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4-(4-Nitrobenzyl)morpholine

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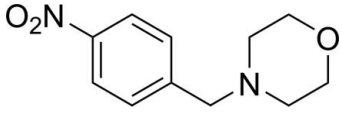
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.137; data-to-parameter ratio = 15.6.

In the title compound, $C_{11}H_{14}N_2O_3$, an intermolecular interaction between a nitro group O atom and a neighboring benzene ring helps to stabilize the crystal structure [N···centroid = 3.933 (2) Å]. No classical hydrogen bonds are observed in the crystal packing.

Related literature

For the biological activity of 4-(4-nitrobenzyl)morpholine derivatives, see: Lan *et al.* (2010); Bavetsias *et al.* (2010). For the synthesis, see: Tsou *et al.* (2008). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{14}N_2O_3$
M_r = 222.24
Monoclinic, $P2_1/c$
a = 6.1371 (2) Å
b = 8.2535 (4) Å
c = 21.9867 (9) Å
β = 94.929 (3)°
V = 1109.58 (8) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 K
0.40 × 0.30 × 0.25 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min} = 0.946, T_{max} = 1.0
6059 measured reflections
2264 independent reflections
1640 reflections with $I > 2\sigma(I)$
R_{int} = 0.018

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.106
S = 1.04
2264 reflections
145 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.12 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2006); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2*.

We thank the Analytical and Testing Center of Sichuan University for the X-ray measurements.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: VM2073).

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Ling-Ling Yang, Ren-Lin Zheng, Guo-Bo Li, Qi-Zheng Sun and Yong-Mei Xie

S1. Comment

4-(4-nitrobenzyl)morpholine derivatives are of great importance owing to their anticancer activity (Lan *et al.*, 2010; Bavetsias *et al.*, 2010). The title compound is one of the key intermediates in our synthetic investigations of anticancer drugs. In this paper, we synthesized the title compound and report its crystal structure. In the title compound, $C_{11}H_{14}N_2O_3$, (Fig. 1), the bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The dihedral angle between the best planes between the phenyl and morpholino rings is 87.78 (10)°. An intermolecular interaction between the nitro group atom O3 and the benzene ring helps to stabilize the crystal structure. The distance O3···Cg(1)^a is 3.647 (2) Å (Fig.2, Cg(1) is the centroid of benzene ring C1-C6, symmetry operation (a): -*x*, -1/2+*y*, 1/2-*z*). There are no classical hydrogen bonds observed in the crystal packing.

S2. Experimental

The title compound was prepared by a method similar to that of Tsou *et al.* (2008). Crystals suitable for X-ray analysis were obtained by slow evaporation from a solution of dichloromethane.

S3. Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 Å, N–H =0.91 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent).

