Supplementary Information

Optimizing through-space interaction for singlet fission by using macrocyclic structures

Zhangxia Wang, Xuexiao Yang, Haibo Ma[*] and Xiaoyu Xie[*]

1. Calculation details

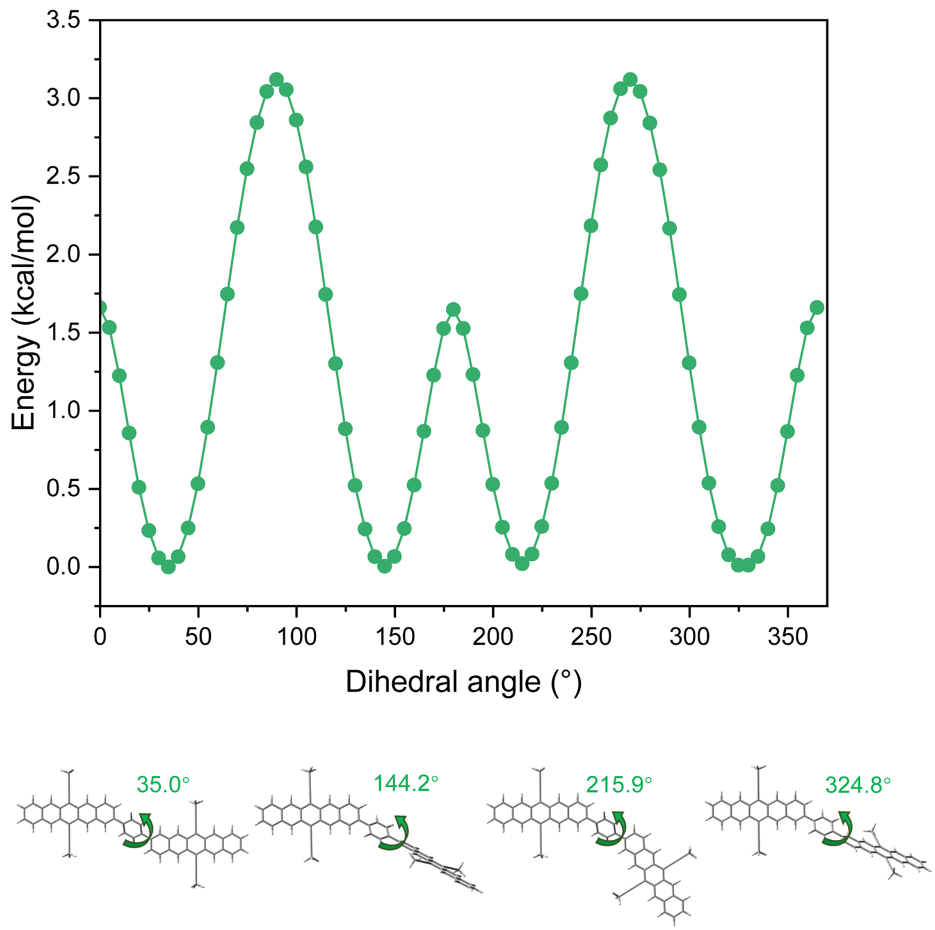


Figure S1. The potential energy surface scan curves of BP1 by scanning the dihedral angle in the range of 0-360°in increments of 5°at the B3LYP/6-31G(d) level.

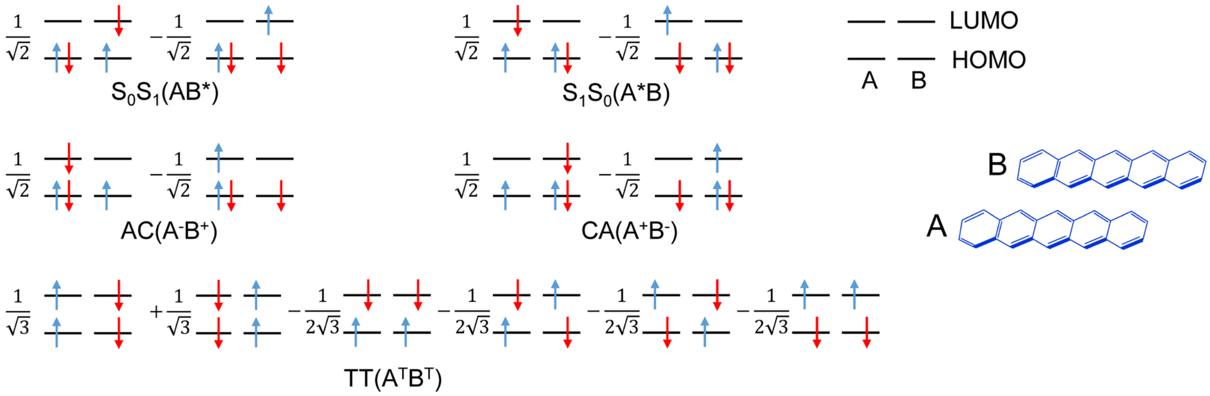


Figure S2. The illustration of diabatic states in bipentacene system as configuration state functions for singlet fission. S_0S_1/S_1S_0: local singlet excited states, CA/AC: charge transfer states and TT: multiexcitonic states, HOMO/LUMO: highest occupied molecular orbital/lowest unoccupied molecular orbital, A/B: two pentacenes.

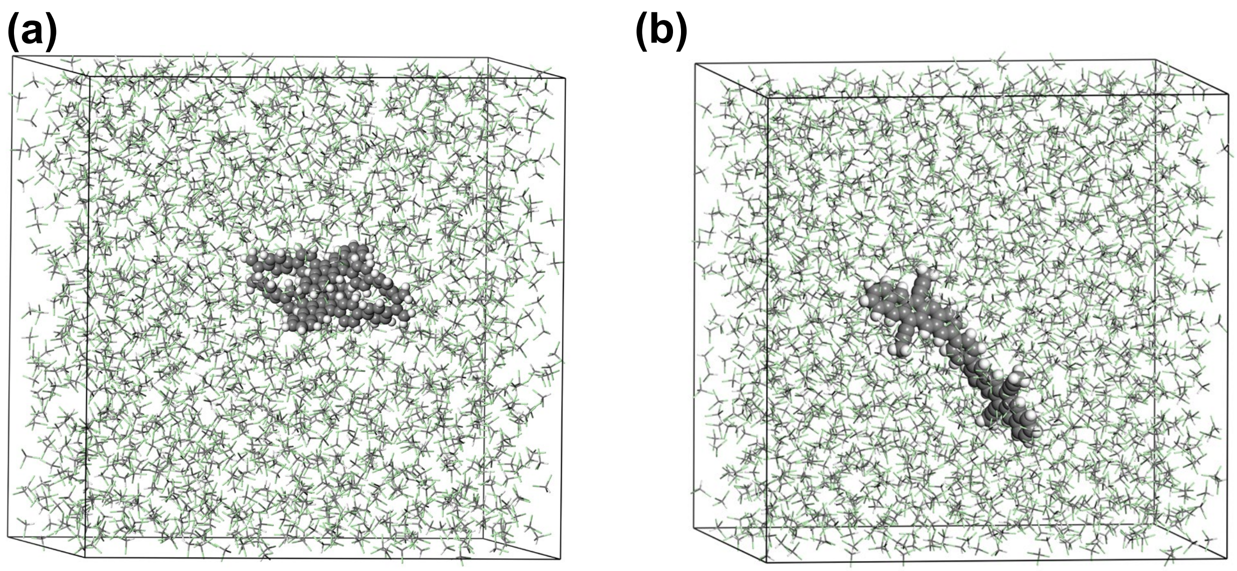


Figure S3. The MD models for (a) BPc and (b) BP1 systems with 2000 chloroform molecules.

Table S1. Parameter values for evaluating FCWD for singlet fission of BP1 and BPcs.

	BP1 (TIPS-Pentacene)			BPc (Pentacene)		
	$S_1 \rightarrow S_0$	$S_0 \rightarrow T_1$	$S_1 \rightarrow T_1$	$S_1 \rightarrow S_0$	$S_0 \rightarrow T_1$	$S_1 \rightarrow T_1$
E_0 (cm^{-1})	15553[1]	6936[2, 3]	8617	17178[5]	6936[3, 4]	10243
$\hbar\omega$ (cm^{-1})	1400	1400	1400	1400	1400	1400
$fwhm$ (cm^{-1})	800	800	800	800	800	800
λ (cm^{-1}) [a]	589	1273	284	767	1510	250
S [a]	0.421	0.909	0.203	0.548	1.079	0.179
$FCWD$ (eV^{-1})		2.162			0.980	

[a] Calculated from DFT and TDDFT-TDA at B3LYP/6-31G* level.

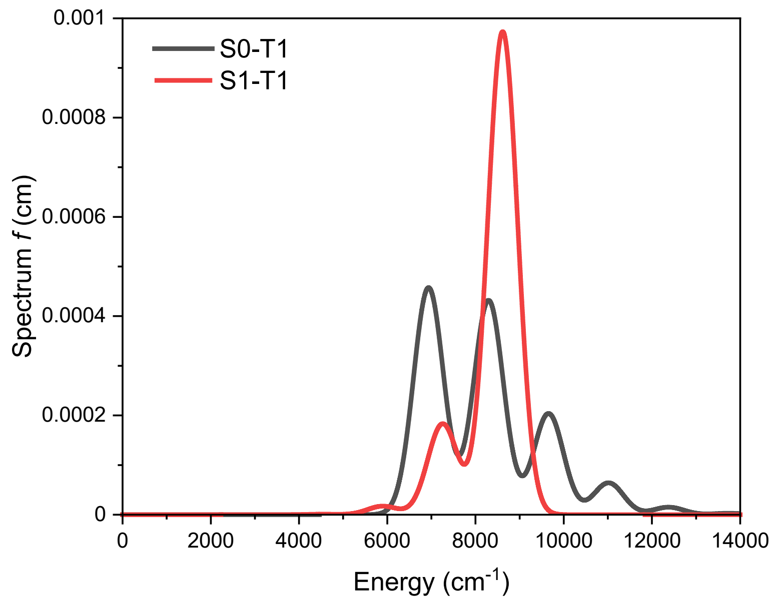


Figure S4. The absorption/emission spectrum (in red/black) of $S_0 \rightarrow T_1/S_1 \rightarrow T_1$ with spectroscopy parameters derived from those of TIPS pentacene to calculate the FCWD value of BP1.

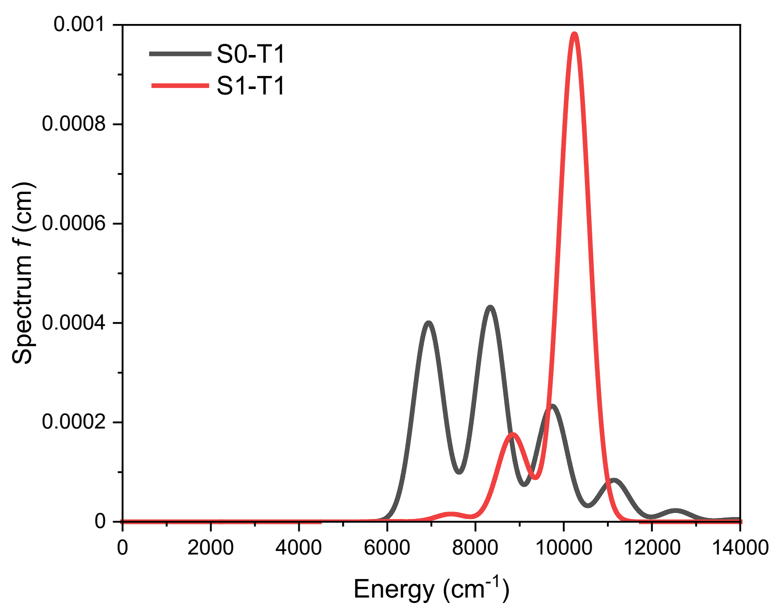


Figure S5. The absorption/emission spectrum (in red/black) of $S_0 \rightarrow T_1/S_1 \rightarrow T_1$ with spectroscopy parameters derived from those of pentacene to calculate the FCWD value of bipentacene macrocycles.

2. Results of equilibrium structures

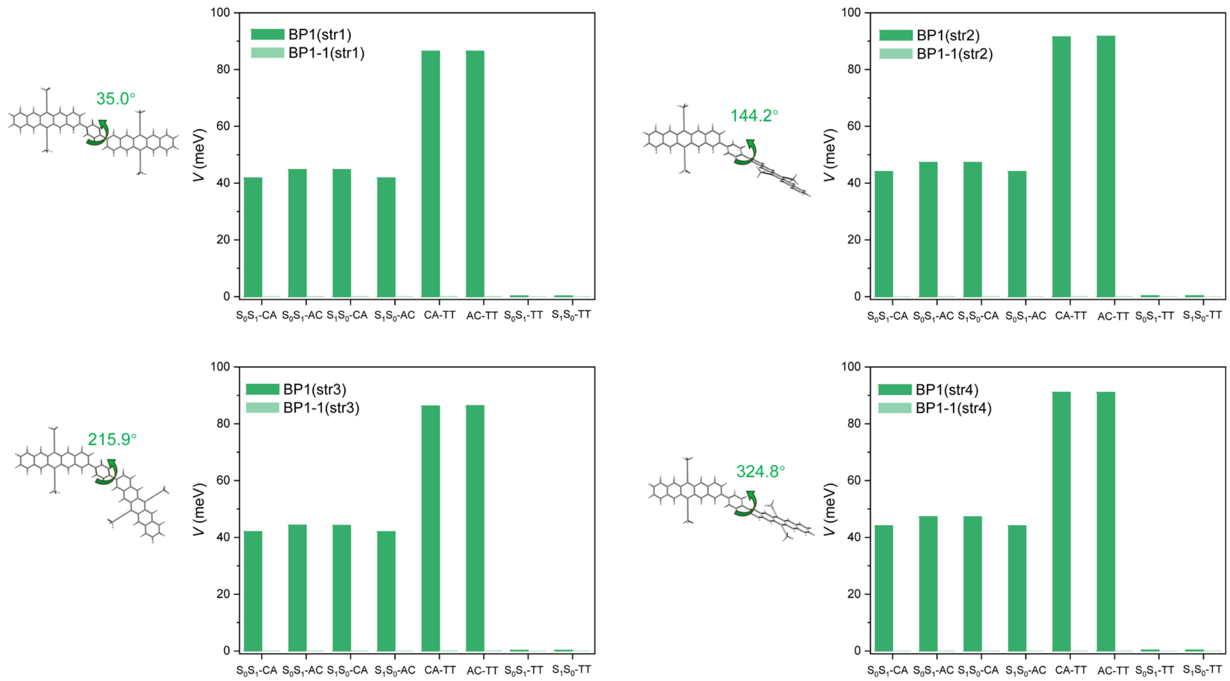


Figure S6. Electronic couplings (absolute values) of four equilibrium BP1 structures.

Table S2. Electronic Hamiltonian elements of four equilibrium BP1 structures (unit: meV)

	S_0S_1	S_1S_0	CA	AC	TT	S_0S_1	S_1S_0	CA	AC	TT
			str1					str1-1		
S_0S_1	3019.16	-4.08	41.80	44.79	0.25	3041.22	-6.37	0.03	0.05	0.00
S_1S_0		3019.46	-44.78	-41.80	0.25		3041.59	-0.05	-0.03	0.00
CA			4674.42	1.38	86.49			4777.24	0.00	0.08
AC				4674.82	-86.49				4777.20	-0.08
TT					2439.00					2344.27
			str2					str2-1		
S_0S_1	3020.16	-6.69	-44.07	47.31	-0.33	3042.35	-3.68	-0.01	0.02	0.00
S_1S_0		3020.87	-47.31	44.08	0.32		3042.30	-0.02	0.01	0.00
CA			4661.99	-1.55	91.51			4765.23	0.00	0.03
AC				4661.63	91.72				4765.61	0.03
TT					2439.38					2342.78
			str3					str3-1		
S_0S_1	3020.18	13.61	-42.03	-44.26	-0.24	3042.53	10.34	-0.03	-0.04	0.00
S_1S_0		3020.90	44.22	42.02	-0.24		3043.03	0.04	0.03	0.00
CA			4652.25	1.33	86.26			4753.96	0.00	0.09
AC				4652.62	-86.37				4754.44	-0.09
TT					2434.09					2340.49
			str4					str4-1		
S_0S_1	3019.50	-0.97	-44.10	47.29	0.32	3041.67	1.76	-0.01	0.02	0.00
S_1S_0		3019.68	-47.28	44.10	-0.32		3041.73	-0.02	0.01	0.00
CA			4665.63	-1.53	-91.09			4769.18	0.00	-0.02
AC				4666.10	-91.06				4770.11	-0.02
TT					2439.12					2343.16

Table S3. Electronic Hamiltonian elements for equilibrium BPc structure. (unit: meV)

	BPc					BPc-1				
	S_0S_1	S_1S_0	CA	AC	TT	S_0S_1	S_1S_0	CA	AC	TT
S_0S_1	3160.63	142.52	68.25	-82.13	0.00	3212.37	136.18	60.96	-87.01	0.00
S_1S_0		3160.64	82.13	-68.25	0.00		3212.53	87.00	-60.96	0.00
CA			3591.95	1.03	0.02			3658.15	1.28	0.01
AC				3592.03	0.01				3658.15	-0.02
TT					2821.06					2884.67

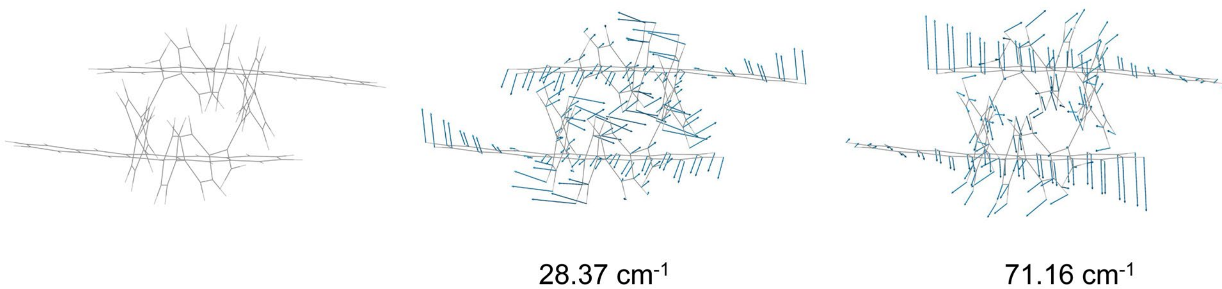


Figure S7. Two low-frequency modes of BPc influent the distance between two pentacene units.

