	691.2	667.4	672.4	671.8
89	704.3	705.7	703.9	667.5	679.9	671.9
90	709.9	708.2	705.1	695.1	691.5	687.9
91	710.2	712.9	709.1	696.3	698.8	694.8
92	717.5	716.2	714.9	709.8	709.9	707.3
93	724.0	722.2	719.6	710.7	713.8	709.3
94	725.2	727.0	723.3	719.9	715.9	710.8
95	764.2	768.0	767.8	753.2	753.1	751.8
96	764.4	773.2	767.8	753.3	756.2	752.2
97	769.0	773.8	771.9	770.0	773.9	771.1
98	771.7	775.5	773.6	770.1	774.1	772.9
99	776.3	776.5	775.3	771.7	774.5	773.0
100	776.5	778.4	776.1	772.9	775.9	773.0
101	777.6	780.2	777.5	773.2	777.1	773.3
102	778.5	781.5	777.7	773.3	780.4	773.6
103	779.5	783.5	784.6	781.0	786.6	785.8
104	791.1	797.6	801.5	781.2	793.7	802.9
105	802.9	803.1	801.6	805.5	806.0	806.3
106	803.0	806.0	803.2	813.4	815.7	814.8
107	812.7	816.0	815.6	816.9	823.7	829.8
108	816.3	821.2	821.2	819.7	832.9	832.0
109	829.3	841.6	843.4	839.6	853.0	852.4
110	864.7	863.4	846.5	876.1	872.3	853.1
111	864.7	867.7	865.8	876.1	879.6	876.4
112	871.4	872.9	865.9	880.8	883.7	876.4
113	915.6	898.5	889.8	909.7	900.1	891.2
114	915.8	917.9	894.8	910.3	914.1	895.1
115	917.4	922.4	915.2	912.5	916.8	910.8
116	918.0	924.0	915.2	912.6	919.1	910.9
117	927.3	929.4	925.4	920.9	923.7	919.5
118	928.4	929.7	927.7	922.2	924.1	921.5
119	930.5	935.1	928.1	924.0	931.6	922.1

120	933.6	936.2	932.4	929.3	931.7	928.9
121	933.9	939.8	933.1	929.3	935.3	929.2
122	936.6	941.3	940.2	933.1	939.1	938.0
123	939.9	946.4	943.1	943.6	945.6	940.5
124	941.9	952.7	947.7	944.8	953.3	945.3
125	956.4	955.8	952.6	955.4	955.6	952.2
126	987.9	987.5	982.0	976.7	980.0	978.2
127	989.5	992.2	991.3	976.7	983.8	978.2
128	989.5	996.7	991.3	996.4	997.0	989.0
129	997.5	999.3	994.1	996.4	999.7	992.4
130	997.9	1000.0	1000.0	1000.5	1005.3	992.5
131	1002.9	1003.3	1002.4	1008.9	1011.8	1011.9
132	1003.1	1007.3	1005.9	1008.9	1016.1	1011.9
133	1003.6	1009.1	1006.9	1017.7	1019.8	1015.2
134	1013.3	1015.8	1008.6	1017.8	1021.2	1020.1
135	1013.3	1020.4	1016.4	1020.8	1022.2	1020.5
136	1034.5	1027.4	1016.4	1067.8	1044.5	1024.3
137	1034.5	1036.8	1034.7	1068.1	1070.8	1067.8
138	1066.6	1037.3	1034.8	1077.5	1072.8	1067.9
139	1072.2	1076.6	1050.4	1092.9	1095.0	1081.2
140	1094.1	1093.5	1092.5	1095.8	1096.0	1092.8
141	1094.7	1097.1	1092.5	1104.5	1109.9	1092.9
142	1105.9	1154.4	1169.2	1120.5	1158.2	1171.8
143	1170.7	1173.2	1170.2	1170.8	1171.4	1171.8
144	1173.2	1177.7	1182.1	1170.8	1176.5	1180.6
145	1181.2	1181.8	1182.2	1174.8	1182.5	1181.5
146	1181.4	1185.5	1203.6	1183.8	1191.3	1192.3
147	1191.9	1198.4	1205.0	1188.5	1192.2	1192.7
148	1210.1	1214.6	1213.7	1208.9	1217.7	1220.5
149	1214.5	1216.4	1215.2	1223.0	1225.2	1220.9
150	1217.8	1223.1	1240.8	1235.7	1241.1	1239.3
151	1222.8	1246.1	1240.8	1238.2	1248.7	1241.6
152	1243.7	1248.5	1243.1	1244.3	1250.9	1245.5
153	1244.8	1252.6	1244.0	1246.7	1252.8	1245.8
154	1248.4	1253.9	1247.2	1250.4	1256.9	1247.6
155	1248.5	1261.4	1255.4	1250.4	1261.2	1255.6
156	1269.8	1269.3	1265.0	1269.8	1276.4	1277.7
157	1271.7	1274.0	1269.0	1276.7	1285.6	1278.2
158	1283.6	1287.3	1282.0	1287.4	1289.8	1284.5
159	1306.1	1318.3	1313.4	1290.6	1292.6	1288.0
160	1326.8	1326.5	1318.6	1291.3	1294.7	1292.9
161	1327.0	1330.5	1325.5	1291.7	1296.7	1295.8
162	1328.8	1333.4	1327.1	1307.4	1312.2	1304.2
163	1337.3	1340.5	1333.0	1310.1	1317.5	1314.4
164	1343.7	1348.0	1343.1	1314.8	1319.0	1316.2
165	1362.5	1362.5	1356.2	1314.8	1321.9	1316.5
166	1363.6	1372.0	1369.7	1329.3	1331.9	1325.3
167	1387.2	1374.5	1373.5	1332.6	1339.5	1336.4
168	1401.5	1396.7	1384.7	1345.3	1347.1	1346.8
169	1411.5	1411.6	1408.3	1378.2	1377.1	1373.9
170	1412.4	1414.9	1412.7	1383.6	1388.9	1386.9

