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9-(1,2,4-Triazol-1-yl)anthracene

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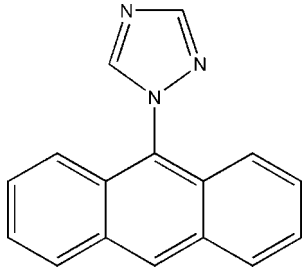
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.062; wR factor = 0.137; data-to-parameter ratio = 11.9.

The title compound, $C_{16}H_{11}N_3$, was obtained by the reaction of 9-bromoanthracene with 1,2,4-triazole in dimethylformamide. The molecule is not planar; the triazole ring makes a dihedral angle of 68.7 (4)° with the anthracene plane.

Related literature

For related literature, see: Fanni *et al.* (2000); Yi *et al.* (2004); Zhang *et al.* (2005).



Experimental

Crystal data

$C_{16}H_{11}N_3$
M_r = 245.28
Triclinic, $P\overline{1}$
a = 8.5580 (17) Å
b = 8.9289 (18) Å
c = 9.0170 (18) Å
α = 63.57 (3)°
β = 75.43 (3)°
γ = 77.80 (3)°
V = 593.2 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.22 × 0.20 × 0.18 mm

Data collection

Rigaku R-AXIS RAPID-S diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.982, T_{max} = 0.985
4470 measured reflections
2053 independent reflections
1624 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.137
S = 1.12
2053 reflections
172 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2138).

References

Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Fanni, S., Murphy, S., Killeen, J. S. & Vos, J. G. (2000). *Inorg. Chem.* **39**, 1320–1321.
Rigaku/MSC (2005). *CrystalClear*. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Yi, L., Ding, B., Zhao, B., Cheng, P., Liao, D. Z., Yan, S. P. & Jiang, Z. H. (2004). *Inorg. Chem.* **43**, 33–43.
Zhang, J. P., Lin, Y. Y., Huang, X. C. & Chen, X. M. (2005). *J. Am. Chem. Soc.* **127**, 5495–5506.

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supplementary materials

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9-(1,2,4-Triazol-1-yl)anthracene

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Comment

In the last few years it has been shown that 1,2,4-triazole and its derivatives are interesting building blocks for supramolecular systems. (Zhang *et al.*, 2005; Yi *et al.* 2004; Fanni *et al.*, 2000). Recently, we synthesized a new rigid triazole-ligand, namely 9-(1,2,4-triazol-1-yl)-anthracene, (I). Here we report the crystal structure of this ligand.

As shown in Fig. 1, the molecule of (I) is not planar; the triazole ring makes a dihedral angle of 68.7 (4)° with the anthracene plane. The C14—N1 bond distance is 1.437 (3) Å, whereas the C—N bond distances in the triazole ring range from 1.315 (3) to 1.356 (3) Å.

Experimental

9-Bromoanthracene (1.29 g, 5.0 mmol), 1,2,4-triazole (0.35 g, 5.0 mmol), 1,10-phenanthroline (0.16 g, 0.88 mmol), anhydrous potassium carbonate (1.24 g, 9.0 mmol), and CuI (0.081 g, 0.043 mmol) were placed in a 50 ml flask with 30 ml dimethylformamide. The mixture was refluxed for 48 h under N_2. After the reaction mixture was cooled to ambient temperature, dichloromethane was added to extract the brown sticky residue. The organic extracts were dried with anhydrous $MgSO_4$ and further purified using a silica gel column (chloroform/ethyl acetate) to obtain a light yellow solid of 9-(1,2,4-triazol-1-yl)-anthracene (I) (yield: 0.49 g, 40%). The yellow powder was recrystallized from a mixture of chloroform and methanol (1:1), which gave single crystals suitable for X-ray diffraction.

Refinement

The H atoms were positioned geometrically and refined using a riding model, with C—H = 0.93 Å and U_{iso}(H) set equal to 1.2U_{eq}(C).

Figures

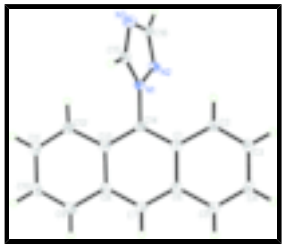

Fig. 1. The molecular structure of the title compound, with displacement ellipsoids drawn at the 30% probability level .

