organic compounds

(±)-1-Methyl-1,3,6-triphenyl-7-(2-phenylpropenyl)-1,2-dihydro-naphthalene

Yongqiang Sui, Charles Barnes and Rainer Glaser*

Department of Chemistry, University of Missouri–Columbia, Missouri 65211, USA
Correspondence e-mail: glaserr@missouri.edu

The crystal structure of the title compound, $C_{38}H_{32}$, presents a novel framework that combines the functionalities of a 1,6-diarene-substituted 1,2-dihydronaphthalene (DHN) with a 1,4-distyrylbenzene (DSB) to form a crossed bis-diarene. The lamellar crystal structure is held together by arene–arene interactions. While the orientations of the phenyl rings of the DSB units alternate within both the R and the S substructures, the homochiral substructures feature opposing polarity along the long axes of the DHN-based diarenes.

Comment

1,2-Dihydronaphthalenes (DHNs, dialin) (Autrey et al., 2003; Gorner et al., 2002; Laarhoven et al., 1985; Woning et al., 1991) and distyrylbenzenes (DSBs) (Bartholomew & Bazan, 2002; Hong et al., 2005; Lupton et al., 2002; Ma et al., 2002; Wang et al., 2003; Marri et al., 2005; Ni et al., 1999; Sarker et al., 2003; Xie et al., 2005) have been attracting increased attention recently because of their optical and optoelectronic properties, and more efficient syntheses of DHN (Maeda et al., 2002) and DSB (Wong et al., 1998) have been sought because of this interest in their properties. The title hydrocarbon, (I), presents a novel framework that combines the functionalities of a bis-arene-substituted DHN and of a substituted DSB.

(I)
Crossed Bis-Diarene with
1,2-Dihydronaphthalene (DHN) Junction
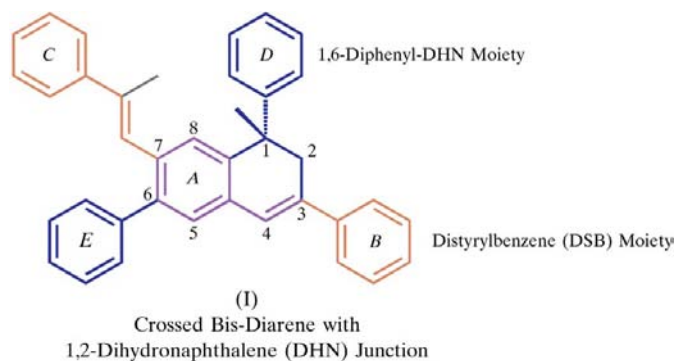
We have relied on arene–arene interactions of diarenes (Ar–spacer–Ar′) as lateral synthons (Lewis et al., 2001) in the

design of polar crystals with layers of parallel beloamphiphiles (Glaser, Knotts & Wu, 2003; Glaser, 2006). We have explored 1,4-diphenylazines (Chen et al., 1995; Lewis et al., 2000a,b), 1,4-diphenylbutadienes (Glaser, Dendi et al., 2003) and biphenyls (Glaser et al., 2006). Facile torsion of the arenes along with conformational flexibility of the spacer (Glaser & Chen, 1998) allow for optimization of arene–arene interactions. Hydrocarbon (I) is a crossed bis-diarene with the ability to engage in arene–arene interactions in every direction, and various types of arene–arene interactions co-operate in the formation of its lamellar crystal architecture.

