Supplementary Material (ESI) for Chemical Communications

Electronic Supplementary Information: Cartesian coordinates, drawings, and total energies of optimized structures (minima on S_0); Tables of X-ray data for cc-DPB consisting of crystallographic parameters, positional parameters, bond distances, bond angles, and torsional angles and .cif file

Photoisomerization of *cis,cis*-1,4-diphenyl-1,3-butadiene in glassy media at 77 K: The Bicycle-Pedal mechanism

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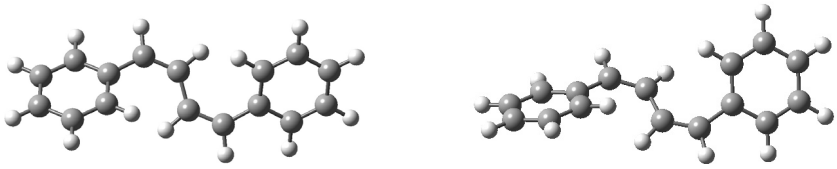
The description of individual conformers from the theoretical calculations utilizes conventional abbreviations: *Z* and *E* denote cis and trans geometries about the CC double bonds, respectively; the letters *c* and *t* refer to s-cis and s-trans geometries about essential CC single bonds, respectively; (-) or (+) indicate the sign of the torsional angle according to the convention of Klyne and Prelog.[1] For extensive calculations on the trans,trans isomer and its X-ray structure see reference 2.

***Table S1*: *cc*-DPB** S_0 min *E* = -618.1528732 a.u. [RB3LYP/6-31+G(d,p)]
conformer: (+)*cZt*(+)*cZ* phenyl angles are +31.0 and +31.9



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C	-0.4935938357,-0.4050232981,5.1280988522
C	0.6619640594,0.3784376041,5.2115074411
H	2.0816645614,1.5673878434,4.1051217476
H	1.0062413793,1.1755465216,1.922021872
H	-1.9945260745,-1.2426975079,3.8351601049
H	-0.927913995,-0.8333261018,6.0270486935
H	1.1295390745,0.564009407,6.174053261
C	-1.2279479006,-0.3876253782,1.430007835
C	-0.702827466,-0.4836055525,0.1819251119
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H	1.4070230852,-0.6618040361,0.6277613507
C	0.5502063887,-0.1060651207,-2.7032893878
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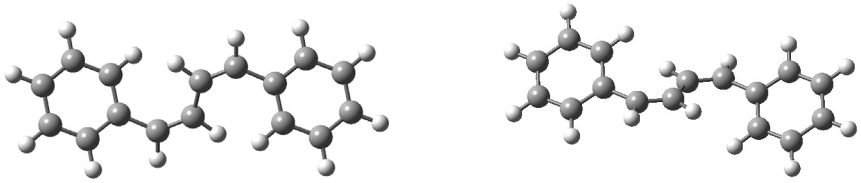
C	0.4935370172,-0.405016917,-5.1281257826
C	1.0951498742,-0.6345636534,-3.8919566342
H	-1.0062101081,1.175389181,-1.9219229864
H	-2.08170926,1.5673226033,-4.1049747352
H	-1.1296403209,0.5640469525,-6.1739827628
H	0.9278266128,-0.833282527,-6.0271081187
H	1.9945189562,-1.2427367742,-3.8352729581

***Table S2*: *cc*-DPB** S_0 min *E* = -618.1504768 [RB3LYP/6-31+G(d,p)] (1.50 kcal/mol higher than above global ***cc*-DPB** minimum
conformer: (-)*cZt*(+)*cZ* phenyl angles are -39.6 and +39.6
Charge = 0 Multiplicity = 1



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C	3.7964696536,-0.8743810955,-0.9986579639
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C	5.2989576896,0.0317475032,0.6683674409
H	4.4613538024,1.567641579,1.9305578444
H	2.2426689747,1.5137933127,0.857167849
H	3.6158319795,-1.5506146936,-1.8304649425
H	5.8464987506,-1.4843535866,-0.7674383874
H	6.2799101294,0.066901546,1.1331780065
C	1.4376030779,-0.1338029652,-1.2169031585
C	0.1849120764,-0.0575386967,-0.6996019479
C	-0.1847535434,0.0607682106,0.6990322596
H	-0.6299963798,-0.1055155651,-1.4154961645
C	-1.4374835112,0.1360400246,1.2164061734
H	1.5036619163,-0.2999286558,-2.2916363948
H	-1.5035623612,0.3025066695,2.2910846128
H	0.6301399569,0.1097202046,1.414874075
C	-2.742798643,0.0612464982,0.5360103261
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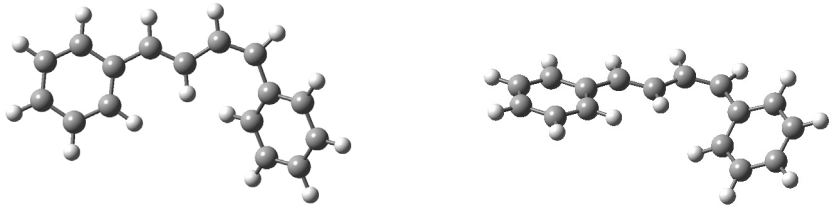
H	-3.617760469,1.5487146139,1.8318547909
H	-5.8486373605,1.4798295912,0.7694681777
H	-6.2801640902,-0.0704344453,-1.1323907326
H	-4.4594794643,-1.5676212418,-1.931594692
H	-2.240611765,-1.5112519457,-0.8588152313

Table S3*: *tc-DPB S_0 min *E* = -618.157194 a.u. [RB3LYP/6-31+G(d,p)]
conformer: (+)*cEtZ*, phenyl angles are +2.6 and +35.4.
Charge = 0 Multiplicity = 1



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C	1.2744617379,0.1174779932,-2.4560037312
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C	3.6249093375,-0.1312729002,-1.9643460641
C	3.9115095242,-0.1689566804,-3.3291605479
C	2.8794409849,-0.0642075649,-4.2646780508
H	0.7505736556,0.1662214213,-4.5379652725
H	0.2440707605,0.2376428108,-2.1362516695
H	4.4342006476,-0.2139477183,-1.2430345979
H	4.939924991,-0.2797333884,-3.6610827613
H	3.0975204576,-0.0920725804,-5.3281683188
C	2.0658860162,0.0407454243,-0.0514735653
C	0.8741777801,0.1224007532,0.5886473037
C	0.7620093731,0.1871310127,2.0305263941
H	-0.0447833521,0.1751062898,0.0120955184
C	-0.3674236541,0.2043155555,2.7839254177
H	2.9656130926,-0.0152879259,0.5620463462
H	-0.2343359704,0.374301538,3.8514199341
H	1.7061535825,0.2800779967,2.5667861467
C	-1.7686218359,0.0568137186,2.3607703977
C	-2.7693899867,0.7559740986,3.0662796989
C	-4.1131041413,0.6509926375,2.7097738413
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H	-2.4807453604,1.3981223132,3.8946204441
H	-4.8627108349,1.2099575842,3.2628472507
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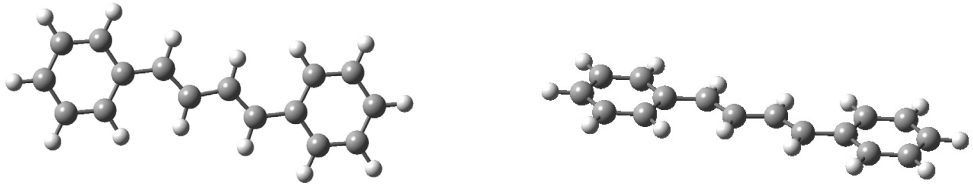
H	-3.8099075784,-1.5659652513,0.1485161429
H	-1.4371760004,-1.3952579354,0.7938354292

***Table S4*: *tt*-DPB** S_0 min *E* = -618.1623714 a.u. [RB3LYP/6-31+G(d,p)]
conformer: *EtE* strictly planar (phenyl angles are 180°).
Charge = 0 Multiplicity = 1



