Supporting Information for

Lowering Inversion Barriers of Buckybowls by Benzannelation of the Rim: Synthesis and Crystal and Molecular Structure of 1,2- Dihydrocyclopenta[b,c] dibenzo[g,m]corannulene

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5,8-Bis(2-bromophenyl)-1,2-dihydrocyclopenta[c,d]fluoranthene (6). A solution of 2g of NaOH in 100 mL of methanol was added to a suspension 1,2-diketopyracene (**4**, 10 mmol) and 1,3-bis(2-bromophenyl)-2-propanone (10mmol) in 130 mL of methanol. The suspension was allowed to stir overnight at room temperature, the dark brown precipitate was separated, washed with methanol and dried to yield almost quantitatively (5.36g) cyclopentadienone **5**, which was used in the next step without further purification.

The crude product **5** (5 mmol) was transferred to a 200 mL thick-wall reaction vessel and 2,5-norbornadiene (20 mL) and acetic anhydride (70 mL) were added. The vessel was sealed and placed in an oil bath at 160^{0}C for 24 h. ***Caution: Due to a possibility of explosion the reaction was carried out in a well ventilated hood behind a heavy-duty safety screen***. After cooling the mixture was poured onto ice and the dark brown solid was separated and chromatographed on silica gel with hexane/DCM (10:1) to provide 2.35g (88%) of **6**. Yellowish needles, mp 278-280^{0}C. ^{1}HNMR (300 MHz, $CDCl_3$) δ 7.81 (2H, d, J = 8.4 Hz), 7.63-7.56 (m, 2H), 7.53-7.49 (m, 2H), 7.42-7.38 (m, 2H), 7.29 (s, 2H), 7.20 (2H, d, J = 7.2 Hz), 6.88 (2H, d, J = 6.8 Hz), 3.44 (s, 4H); ^{13}C NMR (75.4 MHz, $CDCl_3$) δ 146.38, 141.97, 136.89, 133.28, 133.21, 132.01, 131.64,

131.32, 129.60, 127.97, 127.84, 127.80, 124.65, 123.88, 121.01, 32.47. HRMS (EI, 70 eV): Calcd for $C_{30}H_{14}Br_2$: 531.9462, found: 531.9466.

1,2-Dihydro cyclopenta[b,c]dibenzo[g,m]corannulene (3). 2 mmol of **6**, bis(tricyclohexylphosphine)palladium(II) chloride (0.2 mmol) in the presence of DBU (6 mmol) were dissolved in 10 mL of N,N- dimethylacetamide and the mixture was stirred under argon at 145^0C for 2 days. After cooling, the dark mixture was diluted with dichloromethane and washed three times with 10% HCl. The combined organic layers were dried over $MgSO_4$ and the solvents were removed under reduced pressure. Based on integration of benzylic protons ^{1}HNMR of the crude material shows the presence of three products in the ratio of 59% of **3**, 38% of **7** and 3% of **8**. The desired product **3** was isolated by flash chromatography with hexane/DCM (10:1) to give pale yellow solid in 36% yield. Mp. 256 - 258^0C; ^{1}HNMR (300 MHz, $CDCl_3$): 8.67-8.58 (m, 4H), 8.23 (s, 2H), 7.76 (s, 2H), 7.74-7.70 (m, 4H), 3.84, 3.09 (m, 4H). ^{13}C NMR (75.4 MHz, $CDCl_3$): 149.61, 144.15, 138.96, 135.92, 135.26, 134.33, 133.73, 128.18, 127.56, 127.51, 125.17, 125.15, 124.63, 120.35, 32.42. MS (EI, 70 eV) m/z (rel. intensity) 376 (100). HRMS (EI, 70 eV): Calcd for C_{30}H16: 376.1252, found: 376.1258.

Crystallographic Information File (CIF) for **3**.

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C28 C29 1.525(2) . ?
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C29 C30 1.565(3) . ?
C31 C36 1.374(3) . ?
C31 C32 1.377(4) . ?
C32 C33 1.362(3) . ?
C33 C34 1.371(3) . ?
C34 C35 1.403(3) . ?
C35 C36 1.387(3) . ?
C35 C38 1.489(3) . ?

