Bis(9-ethylcarbazol-3-yl)ethane

Erol Asker
Balıkesir University, Balıkesir, Turkey

John Masnovi
Cleveland State University, j.masnovi@csuohio.edu

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In the title compound, C_{30}H_{28}N_{2}, each carbazole skeleton is essentially planar. The planes of the two carbazole ring systems are nearly parallel, with a dihedral angle of 2.33 (19). The crystal packing is stabilized only by van der Waals forces and weak C–H⋯π interactions.

Comment

Polycarbazoles are among the most studied semiconducting polymers, due to their photoconduction properties (Loh et al., 1991; Rocquin & Chevrot, 1997; Li et al., 1998). The conductivities of these polymers are improved by the addition of certain dyes and electron acceptors as dopants (Iwatsuki & Arai, 1977; Hsiao et al., 2001). Upon irradiation, interactions of electron donor-acceptor (EDA) groups along the polymer chain lead to the formation of charge-transfer (CT) complexes. Dicarbazolylalkanes serve as model compounds of related photoconducting polymers for investigating the nature of CT complexation of carbazoles with various electron acceptors, both in solution and in the solid state (Haderski et al., 2000; Rocquin & Chevrot, 1997). We report here the crystal structure of the title compound, (I), which was synthesized to model poly-3-vinyl-N-ethylcarbazole in charge-transfer complexation studies.

The carbazole skeletons in (I) (Fig. 1) are essentially planar with only a slight distortion (r.m.s. deviations of the fitted atoms for both are 0.0436 Å). The interplanar dihedral angle of 2.33 (19)° indicates that the carbazolyl groups are almost parallel. The carbazolyl substituents show an anti conformation with respect to the C12—C12' bond. The geometric parameters in (I) are unexceptional and agree with those of related dicarbazoles reported in the literature (Baker et al., 1991; Asker & Masnovi, 2005). The torsion angles C9a—N—C10—C11 [−86.0 (7)°] and C9a'—N'—C10'—C11' [84.0 (7)°] indicate that the N-ethyl substituents are almost perpendicular to the carbazole planes.

The crystal packing diagram (Fig. 2) shows that the structure is stabilized only by van der Waals forces and weak C—
H · · · π interactions, the strongest of which is C10—H10c · · · Cg1 (H10c · · · Cg1 = 2.73 Å), where Cg1 is the centroid of the pyrrole ring containing N [symmetry code: (i) x − 1/2, y − 1/2, −z]. No intermolecular π–π interactions are observed between the carbazole groups. The carbazole groups of two adjacent molecules are inclined toward each other, preventing such an interaction, possibly due to the orientations of the N-ethyl groups and the methylene chain.

Experimental
The synthesis of the title compound was accomplished via the catalytic hydrogenation of 1,2-bis(9-ethylcarbazol-3-yl)ethene, which was prepared according to a literature procedure, via TiCl4/Zn-catalysed reductive coupling of 9-ethylcarbazole-3-carbaldehyde (Lynch et al., 1997). In a 100 ml round-bottomed flask, a mixture prepared from 1.0 g (2.4 mmol) of 1,2-bis(9-ethylcarbazol-3-yl)ethene, 0.1 g of Pd–C (10%), and 30 ml of tetrahydrofuran was stirred under an H2 atmosphere until the calculated amount of H2 (55 ml) was consumed (about 2 h). The reaction mixture was then filtered and the solvent was evaporated. Column chromatography of the resulting solid, using methanol/hexane (1:9) as eluent, yielded 0.96 g (95.57%) of (I) as colorless crystals (m.p. 454–455 K), 1H NMR (300 MHz, CDCl3):

- H atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.93, 0.96 and 0.97 Å for aromatic, methyl and methylene H atoms, respectively, and with Uiso(H) = 1.5Ueq(C) for the methyl H atoms and 1.2Ueq(C) for the others.
- Data collection: CAD-4-PC Software (Enraf–Nonius, 1993); cell refinement: CAD-4-PC Software; data reduction: DATR2D in NRCVAX (Gabe et al., 1989); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: ORTEP-3 for Windows (Farrugia, 1997) and PLATON (Spek, 2003); software used to prepare material for publication: WinGX publication routines (Farrugia, 1999).

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References

Figure 1
The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 40% probability level.

Figure 2
The molecular packing of (I), viewed down the a axis. H atoms have been omitted for clarity.