3. Decomposition of electronic coupling

The definitions of five diabatic states are shown in Figure S2. Equations 1-8 provide the explicit expressions of the electronic couplings between these states.

$$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle = -F_{h_\mathrm{A}h_\mathrm{B}} - g_{h_\mathrm{A}h_\mathrm{B}h_\mathrm{A}h_\mathrm{A}} - g_{h_\mathrm{A}h_\mathrm{B}h_\mathrm{B}h_\mathrm{B}} - g_{h_\mathrm{A}h_\mathrm{B}l_\mathrm{B}l_\mathrm{B}} + 2g_{h_\mathrm{A}l_\mathrm{B}l_\mathrm{B}h_\mathrm{B}} \tag{1}$$

$$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{AC}\rangle = F_{l_\mathrm{B}l_\mathrm{A}} + 2g_{l_\mathrm{B}l_\mathrm{A}h_\mathrm{A}h_\mathrm{A}} + g_{l_\mathrm{B}l_\mathrm{A}h_\mathrm{B}h_\mathrm{B}} - g_{l_\mathrm{B}h_\mathrm{A}h_\mathrm{A}l_\mathrm{A}} + g_{h_\mathrm{B}l_\mathrm{A}l_\mathrm{B}h_\mathrm{B}} \tag{2}$$

$$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{CA}\rangle = F_{l_\mathrm{A}l_\mathrm{B}} + 2g_{l_\mathrm{A}l_\mathrm{B}h_\mathrm{B}h_\mathrm{B}} + g_{l_\mathrm{A}l_\mathrm{B}h_\mathrm{A}h_\mathrm{A}} - g_{l_\mathrm{A}h_\mathrm{B}h_\mathrm{B}l_\mathrm{B}} + g_{h_\mathrm{A}l_\mathrm{B}l_\mathrm{A}h_\mathrm{A}} \tag{3}$$

$$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{AC}\rangle = F_{h_\mathrm{B}h_\mathrm{A}} + g_{h_\mathrm{B}h_\mathrm{A}h_\mathrm{A}h_\mathrm{A}} + g_{h_\mathrm{B}h_\mathrm{A}l_\mathrm{A}l_\mathrm{A}} + g_{h_\mathrm{B}h_\mathrm{A}h_\mathrm{B}h_\mathrm{B}} - 2g_{h_\mathrm{B}l_\mathrm{A}l_\mathrm{A}h_\mathrm{A}} \tag{4}$$

$$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{TT}\rangle = -\sqrt{3/2}g_{h_\mathrm{A}l_\mathrm{B}l_\mathrm{B}l_\mathrm{A}} + \sqrt{3/2}g_{h_\mathrm{A}h_\mathrm{B}h_\mathrm{B}l_\mathrm{A}} \tag{5}$$

$$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{TT}\rangle = \sqrt{3/2}g_{h_\mathrm{B}l_\mathrm{A}l_\mathrm{A}l_\mathrm{B}} - \sqrt{3/2}g_{h_\mathrm{B}h_\mathrm{A}h_\mathrm{A}l_\mathrm{B}} \tag{6}$$

$$\langle \mathrm{CA}|\hat{H}|\mathrm{TT}\rangle = \sqrt{3/2}\left(F_{h_\mathrm{B}l_\mathrm{A}} + g_{h_\mathrm{B}l_\mathrm{A}h_\mathrm{A}h_\mathrm{A}} + g_{h_\mathrm{B}l_\mathrm{A}h_\mathrm{B}h_\mathrm{B}} + g_{h_\mathrm{B}l_\mathrm{A}l_\mathrm{B}l_\mathrm{B}} - g_{h_\mathrm{B}h_\mathrm{A}h_\mathrm{A}l_\mathrm{A}}\right) \tag{7}$$

$$\langle \mathrm{AC}|\hat{H}|\mathrm{TT}\rangle = \sqrt{3/2}\left(F_{h_\mathrm{A}l_\mathrm{B}} + g_{h_\mathrm{A}l_\mathrm{B}h_\mathrm{A}h_\mathrm{A}} + g_{h_\mathrm{A}l_\mathrm{B}l_\mathrm{A}l_\mathrm{A}} + g_{h_\mathrm{A}l_\mathrm{B}h_\mathrm{B}h_\mathrm{B}} - g_{h_\mathrm{A}h_\mathrm{B}h_\mathrm{B}l_\mathrm{B}}\right) \tag{8}$$

Here, $h_{\mathrm{A/B}}$ stands for HOMO of A/B molecule, and $l_{\mathrm{A/B}}$ stands for LUMO of A/B molecule. The Fock element (F_{ij}) is given by:

$$F_{ij} = h_{ij} + \sum_{a\in \mathrm{occ}} (2g_{iaja} - g_{iaaj}) = h_{ij} + 2J - K$$

$$h_{ij} = \int \Phi_i^*(\mathbf{x})\left(-\frac{1}{2}\nabla^2 - \sum_I \frac{Z_I}{r_I}\right)\Phi_j(\mathbf{x})d\mathbf{x}$$

$$g_{ijkl} = \iint \frac{\Phi_i^*(\mathbf{x_1})\Phi_k^*(\mathbf{x_2})\Phi_j(\mathbf{x_1})\Phi_l(\mathbf{x_2})}{r_{12}}d\mathbf{x_1}d\mathbf{x_2}$$

Here, Z_I is the nuclear charge, r_I is the electron-nuclear separation, r_{12} is the electron-electron separation. $2J$ is the Coulomb term, K is the exchange term, and h_{ij} is one-electron integral. Generally, the couplings can be expressed as $h_{ij} + 2J - K + g$, and the two-electron term (g) is the sum of two-electron integrals of HOMO/LUMO. For example, the two-electron term is $-g_{h_\mathrm{A}h_\mathrm{B}h_\mathrm{A}h_\mathrm{A}} - g_{h_\mathrm{A}h_\mathrm{B}h_\mathrm{B}h_\mathrm{B}} - g_{h_\mathrm{A}h_\mathrm{B}l_\mathrm{B}l_\mathrm{B}} + 2g_{h_\mathrm{A}l_\mathrm{B}l_\mathrm{B}h_\mathrm{B}}$ for $\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle$.

In order to explore the influence of the linker on the couplings, we localize occupied orbitals for BP1 and BPc to analyze the contribution of the linker to Coulomb and exchange interactions in the Fock operator term.

$$\begin{aligned} F_{ij} &= h_{ij} + \sum_{a\in \mathrm{linker}} (2g_{iaja} - g_{iaaj}) + \sum_{b\in \mathrm{core}} (2g_{ibjb} - g_{ibbj}) \\ &= h_{ij} + 2J_{ij}^{\mathrm{l}} - K_{ij}^{\mathrm{l}} + 2J_{ij}^{\mathrm{c}} - K_{ij}^{\mathrm{c}} \end{aligned}$$

Where $2J_{ij}^{\mathrm{l}}$ is the Coulomb term of occupied linker orbitals, and $-K_{ij}^{\mathrm{l}}$ is the exchange terms of occupied linker orbitals. All the data for four equilibrium structures and 10 molecular dynamics snapshots of BP1 are listed in Table S1-S14, and those of BPc are listed in Table S15-S25.

Table S4. Decomposition of electronic coupling of BP1 at equilibrium structure (str1). (meV)

		F				g	V
		h	$2J$ ($2J^{\text{l}}$)	$-K$ ($-K^{\text{l}}$)	total		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BP1	-1843.99	1886.04 (1552.21)	-2.42 (-6.75)	44.47	-2.67	41.80
	BP1-1	-1.41	1.47 (-)	0.03 (-)	0.02	0.01	0.03
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BP1	1063.60	-1018.62 (-1270.11)	4.98 (5.29)	40.01	4.78	44.79
	BP1-1	-0.93	1.02 (-)	0.05 (-)	0.04	0.01	0.05
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BP1	-1063.60	1018.62(1270.11)	-4.98 (-5.29)	-40.01	-4.78	-44.78
	BP1-1	0.93	-1.02 (-)	-0.05 (-)	-0.04	-0.01	-0.05
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BP1	1843.99	-1886.04(1552.21)	2.42 (6.75)	-44.47	2.68	-41.80
	BP1-1	1.41	-1.47 (-)	-0.03 (-)	-0.04	-0.01	-0.03
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BP1	-	-	-	-	0.25	0.25
	BP1-1	-	-	-	-	0.00	0.00
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BP1	-	-	-	-	0.25	0.25
	BP1-1	-	-	-	-	0.00	0.00
$\langle CA\|\hat{H}\|TT\rangle$	BP1	-412.41	456.30 (204.52)	13.65 (-6.33)	30.23	56.25	86.49
	BP1-1	-1.40	1.47 (-)	0.06 (-)	0.02	0.07	0.08
$\langle AC\|\hat{H}\|TT\rangle$	BP1	412.48	-456.35 (204.69)	-13.63 (6.30)	-30.24	-56.25	-86.49
	BP1-1	1.40	-1.47 (-)	-0.06 (-)	-0.02	-0.07	-0.08

Table S5. Energies of five diabatic states of BP1 at equilibrium structure (str1) in eV.

	$E_{S_0S_1}$	$E_{S_1S_0}$	E_{CA}	E_{AC}	E_{TT}
BP1	3.02	3.02	4.67	4.67	2.44
BP1-1	3.04	3.04	4.78	4.78	2.34

Table S6. Decomposition of electronic coupling of BP1 at equilibrium structure (str2). (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J\ (2J^{l})}$	$\boldsymbol{-K\ (-K^{l})}$	**total**		
$\langle S_0S_1\vert\hat{H}\vert CA\rangle$	BP1	2018.76	-2062.98 (-1631.43)	1.49 (-13.31)	-45.72	1.64	-44.07
	BP1-1	0.50	-0.52 (-)	-0.01 (-)	-0.01	0.00	-0.01
$\langle S_0S_1\vert\hat{H}\vert AC\rangle$	BP1	1125.51	-1074.62 (-1282.20)	7.31 (-32.66)	43.58	3.73	47.31
	BP1-1	-0.36	0.39 (-)	0.02 (-)	0.01	0.00	0.02
$\langle S_1S_0\vert\hat{H}\vert CA\rangle$	BP1	-1125.51	1074.62 (1282.20)	-7.31 (32.66)	-43.58	-3.73	-47.31
	BP1-1	0.36	-0.39 (-)	-0.02 (-)	-0.01	0.00	-0.02
$\langle S_1S_0\vert\hat{H}\vert AC\rangle$	BP1	-2018.76	2062.98 (1631.43)	-1.49 (13.31)	45.72	-1.64	44.08
	BP1-1	-0.50	0.52 (-)	0.01 (-)	0.01	0.00	0.01
$\langle S_0S_1\vert\hat{H}\vert TT\rangle$	BP1	-	-	-	-	-0.33	-0.33
	BP1-1	-	-	-	-	0.00	0.00
$\langle S_1S_0\vert\hat{H}\vert TT\rangle$	BP1	-	-	-	-	0.32	0.32
	BP1-1	-	-	-	-	0.00	0.00
$\langle CA\vert\hat{H}\vert TT\rangle$	BP1	-488.56	537.99 (239.59)	17.81 (-11.67)	31.63	59.88	91.51
	BP1-1	-0.52	0.54 (-)	0.02 (-)	0.01	0.02	0.03
$\langle AC\vert\hat{H}\vert TT\rangle$	BP1	-492.50	542.02 (227.67)	17.81 (11.60)	31.71	60.02	91.72
	BP1-1	-0.55	0.57 (-)	0.02 (-)	0.01	0.02	0.03

Table S7. Energies of five diabatic states of BP1 at equilibrium structure (str2). (eV)

	$\boldsymbol{E_{S_0S_1}}$	$\boldsymbol{E_{S_1S_0}}$	$\boldsymbol{E_{CA}}$	$\boldsymbol{E_{AC}}$	$\boldsymbol{E_{TT}}$
BP1	3.02	3.02	4.66	4.66	2.44
BP1-1	3.04	3.04	4.77	4.77	2.34

Table S8. Decomposition of electronic coupling of BP1 at equilibrium structure (str3). (meV)\

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J}$ $(\boldsymbol{2J^{l}})$	$\boldsymbol{-K}$ $(\boldsymbol{-K^{l}})$	**total**		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BP1	1934.99	-1975.38 (-1423.47)	2.97 (4.43)	-43.36	1.33	-42.03
	BP1-1	1.57	-1.63 (-)	-0.03 (-)	-0.02	-0.01	-0.03
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BP1	-1172.68	1128.14 (1138.15)	-3.73 (-4.91)	-40.81	-3.45	-44.26
	BP1-1	0.62	-0.70 (-)	-0.05 (-)	-0.04	-0.01	-0.04
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BP1	1172.68	-1128.14 (-1138.15)	3.73 (4.91)	40.81	3.42	44.22
	BP1-1	-0.62	0.70 (-)	0.05 (-)	0.04	0.01	0.04
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BP1	-1934.99	1975.38 (1423.47)	-2.97 (-4.43)	43.36	-1.34	42.02
	BP1-1	-1.57	1.63 (-)	0.03 (-)	0.02	0.01	0.03
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BP1	-	-	-	-	-0.24	-0.24
	BP1-1	-	-	-	-	0.00	0.00
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BP1	-	-	-	-	-0.24	-0.24
	BP1-1	-	-	-	-	0.00	0.00
$\langle CA\|\hat{H}\|TT\rangle$	BP1	-436.06	480.60 (199.46)	14.89 (-6.67)	29.65	56.61	86.26
	BP1-1	-1.49	1.57 (-)	0.06 (-)	0.02	0.07	0.09
$\langle AC\|\hat{H}\|TT\rangle$	BP1	437.39	-481.98 (-176.79)	-14.88 (7.01)	-29.71	-56.67	-86.37
	BP1-1	1.49	-1.57 (-)	-0.06 (-)	-0.02	-0.07	-0.09

Table S9. Energies of five diabatic states of BP1 at equilibrium structure (str3). (eV)

	$\boldsymbol{E_{S_0S_1}}$	$\boldsymbol{E_{S_1S_0}}$	$\boldsymbol{E_{CA}}$	$\boldsymbol{E_{AC}}$	$\boldsymbol{E_{TT}}$
BP1	3.02	3.02	4.66	4.66	2.44
BP1-1	3.04	3.04	4.77	4.77	2.34

Table S10. Decomposition of electronic coupling of BP1 at equilibrium structure (str4). (meV)

		F				g	V
		h	$2J$ ($2J^{l}$)	$-K$ ($-K^{l}$)	total		
$\langle S_0S_1 \vert \hat{H} \vert CA\rangle$	BP1	1982.80	-2027.55 (-1556.52)	1.45 (4.30)	-46.20	2.10	-44.10
	BP1-1	0.51	-0.53 (-)	-0.01 (-)	-0.01	0.00	-0.01
$\langle S_0S_1 \vert \hat{H} \vert AC\rangle$	BP1	1111.69	-1060.84 (-1240.82)	7.66 (0.04)	43.19	4.10	47.29
	BP1-1	-0.39	0.42 (-)	0.02 (-)	0.01	0.01	0.02
$\langle S_1S_0 \vert \hat{H} \vert CA\rangle$	BP1	-1111.69	1060.84 (1240.82)	-7.66 (-0.04)	-43.19	-4.09	-47.28
	BP1-1	0.39	-0.42 (-)	-0.02 (-)	-0.01	-0.01	-0.02
$\langle S_1S_0 \vert \hat{H} \vert AC\rangle$	BP1	-1982.80	2027.55 (1556.52)	-1.45 (-4.30)	46.20	-2.10	44.10
	BP1-1	-0.51	0.53 (-)	0.01 (-)	0.01	0.00	0.01
$\langle S_0S_1 \vert \hat{H} \vert TT\rangle$	BP1	-	-	-	-	0.32	0.32
	BP1-1	-	-	-	-	0.00	0.00
$\langle S_1S_0 \vert \hat{H} \vert TT\rangle$	BP1	-	-	-	-	-0.32	-0.32
	BP1-1	-	-	-	-	0.00	0.00
$\langle CA \vert \hat{H} \vert TT\rangle$	BP1	494.67	-543.76 (-226.84)	-17.53 (8.18)	-31.56	-59.53	-91.09
	BP1-1	0.44	-0.46 (-)	-0.02 (-)	0.00	-0.02	-0.02
$\langle AC \vert \hat{H} \vert TT\rangle$	BP1	494.33	-543.41 (-231.32)	-17.51 (8.17)	-31.56	-59.50	-91.06
	BP1-1	0.44	-0.47 (-)	-0.02 (-)	0.00	-0.02	-0.02