loop_
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 _geom_angle_atom_site_label_2
 _geom_angle_atom_site_label_3
 _geom_angle
 _geom_angle_site_symmetry_1
 _geom_angle_site_symmetry_3
 _geom_angle_publ_flag
C2 C1 C6 121.80(16) . . ?
C1 C2 C3 120.16(15) . . ?
C4 C3 C2 119.94(17) . . ?
C3 C4 C5 121.69(16) . . ?
C4 C5 C6 118.07(13) . . ?
C4 C5 C14 121.43(14) . . ?
C6 C5 C14 120.38(13) . . ?
C1 C6 C5 118.32(14) . . ?
C1 C6 C7 120.97(14) . . ?
C5 C6 C7 120.63(12) . . ?
C12 C7 C8 117.51(14) . . ?
C12 C7 C6 114.27(13) . . ?
C8 C7 C6 126.77(13) . . ?
C9 C8 C7 120.22(14) . . ?
C8 C9 C10 119.73(14) . . ?
C8 C9 C30 132.35(15) . . ?
C10 C9 C30 106.06(14) . . ?
C11 C10 C28 120.20(14) . . ?
C11 C10 C9 120.60(14) . . ?
C28 C10 C9 114.77(13) . . ?
C10 C11 C12 119.72(13) . . ?
C10 C11 C19 120.12(13) . . ?
C12 C11 C19 110.08(13) . . ?
C7 C12 C11 121.77(13) . . ?
C7 C12 C13 123.05(14) . . ?
C11 C12 C13 106.93(12) . . ?
C14 C13 C18 122.35(13) . . ?
C14 C13 C12 122.74(13) . . ?
C18 C13 C12 108.15(13) . . ?
C13 C14 C15 115.10(12) . . ?
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C15 C14 C5 128.37(14) . . ?
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C18 C17 C16 115.33(13) . . ?
C18 C17 C22 115.53(14) . . ?
C16 C17 C22 127.37(14) . . ?
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C17 C18 C19 122.82(13) . . ?
C13 C18 C19 108.15(13) . . ?
C20 C19 C11 121.38(14) . . ?
C20 C19 C18 123.03(14) . . ?
C11 C19 C18 106.66(13) . . ?
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C19 C20 C27 117.37(14) . . ?
C19 C20 C21 115.00(14) . . ?
C27 C20 C21 125.78(13) . . ?
C26 C21 C22 117.74(14) . . ?
C26 C21 C20 121.69(15) . . ?
C22 C21 C20 120.47(12) . . ?
C23 C22 C21 118.45(13) . . ?
C23 C22 C17 121.17(15) . . ?
C21 C22 C17 120.24(13) . . ?
C24 C23 C22 121.58(17) . . ?
C23 C24 C25 119.87(16) . . ?
C26 C25 C24 120.31(15) . . ?
C25 C26 C21 122.01(17) . . ?
C28 C27 C20 120.47(14) . . ?
C27 C28 C10 119.78(14) . . ?
C27 C28 C29 132.24(15) . . ?
C10 C28 C29 106.15(14) . . ?
C28 C29 C30 105.60(14) . . ?
C9 C30 C29 105.38(14) . . ?
C36 C31 C32 121.3(2) . . ?
C33 C32 C31 118.7(2) . . ?
C32 C33 C34 121.2(2) . . ?
C33 C34 C35 120.8(2) . . ?
C36 C35 C34 117.5(2) . . ?
C36 C35 C38 122.5(2) . . ?
C34 C35 C38 120.0(2) . . ?
C31 C36 C35 120.5(2) . . ?

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_diffrn_reflns_theta_full              28.33
_diffrn_measured_fraction_theta_full   0.959
_refine_diff_density_max    0.156
_refine_diff_density_min   -0.230
_refine_diff_density_rms    0.045
```

Gaussian94 archive files for **3** and **9**.

3, bowl (C_s symmetry)

```
1\1\ISU-SECOND\FOpt\RB3LYP\3-21G\C30H16\ASYGULA\12-Jul-2001\0\\#BECKE3
 LYP/3-21G OPT GEOM=(NODISTANCE,NOANGLE), SCF=DIRECT GUESS=HUCKEL\\cycl
 openta dibezo Corannulene, Cs symmetry\\0,1\C,-0.8487759312,1.06163199
 27,-0.7124236646\C,1.3383916231,1.0499556994,0.\C,-0.8487759312,1.0616
 319927,0.7124236646\C,0.5218073017,1.0359471391,-1.1630447732\C,0.5218
 073017,1.0359471391,1.1630447732\C,-1.8867362091,0.5214980317,-1.44942
 18322\C,-1.8867362091,0.5214980317,1.4494218322\C,0.913377085,0.374824
 5911,-2.3178254212\C,0.913377085,0.3748245911,2.3178254212\C,2.5342766
 658,0.3783656085,0.\C,-3.0448221398,0.1369014573,-0.6966285223\C,-3.04
 48221398,0.1369014573,0.6966285223\C,2.2422679431,-0.2124168301,-2.340
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251405\C,2.2422679431,-0.2124168301,2.340251405\C,-0.1785229122,0.0860
190224,-3.270902092\C,-0.1785229122,0.0860190224,3.270902092\C,-1.5621
538341,0.1697597751,-2.845386895\C,-1.5621538341,0.1697597751,2.845386
895\C,3.0256423432,-0.2206513567,-1.1945054162\C,3.0256423432,-0.22065
13567,1.1945054162\C,0.0922437079,-0.3147660929,-4.5930651429\C,0.0922
437079,-0.3147660929,4.5930651429\C,-2.5685948629,-0.1546005562,-3.774
551643\C,-2.5685948629,-0.1546005562,3.774551643\C,-0.9267259124,-0.62
07286629,-5.4840001526\C,-0.9267259124,-0.6207286629,5.4840001526\C,-2
.2642088639,-0.5403721329,-5.0723099284\C,-2.2642088639,-0.5403721329,
5.0723099284\C,4.254731127,-1.0560934987,-0.7997309065\C,4.254731127,-
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,5.1789994523,-0.6086426239,1.1805576189\H,4.1800385044,-2.0773508632,
-1.1849082191\H,4.1800385044,-2.0773508632,1.1849082191\H,2.543442622,
-0.7942773002,-3.2042580008\H,2.543442622,-0.7942773002,3.2042580008\H
,-3.9059548151,-0.2745476916,-1.21060353\H,-3.9059548151,-0.2745476916
,1.21060353\H,1.1233394506,-0.3617148763,-4.9239479766\H,1.1233394506,
-0.3617148763,4.9239479766\H,-3.6057251737,-0.0836936345,-3.4676146304
\H,-3.6057251737,-0.0836936345,3.4676146304\H,-0.6881272414,-0.9136371
12,-6.4996222945\H,-0.6881272414,-0.913637112,6.4996222945\H,-3.061190
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28H16)]\\@

