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# *N*,*N*,*N*′,*N*′-Tetrabenzylethylenediamine

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**Key indicators**

Single-crystal X-ray study
$T$ = 293 K
Mean $\sigma$(C–C) = 0.004 Å
$R$ factor = 0.045
$wR$ factor = 0.181
Data-to-parameter ratio = 14.8

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

The title compound, $C_{30}H_{32}N_2$, was synthesized from ethylenediamine and benzyl chloride. The molecule occupies a special position on a crystallographic inversion centre.

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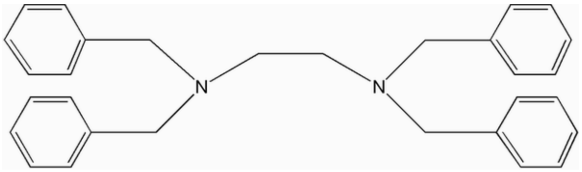
## Comment

Compounds incorporating the 1,2-diamine functionality are currently the topic of studies conducted in several fields (Lucet *et al.*, 1998). In our laboratory, we have recently investigated a new catalyst used in asymmetric synthesis. This compound, *N*,*N*,*N*′,*N*′-tetrabenzylethylenediamine (TBEN), (I), was synthesized by the reaction of ethylenediamine and benzyl chloride. The structure determination of the title compound was undertaken as part of our studies on this catalyst.



(I)

The molecular structure of the title compound is illustrated in Fig. 1. The molecule occupies a special position on a crys-

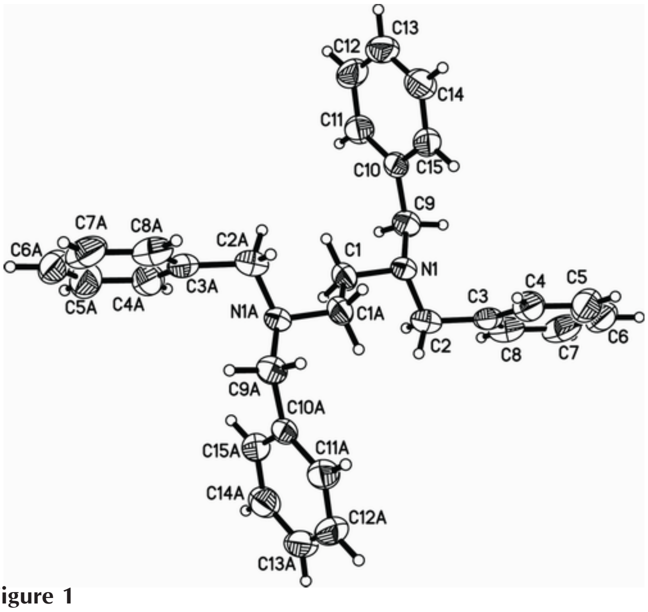


**Figure 1**
View of the title molecule, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level. The suffix A denotes an atom related by the symmetry operator $-x, 2-y, -z$.

tallographic inversion centre. Because of steric hindrance between the vicinal benzene rings, atom C2 has a slightly distorted tetrahedral geometry, with the N1—C2—C3 [113.40 (19)°] and N1—C9—C10 [114.50 (19)°] angles deviating significantly from the regular tetrahedral value (109.5°).

## Experimental

To an ethanol solution of ethylenediamine (1.00 mol), benzyl chloride (4.00 mol) was added dropwise with continuous stirring. The mixture was refluxed for 4 h. After cooling, the white hydrochloride of TBEN was filtered off, washed with ethanol and dried. The solid was then neutralized with 20% sodium hydroxide solution (400 ml) and the resulting oil was extracted; TBEN crystallized on standing. It was recrystallized from hot ethanol (m.p. 367–368 K). IR (KBr, cm$^{-1}$): 3079, 3025, 2949, 2896, 1599, 1492, 1451, 1373, 1243, 1126, 1096, 1068, 1028, 976, 741, 697. $^1$H NMR (CDCl$_3$, $\delta$, p.p.m.): 7.34–7.19 (*m*, 20H), 2(*s*, 8H), 4.81(*s*, 4H). Analysis calculated for $C_{30}H_{32}N_2$: C 85.70, H 7.60, N 6.65%; found: C 85.85, H 7.6, N 6.45%.

### *Crystal data*

$C_{30}H_{32}N_2$
$M_r = 420.58$
Triclinic, $P\overline{1}$
$a = 5.8718\ (19)$ Å
$b = 10.202\ (3)$ Å
$c = 10.629\ (3)$ Å
$\alpha = 97.621\ (6)^\circ$
$\beta = 101.621\ (6)^\circ$
$\gamma = 93.951\ (6)^\circ$
$V = 615.2\ (3)$ Å$^3$

$Z = 1$
$D_x = 1.135$ Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 960 reflections
$\theta = 2.6$–$22.6^\circ$
$\mu = 0.07$ mm$^{-1}$
$T = 293\ (2)$ K
Block, colourless
0.20 × 0.18 × 0.14 mm

### *Data collection*

Bruker SMART CCD area-detector diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
$T_{\min} = 0.926$, $T_{\max} = 0.991$
3224 measured reflections

2166 independent reflections
1283 reflections with $I > 2\sigma(I)$
$R_{\rm int} = 0.028$
$\theta_{\max} = 25.0^\circ$
$h = -6 \rightarrow 6$
$k = -12 \rightarrow 11$
$l = -12 \rightarrow 12$

### *Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.045$
$wR(F^2) = 0.181$
$S = 1.06$
2166 reflections
146 parameters
H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0994P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{\max} = 0.003$
$\Delta\rho_{\max} = 0.13$ e Å$^{-3}$
$\Delta\rho_{\min} = -0.13$ e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.053 (15)

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| N1—C1 | 1.460 (3) | N1—C2 | 1.467 (3) |
| N1—C9 | 1.462 (3) | | |
| C1—N1—C9 | 111.28 (17) | N1—C2—C3 | 113.40 (19) |
| C1—N1—C2 | 111.28 (17) | N1—C9—C10 | 114.15 (19) |
| C9—N1—C2 | 109.35 (19) | | |
| C9—N1—C1—C1$^{\rm i}$ | −162.0 (3) | N1—C2—C3—C8 | −126.5 (3) |
| C2—N1—C1—C1$^{\rm i}$ | 75.8 (3) | C1—N1—C9—C10 | 68.8 (2) |
| C1—N1—C2—C3 | −169.0 (2) | C2—N1—C9—C10 | −167.90 (19) |
| C9—N1—C2—C3 | 67.7 (3) | N1—C9—C10—C15 | 52.2 (3) |
| N1—C2—C3—C4 | 55.4 (3) | N1—C9—C10—C11 | −131.8 (2) |

Symmetry code: (i) $-x, 2-y, -z$.

All H atoms were positioned geometrically and refined as riding (C—H = 0.93–0.97 Å) on the attached C atom. For both CH and CH$_2$ groups, the $U_{\rm iso}$(H) values were set equal to 1.2$U_{\rm eq}$(carrier atom).

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

## References

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