171	1422.6	1420.8	1417.8	1397.0	1398.8	1396.5
172	1429.5	1430.4	1422.6	1397.2	1402.6	1396.8
173	1449.0	1447.0	1447.2	1406.0	1414.6	1414.1
174	1449.3	1451.9	1447.3	1417.6	1420.0	1418.3
175	1453.1	1453.7	1450.5	1418.8	1423.2	1419.7
176	1458.5	1458.5	1451.0	1420.2	1428.9	1432.0
177	1460.4	1464.3	1459.3	1453.3	1455.1	1451.5
178	1461.9	1466.4	1461.3	1454.6	1461.5	1462.5
179	1477.9	1481.3	1488.3	1472.7	1471.8	1466.4
180	1481.0	1494.3	1493.9	1473.2	1477.3	1477.2
181	1495.4	1497.0	1497.8	1499.8	1483.6	1480.8
182	1496.2	1499.3	1498.3	1502.4	1503.2	1492.2
183	1502.7	1506.7	1509.5	1503.0	1508.0	1501.8
184	1506.4	1518.8	1517.0	1503.6	1508.7	1502.9
185	1516.5	1519.9	1520.0	1503.8	1510.0	1503.3
186	1516.8	1527.2	1536.9	1524.2	1516.3	1504.2
187	1557.8	1559.8	1558.5	1527.1	1533.9	1526.9
188	1558.2	1562.1	1562.0	1528.9	1537.4	1532.0
189	1595.4	1597.6	1591.9	1548.0	1555.0	1553.9
190	1596.4	1599.5	1598.1	1550.5	1562.2	1565.2
191	1611.3	1611.8	1608.5	1574.9	1578.8	1575.1
192	1611.4	1614.5	1610.9	1576.0	1581.0	1582.6
193	1630.3	1623.9	1619.5	1618.7	1623.2	1614.6
194	1630.7	1631.2	1628.5	1620.1	1624.3	1621.2
195	1633.1	1632.8	1631.4	1651.5	1641.9	1638.6
196	1651.7	1643.2	1631.8	1653.5	1655.7	1647.4
197	1677.9	1680.5	1676.2	1656.1	1656.3	1654.9
198	1679.2	1683.1	1679.0	1657.3	1660.8	1657.2
199	1686.2	1689.2	1685.4	1660.4	1661.8	1658.1
200	1689.5	1692.7	1692.1	1668.6	1666.9	1659.1
201	1720.5	1725.2	1730.2	1681.1	1687.2	1699.9
202	1729.0	1735.5	1732.6	1689.5	1703.9	1700.5
203	1736.0	1738.2	1736.7	1700.7	1705.1	1700.5
204	1736.3	1740.8	1736.9	1700.7	1706.0	1703.6
205	2242.6	2243.3	2242.6	2188.5	2188.2	2188.8
206	2242.7	2243.3	2242.7	2188.6	2188.7	2188.9
207	2245.3	2245.2	2244.4	2191.2	2190.5	2191.1
208	2245.3	2245.2	2244.4	2191.2	2191.1	2191.1
209	3203.5	3204.3	3203.8	3203.0	3204.0	3203.5
210	3203.5	3204.7	3203.8	3203.0	3204.4	3203.5
211	3206.0	3208.0	3205.6	3205.5	3207.2	3204.8
212	3206.0	3208.3	3206.0	3205.5	3207.3	3205.4
213	3208.3	3209.2	3207.9	3207.6	3208.5	3206.7
214	3208.3	3209.7	3208.4	3207.6	3208.8	3207.7
215	3216.2	3212.1	3208.5	3216.5	3209.7	3207.9
216	3216.6	3217.3	3208.8	3216.8	3216.9	3207.9
217	3222.4	3223.2	3222.7	3220.3	3221.0	3220.8
218	3222.4	3223.5	3222.7	3220.3	3221.2	3220.8
219	3225.0	3224.3	3224.9	3220.8	3221.7	3221.1
220	3225.1	3225.4	3224.9	3220.8	3222.2	3221.2
221	3225.3	3226.0	3225.2	3221.7	3222.2	3222.1

222	3225.4	3226.6	3225.2	3221.7	3222.6	3222.1
223	3227.2	3227.7	3226.5	3222.9	3222.7	3222.9
224	3227.2	3227.8	3226.5	3223.1	3223.9	3223.0
225	3232.7	3228.6	3227.0	3232.9	3224.0	3223.0
226	3233.0	3229.1	3227.1	3233.2	3226.6	3223.1
227	3234.5	3233.9	3229.0	3234.8	3233.9	3226.2
228	3234.6	3235.4	3229.5	3234.8	3235.5	3226.7
229	3246.2	3235.6	3234.8	3244.1	3235.9	3235.3
230	3246.5	3252.1	3234.8	3244.7	3252.6	3235.3
231	3502.9	3500.8	3502.4	3500.8	3499.3	3500.4
232	3503.0	3500.9	3502.4	3500.9	3500.8	3500.6
233	3503.5	3501.4	3502.8	3501.8	3501.1	3500.6
234	3503.6	3503.4	3502.8	3501.9	3502.0	3500.8

Appendix C. NACME calculation

NACME was evaluated at S_0S_0 and ^{1}(TT) state optimized geometries using the NACME subroutine in GAMESS-US[4,5]. Molecular orbitals and the two electronic states were obtained at CASSCF(4o4e)-SA2 level, which were subsequently fed into the NACME subroutine. The electronic configurations of 4o4e active space and NACME are reported.