Table S11. Energies of five diabatic states of BP1 at equilibrium structure (str4). (eV)

	$E_{S_0S_1}$	$E_{S_1S_0}$	E_{CA}	E_{AC}	E_{TT}
BP1	3.02	3.02	4.67	4.67	2.44
BP1-1	3.04	3.04	4.77	4.77	2.34

Table S12. Decomposition of electronic coupling of BPc at equilibrium structure. (meV)

		F				g	V
		h	$2J$ ($2J^{\text{l}}$)	$-K$ ($-K^{\text{l}}$)	total		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	-1832.99	1659.84 (871.80)	73.07 (25.68)	-100.08	31.83	-68.25
	BPc-1	-452.83	295.74 (-)	65.88 (-)	-91.21	30.25	-60.96
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	-635.47	512.03 (348.00)	40.87 (-0.31)	-82.57	0.44	-82.13
	BPc-1	6.87	-131.64 (-)	43.66 (-)	-81.11	-5.90	-87.01
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	-635.47	512.03 (348.00)	40.87 (-0.31)	-82.57	0.44	-82.13
	BPc-1	6.87	-131.64 (-)	43.66 (-)	-81.11	-5.90	-87.00
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	1832.99	-1659.84 (-871.80)	-73.07 (-25.68)	100.08	-31.83	68.25
	BPc-1	452.83	-295.74 (-)	-65.88 (-)	91.21	-30.25	60.96
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	0.00	0.00
	BPc-1	-	-	-	-	0.00	0.00
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	0.00	0.00
	BPc-1	-	-	-	-	0.00	0.00
$\langle CA\|\hat{H}\|TT\rangle$	BPc	0.63	-0.60 (-0.22)	-0.02 (-0.01)	0.01	0.01	0.02
	BPc-1	0.29	-0.26 (-)	-0.02 (-)	0.01	0.00	0.01
$\langle AC\|\hat{H}\|TT\rangle$	BPc	0.99	-0.98 (-0.29)	0.00 (-0.01)	0.01	-0.02	-0.01
	BPc-1	0.22	-0.18 (-)	-0.03 (-)	0.01	0.01	0.02

Table S13. Energies of five diabatic states of BPc at equilibrium structure. (eV)

	$E_{S_0S_1}$	$E_{S_1S_0}$	E_{CA}	E_{AC}	E_{TT}
BPc	3.16	3.16	3.59	3.59	2.82
BPc-1	3.21	3.21	3.66	3.66	2.88

Table S14. Decomposition of electronic coupling of BPc at 0.5 ns in MD simulation. (meV)

		F				g	V
		h	$2J$ $(2J^{\mathrm{l}})$	$-K$ $(-K^{\mathrm{l}})$	total		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	-1146.91	1264.58 (515.29)	-50.78 (-11.04)	66.89	7.24	74.12
	BPc-1	-1162.40	1285.76 (-)	-53.85 (-)	69.51	13.87	83.38
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	-212.40	339.63 (368.60)	-53.47 (-15.88)	73.76	12.86	86.62
	BPc-1	95.05	39.53 (-)	-53.25 (-)	81.33	9.22	90.55
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	-212.40	339.63 (368.60)	-53.47 (-15.88)	73.76	3.28	77.04
	BPc-1	95.05	39.53 (-)	-53.25 (-)	81.33	-1.35	79.98
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	1146.91	-1264.58 (-515.29)	50.78 (11.04)	-66.89	-5.82	-72.70
	BPc-1	1162.40	-1285.76 (-)	53.85 (-)	-69.51	-12.74	-82.25
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.25	-0.25
	BPc-1	-	-	-	-	-0.28	-0.28
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.09	-0.09
	BPc-1	-	-	-	-	-0.12	-0.12
$\langle CA\|\hat{H}\|TT\rangle$	BPc	-722.57	711.74 (420.01)	6.52 (-2.01)	-4.31	9.64	5.34
	BPc-1	-320.31	310.10 (-)	6.53 (-)	-3.68	9.91	6.22
$\langle AC\|\hat{H}\|TT\rangle$	BPc	882.05	-871.66 (-537.00)	-3.25 (1.19)	7.14	-4.98	2.15
	BPc-1	451.62	-440.59 (-)	-3.10 (-)	7.93	-5.96	1.97

Table S15. Energies of five diabatic states of BPc at 0.5 ns in MD simulation. (eV)

	$E_{S_0S_1}$	$E_{S_1S_0}$	E_{CA}	E_{AC}	E_{TT}
BPc	2.72	2.91	3.06	3.23	1.57
BPc-1	2.78	2.98	3.13	3.28	1.64

Table S16. Decomposition of electronic coupling of BPc at 1.0 ns in MD simulation. (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J\ (2J^{l})}$	$\boldsymbol{-K\ (-K^{l})}$	**total**		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	-947.68	1137.62 (219.52)	-70.09 (-1.45)	119.85	-2.76	117.09
	BPc-1	-1075.03	1279.86 (-)	-77.57 (-)	127.26	4.04	131.30
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	1490.20	-1341.48 (-528.23)	-57.82 (-21.35)	90.9	-7.46	83.44
	BPc-1	950.67	-785.94 (-)	-58.23 (-)	106.5	-14.38	92.12
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	1490.20	-1341.48 (-528.23)	-57.82 (-21.35)	90.9	-9.23	81.67
	BPc-1	950.67	-785.94 (-)	-58.23 (-)	106.5	-15.31	91.19
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	947.68	-1137.62 (-219.52)	70.09 (1.45)	-119.85	-5.80	-125.65
	BPc-1	1075.03	-1279.86 (-)	77.57 (-)	-127.26	-13.88	-141.14
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.30	-0.30
	BPc-1	-	-	-	-	-0.21	-0.21
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	0.53	0.53
	BPc-1	-	-	-	-	0.51	0.51
$\langle CA\|\hat{H}\|TT\rangle$	BPc	1234.42	-1257.02 (-562.69)	19.98 (-0.17)	-2.62	-48.62	-51.24
	BPc-1	670.90	-699.73 (-)	23.40 (-)	-5.43	-54.18	-59.61
$\langle AC\|\hat{H}\|TT\rangle$	BPc	132.25	-118.89 (-379.27)	-13.79 (5.32)	-0.43	10.02	9.59
	BPc-1	-243.17	265.76 (-)	-20.08 (-)	2.51	14.29	16.80

Table S17. Energies of five diabatic states of BPc at 1.0 ns in MD simulation. (eV)

	$\boldsymbol{E_{S_0S_1}}$	$\boldsymbol{E_{S_1S_0}}$	$\boldsymbol{E_{CA}}$	$\boldsymbol{E_{AC}}$	$\boldsymbol{E_{TT}}$
BPc	2.74	2.70	2.83	2.97	1.43
BPc-1	2.81	2.78	2.91	3.03	1.52

Table S18. Decomposition of electronic coupling of BPc at 1.5 ns in MD simulation. (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J\ (2J^{\mathrm{l}})}$	$\boldsymbol{-K\ (-K^{\mathrm{l}})}$	**total**		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	1434.71	-1375.42 (-1339.64)	-15.64 (3.05)	43.65	-21.77	21.88
	BPc-1	168.78	-111.46 (-)	-17.36 (-)	39.96	-20.58	19.37
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	-373.19	271.67 (68.14)	33.66 (2.54)	-67.86	19.99	-47.88
	BPc-1	-253.35	147.11 (-)	33.76 (-)	-72.48	22.42	-50.06
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	-373.19	271.67 (68.14)	33.66 (2.54)	-67.86	-8.89	-76.76
	BPc-1	-253.35	147.11 (-)	33.76 (-)	-72.48	-10.39	-82.87
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	-1434.71	1375.42 (1339.64)	15.64 (-3.05)	-43.65	4.80	-38.85
	BPc-1	-168.78	111.46 (-)	17.36 (-)	-39.96	5.79	-34.16
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	0.69	0.69
	BPc-1	-	-	-	-	0.81	0.81
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.27	-0.27
	BPc-1	-	-	-	-	-0.32	-0.32
$\langle CA\|\hat{H}\|TT\rangle$	BPc	-533.98	535.21 (338.45)	-9.13 (0.40)	-7.9	-2.60	-10.50
	BPc-1	-109.51	109.38 (-)	-6.43 (-)	-6.56	-2.13	-8.69
$\langle AC\|\hat{H}\|TT\rangle$	BPc	22.13	-31.78 (-77.36)	6.37 (-1.66)	-3.28	-2.76	-6.04
	BPc-1	-69.08	57.79 (-)	7.07 (-)	-4.22	-3.80	-8.03

Table S19. Energies of five diabatic states of BPc at 1.5 ns in MD simulation. (eV)

	$\boldsymbol{E_{S_0S_1}}$	$\boldsymbol{E_{S_1S_0}}$	$\boldsymbol{E_{CA}}$	$\boldsymbol{E_{AC}}$	$\boldsymbol{E_{TT}}$
BPc	2.72	2.98	3.42	3.38	1.75
BPc-1	2.80	3.06	3.64	3.33	1.83

Table 20. Decomposition of electronic coupling of BPc at 2.0 ns in MD simulation. (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J}$ ($\boldsymbol{2J^{\mathrm{l}}}$)	$\boldsymbol{-K}$ ($\boldsymbol{-K^{\mathrm{l}}}$)	**total**		
$\langle \mathrm{S_0S_1} \| \hat{H} \| \mathrm{CA} \rangle$	BPc	-1142.64	1014.71 (1154.91)	34.95 (2.43)	-92.98	29.12	-63.86
	BPc-1	26.23	-141.68 (-)	30.46 (-)	-84.99	25.14	-59.85
$\langle \mathrm{S_0S_1} \| \hat{H} \| \mathrm{AC} \rangle$	BPc	-860.55	957.35 (601.56)	-34.86 (-3.40)	61.94	-0.72	61.22
	BPc-1	-343.94	444.29 (-)	-34.84 (-)	65.51	-0.63	64.88
$\langle \mathrm{S_1S_0} \| \hat{H} \| \mathrm{CA} \rangle$	BPc	-860.55	957.35 (601.56)	-34.86 (-3.40)	61.94	25.85	87.78
	BPc-1	-343.94	444.29 (-)	-34.84 (-)	65.51	32.21	97.71
$\langle \mathrm{S_1S_0} \| \hat{H} \| \mathrm{AC} \rangle$	BPc	1142.64	-1014.71 (-1154.91)	-34.95 (-2.43)	92.98	-13.12	79.85
	BPc-1	-26.23	141.68 (-)	-30.46 (-)	84.99	-14.30	70.69
$\langle \mathrm{S_0S_1} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-	-	-	-	-0.08	-0.08
	BPc-1	-	-	-	-	-0.08	-0.08
$\langle \mathrm{S_1S_0} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-	-	-	-	-0.31	-0.31
	BPc-1	-	-	-	-	-0.31	-0.31
$\langle \mathrm{CA} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	241.92	-243.50 (-308.75)	4.36 (8.61)	2.78	0.01	2.78
	BPc-1	79.65	-64.93 (-)	-6.23 (-)	8.49	3.55	12.05
$\langle \mathrm{AC} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-655.07	615.67 (797.16)	16.62 (-7.39)	-22.78	-22.53	-45.29
	BPc-1	80.18	-128.58 (-)	24.75 (-)	-23.65	-29.80	-53.45

Table S21. Energies of five diabatic states of BPc at 2.0 ns in MD simulation. (eV)

	$\boldsymbol{E_{\mathrm{S_0S_1}}}$	$\boldsymbol{E_{\mathrm{S_1S_0}}}$	$\boldsymbol{E_{\mathrm{CA}}}$	$\boldsymbol{E_{\mathrm{AC}}}$	$\boldsymbol{E_{\mathrm{TT}}}$
BPc	2.77	2.71	3.21	3.10	1.50
BPc-1	2.84	2.80	3.34	3.13	1.58

Table S22. Decomposition of electronic coupling of BPc at 2.5 ns in MD simulation. (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J}$ ($\boldsymbol{2J^{\mathrm{I}}}$)	$\boldsymbol{-K}$ ($\boldsymbol{-K^{\mathrm{I}}}$)	**total**		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	-349.11	371.55 (38.95)	-10.18 (2.19)	12.26	3.23	15.49
	BPc-1	-286.14	308.29 (-)	-9.97 (-)	12.18	3.36	15.53
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	-428.74	383.03 (153.49)	18.60 (5.75)	-27.11	11.08	-16.03
	BPc-1	-120.06	73.78 (-)	18.58 (-)	-27.7	9.43	-18.27
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	-428.74	383.03 (153.49)	18.60 (5.75)	-27.11	6.62	-20.50
	BPc-1	-120.06	73.78 (-)	18.58 (-)	-27.7	5.19	-22.51
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	349.11	-371.55 (-38.95)	10.18 (-2.19)	-12.26	0.76	-11.50
	BPc-1	286.14	-308.29 (-)	9.97 (-)	-12.18	-0.09	-12.27
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.18	-0.18
	BPc-1	-	-	-	-	-0.19	-0.19
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.49	-0.49
	BPc-1	-	-	-	-	-0.52	-0.52
$\langle CA\|\hat{H}\|TT\rangle$	BPc	755.87	-780.40 (-373.70)	18.32 (5.80)	-6.21	-40.83	-47.04
	BPc-1	545.95	-571.15 (-)	19.17 (-)	-6.03	-44.27	-50.30
$\langle AC\|\hat{H}\|TT\rangle$	BPc	607.79	-581.54 (-510.34)	-11.58 (1.87)	14.67	12.39	27.05
	BPc-1	192.04	-165.71 (-)	-11.27 (-)	15.06	11.81	26.87

Table S23. Energies of five diabatic states of BPc at 2.5 ns in MD simulation. (eV)

	$\boldsymbol{E_{S_0S_1}}$	$\boldsymbol{E_{S_1S_0}}$	$\boldsymbol{E_{CA}}$	$\boldsymbol{E_{AC}}$	$\boldsymbol{E_{TT}}$
BPc	2.76	2.81	3.60	3.54	1.70
BPc-1	2.86	2.89	3.57	3.77	1.81

Table S24. Decomposition of electronic coupling of BPc at 3.0 ns in MD simulation. (meV)

		F				g	V
		h	$2J$ ($2J^{\mathrm{l}}$)	$-K$ ($-K^{\mathrm{l}}$)	total		
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{CA}\rangle$	BPc	1218.31	-1301.44 (259.90)	13.22 (-14.66)	-69.91	2.53	-67.39
	BPc-1	1325.20	-1405.40 (-)	13.26 (-)	-66.94	-1.00	-67.93
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{AC}\rangle$	BPc	-965.47	1010.87 (738.37)	-9.62 (-2.49)	35.78	-3.25	32.52
	BPc-1	-250.86	305.05 (-)	-12.91 (-)	41.28	-6.36	34.91
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{CA}\rangle$	BPc	-965.47	1010.87 (738.37)	-9.62 (-2.49)	35.78	23.46	59.24
	BPc-1	-250.86	305.05 (-)	-12.91 (-)	41.28	24.67	65.94
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{AC}\rangle$	BPc	-1218.31	1301.44 (-259.90)	-13.22 (14.66)	69.91	24.08	94.00
	BPc-1	-1325.20	1405.40 (-)	-13.26 (-)	66.94	24.63	91.56
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{TT}\rangle$	BPc	-	-	-	-	0.64	0.64
	BPc-1	-	-	-	-	0.69	0.69
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{TT}\rangle$	BPc	-	-	-	-	-0.78	-0.78
	BPc-1	-	-	-	-	-0.78	-0.78
$\langle \mathrm{CA}\vert\hat{H}\vert\mathrm{TT}\rangle$	BPc	59.73	-65.01 (-58.46)	-2.60 (-2.15)	-7.88	-5.40	-13.28
	BPc-1	-65.41	52.41 (-)	0.98 (-)	-12.02	-9.13	-21.14
$\langle \mathrm{AC}\vert\hat{H}\vert\mathrm{TT}\rangle$	BPc	962.90	-968.14 (-493.16)	5.64 (5.64)	0.4	-28.43	-28.03
	BPc-1	588.51	-585.45 (-)	0.98 (-)	4.04	-25.32	-21.28

Table S25. Energies of five diabatic states of BPc at 3.0 ns in MD simulation. (eV)

	$E_{\mathrm{S_0S_1}}$	$E_{\mathrm{S_1S_0}}$	E_{CA}	E_{AC}	E_{TT}
BPc	2.78	2.80	3.37	3.34	1.53
BPc-1	2.86	2.86	3.53	3.32	1.61

