Supporting Information

Skeletal Rearrangement of Twisted Polycyclic Aromatic Hydrocarbons under Scholl Reaction Conditions

Shunpei Nobusue, Kazuya Fujita, and Yoshito Tobe*,†

Division of Frontier Materials Science, Graduate School of Engineering Science, Osaka University, 1-3 Machikaneyama, Toyonaka, Osaka 560-8531, Japan

† Present address: The Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki, 567-0047, Japan

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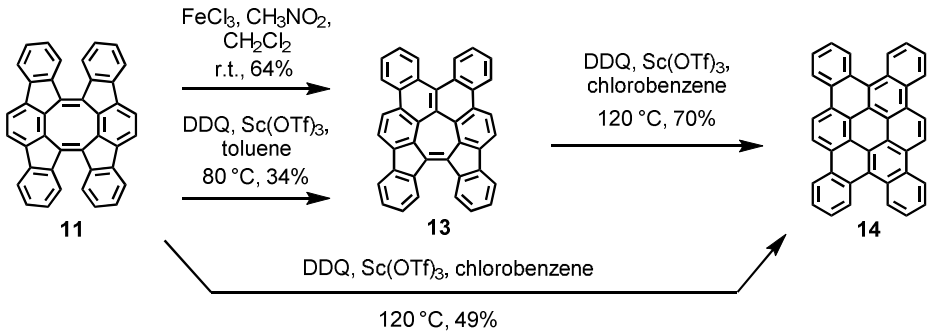
1. General Experimental Methods

^{1}H and ^{13}C NMR spectra were recorded at 30 °C. The chemical shifts were referenced to the residual solvent protons in the ^{1}H NMR (7.26 ppm) and to solvent carbons in the ^{13}C NMR (77.0 ppm). Mass spectral analyses were performed with EI, FAB mode. IR spectra were recorded as a KBr disk. Melting points were measured with a hot-stage apparatus equipped with a thermometer. Column chromatography and TLC were performed with silica gel (70-230 mesh) and precoated silica gel plates, respectively.

All reagents and solvents were obtained from commercial suppliers and used as received without purifications. THF and CH_2Cl_2 were dried with a glasscontour solvent purification system.

DFT calculations were performed with the Gaussian 09 program.[1] All geometry optimizations were carried out at the (R)B3LYP level of density functional theory with the 6-31G(d) basis set. The nature of the stationary points was assessed by means of vibrational frequency analysis. The transition states of the reaction paths were confirmed by intrinsic reaction coordinate (IRC) calculations. In the implicit solvent model by using B3LYP/6-31G(d) method, the CPCM polarizable conductor calculation model was used to the polarizable continuum model (PCM) in the self-consistent reaction field (SCRF) procedure.[2]

2. Synthetic Procedures



Reaction of 11 with $FeCl_3$ in CH_3NO_2 and CH_2Cl_2. A solution of $FeCl_3$ (35.1 mg, 0.216 mmol) in nitromethane (1.2 mL) was added to a solution of **11** (10.3 mg, 20.6 μmol) in CH_2Cl_2 (8 mL). After stirring at room temperature for 1 h under an argon atmosphere, MeOH (4 mL) was added, and the reaction mixture was diluted with water and extracted with $CHCl_3$. The extract was washed with brine and dried over anhydrous $MgSO_4$. After removal of the solvent under reduced pressure, the residue was purified by chromatography (hexanes:$CHCl_3$ = 1:1) followed by recrystallization from hexanes/$CHCl_3$ to afford **13** (8.8 mg, 85%) as a purple solid.

13: mp 211.0–212.0 °C; ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.53 (d, J = 8.4 Hz, 2H), 8.47 (d, J = 7.2 Hz, 2H), 8.45 (d, J = 7.6 Hz, 2H), 8.32 (d, J = 7.6 Hz, 2H), 7.91 (d, J = 8.4 Hz, 2H), 7.81 (d, J = 7.2 Hz, 2H), 7.59 (dd, J = 7.2, 7.2 Hz, 2H), 7.48 (dd, J = 7.2, 7.2 Hz, 2H), 7.42 (dd, J = 7.6, 7.2 Hz, 2H), 7.23 (dd, J = 7.6, 7.2 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ = 141.5, 140.9, 137.1, 137.0, 135.7, 131.3, 130.63, 130.57, 129.9, 129.2, 128.3, 126.81, 126.79, 126.7, 125.60, 125.58, 125.3, 124.1, 123.5, 119.3, 118.6; IR (KBr): 3068, 3011, 2978, 1499, 1470, 1387, 899, 823, 765 cm^{-1}; UV-vis (CH_2Cl_2): λ_{max} (log ε) 560 (3.49), 385 (4.22); MS (FAB): m/z 500.9 [M^+]; HRMS (FAB): m/z calcd for $C_{40}H_{20}$: 500.1565 [M^+]; found: 500.1553. The absorption spectra of **13** in cyclohexane and THF were nearly identical with that in CH_2Cl_2.

Reaction of 11 with DDQ and $Sc(OTf)_3$ at 80 °C. To a solution of **11** (10.0 mg, 20.0 μmol) in toluene (5 mL) was added 2,3-dichloro-5,6-dicyano-1,4-benzoquinone (DDQ) (23.4 mg, 0.103 mmol) and scandium trifluoromethanesulfonate ($Sc(OTf)_3$) (40.3 mg, 81.9 μmol). After stirring at 80 °C for 13 h under a nitrogen atmosphere, the reaction mixture was gradually cooled to room temperature, and $N_2H_4 \cdot H_2O$ (97% solution, 0.5 mL) was added. The reaction mixture was passed through a short silica gel column (CH_2Cl_2). After removal of the solvent under reduced pressure, the residue was recrystallization from hexanes/$CHCl_3$ to afford **13** (3.4 mg, 34%) as a purple solid. The

spectral data are described above.

Reaction of 11 with DDQ and Sc(OTf)$_3$ at 120 °C. To a solution of **11** (8.3 mg, 17 μmol) in chlorobenzene (5 mL) was added DDQ (18.7 mg, 82.4 μmol) and Sc(OTf)$_3$ (40.5 mg, 82.3 μmol). After stirring at 120 °C for 5 h under a nitrogen atmosphere, the reaction mixture was gradually cooled to room temperature. The precipitated solid was filtered and washed with $CHCl_3$ and hexane to afford **14** (4.1 mg, 49%) as an orange solid.

14: ^{1}H NMR (400 MHz, tetrachloroethane-d_2): δ = 9.47 (s, 4H), 9.28 (d, J = 8.0 Hzm 4H), 9.24 (d, J = 7.6 Hz, 4H), 7.98 (dd, J = 7.6, 7.2 Hz, 4H), 7.90 (dd, J = 7.6, 7.2 Hz, 4H); ^{13}C NMR spectrum was not obtained due to poor solubility in common organic solvents; HRMS (EI): m/z calcd for $C_{40}H_{20}$: 500.1565 [M^+]; found: 500.1562. The spectral data of this product agreed with that reported in the literature.[3]

Reaction of 13 with DDQ and Sc(OTf)$_3$ at 120 °C. To a solution of **13** (14.3 mg, 28.5 μmol) in chlorobenzene (5 mL) was added DDQ (26.0 mg, 0.114 mmol) and Sc(OTf)$_3$ (55.7 mg, 0.113 mmol). After stirring at 120 °C for 4 h under an argon atmosphere, the solvent was removed under reduced pressure. The residue was washed with water, MeOH, and $CHCl_3$ to afford **14** (10.0 mg, 70%) as an orange solid. The spectral data are described above.

3. X-ray Crystallographic Analysis of 13

The X-ray diffraction data were collected with an imaging plate diffractometer with graphite monochromated MoK_α radiation. The positional and thermal parameters of non-hydrogen atoms were refined anisotropically on F_2 by the full-matrix least-squares method using SHELXL-2013.[4] Hydrogen atoms were placed at calculated positions and refined "riding" on their corresponding carbon atoms. In the subsequent refinement, the function $\Sigma w(|F_o| - |F_c|)^2$ was minimized, where $|F_o|$ and $|F_c|$ are the observed and calculated structure factor amplitudes, respectively. The agreement indices are defined as $R_1 = \Sigma (||F_o|-|F_c||)/\Sigma|F_o|$ and $wR_2 = [\Sigma w (|F_o|-|F_c|)^2/\Sigma(wF_o^2)^2]^{1/2}$.

