Supplementary Information

Theoretical exploration of NIR-II circularly polarized luminescence in open-shell boron embedded pyrene-naphthalene helicenes

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Table S1 List of abbreviations.

Full form	Abbreviation
Circularly polarized luminescence	CPL
Near infrared	NIR
The second near-infrared window	NIR-II
Near infrared circularly polarized luminescence	NIR-CPL
Emission dissymmetry factor	g_{lum}
Absorption dissymmetry factor	g_{abs}
Huang-Rhys factor	HRF
Interfragment charge transfer	IFCT
Nuclear independent chemical shift	$NICS(1)_{ZZ}$
Root-mean-square displacements	RMSD
Transition electric dipole moment	TEDM
Transition magnetic dipole moment	TMDM

Table S2. Benchmark calculation to get the proper computational level, where the 6-311G** basis set is used for all functionals. The dihedral angle (φ) between the pyrene ring and the naphthalene ring and the computational UV-vis peak for 1-H-*PP* and the experimental UV-vis peaks for 1-CH_3 and 3a are taken as reference.

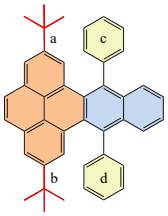
Compounds	Functionals	dihedral angle (°)	S_1 (nm)
1-H-*PP*	B3LYP	32.80	403
	M06-2X	30.17	344
	ωB97XD	30.09	336
	PBE	31.87	487
1-CH_3[a]	experiment	27.69	-
3a[b]	experiment	-	343[c]

[a]From Ref. NPG Asia Materials 2015, 7, e230.

[b]From Ref. Dyes Pigments 2015, 112, 176-182.

[c]Absorption peak in thin film.

Table S3. The first emission peak, *D*, *Sr*, *H*, *t* electron excitation characteristic index, and interfragment charge transfer of different functionals

		B3LYP	M06-2X	ωB97XD	PBE
First emission peak D_1 (nm)		1306	1011	973	2159
D (Å)		2.93	1.63	1.17	4.16
Sr (a.u.)		0.56	0.63	0.71	0.47
H (Å)		3.22	3.59	3.22	3.20
t (Å)		0.66	-1.66	-1.03	1.89
Interfragment charge transfer	pyrene	0.39	0.14	0.09	0.64
	naphthalene	-0.33	-0.11	-0.07	-0.54
	a	-0.01	-0.01	-0.01	0.00
	b	-0.01	-0.01	-0.01	0.00
	c	-0.01	0.00	0.00	-0.04
	d	-0.03	0.00	0.00	-0.05

The results show that PBE significantly overestimates the emission wavelength (2159 nm) and significantly exaggerates the charge transfer character. B3LYP also produces an evident red shift and overestimates the charge transfer contribution. In contrast, ωB97XD yields an emission wavelength comparable to that of M06-2X but slightly underestimates the extent ofcharge transfer in the system. Overall, M06-2X provide a balanced and reliable description both the emission wavelength and charge transfer character, making it more suitable for the system investigated herein. Wu et al.[S1] systematically evaluated the performance of various functionals based on experimental spectra of 71 organic molecules and demonstrated that M06-2X achieves the highest accuracy in predicting excited-state energies, oscillator strengths and exciton reorganization energies, with corresponding R^2 values of 0.948, 0.944 and 0.690, respectively. Using M06-2X as the primary functional, Ulukan et al.[S2] calculated the torsion angles, ΔE_{ST} and spin-orbit coupling of 17 TADF compounds and 2 non-TADF compounds, confirming its capability to accurately describe charge-transfer excited states. Similarly, Chaudhuri et al.[S3] performed a comparative study on a typical D-A-D type TADF molecule and showed that M06-2X can precisely optimize both ground and excited state geometries, as well as accurately predict excited-state energy levels ΔE_{ST}. Moreover, for open-shell triplet systems, M06-2X functional does not suffer from triplet instability and outperforms most global hybrid functionals in calculating triplet excitation energies. In summary, the M06-2X functional is well-suited for describing the ground state, excited state and open-shell charge-transfer systems considered in the present study.

[S1] X. Wu, X. Xie and A. Troisi, Calibration of several first excited state properties for organic molecules through systematic comparison of TDDFT with experimental spectra, *J. Mater. Chem. C,* 2024, **12**, 18886.

[S2] P. Ulukan, E. E. Bas, R. B. Ozek, C. Dal Kaynak, A. Monari, V. Aviyente and S. Catak, Computational descriptor analysis on excited state behaviours of a series of TADF and non-TADF compounds, *Phys. Chem. Chem. Phys.*, 2022, **24**, 16167-16182.

[S3] D. Chaudhuri and C. H. Patterson, TDDFT versus GW/BSE Methods for Prediction of Light Absorption and Emission in a TADF Emitter, *J. Phys. Chem. A*, 2022, **126**, 9627-9643.

Table S4. Relative ground-state Gibbs free energy Δ*G* at 298.15 K for the possible *PP*, *MM*, *PM* and *MP* stereoisomers of B-1, B-2, B-3, B-4, B-5, B-6, B-7, B-8, and B-9. All the energies are in kcal·mol^{-1} and respective to those of B-6-*PP*.

Compounds	Δ*G*	Compounds	Δ*G*
B-1-*PP*/*MM*	15.10	B-1-*MP*/*PM*	16.83
B-2-*PP*/*MM*	19.82	B-2-*MP*/*PM*	21.97
B-3-*PP*/*MM*	22.29	B-3-*MP*/*PM*	24.03
B-4-*PP*/*MM*	9.78	B-4-*MP*/*PM*	-
B-5-*PP*/*MM*	6.41	B-5-*MP*/*PM*	-
B-6-*PP*/*MM*	0.00	B-6-*MP*/*PM*	3.23
B-7-*PP*/*MM*	20.77	B-7-*MP*/*PM*	25.56
B-8-*PP*/*MM*	14.89	B-8-*MP*/*PM*	18.46
B-9-*PP*/*MM*	19.28	B-9-*MP*/*PM*	22.52

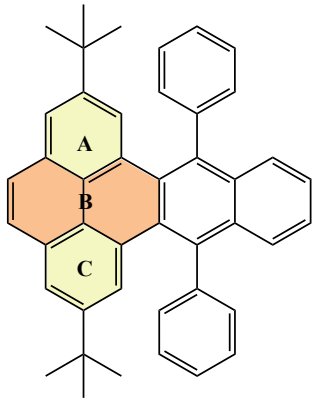


Table S5. Dihedral angles φ (between the pyrene and naphthalene rings), φ_1 and φ_2 (for the two bay regions), φ_3 (between rings A and B), and φ_4 (between rings B and C) for the possible *PP*, *MM*, *PM* and *MP* stereoisomers of the ground states of 1-H, B-1, B-2, B-3, B-4, B-5, B-6, B-7, B-8 and B-9. All angles are expressed in degrees (°).

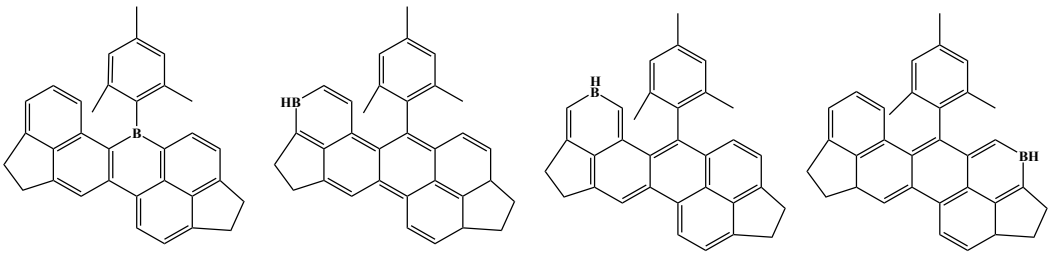
Compounds	$\lvert\varphi\rvert$	$\lvert\varphi_1\rvert$	$\lvert\varphi_2\rvert$	$\lvert\varphi_{3\rvert}$	$\lvert\varphi_4\rvert$	Compounds	$\lvert\varphi\rvert$	$\lvert\varphi_1\rvert$	$\lvert\varphi_2\rvert$	$\lvert\varphi_{3\rvert}$	$\lvert\varphi_4\rvert$	$\Delta\varphi_{MP/PM\text{-}PP/MM}$	$\Delta\lvert\varphi_{1(\text{B-}PP/MM\text{-1-H-}PP/MM)}\rvert+$ $\Delta\lvert\varphi_{2(\text{B-}PP/MM\text{-1-H-}PP/MM)}\rvert/2$
1-H-*PP*/*MM*	30.17	20.26	21.89	6.09	7.04	1-H-*MP*/*PM*	20.85	22.55	25.93	16.53	16.74	-9.32	-
B-1-*PP*/*MM*	32.91	21.18	24.13	7.07	6.23	B-1-*MP*/*PM*	25.21	26.27	28.46	19.83	18.46	-7.7	1.58
B-2-*PP*/*MM*	30.51	23.01	21.31	2.49	11.47	B-2-*MP*/*PM*	21.89	27.55	25.76	20.44	17.67	-8.62	1.67
B-3-*PP*/*MM*	26.23	10.47	29.13	3.22	11.52	B-3-*MP*/*PM*	21.05	21.03	32.77	16.17	18.20	-5.18	8.51
B-4-*PP*/*MM*	29.15	4.20	30.62	3.97	7.71	B-4-*MP*/*PM*	-	-	-	-	-	-	12.39
B-5-*PP*/*MM*	30.90	11.05	29.70	2.14	8.69	B-5-*MP*/*PM*	-	-	-	-	-	-	8.51
B-6-*PP*/*MM*	29.74	16.72	26.53	5.53	6.16	B-6-*MP*/*PM*	18.05	15.06	26.76	12.68	15.93	-11.69	4.09
B-7-*PP*/*MM*	34.23	25.79	21.62	5.97	6.49	B-7-*MP*/*PM*	15.65	19.15	26.21	15.95	17.06	-18.58	2.90
B-8-*PP*/*MM*	32.24	20.34	22.82	6.28	6.40	B-8-*MP*/*PM*	22.14	26.23	22.94	17.03	16.82	-10.1	0.51
B-9-*PP*/*MM*	32.85	21.98	21.89	6.09	7.04	B-9-*MP*/*PM*	22.32	25.07	25.10	19.83	18.46	-10.53	0.86

Table S6. Root-mean-square displacement (RMSD) of geometric structures between the ground state (D_0) and the first excited state (D_1) for compounds B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP*.

	RMSD(Å)
B-1-*PP*	0.05
B-2-*PP*	0.11
B-3-*PP*	0.30
B-4-*PP*	0.13
B-5-*PP*	0.24
B-6-*PP*	0.10
B-7-*PP*	0.19
B-8-*PP*	0.10
B-9-*PP*	0.12

Table S7. Ground-state Gibbs free energy *G* at 298.15 K for B incorporated compound 5 and its isomers.[S4]

Compounds	5	5-1	5-2	5-3
G (Hartree)	-1298.027153	-1297.948259	-1297.969666	-1297.97331



5 5-1 5-2 5-3

The boron-embedded structure at the central 6-position (B-6-*PP*) shares a closely related rigid π-conjugated framework and boron coordination environment with compound 5, which has been experimentally synthesized.[S4] Thermodynamic analysis shows that the central boron-substituted isomer (compound 5) possesses the lowest Gibbs free energy (*G* = -1298.027153 Hartree), compared with its peripheral isomers 5-1 (-1297.948259 Hartree), 5-2 (-1297.969666 Hartree), and 5-3 (-297.973310 Hartree), indicating superior thermodynamic stability. Consistently, within the boron-embedded pyrene-naphthalene derivatives investigated in this work, B-6-*PP* also exhibits the lowest Gibbs free energy among all isomers. These results suggest that the central boron-embedded structure is both thermodynamically favored and experimentally feasible.

[S4] K. Schickedanz, J. Radtke, M. Bolte, H. W. Lerner and M. Wagner, Facile route to quadruply annulated borepins, *J. Am. Chem. Soc.*, 2017, **139**, 2842-2851.

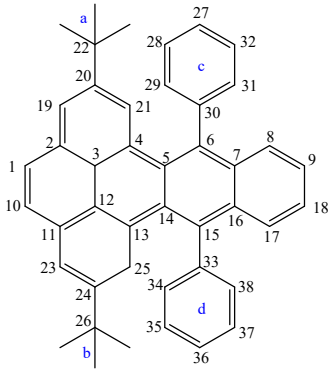


Table S8. Natural population analysis (NPA) charge difference (Δq, in units of e) between the D_1 state and the D_0 state for compounds 1-H-*PP*, B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP* and B-9-*PP*.

No.	Δq									
	1-H-*PP*	B-1-*PP*	B-2-*PP*	B-3-*PP*	B-4-*PP*	B-5-*PP*	B-6-*PP*	B-7-*PP*	B-8-*PP*	B-9-*PP*
1	0.00	-0.17	0.12	0.09	-0.03	0.01	0.01	0.01	0.00	0.00
2	0.01	0.15	-0.23	-0.12	0.15	0.02	0.03	0.00	0.00	-0.01
3	0.00	0.03	-0.04	-0.22	0.05	-0.03	-0.04	0.00	-0.01	0.02
4	0.00	0.02	0.19	0.03	-0.23	0.07	0.02	0.01	-0.01	-0.03
5	-0.01	-0.01	-0.03	0.02	0.07	-0.19	-0.07	0.05	0.02	0.13
6	-0.01	0.02	0.05	0.01	-0.03	-0.18	-0.18	-0.07	-0.03	-0.08
7	0.01	0.00	-0.02	-0.01	0.02	0.14	0.04	-0.13	0.05	0.15
8	0.00	0.00	0.01	0.00	-0.01	-0.07	-0.02	0.09	-0.20	-0.23
9	0.00	0.01	0.00	0.00	0.01	0.08	0.00	-0.05	-0.03	-0.17
10	0.01	-0.28	-0.07	-0.04	0.05	-0.01	0.01	0.03	0.01	0.01
11	-0.01	0.15	0.04	0.00	-0.04	-0.02	-0.01	0.01	0.00	0.01
12	0.00	-0.03	0.04	0.08	-0.01	0.03	0.01	-0.04	0.00	-0.02
13	0.01	0.08	-0.03	-0.04	0.06	0.01	-0.01	0.07	-0.01	0.01

14	-0.01	-0.01	0.01	0.01	-0.03	0.09	0.16	-0.16	0.05	-0.09
15	-0.01	0.03	0.00	0.00	0.02	0.07	-0.20	0.01	-0.08	0.04
16	0.00	0.00	0.01	0.01	-0.02	-0.10	0.06	-0.04	0.19	-0.01
17	0.00	0.01	0.00	0.00	0.01	0.06	-0.02	0.06	-0.28	-0.05
18	0.00	0.00	0.01	0.01	-0.01	-0.09	0.00	-0.01	0.15	0.23
19	-0.01	-0.06	0.06	0.21	-0.27	-0.04	-0.01	0.03	0.03	0.04
20	0.00	0.09	0.11	-0.21	0.16	0.03	0.01	-0.02	-0.01	-0.01
21	0.01	-0.03	-0.27	0.14	-0.01	-0.01	0.04	0.06	0.05	0.04
22	-0.01	-0.01	-0.01	0.02	-0.01	0.00	0.00	0.00	0.00	0.00
23	0.02	-0.08	-0.02	0.02	0.06	0.08	0.07	0.00	0.03	-0.01
24	-0.02	0.13	0.01	-0.03	-0.01	-0.03	-0.03	0.00	-0.01	0.01
25	0.01	-0.12	0.01	0.05	0.00	0.03	0.08	0.02	0.04	0.00
26	0.00	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	0.00	0.00	0.01	0.01	0.00	-0.02	-0.01	0.02	0.00	0.00
28	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
29	0.00	0.00	0.00	0.00	0.02	0.01	0.00	0.03	0.01	0.01
30	-0.01	0.00	0.00	0.00	0.00	0.04	0.05	0.03	0.00	0.01
31	0.01	0.00	0.01	0.01	-0.01	-0.03	-0.01	-0.01	0.00	0.00
32	-0.01	0.00	0.00	0.00	0.00	-0.01	0.00	-0.01	0.00	0.00
33	-0.01	0.00	0.00	0.00	0.00	-0.01	0.03	0.01	0.00	-0.01
34	0.02	0.00	0.00	0.00	0.03	0.04	0.00	0.02	0.01	0.01
35	-0.01	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00	0.00
36	0.00	0.00	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.00
37	-0.01	0.00	0.00	0.00	-0.01	-0.01	-0.01	0.00	0.00	0.00
38	0.00	0.00	0.00	0.00	-0.03	-0.02	-0.01	-0.02	0.00	0.00

Table S9. Interfragment charge transfer (IFCT) and the redistributed IFCT (in units of e) among molecular fragments (pyrene, naphthalene, and four substituents a–d) of compounds 1-H-*PP*, B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP* and B-9-*PP* during the $D_0 \rightarrow D_1$ excitation.

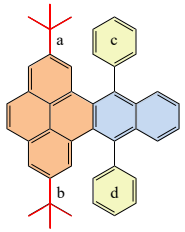
			1-H-*PP*	B-1-*PP*	B-2-*PP*	B-3-*PP*	B-4-*PP*	B-5-*PP*	B-6-*PP*	B-7-*PP*	B-8-*PP*	B-9-*PP*
	Interfragment charge transfer	pyrene	-0.18	0.14	0.16	0.04	0.02	-0.24	-0.42	-0.18	-0.34	-0.23
		naphthalene	0.16	-0.11	-0.14	-0.06	-0.01	0.23	0.39	0.30	0.33	0.23
		a	0.00	-0.01	-0.01	0.02	-0.01	0.00	0.00	0.00	0.00	0.00
		b	0.00	-0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		c	0.02	0.00	-0.01	-0.01	0.01	0.05	0.01	-0.10	0.00	0.01
		d	0.00	-0.01	0.00	0.00	-0.01	-0.03	0.02	-0.02	0.01	0.00
	Transferred electrons between fragments	pyrene -> naphthalene	0.16	-0.11	-0.13	-0.05	-0.01	0.23	0.39	-0.04	0.21	0.33
		pyrene -> a	0.00	-0.01	-0.01	0.02	-0.01	0.00	0.00	0.00	0.00	0.00
		pyrene -> b	0.00	-0.02	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		pyrene -> c	0.01	0.00	-0.01	-0.01	0.01	0.02	0.01	0.00	-0.03	0.00
		pyrene -> d	0.00	-0.01	0.00	0.00	-0.01	-0.01	0.02	0.00	-0.01	0.01
		naphthalene->a	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		naphthalene->b	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		naphthalene->c	0.01	0.00	0.00	0.00	0.00	0.02	0.00	0.00	-0.07	0.00
		naphthalene->d	-0.01	0.00	0.00	0.00	0.00	-0.02	0.00	-0.01	-0.02	0.01
		a-> b	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		a-> c	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		a-> d	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		b-> c	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
		b-> d	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

Table S10. The *D*-index, *Sr*-index, *H*-index, and *t*-index for compounds B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP*.

	1-H-*PP*	B-1-*PP*	B-2-*PP*	B-3-*PP*	B-4-*PP*	B-5-*PP*	B-6-*PP*	B-7-*PP*	B-8-*PP*	B-9-*PP*
D(Å)	0.94	1.63	0.83	0.20	1.03	1.66	1.45	0.55	1.81	1.24
Sr(a.u.)	0.89	0.63	0.70	0.68	0.70	0.66	0.72	0.68	0.70	0.68
H(Å)	3.59	3.01	3.03	3.04	3.08	3.11	3.16	3.06	3.29	3.17
t(Å)	-1.66	-0.26	-1.10	-1.80	-1.20	-0.32	-0.85	-1.46	-0.92	-1.24

Table S11. Atomic spin populations in the first excited state for compounds B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP*.

	B-1-*PP*	B-2-*PP*	B-3-*PP*	B-4-*PP*	B-5-*PP*	B-6-*PP*	B-7-*PP*	B-8-*PP*	B-9-*PP*
1	0.18	-0.05	-0.14	0.07	0.01	0.02	-0.03	0.01	-0.01
2	-0.03	0.19	0.32	-0.14	-0.02	-0.05	0.03	-0.01	0.02
3	-0.01	0.26	0.20	0.17	0.02	0.08	-0.04	0.02	-0.02
4	0.02	-0.18	0.15	0.18	-0.04	-0.09	0.04	-0.03	0.03
5	-0.01	0.04	-0.05	-0.04	0.15	0.34	-0.15	0.12	-0.11
6	0.01	-0.03	0.07	0.06	0.58	0.17	0.29	-0.02	0.25
7	-0.01	0.02	-0.02	-0.02	-0.18	0.08	0.19	0.06	-0.20
8	0.01	-0.01	0.02	0.02	0.20	-0.03	-0.03	0.19	0.57
9	-0.01	0.01	-0.01	-0.01	-0.10	0.10	0.07	0.40	0.19
10	0.60	0.10	0.26	-0.05	-0.01	-0.02	0.02	-0.01	0.01
11	-0.19	0.03	-0.03	0.08	0.00	0.03	-0.06	0.01	-0.03
12	0.15	-0.08	-0.02	-0.05	0.00	-0.03	0.09	-0.01	0.05
13	-0.10	0.10	0.04	0.05	-0.01	0.05	-0.11	0.02	-0.05
14	0.02	-0.03	0.01	0.01	0.03	-0.19	0.41	-0.06	0.21
15	-0.02	0.03	-0.01	0.00	0.00	0.49	-0.07	0.16	-0.08
16	0.01	-0.02	0.02	0.02	0.17	-0.11	0.14	-0.14	0.14
17	-0.01	0.01	-0.01	-0.01	-0.09	0.11	-0.03	0.52	0.04
18	0.00	-0.01	0.02	0.02	0.20	-0.04	0.06	-0.20	-0.01
19	0.04	0.23	-0.18	0.54	0.05	0.11	-0.03	0.03	-0.02
20	0.00	-0.14	0.37	-0.19	-0.03	-0.06	0.03	-0.02	0.02
21	0.03	0.53	-0.09	0.32	0.06	0.12	-0.03	0.03	-0.02
22	0.00	0.00	-0.03	0.01	0.00	0.00	0.00	0.00	0.00
23	0.25	0.00	0.04	-0.05	0.01	-0.04	0.15	-0.01	0.06
24	-0.12	0.07	0.02	0.07	0.00	0.03	-0.07	0.01	-0.03
25	0.25	-0.03	0.02	-0.02	0.01	-0.04	0.14	-0.01	0.06
26	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	0.00	0.00	0.00	0.00	0.04	0.01	0.02	0.00	0.01
28	0.00	0.00	0.00	0.00	-0.02	0.00	-0.01	0.00	0.00
29	0.00	0.00	0.00	0.00	0.05	0.01	0.03	0.00	0.01
30	0.00	0.00	-0.01	0.00	-0.08	-0.02	-0.05	0.00	-0.03
31	0.00	0.00	0.00	0.00	0.04	0.01	0.03	0.00	0.01
32	0.00	0.00	0.00	0.00	-0.02	0.00	-0.01	0.00	-0.01
33	0.00	0.00	0.00	0.00	0.00	-0.06	0.01	-0.02	0.01
34	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.01	0.00
35	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
36	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.00
37	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
38	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.01	-0.01

Table S12. Atomic spin populations in the ground state for compounds B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP*.

	B-1-*PP*	B-2-*PP*	B-3-*PP*	B-4-*PP*	B-5-*PP*	B-6-*PP*	B-7-*PP*	B-8-*PP*	B-9-*PP*
1	0.18	-0.05	-0.14	0.07	0.01	0.02	-0.03	0.01	-0.01
2	-0.03	0.19	0.32	-0.14	-0.02	-0.05	0.03	-0.01	0.02
3	-0.01	0.26	0.20	0.17	0.02	0.08	-0.04	0.02	-0.02
4	0.02	-0.18	0.15	0.18	-0.04	-0.09	0.04	-0.03	0.03
5	-0.01	0.04	-0.05	-0.04	0.15	0.34	-0.15	0.12	-0.11
6	0.01	-0.03	0.07	0.06	0.58	0.17	0.29	-0.02	0.25
7	-0.01	0.02	-0.02	-0.02	-0.18	0.08	0.19	0.06	-0.20
8	0.01	-0.01	0.02	0.02	0.20	-0.03	-0.03	0.19	0.57
9	-0.01	0.01	-0.01	-0.01	-0.10	0.10	0.07	0.40	0.19
10	0.60	0.10	0.26	-0.05	-0.01	-0.02	0.02	-0.01	0.01
11	-0.19	0.03	-0.03	0.08	0.00	0.03	-0.06	0.01	-0.03
12	0.15	-0.08	-0.02	-0.05	0.00	-0.03	0.09	-0.01	0.05
13	-0.10	0.10	0.04	0.05	-0.01	0.05	-0.11	0.02	-0.05
14	0.02	-0.03	0.01	0.01	0.03	-0.19	0.41	-0.06	0.21
15	-0.02	0.03	-0.01	0.00	0.00	0.49	-0.07	0.16	-0.08
16	0.01	-0.02	0.02	0.02	0.17	-0.11	0.14	-0.14	0.14
17	-0.01	0.01	-0.01	-0.01	-0.09	0.11	-0.03	0.52	0.04
18	0.00	-0.01	0.02	0.02	0.20	-0.04	0.06	-0.20	-0.01
19	0.04	0.23	-0.18	0.54	0.05	0.11	-0.03	0.03	-0.02
20	0.00	-0.14	0.37	-0.19	-0.03	-0.06	0.03	-0.02	0.02
21	0.03	0.53	-0.09	0.32	0.06	0.12	-0.03	0.03	-0.02
22	0.00	0.00	-0.03	0.01	0.00	0.00	0.00	0.00	0.00
23	0.25	0.00	0.04	-0.05	0.01	-0.04	0.15	-0.01	0.06
24	-0.12	0.07	0.02	0.07	0.00	0.03	-0.07	0.01	-0.03
25	0.25	-0.03	0.02	-0.02	0.01	-0.04	0.14	-0.01	0.06
26	0.01	-0.01	0.00	0.00	0.00	0.00	0.00	0.00	0.00
27	0.00	0.00	0.00	0.00	0.04	0.01	0.02	0.00	0.01
28	0.00	0.00	0.00	0.00	-0.02	0.00	-0.01	0.00	0.00
29	0.00	0.00	0.00	0.00	0.05	0.01	0.03	0.00	0.01
30	0.00	0.00	-0.01	0.00	-0.08	-0.02	-0.05	0.00	-0.03
31	0.00	0.00	0.00	0.00	0.04	0.01	0.03	0.00	0.01
32	0.00	0.00	0.00	0.00	-0.02	0.00	-0.01	0.00	-0.01
33	0.00	0.00	0.00	0.00	0.00	-0.06	0.01	-0.02	0.01
34	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.01	0.00
35	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
36	0.00	0.00	0.00	0.00	0.00	0.02	0.00	0.01	0.00
37	0.00	0.00	0.00	0.00	0.00	-0.01	0.00	0.00	0.00
38	0.00	0.00	0.00	0.00	0.00	0.03	0.00	0.01	-0.01

Table S13. Excitation energy, wavelength, oscillator strength, and dominant orbital transitions contributions of the $D_1 \rightarrow D_0$ emission transition for compounds B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP*.

Compounds	Excitation energy (eV)	Wavelength (nm)	Oscillator strength	Dominant orbital transitions contributions
B-1-*PP*	1.23	1010.74	0.0094	H-1→S 20.45% H→S 70.68%
B-2-*PP*	0.61	2033.11	0.0065	H-1→S 11.40% H→S 82.11%
B-3-*PP*	0.51	2444.29	0.0134	H→S 94.89%
B-4-*PP*	0.88	1404.69	0.0062	H-1→S 17.57% H→S 74.64%
B-5-*PP*	0.40	3080.78	0.012	H→S 92.69%
B-6-*PP*	1.15	1074.54	0.0289	H→S 86.95%
B-7-*PP*	1.22	1012.83	0.0503	H-1→S 72.32% H→S 10.48%
B-8-*PP*	1.30	953.72	0.022	H-3→S 25.66% H→S 65.33%
B-9-*PP*	0.84	1469.82	0.0034	H→S 75.37%

H represents HOMO, S represents SOMO.

Table S14. Excitation energy, wavelength, oscillator strength, and dominant orbital transitions contributions of the $D_0 \rightarrow D_1$ absorption transition for the optimized *PP*, *MM*, *PM* and *MP* stereoisomers of B-1 B-2, B-3, B-4, B-5, B-6, B-7, B-8, and B-9.

Compounds		Excitation energy/eV	Wavelength /nm	Oscillator strength	Dominant orbital transitions contributions
B-1	B-1-*PP*	1.8731	661.91	0.0078	H-2→S 17.44% H-1→S 23.05% H→S 53.76%
	B-1-*MM*	1.8733	661.86	0.0078	H-2→S 17.44% H-1→S 23.06% H→S 53.75%
	B-1-*MP*	1.8501	670.13	0.0095	H-2→S 10.01% H-1→S 21.30% H→S 62.93%
	B-1-*PM*	1.8502	670.11	0.0095	H-2→S 10.01% H-1→S 21.30% H→S 62.93%
B-2	B-2-*PP*	1.2116	1023.32	0.0110	H-1→S 23.68% H→S 66.54%
	B-2-*MM*	1.2116	1023.27	0.0112	H-1→S 23.68% H→S 66.55%
	B-2-*MP*	1.1908	1041.19	0.0114	H-1→S 17.27% H→S 73.59%
	B-2-*PM*	1.1908	1041.17	0.0114	H-1→S 15.72% H→S 74.86%
B-3	B-3-*PP*	1.0792	1148.87	0.0169	H→S 84.39%
	B-3-*MM*	1.079	1149.09	0.0169	H→S 84.38%
	B-3-*MP*	1.0972	1130.01	0.015	H→S 92.2%
	B-3-*PM*	1.0972	1130.00	0.015	H→S 92.2%
B-4	B-4-*PP*	1.3934	889.77	0.0051	H-1→S 24.86% H→S 63.06%
	B-4-*MM*	1.3935	889.76	0.0051	H-1→S 24.87% H→S 63.05%
	B-4-*MP*	-	-	-	-
	B-4-*PM*	-	-	-	-
B-5	B-5-*PP*	1.4764	839.76	0.0107	H-2→S 13.00% H→S 75.39%
	B-5-*MM*	1.4763	839.86	0.0108	H-2→S 13.00% H→S 75.39%

	B-5-*MP*	-	-	-	-
	B-5-*PM*	-	-	-	-
B-6	B-6-*PP*	1.5608	794.39	0.0343	H→S 83.99%
	B-6-*MM*	1.5607	794.42	0.0343	H→S 83.99%
	B-6-*MP*	1.6154	767.53	0.0385	H→S 85.37%
	B-6-*PM*	1.6154	767.53	0.0385	H→S 85.37%
B-7	B-7-*PP*	0.8557	1448.96	0.0009	H-1→S 11.76% H→S 81.13%
	B-7-*MM*	0.8555	1449.25	0.0009	H-1→S 11.75% H→S 81.14%
	B-7-*MP*	0.8138	1523.47	0.0016	H-1→S 13.80% H→S 77.69%
	B-7-*PM*	0.8137	1523.71	0.0016	H-1→S 13.78% H→S 77.71%
B-8	B-8-*PP*	1.8851	657.72	0.0194	H-3→S 25.04% H→S 61.45%
	B-8-*MM*	1.8852	657.69	0.0194	H-3→S 25.05% H→S 61.4%
	B-8-*MP*	1.9699	629.39	0.0224	H-3→S 25.38% H→S 59.50%
	B-8-*PM*	1.9699	629.4	0.0224	H-3→S 25.38% H→S 59.51%
B-9	B-9-*PP*	1.6206	765.04	0.0059	H-3→S 10.62% H-2→S 11.57% H→S 63.15%
	B-9-*MM*	1.6208	764.97	0.006	H-3→S 10.62% H-2→S 11.57% H→S 63.15%
	B-9-*MP*	1.6841	736.22	0.0055	H-3→S 12.33% H-2→S 16.08% H→S 59.90%
	B-9-*PM*	1.6841	736.19	0.0055	H-3→S 12.33% H-2→S 16.08% H→S 59.90%

Table S15. The transition magnetic dipole moment m, transition electric dipole moment μ, their angle θ, and the dissymmetry factor for boron at various positions and conformations for the $D_0 \rightarrow D_1$ transition.

Compounds	$\lvert m \rvert$ (10^{-20}erg·G^{-1})	$\lvert \mu \rvert$ (10^{-18}esu·cm)	θ (deg)	$\lvert g_{abs} \rvert$ (10^{-3})
1-H-*MM*	0.29	1.67	77.72	1.48
1-H-*PM*/*MP*	0.13	0.80	73.97	1.82
B-1-*MM*	0.77	1.05	92.47	1.27
B-1-*MP*	0.79	1.16	88.38	0.77
B-1-*PM*	0.79	1.16	91.62	0.77
B-2-*MM*	0.90	1.56	96.71	2.71
B-2-*MP*	0.94	1.59	97.58	3.10
B-2-*PM*	0.94	1.59	82.43	3.10
B-3-*MM*	1.37	2.03	92.01	0.95
B-3-*MP*	1.35	1.90	80.14	4.87
B-3-*PM*	1.35	1.90	99.86	4.87
B-4-*MM*	1.13	0.98	85.72	3.43
B-4-*MP*	-	-	-	-
B-4-*PM*	-	-	-	-
B-5-*MM*	0.93	1.39	90.22	0.10
B-5-*MP*	-	-	-	-
B-5-*PM*	-	-	-	-
B-6-*MM*	0.45	2.41	101.01	1.43
B-6-*MP*	0.44	2.51	90.00	0.00
B-6-*PM*	0.44	2.51	90.00	0.00
B-7-*MM*	0.98	0.53	92.12	2.72
B-7-*MP*	0.98	0.72	65.15	22.72
B-7-*PM*	0.98	0.72	114.74	22.62
B-8-*MM*	0.66	1.65	108.05	4.98
B-8-*MP*	0.73	1.73	90.2	5.86
B-8-*PM*	0.73	1.73	89.8	5.86
B-9-*MM*	0.70	0.98	106.88	8.19
B-9-*MP*	0.78	0.93	85.24	2.78
B-9-*PM*	0.78	0.93	94.76	2.78

Table S16. The relative Gibbs free energy (Δ*G*, 298.15K) with respect to the energy of the boron embedding compounds at the 6th position, UV-Vis absorption peak, oscillator strength (*f*), and $|g_{abs}|$ of B-embedded systems in the pyrene anthracene, pyrene tetracene, and pyrene pentacene conjugated frameworks at the 4th, 5th, and 6th positions.