Table S26. Decomposition of electronic coupling of BPc at 3.5 ns in MD simulation. (meV)

		F				***g***	***V***
		$\boldsymbol{h}$	$\boldsymbol{2J\ (2J^{\mathrm{I}})}$	$\boldsymbol{-K\ (-K^{\mathrm{I}})}$	**total**		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	-637.68	711.38 (-161.38)	-23.86 (1.21)	49.84	-1.95	47.89
	BPc-1	-829.14	901.20 (-)	-23.03 (-)	49.03	0.30	49.32
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	625.82	-565.79 (-77.08)	-22.64 (-10.46)	37.39	-13.65	23.73
	BPc-1	405.86	-350.05 (-)	-18.94 (-)	36.87	-13.04	23.82
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	625.82	-565.79 (-77.08)	-22.64 (-10.46)	37.39	-19.54	17.84
	BPc-1	405.86	-350.05 (-)	-18.94 (-)	36.87	-20.68	16.19
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	637.68	-711.38 (161.38)	23.86 (-1.21)	-49.84	-15.36	-65.20
	BPc-1	829.14	-901.20 (-)	23.03 (-)	-49.03	-15.42	-64.45
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-1.33	-1.33
	BPc-1	-	-	-	-	-1.32	-1.32
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	0.30	0.30
	BPc-1	-	-	-	-	0.27	0.27
$\langle CA\|\hat{H}\|TT\rangle$	BPc	44.56	-67.45 (-141.51)	12.96 (3.72)	-9.93	-11.33	-21.26
	BPc-1	60.37	-83.89 (-)	14.09 (-)	-9.43	-16.28	-25.70
$\langle AC\|\hat{H}\|TT\rangle$	BPc	33.32	-82.45 (472.02)	34.68 (-0.60)	-14.45	-48.54	-62.99
	BPc-1	437.85	-487.32 (-)	34.35 (-)	-15.12	-47.84	-62.96

Table S27. Energies of five diabatic states of BPc at 3.5 ns in MD simulation. (eV)

	$\boldsymbol{E_{S_0S_1}}$	$\boldsymbol{E_{S_1S_0}}$	$\boldsymbol{E_{CA}}$	$\boldsymbol{E_{AC}}$	$\boldsymbol{E_{TT}}$
BPc	2.89	2.99	3.48	3.47	2.05
BPc-1	2.96	3.05	3.60	3.49	2.13

Table S28. Decomposition of electronic coupling of BPc at 4.0 ns in MD simulation. (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\mathbf{2}\boldsymbol{J}$ $(\mathbf{2}\boldsymbol{J}^{\mathbf{l}})$	$-\boldsymbol{K}$ $(-\boldsymbol{K}^{\mathbf{l}})$	**total**		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	-2622.36	2670.31 (893.43)	-11.24 (0.71)	36.70	34.98	71.68
	BPc-1	-1992.33	2042.37 (-)	-13.00 (-)	37.05	41.15	78.20
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	-720.17	540.63 (18.21)	64.29 (15.83)	-115.25	20.93	-94.32
	BPc-1	-544.92	359.21 (-)	63.88 (-)	-121.83	22.85	-98.98
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	-720.17	540.63 (18.21)	64.29 (15.83)	-115.25	31.67	-83.58
	BPc-1	-544.92	359.21 (-)	63.88 (-)	-121.83	33.89	-87.94
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	2622.36	-2670.31 (-893.43)	11.24 (-0.71)	-36.70	-25.49	-62.19
	BPc-1	1992.33	-2042.37 (-)	13.00 (-)	-37.05	-30.83	-67.87
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.34	-0.34
	BPc-1	-	-	-	-	-0.33	-0.33
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.38	-0.38
	BPc-1	-	-	-	-	-0.45	-0.45
$\langle CA\|\hat{H}\|TT\rangle$	BPc	2018.94	-1984.75 (-1061.38)	-17.70 (2.02)	16.49	-17.59	-1.11
	BPc-1	961.31	-920.77 (-)	-23.21 (-)	17.33	-12.80	4.53
$\langle AC\|\hat{H}\|TT\rangle$	BPc	1005.52	-970.00 (-405.05)	-11.41 (-3.97)	24.11	6.36	30.46
	BPc-1	558.00	-516.36 (-)	-15.52 (-)	26.12	10.80	36.92

Table S29. Energies of five diabatic states of BPc at 4.0 ns in MD simulation. (eV)

	$\boldsymbol{E}_{\mathbf{S_0S_1}}$	$\boldsymbol{E}_{\mathbf{S_1S_0}}$	$\boldsymbol{E}_{\mathbf{CA}}$	$\boldsymbol{E}_{\mathbf{AC}}$	$\boldsymbol{E}_{\mathbf{TT}}$
BPc	2.67	2.89	3.26	3.34	1.61
BPc-1	2.74	2.94	3.28	3.45	1.68

Table S30. Decomposition of electronic coupling of BPc at 4.5 ns in MD simulation. (meV)

		$\boldsymbol{F}$				$\boldsymbol{g}$	$\boldsymbol{V}$
		$\boldsymbol{h}$	$\boldsymbol{2J}$ $(\boldsymbol{2J^{\mathrm{I}}})$	$\boldsymbol{-K}$ $(\boldsymbol{-K^{\mathrm{I}}})$	total		
$\langle \mathrm{S_0S_1} \| \hat{H} \| \mathrm{CA} \rangle$	BPc	846.92	-1043.01 (17.98)	71.58 (-11.52)	-124.52	1.57	-122.95
	BPc-1	1196.77	-1409.64 (-)	80.44 (-)	-132.43	-7.82	-140.25
$\langle \mathrm{S_0S_1} \| \hat{H} \| \mathrm{AC} \rangle$	BPc	928.84	-731.66 (-190.06)	-80.32 (-25.95)	116.86	-18.12	98.74
	BPc-1	462.43	-250.80 (-)	-80.74 (-)	130.90	-22.43	108.47
$\langle \mathrm{S_1S_0} \| \hat{H} \| \mathrm{CA} \rangle$	BPc	928.84	-731.66 (-190.06)	-80.32 (-25.95)	116.86	-5.58	111.28
	BPc-1	462.43	-250.80 (-)	-80.74 (-)	130.90	-10.02	120.87
$\langle \mathrm{S_1S_0} \| \hat{H} \| \mathrm{AC} \rangle$	BPc	-846.92	1043.01 (-17.98)	-71.58 (11.52)	124.52	4.57	129.09
	BPc-1	-1196.77	1409.64 (-)	-80.44 (-)	132.43	13.07	145.50
$\langle \mathrm{S_0S_1} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-	-	-	-	0.59	0.59
	BPc-1	-	-	-	-	0.58	0.58
$\langle \mathrm{S_1S_0} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-	-	-	-	0.03	0.03
	BPc-1	-	-	-	-	0.05	0.05
$\langle \mathrm{CA} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-340.00	335.05 (232.34)	-2.34 (-1.43)	-7.29	0.89	-6.40
	BPc-1	-132.45	130.67 (-)	-5.07 (-)	-6.85	0.62	-6.23
$\langle \mathrm{AC} \| \hat{H} \| \mathrm{TT} \rangle$	BPc	-391.41	378.10 (178.18)	4.19 (-2.25)	-9.12	1.08	-8.04
	BPc-1	-344.56	329.00 (-)	4.16 (-)	-11.4	0.79	-10.61

Table S31. Energies of five diabatic states of BPc at 4.5 ns in MD simulation. (eV)

	$\boldsymbol{E_{\mathrm{S_0S_1}}}$	$\boldsymbol{E_{\mathrm{S_1S_0}}}$	$\boldsymbol{E_{\mathrm{CA}}}$	$\boldsymbol{E_{\mathrm{AC}}}$	$\boldsymbol{E_{\mathrm{TT}}}$
BPc	2.88	3.00	3.18	3.18	2.08
BPc-1	2.94	3.07	3.22	3.27	2.14

Table S32. Decomposition of electronic coupling of BPc at 5.0 ns in MD simulation. (meV)

		F				g	V
		h	$2J$ ($2J^{\text{I}}$)	$-K$ ($-K^{\text{I}}$)	total		
$\langle S_0S_1\|\hat{H}\|CA\rangle$	BPc	849.94	-958.31 (29.47)	42.13 (-9.61)	-66.27	-6.63	-72.86
	BPc-1	1487.79	-1620.94 (-)	60.72 (-)	-72.43	-20.56	-92.99
$\langle S_0S_1\|\hat{H}\|AC\rangle$	BPc	-844.93	1074.09 (756.43)	-98.34 (-27.66)	130.82	6.14	136.96
	BPc-1	-800.16	1052.32 (-)	-108.06 (-)	144.1	7.71	151.81
$\langle S_1S_0\|\hat{H}\|CA\rangle$	BPc	-844.93	1074.09 (756.43)	-98.34 (-27.66)	130.82	8.45	139.27
	BPc-1	-800.16	1052.32 (-)	-108.06 (-)	144.1	11.48	155.58
$\langle S_1S_0\|\hat{H}\|AC\rangle$	BPc	-849.94	958.31 (-29.47)	-42.13 (9.61)	66.24	9.52	75.75
	BPc-1	-1487.79	1620.94 (-)	-60.72 (-)	72.43	22.91	95.34
$\langle S_0S_1\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.1	-0.1
	BPc-1	-	-	-	-	-0.07	-0.07
$\langle S_1S_0\|\hat{H}\|TT\rangle$	BPc	-	-	-	-	-0.04	-0.04
	BPc-1	-	-	-	-	-0.15	-0.15
$\langle CA\|\hat{H}\|TT\rangle$	BPc	-410.18	415.55 (76.94)	-5.97 (2.47)	-0.6	25.51	24.91
	BPc-1	-325.30	329.61 (-)	-4.07 (-)	0.24	27.76	28.00
$\langle AC\|\hat{H}\|TT\rangle$	BPc	620.76	-611.50 (-281.04)	-4.04 (3.59)	5.22	-3.72	1.51
	BPc-1	381.06	-359.59 (-)	-11.70 (-)	9.77	3.17	12.93

Table S33. Energies of five diabatic states of BPc at 5.0 ns in MD simulation. (eV)

	$E_{S_0S_1}$	$E_{S_1S_0}$	E_{CA}	E_{AC}	E_{TT}
BPc	2.73	2.70	2.97	2.82	1.32
BPc-1	2.67	2.66	2.95	2.91	1.36

Table S34. Effective electronic couplings ($|V_{\text{eff}}|^2$), time constants (τ) of singlet fission in bipentacene systems. $|V_{\text{eff}}|_{10}^2$ is the average effective electronic coupling at 10 molecular dynamics snapshots. The initial states for $|V_{\text{eff}}|_S^2$ (eV^2) and τ_S (fs) calculation are the linear combination of two local excited states with the largest transition dipole.

	$|V_{\text{eff}}|_{10}^2$ (meV^2)	$|V_{\text{eff}}|_S^2$ (meV^2)	τ (ps)	τ_S (ps)	τ_{exp} (ps)
BPc	10.41	9.26	10.3	11.5	13.8
BP1	0.21	0.21	228.8	228.8	20.0

4. Molecular design

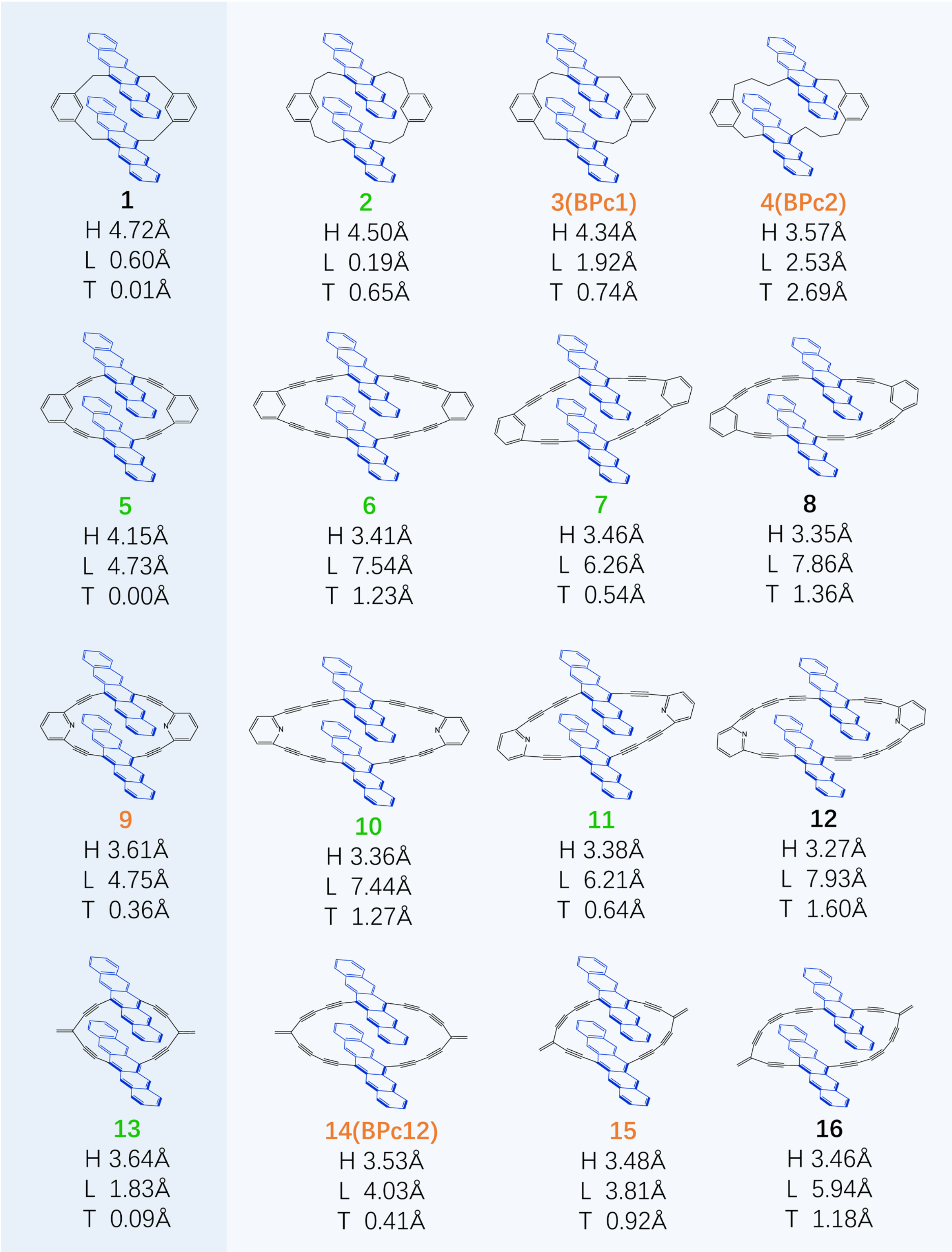
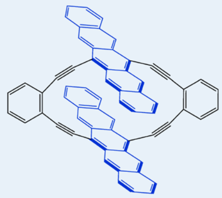
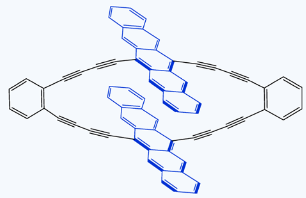


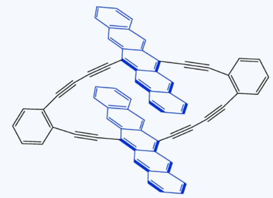
Figure S8



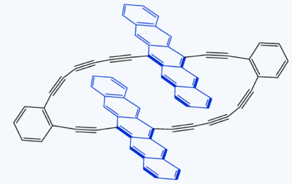
17
H 3.49Å
L 1.55Å
T 0.02Å



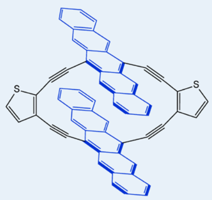
18
H 3.38Å
L 3.66Å
T 0.37Å



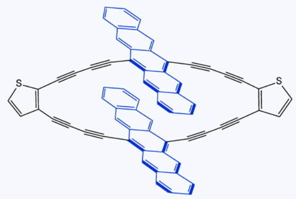
19
H 3.42Å
L 3.42Å
T 1.17Å



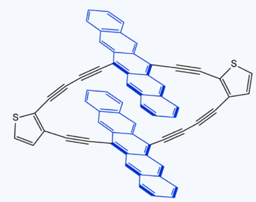
20
H 3.51Å
L 4.36Å
T 3.29Å



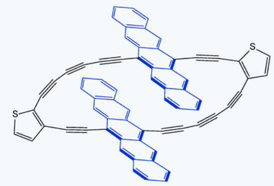
21
H 3.54Å
L 1.74Å
T 0.00Å



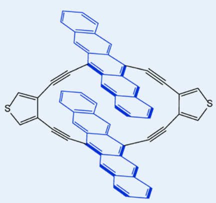
22
H 3.41Å
L 3.71Å
T 0.35Å



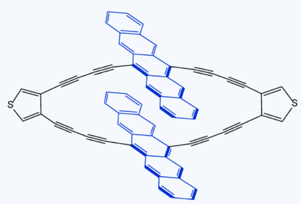
23
H 3.41Å
L 3.56Å
T 1.14Å



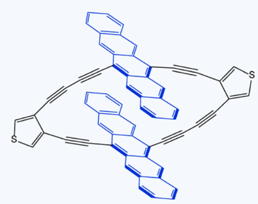
24
H 3.48Å
L 4.67Å
T 3.15Å



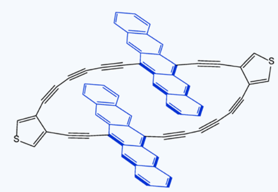
25
H 3.46Å
L 1.50Å
T 0.02Å



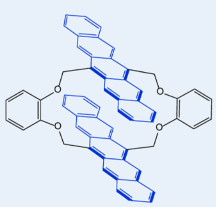
26
H 3.39Å
L 3.66Å
T 0.49Å



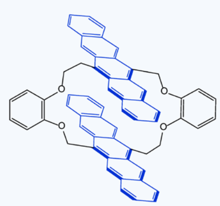
27
H 3.44Å
L 3.43Å
T 1.18Å



28
H 3.51Å
L 4.39Å
T 3.31Å



29
H 3.44Å
L 1.46Å
T 0.37Å



30
H 3.38Å
L 3.48Å
T 0.74Å

Figure S8 (continued)