Becke3LYP/6-31G**//Becke3LYP/321G HF=-1152.88144 hartree

Becke3LYP/321G Zero Point Energy = 226.9 kcal/mol

3, planar (C_{2v} symmetry)

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SCF=(DIRECT) GUESS=HUCKEL OPT GEOM=(NODISTANCE,NOANGLE)\\dibenzo dihydroCPC, pl
anar\\0,1\C,-0.9332056436,0.,-0.7029102614\C,1.1788421728,0.,0.\C,-0.9332056436,
0.,0.7029102614\C,0.4089790219,0.,-1.1422787462\C,0.4089790219,0.,1.1422787462\C
,-2.0299832725,0.,-1.5026964375\C,-2.0299832725,0.,1.5026964375\C,0.9242227699,0
.,-2.4028145136\C,0.9242227699,0.,2.4028145136\C,2.5090660428,0.,0.\C,-3.2545126
865,0.,-0.7076191628\C,-3.2545126865,0.,0.7076191628\C,-1.6338532794,0.,-2.95280
87353\C,-1.6338532794,0.,2.9528087353\C,-0.2062811782,0.,-3.3928819\C,-0.2062811
782,0.,3.3928819\C,2.4188040098,0.,-2.4360394004\C,2.4188040098,0.,2.4360394004\
C,3.180871387,0.,-1.2430691388\C,3.180871387,0.,1.2430691388\C,4.6794363767,0.,-
0.8165688653\C,4.6794363767,0.,0.8165688653\H,-4.2216707196,0.,-1.1985636017\H,-
4.2216707196,0.,1.1985636017\C,-2.6187268999,0.,-3.9534662092\C,-2.6187268999,0.
,3.9534662092\C,0.0480615291,0.,-4.7734976375\C,0.0480615291,0.,4.7734976375\H,2
.9240621162,0.,-3.3956064692\H,2.9240621162,0.,3.3956064692\H,5.2015270571,0.888
8298831,-1.1845511312\H,5.2015270571,0.8888298831,1.1845511312\H,5.2015270571,-0
.8888298831,-1.1845511312\H,5.2015270571,-0.8888298831,1.1845511312\C,-2.3069723
108,0.,-5.3083237465\C,-2.3069723108,0.,5.3083237465\C,-0.9705122527,0.,-5.71928
85334\C,-0.9705122527,0.,5.7192885334\H,-3.6595149076,0.,-3.6479897363\H,-3.6595
149076,0.,3.6479897363\H,1.0811062489,0.,-5.10410793\H,1.0811062489,0.,5.1041079
3\H,-3.1019898357,0.,-6.0446931129\H,-3.1019898357,0.,6.0446931129\H,-0.72673708
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Becke3LYP/6-31G**//Becke3LYP/321G HF=-1152.84978 hartree

Becke3LYP/321G Zero Point Energy = 226.3 kcal/mol, one imaginary frequency: 119*i*

