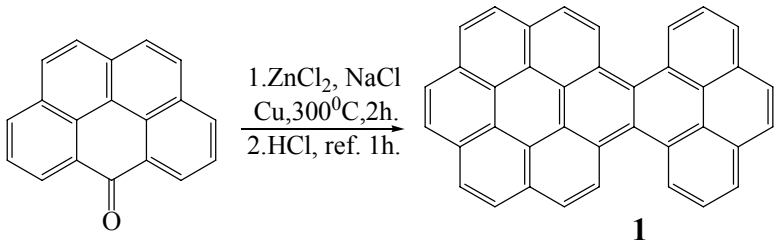
Electronic Supplementary Information

High-performance Single-crystal Field Effect Transistors of Pyreno[4,5-a]coronene

Experimental details

Synthesis of pyreno[4,5-a]coronene: In 1960 E. Clar *et.al*[1] and in 1978 Shoji Fujisawa *et.al*[2] were reported condensation reaction of naphthathrone(benzo[cd]pyren-6-one) at different conditions and isolated series of hydrocarbon isomers. Molecular structure of that compound was assigned only on the basis of UV/Vis spectrum and elemental analysis. Here we introduce a new methodology of condensation reaction of benzo[cd]pyren-6-one to synthesis of pyreno[4,5-a]coronene (Scheme1).



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Scheme 1.

All starting materials were purchased from Aldrich, TCI and Across.

Naphthathrone (**benzo[cd]pyren-6-one):** Benzo[cd]pyren-6-one was obtained by following published procedure.[3]

Pyreno[4,5-a]coronene(1): 7.62g (0.03 mol) of benzo[cd]pyren-6-one was ground up with 6.4g of copper powder and added to a stirred mixture of 41.4g (0.3 mol) zinc chloride and 17.6g (0.3 mol) of sodium chloride at 120 ^{0}C. Reaction mixture was melted and kept at 300 ^{0}C

for 2 h. with constant stirring, then cooled to room temperature and 200 ml of hydrochloric acid (20 %) was added and refluxed for 2 h., insoluble residue was filtered off and washed with water. Residue was refluxed with toluene (200 ml x 5), until solution become almost colorless and solution was isolated by vacuum filtration using filter papers (Whatman, Cat No 1442). The filtrate was combined, dried over $MgSO_4$, passed through a column of silica gel using toluene and evaporation to dryness gave 3.0g (42.1 %) of pure pyreno[4,5-a]coronene as a brownish red crystals.

Instrumentation: ^{1}H NMR spectra were recorded with Bruker AMX 500, proton chemical shifts (δ) are reported in ppm relative to the methine singlet at 7.24 ppm for the residual $CHCl_3$ in the deuteriochloroform. EI-mass spectra were obtained with a JMS-700 double focusing mass spectrometer (JEOL), elemental analysis were done by FlashEA 1112 Series CHNS-O Analyzer. Crystal structure of compound **1** was determined by Bruker X8APEX X-ray diffractometer with Mo Kα radiation (λ = 0.71073 Å).

Molecular structure characterization: Compound **1** was fully characterized by ^{1}H NMR, ^{13}C NMR, DEPT 90, ^{1}H COSY, HETCOR (^{13}C-D), mass and elemental analyses. 500MHz ^{1}H NMR analysis of this compound shows molecule of pyreno[4,5-a]coronene contained one pair of triplet protons with chemical shift at 8.18 ppm, two pairs of singlet protons with the same chemical shift at 8.54 ppm and six pairs of doublet protons with different chemical shifts. 400MHz ^{1}H COSY analysis of compound **1** shows the triplet (J= 7.66 Hz) protons correlate with the neighboring doublets protons of H_2 at 8.36 ppm and H_4 at 9.34 ppm (Fig. S1b). This (H_3) triplet protons at 8.18 ppm belong to the pyrene unit of the compound **1** because of similar chemical shift(8.03 ppm) and the same coupling constant of pyrene molecule. Repulsion between hydrogen atoms of H_5 and H_4 shifted the chemical shift to the 9.52 ppm and 9.34 ppm

respectively. It is interesting that nonequivalent singlet protons of H_1 and H_9 give the same chemical shift at