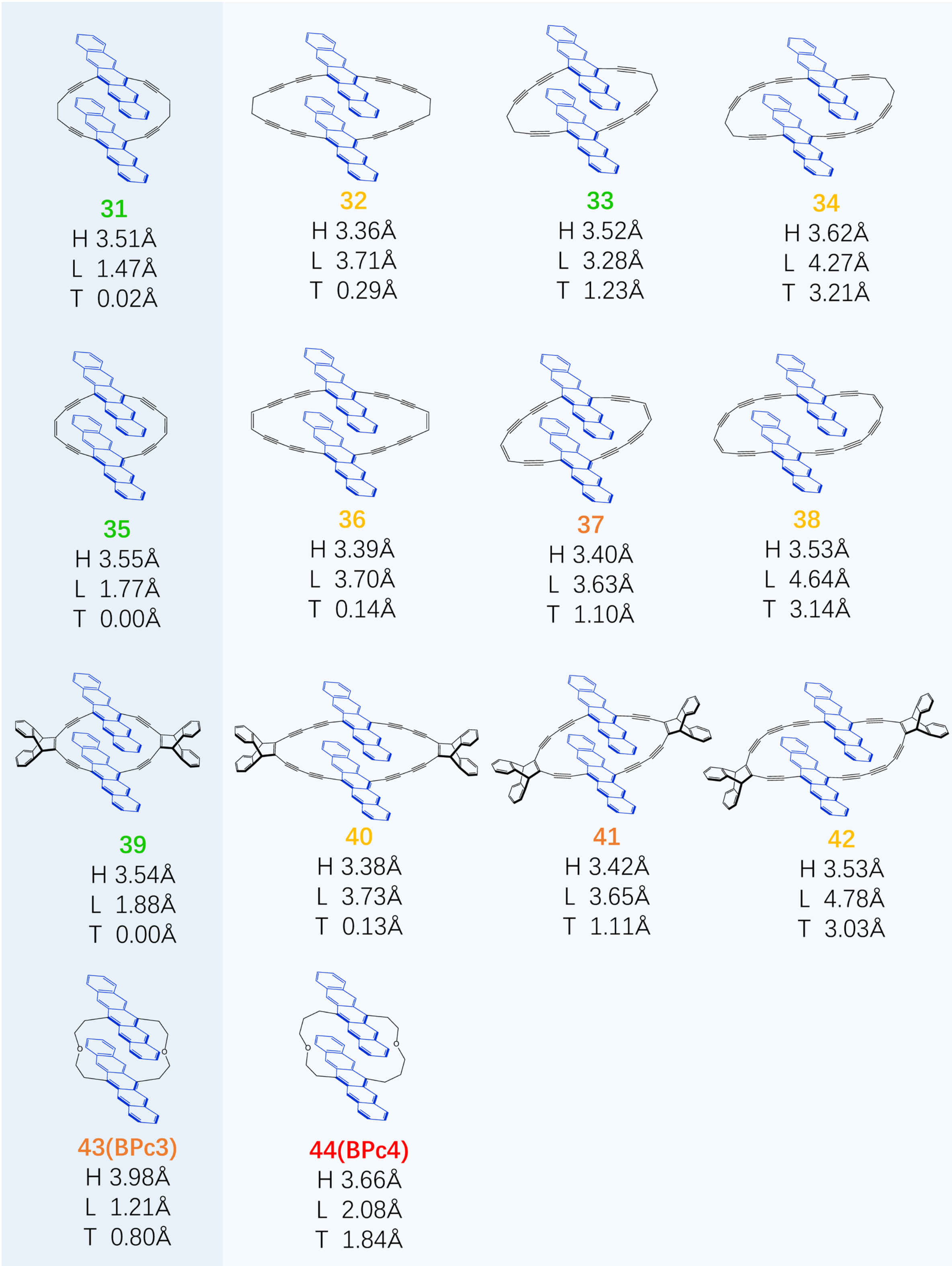
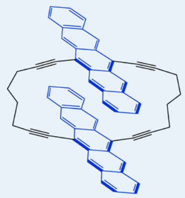
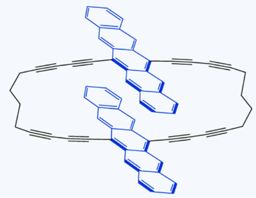


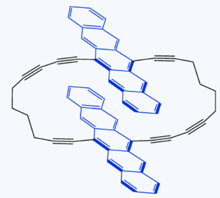
Figure S8 (continued)



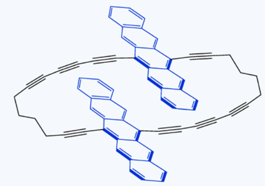
45
H 3.31Å
L 1.11Å
T 0.24Å



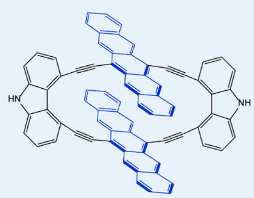
46(BPc13)
H 3.36Å
L 3.56Å
T 0.66Å



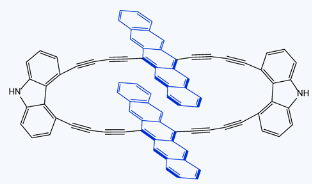
47
H 3.45Å
L 3.57Å
T 1.16Å



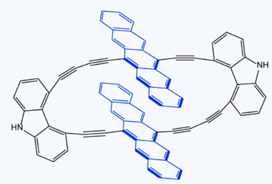
48
H 3.48Å
L 2.36Å
T 3.99Å



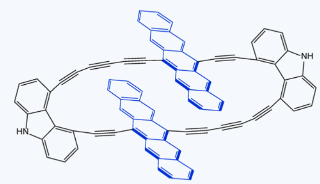
49
H 3.23Å
L 0.98Å
T 0.14Å



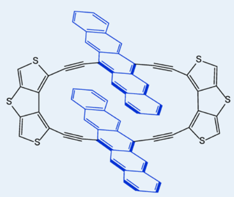
50
H 3.30Å
L 1.11Å
T 0.16Å



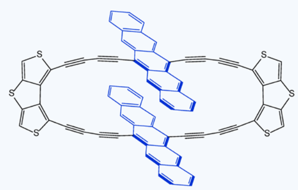
51(BPc5)
H 3.43Å
L 1.54Å
T 1.55Å



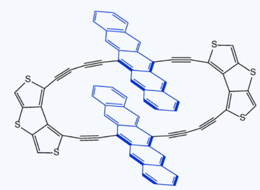
52
H 3.49Å
L 0.84Å
T 4.69Å



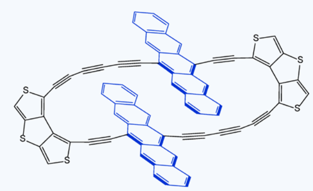
53
H 3.23Å
L 1.10Å
T 0.14Å



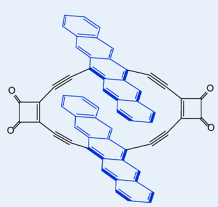
54
H 3.27Å
L 1.14Å
T 0.16Å



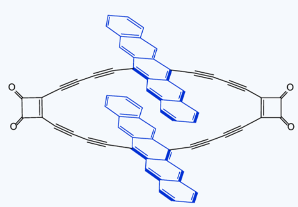
55(BPc6)
H 3.39Å
L 1.89Å
T 1.53Å



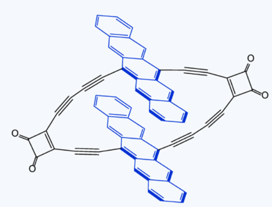
56
H 3.45Å
L 1.07Å
T 4.73Å



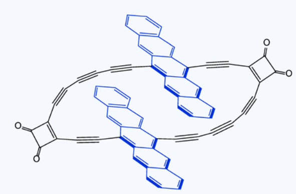
57
H 3.33Å
L 3.32Å
T 0.00Å



58
H 3.39Å
L 3.75Å
T 0.21Å

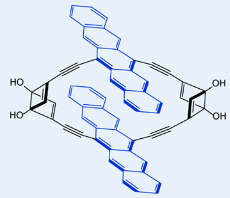


59(BPc10)
H 3.39Å
L 3.87Å
T 1.10Å

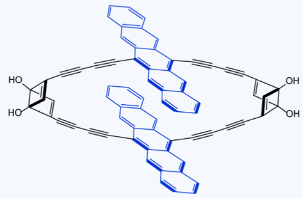


60
H 3.49Å
L 5.03Å
T 2.97Å

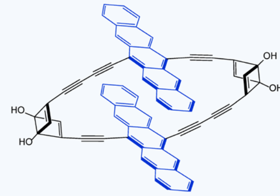
Figure S8 (continued)



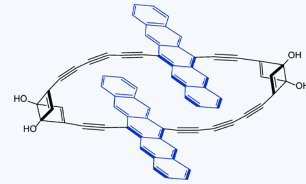
61
H 3.63Å
L 3.99Å
T 0.04Å



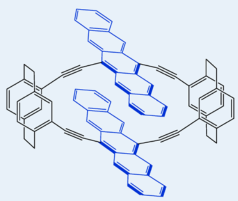
62
H 3.57Å
L 6.20Å
T 0.31Å



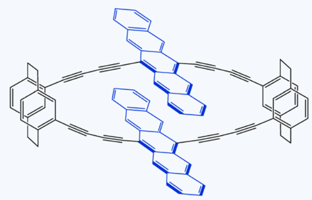
63
H 3.53Å
L 5.99Å
T 0.74Å



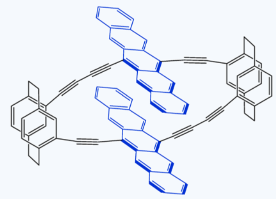
64
H 3.60Å
L 7.60Å
T 1.68Å



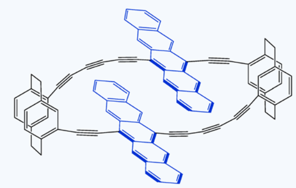
65
H 3.36Å
L 3.52Å
T 0.00Å



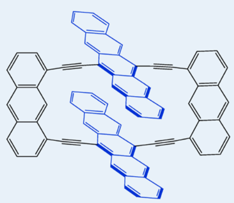
66
H 3.35Å
L 3.64Å
T 0.54Å



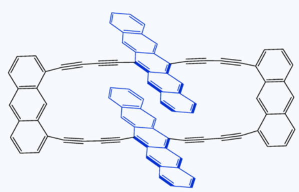
67(BPc11)
H 3.43Å
L 3.64Å
T 1.00Å



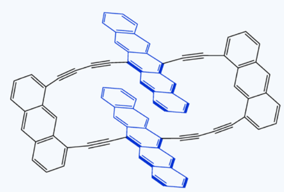
68
H 3.59Å
L 3.47Å
T 3.49Å



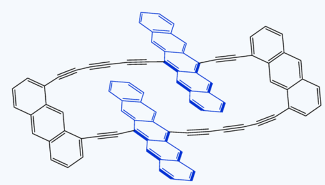
69(BPc14)
H 3.42Å
L 3.80Å
T 0.53Å



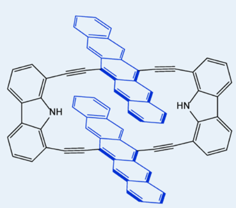
70(BPc15)
H 3.40Å
L 3.68Å
T 0.65Å



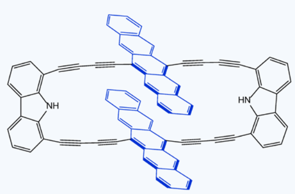
71(BPc16)
H 3.44Å
L 3.78Å
T 1.30Å



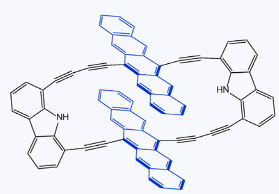
72
H 3.38Å
L 3.75Å
T 3.93Å



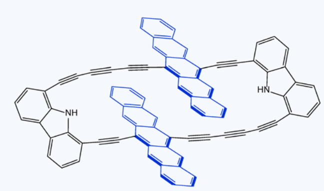
73(BPc17)
H 3.57Å
L 4.65Å
T 0.56Å



74(BPc18)
H 3.44Å
L 3.85Å
T 0.75Å

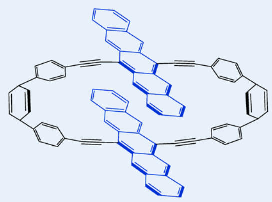


75(BPc19)
H 3.51Å
L 4.91Å
T 1.45Å



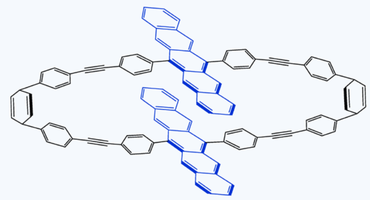
76
H 3.42Å
L 4.77Å
T 3.64Å

Figure S8 (continued)



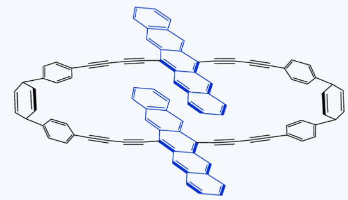
77

H 3.45Å
L 3.55Å
T 0.37Å



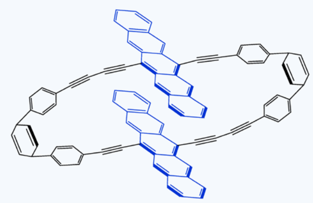
78

H 3.55Å
L 6.10Å
T 0.00Å



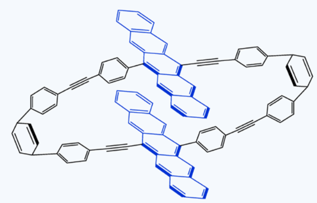
79

H 3.39Å
L 3.46Å
T 0.49Å



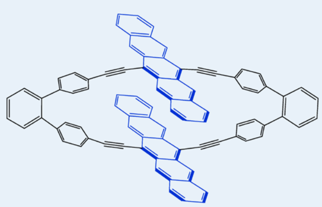
80(BPc7)

H 3.42Å
L 1.63Å
T 1.37Å



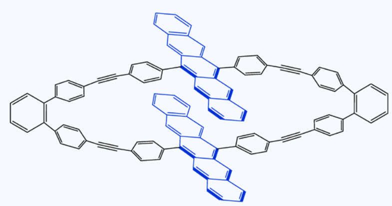
81

H 4.27Å
L 3.54Å
T 2.92Å



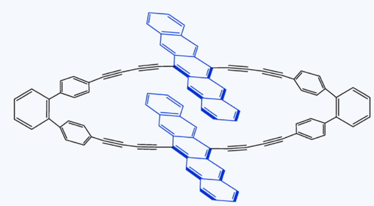
82(BPc9)

H 3.39Å
L 3.76Å
T 0.71Å



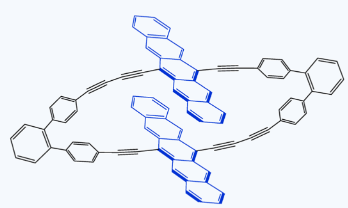
83

H 3.53Å
L 6.13Å
T 0.00Å



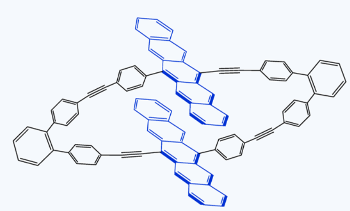
84

H 3.43Å
L 3.76Å
T 0.76Å



85

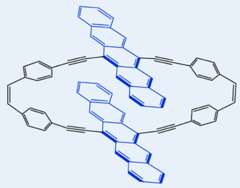
H 3.51Å
L 3.88Å
T 1.21Å



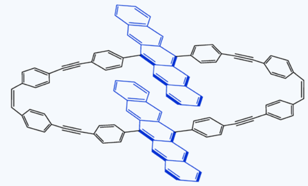
86

H 4.82Å
L 4.09Å
T 4.56Å

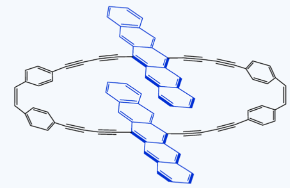
Figure S8 (continued)



