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A new polymorph of *N*,*N*-dibenzylaniline

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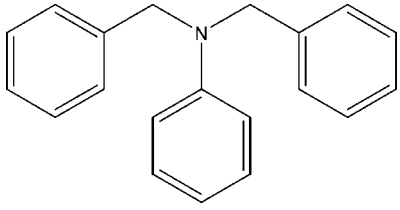
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; R factor = 0.069; wR factor = 0.160; data-to-parameter ratio = 14.6.

The title compound, $C_{20}H_{19}N$, is a second polymorph of *N*,*N*-dibenzylaniline [Bi, Tong & Zhou (2007). *Acta Cryst.* E**63**, o1809–o1810]. The present polymorph and that already reported crystallize in the monoclinic space group $P2_1/n$ with one and two independent molecules, respectively. The molecular conformations in the two polymorphs are slightly different.

Related literature

Bi *et al.* (2007) have reported the crystal structure of another polymorph. For related crystal structures, see also Ianelli *et al.* (1993).



Experimental

Crystal data

$C_{20}H_{19}N$
M_r = 273.36
Monoclinic, $P2_1/n$
a = 8.061 (4) Å
b = 11.529 (6) Å
c = 17.065 (9) Å
β = 91.245 (13)°
V = 1585.6 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Siemens SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.981, T_{max} = 0.987
6429 measured reflections
2797 independent reflections
1858 reflections with $I > 2\sigma(I)$
R_{int} = 0.035

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.069
$wR(F^2)$ = 0.160
S = 1.08
2797 reflections
191 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2328).

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supplementary materials

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A new polymorph of *N*,*N*-dibenzylaniline

H.-B. Tong, M.-S. Zhou, Q.-X. Bi and J.-B. Chao

Comment

We report here the crystal structure of the title compound, (II), which is a second polymorph of *N*,*N*-dibenzylaniline (Bi *et al.*, 2007) (I).

The asymmetric unit of (II) contains one independent molecule (Fig. 1). The C—N bond lengths in (II) agree with those reported for similar compounds (Ianelli *et al.*, 1993). The molecular conformations in (I) and (II) are is slightly different. In (II), the mean plane N1/C1/C8/C15 makes dihedral angles of 90.5 (1), 98.1 (1), 18.3 (1)° with the phenyl rings C2—C7, C9—C14 and C15—C20, respectively.

In the absence of classical hydrogen bonds, the crystal packing is stabilized by van der Waals forces.

Experimental

All manipulations were carried out under argon or *in vacuo* using standard Schlenk techniques. n-Butyllithium(3 ml,1.7*M* in Hexane) was added dropwise to a solution of *N*-benzyl phenyl amine(0.92 g, 5 mmol) in hexane at 273 K, and then the temperature was allowed to rise to room temperature. The mixture was stirred for further 5 h and then simply add benzyl chloride(0.63 g, 5 mmol) to it at 273 K. The mixture was warmed slowly to room temperaturethe solution, and was stirred for further 5 h at room temperature. Then the solvent was removed under vacuum and ether was used to extract the solid. The filtrate was concentrated under a vacuum until colourless crystals of the title compound appeared(1.12 g, yield 82%), suitable for X-ray analysis. Elemental analysis, found: C 87.90, H 6.98, N 5.12%; calculated: C 87.87, H 7.01, N 5.12%.

Refinement

All H atoms were positioned geometrically (C—H = 0.93–0.97 A°) and refined as riding, with U_{iso}(H) = 1.2Ueq(C).

Figures

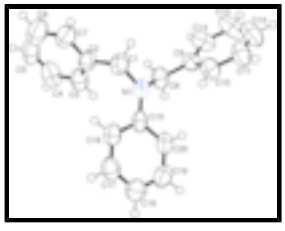


Fig. 1. The asymmetric unit of (II), showing the atom-labelling scheme and displacement ellipsoids drawn at the 50% probability level.