9-(1,2,4-Triazol-1-yl)anthracene

Crystal data

$C_{16}H_{11}N_3$	$Z = 2$
$M_r = 245.28$	$F_{000} = 256$
Triclinic, $P\overline{1}$	$D_x = 1.373$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.5580$ (17) Å	Cell parameters from 1267 reflections
$b = 8.9289$ (18) Å	$\theta = 2.5$–27.9º
$c = 9.0170$ (18) Å	$\mu = 0.08$ mm^{-1}
$\alpha = 63.57$ (3)º	$T = 293$ (2) K
$\beta = 75.43$ (3)º	Block, colorless
$\gamma = 77.80$ (3)º	0.22 × 0.20 × 0.18 mm
$V = 593.2$ (2) Å^3	

Data collection

Rigaku R-AXIS RAPID-S diffractometer	2053 independent reflections
Radiation source: fine-focus sealed tube	1624 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.038$
$T = 293$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 2.5$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -10 \rightarrow 10$
$T_{min} = 0.982$, $T_{max} = 0.985$	$k = -10 \rightarrow 10$
4470 measured reflections	$l = -10 \rightarrow 10$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0545P)^2 + 0.1412P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)] = 0.062$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.137$	$\Delta\rho_{max} = 0.18$ e Å^{-3}
$S = 1.12$	$\Delta\rho_{min} = -0.26$ e Å^{-3}
2053 reflections	Extinction correction: none
172 parameters	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	
Hydrogen site location: inferred from neighbouring sites	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating R-factors(gt) etc. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($Å^2$)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	1.0212 (3)	0.3020 (3)	0.2577 (3)	0.0213 (5)
C2	1.0449 (3)	0.3347 (3)	0.3913 (3)	0.0231 (5)
H2	0.9621	0.3212	0.4842	0.028*
C3	1.1863 (3)	0.3850 (3)	0.3850 (3)	0.0264 (6)
H3	1.1994	0.4054	0.4735	0.032*
C4	1.3144 (3)	0.4070 (3)	0.2444 (3)	0.0277 (6)
H4	1.4107	0.4414	0.2416	0.033*
C5	1.2974 (3)	0.3781 (3)	0.1144 (3)	0.0255 (6)
H5	1.3825	0.3924	0.0234	0.031*
C6	1.1504 (3)	0.3258 (3)	0.1153 (3)	0.0217 (5)
C7	1.1293 (3)	0.2950 (3)	−0.0173 (3)	0.0241 (5)
H7	1.2129	0.3116	−0.1099	0.029*
C8	0.9887 (3)	0.2407 (3)	−0.0157 (3)	0.0219 (5)
C9	0.9710 (3)	0.2043 (3)	−0.1493 (3)	0.0261 (6)
H9	1.0550	0.2197	−0.2414	0.031*
C10	0.8342 (3)	0.1479 (3)	−0.1439 (3)	0.0295 (6)
H10	0.8254	0.1238	−0.2316	0.035*
C11	0.7041 (3)	0.1252 (3)	−0.0056 (3)	0.0291 (6)
H11	0.6101	0.0873	−0.0040	0.035*
C12	0.7148 (3)	0.1578 (3)	0.1245 (3)	0.0269 (6)
H12	0.6280	0.1425	0.2139	0.032*
C13	0.8576 (3)	0.2153 (3)	0.1259 (3)	0.0223 (5)
C14	0.8790 (3)	0.2467 (3)	0.2583 (3)	0.0214 (5)
C15	0.6928 (3)	0.0793 (3)	0.5191 (3)	0.0285 (6)
H15	0.7345	−0.0271	0.5230	0.034*
C16	0.5572 (3)	0.2780 (3)	0.5699 (3)	0.0286 (6)
H16	0.4792	0.3366	0.6233	0.034*
N1	0.7494 (2)	0.2221 (2)	0.4010 (2)	0.0225 (5)
N2	0.6607 (2)	0.3560 (2)	0.4323 (2)	0.0268 (5)
N3	0.5709 (2)	0.1080 (3)	0.6291 (2)	0.0325 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0227 (12)	0.0143 (12)	0.0235 (12)	0.0016 (9)	−0.0051 (10)	−0.0059 (10)
C2	0.0252 (13)	0.0223 (13)	0.0213 (12)	−0.0023 (10)	−0.0015 (10)	−0.0102 (10)
C3	0.0298 (13)	0.0257 (14)	0.0269 (13)	−0.0013 (10)	−0.0082 (10)	−0.0130 (11)
C4	0.0237 (13)	0.0267 (14)	0.0326 (13)	−0.0069 (10)	−0.0063 (10)	−0.0098 (11)
C5	0.0222 (13)	0.0244 (13)	0.0252 (12)	−0.0027 (10)	−0.0013 (10)	−0.0079 (11)
C6	0.0224 (12)	0.0176 (12)	0.0222 (12)	0.0023 (9)	−0.0056 (10)	−0.0069 (10)
C7	0.0226 (12)	0.0241 (13)	0.0222 (12)	−0.0009 (10)	−0.0002 (10)	−0.0093 (10)
C8	0.0231 (12)	0.0195 (12)	0.0209 (12)	0.0005 (10)	−0.0058 (10)	−0.0068 (10)
C9	0.0319 (14)	0.0235 (13)	0.0206 (12)	0.0011 (10)	−0.0054 (10)	−0.0088 (10)
C10	0.0418 (15)	0.0244 (14)	0.0262 (13)	−0.0026 (11)	−0.0123 (11)	−0.0111 (11)
C11	0.0322 (14)	0.0256 (14)	0.0330 (14)	−0.0051 (11)	−0.0128 (11)	−0.0107 (11)
C12	0.0243 (13)	0.0259 (14)	0.0298 (13)	−0.0027 (10)	−0.0036 (10)	−0.0116 (11)
C13	0.0224 (12)	0.0190 (12)	0.0237 (12)	0.0008 (10)	−0.0049 (10)	−0.0083 (10)
C14	0.0199 (12)	0.0185 (12)	0.0221 (12)	−0.0013 (9)	0.0005 (10)	−0.0079 (10)
C15	0.0292 (14)	0.0281 (14)	0.0276 (13)	−0.0074 (11)	−0.0010 (11)	−0.0114 (11)
C16	0.0226 (13)	0.0386 (16)	0.0271 (13)	−0.0038 (11)	−0.0012 (10)	−0.0172 (12)
N1	0.0213 (10)	0.0253 (11)	0.0227 (10)	−0.0040 (8)	0.0003 (8)	−0.0131 (9)
N2	0.0220 (11)	0.0320 (12)	0.0291 (11)	−0.0005 (9)	−0.0001 (9)	−0.0186 (10)
N3	0.0313 (12)	0.0346 (13)	0.0300 (12)	−0.0086 (9)	−0.0001 (9)	−0.0128 (10)