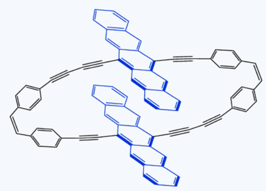
87(BPc8)
H 3.50Å
L 3.88Å
T 0.58Å



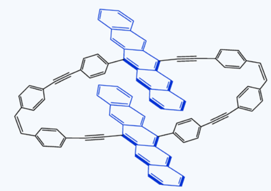
88
H 3.98Å
L 3.93Å
T 0.00Å



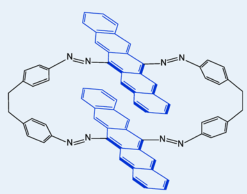
89
H 3.47Å
L 6.06Å
T 0.73Å



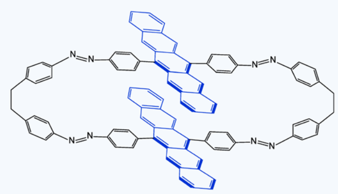
90
H 3.44Å
L 6.20Å
T 0.98Å



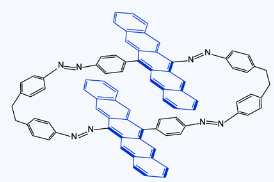
91
H 4.27Å
L 1.76Å
T 3.71Å



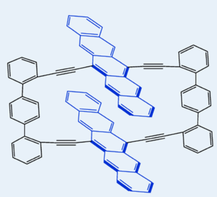
92
H 3.23Å
L 3.49Å
T 0.20Å



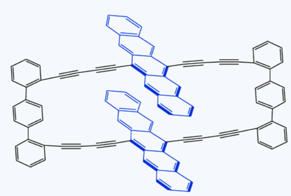
93
H 4.18Å
L 3.18Å
T 0.20Å



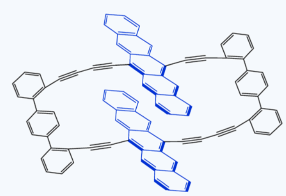
94
H 4.09Å
L 3.95Å
T 3.05Å



95
H 3.45Å
L 5.78Å
T 0.16Å



96
H 3.45Å
L 3.33Å
T 0.64Å



97
H 3.82Å
L 4.51Å
T 2.43Å

Figure S8. The designed bipentacene macrocycles for iSF. In parentheses are the labels of the corresponding molecules in the main text. According to the regions of Fig. 5b in the main text where the slipped distance (T/L) is located, use the same colour label.

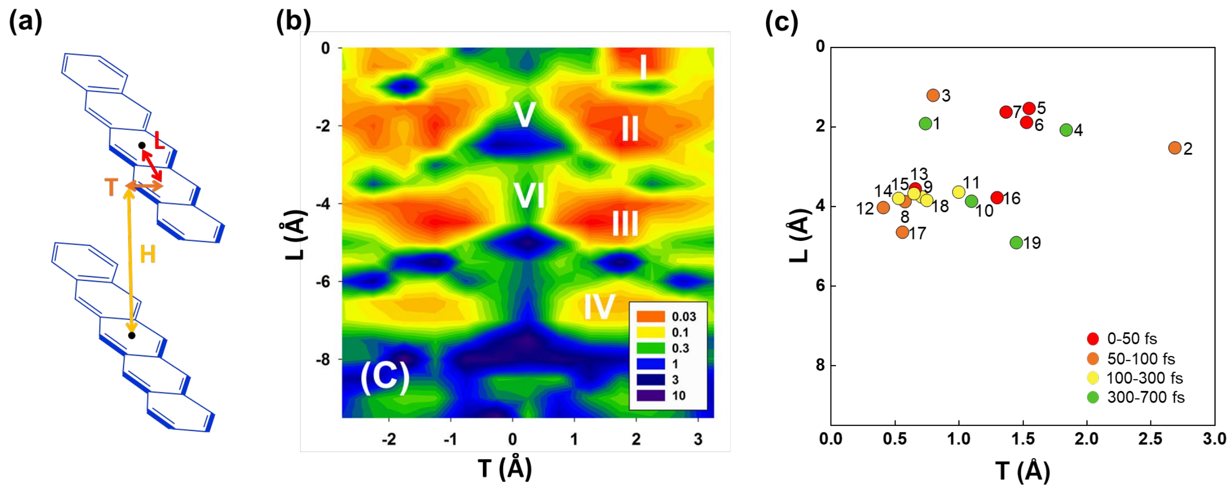


Figure S9. Model molecular packing in designed bipentacene macrocycles. H, L and T are the slipped distances between the centre of mass of the two pentacenes along the vertical, longitudinal and transverse axes, respectively. (b) Relationship between SF time constant (in ps) and pentacene slipped distances (H = 3.4 Å). Reproduced with permission 29. Copyright 2014, American Chemical Society. (c) SF time constants of 19 screened bipentacene macrocycles, calculated with the initial state being the linear combination of two local excited states with the largest transition dipole.

Table S35. Electronic couplings $\langle i|\hat{H}|j\rangle$ ($i \neq j$, meV), energies $\langle i|\hat{H}|i\rangle$ (eV), averaged effective electron couplings $|V_{\text{eff}}|^2_{10}$ (eV^2) and SF time constants τ (fs) of nineteen bipentacene macrocycles. The initial states for $|V_{\text{eff}}|^2_S$ (eV^2) and τ_S (fs) calculation are the linear combination of two local excited states with the largest transition dipole. Variances (eV^4) are calculated by $s^2 = \frac{\sum(V_{\text{eff}}-\bar{V}_{\text{eff}})^2}{N}$.

	0.5 ns	1.0 ns	1.5 ns	2.0 ns	2.5 ns	3.0 ns	3.5 ns	4.0 ns	4.5 ns	5.0 ns
					BPc1					
$\langle S_0S_1|\hat{H}|CA\rangle$	-44.63	46.30	50.26	-35.75	-39.21	42.82	73.90	108.82	20.42	-34.27
$\langle S_0S_1|\hat{H}|AC\rangle$	44.19	141.33	127.52	64.88	57.92	89.44	73.07	110.84	46.16	58.59
$\langle S_1S_0|\hat{H}|CA\rangle$	-43.02	-138.27	-131.18	-61.76	-59.16	-79.36	-69.53	-106.28	-37.88	-57.01
$\langle S_1S_0|\hat{H}|AC\rangle$	40.25	-44.87	-45.42	36.41	38.98	-47.01	-83.73	-119.05	-27.28	31.66
$\langle S_0S_1|\hat{H}|TT\rangle$	-1.20	-0.36	1.24	-1.09	-1.88	-0.80	-2.14	1.74	0.14	-1.70
$\langle S_1S_0|\hat{H}|TT\rangle$	0.49	0.05	0.76	1.18	0.02	-0.93	1.35	-1.65	0.18	1.96
$\langle CA|\hat{H}|TT\rangle$	-62.74	-11.25	137.10	-69.55	-118.20	67.83	114.66	-75.03	-88.28	-99.70
$\langle AC|\hat{H}|TT\rangle$	-10.04	-112.93	20.41	-58.23	0.86	168.87	155.81	-134.75	-147.56	-59.30
$\langle S_0S_1|\hat{H}|S_0S_1\rangle$	2.79	2.67	2.64	2.72	2.76	2.69	2.52	2.59	2.87	2.64
$\langle S_1S_0|\hat{H}|S_1S_0\rangle$	2.83	2.66	2.67	3.00	2.98	2.71	2.81	2.77	2.79	2.85
$\langle CA|\hat{H}|CA\rangle$	3.30	2.87	3.00	3.27	3.31	3.10	3.20	3.30	3.32	3.19
$\langle AC|\hat{H}|AC\rangle$	3.31	2.88	2.96	3.39	3.43	3.05	3.23	3.00	3.29	3.15
$\langle TT|\hat{H}|TT\rangle$	1.86	1.37	1.29	1.87	1.82	1.49	1.57	1.52	1.62	1.55
$|V_{\text{eff}}|^2_{10}$ (variance)					1.82×10^{-4} (4.27×10^{-8})					
τ					587.0					
$|V_{\text{eff}}|^2_S$ (variance)					2.66×10^{-4} (8.66×10^{-8})					

τ_S	401.2									
BPc2										
$\langle S_0S_1\|\hat{H}\|CA\rangle$	31.31	4.64	20.78	-13.23	41.19	0.48	26.01	34.26	23.18	21.37
$\langle S_0S_1\|\hat{H}\|AC\rangle$	158.65	120.31	84.97	85.34	-58.56	151.21	163.26	96.85	145.44	-15.89
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-147.34	-99.73	-67.51	-68.19	83.08	-150.91	-156.50	-115.34	-157.07	56.46
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-27.76	-10.77	-17.77	10.90	-42.22	-2.21	-29.25	-34.47	-21.10	-23.22
$\langle S_0S_1\|\hat{H}\|TT\rangle$	-0.30	1.30	-2.68	-0.72	-1.74	-0.73	-1.29	0.79	-1.78	-47.14
$\langle S_1S_0\|\hat{H}\|TT\rangle$	4.22	-0.77	2.04	0.82	-0.91	-0.26	2.47	-0.39	0.62	-66.26
$\langle CA\|\hat{H}\|TT\rangle$	321.93	154.97	-114.89	-131.87	-4.33	-112.31	247.23	-125.27	103.26	3.11
$\langle AC\|\hat{H}\|TT\rangle$	211.01	75.30	92.51	-11.49	-193.18	-83.76	198.08	-147.64	175.07	35.05
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.80	2.91	2.84	2.95	2.92	2.97	2.76	2.77	3.04	3.09
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	2.80	2.79	2.96	2.95	2.96	3.07	2.81	3.15	3.03	3.35
$\langle CA\|\hat{H}\|CA\rangle$	3.15	3.32	3.35	3.35	3.41	3.54	3.11	3.42	3.47	2.73
$\langle AC\|\hat{H}\|AC\rangle$	3.12	3.16	3.35	3.40	3.26	3.51	3.12	3.43	3.56	3.02
$\langle TT\|\hat{H}\|TT\rangle$	1.55	1.57	1.80	1.89	1.86	2.20	1.45	1.92	2.12	4.72
$\|V_{eff}\|^2_{10}$ (variance)	9.89×10^{-4} (1.60×10^{-6})									
τ	108.1									
$\|V_{eff}\|^2_S$ (variance)	1.25×10^{-3} (3.01×10^{-6})									
τ_S	85.7									
BPc3										
$\langle S_0S_1\|\hat{H}\|CA\rangle$	273.96	238.44	244.26	207.77	231.10	222.63	194.12	237.42	251.79	153.89
$\langle S_0S_1\|\hat{H}\|AC\rangle$	306.66	203.11	200.11	274.16	251.34	288.58	238.55	280.20	202.87	92.51
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-305.25	-202.18	-196.25	-262.03	-258.13	-272.92	-249.80	-257.51	-203.92	-98.18
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-283.10	-244.50	-245.61	-216.73	-222.23	-236.47	-193.82	-265.90	-248.56	-141.65
$\langle S_0S_1\|\hat{H}\|TT\rangle$	-0.46	-0.61	-3.39	-0.24	1.30	0.98	1.80	-5.62	-1.25	2.64
$\langle S_1S_0\|\hat{H}\|TT\rangle$	0.19	0.72	1.77	-1.67	-0.70	-0.85	0.16	3.39	3.33	-2.74
$\langle CA\|\hat{H}\|TT\rangle$	33.41	-1.38	32.71	-83.10	-28.08	68.70	-75.97	65.95	94.08	-96.22
$\langle AC\|\hat{H}\|TT\rangle$	-55.05	-35.42	34.92	86.73	43.43	13.34	-39.05	60.84	-92.17	7.81
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.93	2.78	2.80	3.13	2.89	2.94	2.83	2.71	2.88	3.02
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	2.99	3.01	2.75	2.86	2.84	2.82	2.85	3.13	2.97	2.97
$\langle CA\|\hat{H}\|CA\rangle$	2.89	2.84	2.74	2.92	2.78	2.78	2.78	2.92	2.81	2.72
$\langle AC\|\hat{H}\|AC\rangle$	3.10	2.88	2.68	2.92	2.80	2.73	2.73	2.79	2.88	2.92
$\langle TT\|\hat{H}\|TT\rangle$	1.82	1.66	1.39	1.93	1.52	1.45	1.58	1.79	1.91	1.85
$\|V_{eff}\|^2_{10}$ (variance)	1.14×10^{-3} (3.14×10^{-6})									
τ	94.1									
$\|V_{eff}\|^2_S$ (variance)	1.19×10^{-3} (2.50×10^{-6})									
τ_S	89.7									
BPc4										
$\langle S_0S_1\|\hat{H}\|CA\rangle$	50.06	0.22	5.84	-24.34	96.78	-7.82	62.11	33.07	-31.49	73.12
$\langle S_0S_1\|\hat{H}\|AC\rangle$	-19.08	-37.33	-19.49	-167.76	38.11	40.99	131.55	79.42	71.98	57.28
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-3.53	31.62	24.80	157.31	-46.75	-28.52	-133.51	-78.86	-64.20	-54.68
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-38.37	6.36	-26.34	30.79	-99.04	3.20	-77.42	-32.59	27.58	-75.50
$\langle S_0S_1\|\hat{H}\|TT\rangle$	-5.10	-3.70	-0.57	2.01	2.96	-0.58	-1.18	0.27	1.12	2.07
$\langle S_1S_0\|\hat{H}\|TT\rangle$	0.25	0.08	1.21	-0.45	-0.34	0.24	1.24	-1.05	1.29	-3.27
$\langle CA\|\hat{H}\|TT\rangle$	-103.67	-5.32	111.86	57.93	-6.45	-68.10	2.85	-180.13	133.53	-77.26
$\langle AC\|\hat{H}\|TT\rangle$	186.63	89.98	-170.28	-97.40	-138.91	-176.58	78.02	-211.27	126.44	-41.28
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.75	2.92	2.89	2.90	2.78	2.95	2.83	2.72	2.97	2.71
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	3.04	2.97	2.89	3.03	3.00	3.01	2.92	2.71	3.05	2.99
$\langle CA\|\hat{H}\|CA\rangle$	2.90	2.96	3.01	3.12	2.96	3.33	2.98	2.75	3.17	2.97

