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2-Ethyl-5-nitroaniline

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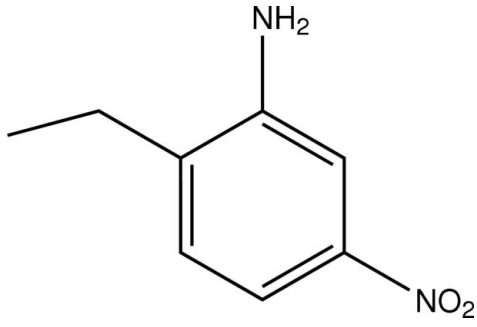
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.055; wR factor = 0.153; data-to-parameter ratio = 13.5.

The molecule of the title compound, $C_8H_{10}N_2O_2$, is nearly planar [maximum deviation of 0.163 (3) Å for one of the O atoms of the NO_2 group]. In the crystal structure, weak intermolecular N—H···N and C—H···O hydrogen bonds link the molecules into chains, forming $R_2^2(10)$ ring motifs.

Related literature

For a related structure, see: Corwin (1955). For bond-length data, see: Allen *et al.* (1987). For ring motifs, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_8H_{10}N_2O_2$
M_r = 166.18
Monoclinic, $C2/c$
a = 23.037 (5) Å
b = 3.9540 (8) Å
c = 18.393 (4) Å
β = 104.51 (3)°
V = 1621.9 (6) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 298 K
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.980, T_{max} = 0.990
2937 measured reflections
1474 independent reflections
906 reflections with $I > 2\sigma(I)$
R_{int} = 0.056
3 standard reflections
frequency: 120 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.153
S = 1.01
1474 reflections
109 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2B···N2^{i}	0.86	2.62	3.423 (3)	156
C7—H7A···O1^{ii}	0.93	2.60	3.417 (4)	147

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

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2644).

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supporting information

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2-Ethyl-5-nitroaniline

Yan Chen, Zheng Fang and Ping Wei

S1. Comment

Some derivatives of aniline are important chemical materials. We report herein the crystal structure of the title compound.

In the molecule of the title compound (Fig. 1), the bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. Ring A (C3-C8) is, of course, planar. Atoms C1, C2, N1, N2, O1 and O2 are -0.067 (3), -0.028 (2), -0.035 (3), -0.055 (3), 0.054 (3) and -0.163 (3) Å away from the ring plane of A, respectively.

In the crystal structure, weak intermolecular N-H···N and C-H···O hydrogen bonds (Table 1) link the molecules into chains, forming $R_2^2(10)$ ring motifs (Fig. 2) (Bernstein *et al.*, 1995). in which they may be effective in the stabilization of the structure.

S2. Experimental

For the preparation of the title compound, 2-ethylaniline (12.1 g) was dissolved in concentrated sulfuric acid (50 ml). The mixture was cooled to 273 K, and nitric acid (6.37 ml) was added in small portions. The mixture was stirred at 295 K for 0.5 h. Then, it was poured into a large volume of ice, used natrium hydroxydatum to neutralize excess acid, filtered, and dried. The compound was crystallized from cyclohexane (Corwin, 1955). Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

S3. Refinement

H atoms were positioned geometrically, with N-H = 0.86 Å (for NH_2) and C-H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with $U_{iso}(H) = xU_{eq}(C,N)$, where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