Crystal data for **13**: Formula $C_{40}H_{20}$, M_r = 500.56, 0.50 × 0.40 × 0.10 mm^3, T = 113(2) K, triclinic, space group *P-1*, a = 14.953(2) Å, b = 15.734(3) Å, c = 17.704(3) Å, α = 78.652(3)°, β = 66.812(3)°, γ = 72.621(3)°, V = 3638.8 (10) Å^3, Z = 6, ρ_{calcd} = 1.371 gcm^{-3}, μ = 0.078 mm^{-1}, $F(000)$ = 1560, $2\theta_{max}$ = 55.0°, R_1 ($I > 2\theta(I)$) = 0.093, wR_2 (all data) = 0.218 and GOF = 1.032 for 16349 reflections and 1155 parameters.

4. Estimation of Association Constant of 13 in Solution

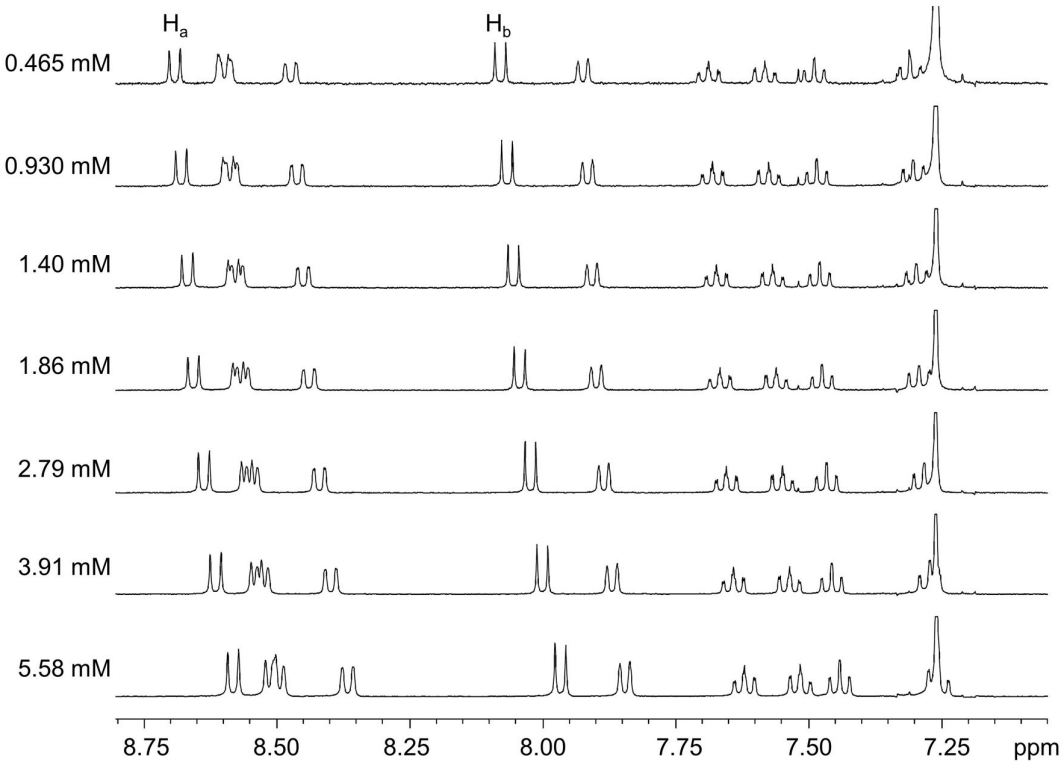


Figure S1. Concentration-dependent ^{1}H NMR spectra of **13** in $CDCl_3$.

The self-aggregation behavior of **13** was investigated quantitatively on the basis of the concentration dependence of the ^{1}H NMR chemical shifts.[5] The ^{1}H NMR spectra of **13** were measured at 0.465, 0.930, 1.40, 1.86, 2.79, 3.91, and 5.58 mM in $CDCl_3$ at 30 °C (Figure S1). The chemical shifts and dilution curves for H_a and H_b are shown in Table S1 and Figure S2, respectively. The association constant (K_2) was determined by assuming that monomer-dimer equilibrium is the predominant process of the self-association. The least-squares curve fitting to equation (1) was carried out to determine K_2, where δ_m and δ_d are chemical shifts of the monomer and dimer, respectively, and C_t is the total concentration of the substrate. Estimated chemical shifts of the protons δ_m, δ_d and association constant K_2 are included in the bottom of Table S1.

$$\delta = \delta_{m} + (\delta_{d} - \delta_{m})\left(1 + \frac{1 - \sqrt{8K_2C_t + 1}}{4K_2C_t}\right) \quad (1)$$

Table S1. ^{1}H NMR dilution data of **13** in $CDCl_3$ at 30 °C, calculated association constants, and calculated chemical shifts for the monomer and dimer.

concentration / mM	H_a / ppm	H_b / ppm
5.58	8.583	7.968
3.91	8.610	8.000
2.79	8.630	8.020
1.86	8.657	8.043
1.40	8.668	8.055
0.930	8.680	8.067
0.465	8.692	8.080
calculated chemical shifts for the proton of the dimer δ_d / ppm	8.708 ± 0.003	8.094 ± 0.002
calculated chemical shifts for the proton of the monomer δ_m / ppm	8.009 ± 0.002	7.235 ± 0.001
association constant K_2 / M^{-1}	24.1 ± 2.9	18.0 ± 1.4

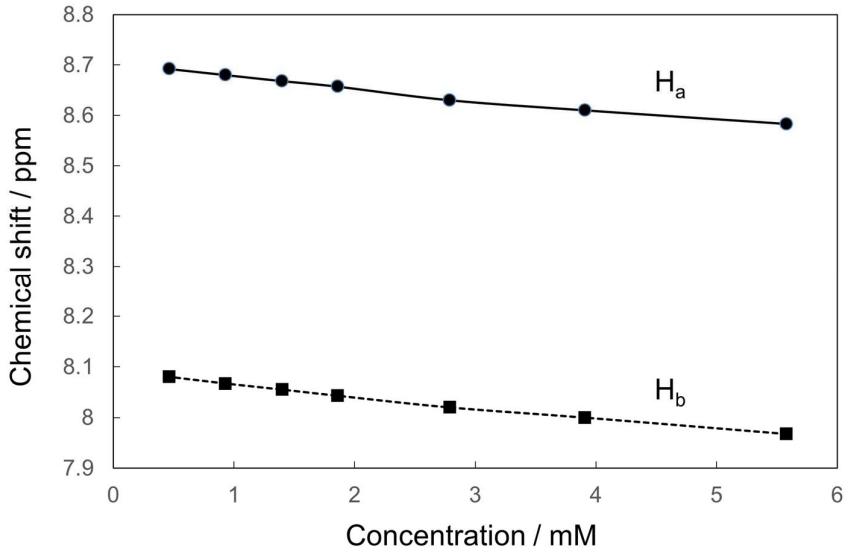


Figure S2. Concentration dependence of ^{1}H NMR chemical shifts for H_a (circle and solid line) and H_b (square and dotted line) of **13** in $CDCl_3$.

5. Cyclic Voltammogram of 13

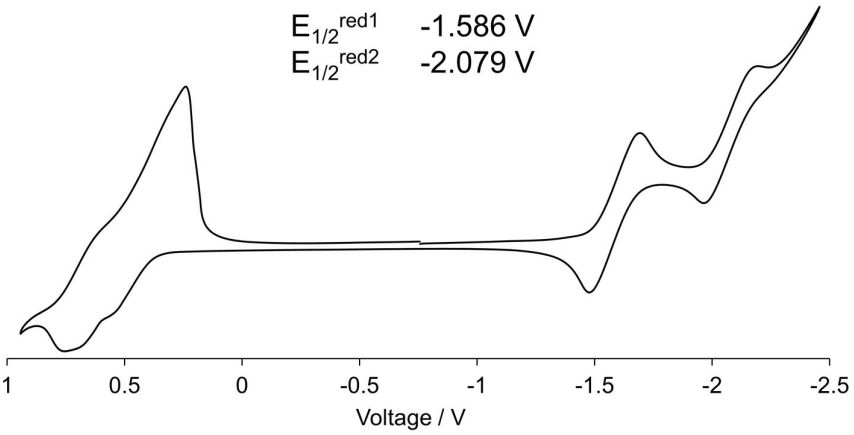


Figure S3. Cyclic voltammogram of **13**. Condition: in CH_2Cl_2 at room temperature, 0.1 M Bu_4NClO_4, working electrode: glassy carbon, counter electrode: Pt. reference electrode: $Ag/AgNO_3$, scan rate: 0.1 V/s, $Fc/Fc^+ = 0$ V.