N,N-dibenzylaniline

Crystal data

$C_{20}H_{19}N$	F_{000} = 584
M_r = 273.36	D_x = 1.145 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 8.061 (4) Å	Cell parameters from 1210 reflections
b = 11.529 (6) Å	θ = 2.4–20.0º
c = 17.065 (9) Å	μ = 0.07 mm^{-1}
β = 91.245 (13)º	T = 293 (2) K
V = 1585.6 (14) Å^3	Block, colourless
Z = 4	0.30 × 0.20 × 0.20 mm

Data collection

Siemens SMART CCD area detector diffractometer	2797 independent reflections
Radiation source: fine-focus sealed tube	1858 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.035
T = 293(2) K	θ_{max} = 25.0º
ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −9→7
T_{min} = 0.981, T_{max} = 0.987	k = −13→13
6429 measured reflections	l = −20→20

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.069	$w = 1/[\sigma^2(F_o^2) + (0.0581P)^2 + 0.3456P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.160	$(\Delta/\sigma)_{max} < 0.001$
S = 1.08	$\Delta\rho_{max}$ = 0.22 e Å^{-3}
2797 reflections	$\Delta\rho_{min}$ = −0.16 e Å^{-3}
191 parameters	Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.014 (2)
Secondary atom site location: difference Fourier map	

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.0735 (3)	0.06758 (18)	0.13394 (12)	0.0613 (6)
C1	0.0455 (3)	0.1689 (2)	0.08584 (15)	0.0666 (7)
H1A	−0.0572	0.2050	0.1017	0.080*
H1B	0.0298	0.1438	0.0319	0.080*
C2	0.1806 (3)	0.2599 (2)	0.08834 (14)	0.0599 (7)
C3	0.3256 (4)	0.2461 (3)	0.13071 (16)	0.0709 (8)
H3	0.3447	0.1785	0.1593	0.085*
C4	0.4449 (4)	0.3343 (3)	0.13072 (17)	0.0867 (10)
H4	0.5439	0.3259	0.1592	0.104*
C5	0.4141 (6)	0.4338 (3)	0.0881 (2)	0.0968 (12)
H5	0.4923	0.4930	0.0882	0.116*
C6	0.2711 (6)	0.4459 (3)	0.0461 (2)	0.1071 (12)
H6	0.2520	0.5129	0.0170	0.129*
C7	0.1555 (4)	0.3605 (3)	0.04629 (17)	0.0822 (9)
H7	0.0573	0.3701	0.0174	0.099*
C8	0.0270 (3)	0.0789 (2)	0.21503 (15)	0.0675 (8)
H8A	0.0513	0.1575	0.2320	0.081*
H8B	0.0962	0.0272	0.2464	0.081*
C9	−0.1526 (3)	0.0532 (2)	0.23217 (14)	0.0563 (6)
C10	−0.2459 (3)	−0.0233 (2)	0.18791 (15)	0.0682 (7)
H10	−0.1999	−0.0574	0.1440	0.082*
C11	−0.4059 (4)	−0.0501 (3)	0.20734 (19)	0.0842 (9)
H11	−0.4673	−0.1020	0.1767	0.101*
C12	−0.4743 (4)	−0.0010 (4)	0.2713 (2)	0.0988 (12)
H12	−0.5820	−0.0201	0.2850	0.119*
C13	−0.3849 (5)	0.0764 (4)	0.3155 (2)	0.1083 (12)
H13	−0.4319	0.1104	0.3592	0.130*
C14	−0.2251 (4)	0.1041 (3)	0.29547 (17)	0.0821 (9)
H14	−0.1656	0.1581	0.3252	0.099*
C15	0.1611 (3)	−0.0270 (2)	0.10677 (14)	0.0551 (6)
C16	0.2536 (3)	−0.0206 (2)	0.03909 (14)	0.0604 (7)
H16	0.2576	0.0490	0.0117	0.073*
C17	0.3388 (3)	−0.1146 (3)	0.01189 (16)	0.0702 (8)

H17	0.3989	−0.1077	−0.0338	0.084*
C18	0.3372 (4)	−0.2186 (3)	0.05075 (19)	0.0763 (8)
H18	0.3965	−0.2818	0.0324	0.092*
C19	0.2454 (4)	−0.2270 (3)	0.11777 (18)	0.0750 (8)
H19	0.2421	−0.2973	0.1445	0.090*
C20	0.1585 (3)	−0.1337 (2)	0.14601 (15)	0.0647 (7)
H20	0.0977	−0.1416	0.1914	0.078*

Atomic displacement parameters (Å^2)