Electronic state configuration of 11BP at S_0S_0 state geometry

1st state

Alpha	Beta	Coefficient
1100	1100	0.8928579
1001	1001	-0.1445765
1001	0110	0.1425141
0110	1001	0.1425141
0110	0110	-0.1404382
1010	1010	-0.1318827
1010	0101	0.1301015
0101	1010	0.1301015
0101	0101	-0.1282238
1010	1100	-0.1095977
1100	1010	-0.1095977
0101	1100	0.0966196
1100	0101	0.0966196
0011	0011	0.0831876

2nd state

Alpha	Beta	Coefficient
1010	1010	0.4436813
1001	1001	-0.4408417
0110	0110	-0.4249361
0101	0101	0.4219003
0011	1100	0.2883815
1100	0011	0.2883815
0110	1001	-0.1442898
1001	0110	-0.1442898
1010	0101	0.1440917
0101	1010	0.1440917

NACME between the 1st and 2nd states of 11BP at S_0S_0 state geometry

ATOM d/dX d/dY d/dZ

C	0.0000551	-0.0001069	0.0000059
C	-0.0000551	0.0001069	0.0000059
C	-0.0000858	-0.0001018	0.0001123
C	0.0000858	0.0001017	0.0001123
C	0.0000919	-0.0001817	-0.0000019
C	-0.0000919	0.0001817	-0.0000019
C	0.0003726	-0.0006146	-0.0000360
C	-0.0003726	0.0006146	-0.0000360
C	-0.0000120	-0.0000329	0.0001093
C	0.0000120	0.0000329	0.0001093
C	0.0001041	-0.0001990	-0.0000079
C	-0.0001042	0.0001990	-0.0000079
C	0.0001293	-0.0000738	-0.0000700
C	-0.0001293	0.0000738	-0.0000700
C	-0.0001208	0.0000537	0.0000752
C	0.0001208	-0.0000537	0.0000752
C	-0.0002350	-0.0003199	0.0002726
C	0.0002350	0.0003199	0.0002726
C	0.0002497	-0.0003520	-0.0001489
C	-0.0002497	0.0003520	-0.0001489
C	0.0000034	-0.0000147	0.0000030
C	-0.0000034	0.0000147	0.0000030
C	0.0000864	-0.0000609	-0.0000457
C	-0.0000864	0.0000609	-0.0000457
C	-0.0000058	-0.0000063	0.0000064
C	0.0000058	0.0000063	0.0000064
C	0.0001201	0.0004287	-0.0002882
C	-0.0001201	-0.0004287	-0.0002882
C	0.0000463	0.0000173	-0.0000425
C	-0.0000463	-0.0000173	-0.0000425
C	-0.0000366	0.0000375	0.0000088
C	0.0000366	-0.0000375	0.0000088
C	-0.0002501	0.0003987	0.0000307
C	0.0002501	-0.0003987	0.0000307
C	-0.0000137	0.0009138	-0.0001578
C	0.0000137	-0.0009138	-0.0001578
C	0.0000212	0.0004441	-0.0001781
C	-0.0000212	-0.0004441	-0.0001781
C	-0.0002481	0.0000879	0.0001546
C	0.0002481	-0.0000879	0.0001546
C	0.0000904	-0.0002053	-0.0000753
C	-0.0000904	0.0002053	-0.0000753
C	0.0000041	-0.0000347	0.0000097
C	-0.0000041	0.0000347	0.0000097
C	-0.0000154	0.0000072	0.0000094
C	0.0000154	-0.0000072	0.0000094
C	0.0001105	0.0004561	-0.0000438
C	-0.0001105	-0.0004561	-0.0000438
C	-0.0003575	-0.0000378	0.0002681
C	0.0003575	0.0000378	0.0002681
C	0.0001331	-0.0002700	0.0000020

C	-0.0001331	0.0002700	0.0000020
H	-0.0000071	0.0000145	-0.0000017
H	0.0000071	-0.0000145	-0.0000017
H	-0.0000125	0.0000286	-0.0000027
H	0.0000125	-0.0000286	-0.0000027
H	0.0000023	0.0000010	-0.0000023
H	-0.0000023	-0.0000010	-0.0000023
H	0.0000044	-0.0000014	-0.0000029
H	-0.0000044	0.0000014	-0.0000029
H	-0.0000010	-0.0000023	0.0000016
H	0.0000010	0.0000023	0.0000016
H	-0.0000003	0.0000047	0.0000047
H	0.0000003	-0.0000047	0.0000047
H	-0.0000027	-0.0000012	0.0000025
H	0.0000027	0.0000012	0.0000025
H	0.0000069	0.0000046	-0.0000085
H	-0.0000069	-0.0000046	-0.0000085
H	0.0000012	0.0000092	-0.0000048
H	-0.0000012	-0.0000092	-0.0000048
H	-0.0000104	0.0000078	0.0000046
H	0.0000104	-0.0000078	0.0000046
H	-0.0000019	0.0000220	0.0000180
H	0.0000019	-0.0000220	0.0000180
H	0.0000195	0.0000375	0.0000135
H	-0.0000195	-0.0000375	0.0000135
H	0.0000124	0.0000056	0.0000050
H	-0.0000124	-0.0000056	0.0000050