C	0.0701429012,-0.0034466878,-5.1818142947
C	-0.0346424637,-0.002500134,-3.7932693792
C	1.1173969219,-0.0029341062,-2.978326728
C	2.3730396554,-0.0044146925,-3.6190084145
C	2.4785610748,-0.0053543465,-5.0100136161
C	1.3265320379,-0.0048719239,-5.8001540579
H	-0.8320480171,-0.0031062557,-5.7871314748
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H	3.2748726842,-0.0048041174,-3.0116504029
H	3.4598893424,-0.0064655292,-5.4759472464
H	1.4035535888,-0.0056316651,-6.8833739113
C	1.0718132462,-0.0020250398,-1.5154185869
C	-0.0268300179,-0.0009510212,-0.7211749041
C	0.0269052626,0.0002291833,0.7211933624
H	-1.0209905324,-0.0008487968,-1.1660590317
C	-1.0717299552,0.0015455142,1.5154316114
H	2.0461521015,-0.001790575,-1.0262629375
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H	1.0210745094,0.0003168874,1.1660701357
C	-1.1173359048,0.0028856361,2.9783373914
C	-2.3730139041,0.0034752962,3.6189337718
C	-2.4786224516,0.0047203725,5.0099320314
C	-1.3266452727,0.0053575459,5.8001372209
C	-0.0702168124,0.0047339782,5.181877344
C	0.0346642347,0.0035005188,3.7933394775
H	-3.2748069884,0.0029693886,3.0115200597
H	-3.4599771342,0.0051753996,5.4758140674
H	-1.4037500132,0.0062794877,6.8833516179
H	0.8319349397,0.0051807885,5.7872494241
H	1.0206585433,0.0030070782,3.3392774417

X-Ray structure. *cis,cis*-1,4-Diphenyl-1,3-butadiene (***cc*-DPB**) was recrystallized from methanol (see ref 13 in manuscript). Crystals were mounted on a nylon loop with glue. The sample temperature was

held at either -100 or -173 ^{o}C for data collection and six full data sets, taken on four different crystals using a Bruker SMART APEX diffractometer at a detector distance of 5 cm, yielded essentially identical results. The number of frames taken was typically 2400 using 0.3 degree omega scans at 20 s frame collection time. The first 50 frames were repeated at the end of data collection and no significant crystal decomposition in the course of the measurements was detected. Integration was performed using the program SAINT which is part of the Bruker suite of programs. Absorption corrections were made using SADABS. XPREP was used to suggest the space groups and the structure was solved by direct methods and refined by SHELXTL. The non-hydrogen atoms were refined anisotropically. Most of the hydrogen atoms could be found during refinement, but in practice, they were computed and placed as a riding model. Selected crystal data are shown in the attached tables. Hydrogen atoms were often omitted in areas of disorder.

Interestingly, depending upon the random selection of reflections, the indexing program in SMART produced: (i) a monoclinic cell of approximate dimensions a = 7.140 Å, b = 7.126 Å, c = 22.660 Å, $\alpha = 90^{o}$, $\beta = 92.132^{o}$, $\gamma = 90^{o}$ with a volume of 1152.49 Å^3, (ii) a triclinic cell with the initial two distances a little over 10 Å doubling the volume of the cell in (i), or (iii) again a monoclinic cell with the initial values above 14 Å quadrupling the cell volume in (i).

Numerous space groups were attempted with each of those three space groups. Also, calculations were done based on the assumption that the monoclinic cells were only accidentally monoclinic. The most chemically reasonable structures were obtained by using space groups P2(1) or P2(1)/c with the smallest cell and Cc with the largest cell. Throughout all the solution attempts–the better space groups and some of the less successful ones–two features recurred. First, it was clear that in the crystal the molecule exists in two fundamentally different conformations–one with the phenyl groups oriented in parallel planes and the other with the phenyl groups oriented in almost perpendicular planes. Second, the packing of the phenyl groups of adjacent molecules was always edge to face.

Thus the structure found for the P2(1) space group, shown in Figure 1S, clearly reveals a form of disorder. The asymmetric unit showed two C_{16} molecules plus extra areas of significant electron density which were treated as carbon atoms. Those carbon atoms of the diene moiety appeared to form a central "chain" composed of less than full atoms. The R value improved noticeably when the site occupancy factor (SOF) value of the "extra" carbons was reduced from 1.0 to 0.5. When the SOF was allowed to refine

freely during least squares refinement, the value remained very close to 0.5. Expansion of the structure around the "chain" of the asymmetric unit, revealed the edge to face packing. The exact kind of molecular arrangement that leads to the disorder seen around the carbon atoms 8 and 9 is not immediately obvious. However, graphic manipulation revealed that the average of a layer of edge to face molecules with parallel phenyl groups with a layer of molecules (again edge to face) with phenyl groups in roughly perpendicular planes yields the observed "chain" pattern. In addition, when the "chain" is extended, one can readily pick out either "parallel" or "perpendicular" molecules.

The problem with the P2(1) space group is that it shows signs that a non-centrosymmetric space group was selected when a centrosymmetric one should have been chosen instead. The latter was often recommended by the program PLATON. Another anomaly concerning the choice of space group is revealed by the carbon-carbon distances in the phenyl rings that are somewhat more irregular than one would expect. However, nothing unusual is revealed by the ellipsoids in Figure 2S.

The same data were also treated using the P2(1)/c space group. This space group yields an asymmetric unit containing a single molecule plus two additional areas of electron density that again must be treated as partial carbon atoms. Expansion of this unit yields the pattern shown in Figure 1S. Bond distances within the phenyl groups are more chemically reasonable in this space group. On the other hand, the *R* values are significantly higher. Both space groups yield almost the same structure without revealing the nature of the disorder and the exact packing. The disorder suggests that the derived carbon carbon bond distances may be subject to greater uncertainty.

Structural relationships emerged more clearly when the unit cell size was allowed to expand. A typical unit cell has the dimensions of 14.276 Å, 14.248 Å, 22.656 Å, 90^{o}, 92.136^{o}, 90^{o} with a volume of 4605.4 $Å^3$. XPREP recommended space groups were used along with several others. The greatest success was achieved with space group number 9, Cc. Its use gives four molecules in the asymmetric unit, two with phenyl groups in parallel planes and two with phenyl groups in almost perpendicular planes. It was not necessary to invoke disorder in order to get the best refinement as the choice of the larger unit cell led to distinct molecules. In each conformer pair the two molecules are enantiomers that are oriented edge to face. Figure 3S shows the complete asymmetric unit and Figures 4aS and 4bS show the pairs of parallel and perpendicular molecules, respectively.

Our enthusiasm for this refinement was tempered somewhat by a relatively high R_1 value of 9.8% and by other problems. A number of the ellipsoids were non positive definite and once again, the carbon-carbon distances around the phenyl rings were not as regular as one would expect. The programs XPREP and PLATON would sometimes (not always) give C2/c as a recommendation. However, meaningful refinements were not obtained with that space group using direct methods or the SHELXTL program XM.

The difficulty in obtaining a more satisfactory *R* value may be related to the fact that none of the crystals used were of high quality. They did not show the desired sharp edges and flat faces. Analysis of our synthetic ***cc*-DPB** (reduction of the corresponding diyne over Lindlar Pd) revealed the presence of about 1% trans,trans isomer. The shapes of the ***cc*-DPB** and the ***tt*-DPB** molecules[2] are sufficiently similar that the latter could fit into the lattice of the former as has been confirmed in our laboratory by the observation of exclusive ***cc*-DPB** to ***tt*-DPB** photoisomerization in a crystal to crystal reaction (see ref 24 in the paper). The atoms would be in similar general positions in the lattice but slightly imperfect placement of atoms could noticeably, but not fatally degrade the quality of the data. We did not notice a degradation of the structure during the time the data was taken, but since the two molecules are so similar, a minor change in isomer composition may not have been detected.