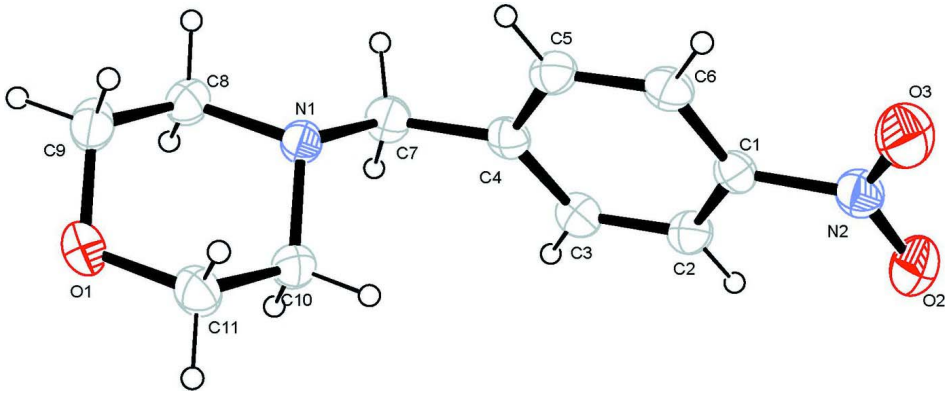

Figure 1

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

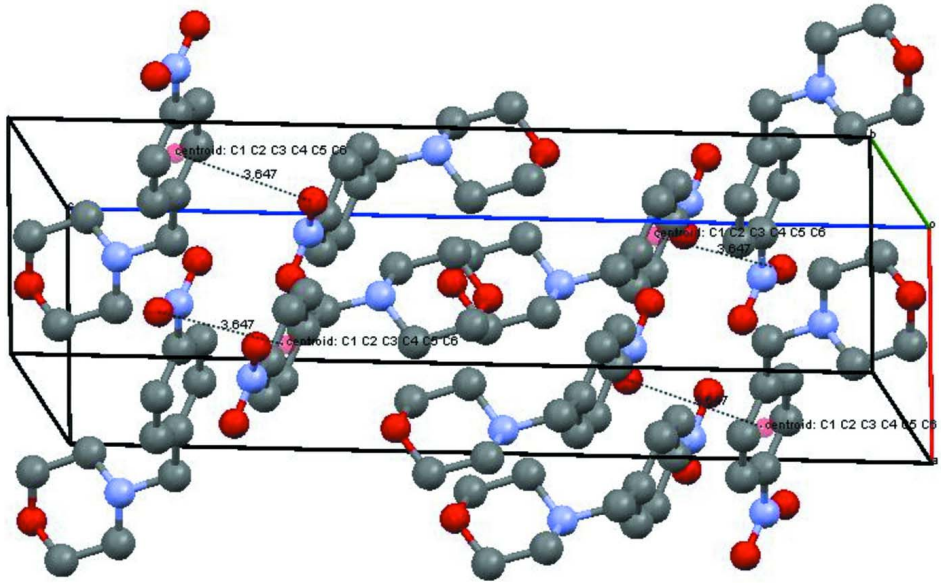

Figure 2

Packing diagram of the title compound showing the intermolecular interaction (dashed lines) between nitro group atom O3 and benzene ring C1-C6 (centroid indicated by pink sphere).

4-(4-Nitrobenzyl)morpholine

Crystal data

$C_{11}H_{14}N_2O_3$
M_r = 222.24
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 6.1371 (2) Å
b = 8.2535 (4) Å
c = 21.9867 (9) Å
β = 94.929 (3)°
V = 1109.58 (8) Å^3
Z = 4

$F(000)$ = 472
D_x = 1.330 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.7107 Å
Cell parameters from 2399 reflections
θ = 3.1–29.2°
μ = 0.10 mm^{-1}
T = 293 K
Block, yellow
0.40 × 0.30 × 0.25 mm

Data collection

Oxford Diffraction Xcalibur Eos diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.0874 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2006)
T_{min} = 0.946, T_{max} = 1.0

6059 measured reflections
2264 independent reflections
1640 reflections with $I > 2\sigma(I)$
R_{int} = 0.018
θ_{max} = 26.4°, θ_{min} = 3.1°
h = −7→7
k = −8→10
l = −25→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.106
S = 1.04

2264 reflections
145 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map	$w = 1/[\sigma^2(F_o^2) + (0.0423P)^2 + 0.1325P]$ where $P = (F_o^2 + 2F_c^2)/3$
Hydrogen site location: inferred from neighbouring sites	$(\Delta/\sigma)_{max} < 0.001$
H-atom parameters constrained	$\Delta\rho_{max} = 0.12$ e Å^{-3}
	$\Delta\rho_{min} = -0.13$ e Å^{-3}

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.40024 (19)	0.31753 (14)	0.53296 (5)	0.0556 (3)
O2	−0.4376 (2)	−0.42771 (17)	0.28701 (7)	0.0751 (4)
O3	−0.1642 (2)	−0.57082 (16)	0.32340 (8)	0.0808 (5)
N1	0.33645 (19)	0.14840 (16)	0.41946 (6)	0.0417 (3)
N2	−0.2491 (2)	−0.44089 (19)	0.30912 (6)	0.0530 (4)
C1	−0.1173 (2)	−0.29260 (19)	0.31894 (7)	0.0413 (4)
C2	−0.2096 (2)	−0.1454 (2)	0.30324 (7)	0.0461 (4)
H2	−0.3521	−0.1392	0.2853	0.055*
C3	−0.0870 (2)	−0.0064 (2)	0.31460 (7)	0.0467 (4)
H3	−0.1484	0.0941	0.3044	0.056*
C4	0.1268 (2)	−0.0148 (2)	0.34109 (7)	0.0420 (4)
C5	0.2166 (2)	−0.1668 (2)	0.35492 (7)	0.0468 (4)
H5	0.3605	−0.1743	0.3718	0.056*
C6	0.0965 (3)	−0.3056 (2)	0.34414 (7)	0.0471 (4)
H6	0.1576	−0.4066	0.3536	0.057*
C7	0.2629 (3)	0.1353 (2)	0.35452 (7)	0.0493 (4)
H7A	0.3893	0.1325	0.3309	0.059*
H7B	0.1771	0.2302	0.3421	0.059*
C8	0.5018 (2)	0.2751 (2)	0.43006 (8)	0.0499 (4)
H8B	0.4409	0.3785	0.4162	0.060*
H8A	0.6256	0.2513	0.4069	0.060*
C9	0.5767 (3)	0.2851 (2)	0.49693 (9)	0.0550 (5)
H9A	0.6451	0.1835	0.5100	0.066*
H9B	0.6853	0.3701	0.5033	0.066*
C10	0.1559 (2)	0.1839 (2)	0.45620 (8)	0.0502 (4)
H10A	0.0466	0.0991	0.4507	0.060*
H10B	0.0879	0.2855	0.4430	0.060*
C11	0.2381 (3)	0.1952 (2)	0.52265 (8)	0.0566 (5)
H11B	0.1165	0.2191	0.5466	0.068*
H11A	0.2992	0.0916	0.5361	0.068*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0660 (7)	0.0481 (7)	0.0523 (7)	−0.0032 (6)	0.0017 (6)	−0.0124 (6)
O2	0.0609 (8)	0.0800 (10)	0.0819 (10)	−0.0136 (7)	−0.0089 (7)	−0.0130 (8)
O3	0.0861 (10)	0.0489 (9)	0.1079 (12)	−0.0023 (7)	0.0107 (8)	0.0089 (8)
N1	0.0422 (7)	0.0462 (8)	0.0372 (7)	−0.0052 (6)	0.0053 (5)	−0.0017 (6)
N2	0.0584 (9)	0.0565 (10)	0.0451 (8)	−0.0045 (7)	0.0101 (7)	−0.0050 (7)
C1	0.0460 (9)	0.0465 (10)	0.0314 (8)	0.0000 (7)	0.0045 (6)	−0.0033 (7)
C2	0.0416 (8)	0.0573 (11)	0.0385 (9)	0.0041 (7)	−0.0026 (7)	−0.0006 (8)
C3	0.0516 (9)	0.0469 (10)	0.0408 (9)	0.0081 (7)	−0.0002 (7)	0.0019 (7)
C4	0.0474 (9)	0.0495 (10)	0.0294 (8)	0.0016 (7)	0.0055 (6)	−0.0017 (7)
C5	0.0399 (8)	0.0607 (12)	0.0394 (9)	0.0034 (8)	−0.0001 (7)	−0.0014 (8)
C6	0.0502 (9)	0.0476 (10)	0.0435 (9)	0.0104 (7)	0.0044 (7)	0.0016 (8)
C7	0.0542 (9)	0.0555 (11)	0.0386 (9)	−0.0047 (8)	0.0065 (7)	0.0027 (8)
C8	0.0463 (9)	0.0492 (11)	0.0546 (11)	−0.0072 (7)	0.0059 (7)	0.0007 (8)
C9	0.0523 (10)	0.0501 (11)	0.0610 (12)	−0.0059 (8)	−0.0047 (8)	−0.0050 (9)
C10	0.0457 (9)	0.0588 (11)	0.0468 (10)	−0.0069 (7)	0.0080 (7)	−0.0067 (8)
C11	0.0632 (11)	0.0609 (12)	0.0472 (10)	−0.0092 (9)	0.0128 (8)	−0.0105 (9)