Electronic state configuration of 11BP at ^{1}(TT) state geometry

1st state

Alpha	Beta	Coefficient
1100	1100	0.7813046
1001	1001	-0.1959759
1001	0110	-0.1933082
0110	1001	-0.1933082
0110	0110	-0.1904170
1010	1010	-0.1689186
1010	0101	-0.1665979
0101	1010	-0.1665979
0011	0011	0.1656073
0101	0101	-0.1641787
1010	1100	0.1523065
1100	1010	0.1523065
0101	1100	0.1349886
1100	0101	0.1349886

2nd state

Alpha	Beta	Coefficient
1010	1010	0.4420759
1001	1001	-0.4396781
0110	0110	-0.4263174
0101	0101	0.4233769
0011	1100	-0.2883512
1100	0011	-0.2883512
1001	0110	0.1442419
0110	1001	0.1442419
1010	0101	-0.1441093
0101	1010	-0.1441093

0011	0101	-0.0678377
0101	0011	-0.0678377
0011	1010	-0.0643004
1010	0011	-0.0643004

NACME between the 1st and 2nd states of 11BP at ^{1}(TT) state geometry

ATOM	d/dX	d/dY	d/dZ
C	0.0000151	-0.0000095	0.0000111
C	-0.0000151	0.0000095	0.0000111
C	-0.0000229	-0.0000686	0.0000258
C	0.0000229	0.0000686	0.0000258
C	0.0000080	0.0000402	-0.0000110
C	-0.0000080	-0.0000402	-0.0000110
C	0.0002763	-0.0007679	0.0000270
C	-0.0002763	0.0007679	0.0000270
C	-0.0003567	-0.0000617	0.0005287
C	0.0003567	0.0000617	0.0005287
C	0.0000957	-0.0001706	-0.0000470
C	-0.0000957	0.0001706	-0.0000470
C	0.0002682	0.0000396	-0.0002175
C	-0.0002682	-0.0000396	-0.0002174
C	-0.0002847	0.0001146	0.0001807
C	0.0002847	-0.0001146	0.0001807
C	-0.0003557	-0.0001753	0.0002780
C	0.0003557	0.0001753	0.0002780
C	0.0002996	-0.0004534	-0.0003000
C	-0.0002996	0.0004534	-0.0003000
C	-0.0000807	-0.0002455	0.0001535
C	0.0000807	0.0002455	0.0001535
C	0.0002218	0.0000887	-0.0002097
C	-0.0002218	-0.0000887	-0.0002097
C	0.0000863	0.0000518	-0.0000889
C	-0.0000863	-0.0000518	-0.0000889
C	-0.0000506	0.0004835	-0.0002073
C	0.0000506	-0.0004835	-0.0002073
C	0.0001182	0.0000380	-0.0001055
C	-0.0001182	-0.0000380	-0.0001055
C	-0.0001978	-0.0001183	0.0001806
C	0.0001978	0.0001183	0.0001806
C	-0.0000068	0.0002725	-0.0001438
C	0.0000068	-0.0002725	-0.0001438
C	0.0005246	0.0010412	-0.0001959
C	-0.0005246	-0.0010412	-0.0001959
C	0.0002775	0.0003604	-0.0003269
C	-0.0002775	-0.0003604	-0.0003269
C	-0.0003449	0.0000050	0.0002700
C	0.0003449	-0.0000050	0.0002700

C	-0.0000259	-0.0001175	-0.0001373
C	0.0000259	0.0001175	-0.0001373
C	0.0000094	-0.0001555	0.0000503
C	-0.0000094	0.0001555	0.0000503
C	-0.0001100	0.0001000	0.0000494
C	0.0001100	-0.0001000	0.0000494
C	0.0002560	0.0004487	-0.0001816
C	-0.0002560	-0.0004487	-0.0001816
C	-0.0002810	-0.0003780	0.0003314
C	0.0002810	0.0003780	0.0003314
C	0.0001044	-0.0001732	0.0000084
C	-0.0001044	0.0001732	0.0000084
H	-0.0000032	0.0000033	-0.0000025
H	0.0000032	-0.0000033	-0.0000025
H	-0.0000068	0.0000255	-0.0000008
H	0.0000068	-0.0000255	-0.0000008
H	-0.0000013	0.0000036	-0.0000006
H	0.0000013	-0.0000036	-0.0000006
H	0.0000017	-0.0000022	-0.0000005
H	-0.0000017	0.0000022	-0.0000005
H	-0.0000014	0.0000001	0.0000011
H	0.0000014	-0.0000001	0.0000011
H	0.0000127	-0.0000020	0.0000069
H	-0.0000127	0.0000020	0.0000069
H	0.0000001	-0.0000041	0.0000015
H	-0.0000001	0.0000041	0.0000015
H	0.0000262	0.0000206	0.0000105
H	-0.0000262	-0.0000206	0.0000105
H	0.0000008	0.0000011	-0.0000022
H	-0.0000008	-0.0000011	-0.0000022
H	-0.0000046	0.0000046	0.0000044
H	0.0000046	-0.0000046	0.0000044
H	0.0000234	0.0000161	0.0000403
H	-0.0000234	-0.0000161	0.0000403
H	0.0000306	0.0000266	0.0000032
H	-0.0000306	-0.0000266	0.0000032
H	-0.0000056	0.0000068	0.0000165
H	0.0000056	-0.0000068	0.0000165