6. Theoretical Calculations of 13

Table S2. Excitation energies of **13** calculated at the B3LYP/6-31G(d) level of theory.

excited state	transition energy / eV (Wavelength / nm)	main CI coefficient	oscillator strength *f*
1	2.06 (603)	0.696 (HOMO - LUMO)	0.0897
2	2.45 (505)	0.700 (HOMO−1 - LUMO)	0.0122
3	2.61 (475)	0.693 (HOMO−2 - LUMO)	0.0012

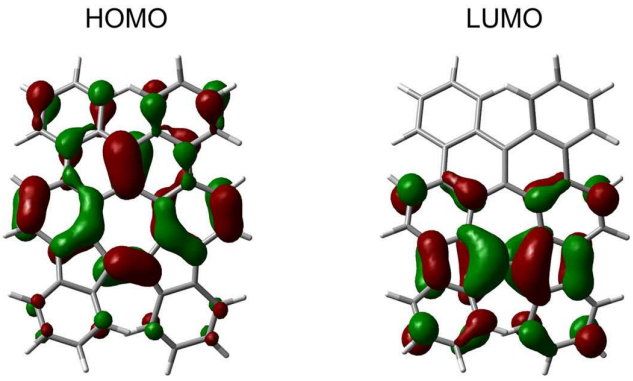
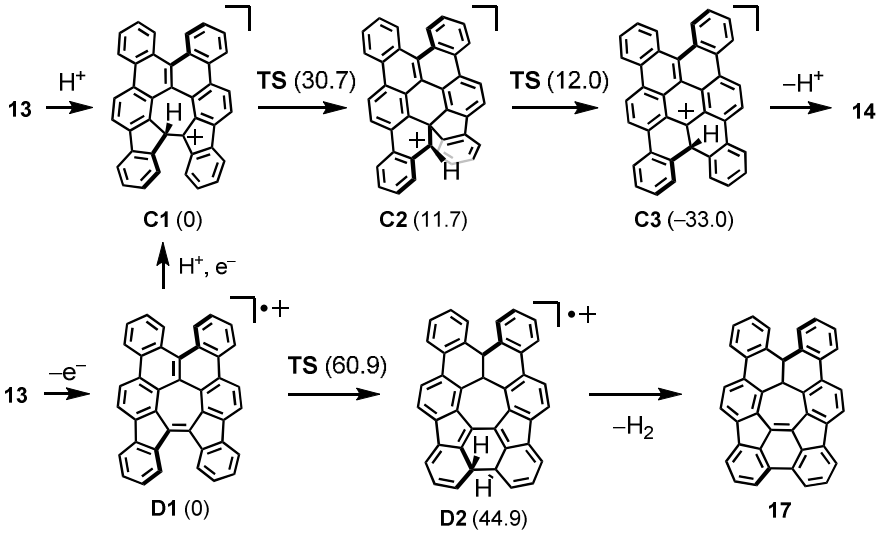


Figure S4. HOMO and LUMO of **13**.

7. Theoretical Calculations of Reaction Pathways



Scheme S1. Calculated energies of intermediates and barriers for isomerization and cyclodehydrogenation reaction pathways for **13**. The calculated energies (kcal/mol) relative to **C1** and **D1** in each reaction are shown in parentheses.

8. References

(1) Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

(2) (a) Jain, R.; Bally, T.; Rablen P. R. *J. Org. Chem.* **2009**, *74*, 4017–4023. (b) Bally, T.; Rablen, P. R. *J. Org. Chem.* **2011**, *76*, 4818–4830. (c) Cossi, M.; Scalmani, G.; Rega, N.; Barone, V. *J. Chem. Phys.* **2002**, *117*, 43–54.

(3) (a) Clar, E.; McAndrew, B. A. *Tetrahedron* **1972**, *28*, 1137–1142. (b) Pola, S.; Kuo, C.-H.; Peng, W.-T.; Islam, M. M.; Chao, I.; Tao, Y.-T. *Chem. Mater.* **2012**, *24*, 2566–2571.

(4) G. M. *Acta Crystallogr. A* **2008**, *64*, 112–122.

(5) Tobe, Y.; Utsumi, N.; Kawabata, K.; Nagano, A.; Adachi, K.; Araki, S.; Sonoda, M.; Hirose, K.; Naemura, K. *J. Am. Chem. Soc.* **2002**, *124*, 5350–5364.

9. ^{1}H and ^{13}C NMR Spectra

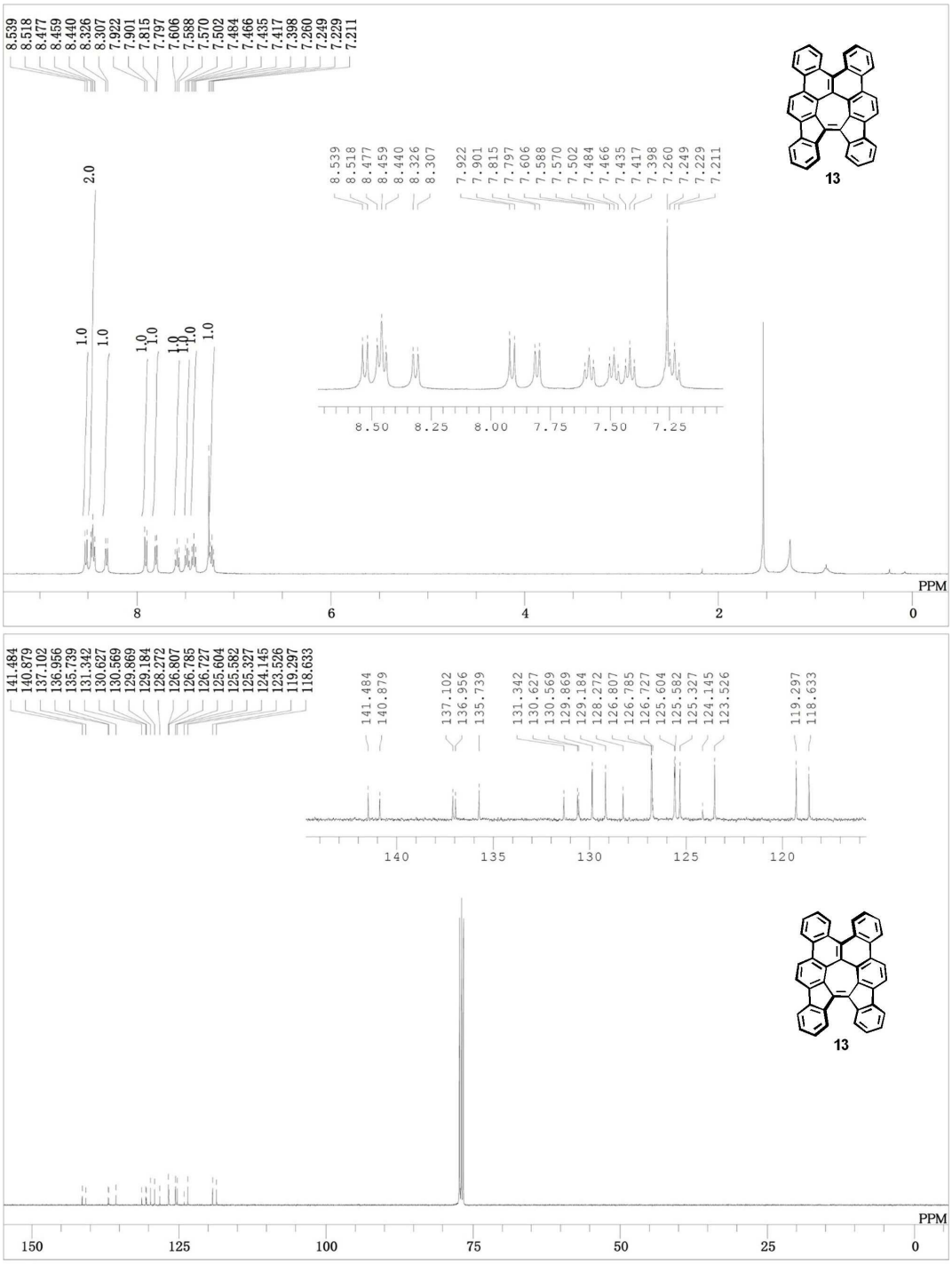


Figure S5. ^{1}H and ^{13}C NMR spectra of **13**.

