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Key indicators

Single-crystal X-ray study T = 293 K Mean σ (C–C) = 0.004 Å R factor = 0.050 wR factor = 0.152 Data-to-parameter ratio = 13.2

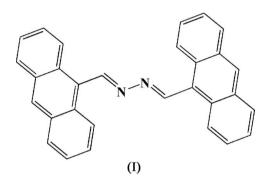
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

N,N'-Bis(9-anthracenylidene)hydrazine

In the title compound, $C_{30}H_{20}N_2$, synthesized by the reaction of anthracene-9-carbaldehyde with hydrazine hydrate, the two independent molecules are each located on a centre of symmetry. Weak π - π interactions between adjacent anthracene rings contribute to the stabilization of the crystal packing. Received 13 April 2006 Accepted 22 April 2006

Comment

Recently, a number of azine compounds containing both a diimine linkage and N—N bonding have been investigated in terms of their crystallography and coordination chemistry (Zheng *et al.*, 2005*a,b*; Duan *et al.*, 2005; Kundu *et al.*, 2005; Kesslen & Euler, 1999; Armstrong *et al.*, 1998; Xu *et al.*, 1997). We report here the crystal structure of the title compound, (I), in which two 9-anthracylidene units are directly linked through the imine N atoms.



The asymmetric unit of (I) contains two half-molecules. Each molecule has an E,E configuration, possessing a crys-

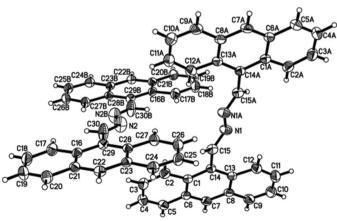


Figure 1

Two independent molecules in (I), showing the atom-labelling scheme and displacement ellipsoids drawn at the 30% probability level. Atoms labelled with the letters A and B are generated by the symmetry codes (1 - x, 1 - y, 1 - z) and (1 - x, 1 - y, 2 - z), respectively.

© 2006 International Union of Crystallography All rights reserved tallographically imposed centre of symmetry at the mid-point of the N-N bond (Fig. 1). This configuration agrees with that commonly found in a number of azine compounds (Zheng et al., 2005a,b; Duan et al., 2005; Şengül et al., 2004, Liu et al., 2004). The N-N bond lengths in the two molecules are 1.420 (3) and 1.383 (4) Å. One of the C=N-N angles $[C15 = N1 - N1 = 111.7 (2)^{\circ}]$ deviates significantly from the ideal sp^2 value of 120° as a consequence of repulsion between the nitrogen lone pairs and the adjacent C=N bond. The two independent molecules adopt different conformations, as can be seen from the significantly different values of the dihedral angles between the anthracene ring and the linkage plane [3.0(4) and 40.5(4)]. The short intermolecular contacts $C2 \cdot \cdot \cdot C6^{i}$ [3.561 (4) Å] and $C16 \cdot \cdot \cdot C22^{ii}$ [3.479 (4) Å] indicate weak π - π interactions, which contribute to the stabilization of the crystal packing [symmetry codes: (i) 2 - x, 1 - y, 1 - z; (ii) 1 - x, 2 - y, 2 - z].

Experimental

The title compound was synthesized by the reaction of anthracene-9carbaldehyde with hydrazine hydrate in refluxing ethanol (Liu *et al.*, 2004). Single crystals suitable for X-ray analysis were obtained by slow evaporation of a tetrahydrofuran solution.

Crystal data

 $\begin{array}{l} C_{30}H_{20}N_2 \\ M_r = 408.48 \\ \text{Triclinic, } P\overline{1} \\ a = 10.198 (3) \text{ Å} \\ b = 10.750 (4) \text{ Å} \\ c = 11.222 (4) \text{ Å} \\ a = 75.111 (5)^{\circ} \\ \beta = 65.663 (5)^{\circ} \\ \gamma = 86.438 (6)^{\circ} \end{array}$ $\begin{array}{l} Data \ collection \\ \text{Bruker SMART CCD area-detector} \end{array}$

diffractometer φ and ω scans Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) $T_{min} = 0.983, T_{max} = 0.992$ $V = 1082.0 \text{ (6) } \text{Å}^{3}$ Z = 2 $D_{x} = 1.254 \text{ Mg m}^{-3}$ Mo K\alpha radiation $\mu = 0.07 \text{ mm}^{-1}$ T = 293 (2) KBlock, colourless $0.24 \times 0.20 \times 0.18 \text{ mm}$

5531 measured reflections 3816 independent reflections 2002 reflections with $I > 2\sigma(I)$ $R_{int} = 0.024$ $\theta_{max} = 25.0^{\circ}$ Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.050$	$w = 1/[\sigma^2(F_o^2) + (0.0773P)^2]$
$wR(F^2) = 0.152$	where $P = (F_o^2 + 2F_c^2)/3$
S = 0.96	$(\Delta/\sigma)_{max} < 0.001$
3816 reflections 289 parameters	$\Delta \rho_{\text{max}} = 0.20 \text{ e } \text{\AA}^{-3}$ $\Delta \rho_{\text{min}} = -0.26 \text{ e } \text{\AA}^{-3}$

All H atoms were positioned geometrically and refined as riding, with C-H = 0.93 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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References

- Armstrong, J. A., Barnes, J. C. & Weakley, T. J. R. (1998). Acta Cryst. C54, 1923–1925.
- Bruker (1997). SMART, SAINT and SHELXTL. Bruker AXS Inc., Madison, Wisconsin, USA.
- Duan, X.-M., Zheng, P.-W. & Zhou, B. (2005). *Acta Cryst.* E61, 03449–03451. Kesslen, E. C. & Euler, W. B. (1999). *Chem. Mater.* 11, 336–340.
- Kundu, N., Chatterjee, P. B., Chaudhury, M. & Tiekink, E. R. T. (2005). Acta Cryst. E61, m1583–m1585.
- Liu, S. L., Chen, Y., Dai, J. F. & Liu, H. W. (2004). Chin. J. Synth. Chem. 12, 219–221.
- Şengül, A., Karadayi, N. & Büyükgüngör, O. (2004). Acta Cryst. C60, 0507– 0508.
- Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.

Sheldrick, G. M. (1997). SHELXS97 and SHELXL97. University of Göttingen, Germany.

Xu, Z., Thompson, L. K. & Miller, D. O. (1997). *Inorg. Chem.* **36**, 3985–3995. Zheng, P.-W., Wang, W. & Duan, X.-M. (2005*a*). *Acta Cryst.* **E61**, 03020–03021. Zheng, P.-W., Wang, W. & Duan, X.-M. (2005*b*). *Acta Cryst.* **E61**, 03485–03486.