Electronic state configuration of 12BP at S_0S_0 state geometry

1st state

Alpha	Beta	Coefficient
1100	1100	0.9106908
1010	1010	-0.1434130
0110	0110	-0.1416441
0101	0101	-0.1406021
1001	1001	-0.1398786

2nd state

Alpha	Beta	Coefficient
1010	1010	0.3831722
0110	0110	-0.3805971
1001	1001	-0.3738209
0101	0101	0.3720515
1100	0011	0.2878450

1001	0110	0.1243257
0110	1001	0.1243257
1010	0101	0.1230672
0101	1010	0.1230672
0011	0011	0.0878062
1001	1010	0.0690028
1010	1001	0.0690028
0110	0101	-0.0684860
0101	0110	-0.0684860

0011	1100	0.2878450
0110	1010	-0.2136310
1010	0110	-0.2136310
0101	1001	0.2085949
1001	0101	0.2085949
0110	1001	-0.1455843
1001	0110	-0.1455843
0101	1010	0.1422607
1010	0101	0.1422607

NACME between the 1st and 2nd states of 12BP at S_0S_0 state geometry

ATOM	d/dX	d/dY	d/dZ
C	0.0012806	-0.0000976	0.0000187
C	0.0001728	-0.0004959	0.0000321
C	-0.0002400	0.0000160	-0.0000156
C	-0.0011782	-0.0011238	0.0000304
C	-0.0002999	-0.0002253	-0.0000093
C	-0.0001995	0.0003175	0.0000074
C	0.0000477	0.0003825	-0.0000132
C	0.0000100	0.0003032	-0.0000080
C	-0.0000055	0.0002251	-0.0000026
C	0.0000108	0.0002734	-0.0000029
H	0.0000010	-0.0000320	0.0000009
H	-0.0000025	-0.0000309	0.0000003
C	-0.0006907	0.0007467	-0.0001447
C	0.0002421	0.0001994	-0.0000018
C	0.0008092	0.0003824	-0.0000217
C	0.0001962	0.0001610	-0.0000023
C	-0.0004043	-0.0008899	-0.0000420
C	-0.0000777	0.0000974	-0.0000022
C	0.0011217	-0.0000903	0.0000901
C	-0.0002840	-0.0002134	0.0000046
H	0.0000077	-0.0000199	0.0000006
H	-0.0000114	-0.0000152	0.0000143
H	-0.0000114	-0.0000185	-0.0000004
H	0.0000096	-0.0000623	-0.0000083
C	-0.0012080	0.0006151	0.0005803
C	0.0000456	-0.0000066	-0.0000007
C	0.0000178	0.0003759	-0.0001049
C	0.0001690	0.0000118	0.0000024
C	-0.0003366	-0.0000560	-0.0002829
C	-0.0000544	0.0001230	-0.0000031
C	0.0019368	-0.0003345	0.0001920
C	-0.0000567	-0.0000865	0.0000000
H	-0.0000073	0.0000033	0.0000002
H	-0.0000112	0.0000233	-0.0000066

H	0.0000048	0.0000049	0.0000001
H	0.0000158	-0.0000192	-0.0000088
H	-0.0000066	0.0000040	-0.0000003
H	-0.0000150	-0.0000006	0.0000617
H	0.0000054	-0.0000033	0.0000002
C	-0.0000861	0.0005625	0.0007390
C	-0.0004571	0.0001085	0.0005379
C	-0.0004722	-0.0008508	-0.0007398
C	0.0000828	-0.0000668	-0.0001625
C	0.0008379	0.0000636	-0.0004708
C	-0.0000317	-0.0001606	-0.0001683
C	0.0000290	0.0000193	0.0000299
C	0.0000064	0.0000529	-0.0000028
C	0.0000620	0.0000728	-0.0000714
C	0.0000718	0.0000434	0.0000026
H	0.0000004	-0.0000386	0.0000207
H	-0.0000045	-0.0000042	-0.0000005
C	0.0000034	0.0001078	0.0001349
C	0.0002006	0.0000206	-0.0000079
C	-0.0000179	0.0000933	0.0001371
C	0.0001835	0.0001100	0.0004472
C	0.0001210	0.0000034	-0.0001025
C	-0.0009311	-0.0013214	-0.0001786
C	-0.0000657	-0.0001506	-0.0001393
C	0.0008691	0.0014326	0.0005414
H	0.0000166	0.0000394	-0.0000309
H	-0.0000023	-0.0000097	0.0000067
H	-0.0000238	-0.0000315	0.0000249
H	-0.0000027	-0.0000022	-0.0000043
C	-0.0000287	0.0000300	0.0000627
C	0.0003951	-0.0008991	-0.0014414
C	-0.0000239	0.0000589	0.0000886
C	-0.0009592	-0.0009725	-0.0004623
C	0.0000962	0.0000270	-0.0000404
C	0.0006851	0.0014928	0.0003715
C	-0.0000588	-0.0000680	-0.0000370
C	-0.0016250	-0.0001819	0.0005209
H	0.0000016	-0.0000013	-0.0000029
H	0.0000142	-0.0000861	0.0000330
H	0.0000013	0.0000008	0.0000000
H	0.0000360	-0.0000415	0.0000335
H	0.0000035	0.0000010	-0.0000018
H	0.0000432	0.0000002	-0.0000043
H	-0.0000034	-0.0000014	0.0000010