We report here the single-crystal structure of (I) (Fig. 1). The systematic name of (I) stresses its 'dihydronaphthalene' nature, and the DSB framework is also highlighted in the scheme above. A search of the Cambridge Structural Database (Allen, 2002) suggests that (I) is the first compound with a framework that combines the DSB and DHN moieties.
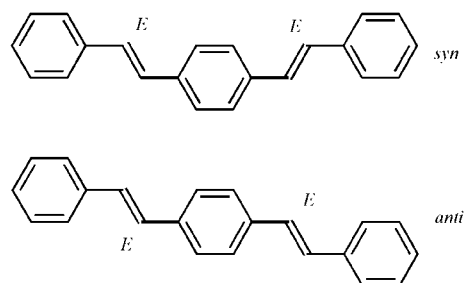
Distyrylbenzene prefers the E configuration at both double bonds so as to place the terminal arenes B and C far from the central arene A, and the same is true in (I). There is, however, a remarkable conformational difference. While DSB itself prefers the $anti$ conformation with regard to the 1,4-exocyclic bonds of arene A (highlighted in bold in the scheme above) (Wu et al., 2003), compound (I) crystallizes in the syn conformation. It is not clear whether this conformation is adopted as a result of intramolecular features (e.g. steric interference by arene E) or to improve intermolecular bonding in the crystal structure.
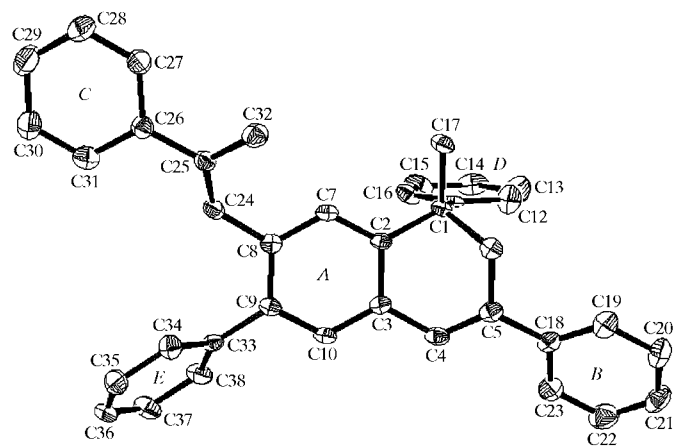

Figure 1
A displacement ellipsoid representation (50% probability) of (I). H atoms have been omitted for clarity.

Molecule (I) has a chiral center at atom C1 and the crystal is a racemate (Jacques *et al.*, 1981; Brock *et al.*, 1991). As can be seen in Fig. 2, layers are formed by the stacking of pure *R* and *S* enantiomers in one layer direction, and stacks of *R* and *S* enantiomers alternate in the second layer direction with double-stack alternation. In addition to the two neighbors with the same configuration in the stack, every molecule is surrounded by two *S* and two *R* enantiomers (and *vice versa*) in the neighboring stacks because of this double-stack alternation.

The stacking distance is very long (7.883 Å) and there are no direct stacking interactions. Instead, the stacks are held together by bridging interactions with molecules in neighboring stacks. All of these intermolecular interactions involve arene–arene bonding, *viz.* pair interactions involving arenes *B* and *C*, and triple interactions involving arenes *A*, *D* and *E*.
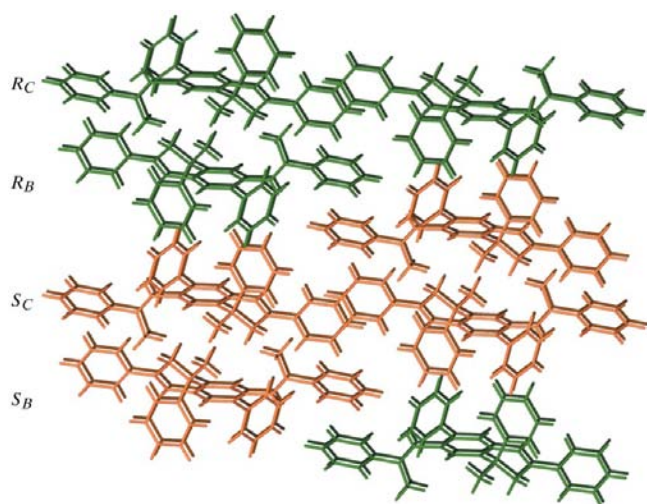

