Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2,2′-(Ethane-1,2-diyl)bis(2*H*-indazole)

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Key indicators

Single-crystal X-ray study
T = 296 K
Mean σ(C–C) = 0.002 Å
R factor = 0.040
wR factor = 0.106
Data-to-parameter ratio = 16.0

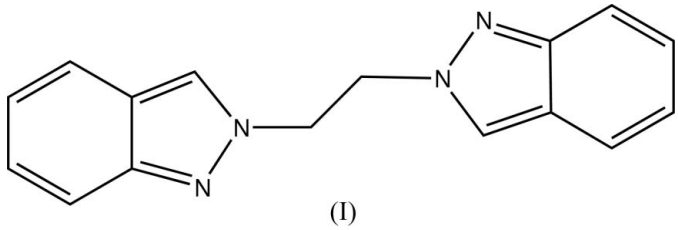
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 15 September 2006
Accepted 27 October 2006

The molecule of the title compound, $C_{16}H_{14}N_4$, lies on an inversion center. The crystal structure is built up by weak C—H···π and π–π interactions involving the indazole ring systems.

Comment

As part of an ongoing study of the synthesis of new macrocyclic and acyclic Schiff base ligands, the title compound, (I), was obtained by accident, instead of the expected acyclic ligand, *N*,*N*′-bis(2-aminobenzyl)ethane-1,2-diamine. A view of the molecular structure of (I) is given in Fig. 1.



(I)

Compound (I) crystallizes with the molecule lying on a center of symmetry located at the mid-point of the central CH_2—CH_2 bond. The molecular dimensions of (I) are within normal ranges (Allen *et al.*, 1987) and are similar to those found in the literature (Shirtcliff *et al.*, 2004; Seela *et al.*, 2004; Keyes *et al.*, 1998; Kimball *et al.*, 2002). The two Csp^2—N bonds [mean value 1.332 (2) Å] are intermediate in length between double (1.265 Å) and single (1.470 Å) bonds. This result indicates delocalization of the double bonds of the five-membered ring.

The crystal structure shows C—H···π interactions (Table 1). There are also weak π–π interactions involving symmetry-related indazole ring systems [molecule at (*x*, *y*, *z*) and molecule at (− *x*, −*y*, 1 − *z*)], with a separation of 3.647 Å

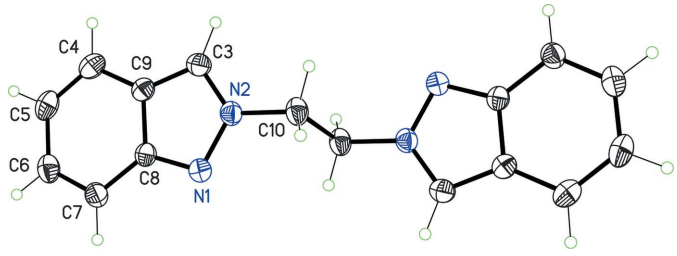


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 30% probability level and H atoms shown as small spheres of arbitrary radii. Unlabeled atoms are related to labeled atoms by the symmetry code (−*x* + 1, −*y* + 1, −*z* + 1)

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between centroids. This distance represents a weak π–π interaction between consecutive parallel molecules [3.35 Å in graphite (Wyckoff, 1963), as one representative example] (Fig. 2).

Experimental

Compound (I) was prepared following published procedures (Elizondo-Martínez *et al.*, 2006; Obregón-Solís *et al.*, 2001), followed by a selective reduction reaction. Prismatic yellow crystals were obtained by recrystallization from ethanol by slow evaporation (yield: 50%). The solid was characterized by elemental analysis and ^{1}H NMR.

Crystal data

$C_{16}H_{14}N_4$
M_r = 262.31
Orthorhombic, *Pbca*
a = 9.8781 (8) Å
b = 6.9451 (5) Å
c = 19.2655 (15) Å
V = 1321.70 (18) Å^3
Z = 4
D_x = 1.318 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 296 (2) K
Prism, pale yellow
0.5 × 0.5 × 0.4 mm

Data collection

Bruker P4 diffractometer
$2\theta/\omega$ scans
Absorption correction: none
4200 measured reflections
1918 independent reflections
1345 reflections with $I > 2\sigma(I)$
R_{int} = 0.024
θ_{max} = 30.0°
3 standard reflections
every 97 reflections
intensity decay: 2.9%

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.106
S = 1.02
1918 reflections
120 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0444P)^2 + 0.1528P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: *SHELXTL-Plus*
Extinction coefficient: 0.0074 (15)

Table 1
C—H···π interactions (Å, °).