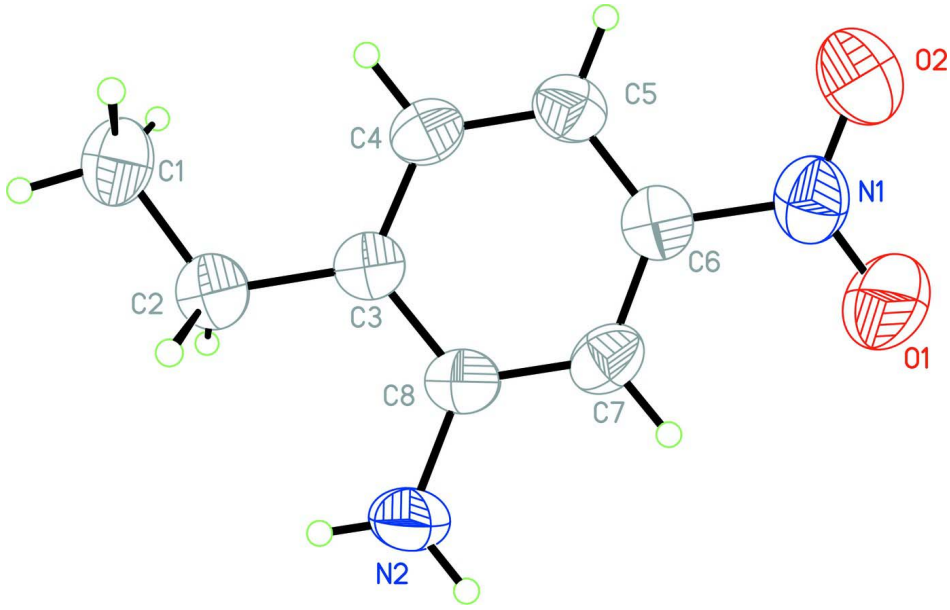

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

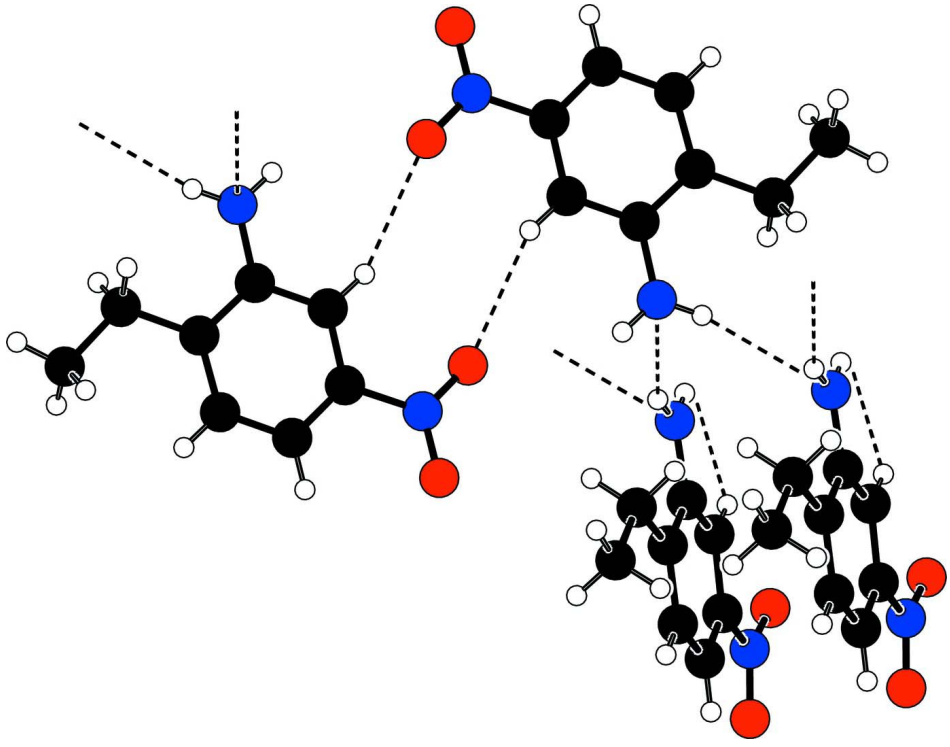

Figure 2

A partial packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

2-Ethyl-5-nitroaniline

Crystal data

$C_8H_{10}N_2O_2$
$M_r = 166.18$
Monoclinic, $C2/c$
Hall symbol: -C 2yc
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$c = 18.393\ (4)$ Å
$\beta = 104.51\ (3)°$
$V = 1621.9\ (6)$ Å^3
$Z = 8$
$F(000) = 704$
$D_x = 1.361$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 10–13°$
$\mu = 0.10$ mm^{-1}
$T = 298$ K
Block, colorless
0.20 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
$T_{min} = 0.980$, $T_{max} = 0.990$
2937 measured reflections
1474 independent reflections
906 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 25.3°$, $\theta_{min} = 1.8°$
$h = -27\rightarrow27$
$k = 0\rightarrow4$
$l = -22\rightarrow22$
3 standard reflections every 120 min
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.153$
$S = 1.01$
1474 reflections
109 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
$w = 1/[\sigma^2(F_o^2) + (0.06P)^2 + P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.21$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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}
O1	0.18034 (10)	0.6924 (7)	−0.09151 (11)	0.0931 (9)
O2	0.08462 (10)	0.6656 (7)	−0.12713 (11)	0.0921 (8)
N1	0.13189 (12)	0.6134 (7)	−0.08113 (12)	0.0598 (6)

N2	0.23320 (8)	0.2602 (7)	0.17155 (11)	0.0643 (8)
H2A	0.2663	0.3390	0.1651	0.077*
H2B	0.2322	0.1704	0.2138	0.077*
C1	0.06424 (11)	−0.1027 (8)	0.20919 (14)	0.0592 (8)