Compounds		ΔG (kcal·mol^{-1})	UV-vis peak (nm)	oscillator strength *f*	$\|g_{abs}\|$ (10^{-3})
Pyrene and naphthalene	B-4	9.65	890	0.0051	3.43
	B-5	6.41	840	0.0107	0.11
	B-6	0.00	794	0.0343	1.43
pyrene anthracene	B-4	13.53	888	0.0097	3.08
	B-5	5.71	762	0.2050	0.94
	B-6	0.00	740	0.0433	1.44
pyrene tetracene	B-4	15.74	895	0.0191	2.45
	B-5	4.54	739	0.0473	0.75
	B-6	0.00	750	0.0319	1.95
pyrene pentacene	B-4	17.16	D_1:1213 D_2:901	D_1:0.0010 D_2:0.0305	1.53
	B-5	4.44	796	0.0075	1.66
	B-6	0.00	D_1:894 D_2:695	D_1:0.0035 D_2:0.1219	1.05

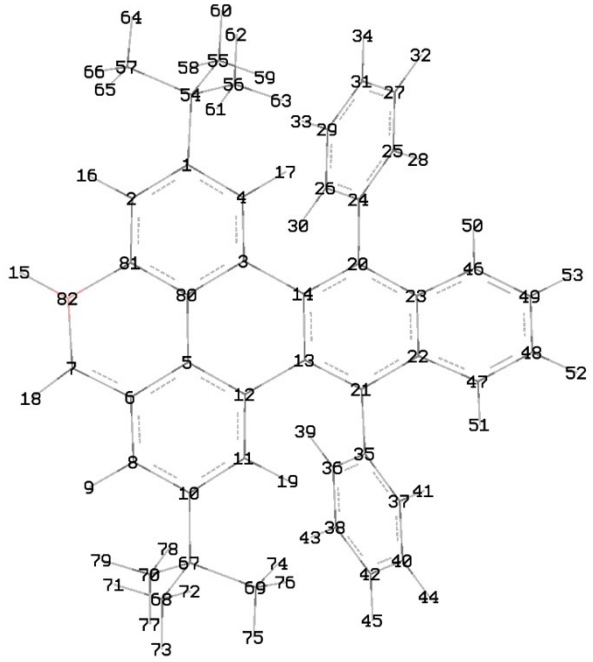


Table S17. Deviations in bond lengths and angles of B-1-*MM*, B-1-*MP*, and B-1-*PM* isomers by comparison with the B-1-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	1.63E-05	5.62E-03	5.61E-03	-	-	-	-	-	-
3	1	-3.06E-05	-5.06E-03	-5.06E-03	3	1	2	-7.17E-04	-3.76E-01	-3.76E-01
4	1	-1.44E-05	-2.97E-03	-2.97E-03	4	1	2	-5.35E-05	2.02E-03	2.05E-03
5	3	-1.28E-05	-7.10E-03	-7.10E-03	5	3	1	2.13E-03	-1.26E+00	-1.26E+00
6	5	-3.25E-05	-1.61E-03	-1.61E-03	6	5	3	-1.57E-03	-2.81E-01	-2.81E-01
7	6	2.21E-05	5.25E-04	5.22E-04	7	6	5	3.99E-04	-1.17E-01	-1.18E-01
8	6	-1.09E-05	6.18E-04	6.19E-04	8	6	5	1.31E-03	-1.89E-01	-1.89E-01

9	8	-2.80E-06	-8.29E-05	-8.24E-05	9	8	6	5.34E-04	4.09E-02	4.10E-02
10	8	-5.00E-06	-6.15E-04	-6.18E-04	10	8	6	-1.30E-03	-2.02E-01	-2.03E-01
11	10	4.50E-06	2.79E-03	2.79E-03	11	10	8	4.51E-04	1.15E-02	1.16E-02
12	5	-1.90E-06	1.52E-03	1.53E-03	12	5	3	8.66E-04	-7.86E-01	-7.86E-01
13	12	3.45E-05	-4.26E-04	-4.31E-04	13	12	5	-1.87E-04	-1.34E+00	-1.34E+00
14	13	-1.69E-05	7.89E-03	7.89E-03	14	13	12	-1.10E-05	8.60E-01	8.60E-01
15	7	-5.40E-06	2.13E-03	2.13E-03	15	7	6	2.26E-04	-2.67E-01	-2.67E-01
16	2	-6.90E-06	2.12E-03	2.12E-03	16	2	1	3.30E-04	-5.05E-01	-5.05E-01
17	4	4.70E-06	-1.60E-03	-1.60E-03	17	4	1	2.83E-04	8.66E-01	8.66E-01
18	7	-3.30E-06	9.20E-06	1.06E-05	18	7	6	6.11E-04	8.74E-02	8.68E-02
19	11	-4.10E-06	2.15E-04	2.17E-04	19	11	10	-2.00E-03	2.20E-01	2.21E-01
20	14	-2.72E-05	-4.99E-04	-4.95E-04	20	14	13	2.19E-03	5.88E-01	5.88E-01
21	13	-1.32E-05	-7.83E-04	-7.79E-04	21	13	12	2.06E-03	-1.75E+00	-1.75E+00
22	21	6.80E-06	8.16E-04	8.16E-04	22	21	13	2.26E-04	9.84E-01	9.83E-01
23	22	-2.61E-05	-2.92E-03	-2.92E-03	23	22	21	2.03E-04	3.67E-01	3.67E-01
24	20	1.15E-05	3.15E-03	3.15E-03	24	20	14	-5.41E-04	1.13E+00	1.13E+00
25	24	-3.13E-03	-2.20E-03	-4.33E-03	25	24	20	-2.11E+00	-7.28E-01	-1.72E+00
26	24	3.11E-03	-1.20E-03	9.34E-04	26	24	20	2.11E+00	3.95E-01	1.38E+00
27	25	8.95E-04	7.90E-04	1.05E-03	27	25	24	-5.74E-02	-7.17E-02	-2.03E-01
28	25	-8.12E-04	2.90E-06	-6.36E-04	28	25	24	-1.27E-01	-1.93E-02	-2.24E-02
29	26	-8.94E-04	1.45E-04	-1.12E-04	29	26	24	5.54E-02	-1.47E-01	-1.51E-02
30	26	8.06E-04	1.74E-04	8.13E-04	30	26	24	1.27E-01	1.04E-01	1.07E-01
31	29	-8.00E-07	1.02E-03	1.02E-03	31	29	26	-4.93E-04	1.68E-02	1.67E-02
32	27	-1.50E-04	2.69E-05	7.85E-05	32	27	25	-6.40E-02	3.42E-02	-5.82E-02
33	29	1.46E-04	2.27E-04	1.75E-04	33	29	26	6.56E-02	7.13E-03	9.99E-02
34	31	1.30E-06	3.44E-05	3.41E-05	34	31	29	-1.16E-03	-1.40E-02	-1.39E-02

35	21	1.91E-05	4.02E-03	4.02E-03	35	21	13	2.14E-03	1.27E+00	1.27E+00
36	35	2.18E-03	5.31E-04	-1.54E-03	36	35	21	1.93E+00	1.37E+00	2.73E-01
37	35	-2.20E-03	-3.74E-03	-1.67E-03	37	35	21	-1.93E+00	-1.66E+00	-5.61E-01
38	36	-2.31E-04	4.70E-04	7.26E-04	38	36	35	5.68E-02	4.98E-03	-1.27E-01
39	36	5.38E-04	8.00E-04	1.80E-04	39	36	35	1.68E-01	9.58E-02	8.54E-02
40	37	2.32E-04	9.63E-04	7.06E-04	40	37	35	-5.94E-02	-1.85E-01	-5.28E-02
41	37	-5.43E-04	-3.60E-04	2.60E-04	41	37	35	-1.68E-01	-8.22E-02	-7.20E-02
42	38	-4.00E-07	9.82E-05	9.69E-05	42	38	36	-2.31E-04	3.51E-02	3.52E-02
43	38	1.29E-04	1.44E-04	2.17E-04	43	38	36	5.14E-02	8.29E-02	-8.27E-03
44	40	-1.32E-04	8.55E-05	1.18E-05	44	40	37	-4.95E-02	-5.94E-02	3.20E-02
45	42	1.30E-06	-2.84E-05	-2.81E-05	45	42	38	-9.72E-04	4.17E-03	4.27E-03
46	23	1.43E-05	1.59E-03	1.58E-03	46	23	22	8.42E-04	1.74E-01	1.74E-01
47	22	1.86E-05	1.63E-03	1.63E-03	47	22	21	4.38E-05	-5.83E-01	-5.83E-01
48	47	-1.73E-05	-8.89E-04	-8.85E-04	48	47	22	-6.64E-04	2.21E-01	2.21E-01
49	46	-1.78E-05	-8.96E-04	-8.93E-04	49	46	23	-7.61E-04	2.20E-01	2.19E-01
50	46	-8.00E-07	-7.72E-04	-7.73E-04	50	46	23	-1.18E-03	2.05E-01	2.05E-01
51	47	-2.20E-06	-8.86E-04	-8.86E-04	51	47	22	-5.66E-04	2.39E-01	2.39E-01
52	48	-6.00E-07	2.59E-05	2.58E-05	52	48	47	1.00E-03	-6.72E-02	-6.71E-02
53	49	-1.00E-06	1.30E-05	1.42E-05	53	49	46	1.37E-03	-4.75E-02	-4.72E-02
54	1	-5.80E-06	-5.08E-04	-5.10E-04	54	1	4	-2.46E-03	3.49E+00	3.48E+00
55	54	5.16E-04	6.37E-04	-6.58E-03	55	54	1	5.81E-01	-3.75E-01	3.17E+00
56	54	-5.32E-04	-7.12E-03	9.95E-05	56	54	1	-5.82E-01	2.59E+00	-9.56E-01
57	54	-1.90E-05	6.10E-03	6.10E-03	57	54	1	1.95E-03	-2.20E+00	-2.20E+00
58	55	-4.72E-04	-8.02E-04	5.18E-04	58	55	54	7.42E-02	7.65E-01	7.89E-01
59	55	3.98E-04	1.28E-03	4.00E-05	59	55	54	1.75E-01	-1.15E+00	9.70E-02
60	55	-4.92E-04	-2.54E-04	-1.26E-03	60	55	54	-2.12E-01	9.42E-03	-7.68E-01

61	56	4.66E-04	9.84E-04	-3.36E-04	61	56	54	-7.35E-02	7.16E-01	6.91E-01
62	56	4.97E-04	-7.62E-04	2.40E-04	62	56	54	2.11E-01	-5.58E-01	2.19E-01
63	56	-4.00E-04	-3.55E-04	8.85E-04	63	56	54	-1.79E-01	-7.90E-02	-1.33E+00
64	57	-2.00E-07	9.57E-04	9.56E-04	64	57	54	4.25E-04	5.19E-01	5.19E-01
65	57	-1.63E-04	-2.29E-04	-1.47E-03	65	57	54	-4.77E-02	-9.65E-01	3.47E-01
66	57	1.65E-04	-1.31E-03	-6.59E-05	66	57	54	4.60E-02	3.94E-01	-9.17E-01
67	10	-1.90E-06	1.71E-04	1.67E-04	67	10	8	-3.04E-04	-3.48E-02	-3.49E-02
68	67	-1.06E-03	-9.05E-04	-2.55E-04	68	67	10	1.03E+00	1.21E+00	-7.95E-02
69	67	-1.33E-05	-1.44E-04	-1.41E-04	69	67	10	1.08E-03	-7.26E-02	-7.25E-02
70	67	1.04E-03	7.82E-04	1.38E-04	70	67	10	-1.03E+00	-1.11E+00	1.78E-01
71	68	-3.71E-04	-6.24E-04	2.96E-04	71	68	67	2.11E-01	3.87E-01	-1.60E-01
72	68	-4.26E-04	-4.12E-04	1.05E-04	72	68	67	2.85E-01	2.94E-01	-7.42E-02
73	68	-2.05E-04	-2.63E-04	1.55E-04	73	68	67	-1.06E-01	-2.08E-01	5.99E-02
74	69	-9.47E-04	-1.70E-03	1.70E-05	74	69	67	-1.77E-01	-1.39E-01	-1.61E-01
75	69	1.80E-06	2.90E-05	2.83E-05	75	69	67	-5.24E-04	2.32E-02	2.27E-02
76	69	9.43E-04	9.63E-04	-7.54E-04	76	69	67	1.76E-01	1.58E-02	3.82E-02
77	70	2.11E-04	3.64E-04	-5.72E-05	77	70	67	1.06E-01	1.65E-01	-1.03E-01
78	70	4.19E-04	5.28E-04	1.08E-05	78	70	67	-2.86E-01	-3.60E-01	8.43E-03
79	70	3.72E-04	6.66E-04	-2.53E-04	79	70	67	-2.12E-01	-3.69E-01	1.78E-01
80	3	-4.20E-05	-2.82E-03	-2.81E-03	80	3	1	1.63E-03	-8.23E-02	-8.23E-02
81	2	-6.70E-06	-5.29E-03	-5.28E-03	81	2	1	-1.12E-03	6.12E-02	6.16E-02
82	7	-5.30E-06	6.33E-04	6.32E-04	82	7	6	2.29E-04	-1.98E-01	-1.98E-01

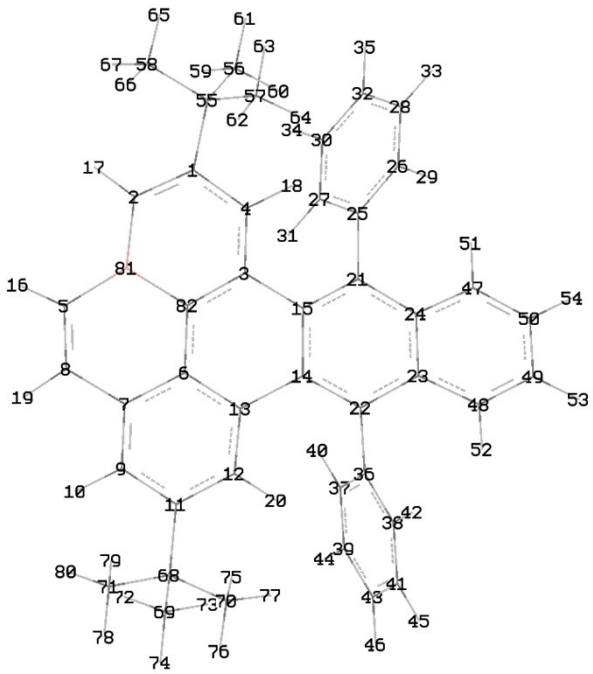


Table S18. Deviations in bond lengths and angles of B-2-*MM*, B-2-*MP*, and B-2-*PM* isomers by comparison with the B-2-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	5.00E-06	-1.81E-03	-1.81E-03	-	-	-	-	-	-
3	1	-5.40E-06	-2.34E-03	-2.34E-03	3	1	2	-1.51E-03	2.62E-01	2.62E-01
4	3	1.05E-05	-7.69E-03	-7.68E-03	4	3	1	2.25E-04	1.87E-01	1.87E-01
5	2	9.10E-06	-1.55E-03	-1.55E-03	5	2	1	1.91E-04	-7.66E-01	-7.67E-01
6	3	-2.07E-05	9.24E-04	9.34E-04	6	3	1	1.50E-03	-1.94E+00	-1.94E+00
7	6	-9.60E-06	-2.04E-04	-2.10E-04	7	6	1	-1.32E-03	-4.66E-02	-4.77E-02
8	5	-2.00E-07	-9.11E-04	-9.13E-04	8	5	2	-1.14E-03	-1.98E+00	-1.99E+00

9	7	1.30E-06	-7.15E-05	-7.19E-05	9	7	6	1.39E-03	-9.60E-02	-9.71E-02
10	9	-9.00E-07	-1.67E-04	-1.64E-04	10	9	7	8.68E-04	3.02E-02	3.07E-02
11	9	4.00E-07	-3.51E-04	-3.52E-04	11	9	7	-1.25E-03	-1.79E-01	-1.78E-01
12	11	3.70E-06	2.32E-03	2.32E-03	12	11	9	2.66E-04	3.63E-02	3.70E-02
13	12	7.00E-07	-2.58E-03	-2.57E-03	13	12	11	1.15E-03	-1.61E-01	-1.62E-01
14	13	1.49E-05	1.28E-03	1.27E-03	14	13	12	3.02E-05	1.43E+00	1.43E+00
15	14	7.10E-06	8.40E-03	8.43E-03	15	14	13	-4.11E-04	7.70E-01	7.70E-01
16	5	1.70E-06	-1.29E-04	-1.31E-04	16	5	2	9.65E-04	6.31E-01	6.32E-01
17	2	3.00E-06	-2.21E-04	-2.19E-04	17	2	1	-1.88E-04	6.09E-02	6.15E-02
18	4	-6.10E-06	-2.30E-04	-2.26E-04	18	4	3	8.39E-04	8.49E-02	8.19E-02
19	8	4.60E-06	-8.00E-05	-7.73E-05	19	8	5	9.40E-04	1.96E-01	1.96E-01
20	12	-7.30E-06	-1.85E-04	-1.86E-04	20	12	11	-2.23E-03	1.35E-01	1.38E-01
21	15	-1.12E-05	-3.17E-03	-3.18E-03	21	15	14	1.02E-03	5.29E-01	5.28E-01
22	14	-3.00E-06	-1.97E-03	-2.00E-03	22	14	13	1.49E-03	-1.69E+00	-1.69E+00
23	22	1.01E-05	2.16E-03	2.19E-03	23	22	14	7.67E-04	9.05E-01	9.06E-01
24	21	-7.00E-07	-2.19E-03	-2.20E-03	24	21	15	5.03E-04	-1.28E-01	-1.29E-01
25	21	8.00E-06	4.30E-03	4.30E-03	25	21	15	2.38E-03	1.80E+00	1.80E+00
26	25	-2.76E-03	-1.76E-03	-4.40E-03	26	25	21	-2.10E+00	-7.42E-01	-1.94E+00
27	25	2.76E-03	-1.64E-03	1.00E-03	27	25	21	2.10E+00	1.55E-01	1.36E+00
28	26	1.06E-03	7.41E-04	1.67E-03	28	26	25	-8.10E-02	-9.71E-02	-2.10E-01
29	26	-7.44E-04	1.87E-04	-6.58E-04	29	26	25	-1.19E-01	-2.33E-02	-5.24E-02
30	27	-1.06E-03	6.07E-04	-3.19E-04	30	27	25	7.99E-02	-1.29E-01	-1.69E-02
31	27	7.43E-04	8.41E-05	9.29E-04	31	27	25	1.18E-01	6.61E-02	9.49E-02
32	30	5.70E-06	7.00E-07	5.40E-06	32	30	27	-1.49E-05	1.32E-02	1.31E-02
33	28	-1.47E-04	2.88E-05	-4.32E-05	33	28	26	-7.80E-02	2.97E-02	-7.59E-02
34	30	1.48E-04	1.06E-04	1.78E-04	34	30	27	7.89E-02	2.74E-03	1.09E-01

35	32	2.00E-06	-2.33E-05	-2.23E-05	35	32	30	-9.72E-04	-4.77E-03	-5.13E-03
36	22	8.00E-06	4.19E-03	4.20E-03	36	22	14	2.84E-03	1.41E+00	1.40E+00
37	36	2.43E-03	8.05E-04	-1.50E-03	37	36	22	1.89E+00	1.35E+00	2.60E-01
38	36	-2.43E-03	-3.92E-03	-1.62E-03	38	36	22	-1.89E+00	-1.64E+00	-5.47E-01
39	37	-3.70E-04	4.03E-04	7.52E-04	39	37	36	6.11E-02	1.50E-02	-1.11E-01
40	37	6.11E-04	8.02E-04	1.60E-04	40	37	36	1.35E-01	9.13E-02	7.82E-02
41	38	3.75E-04	1.13E-03	7.78E-04	41	38	36	-6.18E-02	-1.72E-01	-4.61E-02
42	38	-6.10E-04	-4.51E-04	1.93E-04	42	38	36	-1.35E-01	-5.64E-02	-4.36E-02
43	39	5.00E-07	1.76E-04	1.80E-04	43	39	37	4.19E-05	3.35E-02	3.35E-02
44	39	1.17E-04	1.32E-04	1.78E-04	44	39	37	6.10E-02	7.82E-02	-1.14E-02
45	41	-1.14E-04	6.26E-05	1.65E-05	45	41	38	-6.07E-02	-7.24E-02	1.82E-02
46	43	2.20E-06	-3.60E-05	-3.44E-05	46	43	39	-3.08E-05	2.87E-03	2.19E-03
47	24	2.20E-06	9.54E-04	9.44E-04	47	24	21	-1.09E-03	-4.13E+00	-4.12E+00
48	23	1.04E-05	8.65E-04	8.60E-04	48	23	22	1.13E-03	-5.48E-01	-5.47E-01
49	48	-2.40E-06	-3.41E-04	-3.32E-04	49	48	23	2.79E-04	2.13E-01	2.13E-01
50	47	-1.20E-06	-1.73E-04	-1.71E-04	50	47	24	-2.36E-04	1.92E-01	1.92E-01
51	47	1.60E-06	-5.99E-04	-5.96E-04	51	47	24	-9.67E-04	2.84E-01	2.83E-01
52	48	-1.60E-06	-8.31E-04	-8.33E-04	52	48	23	3.41E-05	2.50E-01	2.51E-01
53	49	2.10E-06	1.79E-05	1.79E-05	53	49	48	-2.37E-04	-6.58E-02	-6.64E-02
54	50	6.00E-07	2.95E-05	2.80E-05	54	50	47	3.10E-04	-7.36E-02	-7.37E-02
55	1	6.00E-07	-3.28E-04	-3.32E-04	55	1	2	5.37E-04	-2.55E-01	-2.57E-01
56	55	1.92E-03	-1.18E-03	2.00E-03	56	55	1	6.51E-01	3.67E-01	2.95E-01
57	55	-1.90E-03	8.48E-05	-3.09E-03	57	55	1	-6.50E-01	-3.55E-01	-2.80E-01
58	55	-4.00E-07	4.91E-05	4.51E-05	58	55	1	-1.76E-03	5.00E-02	4.59E-02
59	56	-4.61E-04	2.31E-05	-4.78E-04	59	56	55	7.78E-02	1.05E-01	7.10E-02
60	56	1.03E-03	-9.00E-04	1.05E-03	60	56	55	3.70E-01	-6.18E-02	2.93E-01

61	56	-5.85E-04	3.64E-05	-5.49E-04	61	56	55	-3.62E-01	-1.39E-02	-3.38E-01
62	57	4.61E-04	-1.67E-05	4.85E-04	62	57	55	-7.47E-02	-5.65E-03	3.06E-02
63	57	5.91E-04	3.50E-05	6.22E-04	63	57	55	3.61E-01	2.35E-02	3.46E-01
64	57	-1.02E-03	3.09E-05	-1.92E-03	64	57	55	-3.72E-01	-7.64E-02	-4.32E-01
65	58	1.40E-06	1.30E-05	1.17E-05	65	58	55	3.23E-04	-4.07E-02	-4.01E-02
66	58	-2.13E-04	-1.14E-04	-1.65E-04	66	58	55	-7.12E-02	4.02E-02	-8.48E-02
67	58	2.18E-04	4.89E-05	1.03E-04	67	58	55	7.09E-02	-1.22E-02	1.11E-01
68	11	1.60E-06	-1.97E-04	-1.94E-04	68	11	9	-3.95E-04	-4.90E-02	-4.96E-02
69	68	-8.61E-04	-7.01E-04	-1.08E-04	69	68	11	8.06E-01	1.10E+00	-2.63E-01
70	68	-1.00E-07	-3.62E-04	-3.68E-04	70	68	11	-6.64E-04	-4.77E-02	-4.78E-02
71	68	8.61E-04	7.65E-04	1.78E-04	71	68	11	-8.06E-01	-1.08E+00	2.88E-01
72	69	-2.18E-04	-5.47E-04	3.16E-04	72	69	68	1.09E-01	3.48E-01	-1.60E-01
73	69	-3.40E-04	-3.23E-04	2.22E-04	73	69	68	2.24E-01	2.44E-01	-1.02E-01
74	69	-1.49E-04	-2.46E-04	1.07E-04	74	69	68	-4.93E-02	-1.94E-01	6.52E-02
75	70	-7.24E-04	-1.58E-03	3.78E-05	75	70	68	-1.27E-01	-1.27E-01	-1.23E-01
76	70	2.30E-06	6.40E-06	8.30E-06	76	70	68	2.92E-04	1.60E-02	1.62E-02
77	70	7.30E-04	7.63E-04	-8.56E-04	77	70	68	1.28E-01	2.40E-03	-9.89E-04
78	71	1.54E-04	2.60E-04	-9.51E-05	78	71	68	4.95E-02	1.17E-01	-1.42E-01
79	71	3.39E-04	5.60E-04	1.75E-05	79	71	68	-2.23E-01	-3.26E-01	1.82E-02
80	71	2.24E-04	5.43E-04	-3.22E-04	80	71	68	-1.10E-01	-2.75E-01	2.33E-01
81	2	-2.20E-06	-2.22E-03	-2.20E-03	81	2	1	7.46E-04	-2.80E-01	-2.80E-01
82	3	-2.31E-05	6.10E-03	6.09E-03	82	3	1	1.37E-03	-5.27E-01	-5.27E-01

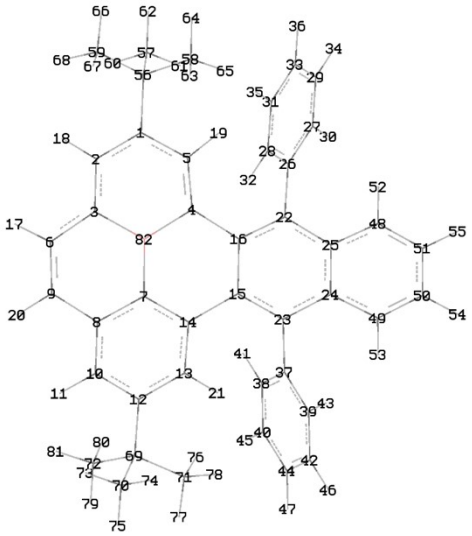


Table S19. Deviations in bond lengths and angles of B-3-*MM*, B-3-*MP*, and B-3-*PM* isomers by comparison with the B-3-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
1	2	0.00E+00	1.90E-02	1.90E-02	-	-	-	-	-	-
1	5	0.00E+00	-1.67E-02	-1.67E-02	2	1	5	-4.00E-04	-7.93E-02	-7.93E-02
1	56	0.00E+00	1.50E-03	1.50E-03	2	1	56	-2.70E-03	-3.99E+00	-3.99E+00
2	3	0.00E+00	-1.51E-02	-1.51E-02	5	1	56	3.10E-03	4.08E+00	4.08E+00
2	18	0.00E+00	2.60E-03	2.60E-03	1	2	3	9.00E-04	6.53E-01	6.53E-01
3	6	0.00E+00	1.07E-02	1.07E-02	1	2	18	-2.10E-03	-1.13E+00	-1.13E+00
3	82	0.00E+00	-4.00E-04	-4.00E-04	3	2	18	1.30E-03	3.27E-01	3.27E-01
4	5	0.00E+00	8.20E-03	8.20E-03	2	3	6	2.00E-03	9.72E-02	9.72E-02
4	16	0.00E+00	-5.30E-03	-5.30E-03	2	3	82	-1.00E-03	-3.76E-01	-3.76E-01
4	82	0.00E+00	1.70E-03	1.70E-03	6	3	82	-8.00E-04	1.00E-02	1.00E-02
5	19	0.00E+00	-2.30E-03	-2.30E-03	5	4	16	-7.00E-03	4.24E-01	4.24E-01

6	9	1.00E-04	-7.10E-03	-7.10E-03	5	4	82	2.80E-03	6.74E-01	6.74E-01
6	17	0.00E+00	-1.00E-04	-1.00E-04	16	4	82	3.00E-03	-7.15E-01	-7.15E-01
7	8	0.00E+00	-4.00E-04	-4.00E-04	1	5	4	-2.60E-03	-9.15E-01	-9.15E-01
7	14	0.00E+00	2.90E-03	2.90E-03	1	5	19	6.50E-03	1.47E+00	1.47E+00
7	82	0.00E+00	1.20E-03	1.20E-03	4	5	19	-4.00E-03	-5.52E-01	-5.52E-01
8	9	0.00E+00	4.60E-03	4.60E-03	3	6	9	-3.00E-04	-4.21E-01	-4.21E-01
8	10	0.00E+00	-1.00E-04	-1.00E-04	3	6	17	3.00E-04	-1.40E-03	-1.40E-03
9	20	0.00E+00	0.00E+00	0.00E+00	9	6	17	0.00E+00	3.13E-01	3.13E-01
10	11	0.00E+00	-1.00E-04	-1.00E-04	8	7	14	1.70E-03	-1.72E-01	-1.72E-01
10	12	0.00E+00	-5.00E-04	-5.00E-04	8	7	82	-1.10E-03	-2.89E-01	-2.89E-01
12	13	0.00E+00	1.30E-03	1.30E-03	14	7	82	2.00E-04	-6.95E-01	-6.95E-01
12	69	0.00E+00	0.00E+00	0.00E+00	7	8	9	1.00E-04	1.83E-01	1.83E-01
13	14	0.00E+00	-3.20E-03	-3.20E-03	7	8	10	-9.00E-04	-6.58E-02	-6.58E-02
13	21	-1.00E-04	2.00E-04	2.00E-04	9	8	10	9.00E-04	-2.07E-01	-2.07E-01
14	15	0.00E+00	2.00E-04	2.00E-04	6	9	8	5.00E-04	-3.71E-01	-3.71E-01
15	16	0.00E+00	2.50E-03	2.50E-03	6	9	20	-5.00E-04	2.27E-01	2.27E-01
15	23	0.00E+00	-1.80E-03	-1.80E-03	8	9	20	1.00E-04	5.40E-02	5.40E-02
16	22	0.00E+00	-2.00E-04	-2.00E-04	8	10	11	0.00E+00	-6.63E-02	-6.63E-02
22	25	0.00E+00	1.20E-03	1.20E-03	8	10	12	2.00E-04	5.52E-02	5.52E-02
22	26	0.00E+00	3.30E-03	3.30E-03	11	10	12	-3.00E-04	-5.58E-02	-5.58E-02
23	24	0.00E+00	1.50E-03	1.50E-03	10	12	13	8.00E-04	8.00E-04	8.00E-04
23	37	0.00E+00	1.80E-03	1.80E-03	10	12	69	-2.40E-03	7.20E-03	7.20E-03
24	25	1.00E-04	-1.30E-03	-1.30E-03	13	12	69	1.60E-03	-5.30E-03	-5.30E-03
24	49	0.00E+00	1.00E-04	1.00E-04	12	13	14	-1.00E-04	-1.79E-01	-1.79E-01
25	48	0.00E+00	7.00E-04	7.00E-04	12	13	21	0.00E+00	1.94E-01	1.94E-01
26	27	-2.30E-03	-2.00E-03	-2.40E-03	14	13	21	0.00E+00	-1.21E-02	-1.21E-02

26	28	2.40E-03	-1.00E-04	3.00E-04	7	14	13	-8.00E-04	1.94E-01	1.94E-01
27	29	3.00E-04	4.00E-04	1.00E-03	7	14	15	2.50E-03	-8.47E-01	-8.47E-01
27	30	-8.00E-04	-6.00E-04	-2.00E-04	13	14	15	-1.90E-03	7.27E-01	7.27E-01
28	31	-3.00E-04	7.00E-04	1.00E-04	14	15	16	-1.20E-03	4.92E-02	4.92E-02
28	32	8.00E-04	6.00E-04	2.00E-04	14	15	23	3.30E-03	-7.24E-01	-7.24E-01
29	33	-9.00E-04	-9.00E-04	-4.00E-04	16	15	23	-2.10E-03	5.35E-01	5.35E-01
29	34	0.00E+00	0.00E+00	1.00E-04	4	16	15	-2.10E-03	3.30E-01	3.30E-01
31	33	9.00E-04	5.00E-04	0.00E+00	4	16	22	1.40E-03	-1.13E+00	-1.13E+00
31	35	0.00E+00	1.00E-04	0.00E+00	15	16	22	1.50E-03	5.93E-01	5.93E-01
33	36	0.00E+00	-1.00E-04	-1.00E-04	16	22	25	-2.80E-03	3.90E-01	3.90E-01
37	38	2.60E-03	1.60E-03	-9.00E-04	16	22	26	1.70E-03	1.35E+00	1.35E+00
37	39	-2.60E-03	-3.50E-03	-1.00E-03	25	22	26	1.10E-03	-1.90E+00	-1.90E+00
38	40	-4.00E-04	0.00E+00	2.00E-04	15	23	24	-1.20E-03	4.56E-01	4.56E-01
38	41	7.00E-04	8.00E-04	1.00E-04	15	23	37	-2.70E-03	5.69E-01	5.69E-01
39	42	4.00E-04	6.00E-04	4.00E-04	24	23	37	4.20E-03	-1.14E+00	-1.14E+00
39	43	-7.00E-04	-6.00E-04	1.00E-04	23	24	25	4.00E-04	2.81E-01	2.81E-01
40	44	7.00E-04	6.00E-04	2.00E-04	23	24	49	-8.00E-04	-3.67E-01	-3.67E-01
40	45	2.00E-04	2.00E-04	1.00E-04	25	24	49	3.00E-04	7.11E-02	7.11E-02
42	44	-7.00E-04	-5.00E-04	-1.00E-04	22	25	24	-2.00E-04	2.98E-01	2.98E-01
42	46	-2.00E-04	-1.00E-04	0.00E+00	22	25	48	1.70E-03	-4.29E-01	-4.29E-01
44	47	0.00E+00	0.00E+00	0.00E+00	24	25	48	-1.50E-03	1.09E-01	1.09E-01
48	51	0.00E+00	-3.00E-04	-3.00E-04	22	26	27	-1.26E+00	-5.11E-01	-1.03E+00
48	52	0.00E+00	-2.00E-04	-2.00E-04	22	26	28	1.26E+00	2.30E-01	7.52E-01
49	50	0.00E+00	0.00E+00	0.00E+00	27	26	28	-2.30E-03	9.98E-02	9.98E-02
49	53	0.00E+00	-4.00E-04	-4.00E-04	26	27	29	-2.99E-02	-4.37E-02	-8.32E-02
50	51	-1.00E-04	-1.30E-03	-1.30E-03	26	27	30	-8.53E-02	2.39E-02	-1.89E-02

50	54	0.00E+00	0.00E+00	0.00E+00	29	27	30	1.19E-01	2.30E-02	1.06E-01
51	55	0.00E+00	0.00E+00	0.00E+00	26	28	31	3.26E-02	-5.14E-02	-1.19E-02
56	57	1.00E-03	-7.90E-03	4.00E-04	26	28	32	8.52E-02	6.64E-02	1.09E-01
56	58	-1.00E-03	-6.00E-04	-8.90E-03	31	28	32	-1.21E-01	-1.45E-02	-9.74E-02
56	59	0.00E+00	8.20E-03	8.20E-03	27	29	33	9.53E-02	2.84E-02	9.57E-02
57	60	-2.00E-04	-1.50E-03	2.00E-04	27	29	34	-3.99E-02	-2.16E-02	-4.98E-02
57	61	4.00E-04	1.70E-03	6.00E-04	33	29	34	-5.52E-02	-7.20E-03	-4.70E-02
57	62	-5.00E-04	-4.00E-04	-1.20E-03	28	31	33	-9.45E-02	6.00E-04	-6.67E-02
58	63	2.00E-04	4.00E-04	-1.30E-03	28	31	35	3.84E-02	-1.04E-02	1.78E-02
58	64	5.00E-04	-7.00E-04	1.00E-04	33	31	35	5.59E-02	8.50E-03	4.83E-02
58	65	-4.00E-04	2.00E-04	1.30E-03	29	33	31	-1.00E-03	-2.59E-02	-2.59E-02
59	66	0.00E+00	1.00E-03	1.00E-03	29	33	36	3.65E-02	2.32E-02	3.85E-02
59	67	-3.00E-04	-2.00E-04	-2.00E-03	31	33	36	-3.54E-02	2.30E-03	-1.30E-02
59	68	3.00E-04	-1.70E-03	1.00E-04	23	37	38	1.73E+00	1.41E+00	1.62E-01
69	70	-8.00E-04	-7.00E-04	-1.00E-04	23	37	39	-1.73E+00	-1.57E+00	-3.26E-01
69	71	0.00E+00	0.00E+00	0.00E+00	38	37	39	-1.00E-03	1.32E-01	1.32E-01
69	72	8.00E-04	7.00E-04	1.00E-04	37	38	40	4.94E-02	6.50E-03	-8.62E-02
70	73	-7.00E-04	-9.00E-04	1.00E-04	37	38	41	1.78E-01	1.53E-01	5.46E-02
70	74	-6.00E-04	-6.00E-04	0.00E+00	40	38	41	-2.25E-01	-1.53E-01	3.13E-02
70	75	-3.00E-04	-3.00E-04	1.00E-04	37	39	42	-4.83E-02	-1.35E-01	-4.26E-02
71	76	-1.10E-03	-1.40E-03	0.00E+00	37	39	43	-1.78E-01	-1.23E-01	-2.50E-02
71	77	0.00E+00	0.00E+00	0.00E+00	42	39	43	2.24E-01	2.55E-01	7.10E-02
71	78	1.10E-03	1.10E-03	-3.00E-04	38	40	44	-1.10E-01	-1.36E-01	1.53E-02
72	79	3.00E-04	4.00E-04	0.00E+00	38	40	45	6.62E-02	9.12E-02	-4.40E-03
72	80	6.00E-04	6.00E-04	0.00E+00	44	40	45	4.10E-02	4.31E-02	-1.09E-02
72	81	7.00E-04	8.00E-04	-2.00E-04	39	42	44	1.10E-01	1.25E-01	-2.56E-02