Electronic state configuration of 12BP at ^{1}(TT) state geometry

1st state

Alpha	Beta	Coefficient

2nd state

Alpha	Beta	Coefficient

1100	1100	0.7964018
1010	1010	-0.2678294
0101	0101	-0.2595023
0011	0011	0.1706522
0110	1010	-0.1557937
1010	0110	-0.1557937
0101	1001	0.1515593
1001	0101	0.1515593
0101	1100	0.1342408
1100	0101	0.1342408
0110	0110	-0.1060857
1001	1001	-0.1039482
1001	1100	-0.0777939
1100	1001	-0.0777939
0011	1010	-0.0634450
1010	0011	-0.0634450
1001	0110	0.0580375
0110	1001	0.0580375
1010	0101	0.0571553
0101	1010	0.0571553

1001	1010	0.3578882
1010	1001	0.3578882
0101	0110	-0.3555097
0110	0101	-0.3555097
1001	0110	-0.3296293
0110	1001	-0.3296293
1100	0011	0.2877208
0011	1100	0.2877208
1010	1010	0.1441222
0110	0110	-0.1430314
1001	1001	-0.1383662
0101	0101	0.1375202
1010	0110	-0.0752193
0110	1010	-0.0752193
1001	0101	0.0722311
0101	1001	0.0722311

NACME between the 1st and 2nd states of 12BP at ^{1}(TT) state geometry

ATOM	d/dX	d/dY	d/dZ
C	0.0018178	0.0002325	0.0000127
C	0.0001430	-0.0002555	0.0000423
C	-0.0005219	0.0000079	-0.0000278
C	-0.0016377	-0.0012985	0.0000616
C	-0.0005400	-0.0001425	-0.0000266
C	-0.0001323	0.0003210	0.0000265
C	0.0000622	0.0003942	-0.0000251
C	0.0000089	0.0002059	-0.0000016
C	-0.0000126	0.0001163	-0.0000003
C	0.0000149	0.0002422	-0.0000007
H	0.0000018	-0.0000248	0.0000017
H	-0.0000037	-0.0000248	0.0000003
C	-0.0010564	0.0009067	-0.0002261
C	0.0006200	0.0001938	0.0000036
C	0.0013895	0.0004619	-0.0000605
C	0.0005015	0.0001065	0.0000043
C	-0.0006622	-0.0014031	-0.0000406
C	-0.0003769	0.0003162	-0.0000143
C	0.0015013	0.0000056	0.0000851
C	-0.0005725	-0.0004064	0.0000057
H	0.0000045	-0.0000148	0.0000011

H	-0.0000078	-0.0000103	0.0000245
H	-0.0000096	-0.0000160	-0.0000013
H	0.0000069	-0.0000725	-0.0000124
C	-0.0018620	0.0009421	0.0009698
C	0.0002502	-0.0000301	0.0000021
C	0.0002683	0.0006285	-0.0001394
C	0.0003397	0.0000334	0.0000046
C	-0.0006494	-0.0002739	-0.0005026
C	-0.0001467	0.0003021	-0.0000059
C	0.0030112	-0.0004440	0.0004158
C	-0.0001538	-0.0002720	0.0000000
H	-0.0000082	0.0000015	0.0000004
H	-0.0000084	0.0000239	-0.0000429
H	0.0000013	0.0000059	0.0000002
H	0.0000178	-0.0000249	-0.0000006
H	-0.0000063	0.0000110	-0.0000005
H	-0.0000172	0.0000019	0.0000996
H	0.0000039	-0.0000084	0.0000004
C	-0.0000649	0.0008581	0.0010969
C	-0.0004505	0.0001889	0.0006539
C	-0.0003658	-0.0011395	-0.0010950
C	0.0001220	-0.0002104	-0.0004071
C	0.0009484	0.0001550	-0.0004313
C	0.0000985	-0.0002647	-0.0004019
C	0.0000287	0.0000040	0.0000435
C	-0.0000787	0.0000150	-0.0000021
C	0.0000247	0.0000724	-0.0001225
C	0.0001034	0.0000633	0.0000032
H	0.0000110	-0.0000595	0.0000356
H	-0.0000047	-0.0000047	-0.0000009
C	-0.0000855	0.0002986	0.0004421
C	0.0002404	-0.0000407	-0.0000848
C	-0.0001525	0.0002463	0.0004247
C	0.0001843	0.0002842	0.0009373
C	0.0003961	-0.0000223	-0.0003550
C	-0.0014575	-0.0020388	-0.0003479
C	-0.0001592	-0.0004129	-0.0003944
C	0.0014324	0.0021080	0.0007895
H	0.0000227	0.0000792	-0.0000525
H	0.0000018	-0.0000131	0.0000088
H	-0.0000333	-0.0000332	0.0000289
H	-0.0000035	-0.0000028	-0.0000046
C	-0.0001059	0.0001117	0.0002264
C	0.0006537	-0.0013837	-0.0022189
C	-0.0000605	0.0001613	0.0002435
C	-0.0015652	-0.0015236	-0.0009469
C	0.0002819	0.0000796	-0.0001209
C	0.0010229	0.0023943	0.0006136
C	-0.0001883	-0.0002155	-0.0001163
C	-0.0025192	-0.0003459	0.0008624
H	0.0000009	-0.0000031	-0.0000043