$\langle \mathrm{AC}|\hat{H}|\mathrm{AC}\rangle$	2.80	3.12	2.98	3.14	2.91	3.23	2.92	2.61	3.18	2.94
$\langle \mathrm{TT}|\hat{H}|\mathrm{TT}\rangle$	1.73	1.89	1.70	1.94	1.63	2.04	1.76	1.15	2.18	1.59
$|V_{\mathrm{eff}}|^2_{10}$ (variance)	2.17×10^{-4} (6.76×10^{-8})									
τ	493.7									
$|V_{\mathrm{eff}}|^2_{S}$ (variance)	2.60×10^{-4} (1.65×10^{-7})									
τ_S	410.9									
BPc5										
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle$	-130.74	-91.43	-58.16	20.19	5.06	-27.25	-34.26	-23.70	-99.64	-20.29
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{AC}\rangle$	287.22	262.74	142.26	47.47	310.18	49.40	257.96	246.04	285.83	303.12
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{CA}\rangle$	-296.38	-266.99	-125.27	-58.13	-295.10	-25.48	-253.63	-246.11	-287.16	-305.06
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{AC}\rangle$	136.03	77.33	78.62	11.42	-5.90	-9.04	21.51	30.80	99.82	12.73
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{TT}\rangle$	2.90	0.95	-1.38	6.50	-2.00	-6.58	-3.85	2.63	2.19	-4.29
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{TT}\rangle$	-2.37	2.57	1.00	-4.65	3.07	10.24	2.87	-3.60	-4.51	5.04
$\langle \mathrm{CA}|\hat{H}|\mathrm{TT}\rangle$	188.63	-243.23	-60.17	-18.77	11.63	-34.58	-197.56	168.38	181.63	-141.44
$\langle \mathrm{AC}|\hat{H}|\mathrm{TT}\rangle$	202.63	-268.70	-90.85	31.67	-327.26	-113.69	-117.97	228.56	248.66	-196.05
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{S_0S_1}\rangle$	2.87	2.88	2.75	3.20	3.08	3.09	2.97	2.94	2.77	2.89
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{S_1S_0}\rangle$	3.26	3.29	3.16	3.04	2.96	3.26	3.11	3.29	3.11	3.30
$\langle \mathrm{CA}|\hat{H}|\mathrm{CA}\rangle$	3.20	3.20	2.97	3.10	2.85	3.26	3.22	3.14	3.00	3.15
$\langle \mathrm{AC}|\hat{H}|\mathrm{AC}\rangle$	3.19	3.20	3.16	3.20	3.21	3.21	3.06	3.31	2.99	3.04
$\langle \mathrm{TT}|\hat{H}|\mathrm{TT}\rangle$	2.11	2.14	1.66	2.31	1.91	2.56	2.25	2.22	1.73	2.14
$|V_{\mathrm{eff}}|^2_{10}$ (variance)	5.08×10^{-3} (6.01×10^{-5})									
τ	21.0									
$|V_{\mathrm{eff}}|^2_{S}$ (variance)	4.23×10^{-3} (1.25×10^{-5})									
τ_S	25.2									
BPc6										
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle$	-26.10	-20.59	44.70	-17.38	43.76	-124.24	-49.92	50.90	-0.97	-99.05
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{AC}\rangle$	296.50	-46.29	260.57	296.25	181.15	336.39	232.91	391.29	300.17	285.66
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{CA}\rangle$	-293.22	27.84	-273.91	-309.79	-194.51	-327.10	-222.88	-393.64	-290.16	-300.90
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{AC}\rangle$	27.50	42.39	-45.54	20.39	-39.33	119.12	62.29	-43.65	9.95	99.20
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{TT}\rangle$	-4.83	-2.62	-1.33	-1.41	0.97	-6.12	-2.97	-7.65	2.20	2.42
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{TT}\rangle$	4.42	-2.78	3.91	0.15	-2.06	3.36	4.21	3.48	-6.47	-4.20
$\langle \mathrm{CA}|\hat{H}|\mathrm{TT}\rangle$	-205.33	-51.05	-154.19	-291.72	89.79	-254.82	-110.75	-354.62	121.76	202.63
$\langle \mathrm{AC}|\hat{H}|\mathrm{TT}\rangle$	-199.52	17.60	-224.71	5.65	184.15	-276.63	-131.56	-259.19	321.45	195.36
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{S_0S_1}\rangle$	2.72	2.68	2.73	2.71	2.74	2.74	2.73	2.89	2.65	2.82
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{S_1S_0}\rangle$	2.81	2.91	2.93	2.80	2.90	2.67	2.71	2.84	2.72	2.75
$\langle \mathrm{CA}|\hat{H}|\mathrm{CA}\rangle$	2.63	2.80	2.76	2.63	2.84	2.54	2.63	2.80	2.40	2.78
$\langle \mathrm{AC}|\hat{H}|\mathrm{AC}\rangle$	2.70	2.68	2.84	2.59	2.92	2.50	2.56	2.62	2.55	2.61
$\langle \mathrm{TT}|\hat{H}|\mathrm{TT}\rangle$	1.15	1.11	1.16	0.77	1.13	0.70	0.98	1.48	0.70	0.91
$|V_{\mathrm{eff}}|^2_{10}$ (variance)	9.24×10^{-3} (3.25×10^{-4})									
τ	11.6									
$|V_{\mathrm{eff}}|^2_{S}$ (variance)	1.38×10^{-2} (7.39×10^{-4})									
τ_S	7.8									
BPc7										
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle$	71.11	66.04	125.67	-94.57	210.87	72.04	112.27	125.93	36.17	109.35
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{AC}\rangle$	337.29	271.15	79.86	266.95	-257.59	-172.83	-180.15	-252.93	403.76	60.17
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{CA}\rangle$	-353.16	-257.18	-71.71	-262.67	243.19	185.63	199.43	254.57	-374.66	-56.48
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{AC}\rangle$	-72.68	-42.77	-127.35	112.32	-215.81	-83.33	-132.51	-119.65	-44.33	-104.19
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{TT}\rangle$	0.51	1.57	0.72	-7.56	2.38	-4.47	5.40	7.24	0.91	0.92

$\langle S_1S_0\|\hat{H}\|TT\rangle$	-5.84	-5.80	-0.77	3.88	-1.26	1.62	-3.51	-4.22	-2.91	-1.31
$\langle CA\|\hat{H}\|TT\rangle$	71.28	122.53	-4.82	-331.46	-311.92	116.82	-221.59	-237.57	250.37	46.09
$\langle AC\|\hat{H}\|TT\rangle$	270.90	-65.95	-27.48	-250.16	-268.38	216.07	-77.48	-118.01	212.37	-107.31
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.70	2.93	2.95	2.79	3.00	2.89	3.00	3.05	2.98	2.83
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	2.95	2.90	3.03	2.80	3.01	3.03	3.02	2.85	3.11	2.88
$\langle CA\|\hat{H}\|CA\rangle$	2.79	2.78	3.30	2.73	3.20	3.08	3.31	3.08	3.22	3.03
$\langle AC\|\hat{H}\|AC\rangle$	2.95	2.91	3.10	2.81	3.25	2.98	3.10	2.96	3.19	3.10
$\langle TT\|\hat{H}\|TT\rangle$	1.63	1.74	2.09	1.38	2.07	1.88	2.11	1.80	2.32	1.71
$\|V_{\text{eff}}\|^2_{10}$ (variance)	5.79×10^{-3} (1.20×10^{-4})									
τ	18.4									
$\|V_{\text{eff}}\|^2_{S}$ (variance)	8.22×10^{-3} (2.28×10^{-4})									
τ_S	13.0									
BPc8										
$\langle S_0S_1\|\hat{H}\|CA\rangle$	299.42	290.39	339.61	381.02	1.76	300.92	160.56	336.38	267.92	247.35
$\langle S_0S_1\|\hat{H}\|AC\rangle$	227.82	-28.79	292.80	296.07	269.56	349.73	377.24	-70.12	376.07	344.07
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-230.95	45.22	-310.01	-296.31	-312.63	-309.86	-344.60	79.41	-403.15	-346.57
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-289.72	-300.87	-324.84	-383.52	-0.67	-280.22	-161.97	-340.37	-261.98	-228.46
$\langle S_0S_1\|\hat{H}\|TT\rangle$	-2.89	3.96	1.88	1.16	2.79	-0.68	-0.22	3.88	-7.15	8.82
$\langle S_1S_0\|\hat{H}\|TT\rangle$	0.92	-2.39	1.29	3.51	0.05	-7.64	1.31	1.79	-9.76	-0.07
$\langle CA\|\hat{H}\|TT\rangle$	-77.23	-130.80	68.73	-15.60	-27.58	90.95	-0.07	-113.39	-9.96	-13.52
$\langle AC\|\hat{H}\|TT\rangle$	101.96	-1.01	-95.46	-10.06	108.67	-43.00	37.82	-24.93	31.37	192.52
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.74	2.93	2.80	2.75	2.78	2.88	2.96	2.88	2.81	2.66
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	3.13	2.96	2.83	2.76	3.03	2.96	2.90	2.94	3.02	2.67
$\langle CA\|\hat{H}\|CA\rangle$	3.04	3.15	2.89	2.87	3.03	3.09	3.10	3.06	2.96	2.61
$\langle AC\|\hat{H}\|AC\rangle$	3.12	3.10	2.85	2.91	2.89	3.03	3.13	3.11	2.94	2.78
$\langle TT\|\hat{H}\|TT\rangle$	2.03	2.02	1.70	1.77	1.83	2.09	2.09	1.91	1.89	1.27
$\|V_{\text{eff}}\|^2_{10}$ (variance)	1.03×10^{-3} (2.68×10^{-6})									
τ	103.8									
$\|V_{\text{eff}}\|^2_{S}$ (variance)	1.23×10^{-3} (3.50×10^{-6})									
τ_S	86.8									
BPc9										
$\langle S_0S_1\|\hat{H}\|CA\rangle$	346.89	182.98	366.98	318.94	235.88	36.89	309.97	334.25	284.11	288.21
$\langle S_0S_1\|\hat{H}\|AC\rangle$	212.58	78.74	-32.32	83.37	-178.20	-263.29	43.52	11.64	-118.03	145.60
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-234.27	-81.33	57.04	-79.56	158.80	261.02	-31.79	18.81	148.26	-144.09
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-344.41	-180.04	-383.74	-329.88	-246.28	-46.54	-320.10	-332.49	-255.00	-312.33
$\langle S_0S_1\|\hat{H}\|TT\rangle$	4.73	-0.19	0.67	-0.66	-1.23	0.73	-6.62	-2.20	-1.79	1.15
$\langle S_1S_0\|\hat{H}\|TT\rangle$	-3.62	-1.81	-2.60	-3.14	0.31	-6.10	-5.04	-0.05	3.66	2.05
$\langle CA\|\hat{H}\|TT\rangle$	15.54	-33.07	-108.04	50.59	38.07	-53.06	133.43	-5.62	162.87	-84.11
$\langle AC\|\hat{H}\|TT\rangle$	2.25	-31.22	6.44	-164.72	60.74	-125.12	-103.60	140.59	84.56	32.19
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.80	2.68	2.76	2.79	2.69	2.62	2.78	2.70	2.66	2.86
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	2.49	2.94	2.83	2.75	2.78	2.63	2.98	2.85	3.01	2.85
$\langle CA\|\hat{H}\|CA\rangle$	2.83	3.08	2.89	2.99	2.93	2.93	3.07	2.99	2.91	2.98
$\langle AC\|\hat{H}\|AC\rangle$	2.60	3.11	2.81	2.73	2.93	2.95	3.19	2.82	2.98	3.10
$\langle TT\|\hat{H}\|TT\rangle$	1.09	1.35	1.21	1.03	1.13	1.09	1.32	1.16	1.38	1.58
$\|V_{\text{eff}}\|^2_{10}$ (variance)	7.08×10^{-4} (9.54×10^{-7})									
τ	150.9									
$\|V_{\text{eff}}\|^2_{S}$ (variance)	5.49×10^{-4} (2.35×10^{-7})									
τ_S	194.8									

BPc10										
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{CA}\rangle$	29.33	66.97	-61.75	-53.39	-85.49	-12.81	99.63	50.18	36.15	-11.32
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{AC}\rangle$	146.42	-85.09	-195.06	-119.10	158.48	-157.34	75.07	-199.74	-101.86	-75.22
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{CA}\rangle$	-133.59	88.82	185.44	124.71	-143.80	116.95	-82.39	212.57	100.99	67.74
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{AC}\rangle$	-21.46	-60.88	37.24	76.98	75.24	-2.56	-116.44	-75.84	-76.95	-6.48
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{TT}\rangle$	5.93	-1.40	2.49	2.98	-6.56	0.84	0.82	-6.19	4.94	2.58
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{TT}\rangle$	-0.55	1.15	-2.46	-3.20	5.55	1.15	0.61	1.27	-1.52	-2.42
$\langle \mathrm{CA}\|\hat{H}\|\mathrm{TT}\rangle$	62.05	76.12	25.56	90.64	-157.45	-82.17	16.06	72.33	-178.73	10.00
$\langle \mathrm{AC}\|\hat{H}\|\mathrm{TT}\rangle$	20.70	83.59	-5.86	-62.79	-140.78	-4.14	0.54	54.61	50.69	-37.56
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{S_0S_1}\rangle$	2.79	3.03	2.87	2.85	2.59	2.97	2.93	2.84	2.85	2.94
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{S_1S_0}\rangle$	3.15	2.76	3.16	2.79	2.84	2.63	2.78	3.26	2.95	2.95
$\langle \mathrm{CA}\|\hat{H}\|\mathrm{CA}\rangle$	3.05	3.04	3.13	2.93	2.88	3.07	3.11	3.15	3.23	3.24
$\langle \mathrm{AC}\|\hat{H}\|\mathrm{AC}\rangle$	3.22	3.17	2.97	2.78	2.80	3.11	3.09	3.29	2.96	3.10
$\langle \mathrm{TT}\|\hat{H}\|\mathrm{TT}\rangle$	2.10	1.79	2.05	1.68	1.45	1.57	1.66	2.31	2.07	2.20
$\|V_{\mathrm{eff}}\|^2_{10}$ (variance)	1.71×10^{-4} (9.77×10^{-8})									
τ	624.9									
$\|V_{\mathrm{eff}}\|^2_{S}$ (variance)	3.98×10^{-5} (1.42×10^{-9})									
τ_S	2688.2									
BPc11										
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{CA}\rangle$	34.22	55.95	153.53	117.55	84.45	20.15	-71.14	157.04	79.03	52.88
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{AC}\rangle$	-44.03	-7.31	-224.02	-237.38	-181.42	190.67	-33.91	-122.01	-161.68	-124.71
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{CA}\rangle$	36.08	21.95	214.96	248.11	177.05	-170.39	5.48	144.67	181.92	144.79
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{AC}\rangle$	-48.68	-54.46	-131.03	-110.99	-75.37	9.22	48.54	-149.83	-80.47	-30.69
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{TT}\rangle$	0.13	-1.04	1.33	0.49	-1.36	8.84	2.41	-1.84	0.38	-1.47
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{TT}\rangle$	-2.20	3.67	-2.14	1.41	2.82	-3.21	5.43	3.25	-1.49	3.26
$\langle \mathrm{CA}\|\hat{H}\|\mathrm{TT}\rangle$	-22.91	14.88	-121.59	131.97	71.59	166.08	-65.33	148.73	-71.80	-18.79
$\langle \mathrm{AC}\|\hat{H}\|\mathrm{TT}\rangle$	15.61	22.53	-220.44	144.61	77.45	35.50	-49.93	174.96	-166.81	119.13
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{S_0S_1}\rangle$	2.87	2.82	2.92	2.95	3.11	2.98	2.89	2.91	2.75	2.84
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{S_1S_0}\rangle$	2.87	2.80	3.03	3.00	2.88	2.94	2.91	2.99	2.77	2.88
$\langle \mathrm{CA}\|\hat{H}\|\mathrm{CA}\rangle$	3.11	2.92	3.20	3.26	3.21	3.10	3.02	3.17	2.92	2.91
$\langle \mathrm{AC}\|\hat{H}\|\mathrm{AC}\rangle$	3.03	2.94	3.15	2.99	3.06	3.02	3.03	3.17	2.90	3.06
$\langle \mathrm{TT}\|\hat{H}\|\mathrm{TT}\rangle$	1.75	1.57	2.00	1.98	2.02	1.92	1.94	1.99	1.26	1.71
$\|V_{\mathrm{eff}}\|^2_{10}$ (variance)	3.33×10^{-4} (2.66×10^{-7})									
τ	320.9									
$\|V_{\mathrm{eff}}\|^2_{S}$ (variance)	4.07×10^{-4} (2.46×10^{-7})									
τ_S	262.9									
BPc12										
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{CA}\rangle$	320.48	144.98	331.49	283.57	350.94	283.73	120.80	292.14	364.64	213.92
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{AC}\rangle$	219.00	366.30	270.06	175.41	176.26	274.20	233.01	271.46	282.81	302.36
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{CA}\rangle$	-209.51	-357.12	-289.71	-137.60	-191.98	-272.28	-260.42	-301.57	-229.86	-312.05
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{AC}\rangle$	-316.11	-141.81	-333.90	-283.45	-371.18	-297.63	-136.70	-325.39	-323.84	-193.24
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{TT}\rangle$	3.10	-1.12	-0.53	2.76	1.17	-1.51	3.54	1.83	4.82	1.74
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{TT}\rangle$	-0.29	-2.63	2.08	7.33	1.87	4.83	-1.26	0.02	3.01	1.41
$\langle \mathrm{CA}\|\hat{H}\|\mathrm{TT}\rangle$	-62.98	54.40	17.72	17.45	-96.95	-73.20	-6.67	20.30	17.37	40.19
$\langle \mathrm{AC}\|\hat{H}\|\mathrm{TT}\rangle$	-32.18	-85.80	-48.11	-44.65	54.23	120.66	43.95	-125.08	51.68	-75.06
$\langle \mathrm{S_0S_1}\|\hat{H}\|\mathrm{S_0S_1}\rangle$	2.94	2.78	2.81	3.06	2.88	2.92	2.93	2.71	2.88	2.90
$\langle \mathrm{S_1S_0}\|\hat{H}\|\mathrm{S_1S_0}\rangle$	2.97	3.03	2.90	2.93	2.80	2.98	2.89	3.02	2.83	2.90
$\langle \mathrm{CA}\|\hat{H}\|\mathrm{CA}\rangle$	3.00	3.00	2.92	3.19	2.87	3.20	3.19	2.86	2.87	3.04
$\langle \mathrm{AC}\|\hat{H}\|\mathrm{AC}\rangle$	3.16	3.03	2.91	3.17	3.03	3.05	2.98	3.14	3.11	2.99

