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An orthorhombic modification of 4,4′-diaminobenzophenone

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Key indicators

Single-crystal X-ray study
T = 291 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.088
Data-to-parameter ratio = 7.6

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

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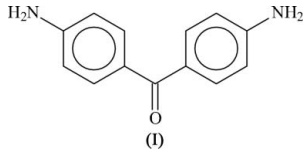
The molecule of the title compound, $C_{13}H_{12}N_2O$, uses one of its amine groups to hydrogen bond to two other molecules, affording a layer motif in the crystal structure.

Comment

The crystal structure of 4,4′-diaminobenzophenone, (I), was reported in the trigonal space group $P3_1$ (Velden & Noordik, 1980); the compound adopts a linear hydrogen-bonded chain structure. The orthorhombic modification also has the atoms of the molecule lying in general positions, but the less densely packed structure features hydrogen bonds that give rise to a hydrogen-bonded layer motif (Fig. 1). Only one amine group is involved in the interactions.



(I)

Experimental

A mixture of cadmium acetate dihydrate (0.133 g, 0.5 mmol) and 4,4′-diaminobenzophenone-3,3′-dicarboxylic acid (0.075 g, 0.25 mmol) in water (16 ml) was placed in a 25 ml Teflon-lined stainless steel Parr bomb. The bomb was heated to 433 K for 72 h. It was cooled to room temperature over 3 d to furnish orange prismatic crystals.

Crystal data

$C_{13}H_{12}N_2O$
M_r = 212.25
Orthorhombic, $P2_12_12_1$
a = 5.4982 (5) Å
b = 8.1110 (7) Å
c = 24.306 (2) Å
V = 1084.0 (2) Å^3
Z = 4
D_x = 1.301 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 291 (2) K
Prism, orange
0.40 × 0.30 × 0.08 mm

Data collection

Rigaku Mercury CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2000)
T_{min} = 0.702, T_{max} = 1.000
8288 measured reflections
1470 independent reflections
1416 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.088
S = 1.02
1470 reflections
193 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0594P)^2 + 0.165P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n1···O1^{i}	0.86 (1)	2.08 (1)	2.917 (2)	165 (2)
N1—H1n2···O1^{ii}	0.86 (1)	2.27 (1)	3.047 (2)	152 (2)

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

In the absence of significant anomalous scattering effects, Friedel pairs were merged. H atoms were located in difference Fourier maps and refined with distance restraints of N—H = 0.85 (1) Å and C—H = 0.95 (1) Å; their displacement parameters were freely refined.

Data collection: *CrystalClear* (Rigaku/MSC, 2000); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXL97*.

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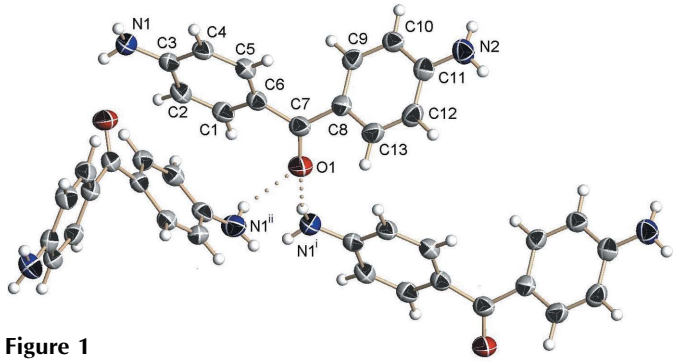

Figure 1
Three molecules of (I), with displacement ellipsoids drawn at the 50% probability level and H atoms shown as spheres of arbitrary radii. [Symmetry codes: (i) $x, 1+y, z$; (ii) $\frac{1}{2}+x, \frac{1}{2}-y, -z$.] Dotted lines indicate hydrogen bonds.

References

Bruker (1998). *SHELXTL*. Bruker AXS Inc., Madison, Wisconsin, USA.
Rigaku/MSC (2000). *CrystalClear*. Version 1.3.6. Rigaku/MSC, The Woodlands, Texas, USA.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXL97*. University of Göttingen, Germany.
Velden, G. P. M. van der & Noordik, J. H. (1980). *J. Cryst. Mol. Struct.* **10**, 83–92.