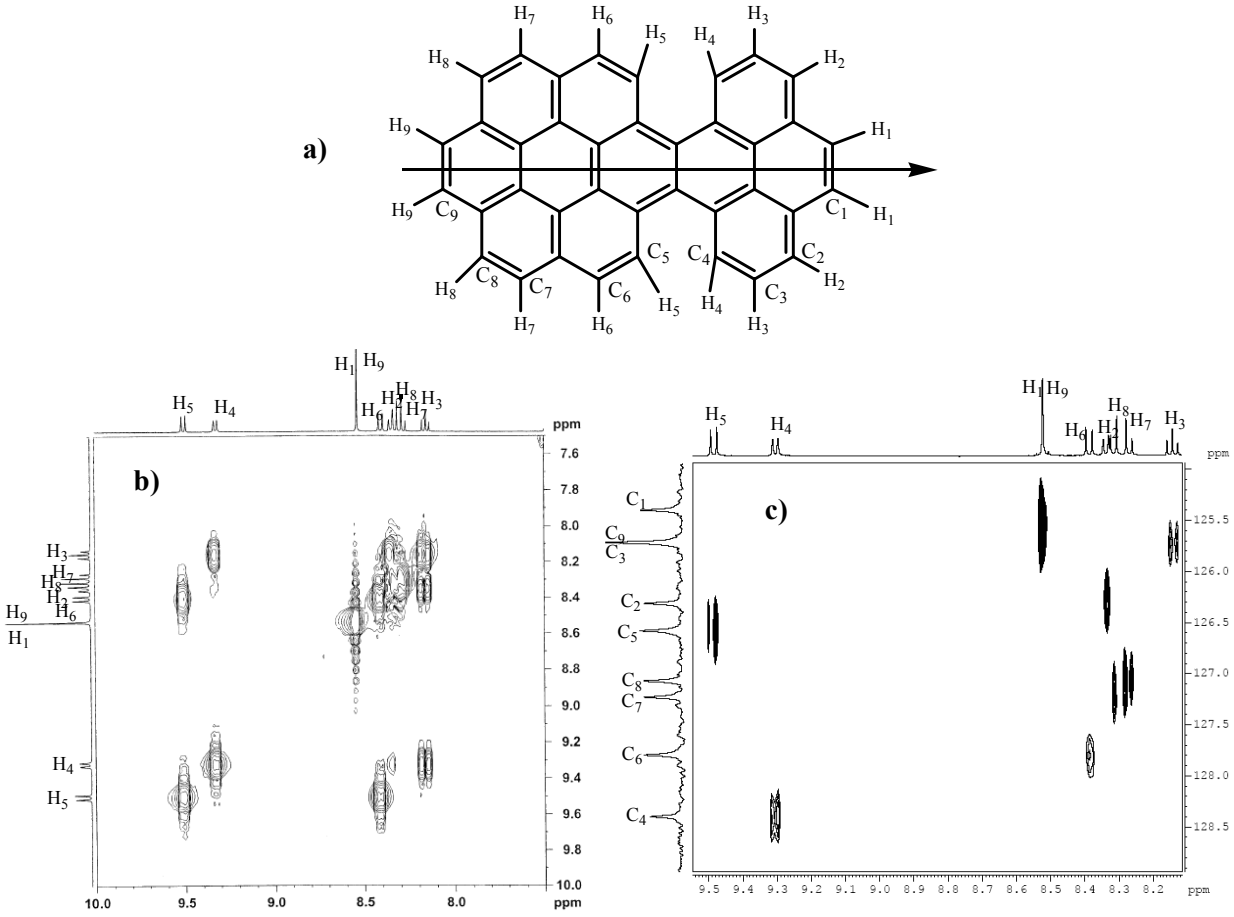


Fig. S1 a) Molecular structure, **b**) 400 MHz ^{1}H COSY NMR, and **c**) 500 MHz HETCOR(^{13}C-D) NMR spectra of pyreno[4,5-a]coronene.