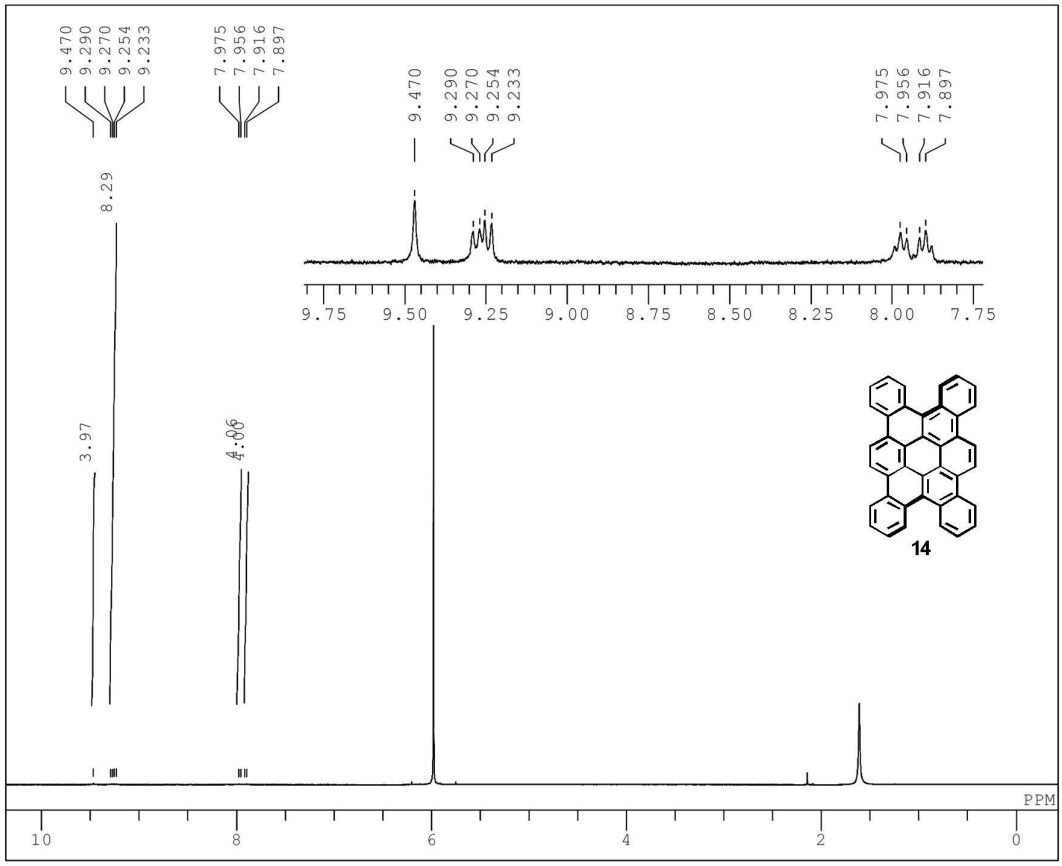
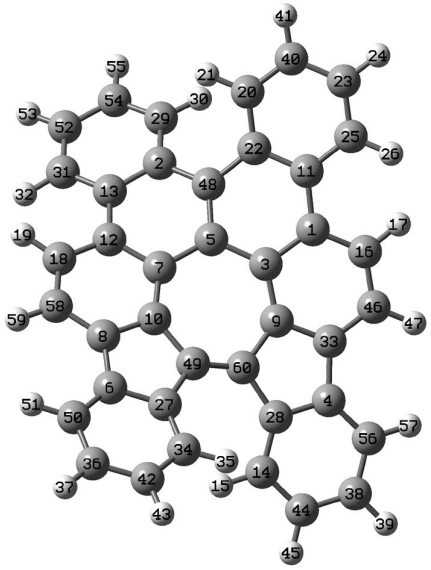


Figure S6. ^{1}H NMR spectrum of **14**.

10. Computational Results

10-1. Cartesian coordinates for optimized geometry of **13**.



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5	C	-1.21824	-3E-06	0.000007
6	C	2.72925	-2.80694	0.747974
7	C	-0.54335	-1.30532	-0.09628
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9	C	0.831545	1.544163	-0.18873
10	C	0.831551	-1.54416	0.188726
11	C	-2.70721	2.338729	0.800296
12	C	-1.3423	-2.47992	-0.32644
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14	C	4.430847	1.115002	-1.10824
15	H	4.754173	0.081042	-1.13056
16	C	-0.81505	3.772557	0.124526
17	H	-1.47037	4.628397	0.237202
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no.	atom	X	Y	Z
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35	H	4.754156	-0.08103	1.130614
36	C	4.885173	-3.45789	1.580048
37	H	5.570969	-4.22516	1.929167
38	C	4.885165	3.457894	-1.58005
39	H	5.570959	4.225172	-1.92917
40	C	-5.29875	1.953603	1.824682
41	H	-6.28285	1.787034	2.254159
42	C	5.291905	-2.11838	1.559341
43	H	6.286129	-1.85158	1.906937
44	C	5.291909	2.118391	-1.55931
45	H	6.286139	1.851594	-1.90689
46	C	0.493488	3.975049	-0.26175
47	H	0.873692	4.977046	-0.43936
48	C	-2.62727	-6E-06	0.000011
49	C	2.001424	-0.64684	0.218672

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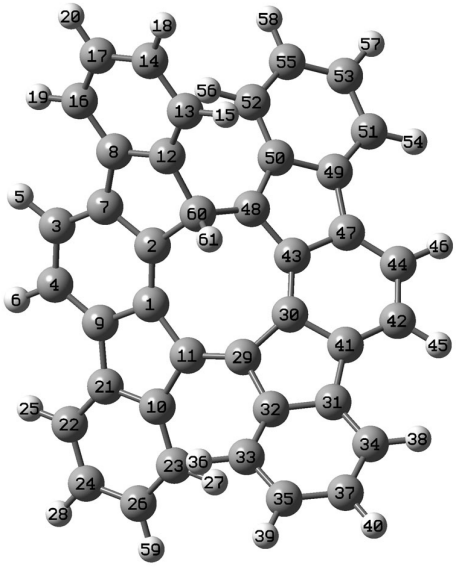
10-2. Cartesian coordinates for optimized geometry of **A1**.



no.	atom	X	Y	Z
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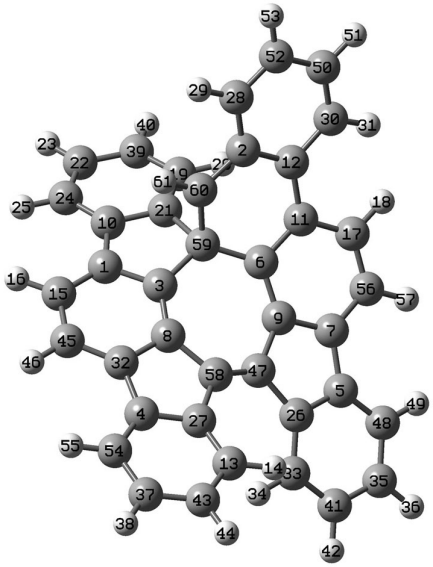
58	H	5.886187	1.260329	1.853253
59	H	-5.9559	-2.21339	1.598503
60	C	1.475308	-0.26424	-1.0319
61	H	0.84429	0.078199	-1.86346

10-3. Cartesian coordinates for optimized geometry of **A2**.



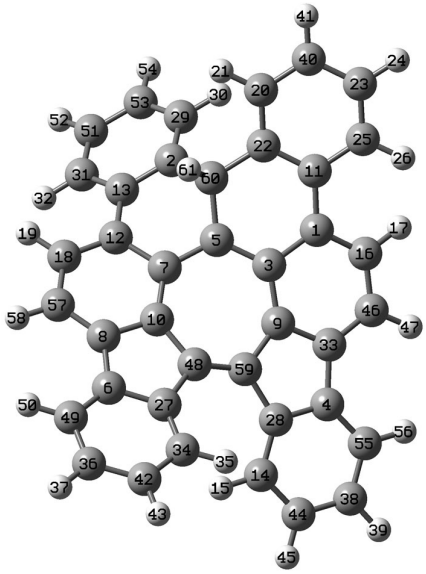
no.	atom	X	Y	Z
1	C	-0.83553	-2.74204	-0.63631
2	C	-3.2963	0.182409	1.421976
3	C	-0.27303	-1.55962	-0.1015
4	C	3.145638	-2.46685	0.697939
5	C	2.008857	3.08916	-0.72476
6	C	-0.91582	0.991367	-0.01299
7	C	0.597468	2.845222	-0.46954
8	C	1.060558	-1.54038	0.241176
9	C	0.391518	1.453741	-0.2474
10	C	-2.0984	-2.3957	-1.26982
11	C	-1.93823	1.952935	0.276667
12	C	-3.1499	1.543366	0.998321
13	C	4.463319	-0.512	1.295698
14	H	4.572406	0.55777	1.433181
15	C	-0.12138	-3.94739	-0.63004
16	H	-0.56163	-4.85385	-1.03476
17	C	-1.68881	3.320452	0.033411
18	H	-2.46595	4.054287	0.20774
19	C	-3.48254	-0.3959	-1.67005
20	H	-3.71675	0.645741	-1.48036