Geometric parameters (Å, °)

C1—C14	1.405 (3)	C9—H9	0.9300
C1—C2	1.428 (3)	C10—C11	1.417 (3)
C1—C6	1.435 (3)	C10—H10	0.9300
C2—C3	1.357 (3)	C11—C12	1.356 (3)
C2—H2	0.9300	C11—H11	0.9300
C3—C4	1.420 (3)	C12—C13	1.427 (3)
C3—H3	0.9300	C12—H12	0.9300
C4—C5	1.354 (3)	C13—C14	1.402 (3)
C4—H4	0.9300	C14—N1	1.437 (3)
C5—C6	1.429 (3)	C15—N3	1.315 (3)
C5—H5	0.9300	C15—N1	1.336 (3)
C6—C7	1.399 (3)	C15—H15	0.9300
C7—C8	1.384 (3)	C16—N2	1.322 (3)
C7—H7	0.9300	C16—N3	1.356 (3)
C8—C9	1.429 (3)	C16—H16	0.9300
C8—C13	1.438 (3)	N1—N2	1.377 (3)
C9—C10	1.351 (3)		
C14—C1—C2	123.7 (2)	C9—C10—C11	120.5 (2)
C14—C1—C6	118.1 (2)	C9—C10—H10	119.8
C2—C1—C6	118.2 (2)	C11—C10—H10	119.8
C3—C2—C1	121.0 (2)	C12—C11—C10	120.8 (2)
C3—C2—H2	119.5	C12—C11—H11	119.6