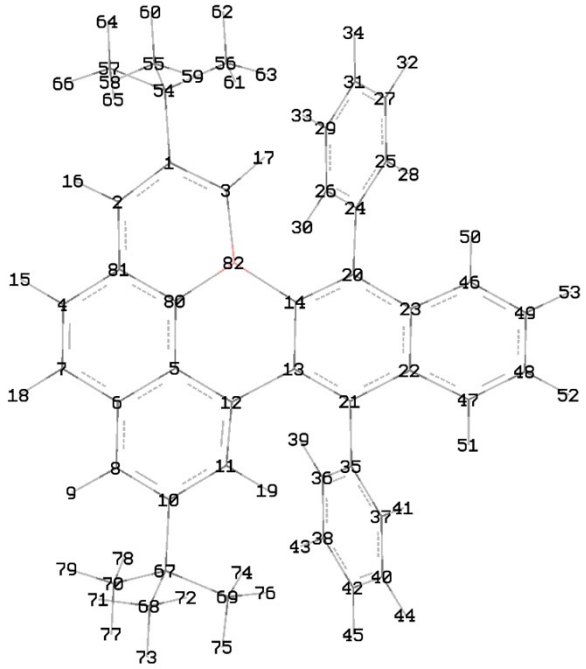


Table S20. Deviations in bond lengths and angles of B-4-*MM*, B-4-*MP*, and B-4-*PM* isomers by comparison with the B-4-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	4.30E-06	-	-	-	-	-	-	-	-
3	1	-8.60E-06	-	-	3	1	2	-3.38E-05	-	-
4	2	4.00E-07	-	-	4	2	1	2.12E-04	-	-
5	4	1.11E-05	-	-	5	4	2	-1.69E-04	-	-
6	5	-6.90E-06	-	-	6	5	4	-3.28E-04	-	-
7	4	-2.80E-06	-	-	7	4	2	-2.72E-04	-	-
8	6	3.70E-06	-	-	8	6	5	3.78E-04	-	-

9	8	-2.80E-06	-	-	9	8	6	-6.13E-04	-	-
10	8	-2.40E-06	-	-	10	8	6	-4.22E-04	-	-
11	10	3.00E-07	-	-	11	10	8	-9.71E-05	-	-
12	11	5.00E-07	-	-	12	11	10	3.68E-04	-	-
13	12	5.00E-06	-	-	13	12	11	2.50E-04	-	-
14	13	9.00E-07	-	-	14	13	12	-5.52E-05	-	-
15	4	-2.80E-06	-	-	15	4	2	-6.43E-04	-	-
16	2	-2.20E-06	-	-	16	2	1	8.77E-05	-	-
17	3	-2.20E-06	-	-	17	3	1	2.63E-04	-	-
18	7	-1.60E-06	-	-	18	7	4	1.10E-03	-	-
19	11	-2.90E-06	-	-	19	11	10	-1.62E-03	-	-
20	14	-2.20E-06	-	-	20	14	13	-2.25E-04	-	-
21	13	-5.40E-06	-	-	21	13	12	-1.26E-04	-	-
22	21	5.30E-06	-	-	22	21	13	2.16E-04	-	-
23	22	-4.30E-06	-	-	23	22	21	-3.24E-04	-	-
24	20	-3.10E-06	-	-	24	20	14	7.04E-04	-	-
25	24	-2.25E-03	-	-	25	24	20	-9.97E-01	-	-
26	24	2.25E-03	-	-	26	24	20	9.97E-01	-	-
27	25	1.07E-03	-	-	27	25	24	1.68E-02	-	-
28	25	-6.31E-04	-	-	28	25	24	-1.39E-01	-	-
29	26	-1.07E-03	-	-	29	26	24	-1.67E-02	-	-
30	26	6.29E-04	-	-	30	26	24	1.39E-01	-	-
31	29	-2.00E-07	-	-	31	29	26	-6.00E-05	-	-
32	27	-3.35E-05	-	-	32	27	25	-2.50E-02	-	-
33	29	3.32E-05	-	-	33	29	26	2.53E-02	-	-
34	31	-9.00E-07	-	-	34	31	29	1.01E-04	-	-

35	21	5.70E-06	-	-	35	21	13	-1.97E-04	-	-
36	35	1.92E-03	-	-	36	35	21	1.52E+00	-	-
37	35	-1.93E-03	-	-	37	35	21	-1.52E+00	-	-
38	36	6.19E-04	-	-	38	36	35	8.14E-02	-	-
39	36	7.32E-04	-	-	39	36	35	1.58E-01	-	-
40	37	-6.17E-04	-	-	40	37	35	-8.24E-02	-	-
41	37	-7.35E-04	-	-	41	37	35	-1.59E-01	-	-
42	40	-3.30E-06	-	-	42	40	37	-1.79E-04	-	-
43	38	1.09E-04	-	-	43	38	36	5.22E-02	-	-
44	40	-1.09E-04	-	-	44	40	37	-5.14E-02	-	-
45	42	-2.00E-07	-	-	45	42	40	2.19E-04	-	-
46	23	4.40E-06	-	-	46	23	22	-3.58E-04	-	-
47	22	4.00E-06	-	-	47	22	21	-1.01E-04	-	-
48	47	-5.20E-06	-	-	48	47	22	-3.49E-04	-	-
49	46	-5.50E-06	-	-	49	46	23	-3.77E-05	-	-
50	46	-9.00E-07	-	-	50	46	23	-4.69E-04	-	-
51	47	-2.30E-06	-	-	51	47	22	-5.30E-04	-	-
52	48	-7.00E-07	-	-	52	48	47	6.87E-04	-	-
53	49	1.00E-07	-	-	53	49	46	4.55E-04	-	-
54	1	-3.90E-06	-	-	54	1	3	7.73E-05	-	-
55	54	3.06E-04	-	-	55	54	1	6.49E-01	-	-
56	54	-3.01E-04	-	-	56	54	1	-6.50E-01	-	-
57	54	-2.80E-06	-	-	57	54	1	-4.55E-05	-	-
58	55	-2.58E-04	-	-	58	55	54	8.11E-02	-	-
59	55	8.30E-06	-	-	59	55	54	4.53E-01	-	-
60	55	-3.85E-04	-	-	60	55	54	-2.15E-01	-	-

61	56	2.56E-04	-	-	61	56	54	-8.09E-02	-	-
62	56	3.84E-04	-	-	62	56	54	2.15E-01	-	-
63	56	-9.10E-06	-	-	63	56	54	-4.53E-01	-	-
64	57	-1.00E-06	-	-	64	57	54	2.33E-04	-	-
65	57	-2.96E-04	-	-	65	57	54	1.26E-01	-	-
66	57	2.96E-04	-	-	66	57	54	-1.26E-01	-	-
67	10	-2.70E-06	-	-	67	10	8	2.63E-03	-	-
68	67	-1.15E-03	-	-	68	67	10	1.53E+00	-	-
69	67	3.30E-06	-	-	69	67	10	-6.74E-04	-	-
70	67	1.15E-03	-	-	70	67	10	-1.53E+00	-	-
71	68	-9.36E-04	-	-	71	68	67	6.36E-01	-	-
72	68	-6.65E-04	-	-	72	68	67	3.85E-01	-	-
73	68	-5.22E-04	-	-	73	68	67	-2.75E-01	-	-
74	69	-1.20E-03	-	-	74	69	67	1.40E-02	-	-
75	69	9.00E-07	-	-	75	69	67	-5.86E-05	-	-
76	69	1.20E-03	-	-	76	69	67	-1.32E-02	-	-
77	70	5.21E-04	-	-	77	70	67	2.75E-01	-	-
78	70	6.63E-04	-	-	78	70	67	-3.84E-01	-	-
79	70	9.33E-04	-	-	79	70	67	-6.35E-01	-	-
80	5	2.20E-06	-	-	80	5	4	-8.18E-05	-	-
81	80	-2.10E-06	-	-	81	80	5	1.09E-04	-	-
82	80	-3.60E-06	-	-	82	80	5	1.23E-04	-	-

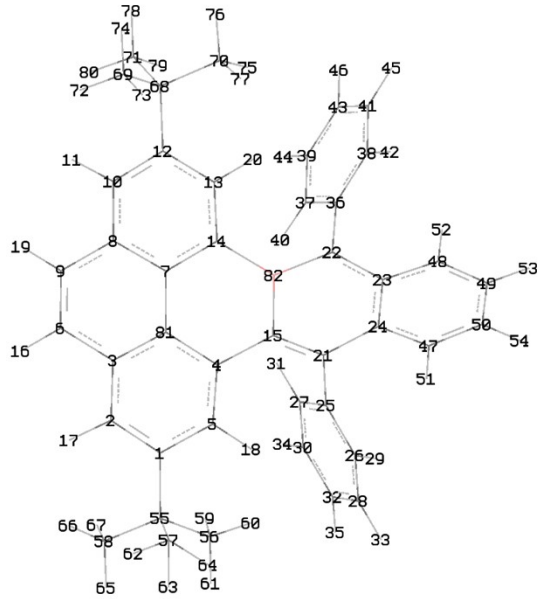


Table S21. Deviations in bond lengths and angles of B-5-*MM*, B-5-*MP*, and B-5-*PM* isomers by comparison with the B-5-*PP* structure.

Atom1	Atom2	Δr_{MM-PP} (Å)	Δr_{PM-PP} (Å)	Δr_{MP-PP} (Å)	Atom1	Atom2	Atom3	ΔA_{MM-PP} (°)	ΔA_{PM-PP} (°)	ΔA_{MP-PP} (°)
2	1	6.00E-07	-	-	-	-	-	-	-	-
3	1	1.00E-07	-	-	3	1	2	-1.16E-05	-	-
4	3	-5.00E-07	-	-	4	3	1	-3.76E-05	-	-
5	2	2.40E-06	-	-	5	2	1	-2.13E-05	-	-
6	3	-1.00E-07	-	-	6	3	1	3.30E-05	-	-
7	6	-7.00E-07	-	-	7	6	3	1.10E-04	-	-
8	5	1.00E-07	-	-	8	5	2	-7.07E-05	-	-
9	7	2.00E-07	-	-	9	7	6	-8.10E-06	-	-

10	9	2.00E-07	-	-	10	9	7	-5.54E-05	-	-
11	9	-3.00E-07	-	-	11	9	7	5.60E-05	-	-
12	11	1.00E-06	-	-	12	11	9	-3.12E-05	-	-
13	12	2.00E-07	-	-	13	12	11	-7.38E-05	-	-
14	13	-2.20E-06	-	-	14	13	12	3.10E-06	-	-
15	5	1.00E-06	-	-	15	5	2	8.13E-05	-	-
16	2	3.00E-07	-	-	16	2	1	-1.05E-04	-	-
17	4	2.00E-07	-	-	17	4	3	-5.67E-05	-	-
18	8	2.00E-07	-	-	18	8	5	-6.30E-05	-	-
19	12	6.00E-07	-	-	19	12	11	2.06E-04	-	-
20	14	-2.40E-06	-	-	20	14	13	3.59E-05	-	-
21	14	1.20E-06	-	-	21	14	13	-8.18E-05	-	-
22	21	-7.00E-07	-	-	22	21	14	-1.40E-04	-	-
23	20	-1.00E-07	-	-	23	20	14	6.32E-05	-	-
24	20	1.20E-06	-	-	24	20	14	-1.62E-04	-	-
25	24	-1.39E-03	-	-	25	24	20	-2.27E+00	-	-
26	24	1.39E-03	-	-	26	24	20	2.27E+00	-	-
27	25	-9.81E-04	-	-	27	25	24	6.23E-02	-	-
28	25	-3.01E-04	-	-	28	25	24	-1.01E-01	-	-
29	26	9.83E-04	-	-	29	26	24	-6.25E-02	-	-
30	26	3.00E-04	-	-	30	26	24	1.01E-01	-	-
31	27	-9.00E-07	-	-	31	27	25	6.20E-06	-	-
32	27	-9.42E-05	-	-	32	27	25	6.60E-03	-	-
33	29	9.54E-05	-	-	33	29	26	-6.60E-03	-	-
34	31	0.00E+00	-	-	34	31	27	1.00E-07	-	-
35	21	-1.20E-06	-	-	35	21	14	-1.32E-04	-	-

36	35	2.87E-03	-	-	36	35	21	1.65E+00	-	-
37	35	-2.87E-03	-	-	37	35	21	-1.65E+00	-	-
38	36	-3.43E-04	-	-	38	36	35	5.61E-02	-	-
39	36	8.06E-04	-	-	39	36	35	2.34E-01	-	-
40	37	3.43E-04	-	-	40	37	35	-5.60E-02	-	-
41	37	-8.07E-04	-	-	41	37	35	-2.34E-01	-	-
42	38	2.00E-07	-	-	42	38	36	-4.87E-05	-	-
43	38	1.04E-04	-	-	43	38	36	7.38E-02	-	-
44	40	-1.05E-04	-	-	44	40	37	-7.38E-02	-	-
45	42	-1.20E-06	-	-	45	42	38	1.11E-05	-	-
46	23	-1.80E-06	-	-	46	23	20	4.96E-05	-	-
47	22	3.00E-07	-	-	47	22	21	-7.07E-05	-	-
48	47	-9.00E-07	-	-	48	47	22	-3.64E-05	-	-
49	46	1.20E-06	-	-	49	46	23	-3.97E-05	-	-
50	46	-7.00E-07	-	-	50	46	23	7.73E-05	-	-
51	47	-5.00E-07	-	-	51	47	22	-4.73E-05	-	-
52	48	-4.00E-07	-	-	52	48	47	8.19E-05	-	-
53	49	1.00E-07	-	-	53	49	46	-8.90E-06	-	-
54	1	-1.00E-06	-	-	54	1	2	3.35E-05	-	-
55	54	3.20E-04	-	-	55	54	1	3.18E-01	-	-
56	54	-3.20E-04	-	-	56	54	1	-3.18E-01	-	-
57	54	3.00E-07	-	-	57	54	1	-4.23E-05	-	-
58	55	-3.27E-04	-	-	58	55	54	1.17E-01	-	-
59	55	9.15E-05	-	-	59	55	54	5.59E-02	-	-
60	55	-3.69E-04	-	-	60	55	54	-1.15E-01	-	-
61	56	3.27E-04	-	-	61	56	54	-1.17E-01	-	-

62	56	3.69E-04	-	-	62	56	54	1.16E-01	-	-
63	56	-9.13E-05	-	-	63	56	54	-5.59E-02	-	-
64	57	4.00E-07	-	-	64	57	54	-3.91E-05	-	-
65	57	-1.47E-04	-	-	65	57	54	2.76E-02	-	-
66	57	1.46E-04	-	-	66	57	54	-2.76E-02	-	-
67	11	5.00E-07	-	-	67	11	9	1.75E-04	-	-
68	67	-1.11E-03	-	-	68	67	11	1.32E+00	-	-
69	67	-2.00E-07	-	-	69	67	11	-6.42E-05	-	-
70	67	1.11E-03	-	-	70	67	11	-1.32E+00	-	-
71	68	-6.45E-04	-	-	71	68	67	4.50E-01	-	-
72	68	-6.19E-04	-	-	72	68	67	3.55E-01	-	-
73	68	-3.77E-04	-	-	73	68	67	-2.17E-01	-	-
74	69	-8.16E-04	-	-	74	69	67	5.47E-02	-	-
75	69	5.00E-07	-	-	75	69	67	-7.00E-06	-	-
76	69	8.15E-04	-	-	76	69	67	-5.47E-02	-	-
77	70	3.77E-04	-	-	77	70	67	2.17E-01	-	-
78	70	6.19E-04	-	-	78	70	67	-3.55E-01	-	-
79	70	6.46E-04	-	-	79	70	67	-4.50E-01	-	-
80	3	-9.00E-07	-	-	80	3	1	3.78E-05	-	-
81	2	2.00E-07	-	-	81	2	1	2.22E-05	-	-
82	14	-1.40E-06	-	-	82	14	13	-1.00E-06	-	-

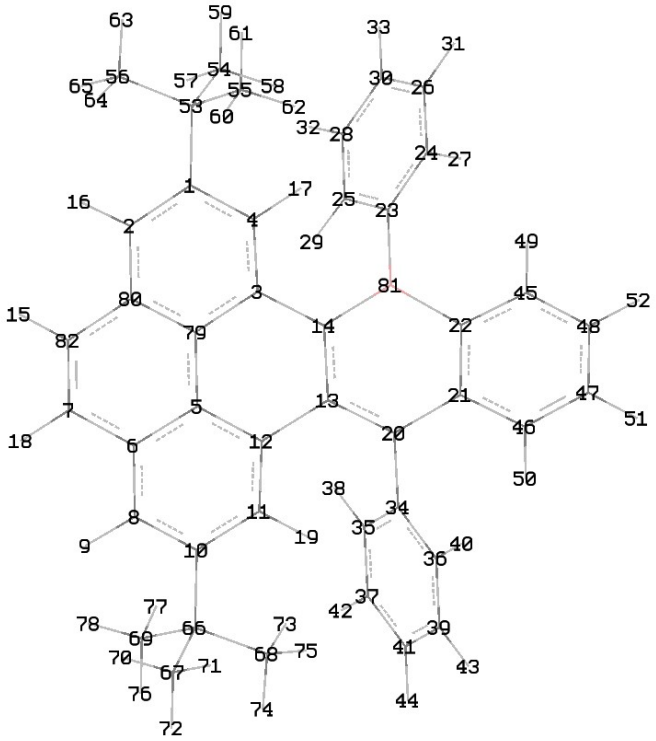


Table S22. Deviations in bond lengths and angles of B-6-*MM*, B-6-*MP*, and B-6-*PM* isomers by comparison with the B-6-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	1.04E-05	5.29E-03	5.29E-03	-	-	-	-	-	-
3	1	5.90E-06	-3.48E-04	-3.48E-04	3	1	2	-4.34E-04	-1.71E-01	-1.71E-01
4	1	-1.36E-05	-5.09E-03	-5.09E-03	4	1	2	-1.82E-04	1.13E-02	1.13E-02
5	3	-2.20E-06	-4.68E-03	-4.68E-03	5	3	1	1.74E-04	-6.97E-01	-6.97E-01
6	5	7.00E-07	2.23E-04	2.23E-04	6	5	3	2.41E-04	-1.77E-01	-1.77E-01

7	6	-4.90E-06	1.31E-03	1.31E-03	7	6	5	6.28E-04	6.36E-02	6.36E-02
8	6	2.80E-06	-1.82E-03	-1.81E-03	8	6	5	8.02E-04	-5.74E-02	-5.74E-02
9	8	-2.00E-06	-1.78E-04	-1.78E-04	9	8	6	-1.44E-04	4.17E-02	4.17E-02
10	8	-3.70E-06	1.02E-03	1.02E-03	10	8	6	-4.52E-04	-1.56E-01	-1.56E-01
11	10	2.80E-06	-3.51E-04	-3.50E-04	11	10	8	-4.00E-04	-2.39E-02	-2.39E-02
12	11	-4.90E-06	1.61E-03	1.61E-03	12	11	10	9.16E-04	2.15E-02	2.15E-02
13	12	-1.20E-06	1.27E-03	1.27E-03	13	12	11	9.08E-04	1.13E+00	1.13E+00
14	13	2.70E-05	3.28E-03	3.28E-03	14	13	12	-8.17E-04	3.98E-01	3.98E-01
15	7	-3.50E-06	-8.14E-05	-8.19E-05	15	7	6	4.27E-04	-2.57E-01	-2.57E-01
16	2	-1.00E-07	1.81E-03	1.81E-03	16	2	1	-7.27E-04	-4.35E-01	-4.35E-01
17	4	9.00E-07	-4.27E-03	-4.27E-03	17	4	1	8.69E-04	3.17E-01	3.17E-01
18	7	-2.00E-07	-3.01E-05	-3.04E-05	18	7	6	-6.96E-04	3.89E-02	3.89E-02
19	11	-3.70E-06	-3.98E-04	-3.99E-04	19	11	10	-9.61E-04	-1.00E-01	-1.00E-01
20	13	-4.46E-05	4.97E-03	4.97E-03	20	13	12	8.65E-04	-1.72E+00	-1.72E+00
21	20	3.19E-05	-9.53E-04	-9.54E-04	21	20	13	7.98E-04	6.06E-01	6.06E-01
22	21	-3.70E-06	-1.89E-03	-1.89E-03	22	21	20	-4.54E-04	1.86E-01	1.86E-01
23	22	-5.40E-05	-6.01E-02	-6.01E-02	23	22	21	2.38E-03	7.31E-01	7.32E-01
24	23	1.19E-04	-1.93E-03	-5.67E-04	24	23	22	2.65E+01	4.15E+00	1.70E+01
25	23	-1.25E-04	-6.82E-04	-2.05E-03	25	23	22	-2.65E+01	-9.44E+00	-2.23E+01
26	24	-2.19E-03	5.21E-04	-1.49E-03	26	24	23	5.42E-02	5.86E-04	-3.35E-02
27	24	-1.48E-04	3.52E-04	1.18E-04	27	24	23	-2.82E-01	-2.43E-02	-1.47E-01
28	25	2.19E-03	7.02E-04	2.71E-03	28	25	23	-5.54E-02	-8.80E-02	-5.40E-02
29	25	1.49E-04	2.66E-04	5.00E-04	29	25	23	2.83E-01	1.36E-01	2.59E-01
30	26	1.00E-06	-4.08E-04	-4.07E-04	30	26	24	3.77E-04	4.09E-02	4.09E-02
31	26	-1.06E-04	1.85E-05	1.44E-04	31	26	24	8.16E-04	-4.17E-02	-5.31E-02
32	28	1.07E-04	2.51E-04	1.25E-04	32	28	25	4.72E-04	-5.28E-02	-4.14E-02

33	30	2.00E-07	-1.00E-04	-1.01E-04	33	30	26	-1.55E-04	6.94E-02	6.95E-02
34	20	1.04E-05	2.38E-03	2.38E-03	34	20	13	4.29E-03	4.27E-01	4.27E-01
35	34	2.18E-03	1.61E-03	-7.32E-04	35	34	20	1.39E+00	1.75E+00	-3.96E-01
36	34	-2.19E-03	-2.92E-03	-5.71E-04	36	34	20	-1.40E+00	-1.79E+00	3.55E-01
37	35	2.30E-04	3.09E-04	3.13E-04	37	35	34	5.73E-02	6.90E-02	-1.44E-02
38	35	5.09E-04	6.85E-04	1.04E-04	38	35	34	8.96E-02	9.56E-02	2.05E-02
39	36	-2.26E-04	8.32E-05	8.01E-05	39	36	34	-5.86E-02	-7.25E-02	1.10E-02
40	36	-5.11E-04	-4.08E-04	1.73E-04	40	36	34	-8.93E-02	-6.87E-02	6.38E-03
41	37	-4.00E-06	-1.86E-04	-1.86E-04	41	39	36	-1.97E-04	2.26E-02	2.26E-02
42	37	1.19E-04	1.82E-04	8.73E-05	42	37	35	6.36E-02	4.73E-02	-1.34E-02
43	39	-1.20E-04	-3.20E-05	6.29E-05	43	39	36	-6.31E-02	-7.67E-02	-1.60E-02
44	41	-1.00E-07	-1.37E-05	-1.32E-05	44	41	39	9.54E-05	1.98E-02	1.98E-02
45	22	-1.00E-06	1.73E-03	1.73E-03	45	22	21	-5.08E-04	9.31E-02	9.31E-02
46	21	-8.10E-06	2.86E-03	2.86E-03	46	21	20	-7.23E-04	-5.38E-02	-5.38E-02
47	46	-1.60E-06	-1.63E-03	-1.63E-03	47	46	21	-6.14E-04	2.06E-01	2.06E-01
48	45	-3.20E-06	-1.78E-03	-1.78E-03	48	45	22	-2.98E-04	1.93E-01	1.93E-01
49	45	-1.90E-06	-1.92E-04	-1.94E-04	49	45	22	4.74E-04	-1.14E-03	-1.12E-03
50	46	1.50E-06	-1.19E-03	-1.19E-03	50	46	21	3.52E-04	2.41E-01	2.41E-01
51	47	1.30E-06	1.46E-05	1.51E-05	51	47	46	4.19E-04	-5.02E-02	-5.03E-02
52	48	-3.00E-07	-6.70E-06	-7.30E-06	52	48	45	2.81E-04	2.36E-02	2.35E-02
53	1	3.30E-06	6.92E-04	6.93E-04	53	1	4	-9.77E-04	-1.41E+00	-1.41E+00
54	53	-2.37E-04	-1.94E-04	-6.16E-03	54	53	1	2.01E-01	-5.93E-01	2.94E+00
55	53	2.45E-04	-5.92E-03	5.00E-05	55	53	1	-2.00E-01	2.75E+00	-7.91E-01
56	53	-2.10E-06	6.11E-03	6.11E-03	56	53	1	-5.66E-04	-2.06E+00	-2.06E+00
57	54	-3.58E-04	-4.89E-04	3.95E-04	57	54	53	7.76E-02	7.26E-01	7.79E-01
58	54	-2.60E-04	6.53E-04	-4.48E-05	58	54	53	-3.51E-01	-1.48E+00	1.85E-02

59	54	-3.06E-04	-1.53E-04	-1.06E-03	59	54	53	-3.27E-02	1.76E-01	-6.75E-01
60	55	3.55E-04	7.49E-04	-1.33E-04	60	55	53	-7.73E-02	7.02E-01	6.49E-01
61	55	3.07E-04	-7.48E-04	1.53E-04	61	55	53	3.21E-02	-6.44E-01	2.07E-01
62	55	2.53E-04	2.08E-04	9.05E-04	62	55	53	3.50E-01	3.70E-01	-1.13E+00
63	56	-1.00E-06	9.81E-04	9.82E-04	63	56	53	2.78E-04	4.48E-01	4.48E-01
64	56	-6.59E-05	-4.67E-04	-1.42E-03	64	56	53	-1.16E-01	-9.72E-01	4.52E-01
65	56	6.44E-05	-1.36E-03	-4.02E-04	65	56	53	1.15E-01	5.67E-01	-8.56E-01
66	10	3.50E-06	8.04E-05	8.06E-05	66	10	8	-3.63E-04	-1.35E-01	-1.35E-01
67	66	-8.26E-04	-5.74E-04	-1.17E-04	67	66	10	1.17E+00	1.30E+00	-5.25E-02
68	66	-2.10E-06	-2.93E-04	-2.94E-04	68	66	10	2.79E-03	-3.25E-02	-3.26E-02
69	66	8.27E-04	7.13E-04	2.57E-04	69	66	10	-1.17E+00	-1.22E+00	1.30E-01
70	67	-5.60E-04	-7.75E-04	2.36E-04	70	67	66	3.64E-01	5.25E-01	-1.32E-01
71	67	-5.21E-04	-5.17E-04	1.06E-04	71	67	66	3.17E-01	3.42E-01	-2.19E-02
72	67	-3.01E-04	-3.79E-04	1.22E-04	72	67	66	-1.83E-01	-2.80E-01	2.90E-02
73	68	-9.57E-04	-1.76E-03	5.25E-05	73	68	66	-2.52E-02	-4.11E-02	-8.33E-02
74	68	-4.00E-07	2.10E-05	2.24E-05	74	68	66	-4.67E-04	2.74E-02	2.74E-02
75	68	9.56E-04	1.01E-03	-7.99E-04	75	68	66	2.60E-02	-5.80E-02	-1.58E-02
76	69	3.01E-04	4.23E-04	-7.72E-05	76	69	66	1.84E-01	2.13E-01	-9.57E-02
77	69	5.21E-04	6.26E-04	3.20E-06	77	69	66	-3.16E-01	-3.39E-01	2.53E-02
78	69	5.58E-04	7.95E-04	-2.16E-04	78	69	66	-3.65E-01	-4.98E-01	1.60E-01
79	3	1.40E-06	-1.79E-03	-1.80E-03	79	3	1	9.86E-05	-1.80E-01	-1.80E-01
80	2	-1.24E-05	-6.91E-03	-6.91E-03	80	2	1	5.50E-04	3.58E-02	3.58E-02
81	22	6.60E-06	-1.94E-01	-1.94E-01	81	7	6	5.01E-05	2.30E+00	2.30E+00
82	7	-1.60E-06	1.93E-01	1.93E-01	82	22	21	3.57E-04	-2.16E+00	-2.16E+00

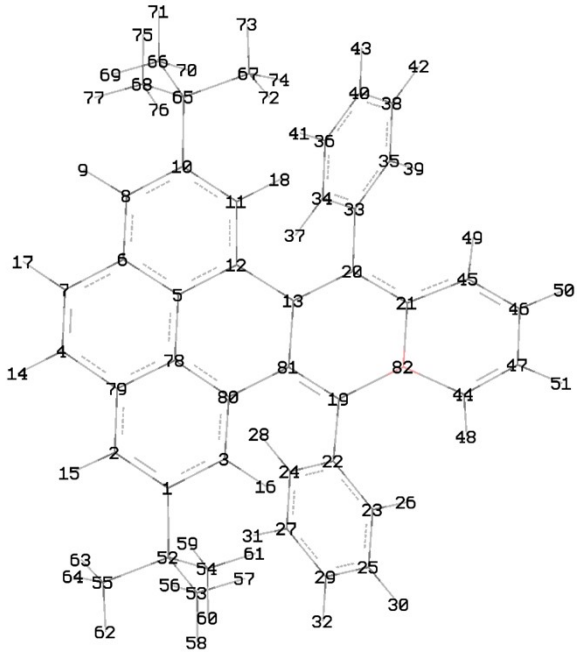


Table S23. Deviations in bond lengths and angles of B-7-*MM*, B-7-*MP*, and B-7-*PM* isomers by comparison with the B-7-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	1.10E-06	-9.41E-04	-9.32E-04	-	-	-	-	-	-
3	1	7.80E-06	8.12E-04	8.00E-04	3	1	2	-3.61E-04	3.62E-02	3.62E-02
4	2	1.30E-05	-6.61E-03	-6.63E-03	4	2	1	-7.67E-04	-5.91E-01	-5.91E-01
5	4	-2.12E-05	-1.78E-03	-1.74E-03	5	4	2	1.19E-04	-2.97E-01	-2.96E-01
6	5	2.20E-06	1.11E-03	1.13E-03	6	5	4	8.06E-04	-1.71E-01	-1.71E-01
7	4	2.11E-05	-1.02E-03	-1.01E-03	7	4	2	-3.07E-04	-1.09E+00	-1.09E+00
8	6	1.59E-05	-1.60E-03	-1.61E-03	8	6	5	3.13E-04	-2.74E-02	-2.66E-02
9	8	-2.20E-06	-1.66E-04	-1.67E-04	9	8	6	-2.17E-03	1.24E-03	5.79E-04

10	8	-4.50E-06	1.92E-04	1.93E-04	10	8	6	-2.59E-04	-1.70E-01	-1.71E-01
11	10	2.90E-06	4.07E-04	4.10E-04	11	10	8	-5.28E-04	-1.05E-01	-1.05E-01
12	11	-3.40E-06	-2.94E-04	-2.86E-04	12	11	10	1.25E-03	-1.11E-02	-9.16E-03
13	12	-2.87E-05	1.65E-03	1.67E-03	13	12	11	-6.21E-04	1.17E+00	1.17E+00
14	4	1.10E-06	-5.59E-05	-5.68E-05	14	4	2	3.95E-03	1.15E-01	1.15E-01
15	2	-1.80E-06	-1.32E-04	-1.32E-04	15	2	1	1.67E-03	1.30E-01	1.31E-01
16	3	1.48E-05	-2.17E-03	-2.17E-03	16	3	1	1.50E-03	-6.10E-01	-6.12E-01
17	7	-1.00E-07	-5.94E-05	-5.83E-05	17	7	4	-3.49E-03	1.60E-01	1.60E-01
18	11	6.60E-06	3.96E-05	3.26E-05	18	11	10	-1.07E-03	5.93E-02	5.53E-02
19	13	2.16E-05	1.45E-02	1.44E-02	19	13	12	-2.04E-03	6.92E+00	6.92E+00
20	13	-4.62E-05	5.97E-03	6.05E-03	20	13	12	5.88E-04	-2.21E+00	-2.22E+00
21	20	2.78E-05	2.10E-04	1.85E-04	21	20	13	-2.23E-03	1.13E+00	1.13E+00
22	19	-1.31E-05	2.40E-03	2.36E-03	22	19	13	3.04E-03	2.44E+00	2.43E+00
23	22	1.45E-03	-7.26E-04	3.30E-04	23	22	19	-6.93E-01	4.87E-01	-1.57E+00
24	22	-1.45E-03	-1.15E-03	-2.19E-03	24	22	19	6.93E-01	-8.71E-01	1.19E+00
25	23	-3.53E-03	-3.46E-04	-2.47E-03	25	23	22	5.51E-02	-4.19E-02	-6.10E-02
26	23	-3.62E-05	3.46E-04	-2.45E-05	26	23	22	-2.04E-01	-1.64E-02	-1.84E-01
27	24	3.53E-03	1.08E-03	3.20E-03	27	24	22	-5.37E-02	-1.16E-01	-9.69E-02
28	24	4.36E-05	1.59E-05	3.84E-04	28	24	22	2.03E-01	2.21E-02	1.89E-01
29	25	1.20E-06	5.37E-04	5.20E-04	29	25	23	1.87E-04	7.72E-03	8.43E-03
30	25	-2.60E-05	1.55E-05	5.90E-06	30	25	23	1.90E-02	-3.24E-03	-3.55E-02
31	27	2.54E-05	3.16E-05	4.19E-05	31	27	24	-2.00E-02	-5.64E-02	-2.36E-02
32	29	-6.00E-07	-1.25E-04	-1.23E-04	32	29	25	8.08E-04	1.82E-03	1.80E-03
33	20	-3.73E-05	4.38E-03	4.38E-03	33	20	13	2.09E-04	1.05E+00	1.04E+00
34	33	8.19E-04	-3.36E-04	-1.13E-03	34	33	20	1.02E+00	1.23E+00	-3.30E-01
35	33	-8.12E-04	-1.95E-03	-1.15E-03	35	33	20	-1.02E+00	-1.34E+00	2.15E-01