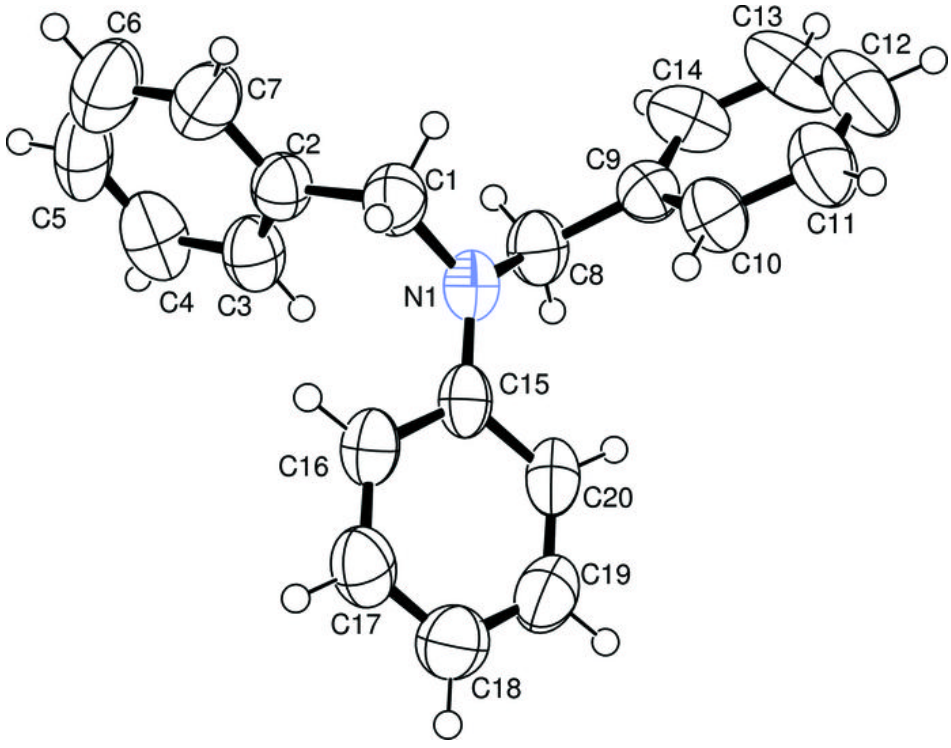
	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0607 (14)	0.0637 (14)	0.0599 (13)	−0.0101 (11)	0.0090 (10)	0.0072 (11)
C1	0.0600 (17)	0.0689 (17)	0.0708 (17)	−0.0068 (14)	0.0003 (13)	0.0072 (14)
C2	0.0665 (18)	0.0565 (15)	0.0572 (16)	−0.0084 (13)	0.0077 (13)	−0.0049 (12)
C3	0.0702 (19)	0.0755 (19)	0.0674 (17)	−0.0185 (16)	0.0059 (14)	−0.0090 (14)
C4	0.081 (2)	0.111 (3)	0.0683 (19)	−0.031 (2)	0.0109 (16)	−0.030 (2)
C5	0.121 (3)	0.081 (2)	0.090 (2)	−0.050 (2)	0.037 (2)	−0.018 (2)
C6	0.139 (4)	0.074 (2)	0.109 (3)	−0.028 (3)	0.021 (3)	0.005 (2)
C7	0.099 (2)	0.0647 (19)	0.083 (2)	−0.0072 (18)	0.0071 (17)	0.0064 (16)
C8	0.0644 (18)	0.0748 (18)	0.0631 (17)	−0.0161 (14)	−0.0009 (13)	−0.0043 (14)
C9	0.0541 (16)	0.0624 (16)	0.0523 (14)	0.0022 (13)	−0.0016 (12)	0.0036 (13)
C10	0.0585 (18)	0.0820 (19)	0.0640 (17)	−0.0064 (15)	0.0021 (13)	−0.0050 (15)
C11	0.0551 (19)	0.108 (2)	0.090 (2)	−0.0116 (17)	−0.0011 (16)	0.0071 (19)
C12	0.0516 (19)	0.154 (3)	0.091 (2)	0.007 (2)	0.0077 (18)	0.023 (2)
C13	0.067 (2)	0.176 (4)	0.083 (2)	0.031 (2)	0.0105 (18)	−0.015 (2)
C14	0.069 (2)	0.099 (2)	0.078 (2)	0.0170 (17)	−0.0051 (16)	−0.0199 (17)
C15	0.0493 (15)	0.0623 (16)	0.0537 (14)	−0.0189 (13)	−0.0023 (12)	0.0026 (13)
C16	0.0624 (17)	0.0643 (16)	0.0545 (15)	−0.0183 (14)	0.0000 (13)	0.0021 (13)
C17	0.0650 (19)	0.078 (2)	0.0683 (18)	−0.0194 (15)	0.0073 (14)	−0.0104 (16)
C18	0.0677 (19)	0.069 (2)	0.092 (2)	−0.0075 (15)	−0.0011 (16)	−0.0085 (17)
C19	0.0684 (19)	0.0638 (19)	0.092 (2)	−0.0126 (16)	−0.0091 (17)	0.0166 (16)
C20	0.0570 (17)	0.0717 (18)	0.0655 (16)	−0.0185 (15)	0.0018 (13)	0.0141 (14)