C1—C2—H2	119.5	C10—C11—H11	119.6
C2—C3—C4	120.6 (2)	C11—C12—C13	120.9 (2)
C2—C3—H3	119.7	C11—C12—H12	119.5
C4—C3—H3	119.7	C13—C12—H12	119.5
C5—C4—C3	120.5 (2)	C14—C13—C12	123.9 (2)
C5—C4—H4	119.7	C14—C13—C8	117.8 (2)
C3—C4—H4	119.7	C12—C13—C8	118.2 (2)
C4—C5—C6	120.8 (2)	C13—C14—C1	123.0 (2)
C4—C5—H5	119.6	C13—C14—N1	118.69 (19)
C6—C5—H5	119.6	C1—C14—N1	118.35 (19)
C7—C6—C5	122.1 (2)	N3—C15—N1	111.6 (2)
C7—C6—C1	119.1 (2)	N3—C15—H15	124.2
C5—C6—C1	118.8 (2)	N1—C15—H15	124.2
C8—C7—C6	122.4 (2)	N2—C16—N3	116.3 (2)
C8—C7—H7	118.8	N2—C16—H16	121.8
C6—C7—H7	118.8	N3—C16—H16	121.8
C7—C8—C9	121.8 (2)	C15—N1—N2	109.22 (18)
C7—C8—C13	119.6 (2)	C15—N1—C14	129.43 (19)
C9—C8—C13	118.6 (2)	N2—N1—C14	121.35 (17)
C10—C9—C8	121.0 (2)	C16—N2—N1	101.12 (19)
C10—C9—H9	119.5	C15—N3—C16	101.70 (19)
C8—C9—H9	119.5		
C14—C1—C2—C3	178.8 (2)	C9—C8—C13—C14	178.1 (2)
C6—C1—C2—C3	−0.7 (3)	C7—C8—C13—C12	−179.4 (2)
C1—C2—C3—C4	0.2 (3)	C9—C8—C13—C12	−1.1 (3)
C2—C3—C4—C5	0.1 (4)	C12—C13—C14—C1	179.5 (2)
C3—C4—C5—C6	0.3 (3)	C8—C13—C14—C1	0.3 (3)
C4—C5—C6—C7	180.0 (2)	C12—C13—C14—N1	−0.8 (3)
C4—C5—C6—C1	−0.9 (3)	C8—C13—C14—N1	179.99 (19)
C14—C1—C6—C7	0.6 (3)	C2—C1—C14—C13	179.9 (2)
C2—C1—C6—C7	−179.8 (2)	C6—C1—C14—C13	−0.5 (3)
C14—C1—C6—C5	−178.5 (2)	C2—C1—C14—N1	0.2 (3)
C2—C1—C6—C5	1.1 (3)	C6—C1—C14—N1	179.79 (18)
C5—C6—C7—C8	178.5 (2)	N3—C15—N1—N2	−0.1 (3)
C1—C6—C7—C8	−0.6 (3)	N3—C15—N1—C14	−179.2 (2)
C6—C7—C8—C9	−177.8 (2)	C13—C14—N1—C15	68.5 (3)
C6—C7—C8—C13	0.4 (3)	C1—C14—N1—C15	−111.7 (3)
C7—C8—C9—C10	178.5 (2)	C13—C14—N1—N2	−110.6 (2)
C13—C8—C9—C10	0.3 (3)	C1—C14—N1—N2	69.2 (3)
C8—C9—C10—C11	0.6 (3)	N3—C16—N2—N1	−0.2 (3)
C9—C10—C11—C12	−0.7 (4)	C15—N1—N2—C16	0.1 (2)
C10—C11—C12—C13	−0.2 (4)	C14—N1—N2—C16	179.39 (19)
C11—C12—C13—C14	−178.0 (2)	N1—C15—N3—C16	0.0 (3)
C11—C12—C13—C8	1.1 (3)	N2—C16—N3—C15	0.1 (3)
C7—C8—C13—C14	−0.2 (3)		

Fig. 1