Cg is the centroid of the C4–C9 benzene ring.

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5···Cg^{i}	0.962 (16)	2.928 (15)	3.7523 (15)	144.4 (11)
C10—H10B···Cg^{ii}	0.979 (15)	2.868 (15)	3.6421 (14)	136.6 (10)

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x+1, -y, -z+1$.

All H atoms were found in difference maps and were refined isotropically.

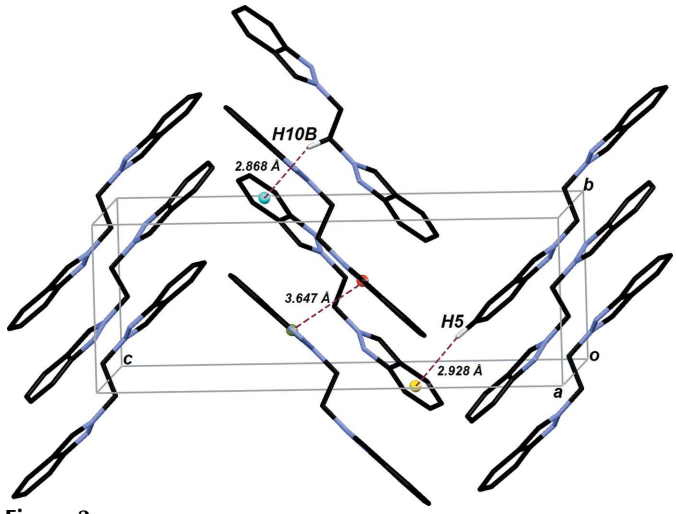

Figure 2
The packing of (I), showing the C—H···π and π–π interactions between indazole ring systems. H atoms not involved in the interactions have been omitted.

Data collection: *XSCANS* (Siemens, 1996); cell refinement: *XSCANS*; data reduction: *SHELXTL-Plus* (Siemens, 1996); program(s) used to solve structure: *SHELXTL-Plus*; program(s) used to refine structure: *SHELXTL-Plus*; molecular graphics: *SHELXTL-Plus* and *MERCURY* (Bruno *et al.*, 2002); software used to prepare material for publication: *SHELXTL-Plus*.

We thank Dr Sylvain Bernès for data collection at the Instituto de Ciencias, BUAP, Puebla, Mexico, and for his valuable comments on this paper.

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst.* B**58**, 389–397.
Elizondo-Martínez, P., Nájera-Martínez, B. & Rodríguez de Barbarín, C. (2006). *Adv. Tech. Mat. Mat. Proc. J.* **8**, 41–44.
Keyes, M. C., Chamberlain, B. M., Caltagirone, S. A., Halfen, J. A. & Tolman, W. B. (1998). *Organometallics*, **17**, 1984–1992.
Kimball, D. B., Weakley, T. J. R., Herges, R. & Haley, M. M. (2002). *J. Am. Chem. Soc.* **124**, 13463–13473.
Obregón-Solís, E., Rodríguez de Barbarín, C., Elizondo de Cota, P. & Nájera-Martínez, B. (2001). *CIENCIA UANL*, **4**, 435–440. (In Spanish.)
Seela, F., Peng, X.-H., Eickmeier, H. & Reuter, H. (2004). *Acta Cryst.* C**60**, o94–o97.
Shirtcliff, L. D., Weakley, T. J. R., Haley, M. M., Kohler, F. & Herges, R. (2004). *J. Org. Chem.* **69**, 6979–6985.
Siemens (1996). *XSCANS User's Manual* (Version 2.21) and *SHELXTL-Plus* (Version 5.10). Siemens Analytical X-ray Instruments Inc. Madison, Wisconsin, USA.
Wyckoff, R. W. G. (1963). *Geometrical Structures*, p. 83. New York: Interscience Publishers.