36	34	1.21E-03	1.59E-03	3.63E-04	36	34	33	4.17E-02	5.72E-02	-2.00E-02
37	34	3.93E-05	3.54E-04	1.70E-04	37	34	33	-9.08E-02	-9.13E-02	-3.95E-03
38	35	-1.22E-03	-8.53E-04	3.81E-04	38	35	33	-3.89E-02	-6.09E-02	1.66E-02
39	35	-3.26E-05	1.35E-04	3.16E-04	39	35	33	8.92E-02	8.73E-02	3.75E-04
40	38	-3.50E-06	-1.69E-04	-1.66E-04	40	38	35	6.78E-04	4.71E-04	9.19E-04
41	36	1.54E-04	2.35E-04	1.82E-04	41	36	34	1.83E-02	7.11E-03	-3.22E-02
42	38	-1.52E-04	2.92E-05	8.47E-05	42	38	35	-2.02E-02	-5.16E-02	-1.20E-02
43	40	-1.90E-06	-9.80E-06	-8.80E-06	43	40	38	4.71E-05	3.73E-02	3.76E-02
44	21	-7.40E-06	4.69E-03	4.64E-03	44	21	20	2.19E-03	1.14E+00	1.14E+00
45	21	-3.78E-05	2.00E-03	2.02E-03	45	21	20	-1.38E-03	-1.72E-01	-1.72E-01
46	45	2.75E-05	-8.50E-04	-8.57E-04	46	45	21	1.38E-03	3.10E-01	3.09E-01
47	44	1.41E-05	-1.11E-03	-1.10E-03	47	44	21	7.36E-04	1.95E-01	1.95E-01
48	44	1.20E-06	-9.05E-04	-9.04E-04	48	44	21	2.05E-03	3.89E-01	3.93E-01
49	45	4.00E-06	-1.26E-03	-1.27E-03	49	45	21	4.52E-03	2.27E-01	2.28E-01
50	46	-6.00E-07	8.00E-06	8.50E-06	50	46	45	-4.93E-03	-1.20E-01	-1.19E-01
51	47	-1.50E-06	-6.93E-05	-6.89E-05	51	47	44	-4.63E-03	-8.51E-05	-2.18E-03
52	1	-3.60E-06	3.44E-04	3.48E-04	52	1	2	1.28E-03	-2.72E-01	-2.73E-01
53	52	-2.89E-04	-1.57E-03	-6.88E-05	53	52	1	7.11E-02	3.30E-01	-1.77E-01
54	52	2.74E-04	2.12E-04	-1.29E-03	54	52	1	-7.27E-02	-2.48E-01	2.61E-01
55	52	1.16E-05	7.54E-05	7.59E-05	55	52	1	3.65E-03	1.60E-02	1.49E-02
56	53	-4.11E-04	3.43E-05	-4.37E-04	56	53	52	1.72E-02	1.33E-01	6.05E-02
57	53	-3.98E-04	-9.28E-04	-1.73E-04	57	53	52	-3.73E-01	-2.20E-01	-4.58E-01
58	53	-2.99E-04	8.86E-05	-2.36E-04	58	53	52	-1.51E-02	3.02E-02	-1.59E-02
59	54	4.12E-04	-2.28E-05	4.47E-04	59	54	52	-1.71E-02	4.36E-02	1.17E-01
60	54	2.99E-04	5.89E-05	3.87E-04	60	54	52	1.57E-02	-1.74E-03	4.40E-02
61	54	3.98E-04	2.25E-04	-5.28E-04	61	54	52	3.69E-01	-8.52E-02	1.53E-01

62	55	-3.00E-07	-1.70E-05	-1.69E-05	62	55	52	-1.28E-03	-4.26E-02	-4.22E-02
63	55	-2.10E-06	-7.63E-05	6.84E-05	63	55	52	-1.08E-01	6.62E-02	-1.19E-01
64	55	-4.50E-06	6.43E-05	-7.83E-05	64	55	52	1.07E-01	-1.07E-02	1.74E-01
65	10	-4.00E-06	7.28E-05	7.58E-05	65	10	8	4.46E-03	-1.48E-01	-1.49E-01
66	65	-1.06E-03	-6.41E-04	-2.88E-04	66	65	10	1.02E+00	1.19E+00	-8.25E-02
67	65	-8.70E-06	-4.44E-04	-4.42E-04	67	65	10	-4.34E-03	-4.76E-02	-4.57E-02
68	65	1.07E-03	7.76E-04	4.26E-04	68	65	10	-1.01E+00	-1.09E+00	1.78E-01
69	66	-3.30E-04	-6.06E-04	3.36E-04	69	66	65	2.00E-01	4.12E-01	-1.78E-01
70	66	-4.34E-04	-3.97E-04	6.24E-05	70	66	65	3.09E-01	3.30E-01	-5.35E-02
71	66	-2.13E-04	-2.79E-04	1.79E-04	71	66	65	-9.43E-02	-2.19E-01	4.11E-02
72	67	-6.83E-04	-1.74E-03	6.92E-05	72	67	65	-1.13E-01	-1.48E-01	-1.36E-01
73	67	-3.00E-06	3.82E-05	3.77E-05	73	67	65	-4.02E-04	2.94E-02	2.90E-02
74	67	6.84E-04	7.47E-04	-1.07E-03	74	67	65	1.11E-01	-2.42E-02	-3.58E-02
75	68	2.12E-04	3.87E-04	-6.94E-05	75	68	65	9.38E-02	1.33E-01	-1.27E-01
76	68	4.36E-04	4.93E-04	3.69E-05	76	68	65	-3.09E-01	-3.63E-01	2.13E-02
77	68	3.27E-04	6.55E-04	-2.83E-04	77	68	65	-2.01E-01	-3.75E-01	2.15E-01
78	5	-2.01E-05	-9.37E-04	-9.60E-04	78	5	4	-5.84E-04	2.28E-01	2.27E-01
79	2	1.27E-05	-1.51E-03	-1.53E-03	79	2	1	8.23E-04	-2.89E-01	-2.89E-01
80	3	-1.52E-05	1.92E-03	1.94E-03	80	3	1	-3.73E-04	2.76E-01	2.77E-01
81	19	-4.37E-05	5.84E-03	5.91E-03	81	19	13	3.24E-04	-3.62E-01	-3.63E-01
82	44	-4.30E-06	7.56E-04	7.59E-04	82	44	21	1.04E-03	-2.58E-01	-2.58E-01

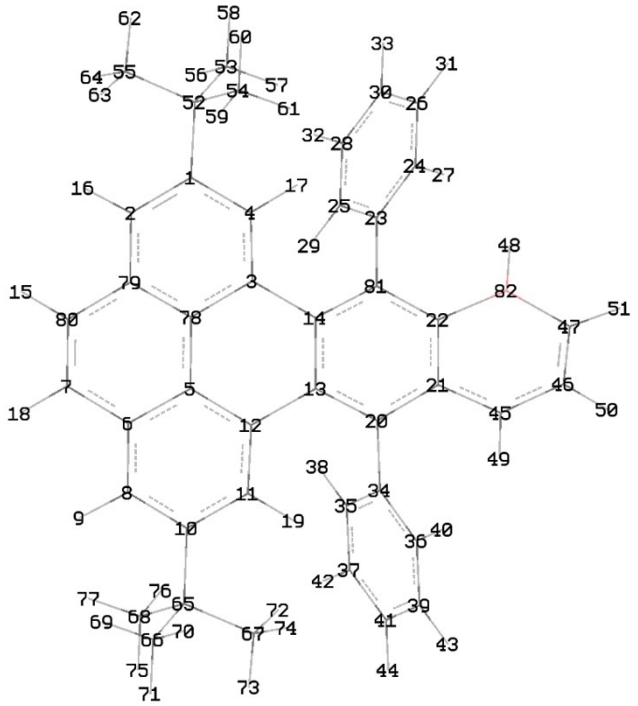


Table S24. Deviations in bond lengths and angles of B-8-*MM*, B-8-*MP*, and B-8-*PM* isomers by comparison with the B-8-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	1.22E-05	4.38E-03	4.37E-03	-	-	-	-	-	-
3	1	5.00E-07	-3.37E-03	-3.37E-03	3	1	2	-3.50E-04	-3.79E-01	-3.79E-01
4	3	1.15E-05	4.52E-03	4.51E-03	4	3	1	-2.89E-04	1.03E-01	1.03E-01
5	3	-2.20E-06	-7.23E-03	-7.24E-03	5	3	1	4.55E-04	-7.53E-01	-7.53E-01
6	5	3.20E-06	-1.25E-03	-1.25E-03	6	5	3	-5.03E-04	-4.09E-01	-4.10E-01
7	6	1.34E-05	1.54E-03	1.55E-03	7	6	5	-3.50E-04	1.88E-01	1.88E-01
8	6	-1.17E-05	-5.63E-04	-5.68E-04	8	6	5	7.76E-04	-9.03E-03	-9.14E-03

9	8	-3.00E-07	-2.62E-04	-2.62E-04	9	8	6	4.90E-04	4.19E-02	4.25E-02
10	8	1.33E-05	-1.04E-03	-1.04E-03	10	8	6	-3.50E-04	-2.91E-01	-2.91E-01
11	10	-8.30E-06	1.75E-03	1.74E-03	11	10	8	-2.13E-04	3.63E-02	3.65E-02
12	11	1.24E-05	3.52E-04	3.56E-04	12	11	10	5.55E-04	9.46E-02	9.42E-02
13	12	7.10E-06	4.95E-03	4.94E-03	13	12	11	-4.32E-04	1.88E+00	1.88E+00
14	13	-1.87E-05	8.78E-03	8.78E-03	14	13	12	9.48E-04	4.54E-01	4.54E-01
15	7	-3.70E-06	4.25E-04	4.28E-04	15	7	6	5.68E-04	-3.12E-01	-3.12E-01
16	2	1.10E-06	1.85E-03	1.85E-03	16	2	1	-3.63E-04	-4.79E-01	-4.79E-01
17	4	-9.20E-06	-2.28E-03	-2.27E-03	17	4	3	9.15E-04	-2.65E-01	-2.65E-01
18	7	1.90E-06	-3.61E-05	-3.72E-05	18	7	6	-3.77E-04	1.65E-02	1.61E-02
19	11	-6.10E-06	-1.65E-03	-1.65E-03	19	11	10	-6.81E-04	-3.39E-01	-3.38E-01
20	13	2.57E-05	-1.06E-03	-1.06E-03	20	13	12	-1.00E-03	-1.24E+00	-1.24E+00
21	20	-1.63E-05	2.66E-03	2.65E-03	21	20	13	6.91E-04	1.01E+00	1.01E+00
22	21	1.36E-05	-4.34E-03	-4.35E-03	22	21	20	-1.80E-03	5.47E-01	5.49E-01
23	22	-9.71E-05	-2.22E-02	-2.22E-02	23	22	21	4.04E-03	1.24E+00	1.24E+00
24	23	-3.03E-04	-1.85E-03	-2.40E-03	24	23	22	2.71E+01	3.58E+00	2.06E+01
25	23	3.02E-04	-2.09E-03	-1.54E-03	25	23	22	-2.71E+01	-6.53E+00	-2.35E+01
26	24	-1.02E-03	-1.20E-04	-2.47E-04	26	24	23	-1.09E-01	-5.75E-02	-2.31E-01
27	24	-4.45E-04	-1.13E-04	-2.69E-04	27	24	23	2.87E-02	3.48E-03	1.27E-01
28	25	1.03E-03	7.70E-04	8.91E-04	28	25	23	1.07E-01	-1.24E-01	5.08E-02
29	25	4.47E-04	1.74E-04	3.30E-04	29	25	23	-2.88E-02	9.83E-02	-2.55E-02
30	26	-3.10E-06	1.22E-04	1.23E-04	30	26	24	-2.08E-04	-1.35E-03	-1.31E-03
31	26	-1.23E-05	8.16E-05	2.80E-04	31	26	24	-4.63E-02	2.61E-02	-5.18E-02
32	28	1.47E-05	2.95E-04	9.53E-05	32	28	25	4.70E-02	-5.05E-03	7.26E-02
33	30	2.70E-06	2.40E-05	2.39E-05	33	30	26	-1.48E-04	3.49E-02	3.51E-02
34	20	-3.10E-06	5.27E-03	5.26E-03	34	20	13	1.92E-04	1.61E+00	1.61E+00

35	34	1.46E-03	-2.47E-05	-2.09E-03	35	34	20	1.33E+00	1.01E+00	-4.33E-02
36	34	-1.46E-03	-3.56E-03	-1.49E-03	36	34	20	-1.33E+00	-1.37E+00	-3.23E-01
37	35	9.66E-04	1.43E-03	1.54E-03	37	35	34	9.35E-02	1.52E-02	-1.13E-01
38	35	5.84E-04	7.02E-04	1.01E-04	38	35	34	3.44E-02	3.05E-02	5.02E-02
39	36	-9.60E-04	5.81E-04	4.76E-04	39	36	34	-9.37E-02	-2.07E-01	-7.84E-02
40	36	-5.84E-04	-4.84E-04	1.17E-04	40	36	34	-3.47E-02	1.58E-02	-3.92E-03
41	39	-5.30E-06	3.36E-04	3.35E-04	41	39	36	-2.15E-05	1.94E-03	2.05E-03
42	37	5.05E-05	8.04E-05	1.67E-04	42	37	35	6.10E-02	7.70E-02	-7.00E-03
43	39	-4.82E-05	1.17E-04	3.12E-05	43	39	36	-6.13E-02	-6.83E-02	1.57E-02
44	41	2.40E-06	-5.27E-05	-5.29E-05	44	41	39	-6.07E-05	1.36E-02	1.35E-02
45	21	2.67E-05	4.53E-03	4.54E-03	45	21	20	3.30E-03	-7.81E-01	-7.82E-01
46	45	-3.50E-06	-1.34E-03	-1.35E-03	46	45	21	-1.48E-04	5.01E-01	5.01E-01
47	46	2.40E-06	-1.80E-03	-1.80E-03	47	46	45	7.47E-04	1.90E-02	1.85E-02
48	47	5.18E-05	-1.43E-02	-1.43E-02	48	47	46	-6.00E-04	1.56E-01	1.57E-01
49	45	9.00E-07	-1.43E-03	-1.43E-03	49	45	21	-1.64E-03	3.40E-01	3.39E-01
50	46	3.90E-06	4.23E-05	4.22E-05	50	46	45	-8.44E-04	-1.21E-01	-1.20E-01
51	47	2.90E-06	-5.60E-05	-5.65E-05	51	47	46	1.47E-03	1.61E-01	1.61E-01
52	1	3.60E-06	1.25E-03	1.25E-03	52	1	2	7.46E-04	-3.35E+00	-3.35E+00
53	52	5.04E-04	5.23E-04	-6.15E-03	53	52	1	3.08E-01	-5.76E-01	3.07E+00
54	52	-5.02E-04	-6.64E-03	3.47E-05	54	52	1	-3.08E-01	2.76E+00	-8.85E-01
55	52	0.00E+00	6.12E-03	6.11E-03	55	52	1	3.22E-04	-2.02E+00	-2.02E+00
56	53	-4.27E-04	-5.64E-04	4.47E-04	56	53	52	5.97E-02	6.70E-01	7.62E-01
57	53	2.88E-04	1.31E-03	-6.82E-05	57	53	52	-2.87E-02	-1.35E+00	3.58E-03
58	53	-4.29E-04	-1.22E-04	-1.19E-03	58	53	52	-1.37E-01	1.16E-01	-7.46E-01
59	54	4.30E-04	8.75E-04	-1.38E-04	59	54	52	-5.92E-02	7.03E-01	6.10E-01
60	54	4.32E-04	-7.57E-04	3.06E-04	60	54	52	1.36E-01	-6.10E-01	2.52E-01

61	54	-2.78E-04	-3.51E-04	1.03E-03	61	54	52	2.79E-02	3.21E-02	-1.33E+00
62	55	2.40E-06	9.64E-04	9.64E-04	62	55	52	2.07E-04	4.48E-01	4.48E-01
63	55	-1.02E-04	-4.07E-04	-1.58E-03	63	55	52	-7.98E-02	-9.46E-01	4.89E-01
64	55	1.06E-04	-1.47E-03	-3.02E-04	64	55	52	7.98E-02	5.67E-01	-8.66E-01
65	10	9.70E-06	2.06E-04	2.06E-04	65	10	8	5.66E-05	-5.84E-02	-5.98E-02
66	65	-9.54E-04	-8.08E-04	-1.81E-04	66	65	10	9.38E-01	1.31E+00	-2.63E-01
67	65	-1.20E-06	-4.61E-04	-4.65E-04	67	65	10	-9.86E-04	-7.02E-02	-6.92E-02
68	65	9.50E-04	7.86E-04	1.56E-04	68	65	10	-9.36E-01	-1.20E+00	3.71E-01
69	66	-3.24E-04	-7.04E-04	3.71E-04	69	66	65	1.99E-01	5.04E-01	-2.41E-01
70	66	-4.30E-04	-4.06E-04	2.02E-04	70	66	65	2.64E-01	2.77E-01	-6.57E-02
71	66	-1.86E-04	-3.29E-04	1.70E-04	71	66	65	-9.75E-02	-2.65E-01	1.24E-01
72	67	-6.41E-04	-1.93E-03	1.55E-04	72	67	65	-7.91E-02	-5.19E-02	-1.18E-01
73	67	2.40E-06	6.73E-05	6.84E-05	73	67	65	4.39E-04	3.49E-02	3.47E-02
74	67	6.46E-04	8.00E-04	-1.29E-03	74	67	65	7.91E-02	-3.96E-02	2.70E-02
75	68	1.94E-04	3.61E-04	-1.39E-04	75	68	65	9.72E-02	2.22E-01	-1.67E-01
76	68	4.29E-04	6.30E-04	2.38E-05	76	68	65	-2.62E-01	-3.29E-01	1.17E-02
77	68	3.29E-04	7.02E-04	-3.78E-04	77	68	65	-2.00E-01	-4.44E-01	3.03E-01
78	3	-1.05E-05	-3.92E-03	-3.93E-03	78	3	1	3.19E-04	1.17E-02	1.18E-02
79	2	-1.38E-05	-5.48E-03	-5.48E-03	79	2	1	-2.87E-04	1.25E-01	1.25E-01
80	7	-7.00E-06	-1.25E-03	-1.25E-03	80	7	6	4.93E-04	-1.91E-01	-1.91E-01
81	22	-1.09E-05	2.97E-03	2.96E-03	81	22	21	5.19E-04	3.71E-01	3.70E-01
82	47	-3.60E-06	-1.78E-03	-1.79E-03	82	47	46	-8.39E-04	-1.66E-01	-1.65E-01

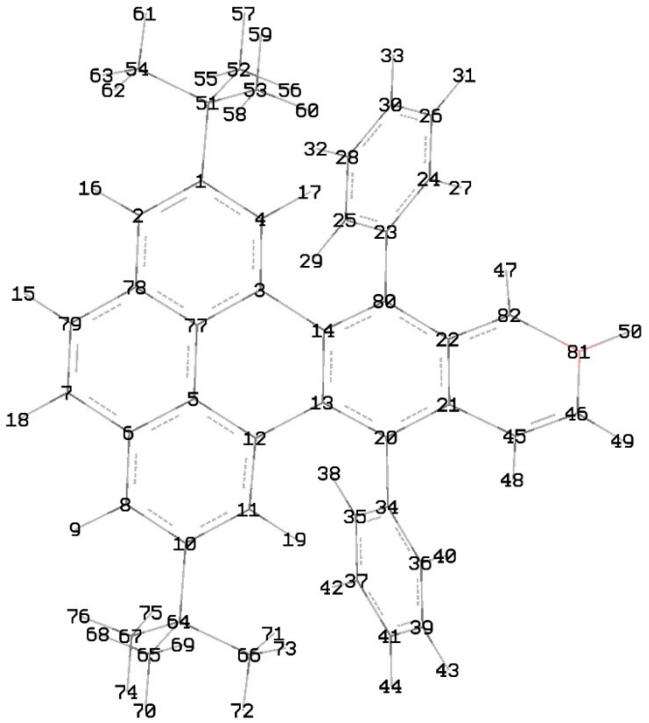


Table S25. Deviations in bond lengths and angles of B-9-*MM*, B-9-*MP*, and B-9-*PM* isomers by comparison with the B-9-*PP* structure.

Atom1	Atom2	$\Delta r_{MM\text{-}PP}$ (Å)	$\Delta r_{PM\text{-}PP}$ (Å)	$\Delta r_{MP\text{-}PP}$ (Å)	Atom1	Atom2	Atom3	$\Delta A_{MM\text{-}PP}$ (°)	$\Delta A_{PM\text{-}PP}$ (°)	$\Delta A_{MP\text{-}PP}$ (°)
2	1	5.40E-06	4.02E-03	4.01E-03	-	-	-	-	-	-
3	1	-1.75E-05	-1.55E-03	-1.55E-03	3	1	2	-1.13E-04	-2.98E-01	-2.98E-01
4	3	8.50E-06	5.15E-03	5.14E-03	4	3	1	2.04E-04	4.49E-02	4.49E-02
5	3	-7.60E-06	-6.04E-03	-6.05E-03	5	3	1	5.29E-04	-9.46E-01	-9.46E-01
6	5	-3.80E-06	-1.10E-03	-1.10E-03	6	5	3	-8.92E-04	-3.45E-01	-3.46E-01
7	6	1.06E-05	1.46E-03	1.45E-03	7	6	5	2.72E-04	1.12E-01	1.13E-01

8	6	-1.19E-05	-6.45E-04	-6.41E-04	8	6	5	7.71E-04	-4.73E-02	-4.73E-02
9	8	6.00E-07	-2.85E-04	-2.82E-04	9	8	6	8.76E-04	4.18E-02	4.17E-02
10	8	4.90E-06	-7.02E-04	-7.01E-04	10	8	6	-5.93E-04	-2.83E-01	-2.84E-01
11	10	-9.70E-06	1.72E-03	1.72E-03	11	10	8	4.90E-04	4.83E-03	4.79E-03
12	11	7.00E-06	-3.68E-04	-3.67E-04	12	11	10	2.65E-04	1.02E-02	1.04E-02
13	12	2.00E-07	5.03E-03	5.02E-03	13	12	11	-4.50E-04	1.89E+00	1.89E+00
14	13	-1.84E-05	7.67E-03	7.70E-03	14	13	12	1.58E-03	5.48E-01	5.48E-01
15	7	-5.90E-06	2.87E-04	2.93E-04	15	7	6	3.15E-04	-3.53E-01	-3.54E-01
16	2	1.30E-06	1.83E-03	1.83E-03	16	2	1	-4.23E-04	-4.44E-01	-4.43E-01
17	4	-3.80E-06	-2.93E-03	-2.93E-03	17	4	3	4.30E-04	-1.71E-01	-1.69E-01
18	7	5.00E-07	-3.22E-05	-3.36E-05	18	7	6	-7.09E-04	5.37E-02	5.36E-02
19	11	-6.40E-06	-9.77E-04	-9.89E-04	19	11	10	-6.71E-04	-1.74E-01	-1.75E-01
20	13	1.82E-05	-2.41E-03	-2.43E-03	20	13	12	8.67E-05	-1.54E+00	-1.54E+00
21	20	-1.83E-05	4.30E-03	4.31E-03	21	20	13	9.46E-04	1.07E+00	1.07E+00
22	21	8.50E-06	-5.44E-03	-5.44E-03	22	21	20	2.62E-04	5.31E-01	5.32E-01
23	22	-8.13E-05	-2.61E-02	-2.61E-02	23	22	21	1.39E-03	1.39E+00	1.39E+00
24	23	-1.86E-03	-1.87E-03	-3.83E-03	24	23	22	2.58E+01	4.30E+00	1.85E+01
25	23	1.85E-03	-1.97E-03	-9.00E-07	25	23	22	-2.58E+01	-7.36E+00	-2.15E+01
26	24	-5.01E-04	3.07E-04	3.49E-04	26	24	23	-4.81E-02	-4.44E-02	-1.71E-01
27	24	-4.81E-04	1.01E-04	-3.52E-04	27	24	23	-5.87E-02	2.94E-03	3.88E-02
28	25	4.99E-04	8.33E-04	7.92E-04	28	25	23	4.67E-02	-1.23E-01	3.10E-03
29	25	4.79E-04	1.30E-04	5.82E-04	29	25	23	5.91E-02	9.70E-02	6.16E-02
30	28	8.00E-06	1.70E-04	1.76E-04	30	28	25	-1.15E-04	-1.37E-01	-1.37E-01
31	26	-4.61E-05	5.55E-05	1.91E-04	31	26	24	-3.46E-02	2.52E-02	-4.50E-02
32	28	4.53E-05	2.37E-04	1.00E-04	32	28	25	3.44E-02	-1.00E-02	5.97E-02
33	30	4.00E-07	-6.90E-06	-7.20E-06	33	30	28	-5.85E-04	1.12E-02	1.11E-02

34	20	-3.10E-06	4.66E-03	4.68E-03	34	20	13	5.20E-04	1.55E+00	1.55E+00
35	34	1.60E-03	2.55E-04	-2.03E-03	35	34	20	1.51E+00	1.10E+00	8.86E-02
36	34	-1.60E-03	-3.63E-03	-1.35E-03	36	34	20	-1.51E+00	-1.42E+00	-4.14E-01
37	35	4.42E-04	8.24E-04	1.27E-03	37	35	34	7.95E-02	1.55E-02	-1.17E-01
38	35	4.23E-04	5.65E-04	7.63E-05	38	35	34	-1.71E-02	-3.92E-02	3.54E-02
39	36	-4.43E-04	8.23E-04	3.85E-04	39	36	34	-8.07E-02	-1.96E-01	-6.46E-02
40	36	-4.25E-04	-3.45E-04	1.39E-04	40	36	34	1.71E-02	5.18E-02	-2.22E-02
41	39	-4.00E-06	2.59E-04	2.59E-04	41	39	36	-1.13E-04	1.59E-01	1.59E-01
42	37	5.33E-05	9.11E-05	2.02E-04	42	37	35	3.08E-02	6.17E-02	-1.06E-02
43	39	-5.39E-05	1.48E-04	3.71E-05	43	39	36	-3.06E-02	-4.12E-02	3.08E-02
44	41	1.40E-06	-4.68E-05	-4.67E-05	44	41	39	-6.37E-04	1.15E-02	1.14E-02
45	21	2.03E-05	3.85E-03	3.87E-03	45	21	20	5.03E-04	-8.12E-01	-8.12E-01
46	45	-5.70E-06	-4.53E-04	-4.55E-04	46	45	21	6.24E-04	6.85E-01	6.86E-01
47	22	-2.00E-06	7.23E-03	7.23E-03	47	22	21	6.90E-05	2.86E-01	2.86E-01
48	45	2.80E-06	-1.88E-03	-1.89E-03	48	45	21	-2.36E-03	2.90E-01	2.90E-01
49	46	-1.00E-07	-2.89E-05	-3.05E-05	49	46	45	5.65E-04	-2.05E-01	-2.05E-01
50	46	1.45E-05	-1.73E-04	-1.75E-04	50	46	45	-1.17E-03	6.73E-02	6.60E-02
51	1	-1.70E-05	1.44E-03	1.44E-03	51	1	2	5.55E-04	-3.34E+00	-3.34E+00
52	51	5.87E-04	6.04E-04	-6.11E-03	52	51	1	2.41E-01	-6.18E-01	3.06E+00
53	51	-6.05E-04	-6.69E-03	1.20E-05	53	51	1	-2.44E-01	2.82E+00	-8.63E-01
54	51	-6.00E-07	6.16E-03	6.15E-03	54	51	1	3.68E-04	-2.02E+00	-2.02E+00
55	52	-4.96E-04	-6.34E-04	4.31E-04	55	52	51	3.77E-02	6.33E-01	7.72E-01
56	52	3.85E-04	1.46E-03	-1.29E-04	56	52	51	8.86E-03	-1.30E+00	2.02E-02
57	52	-4.15E-04	-1.02E-04	-1.18E-03	57	52	51	-1.33E-01	1.38E-01	-7.43E-01
58	53	4.98E-04	9.26E-04	-1.38E-04	58	53	51	-3.84E-02	7.33E-01	5.96E-01
59	53	4.14E-04	-7.68E-04	3.11E-04	59	53	51	1.33E-01	-6.10E-01	2.72E-01

60	53	-3.78E-04	-5.12E-04	1.08E-03	60	53	51	-9.45E-03	8.46E-03	-1.31E+00
61	54	1.10E-06	9.44E-04	9.44E-04	61	54	51	-4.33E-04	4.39E-01	4.38E-01
62	54	-5.22E-05	-3.72E-04	-1.61E-03	62	54	51	-7.29E-02	-9.42E-01	5.08E-01
63	54	5.50E-05	-1.56E-03	-3.24E-04	63	54	51	7.31E-02	5.80E-01	-8.69E-01
64	10	-6.40E-06	1.80E-04	1.92E-04	64	10	8	-1.01E-03	-2.43E-02	-2.78E-02
65	64	-9.57E-04	-7.88E-04	-2.15E-04	65	64	10	9.42E-01	1.35E+00	-2.65E-01
66	64	-3.10E-06	-3.12E-04	-3.17E-04	66	64	10	-9.80E-04	-9.60E-02	-9.04E-02
67	64	9.38E-04	7.52E-04	1.58E-04	67	64	10	-9.42E-01	-1.21E+00	3.94E-01
68	65	-3.40E-04	-7.33E-04	4.36E-04	68	65	64	2.16E-01	5.32E-01	-2.62E-01
69	65	-4.09E-04	-3.76E-04	1.88E-04	69	65	64	2.69E-01	2.90E-01	-8.38E-02
70	65	-2.04E-04	-3.42E-04	1.99E-04	70	65	64	-1.03E-01	-2.82E-01	1.23E-01
71	66	-8.47E-04	-2.11E-03	1.11E-04	71	66	64	-9.67E-02	-5.64E-02	-1.62E-01
72	66	7.00E-07	5.44E-05	5.50E-05	72	66	64	2.59E-04	2.75E-02	2.74E-02
73	66	8.52E-04	9.59E-04	-1.26E-03	73	66	64	9.65E-02	-6.83E-02	4.03E-02
74	67	2.09E-04	4.06E-04	-1.35E-04	74	67	64	1.02E-01	2.26E-01	-1.78E-01
75	67	4.04E-04	5.92E-04	2.61E-05	75	67	64	-2.67E-01	-3.53E-01	2.02E-02
76	67	3.44E-04	7.81E-04	-3.86E-04	76	67	64	-2.18E-01	-4.84E-01	3.11E-01
77	3	-1.37E-05	-2.61E-03	-2.62E-03	77	3	1	3.91E-04	-1.26E-01	-1.25E-01
78	2	-1.50E-05	-5.58E-03	-5.57E-03	78	2	1	-3.99E-04	6.59E-02	6.57E-02
79	7	-9.70E-06	-1.28E-03	-1.27E-03	79	7	6	3.46E-04	-2.38E-01	-2.38E-01
80	14	-7.00E-07	6.62E-04	6.20E-04	80	14	13	1.30E-03	9.17E-01	9.17E-01
81	46	2.60E-06	-3.97E-03	-3.98E-03	81	46	45	-5.41E-04	3.90E-02	3.78E-02
82	22	-5.50E-06	6.30E-03	6.26E-03	82	22	21	-6.24E-05	1.75E-01	1.75E-01

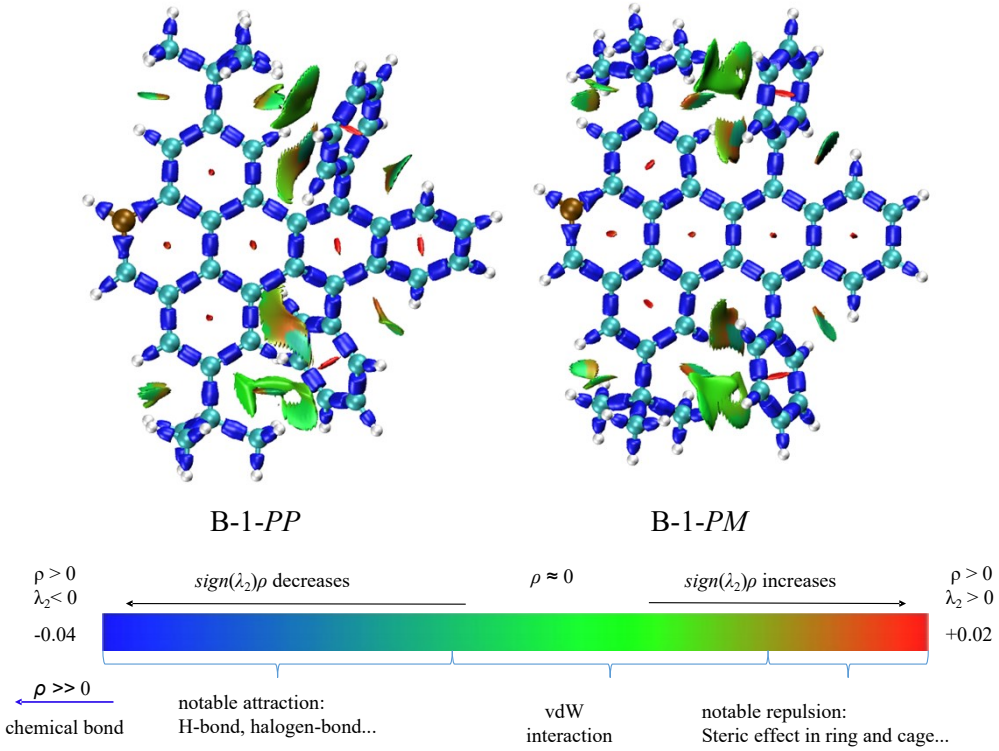


Figure S1. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-1-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

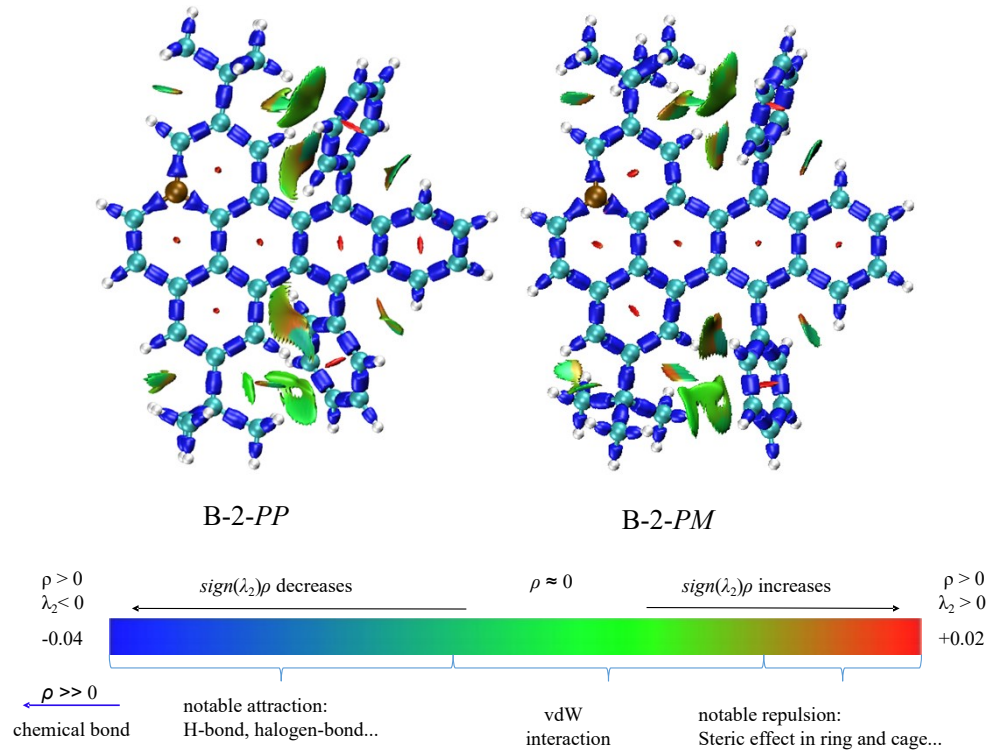


Figure S2. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-2-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

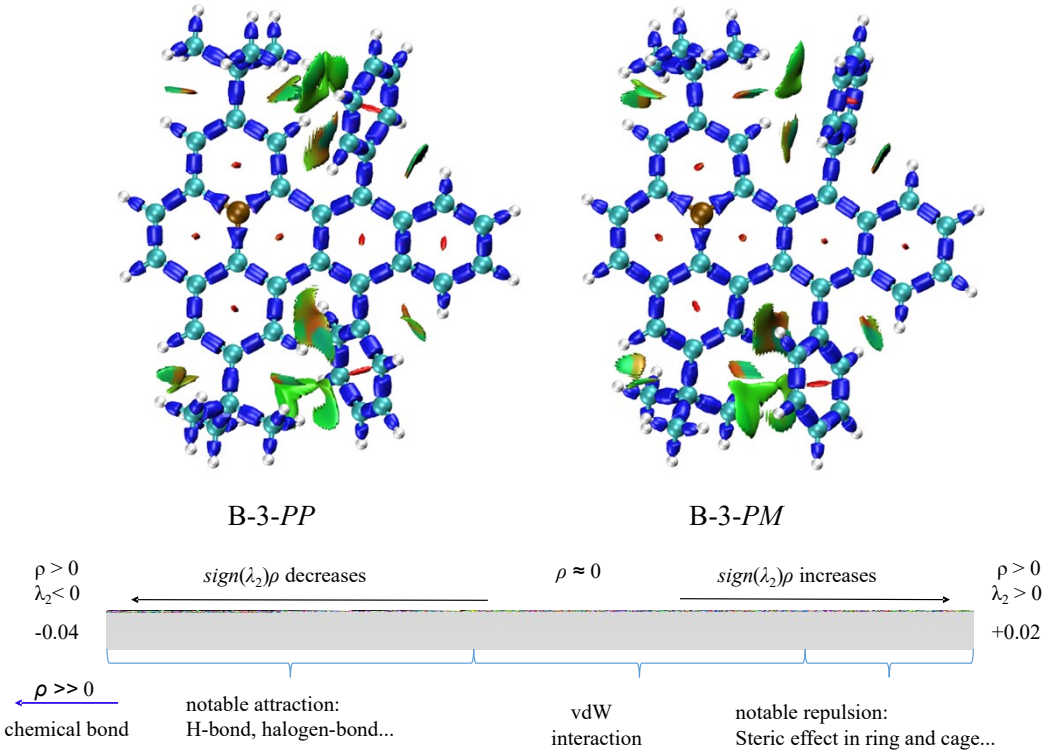


Figure S3. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-3-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

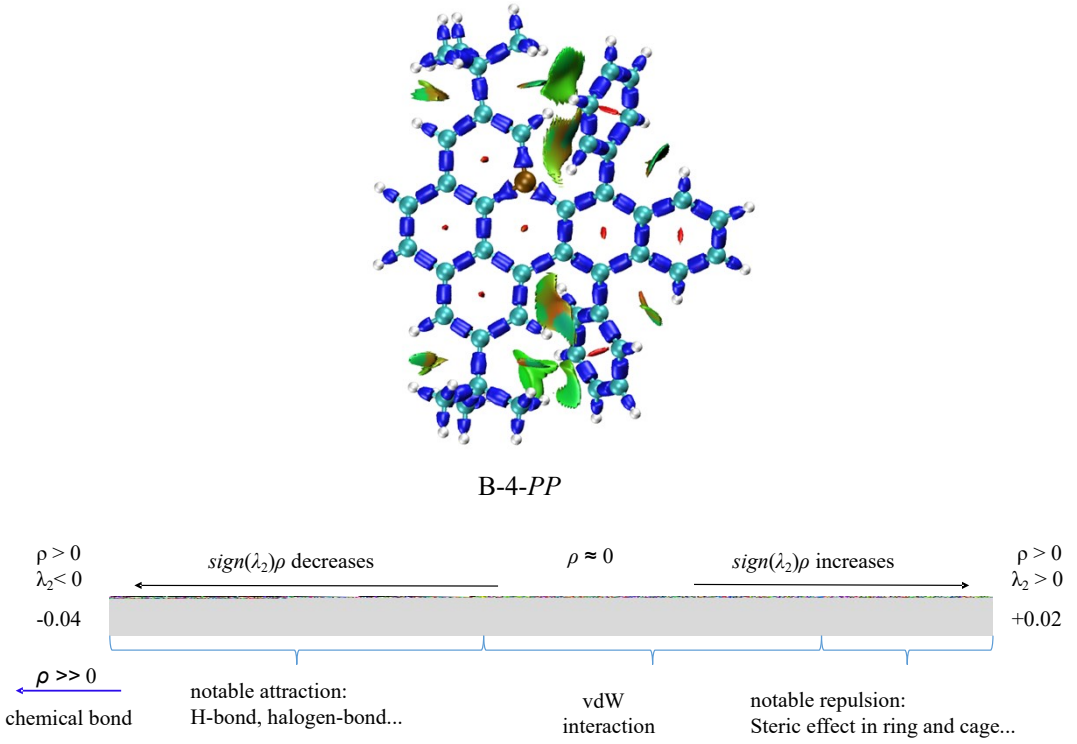
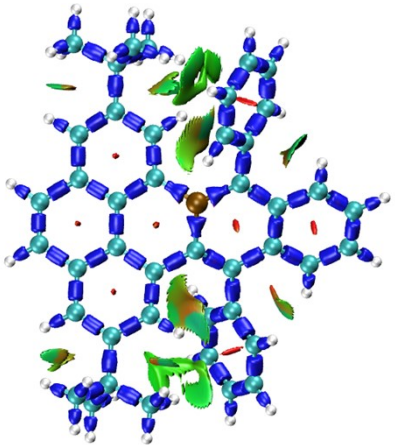


Figure S4. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-4-*PP*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.