no.	atom	X	Y	Z
32	C	1.77922	-2.77022	0.273391
33	C	4.06992	1.818486	-0.8473
34	H	4.622603	0.889351	-0.78952
35	C	4.028268	4.190391	-1.4037
36	H	4.555486	5.080798	-1.73256
37	C	5.374882	-2.75666	1.539924
38	H	6.195929	-3.40364	1.83377
39	C	-4.24716	-1.13787	-2.55756
40	H	-5.06719	-0.66437	-3.08771
41	C	4.71881	2.978701	-1.27667
42	H	5.775338	2.935296	-1.5241
43	C	5.500242	-1.36954	1.675838
44	H	6.41277	-0.95087	2.089615
45	C	1.180032	-3.96829	-0.12267
46	H	1.740518	-4.89802	-0.10664
47	C	1.745178	0.824364	-0.13852
48	C	2.659838	4.250494	-1.13877
49	H	2.114174	5.179955	-1.27523
50	C	-5.20217	2.034672	2.220627
51	H	-5.95132	2.762749	2.518159

21	C	-2.39857	-1.02055	-1.03112
22	C	-3.97487	-2.50382	-2.76964
23	H	-4.60216	-3.07003	-3.45185
24	C	-2.91217	-3.1378	-2.13151
25	H	-2.70011	-4.18453	-2.32635
26	C	2.707979	1.874494	-0.53456
27	C	3.288409	-1.05471	0.770782
28	C	-4.36736	-0.21306	2.264198
29	H	-4.43825	-1.25396	2.56799
30	C	-4.1518	2.443941	1.40823
31	H	-4.11378	3.483924	1.108918

52	C	-5.31039	0.705782	2.672074
53	H	-6.13198	0.410208	3.315922
54	C	4.189016	-3.31649	1.058028
55	H	4.079347	-4.39526	0.991089
56	C	-0.44897	3.762005	-0.39216
57	H	-0.27892	4.817034	-0.583
58	C	2.015419	-0.42753	0.34857
59	C	-1.30877	-0.45906	-0.02019
60	C	-2.39576	-0.78797	0.937365
61	H	-2.48046	-1.81395	1.281119

10-4. Cartesian coordinates for optimized geometry of **A3**.



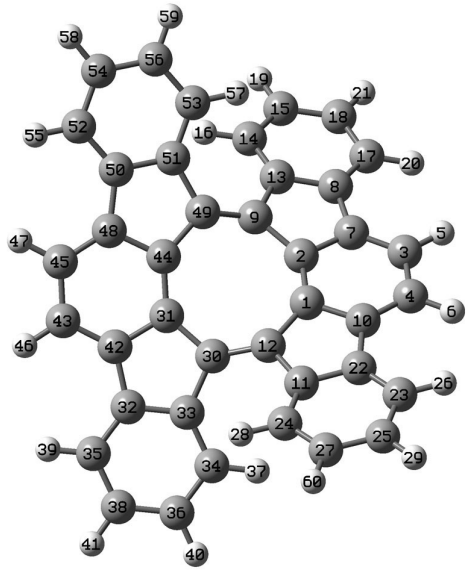
no.	atom	X	Y	Z
1	C	1.595984	2.276742	-0.29562
2	C	3.233577	-1.26481	0.567433
3	C	0.640118	1.176522	-0.1672
4	C	-2.46435	2.939523	0.841912
5	C	1.135762	-0.14848	-0.20502
6	C	-2.96382	-2.65957	-0.73753
7	C	0.393078	-1.35165	0.049716
8	C	-1.56888	-2.80577	-0.31724

no.	atom	X	Y	Z
32	H	2.438039	-4.09935	2.291342
33	C	-1.04187	2.860817	0.526611
34	C	-4.48611	-0.84163	-1.28706
35	H	-4.70929	0.214077	-1.39072
36	C	-5.13694	-3.16183	-1.61715
37	H	-5.87833	-3.88619	-1.94066
38	C	-4.56724	3.748275	1.659123
39	H	-5.17802	4.55039	2.062203

9	C	-0.71477	1.526045	0.168001
10	C	-0.99565	-1.50375	-0.19894
11	C	2.923063	2.058407	-0.88048
12	C	1.129762	-2.54254	0.431872
13	C	2.486625	-2.38215	0.978067
14	C	-4.36307	1.429222	0.949056
15	H	-4.80876	0.448089	0.844998
16	C	1.221376	3.554427	0.1143
17	H	1.953572	4.352091	0.105885
18	C	0.515262	-3.78637	0.366944
19	H	1.084196	-4.67201	0.628494
20	C	4.628226	0.518386	-1.66457
21	H	4.980153	-0.50195	-1.79129
22	C	3.403295	0.748938	-1.02656
23	C	4.926693	2.889177	-1.98912
24	H	5.506779	3.723048	-2.37215
25	C	3.703879	3.124641	-1.37842
26	H	3.336464	4.143027	-1.32801
27	C	-3.26406	-1.27636	-0.76708
28	C	-3.03046	1.667086	0.597162
29	C	4.487925	-1.02209	1.121124
30	H	5.062804	-0.15589	0.814478
31	C	3.020256	-3.25308	1.940219

40	C	5.394146	1.578527	-2.13728
41	H	6.340679	1.386753	-2.63336
42	C	-5.41866	-1.79482	-1.70734
43	H	-6.36965	-1.46732	-2.11589
44	C	-5.12289	2.477643	1.474081
45	H	-6.15801	2.298676	1.74833
46	C	-0.07628	3.851713	0.537874
47	H	-0.32328	4.864746	0.842613
48	C	-2.06774	-0.53658	-0.32606
49	C	-3.89733	-3.6064	-1.14255
50	H	-3.67099	-4.66839	-1.11435
51	C	4.280092	-3.01359	2.483847
52	H	4.682633	-3.68896	3.232526
53	C	5.008825	-1.89429	2.081817
54	H	5.980283	-1.68849	2.521225
55	C	-3.22362	3.985681	1.356282
56	H	-2.78503	4.962387	1.539685
57	C	-0.81941	-3.93305	-0.04808
58	H	-1.25562	-4.92504	-0.12199
59	C	-1.95673	0.7708	0.120945
60	C	2.592446	-0.41811	-0.54271
61	H	2.528323	-1.10379	-1.40573

10-5. Cartesian coordinates for optimized geometry of **B1**.



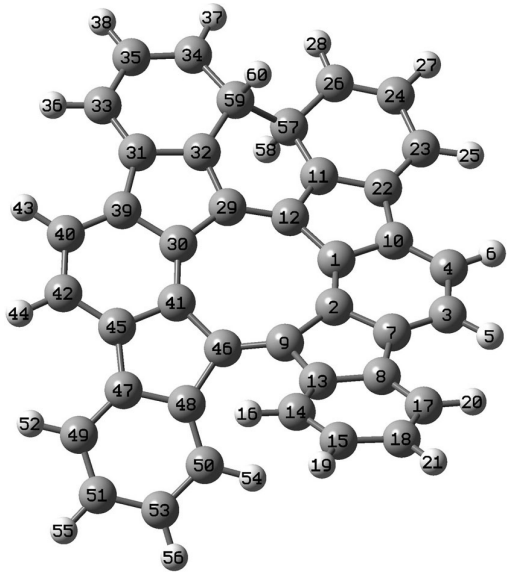
no.	atom	X	Y	Z
1	C	0.672605	1.660834	0.211884
2	C	-0.67261	1.660834	-0.21188
3	C	-0.65341	4.132039	-0.25858
4	C	0.653409	4.132039	0.258584
5	H	-1.16069	5.071754	-0.4549
6	H	1.160687	5.071754	0.454897
7	C	-1.29438	2.926999	-0.48422
8	C	-2.65657	2.687835	-0.95978
9	C	-1.7302	0.645246	-0.26819
10	C	1.294381	2.926999	0.484219
11	C	2.921616	1.306211	0.829756
12	C	1.7302	0.645246	0.268185
13	C	-2.92162	1.306211	-0.82976
14	C	-4.10998	0.774262	-1.34525
15	C	-5.0419	1.63812	-1.92501
16	H	-4.31104	-0.29011	-1.30835
17	C	-3.58893	3.549066	-1.52503
18	C	-4.79308	3.013018	-1.99967
19	H	-5.96587	1.235292	-2.32797
20	H	-3.3883	4.612145	-1.62117

