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1,5-Dicyanoanthraquinone

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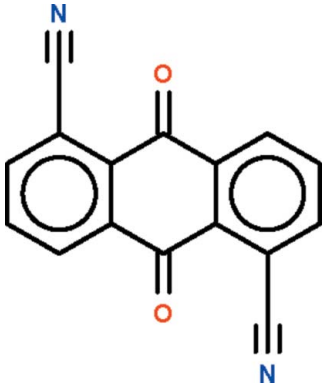
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.053; wR factor = 0.149; data-to-parameter ratio = 11.0.

The complete molecule of the title compound, $C_{16}H_6N_2O_2$, which is generated by a crystallographic inversion centre, is almost planar (r.m.s. deviation = 0.04 Å). In the crystal, adjacent molecules are stacked along the *a* axis, with a shortest centroid–centroid separation of 3.826 (2) Å.

Related literature

For the synthesis, see: Casey *et al.* (1999); Coulson (1930*a*,*b*). For some applications of anthraquinones, see: Alagesan & Samuelson (1997); Chang *et al.* (1996); Cheng *et al.* (1994); Kuritani *et al.* (1973); Lin *et al.* (1995).



Experimental

Crystal data

$C_{16}H_6N_2O_2$
M_r = 258.23
Monoclinic, $P2_1/c$
a = 3.8256 (10) Å
b = 7.0183 (19) Å
c = 21.249 (6) Å
β = 91.064 (4)°
V = 570.4 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.35 × 0.06 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
4238 measured reflections
1013 independent reflections
600 reflections with $I > 2\sigma(I)$
R_{int} = 0.048

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.149
S = 1.06
1013 reflections
92 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5350).

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supporting information

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1,5-Dicyanoanthraquinone

Mahsa Armaghan, Mostafa M. Amini and Seik Weng Ng

S1. Comment

The title substituted anthraquinone (Scheme I, Fig. 1) was synthesized to study its ability to absorb sulfur from oil when immobilized on silica surface (MCM-41). Anthraquinones are a class of anthracene derivatives having useful industrial applications (Alagesan & Samuelson, 1997; Chang *et al.*, 1996; Cheng *et al.*, 1994; Kuritani *et al.*, 1973; Lin *et al.*, 1995). However, they are usually only sparingly soluble in common oragnic solvents. In the present study, the synthesis involves the exchange of chlorine of 1,5-dichloroanthraquinone with the cyanide of copper cyanide (Coulson, 1930; Casey *et al.*, 1999). The compound is somewhat soluble in DMSO but the recrystallized product is a yellow powder. Crystals were ultimately obtained by diffusing methanol into a DMSO solution of the compound.

The molecule of 1,5-dicyanoanthraquinone, which lies about a center-of-inversion, is planar (max. r.m.s.deviation 0.04 Å). Adjacent molecules are stacked over each other along the *a*-axis of the monoclinic unit cell; the distance is that of the *a*-axial length itself (Fig. 2).

S2. Experimental

1,5-Dicyanoanthraquinone was prepared by using a reported procedure by reacting 1,5-dichloroanthraquinone with benzyl cyanide in presence of cuprous cyanide (Coulson, 1930a,b; Casey *et al.*, 1999). The compound is sparingly soluble in common solvents; yellow prisms of (I) were obtained by the slow diffusion of methanol into a DMSO solution of the compound; m.p.> 633 K, decompose).

S3. Refinement

Carbon-bound H-atoms were placed in calculated positions (C—H 0.93 Å) and were included in the refinement in the riding model approximation, with U(H) set to 1.2U(C).