B-5-*PP*

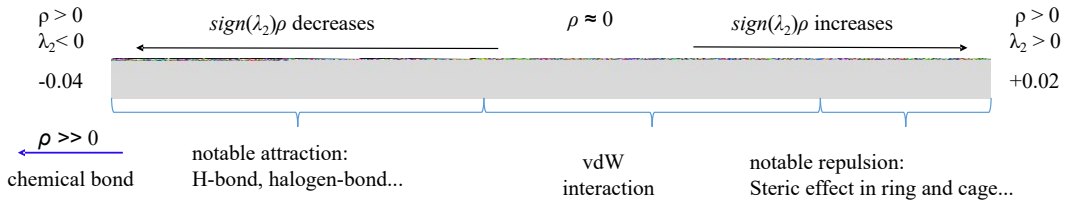
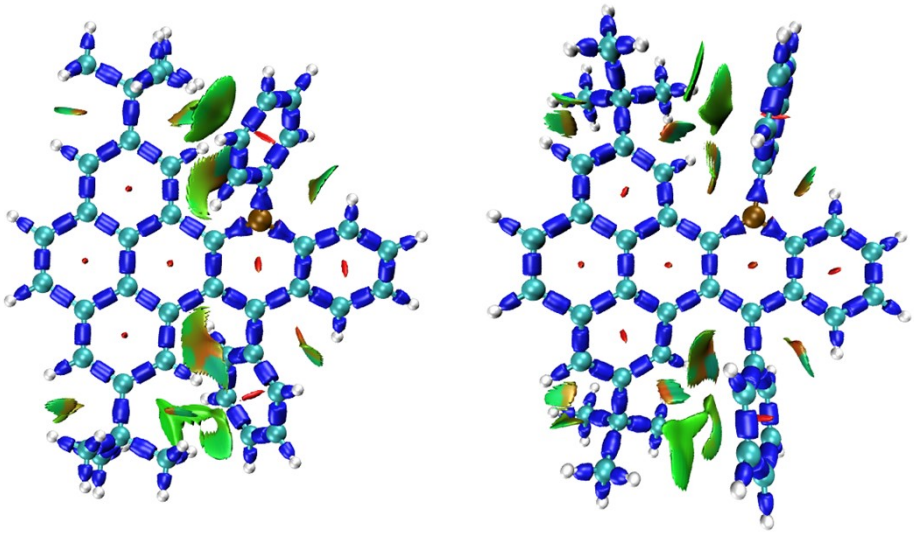


Figure S5. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-5-*PP*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.



B-6-*PP* B-6-*PM*

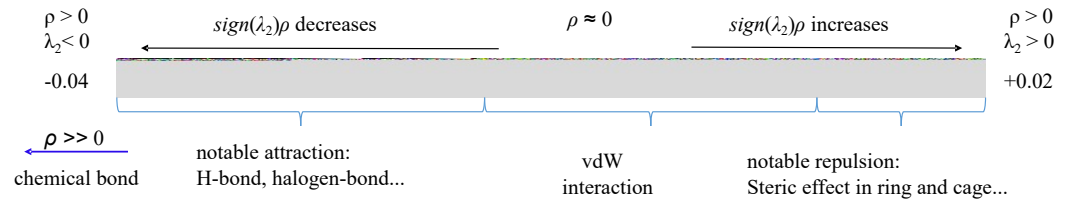


Figure S6. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-6-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

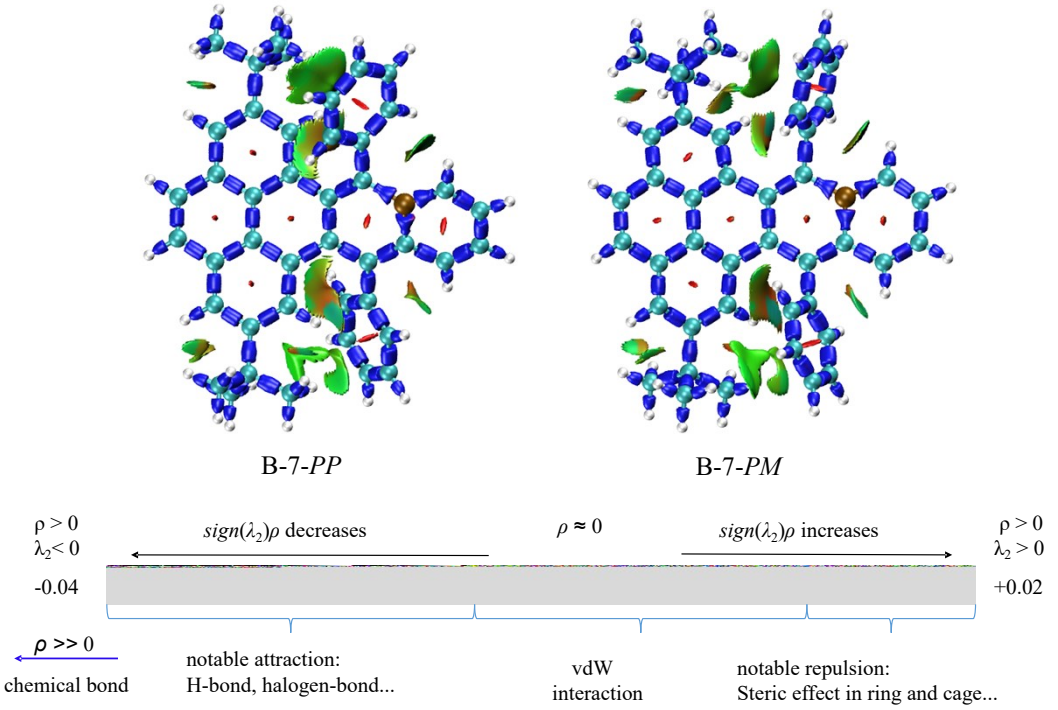


Figure S7. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-7-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

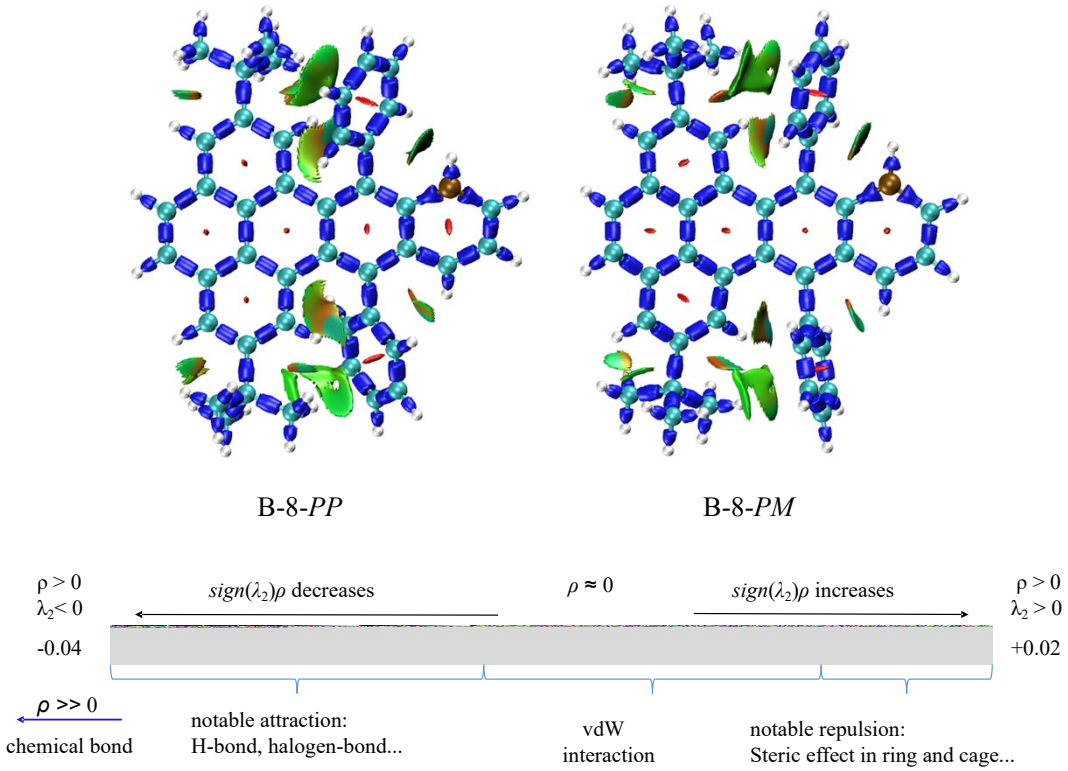


Figure S8. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-8-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

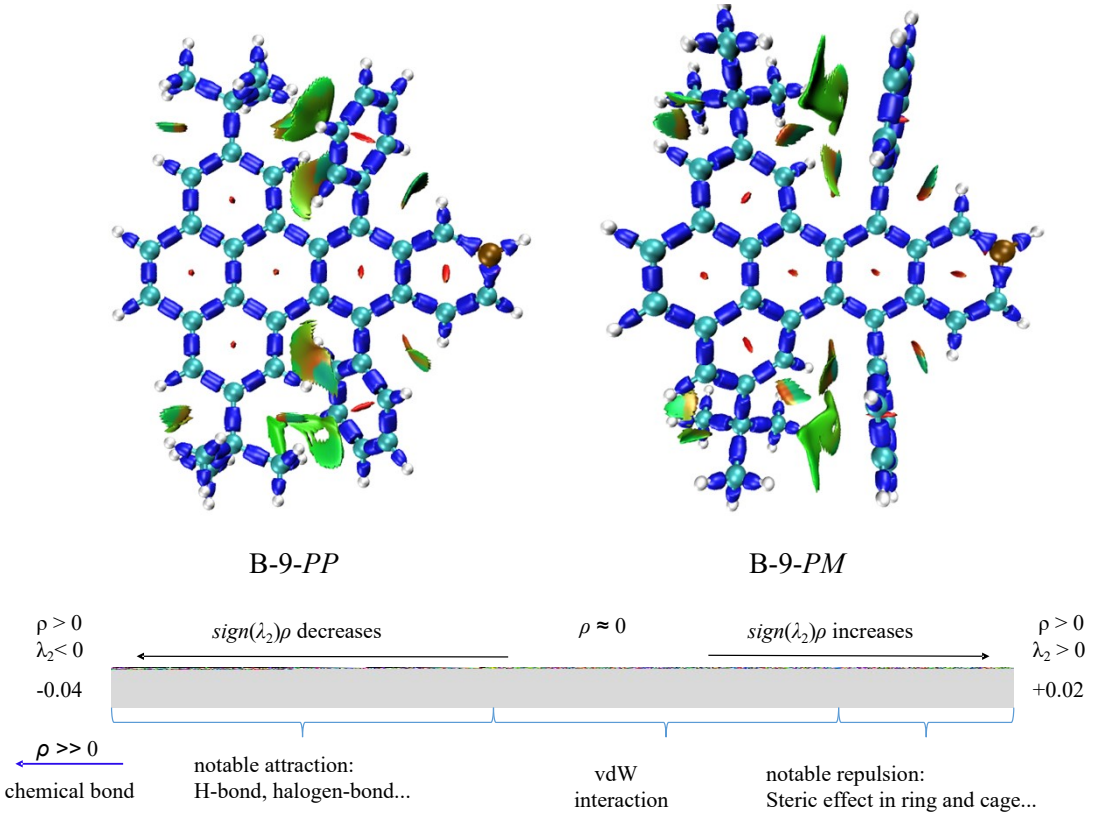


Figure S9. Interaction region indicator (IRI) of chemical bonds and weak interactions for compound B-9-*PP*/*PM*, which were computed by Gaussian 09 at M06-2X/6-311G** level and plotted by Multiwfn and VMD programs. The IRI isovalue is 1.

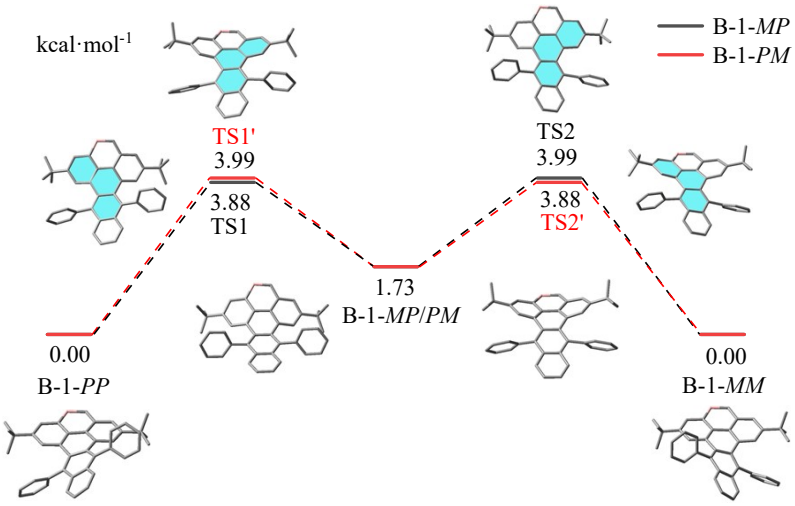


Figure S10. Racemization pathway of B-1 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

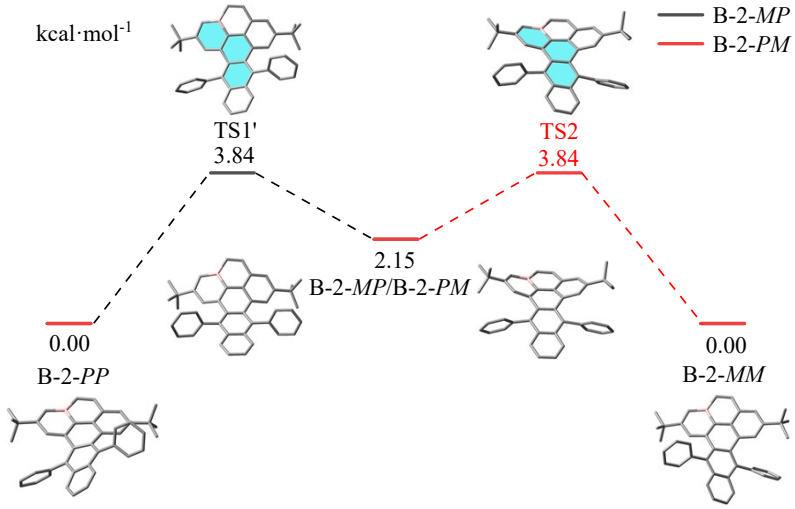


Figure S11. Racemization pathway of B-2 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

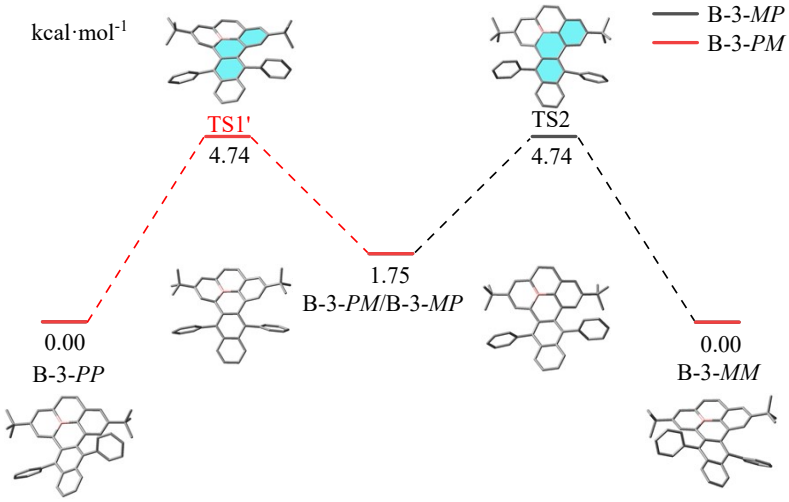


Figure S12. Racemization pathway of B-3 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

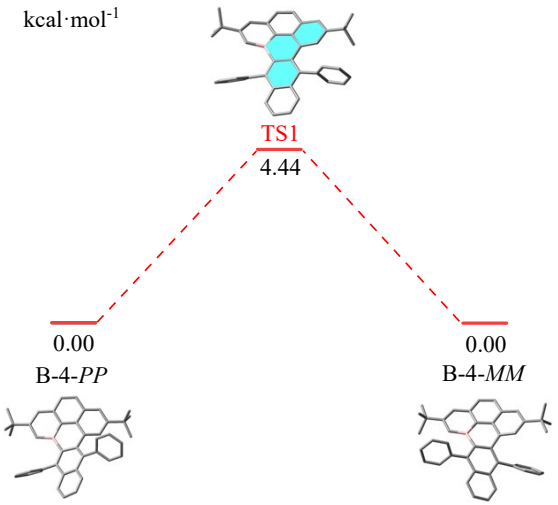


Figure S13. Racemization pathway of B-4 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

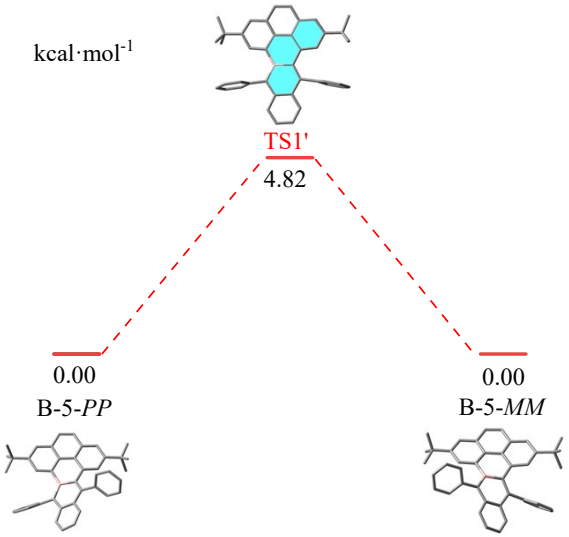


Figure S14. Racemization pathway of B-5 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

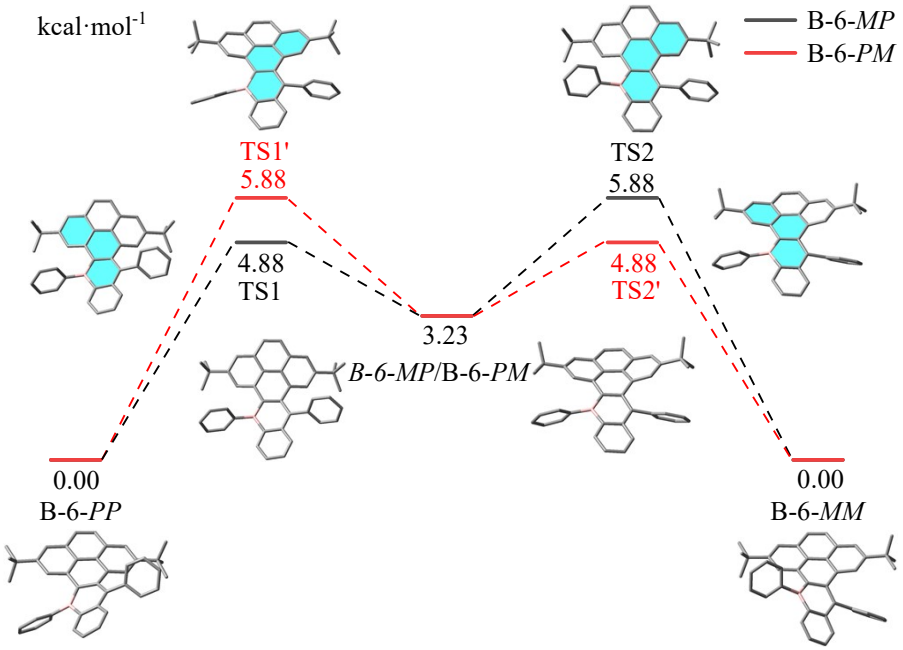


Figure S15. Racemization pathway of B-6 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

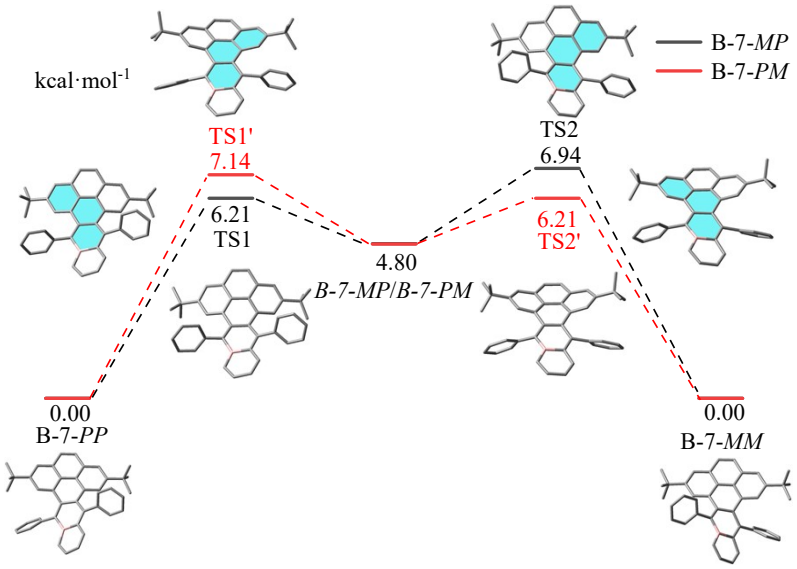


Figure S16. Racemization pathway of B-7 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

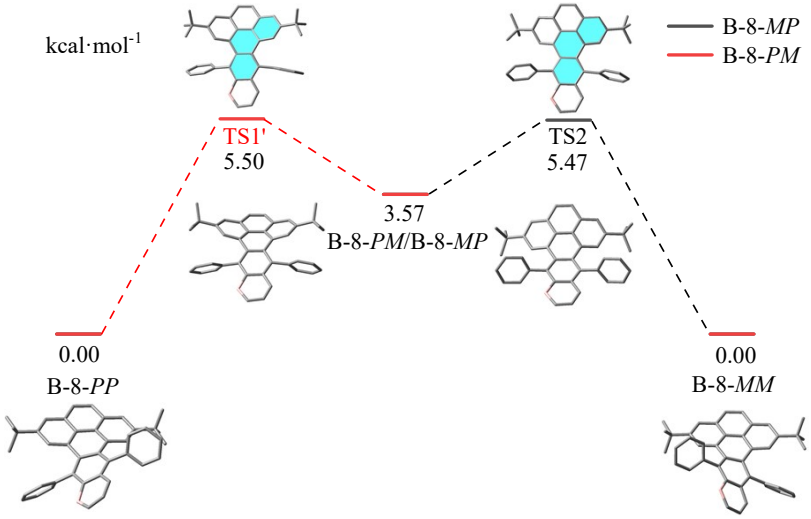


Figure S17. Racemization pathway of B-8 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

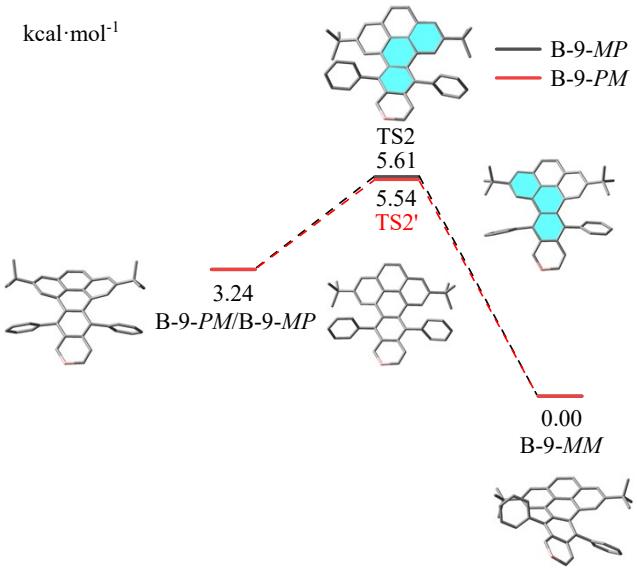


Figure S18. Racemization pathway of B-9 calculated at the M06-2X/6-311G** level. The relative Gibbs free energies of the stationary points are given in kcal·mol^{-1}.

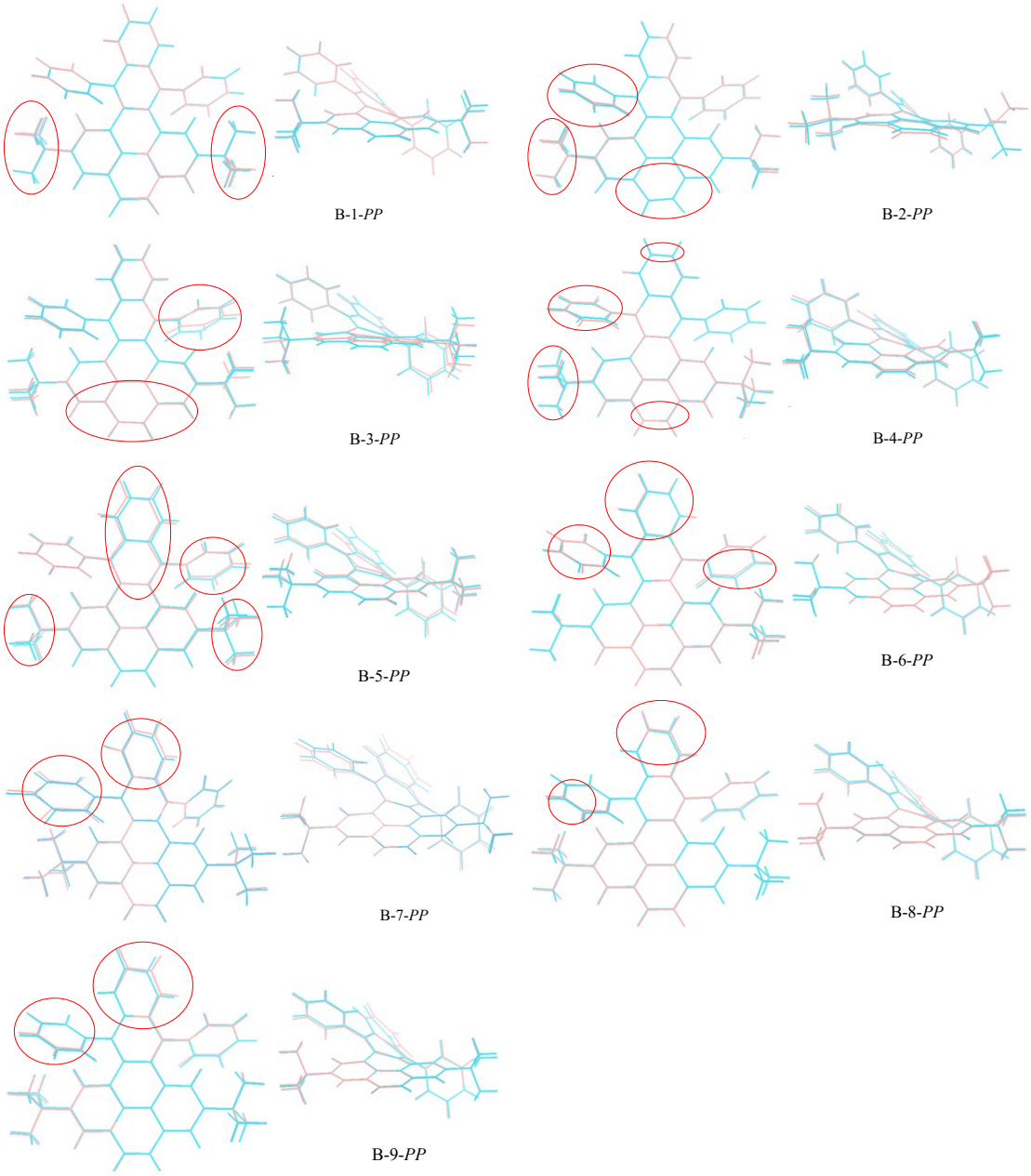


Figure S19. Structural overlays comparing the ground (D_0, blue) and first excited (D_1, pink) states for compounds B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP* optimized at the M06−2X/6‑311G** level.

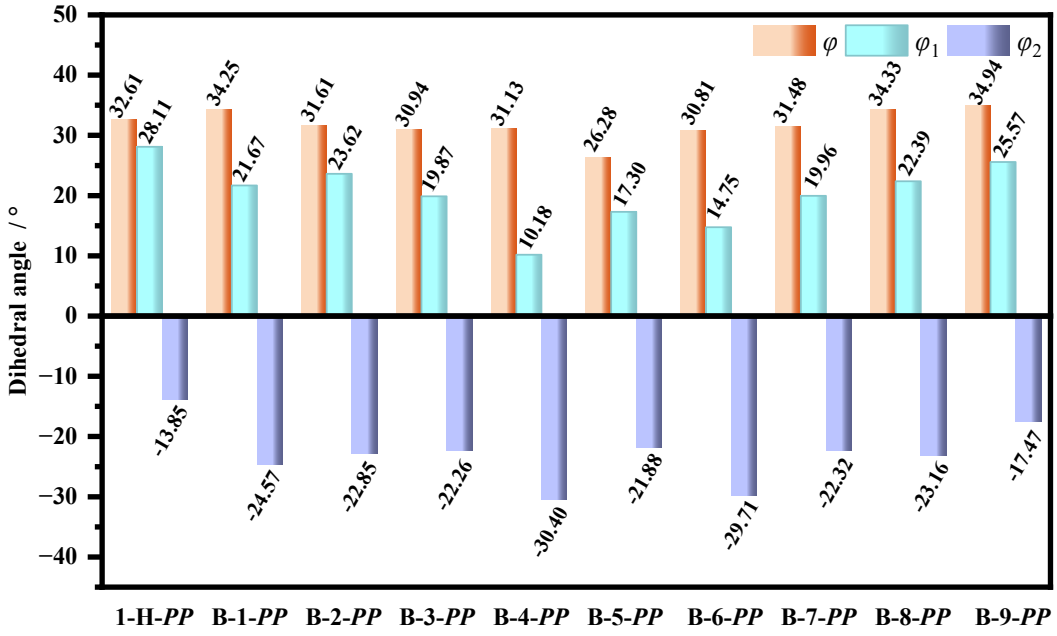


Figure S20. The dihedral angles φ between the pyrene and naphthalene rings in the second excited states, as well as the dihedral angles φ_1 and φ_2 between the two bay regions for compounds 1-H-*PP*, B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP* and B-9-*PP*.