H1A	0.0687	−0.1949	0.2586	0.089*
H1B	0.0479	−0.2721	0.1723	0.089*
H1C	0.0377	0.0881	0.2025	0.089*
C2	0.12500 (10)	0.0091 (7)	0.19996 (12)	0.0489 (7)
H2C	0.1413	0.1738	0.2388	0.059*
H2D	0.1515	−0.1852	0.2087	0.059*
C3	0.12627 (10)	0.1609 (6)	0.12529 (12)	0.0406 (6)
C4	0.07514 (10)	0.1952 (7)	0.06693 (13)	0.0458 (6)
H4A	0.0388	0.1174	0.0738	0.055*
C5	0.07620 (11)	0.3397 (7)	−0.00061 (13)	0.0479 (7)
H5A	0.0413	0.3608	−0.0389	0.058*
C6	0.13008 (10)	0.4519 (7)	−0.01007 (12)	0.0445 (6)
C7	0.18252 (10)	0.4228 (7)	0.04537 (13)	0.0476 (7)
H7A	0.2185	0.4993	0.0372	0.057*
C8	0.18102 (10)	0.2780 (7)	0.11353 (12)	0.0442 (6)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0812 (15)	0.132 (2)	0.0759 (14)	−0.0154 (16)	0.0390 (12)	0.0189 (15)
O2	0.0889 (15)	0.121 (2)	0.0588 (12)	−0.0001 (15)	0.0045 (11)	0.0277 (14)
N1	0.0728 (16)	0.0621 (16)	0.0473 (12)	−0.0051 (14)	0.0201 (12)	−0.0025 (12)
N2	0.0382 (11)	0.101 (2)	0.0502 (12)	−0.0073 (13)	0.0052 (9)	−0.0046 (14)
C1	0.0702 (18)	0.0533 (18)	0.0597 (16)	−0.0030 (15)	0.0266 (13)	0.0046 (14)
C2	0.0550 (15)	0.0431 (16)	0.0493 (14)	0.0009 (12)	0.0142 (12)	−0.0057 (12)
C3	0.0433 (13)	0.0346 (14)	0.0441 (13)	0.0014 (11)	0.0115 (10)	−0.0080 (11)
C4	0.0402 (13)	0.0443 (16)	0.0529 (14)	−0.0059 (12)	0.0117 (11)	−0.0044 (13)
C5	0.0455 (14)	0.0474 (16)	0.0471 (14)	−0.0007 (13)	0.0044 (11)	−0.0016 (13)
C6	0.0526 (14)	0.0411 (15)	0.0415 (13)	0.0020 (12)	0.0148 (11)	−0.0082 (12)
C7	0.0438 (13)	0.0515 (17)	0.0519 (14)	−0.0063 (13)	0.0202 (11)	−0.0094 (13)
C8	0.0394 (13)	0.0479 (16)	0.0448 (13)	0.0022 (12)	0.0097 (10)	−0.0105 (12)