9, bowl (C_s symmetry)


```
1\1\ISU-FIRST\FOpt\RB3LYP\3-21G\C22H12\ASYGULA\16-Jul-2001\0\\#BECKE3L
 YP/3-21G OPT SCF=DIRECT GUESS=HUCKEL GEOM=(NODISTANCE,NOANGLE)\\dihydr
 oCPC, bowl Cs, becke3lyp/3-21g\\0,1\C,-1.3840459687,-0.9192466667,-0.7
 167675148\C,0.7969247926,-0.9386093002,0.\C,-1.3840459687,-0.919246666
 7,0.7167675148\C,-0.0257348063,-0.9077529892,-1.1634111327\C,-0.025734
 8063,-0.9077529892,1.1634111327\C,-2.4065149958,-0.3300780592,-1.44839
 347\C,-2.4065149958,-0.3300780592,1.44839347\C,0.368445451,-0.22496918
 81,-2.3159336306\C,0.368445451,-0.2249691881,2.3159336306\C,1.98929213
 64,-0.2675293887,0.\C,-3.5805268614,0.0483896307,-0.6925461084\C,-3.58
 05268614,0.0483896307,0.6925461084\C,-2.0427444016,0.1099985731,-2.779
 3608173\C,-2.0427444016,0.1099985731,2.7793608173\C,-0.7211463846,0.16
 97619426,-3.1880951802\C,-0.7211463846,0.1697619426,3.1880951802\C,1.7
 172308094,0.3288523328,-2.3437251548\C,1.7172308094,0.3288523328,2.343
 7251548\C,2.4959267598,0.3227764207,-1.1979945489\C,2.4959267598,0.322
 7764207,1.1979945489\C,3.7454686599,1.1263125528,-0.7999871999\C,3.745
 4686599,1.1263125528,0.7999871999\H,-4.4424329936,0.4440336971,-1.2198
 127767\H,-4.4424329936,0.4440336971,1.2198127767\H,-2.8127919293,0.511
 2989085,-3.430266709\H,-2.8127919293,0.5112989085,3.430266709\H,-0.488
 4137986,0.6229696455,-4.1463587423\H,-0.4884137986,0.6229696455,4.1463
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 7285,3.2173166572\H,4.6581445276,0.6536183531,-1.1783822138\H,4.658144
 5276,0.6536183531,1.1783822138\H,3.7003178039,2.1490674359,-1.18575199
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```


Becke3LYP/6-31G**//Becke3LYP/321G HF=-845.57210hartree

Becke3LYP/321G Zero Point Energy = 167.6 kcal/mol

9, planar (C_{2v} symmetry)


```
1\1\ISU-FIRST\FOpt\RB3LYP\3-21G\C22H12\ASYGULA\16-Jul-2001\0\\#BECKE3L
 YP/3-21G SCF=(DIRECT) GUESS=HUCKEL OPT GEOM=(NODISTANCE,NOANGLE)\\dihy
 droCPC, planar C2v by becke3LYP 3-21g\\0,1\C,-1.4666272354,0.,-0.70514
 33082\C,0.6359378787,0.,0.\C,-1.4666272354,0.,0.7051433082\C,-0.136836
 2625,0.,-1.1406067336\C,-0.1368362625,0.,1.1406067336\C,-2.5588197098,
 0.,-1.5166506698\C,-2.5588197098,0.,1.5166506698\C,0.3647741585,0.,-2.
 4133206805\C,0.3647741585,0.,2.4133206805\C,1.9605735748,0.,0.\C,-3.79
 20925332,0.,-0.7046083404\C,-3.7920925332,0.,0.7046083404\C,-2.1298597
 222,0.,-2.9339358803\C,-2.1298597222,0.,2.9339358803\C,-0.7809188683,0
 .,-3.3527846157\C,-0.7809188683,0.,3.3527846157\C,1.8703698116,0.,-2.4
 429475808\C,1.8703698116,0.,2.4429475808\C,2.6300255057,0.,-1.24953446
 83\C,2.6300255057,0.,1.2495344683\C,4.1291619424,0.,-0.8177016417\C,4.
 1291619424,0.,0.8177016417\H,-4.758453919,0.,-1.1976871131\H,-4.758453
 919,0.,1.1976871131\H,-2.882673007,0.,-3.7152976223\H,-2.882673007,0.,
 3.7152976223\H,-0.6012122799,0.,-4.4228064763\H,-0.6012122799,0.,4.422
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 ,4.651894059,0.8888318459,-1.1847644664\H,4.651894059,0.8888318459,1.1
 847644664\H,4.651894059,-0.8888318459,-1.1847644664\H,4.651894059,-0.8
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888318459,1.1847644664\\Version=IBM-RS6000-G94RevE.2\State=1-A1\HF=-84
0.8441484\RMSD=6.994e-09\RMSF=6.425e-05\Dipole=0.4784936,0.,0.\PG=C02V
[C2(C1C1),SGV(C20H8),X(H4)]\\@

Becke3LYP/6-31G**//Becke3LYP/321G HF=-845.53291hartree

Becke3LYP/321G Zero Point Energy = 167.1 kcal/mol, one imaginary frequency: 141*i*