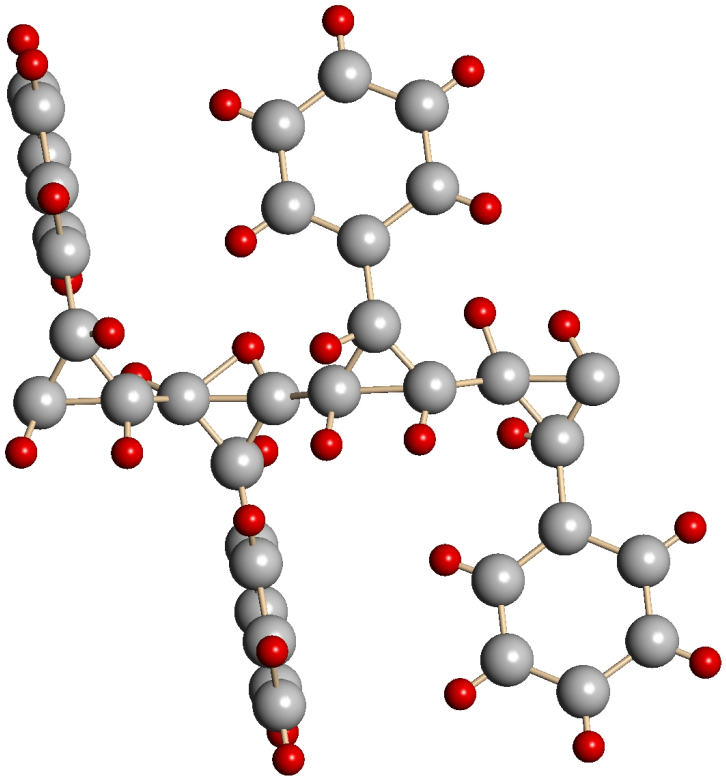


Figure S1. "Chain" structure solved with P2(1) space group.

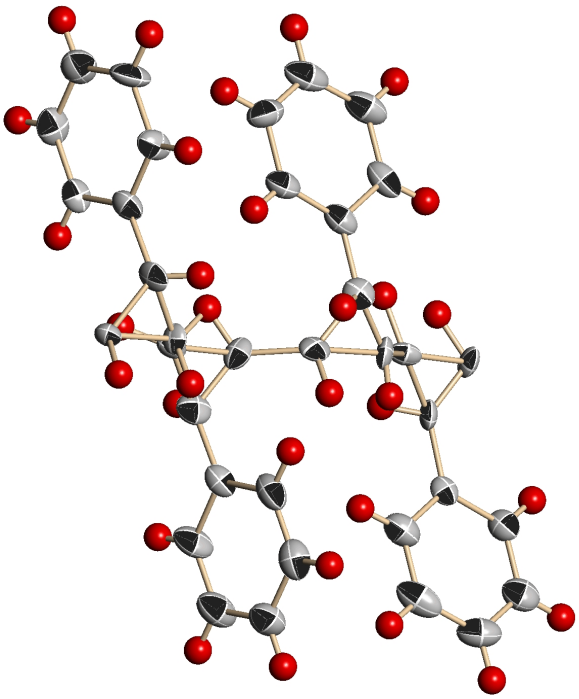


Figure S2. Ellipsoids of P2(1) structure.

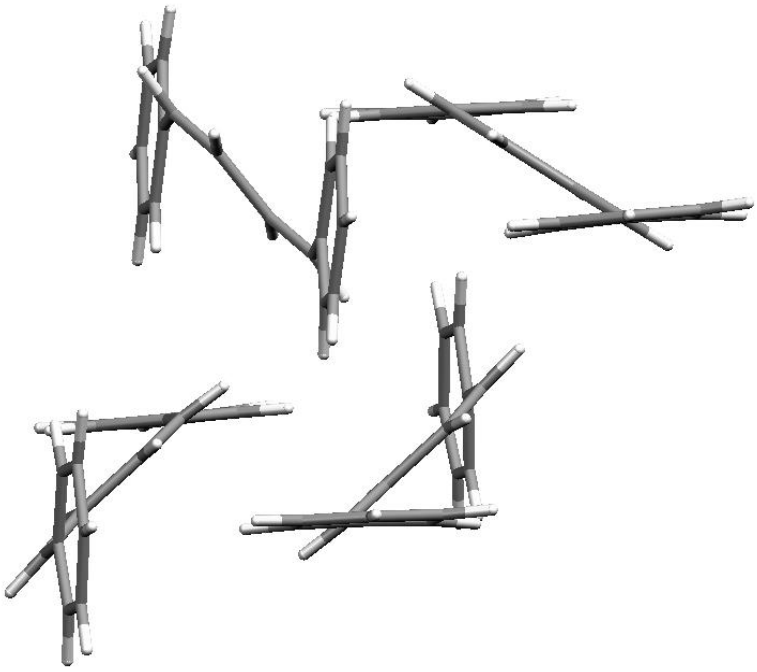


Figure S3. Four molecules in asymmetric unit viewed roughly end on, solved as Cc using large unit cell.

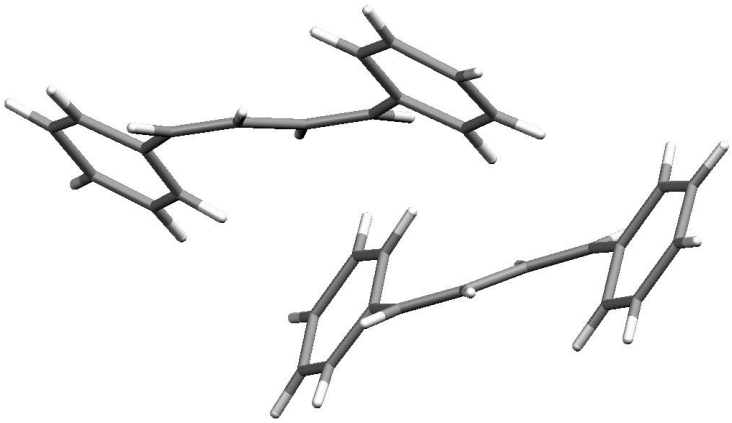


Figure S4a. Two edge to face molecules with phenyl groups in parallel planes.

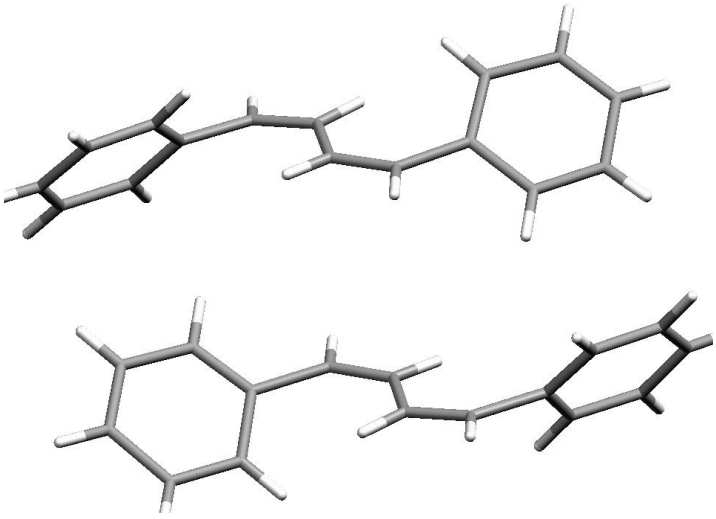
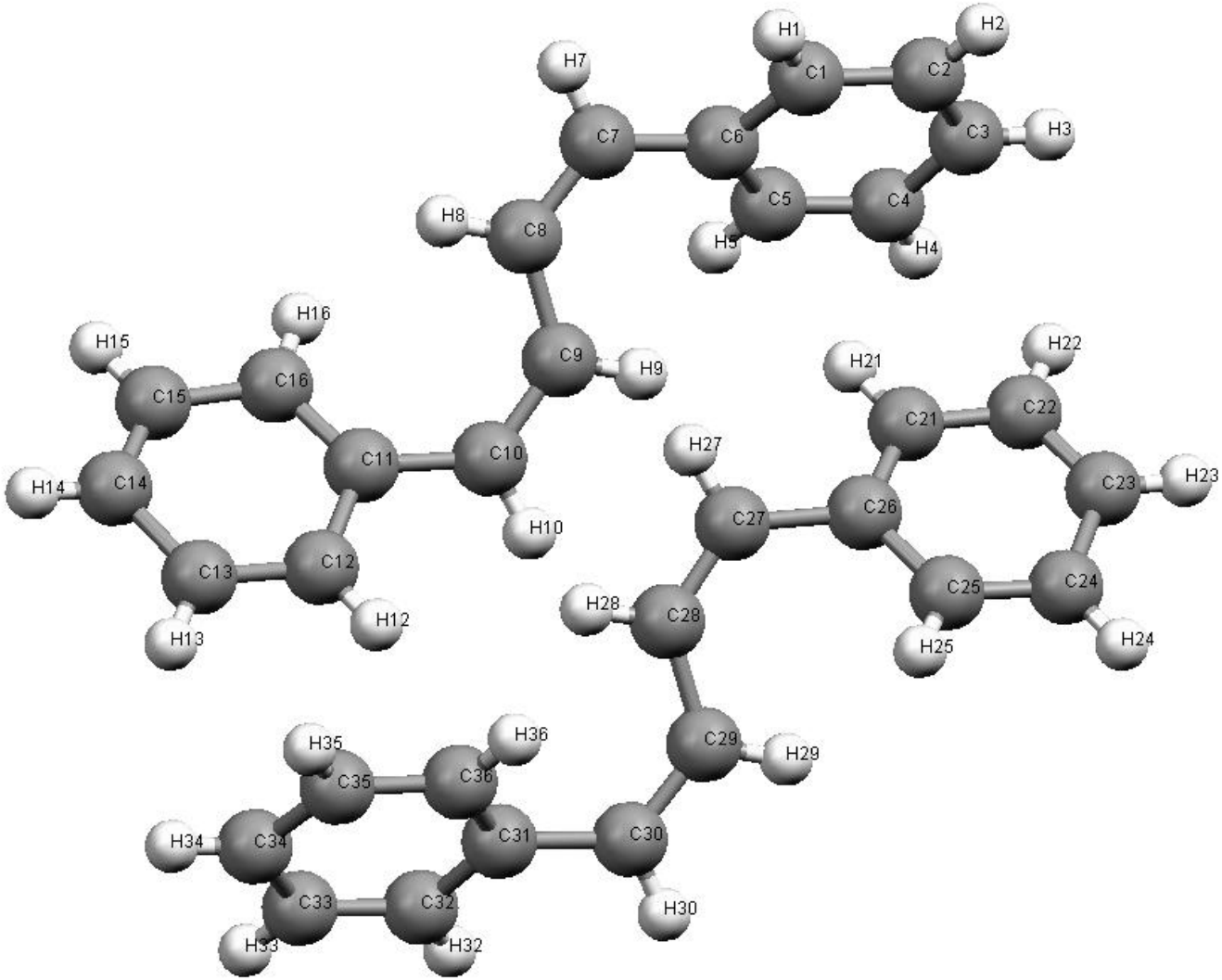