no.	atom	X	Y	Z
31	C	0.672605	-1.66083	-0.21188
32	C	2.656566	-2.68784	-0.95978
33	C	2.921616	-1.30621	-0.82976
34	C	4.109979	-0.77426	-1.34525
35	C	3.588928	-3.54907	-1.52503
36	C	5.0419	-1.63812	-1.92501
37	H	4.311042	0.290106	-1.30835
38	C	4.793077	-3.01302	-1.99967
39	H	3.388301	-4.61215	-1.62117
40	H	5.965868	-1.23529	-2.32797
41	H	5.531561	-3.66986	-2.44947
42	C	1.294381	-2.927	-0.48422
43	C	0.653409	-4.13204	-0.25858
44	C	-0.67261	-1.66083	0.211884
45	C	-0.65341	-4.13204	0.258584
46	H	1.160687	-5.07175	-0.4549
47	H	-1.16069	-5.07175	0.454897
48	C	-1.29438	-2.927	0.484219
49	C	-1.7302	-0.64525	0.268185
50	C	-2.65657	-2.68784	0.959783

21	H	-5.53156	3.669859	-2.44947
22	C	2.656566	2.687835	0.959783
23	C	3.588928	3.549066	1.525028
24	C	4.109979	0.774262	1.345251
25	C	4.793077	3.013018	1.999673
26	H	3.388301	4.612145	1.621167
27	C	5.0419	1.63812	1.92501
28	H	4.311042	-0.29011	1.308353
29	H	5.531561	3.669859	2.449466
30	C	1.7302	-0.64525	-0.26819

51	C	-2.92162	-1.30621	0.829756
52	C	-3.58893	-3.54907	1.525028
53	C	-4.10998	-0.77426	1.345251
54	C	-4.79308	-3.01302	1.999673
55	H	-3.3883	-4.61215	1.621167
56	C	-5.0419	-1.63812	1.92501
57	H	-4.31104	0.290106	1.308353
58	H	-5.53156	-3.66986	2.449466
59	H	-5.96587	-1.23529	2.327973
60	H	5.965868	1.235292	2.327973

10-6. Cartesian coordinates for optimized geometry of **B2**.



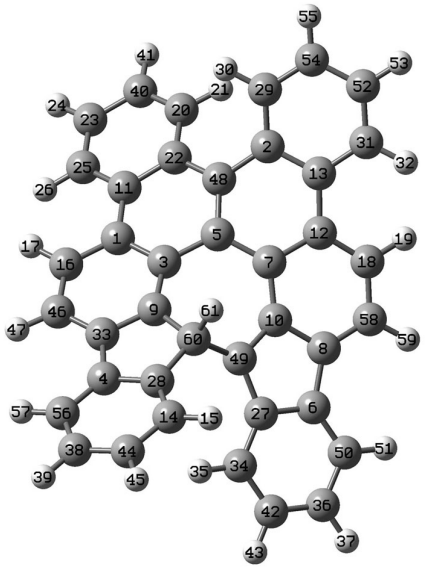
no.	atom	X	Y	Z
1	C	0.000106	1.740948	0.628698
2	C	0.229959	1.705392	-0.7505
3	C	0.337429	4.186844	-0.72846
4	C	0.07396	4.208882	0.64428
5	H	0.479312	5.117256	-1.26951
6	H	0.013051	5.153922	1.176177
7	C	0.434687	2.970056	-1.39619
8	C	0.797084	2.734395	-2.78638
9	C	0.235958	0.649633	-1.80859

31	C	0.227408	-2.73785	2.74488
32	C	0.248584	-1.32806	2.90353
33	C	0.23105	-3.53934	3.866421
34	C	0.290226	-1.60072	5.371951
35	C	0.245861	-2.94537	5.180849
36	H	0.175691	-4.62124	3.783571
37	H	0.321743	-1.19479	6.378853
38	H	0.210909	-3.6087	6.039894
39	C	0.070861	-3.00111	1.309816

10	C	-0.07086	3.001105	1.309816
11	C	-0.24858	1.328057	2.90353
12	C	-0.07531	0.699663	1.655622
13	C	0.723555	1.346191	-3.02906
14	C	1.250915	0.839966	-4.22424
15	C	1.744406	1.724212	-5.18334
16	H	1.285654	-0.22602	-4.41349
17	C	1.27574	3.621993	-3.74993
18	C	1.734889	3.10829	-4.96239
19	H	2.15005	1.331009	-6.11077
20	H	1.321477	4.689404	-3.55356
21	H	2.116763	3.780189	-5.72522
22	C	-0.22741	2.737845	2.74488
23	C	-0.23105	3.539342	3.866421
24	C	-0.24586	2.945373	5.180849
25	H	-0.17569	4.621242	3.783571
26	C	-0.29023	1.60072	5.371951
27	H	-0.21091	3.6087	6.039894
28	H	-0.32174	1.194787	6.378853
29	C	0.075306	-0.69966	1.655622
30	C	-0.00011	-1.74095	0.628698

40	C	-0.07396	-4.20888	0.64428
41	C	-0.22996	-1.70539	-0.7505
42	C	-0.33743	-4.18684	-0.72846
43	H	-0.01305	-5.15392	1.176177
44	H	-0.47931	-5.11726	-1.26951
45	C	-0.43469	-2.97006	-1.39619
46	C	-0.23596	-0.64963	-1.80859
47	C	-0.79708	-2.7344	-2.78638
48	C	-0.72356	-1.34619	-3.02906
49	C	-1.27574	-3.62199	-3.74993
50	C	-1.25092	-0.83997	-4.22424
51	C	-1.73489	-3.10829	-4.96239
52	H	-1.32148	-4.6894	-3.55356
53	C	-1.74441	-1.72421	-5.18334
54	H	-1.28565	0.226022	-4.41349
55	H	-2.11676	-3.78019	-5.72522
56	H	-2.15005	-1.33101	-6.11077
57	C	-0.43469	0.650377	4.218921
58	H	-1.48876	0.301876	4.258624
59	C	0.434687	-0.65038	4.218921
60	H	1.488758	-0.30188	4.258624

10-7. Cartesian coordinates for optimized geometry of **C1**.



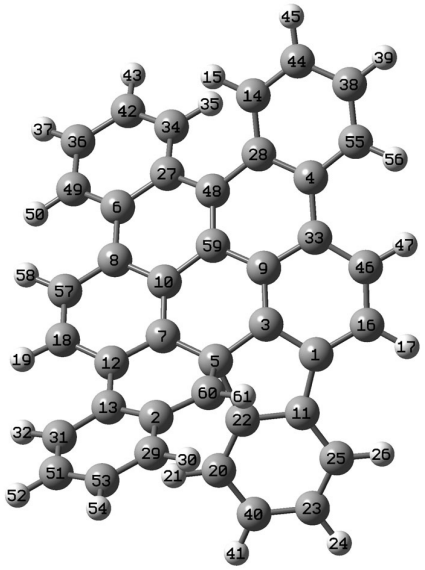
no.	atom	X	Y	Z
1	C	1.083208	-2.4629	0.551126
2	C	3.418756	0.907393	-0.76593
3	C	0.444067	-1.28073	0.059376
4	C	-2.97958	-2.43056	-0.69858
5	C	1.228549	-0.06433	-0.14508
6	C	-2.51367	2.727327	1.082633
7	C	0.673459	1.262977	-0.1264
8	C	-1.07893	2.816289	0.756039
9	C	-0.91806	-1.39367	-0.27595
10	C	-0.68995	1.558258	0.187538
11	C	2.504436	-2.43442	0.86274
12	C	1.55402	2.405303	-0.17137
13	C	2.888248	2.222143	-0.72861
14	C	-4.20602	-0.75641	-1.96764
15	H	-4.27855	0.230769	-2.41631
16	C	0.326096	-3.64231	0.723635
17	H	0.815134	-4.53996	1.08063
18	C	1.119636	3.63748	0.314171
19	H	1.819127	4.466738	0.333261
20	C	4.658419	-1.26294	0.84215

no.	atom	X	Y	Z
32	H	3.22714	4.287375	-1.27389
33	C	-1.64787	-2.58692	-0.11177
34	C	-4.31488	1.098498	0.797146
35	H	-4.68952	0.143541	0.452043
36	C	-4.70526	3.217834	1.923875
37	H	-5.38356	3.89418	2.435235
38	C	-5.17258	-2.94708	-1.52915
39	H	-5.99844	-3.6425	-1.64549
40	C	5.254052	-2.30877	1.51578
41	H	6.298314	-2.24379	1.804787
42	C	-5.16843	1.983834	1.474522
43	H	-6.20229	1.700986	1.645088
44	C	-5.25712	-1.67118	-2.10163
45	H	-6.14459	-1.3911	-2.66128
46	C	-1.02003	-3.71994	0.408272
47	H	-1.55466	-4.65834	0.518887
48	C	2.647576	-0.17426	-0.1637
49	C	-1.85583	0.802573	-0.04198
50	C	-3.36273	3.604465	1.726567
51	H	-3.01624	4.570264	2.082677