8.54 ppm. In addition, we have analyzed the molecule using HETCOR technique. The result shows that the singlet protons of H_1 and H_9 bonded with unsymmetrical carbon atoms of C_1 at 125.606 ppm and C_9 at 125.921 ppm, respectively (Fig. S1c). Unexpectedly C_3 and C_9 carbon atoms also give the same peaks at 125.921 ppm. ^{13}C NMR and DEPT 90 spectra of this compound shows molecule of **1** contains ten pairs of quaternary carbon atoms and nine pairs of tertiary(CH) carbon atoms. Thus, the structure of pyreno[4,5-a]coronene is completely assigned by this methods.

An analytical sample was prepared by vacuum sublimation at 350^0C (10^{-5} Torr) or by vapor phase transfer method (slow sublimation in a copper tube under argon atomosphere) at 400^0C. MS (EI, 70 eV) 474.14 (M^+). ^{1}H NMR (500 MHz, $CDCl_3$) δ = 9.5234- 9.50534(d, 2H, J = 9.03 Hz); 9.33995-9.32463(d, 2H, J = 7.66 Hz), 8.54298 (s, 4H), 8.42311-8.40504(d, 2H, J = 9.03 Hz); 8.36253- 8.34726(d, 2H, J = 7.64 Hz), 8.33915-8.32171(d, 2H, J = 8.72 Hz), 8.29347- 8.27603(d, 2H, J = 8.72 Hz), 8.17929-8.14847(t, 2H, J = 7.66 Hz). Anal.calc. C 96.18 %, H 3.82 %, Found: C 95.7922 %, H 3.7173 %.

Optical and electrochemical properties: Solution of compounds **1** and pentacene were prepared in dichloromethane and the optical properties were investigated by HP 845x UV/Vis spectrophotometer. We observed that the long-wavelength absorption of pentacene completely decays in 40 min, but we do not find any change of UV-vis spectra of pyreno[4,5-a]coronene even after one hour under same condition (Fig. S2a). Cyclic voltammetry were performed to obtain redox potential (Fig. S2b) and HOMO-LUMO level energies of compound **1** using dichloromethane/Bu_4NPF_6 that showed onset of oxidation potential at 0.695 V versus standard calomel electrode (SCE), respectively.

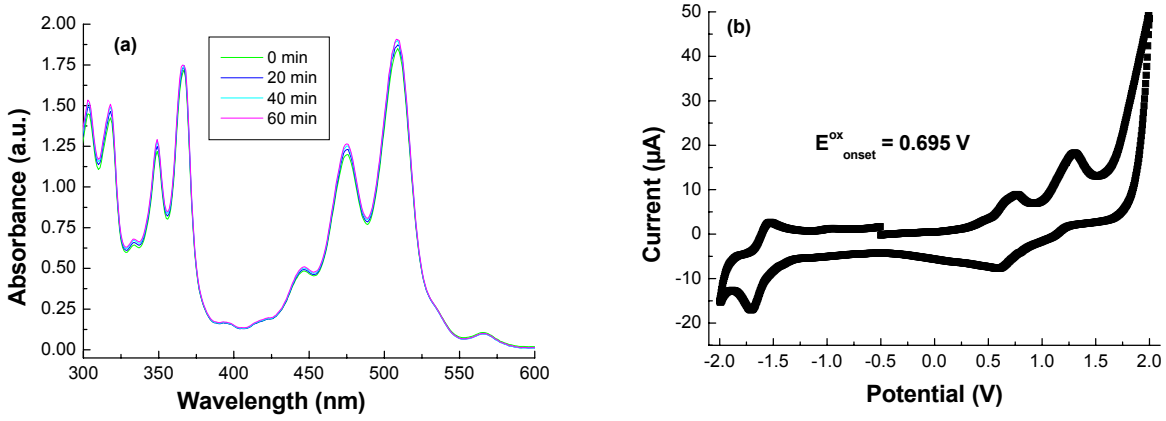


Fig. S2 (**a**) **UV**-vis spectra in $C_2H_2Cl_2$ solution, and (**b**) Cyclic voltammogram of pyreno[4,5-a]coronene.