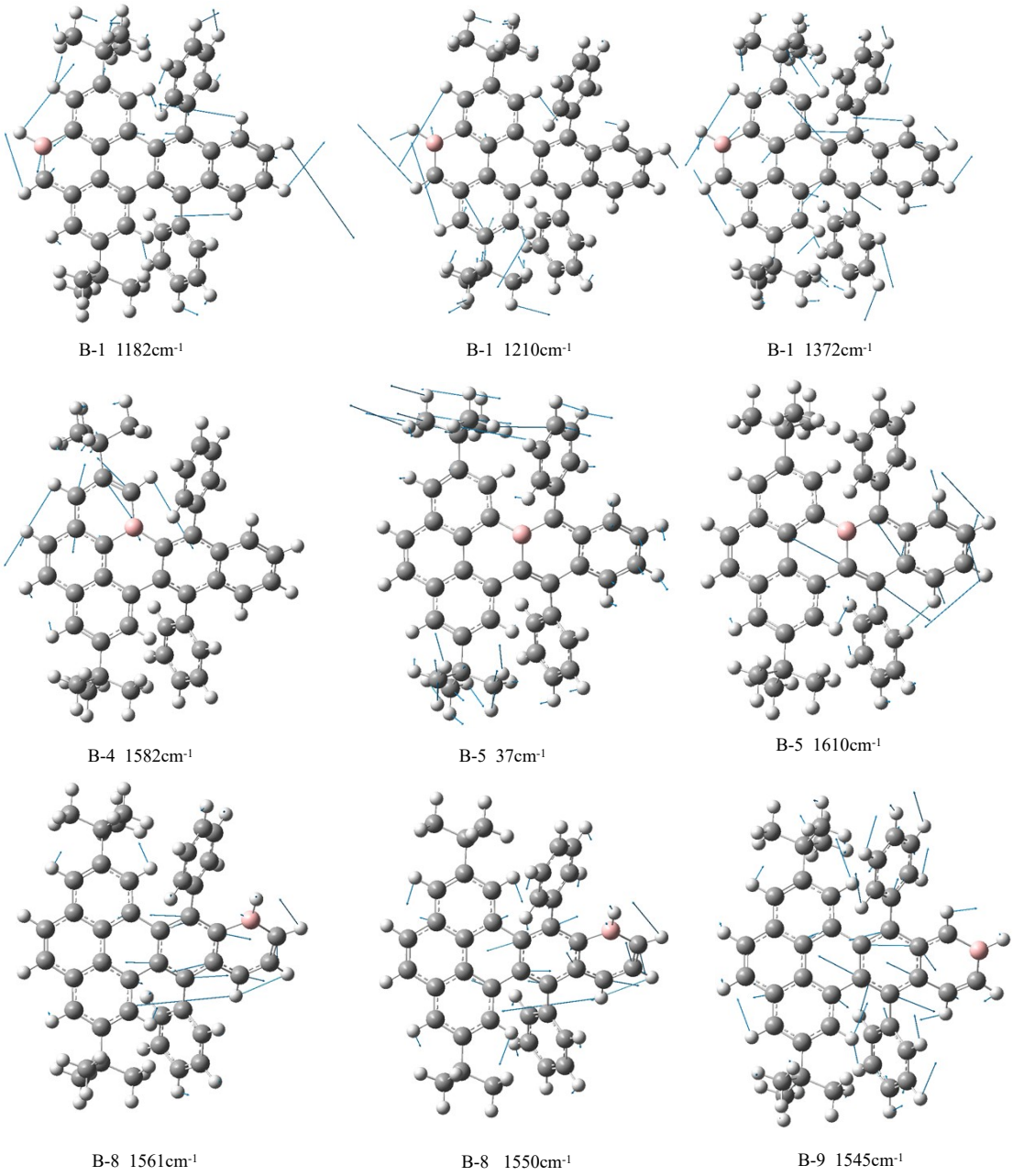


Figure S21. Vibration modes of B-1-*PP*, B-4-*PP*, B-5-*PP*, B-8-*PP* and B-9-*PP*.

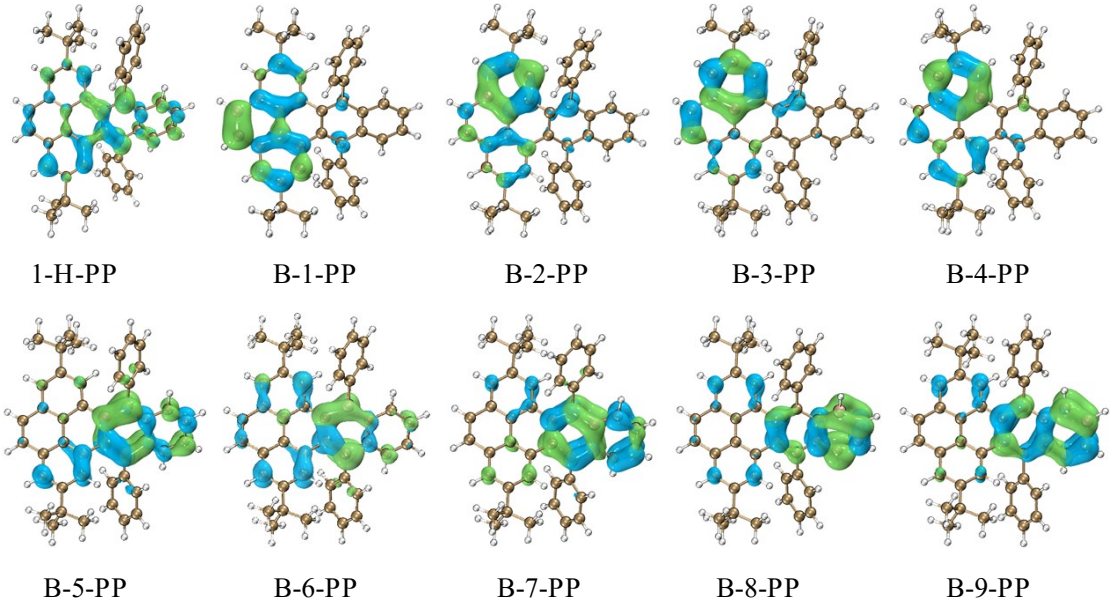


Figure S22. Electron-hole distributions for the $D_0 \rightarrow D_1$ transition of compounds 1-H-*PP*, B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP*(green represents electrons, blue represents holes).

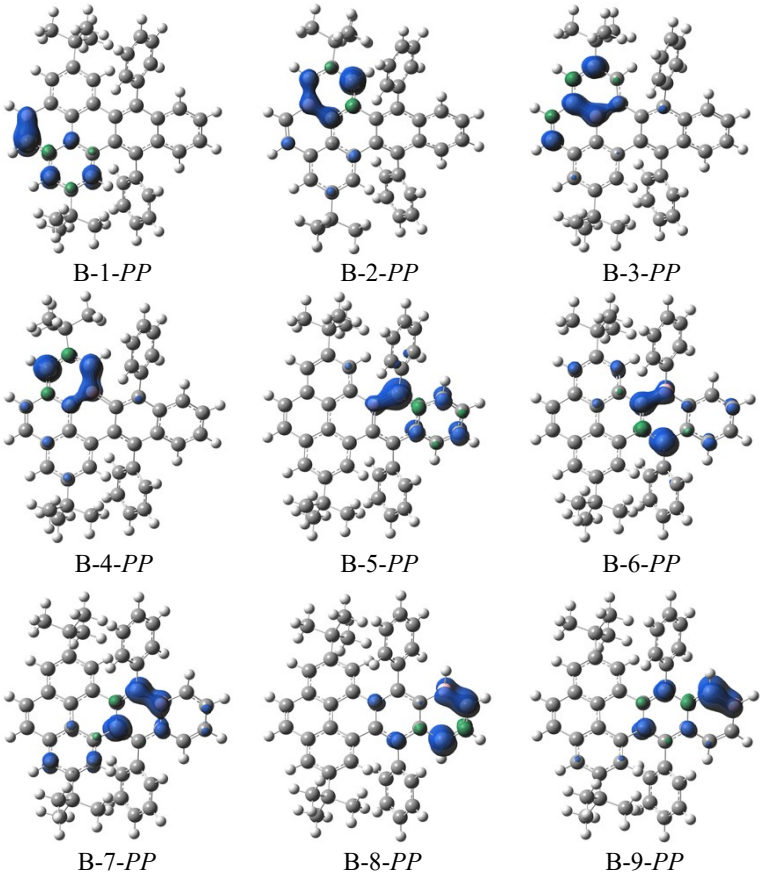


Figure S23. Spin density distributions for the boron embedded compounds in the ground state (blue represents positive spin, green represents negative spin).

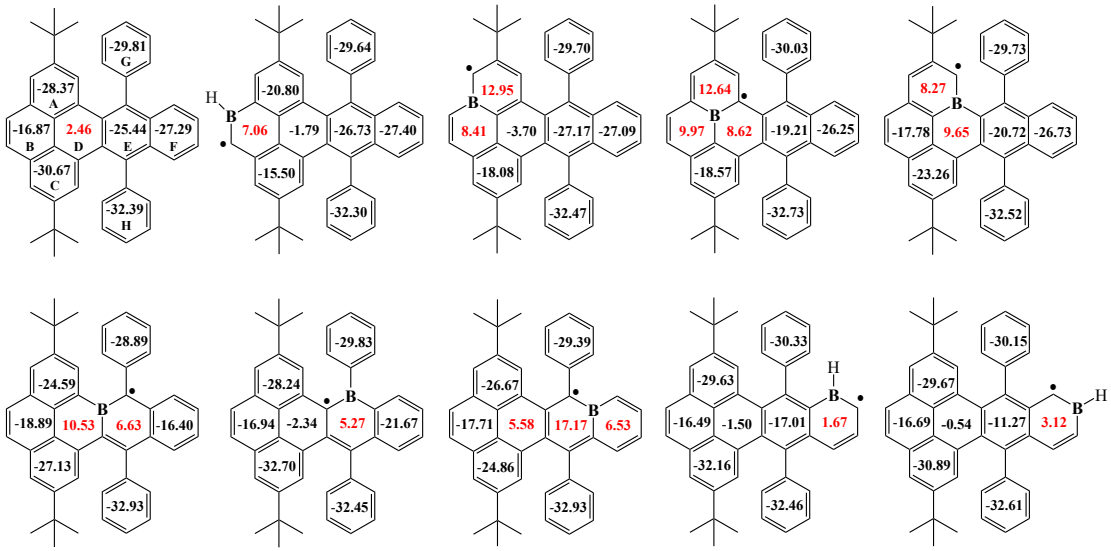


Figure S24. NICS $(1)_{ZZ}$ values (in units of ppm) for compounds 1-H-*PP*, B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP* in the ground state.

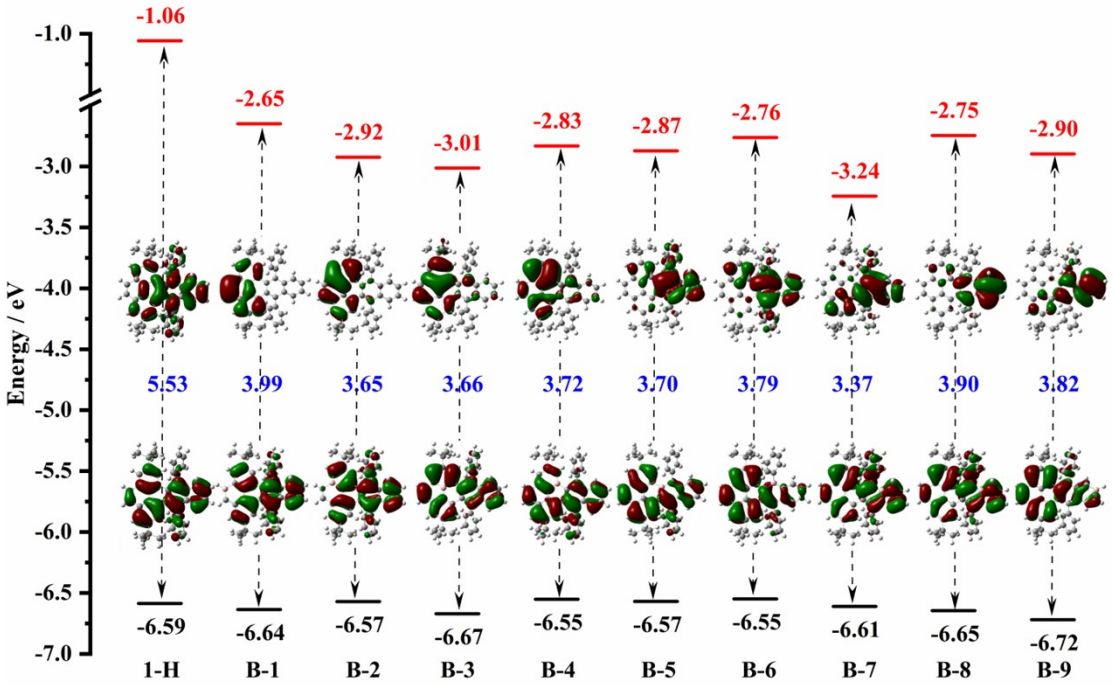


Figure S25. The TD-M06-2X/6-311G** energy levels and β wave-functions for HOMOs and SOMOs of B-1-*PP*, B-2-*PP*, B-3-*PP*, B-4-*PP*, B-5-*PP*, B-6-*PP*, B-7-*PP*, B-8-*PP*, and B-9-*PP* in D_0 state.

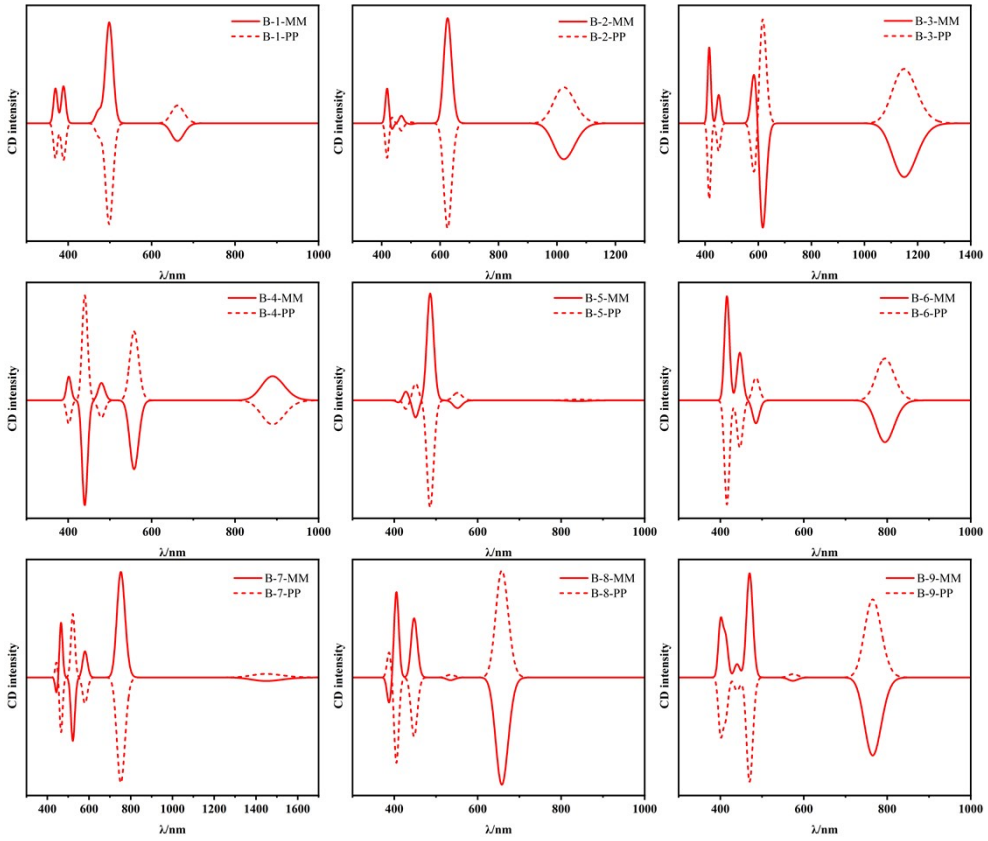


Figure S26. ECD spectra for compounds B-1-*PP*/*MM*, B-2-*PP*/*MM*, B-3-*PP*/*MM*, B-4-*PP*/*MM*, B-5-*PP*/*MM*, B-6-*PP*/*MM*, B-7-*PP*/*MM*, B-8-*PP*/*MM*, B-9-*PP*/*MM*.

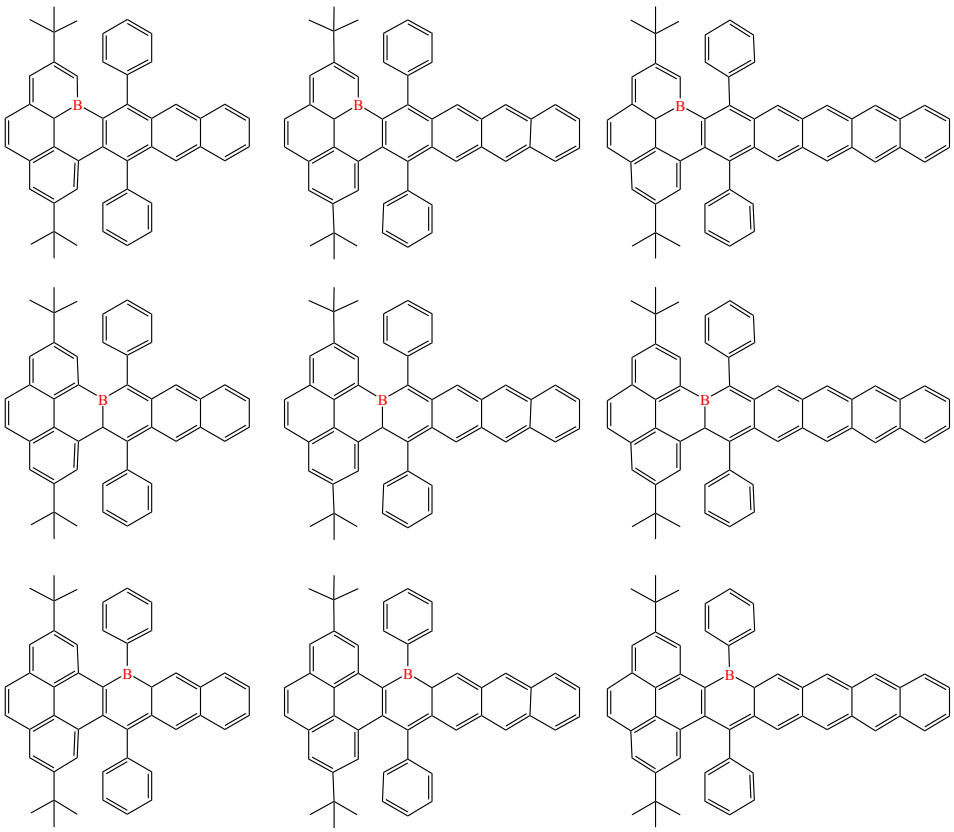


Figure S27. The structures of pyrene anthracene, pyrene tetracene, and pyrene pentacene with boron embedded at the 4, 5, and 6 positions, respectively.

Table S25. Cartesian coordinates for the optimized species at M06-2X/6-311G** level.

1-H-*PP*

Energy (with Zero-point Energy correction) = -1699.337458 (-1698.646072) Hartree

Free energy (298 K) = -1698.712306 Hartree

Zero number of imaginary frequency

0 1

C	-3.42026200	-2.09865600	-0.72279200
C	-2.69272800	-3.26631300	-0.58941500
C	-1.42083300	-0.79248500	-0.14116500
C	-2.76270400	-0.87916700	-0.49343300
C	-0.56299300	-4.44869200	-0.17626700
C	0.74677800	-1.96248800	0.10711400
C	1.45676200	-3.17741600	0.26531100
C	0.75625800	-4.42326800	0.11154200
C	2.82323300	-3.14701800	0.55982400
H	3.34423300	-4.09305000	0.66837700
C	3.49661100	-1.94714200	0.73518300
C	2.78565000	-0.75835000	0.53509800
C	1.44086500	-0.73364400	0.16341800
C	0.70128100	0.53029900	-0.06788900
C	-0.73313700	0.50261600	0.08080700
H	-1.08350200	-5.39099100	-0.30876600
H	-3.15840800	-4.23483400	-0.72650400
H	-3.33346700	0.02642700	-0.61677900
H	1.31844900	-5.34427300	0.22125200
H	3.29844300	0.17517400	0.68847900
C	-1.40685200	1.68949600	0.36134800
C	1.32847200	1.73735100	-0.37176700
C	0.59809900	2.95894000	-0.28027300
C	-0.72796600	2.93774700	0.23572600
C	-2.81534000	1.72318900	0.85781500
C	-3.82353700	2.39175600	0.15616900
C	-3.13177700	1.11919200	2.07527800
C	-5.11557400	2.45960200	0.66425000
H	-3.58508200	2.86025600	-0.79301200
C	-4.42300100	1.19124800	2.58697800
H	-2.35491000	0.59411300	2.61954600
C	-5.41743100	1.86474100	1.88608800
H	-5.88608000	2.97945900	0.10714000
H	-4.65090800	0.72189500	3.53660300
H	-6.42314700	1.92039100	2.28505600
C	2.74021200	1.80714200	-0.85241100
C	3.11005500	1.12640400	-2.01356500

C	3.70633600	2.55876700	-0.17670900
C	4.41566000	1.19060200	-2.48625600
H	2.36569200	0.53758500	-2.53771800
C	5.01098600	2.62751700	-0.65113900
H	3.42808300	3.08467500	0.73042100
C	5.36995000	1.94266600	-1.80812400
H	4.68666100	0.65635100	-3.38917100
H	5.74924900	3.20993900	-0.11252500
H	6.38698500	1.99403000	-2.17806300
C	-1.34754200	4.17957200	0.56137000
C	1.16260200	4.21606200	-0.64445600
C	0.50801900	5.38790400	-0.38602000
C	-0.74453900	5.37043100	0.26699200
H	-2.31401300	4.17637900	1.04595000
H	2.12737600	4.23980700	-1.13177000
H	0.95690200	6.33203500	-0.67038500
H	-1.23504100	6.30225100	0.52167400
C	-4.90519300	-2.07400200	-1.08971900
C	-5.69225800	-1.41315600	0.05377200
C	-5.10065400	-1.25731000	-2.37832700
C	-5.46385000	-3.48099900	-1.31973200
H	-5.56194700	-1.97094300	0.98488500
H	-5.35983100	-0.38787400	0.22798200
H	-6.75886900	-1.38768000	-0.18868400
H	-4.52963800	-1.69172400	-3.20251600
H	-6.15808200	-1.24788500	-2.65724000
H	-4.77957800	-0.22118500	-2.25057800
H	-6.52180600	-3.41341300	-1.58377100
H	-4.94586700	-3.99026300	-2.13658000
H	-5.38359400	-4.09608200	-0.41981900
C	4.98261800	-1.95407500	1.10530900
C	5.77357900	-2.61884200	-0.03423500
C	5.53585600	-0.54029800	1.30747000
C	5.18799600	-2.74762100	2.40582400
H	5.44893800	-3.64818600	-0.20114300
H	5.63726100	-2.06386800	-0.96602000
H	6.84032500	-2.63436600	0.20697800
H	5.01328300	-0.01365600	2.11087900
H	6.59282500	-0.60068400	1.57857700
H	5.45591600	0.05588300	0.39521400
H	6.24717700	-2.75370800	2.67795600
H	4.62394700	-2.29582300	3.22539700
H	4.86202200	-3.78460100	2.30316000
C	-0.66920000	-1.99306400	-0.11287300

C	-1.32050600	-3.23283200	-0.29686300

B-1-*PP*

Energy (with Zero-point Energy correction) = -1686.048077 (-1685.361760) Hartree

Free energy (298 K) = -1685.429361 Hartree

Zero number of imaginary frequency

0 2

C	-3.44041900	-2.08193300	-0.75876500
C	-2.71086700	-3.26388500	-0.64638900
C	-1.41717100	-0.82796200	-0.13684800
C	-2.76940900	-0.89017200	-0.49966000
C	0.75234900	-1.99465800	0.10364700
C	1.50778800	-3.20223300	0.28387400
C	0.90200700	-4.47105300	0.13018700
C	2.87732000	-3.11436500	0.60131200
H	3.42038800	-4.04584800	0.72573800
C	3.52002700	-1.89745300	0.78042900
C	2.77275900	-0.74383200	0.55815800
C	1.42181400	-0.76486400	0.15420100
C	0.68593100	0.49768600	-0.08120700
C	-0.74072500	0.46801200	0.09001500
H	-1.11319800	-5.63908300	-0.40163900
H	-3.18925300	-4.22267100	-0.80827900
H	-3.31887400	0.03083400	-0.61166800
H	1.55513700	-5.32826800	0.27305300
H	3.23974100	0.21181200	0.72639000
C	-1.41127300	1.65447500	0.38685400
C	1.31030400	1.70202100	-0.40574900
C	0.57926300	2.92146300	-0.30701200
C	-0.73429200	2.90071800	0.24384600
C	-2.80698000	1.67860600	0.91723700
C	-3.83063400	2.36919300	0.26005000
C	-3.09787100	1.03292400	2.11989900
C	-5.11086200	2.42022800	0.79860500
H	-3.61425600	2.86647700	-0.67970400
C	-4.37779400	1.08675500	2.66122800
H	-2.31005900	0.48948100	2.62932400
C	-5.38652400	1.78397300	2.00568400
H	-5.89331000	2.95713600	0.27538000
H	-4.58551800	0.58448000	3.59851600
H	-6.38347400	1.82529000	2.42765100
C	2.71115800	1.75850200	-0.91738500
C	3.06406100	1.02142400	-2.04972800
C	3.68762700	2.54363700	-0.29589800

C	4.36167200	1.06345700	-2.54632900
H	2.31247200	0.40760200	-2.53343000
C	4.98345700	2.59175100	-0.79592400
H	3.42525800	3.11110700	0.59063600
C	5.32515600	1.84998300	-1.92272700
H	4.61863900	0.48533800	-3.42599500
H	5.72905100	3.20142000	-0.29919000
H	6.33566700	1.88468800	-2.31190400
C	-1.34343400	4.14443200	0.58456600
C	1.12889900	4.17764000	-0.69815800
C	0.48036400	5.34949000	-0.42744100
C	-0.75081400	5.33383100	0.26658200
H	-2.29386000	4.14252900	1.09983300
H	2.07691200	4.19975300	-1.21740600
H	0.91716500	6.29260000	-0.73308700
H	-1.23341000	6.26649600	0.53293900
C	-4.92207200	-2.03529700	-1.13687500
C	-5.71197200	-1.39581200	0.01677900
C	-5.10239400	-1.18574500	-2.40621200
C	-5.48911600	-3.43240200	-1.40481000
H	-5.59394000	-1.97753800	0.93477400
H	-5.37009800	-0.37850400	0.21845500
H	-6.77655300	-1.35380600	-0.23236000
H	-4.52950500	-1.60444000	-3.23719100
H	-6.15776100	-1.16042100	-2.69194400
H	-4.77364500	-0.15566300	-2.25068900
H	-6.54458300	-3.35034000	-1.67499400
H	-4.96827800	-3.92628900	-2.22909600
H	-5.41944000	-4.06995000	-0.51995800
C	4.99678700	-1.85928000	1.17970000
C	5.82708400	-2.50357500	0.05659800
C	5.50010100	-0.42793500	1.38569600
C	5.20047000	-2.64257400	2.48645900
H	5.53511400	-3.54221400	-0.11393600
H	5.69307400	-1.95402200	-0.87877000
H	6.88893000	-2.48891200	0.31802900
H	4.94657600	0.08435700	2.17768400
H	6.55333200	-0.45267300	1.67576800
H	5.41725600	0.16102100	0.46902900
H	6.25409400	-2.61698700	2.77774100
H	4.60890800	-2.20502100	3.29427200
H	4.90747600	-3.68922900	2.38178300
C	-0.68187400	-2.03214400	-0.13352500
C	-1.34549400	-3.26426000	-0.35221900

B	-0.57052400	-4.59063000	-0.23364400

B-2-*PP*

Energy (with Zero-point Energy correction) = -1686.041708 (-1685.354431) Hartree

Free energy (298 K) = -1685.421846 Hartree

Zero number of imaginary frequency

0 2

C	-3.46225100	-2.16013400	-0.76736900
C	-2.82589400	-3.36300600	-0.63528600
C	-1.38222000	-0.85072800	-0.12855900
C	-2.73573600	-0.94623000	-0.52101100
C	-0.45704000	-4.64301400	-0.10764200
C	0.78276300	-1.97005700	0.11474500
C	1.50989500	-3.18151800	0.28910900
C	0.85401400	-4.48258300	0.17325900
C	2.86383300	-3.12564100	0.57118200
H	3.40094700	-4.06021600	0.70023000
C	3.53866100	-1.90408600	0.72005600
C	2.82452200	-0.73493600	0.50886800
C	1.46270000	-0.73572600	0.15115100
C	0.70326900	0.51201200	-0.07132000
C	-0.72990800	0.45945800	0.08190700
H	-0.83946400	-5.65732000	-0.18888300
H	-3.39127900	-4.27463100	-0.80253300
H	-3.26907600	-0.02449200	-0.69488800
H	1.50753100	-5.34145500	0.31679700
H	3.32586400	0.20688600	0.64853600
C	-1.42619700	1.63398200	0.37328400
C	1.30605800	1.73617700	-0.37400500
C	0.55432500	2.93961600	-0.26941100
C	-0.76952900	2.89190700	0.25641400
C	-2.82895600	1.63133500	0.88673800
C	-3.85160400	2.32862400	0.23423000
C	-3.12319400	0.97714300	2.08487000
C	-5.12812600	2.39216000	0.78051900
H	-3.63397100	2.83177900	-0.70212700
C	-4.40031000	1.04141500	2.63239100
H	-2.33718900	0.42800400	2.59115400
C	-5.40365900	1.75627600	1.98776900
H	-5.90755200	2.93910900	0.26323700
H	-4.60859700	0.53622100	3.56797200
H	-6.39703100	1.80908600	2.41673100
C	2.71028900	1.83075400	-0.87012500

C	3.07822200	1.15554700	-2.03516200
C	3.67190400	2.59639200	-0.20344600
C	4.37790400	1.23947700	-2.52111200
H	2.33748700	0.55614000	-2.55240600
C	4.97058200	2.68358800	-0.69044400
H	3.39522800	3.11689700	0.70725000
C	5.32762600	2.00479900	-1.85180000
H	4.64765400	0.70980800	-3.42705000
H	5.70592600	3.27584000	-0.15865900
H	6.34016400	2.07097900	-2.23157300
C	-1.40098400	4.12289100	0.60714000
C	1.09369400	4.21083600	-0.63044100
C	0.42449300	5.36830300	-0.35308100
C	-0.81918000	5.32436100	0.31920000
H	-2.35856800	4.10082400	1.10833200
H	2.05126300	4.25397000	-1.13042300
H	0.85361500	6.32236200	-0.63464500
H	-1.31803000	6.24605100	0.59373600
C	-4.93622700	-2.00333800	-1.16046600
C	-5.68466100	-1.28743600	-0.02479500
C	-5.04335300	-1.16779700	-2.44837400
C	-5.60676000	-3.35606400	-1.41032500
H	-5.62144000	-1.86410400	0.90184600
H	-5.27135200	-0.29602000	0.16876000
H	-6.74027500	-1.16614100	-0.28585600
H	-4.48844100	-1.64010900	-3.26274100
H	-6.09125100	-1.08284800	-2.74936700
H	-4.65625800	-0.15510900	-2.31404800
H	-6.65194200	-3.19760700	-1.68668100
H	-5.12100900	-3.90011100	-2.22412400
H	-5.58767900	-3.98282300	-0.51558900
C	5.02302900	-1.90371000	1.08811200
C	5.81092100	-2.60685500	-0.03078800
C	5.57948800	-0.48575400	1.24491700
C	5.22588700	-2.65730200	2.41302500
H	5.48349900	-3.63966000	-0.16770200
H	5.67855000	-2.07937100	-0.97888400
H	6.87711300	-2.61973700	0.21250900
H	5.06425400	0.06410800	2.03738000
H	6.63863700	-0.53938300	1.50865200
H	5.49115500	0.08414800	0.31667400
H	6.28534900	-2.65912000	2.68382400
H	4.66492100	-2.17704000	3.21836400
H	4.89572500	-3.69574500	2.34390900

B	-1.32995000	-3.39331100	-0.29116400
C	-0.62908000	-2.02657500	-0.10424000

B-3-*PP*

Energy (with Zero-point Energy correction) = -1686.037016 (-1685.349660) Hartree

Free energy (298 K) = -1685.417907 Hartree

Zero number of imaginary frequency

0 2

C	-3.43849700	-2.22855000	-0.55666700
C	-2.68916900	-3.40571600	-0.63334400
C	-1.30537000	-3.37526600	-0.46831700
C	-1.49210900	-0.74917200	-0.07640600
C	-2.83896600	-0.94385700	-0.27407300
C	-0.45501800	-4.52678000	-0.48635200
C	0.85250500	-1.94948400	-0.07384300
C	1.57539800	-3.15894300	0.00614300
C	0.88529400	-4.41867700	-0.25489600
C	2.91863200	-3.12322000	0.36355700
H	3.48080800	-4.05097400	0.40792000
C	3.53167500	-1.91213800	0.71652500
C	2.79664400	-0.73118300	0.62260100
C	1.46824200	-0.71895200	0.16002800
C	0.68068000	0.54579300	-0.02097400
C	-0.77679500	0.53986200	0.11617700
H	-0.88172900	-5.51075400	-0.66543700
H	-3.18990000	-4.35038000	-0.81687200
H	-3.53824600	-0.12345000	-0.24188900
H	1.49410000	-5.31825100	-0.24866700
H	3.26137300	0.19344400	0.92367500
C	-1.41805200	1.75484600	0.33126700
C	1.32455100	1.73796500	-0.32687600
C	0.61689700	2.98356900	-0.28077700
C	-0.72374200	2.99476900	0.18301100
C	-2.85402500	1.83626600	0.72494200
C	-3.81222900	2.36175900	-0.14552200
C	-3.25105500	1.41197600	1.99296400
C	-5.14654500	2.43996100	0.23773100
H	-3.50393500	2.69662700	-1.13027500
C	-4.58304000	1.50412300	2.38254400
H	-2.50765300	1.00297800	2.66777400
C	-5.53465500	2.01377600	1.50493000
H	-5.88238600	2.83869300	-0.45070100
H	-4.87873400	1.17298500	3.37109500

H	-6.57346000	2.07843000	1.80591200
C	2.74838800	1.77968100	-0.77881200
C	3.13449900	1.07383400	-1.91912100
C	3.71078500	2.52755000	-0.09374800
C	4.45327000	1.10241600	-2.35763300
H	2.39305400	0.48850400	-2.45140500
C	5.02848200	2.56165500	-0.53397500
H	3.42010000	3.07522500	0.79657900
C	5.40494500	1.84557600	-1.66659400
H	4.73696300	0.54539900	-3.24277300
H	5.76386600	3.13975900	0.01334600
H	6.43274200	1.86832900	-2.00871400
C	-1.35596300	4.24705900	0.41854900
C	1.21181300	4.21873700	-0.65597700
C	0.55587200	5.40711700	-0.47039000
C	-0.72887800	5.42427600	0.10947700
H	-2.35101700	4.26528600	0.84222600
H	2.19860000	4.21979600	-1.09734300
H	1.03014000	6.33624700	-0.76296600
H	-1.22716800	6.36822600	0.29491800
C	-4.95659600	-2.23690900	-0.74594400
C	-5.62667600	-1.77404900	0.56141800
C	-5.34031000	-1.27230500	-1.88517400
C	-5.50338900	-3.62428400	-1.09876000
H	-5.37045300	-2.44772900	1.38309500
H	-5.32051800	-0.76439200	0.83981200
H	-6.71384900	-1.77671600	0.43934900
H	-4.84693500	-1.55974000	-2.81693400
H	-6.42169300	-1.30720000	-2.04377900
H	-5.07065900	-0.23916400	-1.65828400
H	-6.58491500	-3.55893000	-1.23773200
H	-5.06816300	-4.00514600	-2.02599800
H	-5.31458400	-4.34753100	-0.30201100
C	4.99537800	-1.92259900	1.16753300
C	5.86741100	-2.37475700	-0.01659900
C	5.47705600	-0.53909000	1.61395200
C	5.17411100	-2.89728800	2.34338900
H	5.59281700	-3.37527800	-0.35817200
H	5.75303200	-1.68409000	-0.85634700
H	6.92094400	-2.39296500	0.27699800
H	4.88636900	-0.15924100	2.45209700
H	6.51777100	-0.60716600	1.94036900
H	5.42749800	0.18495200	0.79750200
H	6.21666900	-2.89574400	2.67317000