$\langle \mathrm{TT}\vert\hat{H}\vert\mathrm{TT}\rangle$	2.04	1.97	1.67	2.20	1.72	2.10	1.97	1.91	1.96	1.86
$\vert V_{\mathrm{eff}}\vert_{10}^2$ (variance)	9.14×10^{-4} (1.11×10^{-6})									
τ	116.9									
$\vert V_{\mathrm{eff}}\vert_{S}^2$ (variance)	1.08×10^{-3} (1.31×10^{-6})									
τ_S	99.4									
BPc13										
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{CA}\rangle$	422.43	-240.95	347.12	-351.85	-80.78	4.21	-163.07	-345.87	126.85	271.88
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{AC}\rangle$	367.84	-378.75	388.22	-454.40	-283.76	-94.90	-306.14	-295.13	72.18	260.91
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{CA}\rangle$	-367.35	377.73	-377.41	475.34	262.13	88.80	324.33	280.60	-78.23	-266.75
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{AC}\rangle$	-424.75	250.13	-336.08	346.78	82.90	-13.29	170.46	320.60	-134.43	-249.32
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{TT}\rangle$	-0.12	-4.04	2.84	-4.53	4.41	-6.47	-0.02	0.70	6.29	-1.57
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{TT}\rangle$	0.88	-3.04	5.98	-7.87	-2.68	4.11	-7.23	-0.71	-4.30	8.49
$\langle \mathrm{CA}\vert\hat{H}\vert\mathrm{TT}\rangle$	132.66	-107.90	-386.23	-143.03	9.74	-31.60	-277.23	-110.89	-343.88	-67.61
$\langle \mathrm{AC}\vert\hat{H}\vert\mathrm{TT}\rangle$	-248.36	86.43	264.66	116.87	-149.18	91.71	292.47	81.36	263.53	223.10
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{S_0S_1}\rangle$	2.79	2.95	2.95	2.87	3.06	2.91	3.10	2.89	2.78	2.85
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{S_1S_0}\rangle$	3.04	2.84	2.97	2.89	2.96	2.92	2.93	2.73	2.92	3.04
$\langle \mathrm{CA}\vert\hat{H}\vert\mathrm{CA}\rangle$	2.66	2.77	2.76	2.74	2.84	2.74	2.90	2.88	2.64	2.59
$\langle \mathrm{AC}\vert\hat{H}\vert\mathrm{AC}\rangle$	2.57	2.74	2.79	2.66	2.92	2.74	2.85	2.65	2.67	2.88
$\langle \mathrm{TT}\vert\hat{H}\vert\mathrm{TT}\rangle$	1.91	1.78	2.04	1.55	2.04	1.81	2.13	1.56	1.80	1.85
$\vert V_{\mathrm{eff}}\vert_{10}^2$ (variance)	1.68×10^{-2} (1.27×10^{-3})									
τ	6.4									
$\vert V_{\mathrm{eff}}\vert_{S}^2$ (variance)	6.40×10^{-3} (7.90×10^{-5})									
τ_S	16.7									
BPc14										
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{CA}\rangle$	-92.39	-80.45	22.75	-206.98	-227.74	-154.33	-112.21	-141.53	-109.48	-117.63
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{AC}\rangle$	265.33	206.66	442.11	138.81	121.12	274.28	324.52	221.82	168.46	272.70
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{CA}\rangle$	-254.84	-213.66	-446.17	-131.51	-110.13	-281.35	-298.06	-234.42	-186.38	-273.81
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{AC}\rangle$	99.61	61.26	-37.24	213.99	250.62	158.78	136.46	111.98	108.70	129.00
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{TT}\rangle$	-6.33	3.19	1.27	-1.36	-2.93	1.49	-2.71	3.08	3.64	-1.11
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{TT}\rangle$	2.12	-1.93	1.72	1.09	1.86	-5.70	3.52	-6.05	-3.93	3.18
$\langle \mathrm{CA}\vert\hat{H}\vert\mathrm{TT}\rangle$	-145.11	147.04	55.29	-196.68	-158.01	0.23	99.53	55.38	136.45	66.62
$\langle \mathrm{AC}\vert\hat{H}\vert\mathrm{TT}\rangle$	98.17	-87.94	-44.35	75.40	-82.67	78.91	-105.85	103.79	-73.07	-85.01
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{S_0S_1}\rangle$	2.91	2.80	3.13	2.85	2.90	3.14	3.46	2.93	2.80	3.18
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{S_1S_0}\rangle$	3.11	3.37	2.94	3.03	3.21	3.04	2.79	3.07	3.16	2.89
$\langle \mathrm{CA}\vert\hat{H}\vert\mathrm{CA}\rangle$	3.04	3.15	3.03	2.88	3.10	3.05	3.18	2.97	3.11	3.02
$\langle \mathrm{AC}\vert\hat{H}\vert\mathrm{AC}\rangle$	2.98	3.16	3.00	2.86	3.00	3.22	3.15	3.21	3.01	2.97
$\langle \mathrm{TT}\vert\hat{H}\vert\mathrm{TT}\rangle$	1.93	2.18	2.19	1.83	2.11	2.24	2.25	2.00	1.95	2.02
$\vert V_{\mathrm{eff}}\vert_{10}^2$ (variance)	4.88×10^{-3} (2.30×10^{-5})									
τ	21.9									
$\vert V_{\mathrm{eff}}\vert_{S}^2$ (variance)	8.12×10^{-4} (5.90×10^{-7})									
τ_S	131.7									
BPc15										
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{CA}\rangle$	-306.69	-16.71	-242.55	-248.95	-20.79	-292.27	-295.87	190.66	-211.29	-299.92
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{AC}\rangle$	-100.74	350.43	80.76	97.68	333.41	5.74	-365.07	415.09	159.52	109.35
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{CA}\rangle$	154.67	-362.53	-64.11	-120.58	-341.28	-26.66	343.32	-377.04	-148.15	-74.07
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{AC}\rangle$	330.22	-6.96	243.63	218.83	21.93	279.92	247.94	-154.93	205.27	267.51
$\langle \mathrm{S_0S_1}\vert\hat{H}\vert\mathrm{TT}\rangle$	1.97	1.40	-7.39	-0.14	0.33	-0.72	-0.90	8.32	-3.22	-3.68
$\langle \mathrm{S_1S_0}\vert\hat{H}\vert\mathrm{TT}\rangle$	1.66	-6.08	6.09	6.18	0.84	1.77	-5.47	5.56	1.94	4.65

$\langle \mathrm{CA}|\hat{H}|\mathrm{TT}\rangle$	149.64	25.14	36.94	116.72	-79.18	-11.47	-77.42	97.58	-95.42	-88.22
$\langle \mathrm{AC}|\hat{H}|\mathrm{TT}\rangle$	-103.88	-47.82	-206.97	-244.43	46.94	-90.19	84.98	-35.27	-22.88	-129.23
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{S_0S_1}\rangle$	2.94	2.85	3.00	3.09	3.00	3.12	3.06	3.15	2.94	2.84
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{S_1S_0}\rangle$	3.25	3.17	3.28	3.27	3.57	3.02	2.69	2.72	3.21	3.30
$\langle \mathrm{CA}|\hat{H}|\mathrm{CA}\rangle$	3.13	3.05	3.13	3.20	3.49	3.14	2.85	3.01	3.10	3.16
$\langle \mathrm{AC}|\hat{H}|\mathrm{AC}\rangle$	3.09	3.08	3.04	3.26	3.35	3.14	2.93	3.08	3.16	3.08
$\langle \mathrm{TT}|\hat{H}|\mathrm{TT}\rangle$	2.26	2.06	2.20	2.53	2.84	2.04	1.72	2.00	2.27	2.18
$|V_{\mathrm{eff}}|^2_{10}$ (variance)	6.29×10^{-3} (1.24×10^{-4})									
τ	17.0									
$|V_{\mathrm{eff}}|^2_{S}$ (variance)	8.11×10^{-4} (4.91×10^{-7})									
τ_S	131.8									
BPc16										
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle$	-33.80	-9.73	36.92	125.19	-109.43	93.55	83.04	-1.67	91.15	-83.23
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{AC}\rangle$	259.73	276.79	251.54	-4.92	317.10	72.75	283.81	268.31	214.89	156.71
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{CA}\rangle$	-259.37	-274.38	-231.70	12.97	-334.98	-53.25	-258.89	-256.59	-175.75	-122.67
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{AC}\rangle$	39.86	-0.74	6.11	-106.59	124.33	-102.30	-54.48	-2.04	-81.17	53.19
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{TT}\rangle$	2.75	-1.86	1.28	2.70	5.01	7.67	2.93	0.00	-4.96	-3.32
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{TT}\rangle$	-1.74	1.86	-4.84	-4.87	-5.84	1.85	1.79	0.87	-3.61	4.52
$\langle \mathrm{CA}|\hat{H}|\mathrm{TT}\rangle$	-107.02	-206.97	-188.64	43.71	-291.99	-30.47	131.94	109.85	-121.11	-60.59
$\langle \mathrm{AC}|\hat{H}|\mathrm{TT}\rangle$	-230.54	-85.43	-51.04	-152.11	-307.81	20.69	120.83	208.63	-61.16	-156.47
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{S_0S_1}\rangle$	2.81	3.00	2.80	2.65	2.82	2.82	2.85	2.85	3.04	2.87
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{S_1S_0}\rangle$	2.85	2.88	2.77	2.80	2.93	2.89	2.83	2.89	2.92	2.95
$\langle \mathrm{CA}|\hat{H}|\mathrm{CA}\rangle$	3.04	3.01	3.04	2.82	3.08	2.84	3.04	2.86	2.97	3.05
$\langle \mathrm{AC}|\hat{H}|\mathrm{AC}\rangle$	2.96	3.13	2.96	2.87	3.04	2.98	2.91	3.07	3.36	2.99
$\langle \mathrm{TT}|\hat{H}|\mathrm{TT}\rangle$	1.60	1.76	1.59	1.37	1.83	1.73	1.73	1.63	2.12	1.76
$|V_{\mathrm{eff}}|^2_{10}$ (variance)	2.71×10^{-3} (7.77×10^{-6})									
τ	39.5									
$|V_{\mathrm{eff}}|^2_{S}$ (variance)	4.31×10^{-3} (1.50×10^{-5})									
τ_S	24.8									
BPc17										
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{CA}\rangle$	414.19	381.76	298.93	212.23	384.56	253.79	290.38	217.95	318.84	254.58
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{AC}\rangle$	201.40	296.90	285.19	290.12	231.95	358.05	285.85	326.13	294.39	290.65
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{CA}\rangle$	-208.34	-320.34	-320.45	-322.99	-222.76	-334.94	-260.73	-328.24	-324.69	-278.03
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{AC}\rangle$	-429.29	-402.03	-331.70	-238.07	-345.05	-229.11	-308.80	-210.45	-353.08	-247.93
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{TT}\rangle$	1.75	-4.38	2.31	-0.46	0.04	-2.01	4.51	-0.24	2.60	-7.46
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{TT}\rangle$	-0.76	-2.26	0.81	1.56	-0.28	4.26	-4.08	6.46	0.47	-1.14
$\langle \mathrm{CA}|\hat{H}|\mathrm{TT}\rangle$	-87.97	4.26	-97.54	27.11	65.13	69.98	-72.66	-61.67	1.37	-63.74
$\langle \mathrm{AC}|\hat{H}|\mathrm{TT}\rangle$	37.18	-100.02	44.91	29.75	-70.65	-111.77	18.37	-15.60	52.26	-12.49
$\langle \mathrm{S_0S_1}|\hat{H}|\mathrm{S_0S_1}\rangle$	2.77	2.72	2.77	2.86	2.90	2.94	2.80	2.73	3.00	2.89
$\langle \mathrm{S_1S_0}|\hat{H}|\mathrm{S_1S_0}\rangle$	3.07	2.79	2.92	2.94	2.85	2.85	2.91	2.83	3.07	2.80
$\langle \mathrm{CA}|\hat{H}|\mathrm{CA}\rangle$	3.05	2.92	2.90	2.99	2.97	2.96	2.86	2.82	3.20	3.00
$\langle \mathrm{AC}|\hat{H}|\mathrm{AC}\rangle$	3.16	2.84	3.11	3.02	3.08	2.93	3.02	2.93	3.19	2.91
$\langle \mathrm{TT}|\hat{H}|\mathrm{TT}\rangle$	2.12	1.91	1.86	1.88	1.88	1.93	1.87	1.65	2.46	1.71
$|V_{\mathrm{eff}}|^2_{10}$ (variance)	1.13×10^{-3} (1.50×10^{-6})									
τ	94.8									
$|V_{\mathrm{eff}}|^2_{S}$ (variance)	1.47×10^{-3} (1.70×10^{-6})									
τ_S	73.0									
BPc18										

$\langle S_0S_1\|\hat{H}\|CA\rangle$	320.35	242.48	315.57	268.59	245.87	244.33	254.14	205.61	320.06	358.65
$\langle S_0S_1\|\hat{H}\|AC\rangle$	264.98	231.93	78.51	377.32	58.99	-153.05	-5.81	-83.81	-5.34	54.94
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-281.14	-263.94	-85.42	-403.54	-67.69	179.17	36.04	79.97	-31.49	-82.35
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-330.43	-267.18	-276.76	-252.89	-254.58	-253.94	-254.49	-198.03	-322.15	-378.85
$\langle S_0S_1\|\hat{H}\|TT\rangle$	-6.39	2.76	3.97	-6.92	1.24	0.62	-2.21	4.48	7.42	2.26
$\langle S_1S_0\|\hat{H}\|TT\rangle$	-6.87	9.72	-5.98	-2.92	0.51	-0.64	-4.81	-0.32	1.04	5.35
$\langle CA\|\hat{H}\|TT\rangle$	84.51	-19.68	-66.18	-92.79	-32.52	-39.93	16.79	-112.94	-59.81	83.70
$\langle AC\|\hat{H}\|TT\rangle$	-97.04	45.25	-21.39	43.73	-53.32	-22.11	-69.93	-70.91	31.39	134.45
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	2.87	2.85	2.82	3.48	2.87	2.85	2.91	2.89	2.71	2.78
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	3.31	3.24	3.21	2.87	3.15	3.21	3.32	3.29	3.12	3.27
$\langle CA\|\hat{H}\|CA\rangle$	3.24	3.32	3.17	3.33	3.33	3.58	3.48	3.41	3.17	3.25
$\langle AC\|\hat{H}\|AC\rangle$	3.22	3.19	3.20	3.37	3.28	3.36	3.41	3.55	3.14	3.24
$\langle TT\|\hat{H}\|TT\rangle$	2.43	2.35	2.09	2.83	1.97	2.11	2.42	2.28	1.95	2.15
$\|V_{\mathrm{eff}}\|^2_{10}$ (variance)					1.34×10^{-3} (7.45×10^{-6})					
τ					80.0					
$\|V_{\mathrm{eff}}\|^2_S$ (variance)					1.02×10^{-3} (1.68×10^{-6})					
τ_S					105.2					
					BPc19					
$\langle S_0S_1\|\hat{H}\|CA\rangle$	95.07	-4.26	19.46	3.47	85.66	60.62	1.18	15.07	-125.65	-74.85
$\langle S_0S_1\|\hat{H}\|AC\rangle$	9.08	97.40	78.64	-41.06	140.53	199.62	178.25	107.04	95.78	125.70
$\langle S_1S_0\|\hat{H}\|CA\rangle$	-10.27	-138.79	-80.29	44.13	-148.65	-162.36	-184.72	-123.12	-119.71	-130.65
$\langle S_1S_0\|\hat{H}\|AC\rangle$	-111.76	18.13	-23.09	7.30	-60.15	-53.37	3.83	-20.66	120.29	79.24
$\langle S_0S_1\|\hat{H}\|TT\rangle$	2.06	-3.43	-0.58	-3.08	2.38	5.02	-1.03	-2.74	3.36	4.29
$\langle S_1S_0\|\hat{H}\|TT\rangle$	-2.65	4.16	2.22	2.10	-8.77	-4.27	1.11	2.37	-4.41	-5.36
$\langle CA\|\hat{H}\|TT\rangle$	-14.60	-127.47	18.94	-17.25	109.62	165.57	-129.68	-44.99	140.20	96.90
$\langle AC\|\hat{H}\|TT\rangle$	-65.15	-121.28	-117.08	5.96	12.15	25.62	-99.91	-42.86	204.51	137.17
$\langle S_0S_1\|\hat{H}\|S_0S_1\rangle$	3.10	2.97	2.91	3.00	2.81	3.06	2.80	3.09	2.90	2.81
$\langle S_1S_0\|\hat{H}\|S_1S_0\rangle$	2.91	3.03	3.34	3.21	3.19	3.15	3.29	3.26	2.98	3.27
$\langle CA\|\hat{H}\|CA\rangle$	3.37	3.37	3.45	3.56	3.26	3.31	3.39	3.57	3.49	3.45
$\langle AC\|\hat{H}\|AC\rangle$	3.42	3.39	3.72	3.59	3.39	3.37	3.43	3.51	3.15	3.35
$\langle TT\|\hat{H}\|TT\rangle$	2.22	2.11	2.32	2.47	2.20	2.22	2.12	2.43	1.89	2.24
$\|V_{\mathrm{eff}}\|^2_{10}$ (variance)					2.24×10^{-4} (1.41×10^{-7})					
τ					476.3					
$\|V_{\mathrm{eff}}\|^2_S$ (variance)					2.25×10^{-4} (8.42×10^{-8})					
τ_S					474.7					

References

1． A. D. Platt, J. Day, S. Subramanian, J. E. Anthony and O. Ostroverkhova. *J. Phys. Chem. C*, 2009, **113**, 14006-14014.

2． B. J. Walker, A. J. Musser, D. Belijonne and R. H. Friend, *Nat. Chem.*, **2013**, 5, 1019-1024.

3． A. A. Bakulin, S. E. Morgan, T. B. Kehoe, M. W. Wilson, A. W. Chin, D. Zigmantas, D. Egorova and A. Rao, *Nat. Chem.*, 2016, **8**, 16–23.

4．T. Zeng, R. Hoffmann and N. Ananth, *J. Am. Chem. Soc.*, 2014, **136**, 5755–5764.

5．M. B. Smith and J. Michl, *Chem. Rev.*, 2010, **110**, 6891–6936.