Crystal growth and structure analysis: In the range of ~ 1.0 - 1.5 cm long and ~ 0.30 - 0.06 mm wide needle like single-crystals of pyreno[4,5-a]coronene were grown by physical vapour transport method[4] in a stream (30cc/min) of highly pure argon at 400^0C(Fig. S3a). To investigate the molecular structure and intermolecular interactions in the solid state, we performed single-crystal structure analysis using Bruker X8APEX X-ray diffractometer with Mo Kα radiation (λ = 0.71073 Å). The data were collected at 150.0(2) K and the structure was solved by SHELX 97 program. The growth direction of single-crystals was confirmed by X-ray structure analysis and was determined short b-axis along the [-100] direction (Fig. S3b).

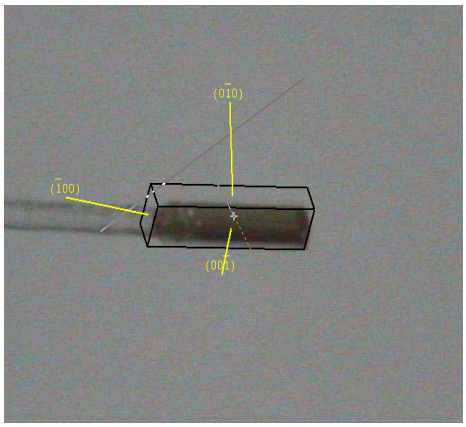
a)  **b)** 

Fig. S3 (**a**) Digital image of single-crystals (**b**) Unit cell exhibiting long a-axis along the (00-1), short b-axis along (-100) and c-axis along (0-10) .

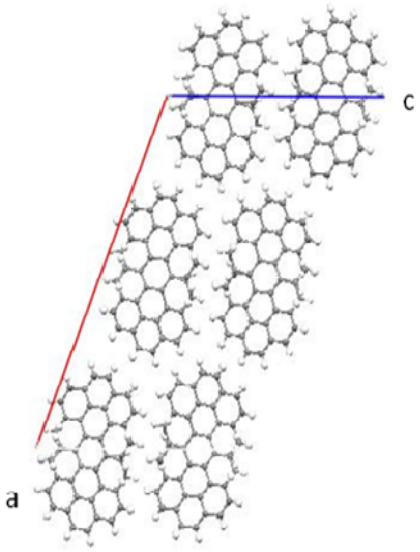


Fig. S4 Unit cell of a pyreno[4,5-a]coronene single-crystal.

References:

1 E. Clar, G. S. Fell, C. T. Ironside and A. Balsillie *Tetrahedron*, 1960, **10**, 26.
2 Sh. Fujisawa, J. Aoki, M. Takekawa and S. Iwashima. *Bull. Chem. Soc. Jpn.*, 1979, **52(7)**, 2159.
3 W. Bradley and F. K. Sutcliffe, *J. Chem. Soc*. 1951, 2118.
4 (a) R. A. Laudise, Ch. Kloc, P. G. Simpkins and T. Siegrist, *J. Cryst. Growth,* 1998, **187**, 449; (b) Roberson, L. B.; Kowalik, J.; Tolbert, L. M.; Kloc, C.; Zeis, R.; Chi, X.; Fleming, R.; Wilkins, C. *J. Am. Chem. Soc.,* 2005, **127**, 3069.15.

Table S1. Crystal data and structure refinement for compound 1.

Identification code	ic13742
Empirical formula	C38 H18
Formula weight	474.52
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic

Space group	C2/c	
Unit cell dimensions	a = 30.567(2) Å	α= 90°.
	b = 3.8084(3) Å	β= 112.436(4)°.
	c = 19.6838(11) Å	γ = 90°.
Volume	2118.0(2) $Å^3$	
Z	4	
Density (calculated)	1.488 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	984	
Crystal size	0.48 x 0.10 x 0.07 mm^3	
Theta range for data collection	1.44 to 25.00°.	
Index ranges	-36<=h<=35, -4<=k<=4, -23<=l<=23	
Reflections collected	4527	
Independent reflections	1871 [R(int) = 0.0443]	
Completeness to theta = 25.00°	99.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.990 and 0.956	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	1871 / 0 / 191	
Goodness-of-fit on F^2	1.014	
Final R indices [I>2sigma(I)]	R1 = 0.0558, wR2 = 0.1379	
R indices (all data)	R1 = 0.0986, wR2 = 0.1762	
Largest diff. peak and hole	0.323 and -0.327 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for compound 1.