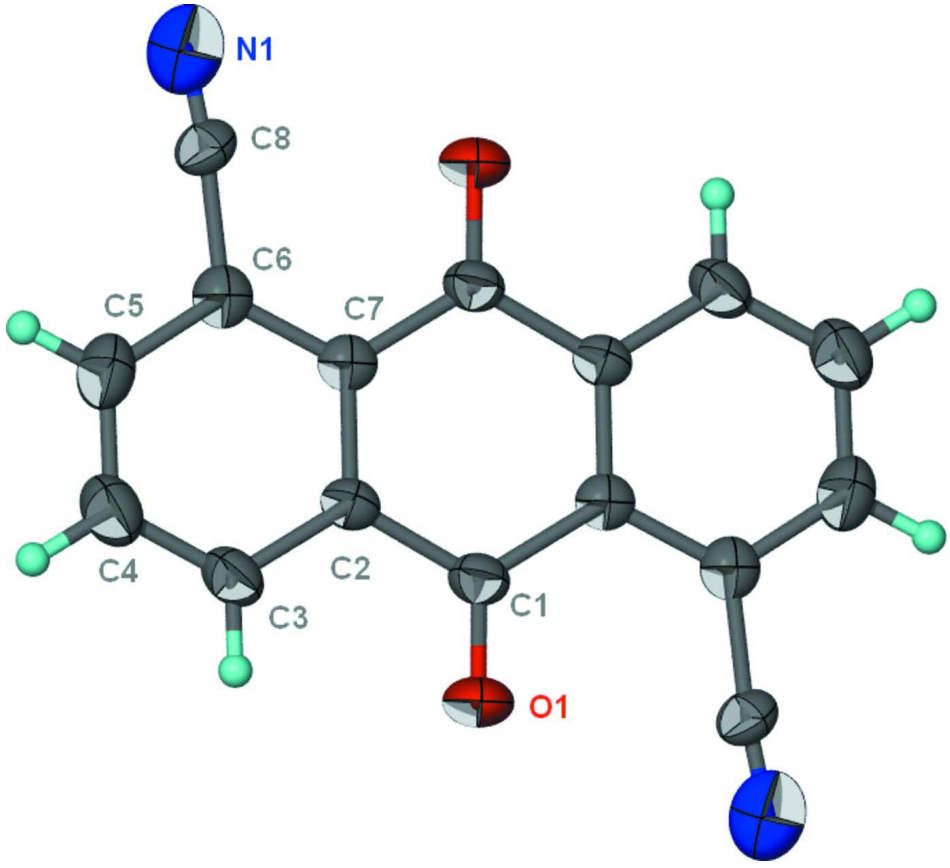

Figure 1

The molecular structure of (I): displacement ellipsoids are drawn at the 50% probability level and H atoms are of arbitrary radius. Unlabelled atoms are generated by the symmetry operation (1–x, 1–y, 1–z).

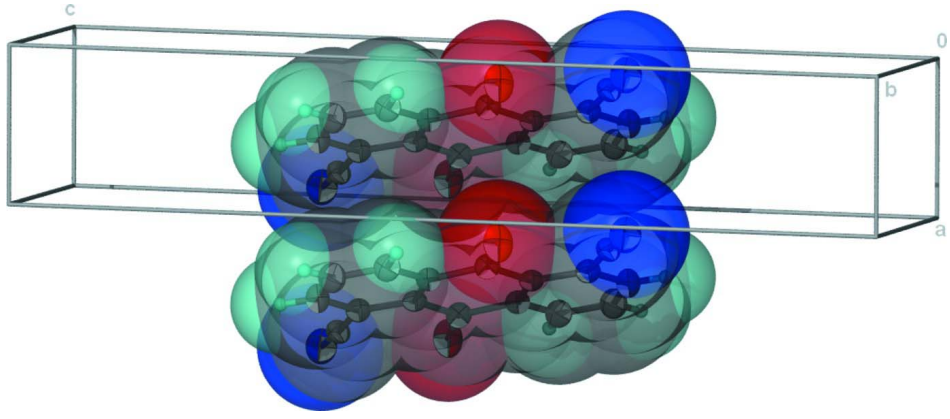

Figure 2

Stacking of the molecules in the unit cell of (I).

1,5-Dicyanoanthraquinone

Crystal data

$C_{16}H_6N_2O_2$
$M_r = 258.23$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 3.8256$ (10) Å
$b = 7.0183$ (19) Å
$c = 21.249$ (6) Å
$\beta = 91.064$ (4)°
$V = 570.4$ (3) Å^3
$Z = 2$
$F(000) = 264$
$D_x = 1.503$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 614 reflections
$\theta = 3.1$–$25.4°$
$\mu = 0.10$ mm^{-1}
$T = 293$ K
Prism, yellow
0.35 × 0.06 × 0.03 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
4238 measured reflections
1013 independent reflections
600 reflections with $I > 2\sigma(I)$
$R_{int} = 0.048$
$\theta_{max} = 25.0°$, $\theta_{min} = 1.9°$
$h = -4 \rightarrow 4$
$k = -8 \rightarrow 8$
$l = -25 \rightarrow 25$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.053$
$wR(F^2) = 0.149$
$S = 1.06$
1013 reflections
92 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0649P)^2 + 0.1468P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.19$ e Å^{-3}
$\Delta\rho_{min} = -0.18$ e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.033 (9)