H	4.54570200	-2.60155800	3.18700400
H	4.91270300	-3.92112600	2.06966900
B	-0.64558800	-2.01068700	-0.23639800

B-4-*PP*

Energy (with Zero-point Energy correction) = -1686.057713 (-1685.369977) Hartree

Free energy (298 K) = -1685.438045 Hartree

Zero number of imaginary frequency

0 2

C	-3.62469500	-2.00427100	-0.55879500
C	-2.80498000	-3.16066200	-0.59533700
C	-3.05457500	-0.77984900	-0.28194100
C	0.67616100	-1.95141900	0.02226700
C	1.37802600	-3.18765000	0.08299400
C	0.66656100	-4.39796700	-0.18138200
C	2.74129900	-3.20368700	0.42224400
H	3.25144300	-4.16136400	0.44746500
C	3.40789100	-2.04096100	0.75349100
C	2.70761000	-0.82075000	0.64647500
C	1.39313900	-0.73407900	0.21644500
C	0.72203800	0.58661000	0.03277400
C	-0.71052800	0.66730800	0.22480300
H	-1.20092800	-5.31212300	-0.62707000
H	-3.26641800	-4.12469600	-0.78732700
H	-3.71940800	0.07278600	-0.27513900
H	1.21747800	-5.33241600	-0.16560700
H	3.22400700	0.08836000	0.90856000
C	1.43608500	1.72735200	-0.32045900
C	0.79747300	3.01069300	-0.27503800
C	-0.53355500	3.11460900	0.21332000
C	-2.71924600	2.03465800	0.79648100
C	-3.64912300	2.67416100	-0.02892100
C	-3.15723800	1.46759900	1.99372900
C	-4.99137000	2.72409300	0.32604500
H	-3.31416300	3.10980400	-0.96408200
C	-4.49913500	1.52647500	2.35532200
H	-2.43716700	0.97082900	2.63392900
C	-5.41948500	2.15101000	1.52096700
H	-5.70523800	3.20611400	-0.33148400
H	-4.82559800	1.08040800	3.28730500
H	-6.46650900	2.19016500	1.79745800
C	2.84519000	1.67457400	-0.81437900
C	3.15641400	0.92449600	-1.94986200

C	3.87135100	2.37094100	-0.16896900
C	4.46199400	0.86134200	-2.42186000
H	2.36595600	0.37780500	-2.45189500
C	5.17668300	2.31463600	-0.64399400
H	3.64019900	2.95139500	0.71811400
C	5.47730400	1.55539100	-1.77049800
H	4.68648600	0.27116600	-3.30257500
H	5.96073300	2.85571400	-0.12714500
H	6.49483000	1.50670700	-2.13946800
C	1.45442800	4.20512000	-0.68309100
C	0.87136400	5.43188300	-0.50787400
H	-2.06809900	4.48527500	0.88605700
H	2.43144600	4.14307700	-1.14145100
H	1.39409100	6.32613600	-0.82594800
H	-0.83501200	6.51364100	0.27380300
C	-5.12412000	-2.19628700	-0.82979500
C	-5.89198500	-0.87268800	-0.77923600
C	-5.31980400	-2.81325200	-2.22535900
C	-5.71764700	-3.13436700	0.23543900
H	-5.81316200	-0.39985900	0.20251900
H	-5.52385900	-0.16474500	-1.52642700
H	-6.94928400	-1.05972400	-0.98339400
H	-4.84203300	-3.79156100	-2.31186900
H	-6.38590200	-2.94371200	-2.43121300
H	-4.89789500	-2.16215100	-2.99486000
H	-6.78899700	-3.26899400	0.06174100
H	-5.25063000	-4.12159900	0.21773800
H	-5.58063300	-2.71297100	1.23438500
C	4.88116100	-2.09458000	1.16860000
C	5.71344000	-2.54672500	-0.04374800
C	5.40542600	-0.73031300	1.62745900
C	5.06460500	-3.09424700	2.32205900
H	5.40635500	-3.53587300	-0.39093200
H	5.59311100	-1.84170800	-0.87068900
H	6.77354200	-2.59181900	0.22242100
H	4.83139100	-0.34339800	2.47399200
H	6.44602000	-0.83187300	1.94535200
H	5.37286800	0.00429300	0.81966600
H	6.11515300	-3.12632000	2.62368600
H	4.46655100	-2.79827300	3.18733400
H	4.76889300	-4.10542000	2.03647200
C	-1.28910500	1.91838500	0.40316200
C	-1.08637100	4.40535400	0.43840900
C	-0.39913600	5.53801000	0.09566300

C	-0.66912800	-4.38664400	-0.43215600
C	-1.39878400	-3.15608400	-0.40705100
C	-0.72804700	-1.94523000	-0.17795800
B	-1.53502500	-0.64420000	-0.02641900

B-5-*PP*

Energy (with Zero-point Energy correction) = -1686.063472 (-1685.375525) Hartree

Free energy (298 K) = -1685.444349 Hartree

Zero number of imaginary frequency

0 2

C	-3.41352800	-2.23689300	-0.65448600
C	-2.59472100	-3.34670400	-0.69868600
C	-1.45431700	-0.85705600	-0.07539300
C	-2.81416200	-1.00584300	-0.32789000
C	-0.40102500	-4.44748300	-0.47367200
C	0.81024800	-1.93557600	0.05466200
C	1.55981600	-3.13718200	0.09845100
C	0.91755500	-4.38962500	-0.18941700
C	2.92497200	-3.10740900	0.42217600
H	3.46277600	-4.05022000	0.43717000
C	3.56956500	-1.92506900	0.73797900
C	2.82933000	-0.73834300	0.64319500
C	1.49429000	-0.70352700	0.25056300
C	0.75280300	0.56716600	0.08777500
H	-0.88068600	-5.39427800	-0.69772700
H	-3.00042300	-4.32675400	-0.92288500
H	-3.45040200	-0.13203500	-0.28208900
H	1.52274000	-5.28966400	-0.17488700
H	3.31211600	0.19511200	0.88494100
C	-1.52004300	1.85364500	0.44413600
C	1.31715300	1.75649700	-0.29968200
C	0.53479500	3.00239300	-0.32239000
C	-0.81520000	3.05780300	0.16341900
C	-2.92583000	1.90000600	0.89530900
C	-3.92909700	2.50751300	0.12806000
C	-3.29126000	1.25909000	2.08529700
C	-5.25589600	2.47436500	0.54086300
H	-3.66263900	2.98090100	-0.81060900
C	-4.61323300	1.25233400	2.51134100
H	-2.52622000	0.76490800	2.67355100
C	-5.60081100	1.85635100	1.73900100
H	-6.02115300	2.93345700	-0.07381000
H	-4.87545200	0.76099900	3.44076700
H	-6.63432900	1.83600400	2.06322500

C	2.73969100	1.85523900	-0.75256300
C	3.15497600	1.15693200	-1.88651700
C	3.67580300	2.62001600	-0.05057900
C	4.47929300	1.21348400	-2.30601500
H	2.43359100	0.55358700	-2.42604800
C	4.99985900	2.67789500	-0.46958300
H	3.36030400	3.16288000	0.83430700
C	5.40600300	1.97285300	-1.59882000
H	4.78744100	0.66322000	-3.18720900
H	5.71626300	3.26781900	0.09008700
H	6.43840700	2.01517600	-1.92478700
C	-1.42138800	4.33246300	0.32698400
C	1.11165100	4.19413200	-0.78670500
C	0.45867300	5.41271000	-0.68834600
C	-0.80182400	5.48887800	-0.08933400
H	-2.39912400	4.38748400	0.78682900
H	2.09803700	4.16998000	-1.22840000
H	0.94205200	6.30875800	-1.05881400
H	-1.29271200	6.44604000	0.03711500
C	-4.91850500	-2.28676600	-0.92066600
C	-5.66718600	-1.83169200	0.34326700
C	-5.26292900	-1.33836700	-2.08171500
C	-5.39171900	-3.69560900	-1.28911200
H	-5.43378500	-2.48767300	1.18593600
H	-5.39632100	-0.81120300	0.62308900
H	-6.74729000	-1.86056500	0.17118100
H	-4.72574000	-1.62632900	-2.98872700
H	-6.33618800	-1.37588900	-2.28900700
H	-5.00323300	-0.30400400	-1.84524600
H	-6.46751000	-3.68063600	-1.47917300
H	-4.89620800	-4.06136800	-2.19228200
H	-5.20621700	-4.40573500	-0.47916500
C	5.05249400	-1.93351900	1.11880000
C	5.86993000	-2.38411700	-0.10379600
C	5.54857300	-0.54721400	1.54190000
C	5.28798200	-2.90789100	2.28401400
H	5.58191100	-3.38655500	-0.42834100
H	5.71184100	-1.69691300	-0.93932800
H	6.93672100	-2.39689600	0.13829500
H	4.98779300	-0.16523500	2.39942900
H	6.60097900	-0.61172900	1.82952500
H	5.46756900	0.17466300	0.72563500
H	6.34584300	-2.91094300	2.56133900
H	4.70321300	-2.61114400	3.15807900

H	5.00828600	-3.93002100	2.02175700
C	-0.61850300	-2.00855900	-0.17520700
C	-1.20824300	-3.26034400	-0.45583300
B	-0.78369600	0.51458600	0.20831400

B-6-*PP*

Energy (with Zero-point Energy correction) = -1686.073100 (-1685.385307) Hartree

Free energy (298 K) = -1685.453423 Hartree

Zero number of imaginary frequency

0 2

C	3.38641600	-2.13218200	0.76893000
C	2.62024900	-3.28991100	0.74596200
C	1.38247900	-0.81445700	0.22731000
C	2.74889600	-0.91523300	0.50964100
C	-0.79347500	-1.95135500	0.00452300
C	-1.53092100	-3.15786100	-0.10588300
C	-0.86526200	-4.40710300	0.15012400
C	-2.87732800	-3.10938800	-0.47116200
H	-3.42332600	-4.04487300	-0.54017800
C	-3.50144200	-1.90520400	-0.77674500
C	-2.76961900	-0.72449700	-0.62132800
C	-1.44711900	-0.70844400	-0.17085000
C	-0.67571500	0.53684400	0.04129400
C	0.74167800	0.46784900	-0.00149100
H	0.94514700	-5.39555500	0.64422600
H	3.07298500	-4.25880300	0.92044800
H	3.33665600	-0.01101100	0.54531600
H	-1.44883100	-5.31934000	0.08936700
H	-3.24328900	0.21102500	-0.86805200
C	-1.30774900	1.77315200	0.34413400
C	-0.58526700	3.03498700	0.36009600
C	0.75815300	3.09158900	-0.09742400
C	2.96508900	1.76691000	-0.95264500
C	4.04140700	2.47490200	-0.39738500
C	3.20785900	1.04053700	-2.12814200
C	5.30140300	2.46131500	-0.98950000
H	3.89698100	3.03293500	0.52278700
C	4.45586700	1.04702700	-2.74027300
H	2.40301800	0.46013100	-2.56861500
C	5.50851100	1.75710400	-2.17082000
H	6.11912500	3.00627300	-0.53189400
H	4.61134100	0.48772100	-3.65560000
H	6.48558500	1.75393600	-2.63945100

C	-2.72958200	1.80956000	0.78489000
C	-3.13284300	1.07058100	1.89967300
C	-3.68034300	2.58408000	0.11129700
C	-4.45447400	1.09979700	2.32717600
H	-2.40211300	0.46387700	2.42254700
C	-5.00270500	2.61135500	0.53741200
H	-3.37634900	3.15629600	-0.75859900
C	-5.39429500	1.86831500	1.64699300
H	-4.75043900	0.52217700	3.19481000
H	-5.72898200	3.20793700	-0.00194000
H	-6.42521600	1.88852400	1.97954700
C	1.36898200	4.34580400	-0.23629000
C	-1.20122500	4.22747800	0.79889500
C	-0.55035400	5.44384200	0.69551700
C	0.72924900	5.51524300	0.14538100
H	2.37107800	4.39872000	-0.64518100
H	-2.19310400	4.20295000	1.22791900
H	-1.04646300	6.34454500	1.03781200
H	1.22497400	6.47241700	0.03581000
C	4.89030400	-2.12546600	1.05150800
C	5.62276600	-1.48829600	-0.14168500
C	5.16502200	-1.29515800	2.31664100
C	5.44146500	-3.53753500	1.26784400
H	5.42853400	-2.05016600	-1.05907000
H	5.30536500	-0.45631200	-0.30837300
H	6.70155000	-1.48409200	0.03984300
H	4.63785500	-1.71415200	3.17732800
H	6.23649600	-1.29082400	2.53572600
H	4.84383800	-0.25873400	2.19160800
H	6.51610700	-3.48338500	1.45663700
H	4.97531500	-4.02407600	2.12867200
H	5.28809100	-4.16655700	0.38710100
C	-4.96376300	-1.90264400	-1.23145400
C	-5.83861700	-2.41772600	-0.07586800
C	-5.45042100	-0.50090800	-1.61123100
C	-5.13067600	-2.82004500	-2.45375500
H	-5.56104400	-3.43328700	0.21499500
H	-5.73052300	-1.77117000	0.79900100
H	-6.89102700	-2.42507600	-0.37388000
H	-4.85724800	-0.07668400	-2.42607000
H	-6.48901700	-0.55738900	-1.94637600
H	-5.40907800	0.18233900	-0.75967000
H	-6.17255800	-2.81444900	-2.78575400
H	-4.50371200	-2.47738700	-3.28048300

H	-4.85738800	-3.85258200	-2.22798500
C	0.60890500	-2.00605100	0.26388900
C	1.23970900	-3.24738800	0.49866200
B	1.51917100	1.76810900	-0.32677100
C	0.45108900	-4.44915300	0.45272700

B-7-*PP*

Energy (with Zero-point Energy correction) = -1686.040196 (-1685.353056) Hartree

Free energy (298 K) = -1685.420332 Hartree

Zero number of imaginary frequency

0 2

C	3.46038200	-2.00321300	0.82673700
C	2.76301800	-3.18540700	0.64782500
C	2.78306400	-0.79174400	0.60625500
C	0.66035400	-4.39915400	0.14148600
C	-0.66712300	-1.92263000	-0.15284000
C	-1.35874300	-3.13954800	-0.34913700
C	-0.64994800	-4.38081100	-0.19173900
C	-2.71767600	-3.11393300	-0.68311700
H	-3.22594800	-4.06282700	-0.82327500
C	-3.40607900	-1.91745400	-0.85550900
C	-2.72063000	-0.72750700	-0.61163400
C	-1.37653400	-0.69126400	-0.20388200
C	-0.68252500	0.55914900	0.08183300
H	1.18385300	-5.33964900	0.27468500
H	3.24894200	-4.14479700	0.77823600
H	3.32049200	0.13311500	0.75712500
H	-1.19823900	-5.30541100	-0.33530700
H	-3.23856000	0.20495700	-0.75839500
C	1.41615100	1.71322700	-0.40816200
C	-1.39901200	1.77485200	0.41419100
C	-0.77193900	3.00524900	0.29625100
C	2.79373800	1.71962900	-0.95691600
C	3.77038500	2.58429300	-0.44946500
C	3.12699200	0.90477100	-2.04687100
C	5.04638900	2.61939700	-1.00282200
H	3.52435100	3.22428700	0.39069400
C	4.39384600	0.95545100	-2.61107700
H	2.37582500	0.23487500	-2.45047200
C	5.36102300	1.81064200	-2.08938700
H	5.79263100	3.28679800	-0.58785100
H	4.62844200	0.32478500	-3.46059000
H	6.35132400	1.84606800	-2.52730400

C	-2.77848200	1.69026900	0.97952400
C	-3.03672200	0.87007200	2.08133900
C	-3.82936900	2.43844500	0.43955700
C	-4.31158800	0.79872900	2.62809100
H	-2.22945500	0.28193200	2.50375400
C	-5.10521600	2.36864200	0.98730000
H	-3.64070300	3.06562800	-0.42482000
C	-5.35093900	1.54702900	2.08256300
H	-4.49373700	0.15993400	3.48414600
H	-5.90945800	2.95005600	0.55192800
H	-6.34536500	1.49023400	2.50883500
C	1.19323800	4.44280500	-0.67839800
C	-1.37744300	4.25481600	0.70223000
C	-0.77867800	5.43715800	0.41751000
C	0.47441800	5.53260900	-0.30456600
H	2.13111500	4.60429800	-1.20196000
H	-2.31337200	4.25883100	1.24876300
H	-1.25151700	6.35997400	0.73559400
H	0.83391600	6.53522300	-0.52378800
C	4.93258000	-1.95069700	1.23768400
C	5.72643100	-1.17995800	0.16896200
C	5.05478500	-1.22295800	2.58711300
C	5.53935700	-3.34894300	1.38346600
H	5.63847100	-1.66854400	-0.80500000
H	5.37047700	-0.15314600	0.05821600
H	6.78464300	-1.14280200	0.44352600
H	4.48852600	-1.74644700	3.36136400
H	6.10332100	-1.17993400	2.89476800
H	4.68029700	-0.19902100	2.52584900
H	6.58994000	-3.26114200	1.66974900
H	5.02985100	-3.92985900	2.15662700
H	5.49413100	-3.90491100	0.44341500
C	-4.88146500	-1.94127600	-1.26349500
C	-5.68824300	-2.63590000	-0.15315300
C	-5.44988800	-0.53223300	-1.45581600
C	-5.04175000	-2.71639000	-2.58125100
H	-5.35327200	-3.66334700	0.00562300
H	-5.58257000	-2.09309300	0.78974500
H	-6.74833800	-2.66331400	-0.42035500
H	-4.91481700	0.01539500	-2.23662600
H	-6.49807800	-0.60358500	-1.75596400
H	-5.40388100	0.04845700	-0.53112300
H	-6.09368600	-2.73401100	-2.87892500
H	-4.46577900	-2.24243700	-3.37971100

H	-4.70331500	-3.75038800	-2.48815300
C	0.73345400	-1.94733100	0.12615600
C	1.39910600	-3.17853900	0.31205600
C	1.45616300	-0.73626300	0.20617600
C	0.76300900	0.54709200	-0.04270500
B	0.64644200	3.05935800	-0.31344300

B-8-*PP*

Energy (with Zero-point Energy correction) = -1686.047932 (-1685.362130) Hartree

Free energy (298 K) = -1685.429697 Hartree

Zero number of imaginary frequency

0 2

C	-3.43444400	-2.05286900	-0.75538000
C	-2.71359500	-3.22947400	-0.63582600
C	-1.42700000	-0.77150900	-0.15236200
C	-2.77204900	-0.84265500	-0.50784600
C	0.72777300	-1.95888400	0.09297100
C	1.43325000	-3.17955900	0.23614100
C	0.72612200	-4.41946100	0.06055100
C	2.79688100	-3.15628400	0.53748900
H	3.31568700	-4.10475600	0.63446500
C	3.47448200	-1.95966900	0.73458400
C	2.77053900	-0.76635900	0.54988800
C	1.42569400	-0.73307700	0.17367300
C	0.68731700	0.52887700	-0.03842900
C	-0.73019400	0.50591700	0.08066100
H	-1.11700000	-5.37140800	-0.37935600
H	-3.18744700	-4.19197100	-0.78661000
H	-3.33485700	0.07031300	-0.61730100
H	1.28258100	-5.34513300	0.15929400
H	3.28483200	0.16366100	0.72018200
C	1.32099700	1.75398200	-0.34265800
C	0.58016700	2.95689300	-0.27866000
C	-0.74720800	2.95266200	0.25094500
C	-2.79687200	1.72535400	0.91282000
C	-3.81341300	2.45265900	0.28998600
C	-3.08908700	1.03201000	2.08894400
C	-5.09160700	2.49536700	0.83568000
H	-3.59429700	2.98604200	-0.62889700
C	-4.36295800	1.08327600	2.64138400
H	-2.30569700	0.45982500	2.57350300
C	-5.36781000	1.81678200	2.01790500
H	-5.86899900	3.06505600	0.34051000

H	-4.57085000	0.55110400	3.56204700
H	-6.36146500	1.85423500	2.44808000
C	2.73363200	1.81203300	-0.81810000
C	3.11309600	1.10703800	-1.96235900
C	3.69178900	2.58246300	-0.15266300
C	4.42034000	1.16897400	-2.42912700
H	2.37521800	0.50351100	-2.47897200
C	4.99969700	2.64590900	-0.62021400
H	3.40480800	3.12590200	0.74130600
C	5.36774100	1.93896000	-1.76034500
H	4.69893300	0.61843600	-3.31982200
H	5.73202900	3.24311300	-0.08994300
H	6.38672500	1.98652800	-2.12528800
C	1.14290800	4.19312200	-0.73658300
C	0.53298100	5.44066500	-0.55428700
C	-0.65658200	5.57416000	0.13163600
H	-2.32804000	4.40092100	1.34700400
H	2.08188900	4.15925800	-1.27282000
H	1.04770200	6.30899900	-0.95564900
H	-1.04526600	6.57713800	0.28068000
C	-4.91773500	-2.01445300	-1.12859500
C	-5.70456700	-1.34593700	0.01074000
C	-5.09774300	-1.19585100	-2.41821800
C	-5.48847700	-3.41614100	-1.36144200
H	-5.58091500	-1.90171900	0.94394900
H	-5.36833500	-0.32173800	0.18455800
H	-6.76998900	-1.31559200	-0.23592000
H	-4.52906600	-1.63762500	-3.24014900
H	-6.15383000	-1.17303700	-2.70124800
H	-4.76384100	-0.16403000	-2.28889200
H	-6.54524400	-3.33837700	-1.62717800
H	-4.97444100	-3.92919200	-2.17843900
H	-5.41546000	-4.03312200	-0.46215600
C	4.95886800	-1.97783000	1.11013700
C	5.75129400	-2.62539200	-0.03829000
C	5.51546800	-0.56928500	1.33869500
C	5.15722500	-2.79424900	2.39750100
H	5.42350400	-3.65040400	-0.22463400
H	5.62047700	-2.05343200	-0.96057400
H	6.81703700	-2.64929100	0.20638600
H	4.99245700	-0.05594000	2.15032000
H	6.57150400	-0.63748800	1.61128200
H	5.43984700	0.04350900	0.43694400
H	6.21537400	-2.80788500	2.67312100

H	4.59161200	-2.35511900	3.22283000
H	4.82915700	-3.82851900	2.27601100
C	-0.68380300	-1.97871400	-0.13709300
C	-1.34356600	-3.21202600	-0.33947000
C	-0.59227800	-4.43365100	-0.23225000
C	-1.40333800	1.72242300	0.37883900
B	-1.37198900	4.32220900	0.64710900

B-9-*PP*

Energy (with Zero-point Energy correction) = -1686.041128 (-1685.355265) Hartree

Free energy (298 K) = -1685.422702 Hartree

Zero number of imaginary frequency

0 2

C	-3.45177400	-2.03280800	-0.74679300
C	-2.74021400	-3.21074200	-0.59557600
C	-1.44199200	-0.75220700	-0.15590700
C	-2.78282000	-0.82059100	-0.52032200
C	0.70428900	-1.94265000	0.12445400
C	1.40234900	-3.16352100	0.29311000
C	0.68961000	-4.40358400	0.14351700
C	2.76646100	-3.14228600	0.59344500
H	3.27856700	-4.09203200	0.71118900
C	3.45417600	-1.94647900	0.76248800
C	2.76005200	-0.75345900	0.54903400
C	1.41181300	-0.71774000	0.17562100
C	0.68599300	0.53980300	-0.05945200
C	-0.73447400	0.52632800	0.06208200
H	-1.15664700	-5.35616000	-0.28210100
H	-3.21901800	-4.17319900	-0.72939600
H	-3.33827400	0.09399700	-0.65472300
H	1.24168300	-5.32934800	0.26334800
H	3.28217100	0.17627100	0.69498100
C	1.33551100	1.76869500	-0.37527400
C	0.63657700	2.97389000	-0.28754600
C	-0.69040200	2.97395200	0.26630700
C	-2.78656400	1.76442200	0.87964500
C	-3.78634700	2.49689900	0.23243000
C	-3.10358000	1.08603500	2.05822900
C	-5.07301500	2.55330500	0.75596800
H	-3.54637500	3.02289500	-0.68534700
C	-4.38726800	1.15097800	2.58676100
H	-2.33292400	0.51172800	2.56001700
C	-5.37486100	1.88631700	1.93923600

H	-5.83770400	3.12344400	0.24201100
H	-4.61571500	0.62758300	3.50748300
H	-6.37563900	1.93498000	2.35124100
C	2.73963300	1.78422100	-0.88493600
C	3.07233600	1.05048900	-2.02500200
C	3.73439400	2.53401900	-0.25126300
C	4.37076600	1.06457200	-2.51998000
H	2.30607100	0.46224700	-2.51753500
C	5.03269600	2.55113700	-0.74771400
H	3.48265400	3.10201700	0.63795200
C	5.35488000	1.81515800	-1.88353900
H	4.61332200	0.49220200	-3.40741800
H	5.79333400	3.13517500	-0.24329900
H	6.36665100	1.82638900	-2.27082800
C	1.23831100	4.23549800	-0.71588300
C	0.71596100	5.45165200	-0.43681900
H	-2.19086100	4.14657900	1.22516300
H	2.14954400	4.15469600	-1.29764600
H	1.24706000	6.31940900	-0.81704400
H	-1.05652900	6.57119400	0.74520500
C	-4.93085800	-1.99363000	-1.13609300
C	-5.72498400	-1.29036300	-0.02315600
C	-5.09104000	-1.20780000	-2.44852400
C	-5.50981200	-3.39671900	-1.33839800
H	-5.61410100	-1.82155500	0.92586800
H	-5.38418900	-0.26391200	0.12617400
H	-6.78763700	-1.26031300	-0.28133800
H	-4.51785900	-1.67584500	-3.25252800
H	-6.14393300	-1.18381900	-2.74301800
H	-4.74941800	-0.17576300	-2.34329800
H	-6.56350500	-3.31817500	-1.61579300
H	-4.99233400	-3.93398100	-2.13738200
H	-5.44935100	-3.99114000	-0.42313700
C	4.93824900	-1.96951900	1.13864400
C	5.72468100	-2.64816000	0.00410400
C	5.50675000	-0.56139900	1.33738800
C	5.12915900	-2.76011800	2.44316200
H	5.38862400	-3.67429200	-0.16023500
H	5.59856300	-2.09486400	-0.93012100
H	6.79015700	-2.67567600	0.24930600
H	4.98591200	-0.02506100	2.13548200
H	6.56117500	-0.63304800	1.61509900
H	5.43986900	0.03132300	0.42183700
H	6.18710100	-2.77671000	2.71912100

H	4.56749200	-2.29859000	3.25891600
H	4.79280100	-3.79412400	2.34401300
C	-0.70652900	-1.96153200	-0.10939200
C	-1.37202400	-3.19527700	-0.28994100
C	-0.62796100	-4.41801400	-0.15304200
C	-1.38835100	1.73317800	0.36454300
B	-0.57610000	5.54263400	0.38369900
C	-1.25315100	4.19843400	0.68426500

1-H-*PP*-S1

Energy (with Zero-point Energy correction) = -1699.216953 (-1698.528874) Hartree

Free energy (298 K) = -1698.595057 Hartree

Zero number of imaginary frequency

0 1

C	-3.40496900	-2.11045900	-0.72368300
C	-2.69783700	-3.26759500	-0.44770200
C	-1.43174400	-0.76577800	-0.15299300
C	-2.74844600	-0.87362100	-0.57173500
C	-0.58609100	-4.41386400	0.14208700
C	0.70272800	-1.91230400	0.28503700
C	1.42980300	-3.10379500	0.50096300
C	0.73748100	-4.35720700	0.43615900
C	2.81001600	-3.04425900	0.74875900
H	3.34102600	-3.97841600	0.90066500
C	3.49270300	-1.82548500	0.82343900
C	2.78708600	-0.65794700	0.58033800
C	1.39426600	-0.65268000	0.24447800
C	0.68822500	0.53349100	-0.08781900
C	-0.74677900	0.52744900	0.02896800
H	-1.09577700	-5.36866100	0.07215100
H	-3.16841900	-4.24027200	-0.52452700
H	-3.29810600	0.02807600	-0.79898400
H	1.30379700	-5.26635600	0.60694500
H	3.28095400	0.29056200	0.70692600
C	-1.38862900	1.71127800	0.35605800
C	1.36996100	1.78473600	-0.40110300
C	0.67552900	3.01365000	-0.16720500
C	-0.65687600	2.96907600	0.35695500
C	-2.81037300	1.75092200	0.79726900
C	-3.76997500	2.49299000	0.09968900
C	-3.20097800	1.07221800	1.95447500
C	-5.08386300	2.55603800	0.54975900
H	-3.47500700	3.02373700	-0.79940400

C	-4.51312300	1.14027300	2.40814400
H	-2.46279400	0.49248300	2.49730000
C	-5.45851700	1.88461600	1.71009900
H	-5.81491900	3.13269200	-0.00480500
H	-4.79640400	0.61314700	3.31158000
H	-6.48105800	1.93747900	2.06420000
C	2.68241800	1.73460700	-1.01594100
C	2.99984600	0.69910900	-1.93293400
C	3.73034700	2.62703400	-0.67230200
C	4.25527600	0.61244900	-2.51819300
H	2.22605300	-0.00529100	-2.21304000
C	4.98301700	2.51865800	-1.24405200
H	3.56234500	3.36349400	0.10311100
C	5.25460400	1.51997100	-2.18679600
H	4.45203000	-0.17459300	-3.23700500
H	5.76795500	3.20107900	-0.93913500
H	6.23738900	1.44427300	-2.63579000
C	-1.25453100	4.16461900	0.77985100
C	1.20363700	4.28682200	-0.48953400
C	0.56315000	5.45596000	-0.11375100
C	-0.64429200	5.39744000	0.57583100
H	-2.22569600	4.13172300	1.25484600
H	2.12028800	4.35604500	-1.05640900
H	1.00826200	6.41245100	-0.36016300
H	-1.13134000	6.30343000	0.91469200
C	-4.86487700	-2.11195200	-1.17804800
C	-5.70523300	-1.29873900	-0.17947700
C	-4.96150100	-1.46358900	-2.56977300
C	-5.44104700	-3.52812000	-1.26233900
H	-5.63774300	-1.72865700	0.82337500
H	-5.37036000	-0.26124300	-0.12025800
H	-6.75527600	-1.29848500	-0.48647200
H	-4.36046000	-2.01577000	-3.29632800
H	-6.00090400	-1.46284900	-2.90984500
H	-4.61217700	-0.42901900	-2.55568900
H	-6.48313000	-3.47716600	-1.58618400
H	-4.89616900	-4.14190300	-1.98423400
H	-5.41710100	-4.02878800	-0.29098600
C	4.99193600	-1.81528200	1.13165200
C	5.72882200	-2.51319200	-0.02431200
C	5.54478600	-0.39256000	1.26028300
C	5.26159700	-2.56449300	2.44622300
H	5.39726800	-3.54686500	-0.14680700
H	5.54714600	-1.98253900	-0.96281300

H	6.80581200	-2.52181600	0.16629200
H	5.05530900	0.15677900	2.06923600
H	6.61317300	-0.43910300	1.48506700
H	5.42015000	0.17163000	0.33222300
H	6.33173200	-2.55183700	2.67054200
H	4.73036400	-2.09045600	3.27512900
H	4.94400000	-3.60781900	2.39358200
C	-0.68707900	-1.96591300	0.02553500
C	-1.34084300	-3.22143400	-0.09218800

B-1-*PP*-D_1

Energy (with Zero-point Energy correction) = -1685.991043 (-1685.304617) Hartree

Free energy (298 K) = -1685.372732 Hartree

Zero number of imaginary frequency

0 2

C	-3.39583100	-2.11227400	-0.76286900
C	-2.68022500	-3.28935400	-0.62117100
C	-1.41223400	-0.80684400	-0.13200800
C	-2.72722100	-0.87991000	-0.51435600
C	0.73393200	-2.00159700	0.08441300
C	1.48733900	-3.25453800	0.23387700
C	0.89092300	-4.51991000	0.08429600
C	2.84544400	-3.12925000	0.58066900
H	3.40561500	-4.04909000	0.70560300
C	3.46935000	-1.90842800	0.78954100
C	2.73984900	-0.71247000	0.58423400
C	1.42706400	-0.73303400	0.16993500
C	0.68909100	0.52063600	-0.08385400
C	-0.74011800	0.48961600	0.09341400
H	-1.14357600	-5.67055500	-0.34552200
H	-3.16413000	-4.24606800	-0.77310000
H	-3.29159200	0.02909300	-0.64447800
H	1.56799100	-5.36199000	0.20981700
H	3.22984600	0.22964200	0.75206100
C	-1.41137400	1.66892700	0.39137600
C	1.31049200	1.72271600	-0.41016100
C	0.57574000	2.94640900	-0.30662200
C	-0.73441900	2.92302500	0.24673000
C	-2.81046500	1.69203900	0.91232800
C	-3.83032600	2.37196800	0.23874900
C	-3.10791600	1.05790000	2.11948400
C	-5.11560600	2.42290200	0.76582500
H	-3.60795900	2.86174100	-0.70359800
C	-4.39254500	1.11240000	2.64895600

H	-2.32247900	0.52328300	2.64170100
C	-5.39866800	1.79817200	1.97696900
H	-5.89549500	2.95164800	0.23071600
H	-4.60593400	0.62001200	3.59013300
H	-6.39905200	1.84038200	2.39050600
C	2.71090600	1.78240600	-0.91944000
C	3.06371900	1.05509900	-2.05787300
C	3.68645200	2.55719700	-0.28468100
C	4.36385400	1.09379700	-2.54600000
H	2.31174000	0.44917100	-2.55066600
C	4.98668100	2.59801000	-0.77427000
H	3.42283200	3.11701000	0.60633500
C	5.32976100	1.86453300	-1.90575200
H	4.62230300	0.52325800	-3.43005600
H	5.73388000	3.19589200	-0.26590600
H	6.34335700	1.89422700	-2.28712100
C	-1.34809200	4.15970400	0.58345600
C	1.12751800	4.19922200	-0.68962000
C	0.47646300	5.37310400	-0.41659400
C	-0.75477800	5.35390100	0.26843500
H	-2.30239600	4.15572500	1.09150000
H	2.07893000	4.22306700	-1.20239500
H	0.91583700	6.31703700	-0.71545400
H	-1.24211400	6.28465800	0.53255800
C	-4.86950100	-2.06223000	-1.14319900
C	-5.65114800	-1.38905700	0.00003900
C	-5.03454300	-1.23124200	-2.42927000
C	-5.45326900	-3.45639000	-1.38592400
H	-5.54142000	-1.95521600	0.92843500
H	-5.30433700	-0.37012200	0.18310500
H	-6.71393500	-1.34465600	-0.25486900
H	-4.46511100	-1.67169400	-3.25106000
H	-6.08944100	-1.20502100	-2.71546000
H	-4.69967600	-0.20060300	-2.29386800
H	-6.50682000	-3.36457300	-1.65971900
H	-4.93698800	-3.97175000	-2.19933000
H	-5.39286300	-4.07774700	-0.48946800
C	4.94257500	-1.87721900	1.18848100
C	5.76727800	-2.49034600	0.04088600
C	5.45571400	-0.45569300	1.43929700
C	5.14627600	-2.70323300	2.47097700
H	5.48012300	-3.52500000	-0.15406800
H	5.62603000	-1.91641000	-0.87856900
H	6.82940800	-2.47233700	0.30063500

H	4.90155200	0.03785300	2.24226500
H	6.50619700	-0.50070600	1.73610800
H	5.38746600	0.16071800	0.53975100
H	6.20045200	-2.67687200	2.75972600
H	4.55389500	-2.29316700	3.29229000
H	4.85958500	-3.74676800	2.33433500
C	-0.64500800	-2.03674300	-0.10433300
C	-1.31703000	-3.30883500	-0.30199200
B	-0.54566800	-4.64491800	-0.19743100