Figure 2
Homochiral stacks of *R* and *S* enantiomers alternating in layers of (I).
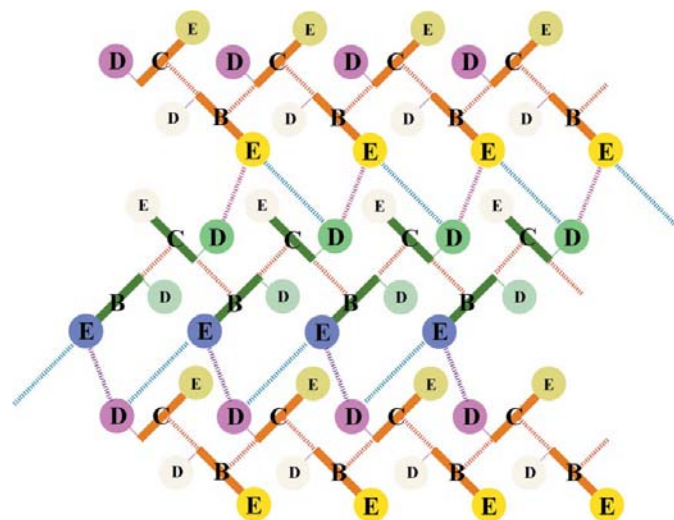

Figure 3
The *D*-to-*E* orientation and polarity of the *R* and *S* substructures. A Newman-type projection of a layer of (±)-(I); arenes *B* and *C* are shown side-on, and arenes *D* and *E* as circles; the smaller font sizes (and fainter colors) indicate arenes *D* and *E* that are farther away.

The long axes of the DSB units are more or less perpendicular to the layer surfaces. For a molecule with a given *B*-to-*C* direction, all of its next neighbors in neighboring stacks are oriented in the opposite direction (see Fig. 3). The homochiral double stacks, together with this alternation of the orientations, results in the four-stack repeating unit $\{R_C R_B S_C S_B\}$. In contrast, the *D*-to-*E* direction is the same for all the molecules in every homochiral double stack, and the *D*-to-*E* direction alternates between the homochiral double stacks. While the DSB units alternate within both the *R* and the *S* substructures, the homochiral substructures feature opposing polarity along the long axes of the DHN-based diarenes.

Experimental

The crude product of the synthesis (Sui & Glaser, 2006) was purified by crystallization induced by slow diffusion of hexanes into an ethyl acetate solution. Single crystals suitable for X-ray analysis were grown by repeated recrystallization at room temperature.

Crystal data

$C_{38}H_{32}$	Mo $K\alpha$ radiation
$M_r = 488.64$	Cell parameters from 6938
Monoclinic, $P2_1/n$	reflections
$a = 16.7069\ (7)$ Å	$\theta = 2.5–27.1°$
$b = 7.8826\ (3)$ Å	$\mu = 0.07$ mm^{-1}
$c = 21.2218\ (8)$ Å	$T = 173\ (2)$ K
$\beta = 104.129\ (1)°$	Prism, colorless
$V = 2710.23\ (18)$ Å^3	$0.35 \times 0.35 \times 0.25$ mm
$Z = 4$	
$D_x = 1.198$ Mg m^{-3}	

Data collection

Bruker SMART CCD area-detector diffractometer	5965 independent reflections
	4592 reflections with $I > 2\sigma(I)$
ω scans	$R_{int} = 0.030$
Absorption correction: multi-scan (Blessing, 1995)	$\theta_{max} = 27.1°$
	$h = -21 \rightarrow 21$
$T_{min} = 0.92$, $T_{max} = 0.98$	$k = -10 \rightarrow 10$
18791 measured reflections	$l = -27 \rightarrow 21$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0492P)^2 + 0.6288P]$
$R[F^2 > 2\sigma(F^2)] = 0.045$	
$wR(F^2) = 0.114$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.03$	$(\Delta/\sigma)_{max} < 0.001$
5965 reflections	$\Delta\rho_{max} = 0.24$ e Å^{-3}
345 parameters	$\Delta\rho_{min} = -0.15$ e Å^{-3}
H-atom parameters constrained	

H atoms were placed at calculated positions and included in the refinement using a riding model.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *CIFTAB* in *SHELXL97*.

organic compounds

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