21	H	5.236587	-0.36979	0.646881
22	C	3.28609	-1.30437	0.467398
23	C	4.493014	-3.43871	1.856717
24	H	4.951691	-4.26304	2.394623
25	C	3.14495	-3.48802	1.548105
26	H	2.575561	-4.34895	1.875717
27	C	-2.98314	1.471127	0.601403
28	C	-3.0785	-1.13913	-1.25029
29	C	4.64284	0.685725	-1.43636
30	H	5.011357	-0.32661	-1.55558
31	C	3.632111	3.280805	-1.27914

52	C	4.853745	3.046451	-1.89493
53	H	5.404323	3.873398	-2.33298
54	C	5.349125	1.739486	-1.99587
55	H	6.276333	1.546636	-2.52652
56	C	-4.03194	-3.34121	-0.82882
57	H	-3.96441	-4.34029	-0.40788
58	C	-0.17982	3.850373	0.827042
59	H	-0.45264	4.824315	1.22129
60	C	-1.80323	-0.36813	-0.97299
61	H	-1.33971	-0.02807	-1.91162

10-8. Cartesian coordinates for optimized geometry of **C2**.



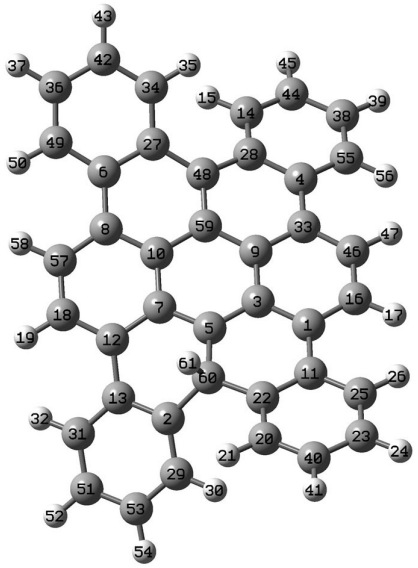
no.	atom	X	Y	Z
1	C	-1.01849	-2.7759	-0.32065
2	C	-3.51861	0.511416	1.292013
3	C	-0.52127	-1.53958	0.09129
4	C	3.099676	-2.15947	0.625239
5	C	-1.55301	-0.45927	0.057074
6	C	2.310704	2.621454	-0.62263
7	C	-1.01223	0.926331	-0.05458
8	C	0.89123	2.436575	-0.3705

no.	atom	X	Y	Z
32	H	-3.95697	3.814031	0.518378
33	C	1.70474	-2.42465	0.315372
34	C	4.547052	1.687444	-0.89062
35	H	5.216737	0.837572	-0.88406
36	C	4.140988	3.995683	-1.4678
37	H	4.498119	4.94679	-1.85081
38	C	5.249316	-2.90766	1.494525
39	H	5.893299	-3.712	1.836827

9	C	0.835854	-1.30049	0.252304
10	C	0.392571	1.121469	-0.16745
11	C	-2.31371	-2.54022	-0.95058
12	C	-1.87659	2.018851	0.145315
13	C	-3.1983	1.799593	0.743413
14	C	4.867481	-0.55506	1.097807
15	H	5.210214	0.468022	1.188814
16	C	-0.16387	-3.89325	-0.29694
17	H	-0.51264	-4.87711	-0.59593
18	C	-1.35471	3.322063	-0.0392
19	H	-1.9889	4.190815	0.092518
20	C	-3.7537	-0.62903	-1.57089
21	H	-4.02169	0.418807	-1.48661
22	C	-2.64996	-1.14609	-0.87351
23	C	-4.19556	-2.85843	-2.41751
24	H	-4.81078	-3.51641	-3.02427
25	C	-3.11429	-3.39091	-1.71415
26	H	-2.87942	-4.44821	-1.78959
27	C	3.211403	1.524676	-0.45
28	C	3.577747	-0.81187	0.580463
29	C	-4.68974	0.328732	2.068903
30	H	-4.89796	-0.65498	2.480934
31	C	-4.13321	2.831821	0.941058

40	C	-4.50143	-1.48657	-2.36653
41	H	-5.33587	-1.09795	-2.94108
42	C	5.006488	2.894433	-1.38574
43	H	6.033895	2.980583	-1.72665
44	C	5.689085	-1.57778	1.545145
45	H	6.669107	-1.34195	1.949101
46	C	1.161778	-3.71118	0.077225
47	H	1.815308	-4.5761	0.094989
48	C	2.709982	0.260754	0.077695
49	C	2.815046	3.850313	-1.10679
50	H	2.146168	4.691579	-1.24663
51	C	-5.28954	2.62314	1.68336
52	H	-5.98818	3.444112	1.816168
53	C	-5.56554	1.375567	2.272962
54	H	-6.46565	1.236225	2.862498
55	C	3.966927	-3.18589	1.054977
56	H	3.609055	-4.20919	1.092872
57	C	-0.02528	3.514185	-0.33571
58	H	0.330179	4.529263	-0.46431
59	C	1.33549	0.042805	0.078267
60	C	-2.68323	-0.59656	1.003921
61	H	-2.85178	-1.54857	1.49744

10-9. Cartesian coordinates for optimized geometry of **C3**.



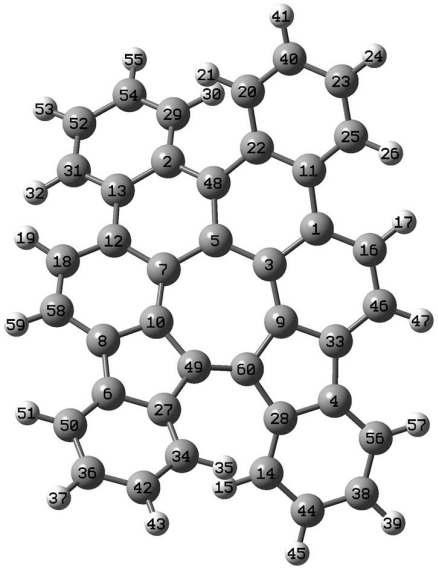
no.	atom	X	Y	Z
1	C	-1.54202	2.365463	-0.20931
2	C	-3.47979	-1.33297	0.354363
3	C	-0.75626	1.164577	-0.15239
4	C	2.727409	2.511849	0.53289
5	C	-1.38269	-0.09276	-0.21062
6	C	2.961616	-2.35224	-0.5121
7	C	-0.63552	-1.28529	-0.06883
8	C	1.534937	-2.43472	-0.23941
9	C	0.670511	1.227147	0.026672
10	C	0.789809	-1.23295	-0.14096
11	C	-2.9763	2.304831	-0.51147
12	C	-1.30887	-2.53161	0.132853
13	C	-2.71902	-2.51199	0.542583
14	C	4.822013	1.321151	0.955447
15	H	5.370609	0.392075	1.036594
16	C	-0.86876	3.578106	-0.02171
17	H	-1.40909	4.51559	-0.04321
18	C	-0.54181	-3.69808	0.070035
19	H	-1.01383	-4.66742	0.183165
20	C	-4.91778	1.017361	-1.19837

no.	atom	X	Y	Z
32	H	-2.71129	-4.49191	1.413825
33	C	1.306367	2.475459	0.228938
34	C	4.944266	-0.98714	-0.93593
35	H	5.407183	-0.01398	-1.0371
36	C	5.036989	-3.37082	-1.28252
37	H	5.587439	-4.25642	-1.58525
38	C	4.687469	3.690509	1.375997
39	H	5.148865	4.612537	1.716442
40	C	-5.64621	2.185092	-1.39932
41	H	-6.66494	2.131515	-1.77106
42	C	5.646646	-2.10781	-1.33632
43	H	6.660866	-2.00571	-1.7097
44	C	5.410492	2.486866	1.403601
45	H	6.423154	2.466557	1.794205
46	C	0.500958	3.62772	0.194125
47	H	0.951073	4.604452	0.329129
48	C	2.86463	0.090119	-0.02536
49	C	3.712991	-3.48237	-0.89577
50	H	3.243151	-4.45843	-0.9323
51	C	-4.57603	-3.50509	1.762605