B-2-*PP*-D_1

Energy (with Zero-point Energy correction) = -1686.008186 (-1685.320313) Hartree

Free energy (298 K) = -1685.388221 Hartree

Zero number of imaginary frequency

0 2

C	-3.40575500	-2.07274600	-0.83031800
C	-2.76741100	-3.32678300	-0.60267400
C	-1.39801300	-0.82039000	-0.15858000
C	-2.72403200	-0.88104400	-0.59955600
C	-0.46898100	-4.63455600	0.02090500
C	0.75725000	-1.98091700	0.14541600
C	1.49758100	-3.20003700	0.34641900
C	0.85973800	-4.48570000	0.27692500
C	2.86994400	-3.12385300	0.62164100
H	3.40837900	-4.05564500	0.76356000
C	3.53225500	-1.91434900	0.73348000
C	2.79823900	-0.73002100	0.50554400
C	1.45960800	-0.73480500	0.15536800
C	0.69547000	0.51686800	-0.05794700
C	-0.74131100	0.46451200	0.11275300
H	-0.86548700	-5.64708200	-0.01424800
H	-3.34417000	-4.22359000	-0.80301600
H	-3.24799000	0.04571000	-0.77327700
H	1.50706700	-5.34473100	0.44030300
H	3.30598800	0.21156900	0.62490700
C	-1.43961300	1.63259500	0.42669100
C	1.27908200	1.73422400	-0.38218500
C	0.52026000	2.94446000	-0.25891000
C	-0.78589000	2.89729800	0.30418600
C	-2.82809300	1.60305300	0.96508300
C	-3.86133000	2.34302700	0.37922900
C	-3.10411000	0.85344700	2.11110900
C	-5.13397400	2.34554800	0.93676000
H	-3.66114500	2.91237200	-0.52210200

C	-4.37605700	0.86002100	2.67064500
H	-2.31031600	0.26912800	2.56252700
C	-5.39284000	1.61011700	2.08977400
H	-5.92483400	2.91893200	0.46788800
H	-4.57184000	0.27808100	3.56318700
H	-6.38420500	1.61454200	2.52654700
C	2.67517200	1.83964800	-0.89938100
C	3.02863000	1.17482900	-2.07466100
C	3.64245300	2.60385000	-0.23972600
C	4.32091500	1.26826800	-2.57793600
H	2.28327700	0.57545900	-2.58518000
C	4.93398500	2.70013000	-0.74422700
H	3.37718900	3.11615000	0.67907200
C	5.27695700	2.03231700	-1.91587400
H	4.58001200	0.74685500	-3.49168700
H	5.67438600	3.29089000	-0.21789300
H	6.28366000	2.10568600	-2.30947600
C	-1.40847100	4.12051600	0.67830600
C	1.04978400	4.21047700	-0.62535700
C	0.38480200	5.37078700	-0.32578700
C	-0.83604000	5.32731700	0.37707800
H	-2.35018000	4.09371400	1.20820200
H	1.99717600	4.25752200	-1.14395600
H	0.80965800	6.32488200	-0.61383700
H	-1.32784200	6.24754600	0.66779300
C	-4.86168600	-1.97097200	-1.30235500
C	-5.68316300	-1.26016000	-0.21159600
C	-4.92907800	-1.15237500	-2.60425500
C	-5.49489400	-3.34030600	-1.56872900
H	-5.63572600	-1.81425900	0.72961400
H	-5.31083400	-0.25187600	-0.02515100
H	-6.73091400	-1.18849500	-0.51927000
H	-4.32450500	-1.61934800	-3.38556800
H	-5.96398500	-1.09934400	-2.95415400
H	-4.56993100	-0.13176500	-2.46141900
H	-6.52342900	-3.20088800	-1.91030300
H	-4.95463200	-3.89004300	-2.34328800
H	-5.52347400	-3.95358700	-0.66516900
C	5.02493500	-1.88712100	1.06832100
C	5.79773800	-2.60280100	-0.05351700
C	5.56915100	-0.45987200	1.18552700
C	5.26682400	-2.61232200	2.40272400
H	5.48199800	-3.64268500	-0.15885400
H	5.63524900	-2.09946700	-1.00999600

H	6.86938400	-2.59357300	0.16496100
H	5.06584100	0.10116100	1.97792500
H	6.63391100	-0.49830900	1.42826900
H	5.45729700	0.09115400	0.24835200
H	6.33208700	-2.59547200	2.64938400
H	4.71770900	-2.12414000	3.21142900
H	4.94782100	-3.65543500	2.35942200
B	-1.32973400	-3.38097700	-0.18768900
C	-0.63235800	-2.03997200	-0.05149100

B-3-*PP*-D_1

Energy (with Zero-point Energy correction) = -1686.008179 (-1685.318902) Hartree

Free energy (298 K) = -1685.386399 Hartree

Zero number of imaginary frequency

0 2

C	-3.49484600	-2.10248200	-0.66157800
C	-2.76144900	-3.29667100	-0.57208000
C	-1.36304600	-3.31014300	-0.35542100
C	-1.45788800	-0.73100500	-0.16630000
C	-2.85066400	-0.87514000	-0.47907600
C	-0.58606100	-4.48286500	-0.22757500
C	0.81560900	-1.96656100	0.01905100
C	1.50246400	-3.19839500	0.17031200
C	0.78191500	-4.42352100	0.02038300
C	2.87798100	-3.17430300	0.48511400
H	3.40989800	-4.11621700	0.58218900
C	3.53487200	-1.97439400	0.70671500
C	2.82205900	-0.76833700	0.54685400
C	1.48231300	-0.73835800	0.14307300
C	0.70837800	0.52625700	-0.04750800
C	-0.75542100	0.51739300	0.06923600
H	-1.05165500	-5.46465900	-0.30128100
H	-3.27949300	-4.24364600	-0.70645300
H	-3.45148100	0.01074500	-0.64630400
H	1.33758600	-5.35092700	0.11772300
H	3.33221800	0.15441700	0.76874800
C	-1.41253400	1.73260500	0.34457000
C	1.33042500	1.73034800	-0.35648900
C	0.60579800	2.96493000	-0.29774800
C	-0.72717100	2.96959900	0.20418100
C	-2.81692500	1.75265500	0.83591400
C	-3.82225000	2.46634800	0.17293600
C	-3.14061800	1.07665100	2.01605700

C	-5.11217900	2.51607900	0.68701200
H	-3.58372000	2.97906000	-0.75271700
C	-4.42846700	1.13691700	2.53641000
H	-2.36866900	0.51198200	2.52642900
C	-5.41595700	1.86095600	1.87765100
H	-5.88059900	3.06815100	0.15887700
H	-4.65992300	0.61608500	3.45782300
H	-6.42024900	1.90497800	2.28166800
C	2.75262400	1.79798300	-0.80909600
C	3.14498600	1.12180100	-1.96541400
C	3.70520500	2.54538700	-0.11026500
C	4.46047200	1.18547800	-2.41030000
H	2.41085000	0.53525000	-2.50629000
C	5.01988400	2.61311000	-0.55647100
H	3.40847500	3.06934200	0.79220900
C	5.40180000	1.93213900	-1.70851200
H	4.74935600	0.65435400	-3.30950600
H	5.74788100	3.19174900	-0.00006900
H	6.42668000	1.98261200	-2.05629900
C	-1.33388600	4.22383800	0.50757400
C	1.18566600	4.20569000	-0.67787900
C	0.53949000	5.39181000	-0.45002700
C	-0.71614500	5.40293700	0.19432600
H	-2.29963000	4.23951100	0.99338000
H	2.15718400	4.21174300	-1.15223900
H	1.00286100	6.32443800	-0.74874200
H	-1.19580700	6.34512200	0.43045600
C	-4.99300500	-2.08956800	-1.00645900
C	-5.77048100	-1.35827600	0.09935100
C	-5.20834800	-1.35681500	-2.34218400
C	-5.57115300	-3.50222200	-1.14173700
H	-5.62666500	-1.85188600	1.06422100
H	-5.44078800	-0.32277000	0.20200200
H	-6.84038700	-1.35006100	-0.13028200
H	-4.65585600	-1.84937800	-3.14603900
H	-6.27054600	-1.35278000	-2.60393900
H	-4.87446300	-0.31799800	-2.28844800
H	-6.63818100	-3.43514700	-1.36659500
H	-5.09574800	-4.05987800	-1.95286800
H	-5.46121600	-4.07246100	-0.21544000
C	5.01898700	-1.98569500	1.09376000
C	5.82743300	-2.57664300	-0.07384000
C	5.55707300	-0.58045000	1.38093400
C	5.22506100	-2.84657800	2.35075200

H	5.51290100	-3.59736000	-0.30246100
H	5.69392600	-1.97027800	-0.97356300
H	6.89222800	-2.59672300	0.17589000
H	5.02146800	-0.10407200	2.20687100
H	6.61133100	-0.64805000	1.66067400
H	5.48334400	0.06535200	0.50273200
H	6.28160700	-2.85005500	2.63299600
H	4.64593300	-2.44967700	3.18805400
H	4.91898900	-3.88199400	2.18939700
B	-0.66433000	-1.99476100	-0.21001000

B-4-*PP*-D_1

Energy (with Zero-point Energy correction) = -1686.014390 (-1685.326450) Hartree

Free energy (298 K) = -1685.394516 Hartree

Zero number of imaginary frequency

0 2

C	-3.62214800	-2.08365200	-0.49580100
C	-2.83536700	-3.21692000	-0.60462000
C	-3.03400700	-0.80573000	-0.18964200
C	0.64127900	-1.93298800	0.00563600
C	1.35900900	-3.16664300	0.02393400
C	0.64636900	-4.38619600	-0.27131000
C	2.70004200	-3.19567800	0.35073900
H	3.21056300	-4.15380700	0.35967600
C	3.39242800	-2.02231100	0.72468200
C	2.71026400	-0.82524800	0.64450400
C	1.36533300	-0.72361800	0.20399500
C	0.72183700	0.59038600	0.03148000
C	-0.71315200	0.67870400	0.19615700
H	-1.20708500	-5.31736200	-0.71669400
H	-3.28999900	-4.18009700	-0.81063100
H	-3.72939200	0.01861300	-0.14316100
H	1.21370000	-5.31098800	-0.30203300
H	3.21261000	0.07977400	0.94496300
C	1.47032700	1.73445300	-0.28611700
C	0.85364900	3.01828400	-0.23581300
C	-0.49375800	3.12487400	0.21339200
C	-2.71275900	2.08943400	0.70248000
C	-3.60610000	2.64241900	-0.21784600
C	-3.19513900	1.65718600	1.93754900
C	-4.95959500	2.74179100	0.08376100
H	-3.23314500	2.97702700	-1.17996700

C	-4.54722600	1.76536500	2.24491700
H	-2.50285000	1.22094300	2.64856100
C	-5.43311600	2.30353700	1.31717100
H	-5.64544700	3.15925100	-0.64414300
H	-4.90983200	1.42425500	3.20750800
H	-6.48816400	2.37967700	1.55252400
C	2.87603200	1.65428100	-0.77949500
C	3.17308200	0.88558600	-1.90754300
C	3.91576300	2.34334300	-0.14571400
C	4.47564700	0.79972100	-2.38453600
H	2.37220000	0.34866000	-2.40365400
C	5.21738100	2.26340800	-0.62573100
H	3.69678400	2.93530800	0.73664000
C	5.50262500	1.48776200	-1.74572900
H	4.68783100	0.19841400	-3.26073200
H	6.01130300	2.79889400	-0.11826100
H	6.51762500	1.42253700	-2.11910900
C	1.52997600	4.21446900	-0.62024100
C	0.95163300	5.44151200	-0.45195800
H	-2.04567800	4.50319700	0.82930600
H	2.51560100	4.14935900	-1.05917000
H	1.48645100	6.33547500	-0.74966000
H	-0.77726600	6.52604600	0.27877600
C	-5.13552000	-2.23506400	-0.69885500
C	-5.89661600	-0.91351400	-0.54819800
C	-5.40180900	-2.78384300	-2.11273900
C	-5.68868000	-3.22248100	0.34584600
H	-5.76925900	-0.48501500	0.44856000
H	-5.56917100	-0.16991600	-1.27919100
H	-6.96294700	-1.09432300	-0.70628000
H	-4.94205600	-3.76222500	-2.26032100
H	-6.47900400	-2.88471300	-2.27370500
H	-5.00241000	-2.10440500	-2.86954400
H	-6.77058400	-3.32452300	0.22156700
H	-5.24008000	-4.21196900	0.24624300
H	-5.49047900	-2.86041200	1.35757000
C	4.84878000	-2.12375800	1.17269200
C	5.69198600	-2.62859600	-0.01144100
C	5.40863900	-0.77125700	1.61961500
C	4.96235800	-3.11095100	2.34672100
H	5.35675500	-3.60902700	-0.35784300
H	5.62701200	-1.92896000	-0.84883200
H	6.74047800	-2.71677500	0.28666800
H	4.84192700	-0.36046100	2.45966700

H	6.44462900	-0.89715700	1.94328200
H	5.39661700	-0.04566700	0.80321500
H	6.00312200	-3.18062000	2.67419500
H	4.35707000	-2.77524100	3.19214500
H	4.63247500	-4.11474200	2.07127300
C	-1.26802100	1.93997900	0.37081600
C	-1.04616700	4.42034800	0.42307500
C	-0.34006400	5.54885000	0.11184100
C	-0.68880900	-4.38964700	-0.49987200
C	-1.45117400	-3.17847600	-0.43458000
C	-0.76423300	-1.92352000	-0.16718300
B	-1.55115600	-0.64452600	0.00487300

B-5-*PP*-D_1

Energy (with Zero-point Energy correction) = -1686.029623 (-1685.338947) Hartree

Free energy (298 K) = -1685.407123 Hartree

Zero number of imaginary frequency

0 2

C	-3.54724300	-2.16959700	-0.59896200
C	-2.77576700	-3.31444000	-0.57695900
C	-1.53820900	-0.81212300	-0.15782500
C	-2.90090300	-0.93435900	-0.37851700
C	-0.61166300	-4.45871700	-0.29966600
C	0.65946500	-1.95096000	0.06668200
C	1.38222500	-3.16416000	0.17253300
C	0.71463000	-4.41623300	-0.03477200
C	2.74732400	-3.14954300	0.49831100
H	3.25779200	-4.10509400	0.56952600
C	3.43752300	-1.96669700	0.76959800
C	2.74536600	-0.77774500	0.61155500
C	1.38943900	-0.70967700	0.18228300
C	0.73376400	0.53051000	-0.09708900
H	-1.11536400	-5.40678500	-0.45517800
H	-3.22096100	-4.29124500	-0.72493100
H	-3.50423800	-0.03530200	-0.39245500
H	1.29952900	-5.32714700	0.02947400
H	3.24587300	0.14944800	0.83731700
C	-1.38142100	1.88808100	0.31754300
C	1.45845300	1.77141100	-0.34993200
C	0.80640900	2.99768600	-0.21969900
C	-0.57542600	3.04827700	0.23838400
C	-2.80286700	2.03641000	0.73817400
C	-3.74369400	2.63856400	-0.10598900

C	-3.24534700	1.51709200	1.95779100
C	-5.08525300	2.70956300	0.25376800
H	-3.41283800	3.03682700	-1.05964200
C	-4.58497800	1.59593900	2.32425700
H	-2.52638300	1.03818400	2.61293400
C	-5.51106500	2.18963400	1.47277000
H	-5.79913800	3.17080300	-0.41908600
H	-4.90756300	1.18486700	3.27400500
H	-6.55613300	2.24321500	1.75391300
C	2.84999200	1.72281500	-0.86511400
C	3.15963600	0.89131200	-1.94834800
C	3.88050400	2.46837700	-0.27617100
C	4.45587900	0.82553100	-2.44246700
H	2.37204700	0.30019600	-2.40127500
C	5.17802400	2.39409700	-0.76576700
H	3.65828500	3.08727200	0.58572800
C	5.46935300	1.57573700	-1.85347800
H	4.67525300	0.18564100	-3.28878500
H	5.96478800	2.96779100	-0.29037100
H	6.48151200	1.51884100	-2.23570300
C	-1.09835200	4.34096800	0.55574500
C	1.44555800	4.23900500	-0.58454900
C	0.87096800	5.44282400	-0.33625500
C	-0.40458600	5.48594100	0.29346500
H	-2.08483400	4.40255700	0.99639500
H	2.40415200	4.20442500	-1.08294200
H	1.37093600	6.36117600	-0.61650900
H	-0.84446200	6.44557500	0.54212500
C	-5.05807200	-2.18235600	-0.83073200
C	-5.75825000	-1.61134000	0.41423600
C	-5.39494100	-1.30468800	-2.04858700
C	-5.59162800	-3.59426600	-1.08847500
H	-5.52924500	-2.21617100	1.29553400
H	-5.44365700	-0.58531900	0.61611600
H	-6.84237500	-1.61169500	0.26666400
H	-4.88830900	-1.67410400	-2.94369400
H	-6.47326800	-1.31994100	-2.23072100
H	-5.09606800	-0.26640200	-1.89036800
H	-6.67021200	-3.55056600	-1.25701000
H	-5.13136600	-4.04182200	-1.97338700
H	-5.41451000	-4.25225400	-0.23381000
C	4.90738600	-2.02228800	1.18893500
C	5.72751500	-2.61069700	0.02832000
C	5.46307900	-0.63299900	1.51308900

C	5.05899400	-2.91178400	2.43351700
H	5.39547600	-3.61906200	-0.22952200
H	5.63202300	-1.98209500	-0.86099700
H	6.78452200	-2.66333600	0.30381800
H	4.91366400	-0.16121500	2.33243900
H	6.50825600	-0.72319000	1.81857300
H	5.42289700	0.02625400	0.64261300
H	6.10795900	-2.94986100	2.73947700
H	4.47185200	-2.51463900	3.26500400
H	4.72943700	-3.93571200	2.24542300
C	-0.75551800	-2.00078900	-0.16302700
C	-1.38664700	-3.25695900	-0.35483000
B	-0.79465000	0.55314800	-0.01263200

B-6-*PP*-D_1

Energy (with Zero-point Energy correction) = -1686.023293 (-1685.335437) Hartree

Free energy (298 K) = -1685.403208 Hartree

Zero number of imaginary frequency

0 2

C	-3.41940100	-2.13139600	-0.74845200
C	-2.66604300	-3.28602200	-0.72600200
C	-1.40337200	-0.79479500	-0.22479900
C	-2.77066100	-0.90312700	-0.50491400
C	0.75065200	-1.94117300	0.02141800
C	1.48786400	-3.13899700	0.14098700
C	0.83434600	-4.38633000	-0.10358600
C	2.84380400	-3.08283400	0.51203700
H	3.38603900	-4.02026800	0.59162100
C	3.47675300	-1.88365200	0.81120800
C	2.74176000	-0.70690500	0.64397400
C	1.41267300	-0.69369100	0.17917400
C	0.68969300	0.53864300	-0.10664400
C	-0.76163400	0.47812600	0.02072900
H	-0.98246100	-5.38080600	-0.58417200
H	-3.11691900	-4.25596200	-0.89605100
H	-3.35172600	0.00475700	-0.56417100
H	1.41637000	-5.29883500	-0.03513300
H	3.20089200	0.23481100	0.89607700
C	1.36486500	1.74696700	-0.41826100
C	0.65695900	2.97998000	-0.36174500
C	-0.68113100	3.04003000	0.16939500
C	-2.96521500	1.79914500	0.94443400
C	-3.99545000	2.50347200	0.30254000

C	-3.29667700	1.11900700	2.12606800
C	-5.28931000	2.53463400	0.81645100
H	-3.77984900	3.03464100	-0.62009700
C	-4.58158500	1.16123400	2.65706200
H	-2.52788700	0.54930200	2.63901600
C	-5.58437300	1.87039200	2.00280700
H	-6.06512500	3.08372600	0.29467400
H	-4.80334700	0.63544700	3.57896700
H	-6.58816000	1.89986600	2.41040900
C	2.78767800	1.74604200	-0.84732000
C	3.21376700	0.92593900	-1.90027700
C	3.74187900	2.56151200	-0.22151300
C	4.54221800	0.91576400	-2.30819300
H	2.48748400	0.29344800	-2.39871800
C	5.06792400	2.56090000	-0.63525500
H	3.43076700	3.19320500	0.60352600
C	5.47546200	1.73459300	-1.67928000
H	4.84709800	0.27516200	-3.12761100
H	5.78752300	3.19760900	-0.13371400
H	6.51020600	1.73060000	-2.00052500
C	-1.26870200	4.31936700	0.34768700
C	1.25194700	4.19879800	-0.82691800
C	0.62345300	5.40108300	-0.66996500
C	-0.64018900	5.47625700	-0.03578800
H	-2.25077700	4.37226000	0.80354400
H	2.20810300	4.16563000	-1.33116200
H	1.09508700	6.30505400	-1.03832400
H	-1.11118000	6.43941500	0.12101800
C	-4.92268400	-2.11180000	-1.02564300
C	-5.64195500	-1.44768000	0.16070500
C	-5.19037300	-1.29600700	-2.30210300
C	-5.48853600	-3.52096700	-1.21957900
H	-5.45156300	-1.99756100	1.08613900
H	-5.31385300	-0.41667600	0.31063300
H	-6.72100900	-1.43440100	-0.01794300
H	-4.67016300	-1.73259300	-3.15830300
H	-6.26236600	-1.28495800	-2.51769100
H	-4.86044400	-0.26070400	-2.19266900
H	-6.56380200	-3.45871200	-1.40145700
H	-5.03364000	-4.02318500	-2.07750200
H	-5.33498000	-4.13942700	-0.33134900
C	4.93864500	-1.87982100	1.26458500
C	5.81018200	-2.39362500	0.10602400
C	5.41716100	-0.47426600	1.63930500

C	5.10843300	-2.79575900	2.48729100
H	5.53308200	-3.40945300	-0.18590300
H	5.70243700	-1.74478500	-0.76714800
H	6.86243200	-2.40242000	0.40327500
H	4.82502700	-0.05165700	2.45581900
H	6.45684500	-0.52399900	1.97114700
H	5.37005900	0.20671600	0.78606500
H	6.15046000	-2.78587600	2.81746400
H	4.48227800	-2.45494500	3.31531000
H	4.84116800	-3.83067300	2.26344100
C	-0.64251800	-1.99481200	-0.25788000
C	-1.27091000	-3.23617500	-0.47752900
B	-1.48108900	1.75918000	0.39439400
C	-0.49050800	-4.43032600	-0.40898000

B-7-*PP*-D_1

Energy (with Zero-point Energy correction) = -1685.987597 (-1685.300987) Hartree

Free energy (298 K) = -1685.368023 Hartree

Zero number of imaginary frequency

0 2

C	-3.46282000	-1.98475500	-0.81935300
C	-2.76677100	-3.16772500	-0.68120000
C	-2.76823000	-0.78099600	-0.58937800
C	-0.65896700	-4.38701700	-0.24911400
C	0.69095600	-1.93812800	0.09405300
C	1.38368900	-3.16297200	0.23656700
C	0.67245600	-4.38353500	0.05351500
C	2.75949600	-3.15840500	0.54271100
H	3.26712900	-4.11283100	0.63579800
C	3.44069300	-1.96894800	0.75521200
C	2.73930000	-0.77037300	0.58786600
C	1.39041700	-0.70889600	0.17390800
C	0.69346500	0.55056300	-0.06737600
H	-1.18685900	-5.32398700	-0.38963900
H	-3.25270100	-4.12429000	-0.83144600
H	-3.28689800	0.15063700	-0.76307500
H	1.21410800	-5.31801500	0.15179300
H	3.24211700	0.15543300	0.81148000
C	-1.46740900	1.70781800	0.38568600
C	1.37026600	1.75975600	-0.35982200
C	0.67995600	2.99254200	-0.30281500
C	-2.80750000	1.65872200	0.98013800
C	-3.84065900	2.51409600	0.55025300

C	-3.08560000	0.78565400	2.05384600
C	-5.08564800	2.49447100	1.15975200
H	-3.64817600	3.18564600	-0.27827300
C	-4.32852300	0.77667100	2.66919100
H	-2.29629100	0.13225600	2.40808600
C	-5.33487500	1.63109200	2.22751200
H	-5.86750500	3.15669000	0.80639600
H	-4.51157500	0.10705400	3.50140200
H	-6.30492500	1.62792400	2.71008500
C	2.79189900	1.75416900	-0.81051500
C	3.18424000	0.98310200	-1.91052500
C	3.75400000	2.54998900	-0.17725100
C	4.49855500	1.00372700	-2.36070400
H	2.44374300	0.36845300	-2.41021100
C	5.06849400	2.57358800	-0.62900200
H	3.45852200	3.14812700	0.67787300
C	5.44598600	1.79948100	-1.72211900
H	4.78237400	0.40464400	-3.21814200
H	5.79979000	3.19362300	-0.12372100
H	6.47022800	1.81717500	-2.07519300
C	-1.33800100	4.45750700	0.46174400
C	1.25094900	4.21078300	-0.77312400
C	0.62854600	5.43536600	-0.59580900
C	-0.62622300	5.56175700	0.04465600
H	-2.28589700	4.64028100	0.96114600
H	2.18825100	4.19302800	-1.32193600
H	1.12649400	6.32938100	-0.95487900
H	-1.01719400	6.56389500	0.19903300
C	-4.93606600	-1.91506000	-1.22165500
C	-5.71581600	-1.14449400	-0.14368800
C	-5.05685000	-1.17667000	-2.56551900
C	-5.55388700	-3.30765000	-1.37352600
H	-5.63043200	-1.64096000	0.82647400
H	-5.34652900	-0.12307600	-0.02718700
H	-6.77426900	-1.09165100	-0.41404200
H	-4.49884200	-1.69916800	-3.34631100
H	-6.10636200	-1.12299000	-2.86751900
H	-4.67502800	-0.15565400	-2.49974200
H	-6.60743100	-3.20944600	-1.64442600
H	-5.06032700	-3.88430600	-2.16017900
H	-5.50032400	-3.87343100	-0.43964300
C	4.92352300	-1.99515000	1.13658100
C	5.71696200	-2.59212400	-0.03829700
C	5.47057200	-0.59320000	1.42064400

C	5.12549400	-2.86108500	2.39037600
H	5.39046600	-3.60916100	-0.26781200
H	5.58588700	-1.98054400	-0.93477900
H	6.78243900	-2.62465600	0.20595200
H	4.94316100	-0.11485000	2.25056700
H	6.52618300	-0.66644300	1.69311000
H	5.39468400	0.05339700	0.54304500
H	6.18283900	-2.87344200	2.66822900
H	4.55355400	-2.46150500	3.23128500
H	4.81187700	-3.89430700	2.22769800
C	-0.70801400	-1.94668100	-0.16726800
C	-1.38561500	-3.16982000	-0.37307000
C	-1.42697700	-0.73029600	-0.18989300
C	-0.74546400	0.53910200	0.09468600
B	-0.75725800	3.06024200	0.21429200

B-8-*PP*-D_1

Energy (with Zero-point Energy correction) = -1685.989435 (-1685.303970) Hartree

Free energy (298 K) = -1685.371525 Hartree

Zero number of imaginary frequency

0 2

C	-3.44191100	-2.00953800	-0.81575600
C	-2.71973000	-3.18181900	-0.71546900
C	-1.42704100	-0.73340300	-0.19002000
C	-2.77630200	-0.80001600	-0.54932900
C	0.72233000	-1.93420900	0.08052900
C	1.41891700	-3.15353700	0.22246600
C	0.71820800	-4.38586900	0.01684600
C	2.78629000	-3.13502800	0.55272900
H	3.29935600	-4.08693300	0.64741100
C	3.46496400	-1.94860300	0.77210500
C	2.76196000	-0.74846800	0.58650600
C	1.42517400	-0.71161000	0.18907500
C	0.71251800	0.54901000	-0.06350700
C	-0.75295800	0.52447700	0.09360000
H	-1.12303000	-5.32711400	-0.46878000
H	-3.19025300	-4.14294900	-0.88443000
H	-3.33323600	0.11949300	-0.64289700
H	1.26848300	-5.31527400	0.11349900
H	3.27151300	0.18392100	0.76471500
C	1.32271700	1.73222700	-0.42085600
C	0.55772000	2.95319700	-0.39242000
C	-0.73990000	2.96292000	0.30523000
C	-2.77857200	1.70266300	1.01435200

C	-3.81300200	2.44694800	0.44235200
C	-3.04529400	0.94688700	2.15755800
C	-5.08335800	2.44145900	1.00593200
H	-3.60985300	3.03902900	-0.44265900
C	-4.31255400	0.94995100	2.72876300
H	-2.24648200	0.36511600	2.60426500
C	-5.33505300	1.69856200	2.15547600
H	-5.87457500	3.02684000	0.55271300
H	-4.49966200	0.37057300	3.62509400
H	-6.32316100	1.70138500	2.60006400
C	2.74530900	1.80094900	-0.86519900
C	3.17162500	1.06460100	-1.97153600
C	3.67012200	2.60498600	-0.19268400
C	4.49724100	1.11687300	-2.38818900
H	2.45651500	0.44276700	-2.49860700
C	4.99474500	2.65908500	-0.60932600
H	3.34045600	3.18905100	0.65960400
C	5.41301200	1.91308700	-1.70776100
H	4.81289300	0.54100800	-3.25017200
H	5.70149600	3.28297600	-0.07501300
H	6.44547100	1.95588800	-2.03353700
C	1.07438800	4.14034200	-0.94203200
C	0.46378500	5.35118100	-0.70876500
C	-0.67784100	5.51028000	0.13315600
H	-2.29660400	4.38769300	1.43476800
H	1.98630100	4.10372600	-1.52194300
H	0.91250600	6.23203600	-1.16361000
H	-1.03679700	6.52563600	0.26942700
C	-4.92534100	-1.96375700	-1.18317000
C	-5.70450100	-1.31323800	-0.02813100
C	-5.10770000	-1.12306600	-2.45818900
C	-5.49613900	-3.36154800	-1.43676800
H	-5.58036300	-1.88650300	0.89431800
H	-5.36503200	-0.29333900	0.16437000
H	-6.77026000	-1.27452900	-0.27099300
H	-4.54425700	-1.55211700	-3.29039400
H	-6.16483700	-1.09371700	-2.73559300
H	-4.77260600	-0.09367800	-2.31390000
H	-6.55385300	-3.27938300	-1.69643300
H	-4.98646000	-3.86074800	-2.26513900
H	-5.42002800	-3.99343000	-0.54806900
C	4.94635800	-1.96920300	1.15857500
C	5.74775100	-2.58190400	-0.00264800
C	5.49102700	-0.56281600	1.42718100

C	5.14059400	-2.81798600	2.42530500
H	5.42660100	-3.60371400	-0.21736400
H	5.61934700	-1.98594300	-0.90992400
H	6.81199800	-2.60652600	0.24746400
H	4.95592700	-0.07245500	2.24506800
H	6.54385700	-0.63215900	1.71075200
H	5.42429400	0.07194600	0.53985300
H	6.19685900	-2.83126600	2.70701700
H	4.56743000	-2.40464200	3.25864200
H	4.82226000	-3.85164500	2.27507200
C	-0.68321800	-1.94643900	-0.18619700
C	-1.33967300	-3.16997800	-0.40713800
C	-0.59960600	-4.39208000	-0.30236600
C	-1.39785800	1.72232400	0.44760200
B	-1.34148600	4.31232600	0.72961000

B-9-*PP*-D_1

Energy (with Zero-point Energy correction) = -1685.995097 (-1685.308848) Hartree

Free energy (298 K) = -1685.376240 Hartree

Zero number of imaginary frequency

0 2

C	-3.38195600	-2.03177600	-0.82055000
C	-2.65309500	-3.19877500	-0.67308300
C	-1.39777600	-0.74002400	-0.16029300
C	-2.73444500	-0.81713900	-0.55107800
C	0.76827500	-1.91775200	0.13352000
C	1.47398100	-3.13145800	0.29734400
C	0.77383500	-4.37387100	0.12371500
C	2.84078200	-3.09874000	0.60614000
H	3.36281700	-4.04355100	0.71801900
C	3.51151400	-1.89833000	0.78090600
C	2.79910200	-0.70705500	0.58079400
C	1.45812900	-0.68834100	0.20584900
C	0.71679500	0.56317500	-0.04492300
C	-0.73551200	0.53897700	0.11847400
H	-1.05808300	-5.33527700	-0.34838300
H	-3.11598100	-4.16529500	-0.83381800
H	-3.29610600	0.09624600	-0.66939300
H	1.32932200	-5.29764400	0.24273200
H	3.30776300	0.23120000	0.72889800
C	1.29168000	1.75698000	-0.41144200
C	0.51950000	2.98331900	-0.34106400
C	-0.77965100	2.98145200	0.35794700

C	-2.81486200	1.66620000	1.00081200
C	-3.84764200	2.39431900	0.40116400
C	-3.09712100	0.91385200	2.14263800
C	-5.13006000	2.37222900	0.93520800
H	-3.63208400	2.98895000	-0.47935400
C	-4.37862000	0.89853200	2.68197900
H	-2.30094700	0.34663200	2.61199100
C	-5.39788400	1.62939800	2.08189300
H	-5.91923900	2.94274300	0.46004700
H	-4.57836200	0.31880300	3.57525900
H	-6.39613600	1.61929500	2.50288900
C	2.69352700	1.84135000	-0.90682300
C	3.08522600	1.08389600	-2.01231600
C	3.63538200	2.66333800	-0.28054400
C	4.39345700	1.13895400	-2.47693100
H	2.35673500	0.44423000	-2.49756900
C	4.94522800	2.71418400	-0.74263000
H	3.33593400	3.25360400	0.57849200
C	5.32784900	1.95211000	-1.84221000
H	4.68291200	0.54901400	-3.33841800
H	5.66739300	3.34809500	-0.24203300
H	6.34821700	1.99347700	-2.20412900
C	1.00373500	4.17162900	-0.85863700
C	0.37006500	5.40836000	-0.59791400
H	-2.28347700	4.08938700	1.35128200
H	1.90917900	4.14765400	-1.45377400
H	0.83950300	6.27661000	-1.05681800
H	-1.34107000	6.55177600	0.60663200
C	-4.85326300	-2.00706200	-1.23690100
C	-5.67781200	-1.35369700	-0.11579000
C	-5.00302700	-1.18220100	-2.52630700
C	-5.40049000	-3.41371700	-1.49410200
H	-5.57738000	-1.91506800	0.81682300
H	-5.35524800	-0.32825100	0.07535100
H	-6.73553100	-1.32950000	-0.39335900
H	-4.40854700	-1.61421000	-3.33502300
H	-6.05079800	-1.16653600	-2.83821700
H	-4.68271700	-0.14795200	-2.38266500
H	-6.44891400	-3.34534800	-1.79258100
H	-4.85611700	-3.91735400	-2.29729300
H	-5.35074800	-4.03459500	-0.59586000
C	4.99875900	-1.89880700	1.14616600
C	5.78738500	-2.55450900	-0.00031500
C	5.54530000	-0.48252100	1.35294700

C	5.21319100	-2.69715100	2.44222100
H	5.46797000	-3.58514100	-0.16937600
H	5.64342300	-1.99666200	-0.92925300
H	6.85522300	-2.56444300	0.23563600
H	5.02457900	0.03642100	2.16233000
H	6.60363600	-0.53949100	1.61865300
H	5.45923200	0.11929300	0.44443700
H	6.27325200	-2.69742100	2.71028900
H	4.64961500	-2.25296300	3.26619400
H	4.89426400	-3.73592100	2.33579500
C	-0.63976700	-1.94231300	-0.12714500
C	-1.28763900	-3.17601500	-0.33595600
C	-0.53910900	-4.39488600	-0.19890200
C	-1.42130400	1.70869900	0.47062100
B	-0.85077700	5.50222600	0.32029200
C	-1.37659300	4.18319900	0.76453400