Figure S4b. Two edge to face molecules with phenyl groups in roughly perpendicular planes.

***Table S5*:** Crystal data and structure refinement for ***cc*-DPB**.

Identification code	***cc*-DPB**	
Empirical formula	$C_{16}H_{14}$	
Formula weight	206.27	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	Cc	
Unit cell dimensions	a = 14.2760(8) Å	α= 90°.
	b = 14.2485(8) Å	β= 92.136(2)°.
	c = 22.6565(13) Å	γ = 90°.
Volume	4605.4(5) $Å^3$	
Z	16	
Density (calculated)	1.190 Mg/m^3	
Absorption coefficient	0.067 mm^{-1}	
F(000)	1760	
Crystal size	0.120 x 0.130 x 0.200 mm^3	
Theta range for data collection	2.02 to 28.31°.	
Index ranges	-19<=h<=19, -18<=k<=18, -30<=l<=30	
Reflections collected	31986	
Independent reflections	11375 [R(int) = 0.0584]	
Completeness to theta = 28.31°	99.9 %	
Absorption correction	None	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11375 / 2 / 578
Goodness-of-fit on F^2	1.155
Final R indices [I>2sigma(I)]	R1 = 0.0980, wR2 = 0.2340
R indices (all data)	R1 = 0.1094, wR2 = 0.2432
Absolute structure parameter	6(10)
Largest diff. peak and hole	0.666 and -0.339 e.$Å^{-3}$


H1
H2
H7
C1
C2
C7
C6
C3
H3
C5
C4
H8
C8
H5
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H15
C9
H9
C16
C15
C21
C22
H21
H22
H27
C11
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C12
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H24
H13
C29
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C36
C35
C31
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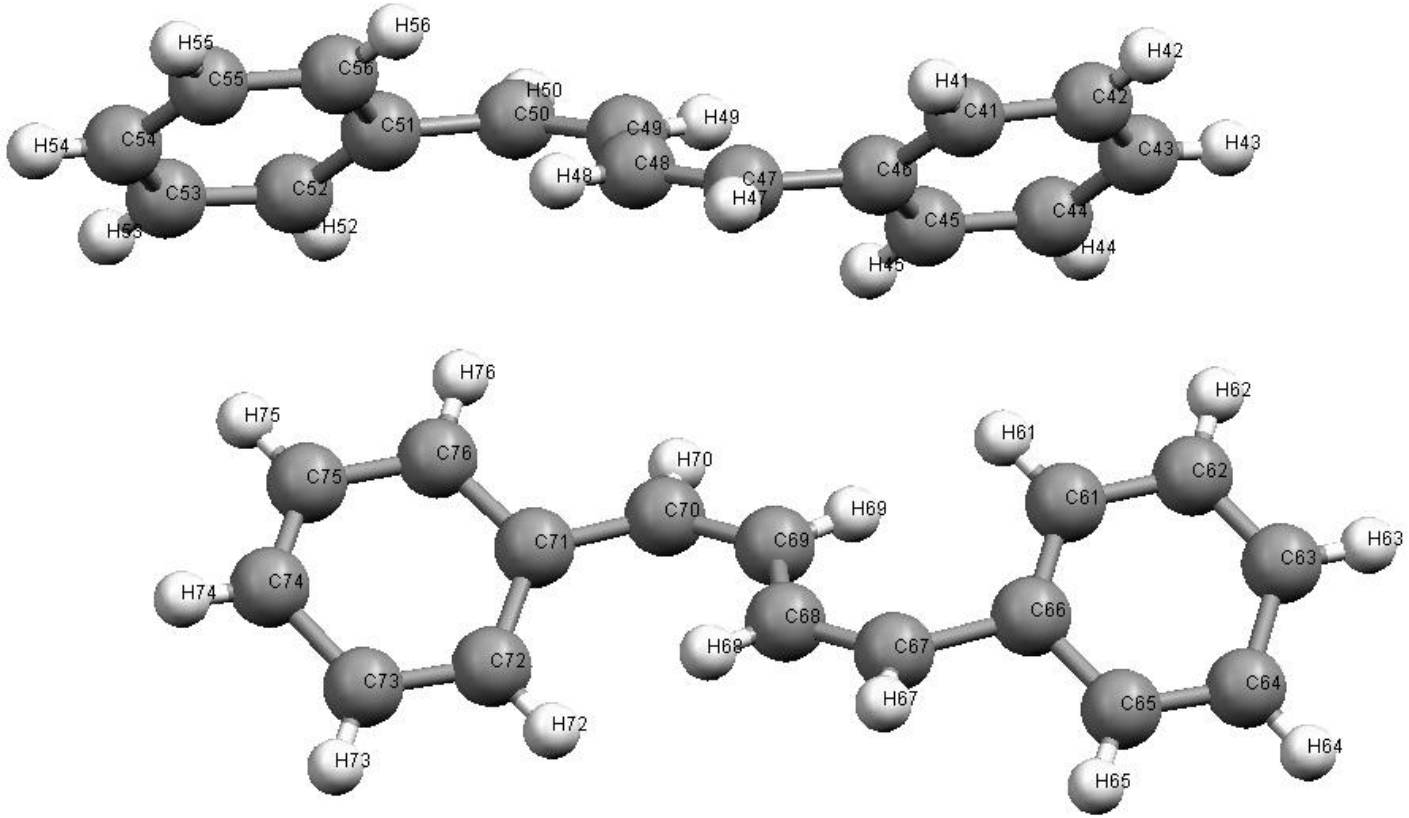
H34
C34
H30
C33
C32
H33
H32


H56
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C56
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C51
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C47
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C67
C72
C73
H72
H73
H67
C66
C65
C64
H64
H65
H62
C62
H61
C61
H63
C63