Geometric parameters (Å, °)

N1—C15	1.385 (3)	C9—C10	1.374 (3)
N1—C1	1.443 (3)	C10—C11	1.374 (4)
N1—C8	1.447 (3)	C10—H10	0.9300
C1—C2	1.512 (3)	C11—C12	1.358 (4)
C1—H1A	0.9700	C11—H11	0.9300
C1—H1B	0.9700	C12—C13	1.365 (5)
C2—C3	1.370 (4)	C12—H12	0.9300
C2—C7	1.377 (4)	C13—C14	1.378 (5)
C3—C4	1.400 (4)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C4—C5	1.378 (5)	C15—C16	1.390 (3)
C4—H4	0.9300	C15—C20	1.401 (3)
C5—C6	1.351 (5)	C16—C17	1.370 (4)
C5—H5	0.9300	C16—H16	0.9300

C6—C7	1.355 (5)	C17—C18	1.370 (4)
C6—H6	0.9300	C17—H17	0.9300
C7—H7	0.9300	C18—C19	1.379 (4)
C8—C9	1.513 (3)	C18—H18	0.9300
C8—H8A	0.9700	C19—C20	1.376 (4)
C8—H8B	0.9700	C19—H19	0.9300
C9—C14	1.371 (3)	C20—H20	0.9300
C15—N1—C1	121.5 (2)	C10—C9—C8	122.3 (2)
C15—N1—C8	122.4 (2)	C9—C10—C11	121.2 (3)
C1—N1—C8	115.5 (2)	C9—C10—H10	119.4
N1—C1—C2	116.2 (2)	C11—C10—H10	119.4
N1—C1—H1A	108.2	C12—C11—C10	120.0 (3)
C2—C1—H1A	108.2	C12—C11—H11	120.0
N1—C1—H1B	108.2	C10—C11—H11	120.0
C2—C1—H1B	108.2	C11—C12—C13	119.9 (3)
H1A—C1—H1B	107.4	C11—C12—H12	120.1
C3—C2—C7	119.1 (3)	C13—C12—H12	120.1
C3—C2—C1	122.7 (2)	C12—C13—C14	120.0 (3)
C7—C2—C1	118.2 (3)	C12—C13—H13	120.0
C2—C3—C4	119.6 (3)	C14—C13—H13	120.0
C2—C3—H3	120.2	C9—C14—C13	120.8 (3)
C4—C3—H3	120.2	C9—C14—H14	119.6
C5—C4—C3	119.2 (3)	C13—C14—H14	119.6
C5—C4—H4	120.4	N1—C15—C16	121.5 (2)
C3—C4—H4	120.4	N1—C15—C20	121.2 (2)
C6—C5—C4	120.6 (3)	C16—C15—C20	117.2 (3)
C6—C5—H5	119.7	C17—C16—C15	121.4 (3)
C4—C5—H5	119.7	C17—C16—H16	119.3
C5—C6—C7	120.2 (4)	C15—C16—H16	119.3
C5—C6—H6	119.9	C16—C17—C18	121.2 (3)
C7—C6—H6	119.9	C16—C17—H17	119.4
C6—C7—C2	121.3 (3)	C18—C17—H17	119.4
C6—C7—H7	119.3	C17—C18—C19	118.3 (3)
C2—C7—H7	119.3	C17—C18—H18	120.8
N1—C8—C9	115.9 (2)	C19—C18—H18	120.8
N1—C8—H8A	108.3	C20—C19—C18	121.4 (3)
C9—C8—H8A	108.3	C20—C19—H19	119.3
N1—C8—H8B	108.3	C18—C19—H19	119.3
C9—C8—H8B	108.3	C19—C20—C15	120.4 (3)
H8A—C8—H8B	107.4	C19—C20—H20	119.8
C14—C9—C10	118.1 (3)	C15—C20—H20	119.8
C14—C9—C8	119.6 (2)		

Fig. 1


C6
C7
C2
C1
C5
C4
C3
N1
C8
C9
C14
C13
C12
C11
C10
C15
C16
C20
C19
C17
C18