H	0.0000210	-0.0001250	0.0000552
H	0.0000032	0.0000003	-0.0000020
H	0.0000493	-0.0000443	0.0000281
H	0.0000092	0.0000043	-0.0000023
H	0.0000568	0.0000022	-0.0000073
H	-0.0000082	-0.0000046	0.0000002

Electronic state configuration of 22BP at S_0S_0 state geometry

1st state

Alpha	Beta	Coefficient
1100	1100	0.9096405
1010	1010	-0.1472976
0101	1010	0.1417689
1010	0101	0.1417689
1001	0110	0.1414110
0110	1001	0.1414110
0110	0110	-0.1407523
1001	1001	-0.1386645
0101	0101	-0.1383968
0011	0011	0.0877260

2nd state

Alpha	Beta	Coefficient
1010	1010	0.4503360
0110	0110	-0.4337356
1001	1001	-0.4279852
0101	0101	0.4142835
0011	1100	0.2864403
1100	0011	0.2864403
1010	0101	0.1444356
0101	1010	0.1444356
1001	0110	-0.1420047
0110	1001	-0.1420047

NACME between the 1st and 2nd states of 22BP at S_0S_0 state geometry

ATOM	d/dX	d/dY	d/dZ
C	-0.0015680	-0.0003560	-0.0003418
C	0.0015680	0.0003560	-0.0003418
C	-0.0059975	0.0007740	-0.0004693
C	0.0059975	-0.0007741	-0.0004693
C	-0.0000244	0.0031539	0.0011150
C	0.0000244	-0.0031539	0.0011150
C	0.0015097	-0.0003721	0.0000752
C	-0.0015097	0.0003721	0.0000752
C	0.0065079	-0.0029429	-0.0001229
C	-0.0065079	0.0029429	-0.0001228
C	0.0016495	0.0009322	0.0005212
C	-0.0016495	-0.0009322	0.0005212
C	-0.0000460	-0.0002065	-0.0000783
C	0.0000460	0.0002064	-0.0000783
C	-0.0002069	0.0001660	0.0000337
C	0.0002069	-0.0001660	0.0000337
C	-0.0000737	0.0002676	0.0000809
C	0.0000737	-0.0002676	0.0000809
C	-0.0000012	0.0000911	0.0000341
C	0.0000012	-0.0000911	0.0000341

H	0.0000075	-0.0000174	-0.0000053
H	-0.0000075	0.0000174	-0.0000053
H	0.0000068	-0.0000265	-0.0000092
H	-0.0000068	0.0000265	-0.0000092
C	-0.0012102	-0.0001136	-0.0002025
C	0.0012102	0.0001136	-0.0002025
C	-0.0027205	-0.0009738	-0.0006528
C	0.0027205	0.0009738	-0.0006528
C	-0.0013712	0.0000337	-0.0001761
C	0.0013712	-0.0000337	-0.0001761
C	0.0025307	0.0014148	0.0010327
C	-0.0025307	-0.0014148	0.0010327
C	0.0012923	-0.0007439	-0.0000944
C	-0.0012923	0.0007439	-0.0000944
C	-0.0045355	0.0007371	-0.0007614
C	0.0045355	-0.0007371	-0.0007614
C	0.0007180	0.0009509	0.0004208
C	-0.0007180	-0.0009509	0.0004208
C	0.0008468	-0.0018201	-0.0005512
C	-0.0008468	0.0018200	-0.0005512
H	0.0000003	-0.0001449	-0.0000334
H	-0.0000003	0.0001449	-0.0000334
H	0.0000124	-0.0000142	-0.0000030
H	-0.0000124	0.0000142	-0.0000030
H	0.0000253	0.0000936	-0.0000177
H	-0.0000253	-0.0000936	-0.0000177
H	0.0000111	-0.0000249	-0.0000070
H	-0.0000111	0.0000249	-0.0000070
C	-0.0006194	-0.0000320	-0.0000874
C	0.0006194	0.0000320	-0.0000874
C	-0.0000652	0.0002169	0.0002818
C	0.0000652	-0.0002169	0.0002818
C	-0.0005392	-0.0001268	-0.0001082
C	0.0005392	0.0001268	-0.0001082
C	0.0056656	0.0018928	0.0001363
C	-0.0056656	-0.0018928	0.0001363
C	0.0004078	-0.0005021	-0.0001220
C	-0.0004078	0.0005021	-0.0001221
C	-0.0066696	-0.0008370	-0.0009454
C	0.0066696	0.0008370	-0.0009454
C	0.0001886	0.0006049	0.0002324
C	-0.0001886	-0.0006049	0.0002324
C	-0.0000665	-0.0006492	0.0009350
C	0.0000665	0.0006492	0.0009350
H	0.0000016	0.0000075	0.0000025
H	-0.0000016	-0.0000075	0.0000025
H	0.0000090	0.0000314	0.0000722
H	-0.0000090	-0.0000314	0.0000722
H	0.0000128	0.0000008	0.0000011
H	-0.0000128	-0.0000008	0.0000011
H	0.0000030	-0.0000198	-0.0000065