***Table S6*:** Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for ***cc*-DPB**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	11443(3)	6557(3)	1676(2)	16(1)
C(2)	11424(3)	6315(4)	1079(2)	26(1)
C(3)	10808(3)	6765(3)	702(2)	12(1)
C(4)	10201(3)	7431(3)	907(2)	15(1)
C(5)	10252(3)	7682(3)	1485(2)	15(1)
C(6)	10861(3)	7256(3)	1900(2)	12(1)
C(7)	10918(3)	7475(3)	2519(2)	19(1)
C(8)	10202(3)	7599(3)	2871(2)	15(1)
C(9)	9224(3)	7446(3)	2709(2)	12(1)
C(10)	8484(3)	7504(3)	3065(2)	14(1)
C(11)	8472(3)	7798(3)	3680(2)	14(1)
C(12)	7785(3)	7334(3)	4048(2)	15(1)
C(13)	7747(3)	7603(3)	4635(2)	20(1)
C(14)	8382(3)	8296(3)	4886(2)	16(1)
C(15)	8951(3)	8705(3)	4545(2)	17(1)
C(16)	9039(3)	8480(3)	3942(2)	17(1)
C(21)	8897(3)	5152(3)	1542(2)	17(1)
C(22)	8940(3)	4947(3)	954(2)	18(1)
C(23)	8403(3)	4281(4)	727(2)	23(1)
C(24)	7753(3)	3763(3)	1096(2)	18(1)
C(25)	7756(3)	3982(3)	1685(2)	11(1)
C(26)	8312(2)	4725(3)	1907(2)	9(1)
C(27)	8271(3)	5005(3)	2546(2)	14(1)
C(28)	7538(3)	5042(3)	2882(2)	15(1)
C(29)	6561(3)	4889(3)	2710(2)	12(1)
C(30)	5842(3)	5014(3)	3068(2)	10(1)
C(31)	5879(3)	5259(3)	3715(2)	17(1)
C(32)	5277(3)	5966(3)	3904(2)	16(1)
C(33)	5316(3)	6216(3)	4495(2)	14(1)
C(34)	5929(3)	5749(4)	4912(2)	24(1)
C(35)	6481(3)	5014(3)	4711(2)	20(1)

C(36)	6475(3)	4767(3)	4111(2)	12(1)
C(41)	6563(3)	6728(3)	1730(2)	12(1)
C(42)	6560(3)	6550(3)	1124(2)	17(1)
C(43)	5896(3)	6942(3)	753(2)	12(1)
C(44)	5252(3)	7563(3)	989(2)	15(1)
C(45)	5289(3)	7752(3)	1589(2)	16(1)
C(46)	5953(2)	7362(3)	1968(2)	6(1)
C(47)	6027(3)	7499(3)	2623(2)	14(1)
C(48)	5957(3)	8293(3)	2928(2)	16(1)
C(49)	5813(3)	9227(3)	2678(2)	13(1)
C(50)	5739(3)	10041(3)	2997(2)	13(1)
C(51)	5779(3)	10208(3)	3640(2)	19(1)
C(52)	5141(3)	10827(3)	3887(2)	15(1)
C(53)	5207(3)	11041(3)	4479(2)	18(1)
C(54)	5901(4)	10601(4)	4855(2)	28(1)
C(55)	6516(4)	9998(3)	4612(2)	25(1)
C(56)	6494(3)	9779(3)	4008(2)	18(1)
C(61)	4041(3)	5221(3)	1640(2)	20(1)
C(62)	4132(3)	5047(3)	1039(2)	18(1)
C(63)	3591(2)	4405(3)	772(2)	9(1)
C(64)	2894(4)	3895(3)	1106(2)	27(1)
C(65)	2842(3)	4077(3)	1692(2)	13(1)
C(66)	3395(3)	4783(3)	1946(2)	10(1)
C(67)	3249(3)	4956(3)	2597(2)	12(1)
C(68)	3293(3)	5764(3)	2906(2)	14(1)
C(69)	3482(3)	6696(3)	2670(2)	16(1)
C(70)	3515(3)	7515(3)	2982(2)	15(1)
C(71)	3387(3)	7705(3)	3595(2)	13(1)
C(72)	2739(3)	7209(3)	3962(2)	11(1)
C(73)	2671(4)	7447(3)	4549(2)	26(1)
C(74)	3280(4)	8168(3)	4817(3)	29(1)
C(75)	3837(3)	8632(3)	4487(2)	13(1)
C(76)	3927(3)	8407(3)	3885(2)	17(1)

***Table S7*:** Bond lengths [Å] and angles [°] for ***cc*-DPB**.

C(1)-C(2)	1.396(6)
C(1)-C(6)	1.403(6)
C(1)-H(1)	0.9500
C(2)-C(3)	1.363(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.377(6)
C(3)-H(3)	0.9500
C(4)-C(5)	1.357(6)
C(4)-H(4)	0.9500
C(5)-C(6)	1.397(6)
C(5)-H(5)	0.9500
C(6)-C(7)	1.436(6)
C(7)-C(8)	1.331(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.447(5)
C(8)-H(8)	0.9500
C(9)-C(10)	1.354(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.456(6)
C(10)-H(10)	0.9500
C(11)-C(16)	1.384(6)
C(11)-C(12)	1.467(6)
C(12)-C(13)	1.389(6)
C(12)-H(12)	0.9500
C(13)-C(14)	1.443(6)
C(13)-H(13)	0.9500
C(14)-C(15)	1.282(7)
C(14)-H(14)	0.9500
C(15)-C(16)	1.414(6)
C(15)-H(15)	0.9500
C(16)-H(16)	0.9500
C(21)-C(26)	1.343(6)
C(21)-C(22)	1.369(6)

C(21)-H(21)	0.9500
C(22)-C(23)	1.313(7)
C(22)-H(22)	0.9500
C(23)-C(24)	1.471(6)
C(23)-H(23)	0.9500
C(24)-C(25)	1.371(6)
C(24)-H(24)	0.9500
C(25)-C(26)	1.405(5)
C(25)-H(25)	0.9500
C(26)-C(27)	1.505(6)
C(27)-C(28)	1.317(6)
C(27)-H(27)	0.9500
C(28)-C(29)	1.450(5)
C(28)-H(28)	0.9500
C(29)-C(30)	1.343(5)
C(29)-H(29)	0.9500
C(30)-C(31)	1.504(5)
C(30)-H(30)	0.9500
C(31)-C(32)	1.402(6)
C(31)-C(36)	1.402(6)
C(32)-C(33)	1.383(5)
C(32)-H(32)	0.9500
C(33)-C(34)	1.427(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.398(7)
C(34)-H(34)	0.9500
C(35)-C(36)	1.404(6)
C(35)-H(35)	0.9500
C(36)-H(36)	0.9500
C(41)-C(46)	1.378(5)
C(41)-C(42)	1.395(6)
C(41)-H(41)	0.9500
C(42)-C(43)	1.364(6)
C(42)-H(42)	0.9500
C(43)-C(44)	1.397(5)
C(43)-H(43)	0.9500

C(44)-C(45)	1.385(5)
C(44)-H(44)	0.9500
C(45)-C(46)	1.372(5)
C(45)-H(45)	0.9500
C(46)-C(47)	1.497(5)
C(47)-C(48)	1.331(6)
C(47)-H(47)	0.9500
C(48)-C(49)	1.458(4)
C(48)-H(48)	0.9500
C(49)-C(50)	1.373(5)
C(49)-H(49)	0.9500
C(50)-C(51)	1.476(6)
C(50)-H(50)	0.9500
C(51)-C(52)	1.399(6)
C(51)-C(56)	1.430(6)
C(52)-C(53)	1.377(5)
C(52)-H(52)	0.9500
C(53)-C(54)	1.426(6)
C(53)-H(53)	0.9500
C(54)-C(55)	1.360(7)
C(54)-H(54)	0.9500
C(55)-C(56)	1.402(7)
C(55)-H(55)	0.9500
C(56)-H(56)	0.9500
C(61)-C(66)	1.331(6)
C(61)-C(62)	1.394(6)
C(61)-H(61)	0.9500
C(62)-C(63)	1.329(6)
C(62)-H(62)	0.9500
C(63)-C(64)	1.465(6)
C(63)-H(63)	0.9500
C(64)-C(65)	1.358(6)
C(64)-H(64)	0.9500
C(65)-C(66)	1.391(5)
C(65)-H(65)	0.9500
C(66)-C(67)	1.517(6)

