Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

4-Anilino-3-nitropyridine

Lynch and McClenaghan

Electronic paper
This paper is published electronically. It meets the data-validation criteria for publication in Acta Crystallographica Section C. The submission has been checked by a Section C Co-editor though the text in the 'Comments' section is the responsibility of the authors.

Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

4-Anilino-3-nitropyridine

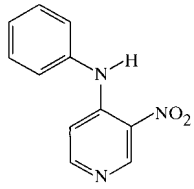
Daniel E. Lynch[a]* and Ian McClenaghan[b]†

[a]School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England, and [b]Spa Contract Synthesis, School of Natural and Environmental Sciences, Coventry University, Coventry CV1 5FB, England
Correspondence e-mail: apx106@coventry.ac.uk

Received 28 September 2000
Accepted 9 October 2000

Data validation number: IUC0000287

The structure of the title compound, $C_{22}H_{18}N_6O_4$, (I), comprises two unique molecules that separately form hydrogen-bonded polymer chains *via* N—H···N interactions. Molecular independence arises due to a difference in the dihedral angles between the linked rings, *i.e.* 52.19 (4) and 46.17 (5)°.



(I)

Experimental

Crystals of (I) were obtained from Spa Contract Synthesis.

Crystal data

$C_{11}H_9N_3O_2$
M_r = 215.21
Monoclinic, $P2_1/c$
a = 9.9036 (2) Å
b = 19.9452 (4) Å
c = 13.6660 (3) Å
β = 133.561 (1)°
V = 1956.12 (7) Å^3
Z = 8
D_x = 1.462 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 9171 reflections
θ = 2.91–27.48°
μ = 0.105 mm^{-1}
T = 150 (2) K
Block, yellow
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius KappaCCD area detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SORTAV*; Blessing, 1995)
T_{min} = 0.969, T_{max} = 0.979
18 006 measured reflections
4333 independent reflections
3232 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.46°
$h = -12 \rightarrow 12$
$k = -25 \rightarrow 22$
$l = -17 \rightarrow 16$
Intensity decay: none

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.120
S = 1.037
4333 reflections
297 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0691P)^2 + 0.1181P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.26 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

Table 1
Hydrogen-bonding geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N41A—H41A···O32A	0.882 (19)	2.012 (17)	2.6434 (14)	127.5 (15)
N41A—H41A···N1A^{i}	0.882 (19)	2.595 (19)	3.3802 (16)	148.8 (15)
N41B—H41B···O32B	0.851 (17)	2.031 (16)	2.6547 (14)	129.4 (14)
N41B—H41B···N1B^{ii}	0.851 (17)	2.638 (17)	3.4064 (16)	150.7 (13)

Symmetry codes: (i) $1+x, \frac{1}{2}-y, \frac{1}{2}+z$; (ii) $x-1, \frac{3}{2}-y, z-\frac{1}{2}$.

All H atoms were included in the refinement at calculated positions as riding, with the C—H distance set to 0.95 Å, except for the two amine protons, which were located in the difference syntheses and for which both positional and displacement parameters were refined.

Data collection: *DENZO* (Otwinowski & Minor, 1997 and *COLLECT* (Hooft, 1998); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO* and *COLLECT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); software used to prepare material for publication: *SHELXL*97.

The authors thank the EPSRC National Crystallography Service (Southampton).

References

Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–37.
Hooft, R. (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods Enzymol.* **276**, 307–326.
Sheldrick, G. M. (1997). *SHELXS*97 and *SHELXL*97. University of Göttingen, Germany.

† Contact e-mail: 106355.1670@compuserve.com.