C(1)-C(16)#1	1.345(3)
C(1)-C(2)	1.429(3)
C(1)-H(1)	0.9500

C(2)-C(3)	1.406(3)
C(2)-C(7)	1.416(3)
C(3)-C(4)	1.365(3)
C(3)-H(3)	0.9500
C(4)-C(5)	1.403(3)
C(4)-H(4)	0.9500
C(5)-C(6)	1.403(3)
C(5)-C(11')	1.414(4)
C(5)-H(5)	0.9500
C(6)-C(7)	1.421(3)
C(6)-C(8)	1.446(3)
C(7)-C(17)#1	1.428(3)
C(8)-C(9)	1.416(3)
C(8)-C(19)#1	1.425(3)
C(9)-C(19)	1.424(3)
C(9)-C(10)	1.448(5)
C(9)-C(10')	1.469(5)
C(10)-C(11)	1.375(7)
C(10)-H(10)	0.9500
C(11)-C(12)	1.414(5)
C(11)-H(11)	0.9500
C(10')-C(11')	1.339(6)
C(10')-H(10')	0.9500
C(11')-H(11')	0.9500
C(12)-C(13)	1.392(3)
C(12)-C(18)	1.399(3)
C(12)-H(12)	0.9500
C(13)-C(14)	1.367(3)
C(13)-H(13)	0.9500
C(14)-C(15)	1.405(3)
C(14)-H(14)	0.9500
C(15)-C(17)	1.416(3)
C(15)-C(16)	1.432(3)
C(16)-C(1)#1	1.345(3)
C(16)-H(16)	0.9500
C(17)-C(18)	1.425(3)

C(17)-C(7)#1	1.428(3)
C(18)-C(19)	1.450(3)
C(19)-C(8)#1	1.425(3)

C(16)#1-C(1)-C(2)	121.0(2)
C(16)#1-C(1)-H(1)	119.5
C(2)-C(1)-H(1)	119.5
C(3)-C(2)-C(7)	119.1(2)
C(3)-C(2)-C(1)	121.7(2)
C(7)-C(2)-C(1)	119.1(2)
C(4)-C(3)-C(2)	120.6(2)
C(4)-C(3)-H(3)	119.7
C(2)-C(3)-H(3)	119.7
C(3)-C(4)-C(5)	120.8(2)
C(3)-C(4)-H(4)	119.6
C(5)-C(4)-H(4)	119.6
C(6)-C(5)-C(4)	120.9(2)
C(6)-C(5)-C(11')	115.1(2)
C(4)-C(5)-C(11')	123.4(2)
C(6)-C(5)-H(5)	119.6
C(4)-C(5)-H(5)	119.6
C(11')-C(5)-H(5)	8.6
C(5)-C(6)-C(7)	118.1(2)
C(5)-C(6)-C(8)	121.5(2)
C(7)-C(6)-C(8)	120.3(2)
C(2)-C(7)-C(6)	120.4(2)
C(2)-C(7)-C(17)#1	119.7(2)
C(6)-C(7)-C(17)#1	119.9(2)
C(9)-C(8)-C(19)#1	119.4(2)
C(9)-C(8)-C(6)	121.83(19)
C(19)#1-C(8)-C(6)	118.80(19)
C(8)-C(9)-C(19)	120.41(19)
C(8)-C(9)-C(10)	124.2(3)
C(19)-C(9)-C(10)	112.5(3)
C(8)-C(9)-C(10')	112.8(3)
C(19)-C(9)-C(10')	124.0(2)