C(67)-C(68)	1.348(6)
C(67)-H(67)	0.9500
C(68)-C(69)	1.461(5)
C(68)-H(68)	0.9500
C(69)-C(70)	1.364(6)
C(69)-H(69)	0.9500
C(70)-C(71)	1.433(6)
C(70)-H(70)	0.9500
C(71)-C(76)	1.411(6)
C(71)-C(72)	1.452(5)
C(72)-C(73)	1.379(6)
C(72)-H(72)	0.9500
C(73)-C(74)	1.464(7)
C(73)-H(73)	0.9500
C(74)-C(75)	1.294(7)
C(74)-H(74)	0.9500
C(75)-C(76)	1.413(6)
C(75)-H(75)	0.9500
C(76)-H(76)	0.9500

C(2)-C(1)-C(6)	122.4(4)
C(2)-C(1)-H(1)	118.8
C(6)-C(1)-H(1)	118.8
C(3)-C(2)-C(1)	118.6(4)
C(3)-C(2)-H(2)	120.7
C(1)-C(2)-H(2)	120.7
C(2)-C(3)-C(4)	120.9(4)
C(2)-C(3)-H(3)	119.6
C(4)-C(3)-H(3)	119.6
C(5)-C(4)-C(3)	119.6(4)
C(5)-C(4)-H(4)	120.2
C(3)-C(4)-H(4)	120.2
C(4)-C(5)-C(6)	123.1(4)
C(4)-C(5)-H(5)	118.5
C(6)-C(5)-H(5)	118.4
C(5)-C(6)-C(1)	115.2(4)

C(5)-C(6)-C(7)	125.1(4)
C(1)-C(6)-C(7)	119.7(4)
C(8)-C(7)-C(6)	126.6(4)
C(8)-C(7)-H(7)	116.7
C(6)-C(7)-H(7)	116.7
C(7)-C(8)-C(9)	125.8(4)
C(7)-C(8)-H(8)	117.1
C(9)-C(8)-H(8)	117.1
C(10)-C(9)-C(8)	127.3(3)
C(10)-C(9)-H(9)	116.3
C(8)-C(9)-H(9)	116.3
C(9)-C(10)-C(11)	128.7(4)
C(9)-C(10)-H(10)	115.6
C(11)-C(10)-H(10)	115.7
C(16)-C(11)-C(10)	125.7(4)
C(16)-C(11)-C(12)	117.8(4)
C(10)-C(11)-C(12)	116.5(4)
C(13)-C(12)-C(11)	118.1(4)
C(13)-C(12)-H(12)	121.0
C(11)-C(12)-H(12)	121.0
C(12)-C(13)-C(14)	121.3(4)
C(12)-C(13)-H(13)	119.3
C(14)-C(13)-H(13)	119.3
C(15)-C(14)-C(13)	118.4(4)
C(15)-C(14)-H(14)	120.8
C(13)-C(14)-H(14)	120.8
C(14)-C(15)-C(16)	124.1(4)
C(14)-C(15)-H(15)	118.0
C(16)-C(15)-H(15)	117.9
C(11)-C(16)-C(15)	120.1(4)
C(11)-C(16)-H(16)	119.9
C(15)-C(16)-H(16)	119.9
C(26)-C(21)-C(22)	123.7(4)
C(26)-C(21)-H(21)	118.2
C(22)-C(21)-H(21)	118.2
C(23)-C(22)-C(21)	119.3(4)

C(23)-C(22)-H(22)	120.3
C(21)-C(22)-H(22)	120.3
C(22)-C(23)-C(24)	120.8(4)
C(22)-C(23)-H(23)	119.6
C(24)-C(23)-H(23)	119.6
C(25)-C(24)-C(23)	117.4(4)
C(25)-C(24)-H(24)	121.3
C(23)-C(24)-H(24)	121.3
C(24)-C(25)-C(26)	120.2(4)
C(24)-C(25)-H(25)	119.9
C(26)-C(25)-H(25)	119.9
C(21)-C(26)-C(25)	118.5(4)
C(21)-C(26)-C(27)	121.3(4)
C(25)-C(26)-C(27)	120.2(4)
C(28)-C(27)-C(26)	128.8(4)
C(28)-C(27)-H(27)	115.6
C(26)-C(27)-H(27)	115.6
C(27)-C(28)-C(29)	128.1(4)
C(27)-C(28)-H(28)	116.0
C(29)-C(28)-H(28)	116.0
C(30)-C(29)-C(28)	124.6(3)
C(30)-C(29)-H(29)	117.7
C(28)-C(29)-H(29)	117.7
C(29)-C(30)-C(31)	128.2(4)
C(29)-C(30)-H(30)	115.9
C(31)-C(30)-H(30)	115.9
C(32)-C(31)-C(36)	121.8(4)
C(32)-C(31)-C(30)	117.8(4)
C(36)-C(31)-C(30)	120.4(4)
C(33)-C(32)-C(31)	118.5(4)
C(33)-C(32)-H(32)	120.7
C(31)-C(32)-H(32)	120.7
C(32)-C(33)-C(34)	121.5(4)
C(32)-C(33)-H(33)	119.2
C(34)-C(33)-H(33)	119.3
C(35)-C(34)-C(33)	118.2(4)

C(35)-C(34)-H(34)	120.9
C(33)-C(34)-H(34)	120.9
C(34)-C(35)-C(36)	121.3(4)
C(34)-C(35)-H(35)	119.3
C(36)-C(35)-H(35)	119.4
C(31)-C(36)-C(35)	118.5(4)
C(31)-C(36)-H(36)	120.8
C(35)-C(36)-H(36)	120.8
C(46)-C(41)-C(42)	121.7(4)
C(46)-C(41)-H(41)	119.2
C(42)-C(41)-H(41)	119.2
C(43)-C(42)-C(41)	120.7(4)
C(43)-C(42)-H(42)	119.7
C(41)-C(42)-H(42)	119.7
C(42)-C(43)-C(44)	118.3(4)
C(42)-C(43)-H(43)	120.9
C(44)-C(43)-H(43)	120.9
C(45)-C(44)-C(43)	119.9(4)
C(45)-C(44)-H(44)	120.0
C(43)-C(44)-H(44)	120.1
C(46)-C(45)-C(44)	122.4(4)
C(46)-C(45)-H(45)	118.8
C(44)-C(45)-H(45)	118.8
C(45)-C(46)-C(41)	116.9(4)
C(45)-C(46)-C(47)	126.0(3)
C(41)-C(46)-C(47)	116.9(3)
C(48)-C(47)-C(46)	128.5(4)
C(48)-C(47)-H(47)	115.8
C(46)-C(47)-H(47)	115.7
C(47)-C(48)-C(49)	125.8(3)
C(47)-C(48)-H(48)	117.1
C(49)-C(48)-H(48)	117.1
C(50)-C(49)-C(48)	125.4(3)
C(50)-C(49)-H(49)	117.3
C(48)-C(49)-H(49)	117.3
C(49)-C(50)-C(51)	130.9(4)

C(49)-C(50)-H(50)	114.6
C(51)-C(50)-H(50)	114.6
C(52)-C(51)-C(56)	119.8(4)
C(52)-C(51)-C(50)	119.6(4)
C(56)-C(51)-C(50)	120.4(4)
C(53)-C(52)-C(51)	120.5(4)
C(53)-C(52)-H(52)	119.8
C(51)-C(52)-H(52)	119.8
C(52)-C(53)-C(54)	120.3(4)
C(52)-C(53)-H(53)	119.8
C(54)-C(53)-H(53)	119.8
C(55)-C(54)-C(53)	118.8(5)
C(55)-C(54)-H(54)	120.6
C(53)-C(54)-H(54)	120.6
C(54)-C(55)-C(56)	122.9(5)
C(54)-C(55)-H(55)	118.5
C(56)-C(55)-H(55)	118.6
C(55)-C(56)-C(51)	117.6(4)
C(55)-C(56)-H(56)	121.2
C(51)-C(56)-H(56)	121.2
C(66)-C(61)-C(62)	121.2(5)
C(66)-C(61)-H(61)	119.4
C(62)-C(61)-H(61)	119.4
C(63)-C(62)-C(61)	119.6(4)
C(63)-C(62)-H(62)	120.2
C(61)-C(62)-H(62)	120.2
C(62)-C(63)-C(64)	120.0(4)
C(62)-C(63)-H(63)	120.0
C(64)-C(63)-H(63)	120.0
C(65)-C(64)-C(63)	118.4(4)
C(65)-C(64)-H(64)	120.8
C(63)-C(64)-H(64)	120.8
C(64)-C(65)-C(66)	119.4(4)
C(64)-C(65)-H(65)	120.3
C(66)-C(65)-H(65)	120.3
C(61)-C(66)-C(65)	121.2(4)