H	-0.0000030	0.0000198	-0.0000065
H	0.0000280	0.0000958	-0.0000800
H	-0.0000280	-0.0000958	-0.0000800
H	0.0000044	0.0000209	0.0000077
H	-0.0000044	-0.0000209	0.0000077
H	-0.0000119	-0.0000488	-0.0001057
H	0.0000119	0.0000488	-0.0001056

Electronic state configuration of 22BP at ^{1}(TT) state geometry

1st state

Alpha	Beta	Coefficient
1100	1100	0.8151804
1010	1010	-0.1995481
1010	0101	0.1924989
0101	1010	0.1924989
1001	0110	0.1921858
0110	1001	0.1921858
0110	0110	-0.1905007
0101	0101	-0.1886688
1001	1001	-0.1880483
0011	0011	0.1802437
1001	1100	-0.0548330
1100	1001	-0.0548330

2nd state

Alpha	Beta	Coefficient
1010	1010	0.4456419
0110	0110	-0.4336001
1001	1001	-0.4291835
0101	0101	0.4188313
1100	0011	0.2865269
0011	1100	0.2865269
0101	1010	0.1448588
1010	0101	0.1448588
0110	1001	-0.1416680
1001	0110	-0.1416680

NACME between the 1st and 2nd states of 22BP at ^{1}(TT) state geometry

ATOM	d/dX	d/dY	d/dZ
C	-0.0016400	0.0000735	-0.0002106
C	0.0016400	-0.0000735	-0.0002106
C	-0.0068314	0.0011975	-0.0004125
C	0.0068314	-0.0011975	-0.0004125
C	-0.0005013	0.0028231	0.0009446
C	0.0005013	-0.0028231	0.0009446
C	0.0024547	0.0001035	0.0003640
C	-0.0024547	-0.0001035	0.0003640
C	0.0072843	-0.0024454	0.0001809
C	-0.0072843	0.0024454	0.0001809
C	0.0024638	0.0007392	0.0005545
C	-0.0024638	-0.0007392	0.0005545
C	-0.0000056	-0.0004815	-0.0001660
C	0.0000056	0.0004815	-0.0001660
C	-0.0002194	0.0002726	0.0000704
C	0.0002194	-0.0002726	0.0000704
C	-0.0000796	0.0003152	0.0000949

C	0.0000796	-0.0003152	0.0000949
C	0.0000684	-0.0002017	-0.0000567
C	-0.0000684	0.0002017	-0.0000567
H	0.0000074	-0.0000171	-0.0000049
H	-0.0000074	0.0000171	-0.0000049
H	0.0000038	-0.0000111	-0.0000048
H	-0.0000038	0.0000111	-0.0000048
C	-0.0023810	-0.0004482	-0.0004663
C	0.0023810	0.0004482	-0.0004663
C	-0.0037683	-0.0012564	-0.0009479
C	0.0037683	0.0012564	-0.0009479
C	-0.0027827	-0.0001147	-0.0004052
C	0.0027827	0.0001147	-0.0004052
C	0.0028157	0.0012360	0.0011015
C	-0.0028157	-0.0012360	0.0011015
C	0.0025575	-0.0013151	-0.0001352
C	-0.0025575	0.0013151	-0.0001352
C	-0.0050370	0.0015640	-0.0006719
C	0.0050370	-0.0015640	-0.0006719
C	0.0017083	0.0018296	0.0008494
C	-0.0017083	-0.0018296	0.0008494
C	0.0014880	-0.0024872	-0.0007271
C	-0.0014880	0.0024872	-0.0007271
H	-0.0000046	-0.0001474	-0.0000393
H	0.0000046	0.0001474	-0.0000393
H	0.0000113	-0.0000166	-0.0000040
H	-0.0000113	0.0000166	-0.0000040
H	0.0000225	0.0001248	-0.0000276
H	-0.0000225	-0.0001248	-0.0000276
H	0.0000131	-0.0000082	-0.0000019
H	-0.0000131	0.0000082	-0.0000019
C	-0.0013323	-0.0000398	-0.0001756
C	0.0013323	0.0000398	-0.0001756
C	-0.0004572	0.0001680	0.0003735
C	0.0004572	-0.0001680	0.0003735
C	-0.0012854	-0.0003105	-0.0002608
C	0.0012854	0.0003105	-0.0002608
C	0.0066524	0.0021618	0.0000424
C	-0.0066523	-0.0021617	0.0000424
C	0.0009053	-0.0011317	-0.0002794
C	-0.0009053	0.0011317	-0.0002794
C	-0.0082200	-0.0003859	-0.0010892
C	0.0082200	0.0003859	-0.0010892
C	0.0004294	0.0013127	0.0005047
C	-0.0004294	-0.0013127	0.0005047
C	0.0001011	-0.0012284	0.0011432
C	-0.0001011	0.0012284	0.0011432
H	0.0000097	0.0000136	0.0000054
H	-0.0000097	-0.0000136	0.0000054
H	0.0000225	0.0000478	0.0000716
H	-0.0000225	-0.0000478	0.0000716

H	0.0000188	-0.0000054	-0.0000006
H	-0.0000188	0.0000054	-0.0000006
H	0.0000098	-0.0000386	-0.0000123
H	-0.0000098	0.0000386	-0.0000123
H	0.0000334	0.0001331	-0.0001058
H	-0.0000334	-0.0001331	-0.0001058
H	0.0000009	0.0000436	0.0000150
H	-0.0000009	-0.0000436	0.0000150
H	-0.0000125	-0.0000529	-0.0001062
H	0.0000125	0.0000529	-0.0001062