C(10)-C(9)-C(10')	35.9(3)
C(11)-C(10)-C(9)	123.6(4)
C(11)-C(10)-H(10)	118.2
C(9)-C(10)-H(10)	118.2
C(10)-C(11)-C(12)	124.1(4)
C(10)-C(11)-H(11)	117.9
C(12)-C(11)-H(11)	117.9
C(11')-C(10')-C(9)	123.5(4)
C(11')-C(10')-H(10')	118.3
C(9)-C(10')-H(10')	118.3
C(10')-C(11')-C(5)	123.7(3)
C(10')-C(11')-H(11')	118.1
C(5)-C(11')-H(11')	118.1
C(13)-C(12)-C(18)	121.0(2)
C(13)-C(12)-C(11)	123.9(3)
C(18)-C(12)-C(11)	113.8(3)
C(13)-C(12)-H(12)	119.5
C(18)-C(12)-H(12)	119.5
C(11)-C(12)-H(12)	12.7
C(14)-C(13)-C(12)	121.2(2)
C(14)-C(13)-H(13)	119.4
C(12)-C(13)-H(13)	119.4
C(13)-C(14)-C(15)	120.2(2)
C(13)-C(14)-H(14)	119.9
C(15)-C(14)-H(14)	119.9
C(14)-C(15)-C(17)	119.3(2)
C(14)-C(15)-C(16)	121.9(2)
C(17)-C(15)-C(16)	118.8(2)
C(1)#1-C(16)-C(15)	121.6(2)
C(1)#1-C(16)-H(16)	119.2
C(15)-C(16)-H(16)	119.2
C(15)-C(17)-C(18)	120.2(2)
C(15)-C(17)-C(7)#1	119.7(2)
C(18)-C(17)-C(7)#1	120.12(19)
C(12)-C(18)-C(17)	118.0(2)
C(12)-C(18)-C(19)	122.2(2)

C(17)-C(18)-C(19)	119.7(2)
C(9)-C(19)-C(8)#1	118.57(19)
C(9)-C(19)-C(18)	122.2(2)
C(8)#1-C(19)-C(18)	119.3(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+1/2

Cartesian coordinates of dimer of an enantiomer from the crystal structure

C	10.317495	1.243823	-1.202845
H	11.201257	1.416344	-0.898310
C	9.213357	1.483372	-0.328463
C	9.399828	1.930859	0.991501
H	10.277375	2.107188	1.309822
C	8.332137	2.114043	1.821308
H	8.474816	2.432425	2.703675
C	7.027966	1.837934	1.384475
H	6.299314	1.954851	1.981975
C	6.786683	1.391208	0.076710
C	7.899015	1.239253	-0.794559
C	5.445500	1.135665	-0.399561
C	4.341362	1.059878	0.483285
C	4.436011	0.654664	1.869508
H	5.293497	0.640573	2.277210
C	3.350520	0.289438	2.630686
H	3.493764	0.099018	3.551792
C	2.032504	0.179376	2.131267
C	0.923281	-0.109301	2.921533
H	1.052681	-0.447868	3.799934
C	-0.347551	0.085308	2.456762
H	-1.091743	-0.095210	3.020129
C	-0.558038	0.552599	1.148092
C	-1.872098	0.778056	0.626371
H	-2.625895	0.594491	1.173430
C	0.558814	0.814617	0.318260
C	1.881349	0.664185	0.827623
C	3.016566	0.952481	-0.026916
C	-2.064220	1.243823	-0.621186
H	-2.947983	1.416344	-0.925721
C	-0.960082	1.483372	-1.495567
C	-1.146554	1.930859	-2.815532
H	-2.024101	2.107188	-3.133853
C	-0.078863	2.114043	-3.645339
H	-0.221542	2.432425	-4.527706