21	H	-5.37359	0.059264	-1.42851
22	C	-3.60402	1.054708	-0.71293
23	C	-5.05628	3.423267	-1.12755
24	H	-5.61635	4.341806	-1.27251
25	C	-3.737	3.478967	-0.70645
26	H	-3.28941	4.453	-0.55089
27	C	3.609137	-1.07791	-0.46432
28	C	3.491823	1.304329	0.45808
29	C	-4.75433	-1.24654	0.910868
30	H	-5.32923	-0.33374	0.817523
31	C	-3.29037	-3.59127	1.24076

52	H	-4.9985	-4.3454	2.304638
53	C	-5.30006	-2.32253	1.615817
54	H	-6.28743	-2.22672	2.05755
55	C	3.366689	3.693294	0.96666
56	H	2.812204	4.622643	1.021586
57	C	0.832661	-3.64806	-0.141
58	H	1.370039	-4.58808	-0.19602
59	C	1.44793	0.03212	-0.06107
60	C	-2.84696	-0.23943	-0.52166
61	H	-2.83254	-0.69969	-1.52975

10-10. Cartesian coordinates for optimized geometry of **D1**.



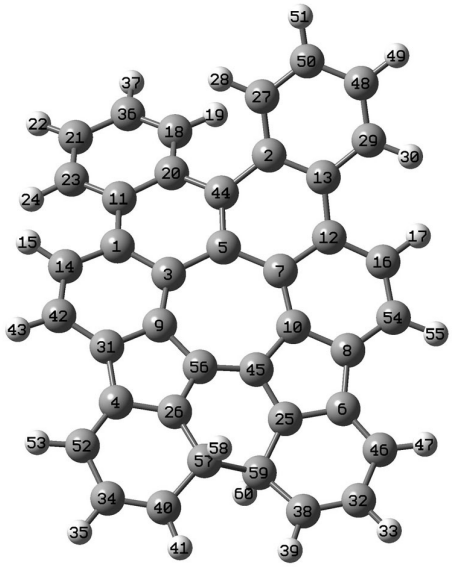
no.	atom	X	Y	Z
1	C	0.531721	2.431327	1.338895
2	C	-0.73972	-1.01411	3.347344
3	C	0.196741	1.279526	0.536599
4	C	-0.61944	2.842128	-2.72572
5	C	0	0	1.195588
6	C	0.619437	-2.84213	-2.72572
7	C	-0.19674	-1.27953	0.536599
8	C	0.229906	-2.87846	-1.31664

no.	atom	X	Y	Z
31	C	-1.77774	-3.21527	3.374698
32	H	-2.03188	-4.14696	2.88207
33	C	-0.22991	2.87846	-1.31664
34	C	1.085358	-1.15221	-4.40976
35	H	1.157211	-0.1188	-4.72756
36	C	1.453387	-3.51217	-4.87165
37	H	1.774527	-4.29071	-5.55701
38	C	-1.45339	3.512167	-4.87165

9	C	-0.08941	1.540506	-0.83823
10	C	0.089407	-1.54051	-0.83823
11	C	1.021084	2.242129	2.697252
12	C	-0.53172	-2.43133	1.338895
13	C	-1.02108	-2.24213	2.697252
14	C	-1.08536	1.15221	-4.40976
15	H	-1.15721	0.118798	-4.72756
16	C	0.409249	3.723984	0.818086
17	H	0.606094	4.572428	1.46284
18	C	-0.40925	-3.72398	0.818086
19	H	-0.60609	-4.57243	1.46284
20	C	1.273888	0.782763	4.64171
21	H	1.140498	-0.18597	5.1079
22	C	0.739716	1.014114	3.347344
23	C	2.261164	2.981429	4.65466
24	H	2.857363	3.741126	5.151034
25	C	1.777739	3.215267	3.374698
26	H	2.031879	4.146958	2.88207
27	C	0.60834	-1.49164	-3.14099
28	C	-0.60834	1.491639	-3.14099
29	C	-1.27389	-0.78276	4.64171
30	H	-1.1405	0.18597	5.1079

39	H	-1.77453	4.290706	-5.55701
40	C	2.020029	1.752348	5.286785
41	H	2.43966	1.550231	6.267243
42	C	1.502003	-2.17358	-5.2707
43	H	1.874356	-1.91939	-6.25827
44	C	-1.502	2.173584	-5.2707
45	H	-1.87436	1.919386	-6.25827
46	C	0	3.963469	-0.49377
47	H	-0.10916	4.980889	-0.8565
48	C	0	0	2.634856
49	C	0.190262	-0.66624	-1.99321
50	C	1.021532	-3.85769	-3.58466
51	H	1.023536	-4.8965	-3.26734
52	C	-2.26116	-2.98143	4.65466
53	H	-2.85736	-3.74113	5.151034
54	C	-2.02003	-1.75235	5.286785
55	H	-2.43966	-1.55023	6.267243
56	C	-1.02153	3.857692	-3.58466
57	H	-1.02354	4.896503	-3.26734
58	C	0	-3.96347	-0.49377
59	H	0.109156	-4.98089	-0.8565
60	C	-0.19026	0.666244	-1.99321

10-11. Cartesian coordinates for optimized geometry of **D2**.



no.	atom	X	Y	Z
1	C	0.314458	2.515318	1.413433
2	C	-0.58464	-1.11335	3.41881
3	C	0.120316	1.332475	0.616999
4	C	-0.17163	2.748767	-2.82177
5	C	0	0	1.269371
6	C	0.171626	-2.74877	-2.82177
7	C	-0.12032	-1.33248	0.616999
8	C	0.07779	-2.9067	-1.34594
9	C	-0.02847	1.610328	-0.76475
10	C	0.028465	-1.61033	-0.76475
11	C	0.713005	2.381941	2.803932
12	C	-0.31446	-2.51532	1.413433
13	C	-0.71301	-2.38194	2.803932
14	C	0.19763	3.800713	0.83323
15	H	0.264193	4.664573	1.483231
16	C	-0.19763	-3.80071	0.83323
17	H	-0.26419	-4.66457	1.483231
18	C	1.135447	0.932904	4.711637
19	H	1.138538	-0.05429	5.156604
20	C	0.584639	1.113351	3.41881

no.	atom	X	Y	Z
31	C	-0.07779	2.906698	-1.34594
32	C	0.021025	-3.02163	-5.24576
33	H	-0.10146	-3.71274	-6.07452
34	C	-0.02103	3.021626	-5.24576
35	H	0.101461	3.712739	-6.07452
36	C	1.720351	1.981657	5.398447
37	H	2.150085	1.81037	6.380828
38	C	0.096282	-1.68776	-5.5025
39	H	0.065212	-1.33178	-6.52856
40	C	-0.09628	1.687758	-5.5025
41	H	-0.06521	1.331775	-6.52856
42	C	0	4.023448	-0.52456
43	H	-0.07132	5.035673	-0.91089
44	C	0	0	2.678052
45	C	0.076988	-0.68437	-1.85553
46	C	0.079609	-3.58564	-3.91061
47	H	-0.00771	-4.66293	-3.79894
48	C	-1.78192	-3.25422	4.811971
49	H	-2.24295	-4.081	5.343898
50	C	-1.72035	-1.98166	5.398447

21	C	1.781916	3.254215	4.811971
22	H	2.242945	4.080996	5.343898
23	C	1.300622	3.442383	3.52883
24	H	1.431473	4.412378	3.063696
25	C	0.209519	-1.35017	-3.07197
26	C	-0.20952	1.350169	-3.07197
27	C	-1.13545	-0.9329	4.711637
28	H	-1.13854	0.054293	5.156604
29	C	-1.30062	-3.44238	3.52883
30	H	-1.43147	-4.41238	3.063696

51	H	-2.15009	-1.81037	6.380828
52	C	-0.07961	3.585644	-3.91061
53	H	0.007712	4.66293	-3.79894
54	C	0	-4.02345	-0.52456
55	H	0.071323	-5.03567	-0.91089
56	C	-0.07699	0.684373	-1.85553
57	C	-0.37221	0.697207	-4.40279
58	H	-1.45186	0.450259	-4.50427
59	C	0.372212	-0.69721	-4.40279
60	H	1.451863	-0.45026	-4.50427