C(61)-C(66)-C(67)	123.7(4)
C(65)-C(66)-C(67)	115.0(4)
C(68)-C(67)-C(66)	129.6(4)
C(68)-C(67)-H(67)	115.2
C(66)-C(67)-H(67)	115.2
C(67)-C(68)-C(69)	126.3(3)
C(67)-C(68)-H(68)	116.8
C(69)-C(68)-H(68)	116.8
C(70)-C(69)-C(68)	126.2(4)
C(70)-C(69)-H(69)	116.9
C(68)-C(69)-H(69)	116.9
C(69)-C(70)-C(71)	131.3(4)
C(69)-C(70)-H(70)	114.3
C(71)-C(70)-H(70)	114.3
C(76)-C(71)-C(70)	119.9(4)
C(76)-C(71)-C(72)	115.3(3)
C(70)-C(71)-C(72)	124.9(4)
C(73)-C(72)-C(71)	120.2(4)
C(73)-C(72)-H(72)	119.9
C(71)-C(72)-H(72)	119.9
C(72)-C(73)-C(74)	120.7(4)
C(72)-C(73)-H(73)	119.7
C(74)-C(73)-H(73)	119.7
C(75)-C(74)-C(73)	119.2(5)
C(75)-C(74)-H(74)	120.4
C(73)-C(74)-H(74)	120.4
C(74)-C(75)-C(76)	121.5(4)
C(74)-C(75)-H(75)	119.2
C(76)-C(75)-H(75)	119.2
C(75)-C(76)-C(71)	122.9(4)
C(75)-C(76)-H(76)	118.6
C(71)-C(76)-H(76)	118.6

***Table S8*:** Anisotropic displacement parameters ($Å^2 x\ 10^3$) for ***cc*-DPB**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	5(2)	20(2)	24(2)	11(2)	-4(2)	6(2)
C(2)	10(2)	43(3)	24(2)	8(2)	7(2)	11(2)
C(3)	12(2)	16(2)	9(2)	-1(2)	-1(1)	2(2)
C(4)	4(2)	19(2)	22(2)	12(2)	-1(1)	8(1)
C(5)	16(2)	12(2)	17(2)	3(2)	-4(2)	5(2)
C(6)	0(2)	15(2)	20(2)	2(2)	0(1)	2(1)
C(7)	9(2)	13(2)	34(3)	-2(2)	-3(2)	-5(1)
C(8)	15(2)	14(2)	15(2)	4(1)	-1(1)	4(1)
C(9)	16(2)	13(2)	6(2)	-4(1)	-1(1)	-2(1)
C(10)	12(2)	12(2)	19(2)	4(2)	4(2)	3(2)
C(11)	16(2)	12(2)	14(2)	8(2)	6(2)	5(2)
C(12)	15(2)	15(2)	13(2)	5(2)	6(2)	2(2)
C(13)	33(2)	10(2)	16(2)	0(2)	9(2)	-1(2)
C(14)	17(2)	11(2)	20(2)	-7(2)	-10(2)	-2(1)
C(15)	27(2)	11(2)	12(2)	-9(2)	-8(2)	10(2)
C(16)	13(2)	23(2)	17(2)	0(2)	-1(2)	-1(2)
C(21)	19(2)	5(2)	28(2)	-1(2)	-3(2)	-3(1)
C(22)	6(2)	26(2)	23(2)	15(2)	10(2)	11(2)
C(23)	21(2)	40(3)	10(2)	7(2)	15(2)	16(2)
C(24)	8(2)	17(2)	28(2)	3(2)	10(2)	-4(2)
C(25)	18(2)	2(2)	14(2)	-2(1)	9(2)	0(1)
C(26)	1(1)	12(2)	14(2)	-8(1)	-3(1)	3(1)
C(27)	11(2)	15(2)	15(2)	-5(2)	-8(2)	-5(2)
C(28)	15(2)	15(2)	16(2)	6(1)	-1(1)	5(1)
C(29)	16(2)	14(2)	7(2)	-6(1)	-1(1)	-2(1)
C(30)	14(2)	15(2)	0(2)	-2(1)	-1(1)	5(1)
C(31)	32(2)	11(2)	9(2)	0(1)	8(2)	-12(2)
C(32)	18(2)	13(2)	16(2)	-4(2)	5(2)	4(2)
C(33)	22(2)	8(2)	13(2)	-5(1)	2(2)	5(2)
C(34)	27(2)	27(2)	19(2)	-2(2)	10(2)	2(2)
C(35)	30(2)	21(2)	9(2)	1(2)	6(2)	-10(2)

C(36)	9(2)	6(2)	22(2)	5(1)	6(2)	0(1)
C(41)	20(2)	3(2)	14(2)	4(1)	2(2)	3(1)
C(42)	14(2)	4(2)	34(2)	0(2)	1(2)	-4(1)
C(43)	20(2)	14(2)	2(1)	-8(1)	-5(1)	-1(2)
C(44)	13(2)	19(2)	12(2)	0(2)	-3(2)	12(2)
C(45)	14(2)	18(2)	15(2)	-10(2)	-3(2)	2(2)
C(46)	2(1)	7(2)	10(2)	-4(1)	-1(1)	4(1)
C(47)	14(2)	12(2)	15(2)	2(1)	-2(2)	-2(1)
C(48)	10(2)	22(2)	15(2)	4(2)	1(1)	1(1)
C(49)	15(2)	11(2)	14(2)	3(1)	2(1)	4(1)
C(50)	10(2)	8(2)	21(2)	4(1)	5(2)	0(1)
C(51)	24(2)	9(2)	23(2)	5(2)	3(2)	-7(2)
C(52)	7(2)	20(2)	17(2)	-5(2)	4(1)	0(1)
C(53)	26(2)	21(2)	7(2)	1(2)	2(2)	8(2)
C(54)	26(2)	29(3)	30(3)	15(2)	9(2)	-3(2)
C(55)	29(3)	19(2)	28(3)	3(2)	-8(2)	-8(2)
C(56)	19(2)	9(2)	26(2)	5(2)	10(2)	-4(2)
C(61)	29(2)	19(2)	12(2)	5(2)	-3(2)	14(2)
C(62)	17(2)	13(2)	22(2)	2(2)	1(2)	4(2)
C(63)	9(2)	16(2)	0(1)	-6(1)	-2(1)	0(1)
C(64)	34(3)	20(2)	27(3)	-9(2)	0(2)	-3(2)
C(65)	14(2)	6(2)	20(2)	-5(2)	0(2)	5(1)
C(66)	7(2)	7(2)	17(2)	-2(1)	-4(1)	5(1)
C(67)	15(2)	14(2)	6(2)	1(1)	-4(1)	0(2)
C(68)	11(2)	23(2)	10(2)	1(2)	1(1)	4(2)
C(69)	12(2)	18(2)	18(2)	-6(2)	-1(1)	4(1)
C(70)	8(2)	7(2)	30(2)	3(2)	1(2)	1(1)
C(71)	22(2)	13(2)	4(2)	3(1)	8(2)	0(2)
C(72)	6(2)	11(2)	18(2)	-3(1)	6(1)	-9(1)
C(73)	36(3)	18(2)	24(2)	6(2)	9(2)	-4(2)
C(74)	37(3)	14(2)	37(3)	9(2)	1(2)	8(2)
C(75)	7(2)	13(2)	19(2)	-3(2)	-5(1)	6(1)
C(76)	11(2)	18(2)	20(2)	5(2)	-1(2)	0(2)

Table 5S. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for ***cc*-DPB**.