Geometric parameters (Å, º)

O1—N1	1.219 (3)	C2—H2C	0.9700
O2—N1	1.218 (3)	C2—H2D	0.9700
N1—C6	1.465 (3)	C3—C4	1.387 (3)
N2—C8	1.395 (3)	C3—C8	1.410 (3)
N2—H2A	0.8600	C4—C5	1.373 (3)
N2—H2B	0.8600	C4—H4A	0.9300
C1—C2	1.517 (3)	C5—C6	1.370 (3)
C1—H1A	0.9600	C5—H5A	0.9300
C1—H1B	0.9600	C6—C7	1.377 (3)
C1—H1C	0.9600	C7—C8	1.387 (3)

C2—C3	1.506 (3)	C7—H7A	0.9300
O2—N1—O1	122.8 (2)	C4—C3—C8	117.9 (2)
O2—N1—C6	118.3 (2)	C4—C3—C2	122.5 (2)
O1—N1—C6	118.9 (2)	C8—C3—C2	119.56 (19)
C8—N2—H2A	120.0	C5—C4—C3	122.5 (2)
C8—N2—H2B	120.0	C5—C4—H4A	118.8
H2A—N2—H2B	120.0	C3—C4—H4A	118.8
C2—C1—H1A	109.5	C6—C5—C4	118.2 (2)
C2—C1—H1B	109.5	C6—C5—H5A	120.9
H1A—C1—H1B	109.5	C4—C5—H5A	120.9
C2—C1—H1C	109.5	C5—C6—C7	122.3 (2)
H1A—C1—H1C	109.5	C5—C6—N1	118.9 (2)
H1B—C1—H1C	109.5	C7—C6—N1	118.8 (2)
C3—C2—C1	116.59 (19)	C6—C7—C8	119.2 (2)
C3—C2—H2C	108.1	C6—C7—H7A	120.4
C1—C2—H2C	108.1	C8—C7—H7A	120.4
C3—C2—H2D	108.1	C7—C8—N2	120.0 (2)
C1—C2—H2D	108.1	C7—C8—C3	120.0 (2)
H2C—C2—H2D	107.3	N2—C8—C3	119.9 (2)
C1—C2—C3—C4	−0.7 (4)	O1—N1—C6—C7	5.9 (4)
C1—C2—C3—C8	178.4 (2)	C5—C6—C7—C8	−0.6 (4)
C8—C3—C4—C5	−0.5 (4)	N1—C6—C7—C8	178.4 (2)
C2—C3—C4—C5	178.7 (3)	C6—C7—C8—N2	−177.1 (2)
C3—C4—C5—C6	0.3 (4)	C6—C7—C8—C3	0.4 (4)
C4—C5—C6—C7	0.3 (4)	C4—C3—C8—C7	0.1 (3)
C4—C5—C6—N1	−178.7 (2)	C2—C3—C8—C7	−179.0 (2)
O2—N1—C6—C5	5.6 (4)	C4—C3—C8—N2	177.6 (2)
O1—N1—C6—C5	−175.1 (3)	C2—C3—C8—N2	−1.5 (4)
O2—N1—C6—C7	−173.4 (2)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*B*···N2^{i}	0.86	2.62	3.423 (3)	156
C7—H7*A*···O1^{ii}	0.93	2.60	3.417 (4)	147

Symmetry codes: (i) −*x*+1/2, *y*−1/2, −*z*+1/2; (ii) −*x*+1/2, −*y*+3/2, −*z*.