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.8448 (7)	0.2052 (3)	0.55023 (10)	0.0691 (8)
N1	0.0797 (10)	0.7591 (5)	0.30574 (16)	0.0837 (11)
C1	0.6782 (8)	0.3375 (4)	0.52815 (13)	0.0407 (7)
C2	0.5829 (7)	0.3390 (4)	0.46013 (12)	0.0373 (7)
C3	0.6669 (8)	0.1823 (4)	0.42375 (14)	0.0473 (8)
H3	0.7752	0.0773	0.4423	0.057*
C4	0.5910 (9)	0.1815 (5)	0.36042 (15)	0.0583 (10)
H4	0.6438	0.0750	0.3364	0.070*
C5	0.4369 (9)	0.3378 (5)	0.33232 (15)	0.0566 (9)
H5	0.3903	0.3369	0.2892	0.068*
C6	0.3504 (7)	0.4968 (4)	0.36757 (13)	0.0430 (8)
C7	0.4220 (7)	0.4985 (4)	0.43270 (12)	0.0373 (7)

C8	0.1889 (8)	0.6593 (5)	0.33253 (14)	0.0424 (8)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.097 (2)	0.0525 (15)	0.0572 (15)	0.0343 (13)	−0.0103 (13)	0.0056 (11)
N1	0.090 (3)	0.093 (3)	0.068 (2)	−0.006 (2)	0.0044 (19)	−0.0029 (19)
C1	0.0450 (18)	0.0323 (16)	0.0450 (17)	0.0043 (13)	0.0016 (13)	0.0035 (13)
C2	0.0383 (17)	0.0308 (16)	0.0427 (16)	0.0014 (12)	0.0011 (12)	0.0016 (12)
C3	0.053 (2)	0.0347 (18)	0.0540 (19)	0.0052 (13)	0.0015 (14)	−0.0067 (14)
C4	0.063 (2)	0.052 (2)	0.060 (2)	0.0047 (16)	0.0011 (17)	−0.0155 (17)
C5	0.058 (2)	0.070 (2)	0.0414 (17)	−0.0024 (17)	−0.0007 (15)	−0.0078 (16)
C6	0.0400 (17)	0.0455 (18)	0.0437 (17)	−0.0032 (14)	0.0028 (12)	−0.0009 (14)
C7	0.0325 (15)	0.0377 (17)	0.0416 (16)	−0.0027 (12)	0.0024 (11)	0.0024 (12)
C8	0.0388 (18)	0.050 (2)	0.0382 (17)	0.0024 (14)	−0.0053 (13)	0.0059 (15)

Geometric parameters (Å, º)

O1—C1	1.216 (3)	C4—C5	1.376 (4)
N1—C8	0.991 (4)	C4—H4	0.9300
C1—C7^{i}	1.475 (4)	C5—C6	1.387 (4)
C1—C2	1.484 (4)	C5—H5	0.9300
C2—C3	1.386 (4)	C6—C7	1.406 (3)
C2—C7	1.399 (4)	C6—C8	1.490 (4)
C3—C4	1.371 (4)	C7—C1^{i}	1.475 (4)
C3—H3	0.9300		
O1—C1—C7^{i}	121.2 (3)	C5—C4—H4	119.9
O1—C1—C2	119.9 (3)	C4—C5—C6	120.8 (3)
C7^{i}—C1—C2	118.8 (2)	C4—C5—H5	119.6
C3—C2—C7	120.5 (3)	C6—C5—H5	119.6
C3—C2—C1	118.8 (2)	C5—C6—C7	119.6 (3)
C7—C2—C1	120.7 (2)	C5—C6—C8	116.5 (3)
C4—C3—C2	120.2 (3)	C7—C6—C8	123.9 (3)
C4—C3—H3	119.9	C2—C7—C6	118.7 (3)
C2—C3—H3	119.9	C2—C7—C1^{i}	120.4 (2)
C3—C4—C5	120.2 (3)	C6—C7—C1^{i}	120.9 (3)
C3—C4—H4	119.9	N1—C8—C6	174.6 (4)
O1—C1—C2—C3	4.2 (4)	C4—C5—C6—C8	179.3 (3)
C7^{i}—C1—C2—C3	−177.9 (3)	C3—C2—C7—C6	−0.5 (4)
O1—C1—C2—C7	−173.6 (3)	C1—C2—C7—C6	177.2 (2)
C7^{i}—C1—C2—C7	4.3 (4)	C3—C2—C7—C1^{i}	177.9 (3)
C7—C2—C3—C4	−0.4 (4)	C1—C2—C7—C1^{i}	−4.4 (4)
C1—C2—C3—C4	−178.2 (3)	C5—C6—C7—C2	0.6 (4)
C2—C3—C4—C5	1.3 (5)	C8—C6—C7—C2	−178.4 (3)

C3—C4—C5—C6	−1.2 (5)	C5—C6—C7—C1^{i}	−177.8 (3)
C4—C5—C6—C7	0.2 (4)	C8—C6—C7—C1^{i}	3.2 (4)

Symmetry code: (i) −*x*+1, −*y*+1, −*z*+1.