	x	y	z	U(eq)
H(1)	11865	6238	1940	20
H(2)	11832	5846	938	31
H(3)	10797	6618	293	15
H(4)	9748	7714	645	18
H(5)	9855	8171	1613	18
H(7)	11529	7539	2695	23
H(8)	10346	7806	3262	18
H(9)	9084	7286	2308	14
H(10)	7895	7331	2890	17
H(12)	7378	6863	3888	18
H(13)	7293	7326	4877	23
H(14)	8379	8446	5295	19
H(15)	9338	9190	4707	20
H(16)	9489	8797	3716	21
H(21)	9304	5623	1702	21
H(22)	9355	5282	712	22
H(23)	8434	4132	319	27
H(24)	7347	3294	932	21
H(25)	7380	3632	1943	13
H(27)	8852	5180	2733	17
H(28)	7665	5187	3286	18
H(29)	6420	4687	2318	14
H(30)	5234	4938	2891	12
H(32)	4851	6267	3633	19
H(33)	4927	6709	4626	17
H(34)	5960	5934	5315	29
H(35)	6869	4675	4986	24
H(36)	6866	4278	3977	15
H(41)	6998	6405	1984	14
H(42)	7024	6152	970	21

H(43)	5872	6797	343	14
H(44)	4789	7855	739	18
H(45)	4839	8167	1744	19
H(47)	6138	6948	2851	16
H(48)	6005	8246	3347	19
H(49)	5766	9276	2260	16
H(50)	5648	10591	2764	15
H(52)	4659	11101	3643	18
H(53)	4790	11485	4639	21
H(54)	5932	10726	5267	34
H(55)	6982	9712	4862	31
H(56)	6937	9362	3849	21
H(61)	4448	5661	1833	24
H(62)	4578	5385	822	21
H(63)	3656	4276	364	10
H(64)	2489	3449	918	33
H(65)	2431	3724	1927	16
H(67)	3105	4414	2820	14
H(68)	3191	5724	3317	17
H(69)	3592	6736	2259	19
H(70)	3646	8055	2752	18
H(72)	2361	6719	3798	14
H(73)	2224	7139	4782	31
H(74)	3266	8295	5229	35
H(75)	4194	9135	4654	16
H(76)	4371	8744	3665	20

Table 6S. Torsion angles [°] for ***cc*-DPB**.

C(6)-C(1)-C(2)-C(3)	-0.9(7)
C(1)-C(2)-C(3)-C(4)	-1.4(7)
C(2)-C(3)-C(4)-C(5)	3.8(7)
C(3)-C(4)-C(5)-C(6)	-4.0(7)
C(4)-C(5)-C(6)-C(1)	1.6(6)
C(4)-C(5)-C(6)-C(7)	-177.8(4)

C(2)-C(1)-C(6)-C(5)	0.9(6)
C(2)-C(1)-C(6)-C(7)	-179.7(4)
C(5)-C(6)-C(7)-C(8)	44.4(7)
C(1)-C(6)-C(7)-C(8)	-135.0(5)
C(6)-C(7)-C(8)-C(9)	6.4(7)
C(7)-C(8)-C(9)-C(10)	175.3(5)
C(8)-C(9)-C(10)-C(11)	4.9(7)
C(9)-C(10)-C(11)-C(16)	34.4(7)
C(9)-C(10)-C(11)-C(12)	-146.6(4)
C(16)-C(11)-C(12)-C(13)	-0.2(6)
C(10)-C(11)-C(12)-C(13)	-179.3(4)
C(11)-C(12)-C(13)-C(14)	-2.0(6)
C(12)-C(13)-C(14)-C(15)	4.2(7)
C(13)-C(14)-C(15)-C(16)	-4.2(7)
C(10)-C(11)-C(16)-C(15)	179.4(4)
C(12)-C(11)-C(16)-C(15)	0.4(6)
C(14)-C(15)-C(16)-C(11)	1.9(7)
C(26)-C(21)-C(22)-C(23)	-1.8(7)
C(21)-C(22)-C(23)-C(24)	0.5(6)
C(22)-C(23)-C(24)-C(25)	-2.0(6)
C(23)-C(24)-C(25)-C(26)	4.7(6)
C(22)-C(21)-C(26)-C(25)	4.4(6)
C(22)-C(21)-C(26)-C(27)	-177.7(4)
C(24)-C(25)-C(26)-C(21)	-5.8(6)
C(24)-C(25)-C(26)-C(27)	176.2(4)
C(21)-C(26)-C(27)-C(28)	143.8(5)
C(25)-C(26)-C(27)-C(28)	-38.3(6)
C(26)-C(27)-C(28)-C(29)	-5.2(7)
C(27)-C(28)-C(29)-C(30)	-174.3(5)
C(28)-C(29)-C(30)-C(31)	-4.9(6)
C(29)-C(30)-C(31)-C(32)	134.0(5)
C(29)-C(30)-C(31)-C(36)	-48.2(6)
C(36)-C(31)-C(32)-C(33)	3.7(6)
C(30)-C(31)-C(32)-C(33)	-178.5(4)
C(31)-C(32)-C(33)-C(34)	-2.1(6)
C(32)-C(33)-C(34)-C(35)	-1.3(7)

C(33)-C(34)-C(35)-C(36)	3.2(7)
C(32)-C(31)-C(36)-C(35)	-1.8(6)
C(30)-C(31)-C(36)-C(35)	-179.5(4)
C(34)-C(35)-C(36)-C(31)	-1.8(6)
C(46)-C(41)-C(42)-C(43)	-5.5(6)
C(41)-C(42)-C(43)-C(44)	3.3(6)
C(42)-C(43)-C(44)-C(45)	-1.1(6)
C(43)-C(44)-C(45)-C(46)	1.1(7)
C(44)-C(45)-C(46)-C(41)	-3.1(6)
C(44)-C(45)-C(46)-C(47)	-177.8(4)
C(42)-C(41)-C(46)-C(45)	5.2(6)
C(42)-C(41)-C(46)-C(47)	-179.6(4)
C(45)-C(46)-C(47)-C(48)	-44.8(7)
C(41)-C(46)-C(47)-C(48)	140.5(4)
C(46)-C(47)-C(48)-C(49)	-1.7(6)
C(47)-C(48)-C(49)-C(50)	179.8(5)
C(48)-C(49)-C(50)-C(51)	-0.1(7)
C(49)-C(50)-C(51)-C(52)	-137.3(5)
C(49)-C(50)-C(51)-C(56)	46.0(6)
C(56)-C(51)-C(52)-C(53)	1.3(6)
C(50)-C(51)-C(52)-C(53)	-175.4(4)
C(51)-C(52)-C(53)-C(54)	-3.0(7)
C(52)-C(53)-C(54)-C(55)	2.7(7)
C(53)-C(54)-C(55)-C(56)	-0.8(7)
C(54)-C(55)-C(56)-C(51)	-0.8(7)
C(52)-C(51)-C(56)-C(55)	0.6(6)
C(50)-C(51)-C(56)-C(55)	177.3(4)
C(66)-C(61)-C(62)-C(63)	-2.8(6)
C(61)-C(62)-C(63)-C(64)	0.9(6)
C(62)-C(63)-C(64)-C(65)	-2.1(6)
C(63)-C(64)-C(65)-C(66)	4.8(6)
C(62)-C(61)-C(66)-C(65)	5.7(6)
C(62)-C(61)-C(66)-C(67)	-178.8(4)
C(64)-C(65)-C(66)-C(61)	-6.8(6)
C(64)-C(65)-C(66)-C(67)	177.4(4)
C(61)-C(66)-C(67)-C(68)	38.3(7)

C(65)-C(66)-C(67)-C(68)	-146.0(4)
C(66)-C(67)-C(68)-C(69)	1.3(7)
C(67)-C(68)-C(69)-C(70)	179.2(5)
C(68)-C(69)-C(70)-C(71)	0.2(7)
C(69)-C(70)-C(71)-C(76)	144.0(5)
C(69)-C(70)-C(71)-C(72)	-34.7(7)
C(76)-C(71)-C(72)-C(73)	1.1(6)
C(70)-C(71)-C(72)-C(73)	179.9(4)
C(71)-C(72)-C(73)-C(74)	-3.0(7)
C(72)-C(73)-C(74)-C(75)	5.1(7)
C(73)-C(74)-C(75)-C(76)	-5.2(7)
C(74)-C(75)-C(76)-C(71)	3.5(6)
C(70)-C(71)-C(76)-C(75)	179.9(4)
C(72)-C(71)-C(76)-C(75)	-1.2(6)

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