Geometric parameters (Å, º)

O1—C9	1.421 (2)	C5—H5	0.9300
O1—C11	1.4218 (19)	C5—C6	1.372 (2)
O2—N2	1.2210 (17)	C6—H6	0.9300
O3—N2	1.2214 (17)	C7—H7A	0.9700
N1—C7	1.4641 (19)	C7—H7B	0.9700
N1—C8	1.4616 (19)	C8—H8B	0.9700
N1—C10	1.456 (2)	C8—H8A	0.9700
N2—C1	1.473 (2)	C8—C9	1.504 (2)
C1—C2	1.372 (2)	C9—H9A	0.9700
C1—C6	1.384 (2)	C9—H9B	0.9700
C2—H2	0.9300	C10—H10A	0.9700
C2—C3	1.383 (2)	C10—H10B	0.9700
C3—H3	0.9300	C10—C11	1.507 (2)
C3—C4	1.3911 (19)	C11—H11B	0.9700
C4—C5	1.393 (2)	C11—H11A	0.9700
C4—C7	1.509 (2)		
O1—C9—C8	111.83 (13)	C4—C3—H3	119.6
O1—C9—H9A	109.3	C4—C5—H5	119.4
O1—C9—H9B	109.3	C4—C7—H7A	109.3
O1—C11—C10	111.71 (14)	C4—C7—H7B	109.3
O1—C11—H11B	109.3	C5—C4—C7	119.67 (13)
O1—C11—H11A	109.3	C5—C6—C1	118.75 (15)
O2—N2—O3	123.32 (15)	C5—C6—H6	120.6
O2—N2—C1	118.31 (15)	C6—C1—N2	118.95 (15)
O3—N2—C1	118.38 (14)	C6—C5—C4	121.20 (14)

N1—C7—C4	111.73 (13)	C6—C5—H5	119.4
N1—C7—H7A	109.3	H7A—C7—H7B	107.9
N1—C7—H7B	109.3	C8—N1—C7	111.09 (12)
N1—C8—H8B	109.6	C8—C9—H9A	109.3
N1—C8—H8A	109.6	C8—C9—H9B	109.3
N1—C8—C9	110.15 (14)	H8B—C8—H8A	108.1
N1—C10—H10A	109.6	C9—O1—C11	109.49 (13)
N1—C10—H10B	109.6	C9—C8—H8B	109.6
N1—C10—C11	110.07 (13)	C9—C8—H8A	109.6
C1—C2—H2	120.6	H9A—C9—H9B	107.9
C1—C2—C3	118.87 (14)	C10—N1—C7	111.73 (12)
C1—C6—H6	120.6	C10—N1—C8	108.57 (13)
C2—C1—N2	119.30 (14)	C10—C11—H11B	109.3
C2—C1—C6	121.76 (15)	C10—C11—H11A	109.3
C2—C3—H3	119.6	H10A—C10—H10B	108.2
C2—C3—C4	120.88 (15)	C11—C10—H10A	109.6
C3—C2—H2	120.6	C11—C10—H10B	109.6
C3—C4—C5	118.51 (15)	H11B—C11—H11A	107.9
C3—C4—C7	121.81 (15)		