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1,4-Diisocyano-2,5-dimethylbenzene

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.002 Å
R factor = 0.048
wR factor = 0.131
Data-to-parameter ratio = 15.1

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

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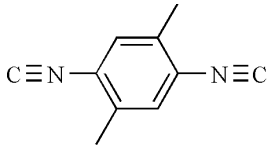
1,4-Diisocyano-2,5-dimethylbenzene, p-$C_6H_2(CH_3)_2(NC)_2$, crystallizes in the monoclinic space group $P2_1/c$. One-half of the molecule is crystallographically independent, with the other half being generated by an inversion centre located at the centre of the molecule.

Comment

In the course of our work on isonitrile-bridged and capped molybedenum complexes, we isolated and structurally characterized 1,4-diisocyano-2,5-dimethylbenzene, (I). The bis-isocyanide is located on a crystallographic inversion centre, with only one-half of the molecule crystallographically independent. Bond lengths and angles are in the expected ranges for aromatic isonitriles.



(I)

Experimental

1,4-Diisocyano-2,5-dimethylbenzene was synthesized from the corresponding formamide by reacting 2,5-dimethyl-*p*-phenylenediamine with 75% formic acid under reflux for two hours. Addition of water precipitated the formamide, which was washed with water until neutral and dried *in vacuo*. The isocyanide was synthesized as described by Efraty *et al.* (1980) for 1,4-diisocyanobenzene. The isocyanide was purified by sublimation *in vacuo*. Single crystals were grown by sublimation *in vacuo*.

Crystal data

$C_{10}H_8N_2$
M_r = 156.18
Monoclinic, $P2_1/c$
a = 3.9754 (9) Å
b = 9.263 (2) Å
c = 11.591 (3) Å
β = 91.690 (4)°
V = 426.64 (17) Å^3
Z = 2
D_x = 1.216 Mg m^{-3}
Mo Kα radiation
Cell parameters from 2218 reflections
θ = 2.8–28.3°
μ = 0.08 mm^{-1}
T = 100 (2) K
Block, colourless
0.3 × 0.2 × 0.2 mm

Data collection

Bruker AXS SMART APEX CCD diffractometer
ω scans
Absorption correction: none
4084 measured reflections
1069 independent reflections
827 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 28.3°
$h = -5 \rightarrow 5$
$k = -12 \rightarrow 12$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0698P)^2 + 0.6662P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > F^2\sigma(F^2)] = 0.048$	$(\Delta/\sigma)_{max} < 0.001$
$wR(F^2) = 0.131$	$\Delta\rho_{max} = 0.32$ e Å^{-3}
$S = 1.03$	$\Delta\rho_{min} = -0.19$ e Å^{-3}
1069 reflections	
71 parameters	
All H-atom parameters refined	

Table 1
Selected geometric parameters (Å, °).

N1—C1	1.1648 (19)	C3—C2	1.3944 (19)
N1—C2	1.4066 (17)	C2—C4^{i}	1.4027 (18)
C3—C4	1.391 (2)	C5—C4	1.5044 (19)
C1—N1—C2	178.26 (14)	C4^{i}—C2—N1	118.59 (12)
C4—C3—C2	120.49 (12)	C3—C4—C2^{i}	116.64 (12)
C3—C2—C4^{i}	122.88 (12)	C3—C4—C5	121.58 (12)
C3—C2—N1	118.53 (12)	C2^{i}—C4—C5	121.79 (13)

Symmetry code: (i) $1-x, 1-y, 1-z$.

All H atoms were located in a difference Fourier map and refined isotropically.

The s.u. values of the cell parameters are derived from the software, and are unreasonably small (Herbstein, 2000).

Data collection: *SMART* (Bruker 1997–2000); cell refinement: *SAINT-Plus* (Bruker 1997–1999); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXL*97; software used to prepare material for publication: *SHELXL*97.

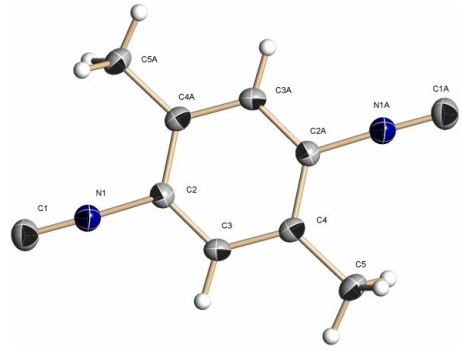


Figure 1
Molecular structure of (I), showing 30% probability displacement ellipsoids.

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