C	1.225309	1.837934	-3.208506
C	1.466591	1.391208	-1.900741
C	0.354260	1.239253	-1.029472
C	2.807774	1.135665	-1.424470
C	3.911912	1.059878	-2.307316
C	3.588977	1.523360	-3.662266
H	4.301807	1.630757	-4.283349
C	2.344703	1.803277	-4.071669
H	2.205414	1.988746	-4.992441
C	6.220770	0.179376	-3.955298
H	5.347179	0.044939	-4.305566
C	7.329993	-0.109301	-4.745564
H	7.200593	-0.447868	-5.623965
C	8.600826	0.085308	-4.280793
H	9.345017	-0.095210	-4.844160
C	8.811313	0.552599	-2.972123
C	10.125372	0.778056	-2.450402
H	10.879170	0.594491	-2.997461
C	7.694461	0.814617	-2.142291
C	6.371925	0.664185	-2.651654
C	5.236708	0.952481	-1.797115
C	10.317495	5.052223	-1.202845
H	11.201257	5.224744	-0.898310
C	9.213357	5.291772	-0.328463
C	9.399828	5.739259	0.991501
H	10.277375	5.915588	1.309822
C	8.332137	5.922443	1.821308
H	8.474816	6.240825	2.703675
C	7.027966	5.646334	1.384475
H	6.299314	5.763251	1.981975
C	6.786683	5.199608	0.076710
C	7.899015	5.047653	-0.794559
C	5.445500	4.944065	-0.399561
C	4.341362	4.868278	0.483285
C	4.436011	4.463064	1.869508
H	5.293497	4.448973	2.277210
C	3.350520	4.097838	2.630686
H	3.493764	3.907418	3.551792
C	2.032504	3.987776	2.131267
C	0.923281	3.699099	2.921533
H	1.052681	3.360532	3.799934
C	-0.347551	3.893708	2.456762
H	-1.091743	3.713190	3.020129
C	-0.558038	4.360999	1.148092
C	-1.872098	4.586456	0.626371
H	-2.625895	4.402891	1.173430
C	0.558814	4.623017	0.318260
C	1.881349	4.472585	0.827623

C	3.016566	4.760881	-0.026916
C	-2.064220	5.052223	-0.621186
H	-2.947983	5.224744	-0.925721
C	-0.960082	5.291772	-1.495567
C	-1.146554	5.739259	-2.815532
H	-2.024101	5.915588	-3.133853
C	-0.078863	5.922443	-3.645339
H	-0.221542	6.240825	-4.527706
C	1.225309	5.646334	-3.208506
C	1.466591	5.199608	-1.900741
C	0.354260	5.047653	-1.029472
C	2.807774	4.944065	-1.424470
C	3.911912	4.868278	-2.307316
C	3.588977	5.331760	-3.662266
H	4.301807	5.439157	-4.283349
C	2.344703	5.611677	-4.071669
H	2.205414	5.797146	-4.992441
C	6.220770	3.987776	-3.955298
H	5.347179	3.853339	-4.305566
C	7.329993	3.699099	-4.745564
H	7.200593	3.360532	-5.623965
C	8.600826	3.893708	-4.280793
H	9.345017	3.713190	-4.844160
C	8.811313	4.360999	-2.972123
C	10.125372	4.586456	-2.450402
H	10.879170	4.402891	-2.997461
C	7.694461	4.623017	-2.142291
C	6.371925	4.472585	-2.651654
C	5.236708	4.760881	-1.797115

Cartesian coordinates of dimer stacked with monomer optimized at the B3LYP/6-31G level**

C	-0.000517	2.842934	-0.011146
H	-0.066776	3.398402	0.914820
C	-0.094337	3.524559	-1.199377
H	-0.199832	4.606164	-1.193978
C	-0.110605	3.531293	-3.691074
H	-0.148044	4.617332	-3.685548
C	-0.098840	2.845415	-4.876902
H	-0.124867	3.382597	-5.821230
C	-0.025418	0.685620	-6.119162
H	-0.045182	1.231991	-7.058370
C	0.025418	-0.685620	-6.119162
H	0.045182	-1.231991	-7.058370
C	0.098840	-2.845415	-4.876902
H	0.124867	-3.382597	-5.821230
C	0.110605	-3.531293	-3.691074
H	0.148044	-4.617332	-3.685548

C	0.094337	-3.524559	-1.199377
H	0.199832	-4.606164	-1.193978
C	0.000517	-2.842934	-0.011146
H	0.066776	-3.398402	0.914820
C	-0.110605	-1.421095	0.036567
C	-0.183145	-0.679940	1.280315
C	0.183145	0.679940	1.280315
C	0.110605	1.421095	0.036567
C	-0.069850	2.845091	-2.443120
C	-0.050682	1.421648	-4.902036
C	0.050682	-1.421648	-4.902036
C	0.069850	-2.845091	-2.443120
C	-0.014060	-0.715170	-1.192099
C	0.014060	0.715170	-1.192099
C	-0.028505	1.424909	-2.432269
C	-0.023897	0.712422	-3.670042
C	0.023897	-0.712422	-3.670042
C	0.028505	-1.424909	-2.432269
C	-0.640311	-1.280160	2.537230
C	-1.466334	-2.417010	2.583076
H	-1.809745	-2.868810	1.662054
C	-1.905492	-2.953611	3.795073
H	-2.547230	-3.829680	3.786553
C	-1.530290	-2.378307	5.000263
H	-1.844634	-2.815235	5.944098
C	-0.372981	-0.568276	6.237745
H	-0.679404	-1.028212	7.173394
C	0.372981	0.568276	6.237745
H	0.679404	1.028212	7.173394
C	1.530290	2.378307	5.000263
H	1.844634	2.815235	5.944098
C	1.905492	2.953611	3.795073
H	2.547230	3.829680	3.786553
C	1.466334	2.417010	2.583076
H	1.809745	2.868810	1.662054
C	0.640311	1.280160	2.537230
C	0.353730	0.621026	3.770364
C	-0.353730	-0.621026	3.770364
C	-0.761720	-1.202586	5.009627
C	0.761720	1.202586	5.009627
C	3.734483	2.098834	-0.011146
H	3.668224	2.654302	0.914820
C	3.640663	2.780459	-1.199377
H	3.535168	3.862064	-1.193978
C	3.624395	2.787193	-3.691074
H	3.586956	3.873232	-3.685548
C	3.636160	2.101315	-4.876902
H	3.610133	2.638497	-5.821230

C	3.709582	-0.058480	-6.119162
H	3.689818	0.487891	-7.058370
C	3.760418	-1.429720	-6.119162
H	3.780182	-1.976091	-7.058370
C	3.833840	-3.589515	-4.876902
H	3.859867	-4.126697	-5.821230
C	3.845605	-4.275393	-3.691074
H	3.883044	-5.361432	-3.685548
C	3.829337	-4.268659	-1.199377
H	3.934832	-5.350264	-1.193978
C	3.735517	-3.587034	-0.011146
H	3.801776	-4.142502	0.914820
C	3.624395	-2.165195	0.036567
C	3.551855	-1.424040	1.280315
C	3.918145	-0.064160	1.280315
C	3.845605	0.676995	0.036567
C	3.665150	2.100991	-2.443120
C	3.684318	0.677548	-4.902036
C	3.785682	-2.165748	-4.902036
C	3.804850	-3.589191	-2.443120
C	3.720940	-1.459270	-1.192099
C	3.749060	-0.028930	-1.192099
C	3.706495	0.680809	-2.432269
C	3.711103	-0.031678	-3.670042
C	3.758897	-1.456522	-3.670042
C	3.763505	-2.169009	-2.432269
C	3.094689	-2.024260	2.537230
C	2.268666	-3.161110	2.583076
H	1.925255	-3.612910	1.662054
C	1.829508	-3.697711	3.795073
H	1.187770	-4.573780	3.786553
C	2.204710	-3.122407	5.000263
H	1.890366	-3.559335	5.944098
C	3.362019	-1.312376	6.237745
H	3.055596	-1.772312	7.173394
C	4.107981	-0.175824	6.237745
H	4.414404	0.284112	7.173394
C	5.265290	1.634207	5.000263
H	5.579634	2.071135	5.944098
C	5.640492	2.209511	3.795073
H	6.282230	3.085580	3.786553
C	5.201334	1.672910	2.583076
H	5.544745	2.124710	1.662054
C	4.375311	0.536060	2.537230
C	4.088730	-0.123074	3.770364
C	3.381270	-1.365126	3.770364
C	2.973280	-1.946686	5.009627
C	4.496720	0.458486	5.009627