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1,3-Dibenzyl-2-phenylimidazolidine

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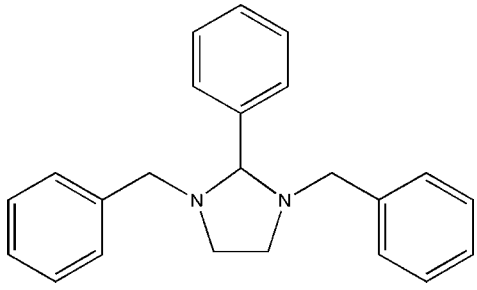
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; R factor = 0.066; wR factor = 0.161; data-to-parameter ratio = 14.8.

In the title compound, $C_{23}H_{24}N_2$, the dihedral angles between the phenyl ring at the 2-position and the other two other phenyl rings are 78.95 (10) and 71.76 (10)°. The imidazolidine ring adopts a slightly distorted envelope conformation. Molecules are linked into chains of rings and a three-dimensional network by C—H···π hydrogen bonds

Related literature

For bond-length data, see: Allen *et al.* (1987). For a related structure, see: Xia *et al.* (2007).



Experimental

Crystal data

$C_{23}H_{24}N_2$
M_r = 328.44
Monoclinic, $P2_1/n$
a = 6.0611 (12) Å
b = 16.0637 (16) Å
c = 19.494 (2) Å
β = 91.545 (2)°
V = 1897.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 298 (2) K
0.68 × 0.21 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.956, T_{max} = 0.993
9261 measured reflections
3344 independent reflections
1682 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.161
S = 1.03
3344 reflections
226 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

*Cg*1 and *Cg*2 are the centroids of the C18–C23 and C11–C16 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···*Cg*1^{i}	0.93	3.07	3.76 (2)	132
C20—H20···*Cg*2^{ii}	0.93	2.85	3.59 (2)	137

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

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

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2158).

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supplementary materials

Acta Cryst. (2007). E**63**, o3666 [**doi:10.1107/S1600536807037026**]

1,3-Dibenzyl-2-phenylimidazolidine

H.-T. Xia, Y.-F. Liu, D.-Q. Wang and B. Li

Comment

As part of our investigation of the crystal structures of ethylenediamine derivatives, we report here the crystal structure of a new ethylenediamine derivative.

The molecular structure of the title compound is illustrated in Fig. 1. In the molecule, the dihedral angles between the phenyl ring (C4–C9) and the other two phenyl rings are 78.95 (10)° (C11–C16) and 71.76 (10)° (C18–C23). The imidazolidine ring adopts a slightly distorted envelope conformation, with C3 as the flap atom. Molecules are linked into chains of rings and a three dimensional network by C—H···π hydrogen bonds (Fig. 2 and Fig. 3).

Experimental

To a solution of benzaldehyde (20 mmol) in methanol (20 ml) ethylenediamine (10 mmol) in methanol (10 ml) was added. The mixed solution was stirred for 10 min and then acetic acid catalyst was added. The reaction mixture was stirred continuously for 10 h at 338 K and then filtered. The solution was allowed to stand, slowly producing crystals of the title compound.

Refinement

All H atoms were located in difference Fourier maps. They were then treated as riding, with C—H distances of 0.93 Å (aryl), 0.97 Å (methylene) and 0.98 Å (methine); U_{iso}(H) = 1.2U_{eq}(C).

Figures

Fig. 1. The molecular structure of the title compound, showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 30% probability level.

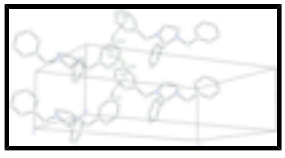

Fig. 2. Part of the crystal structure of the title compound, showing the formation of a hydrogen-bonded (dashed lines) sheet built from three C—H···π interactions. For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry code: (C) 1/2 + *x*, 1/2 − *y*, 1/2 + *z*, (D) 1 + *x*, *y*, *z*, (E) 3/2 + *x*, 1/2 − *y*, 1/2 + *z*].

Fig. 3. The crystal structure of the title compound. Neighbouring sheets are connected by a pair of C—H···π hydrogen bonds (dashed lines). For clarity, H atoms not involved in the hydrogen bonding have been omitted. [Symmetry code: (A) 1/2 − *x*, 1/2 + *y*, 1/2 − *z*, (B) 1 − *x*, 1 − *y*, 1 − *z* (C) 1/2 + *x*, 1/2 − *y*, 1/2 + *z*].

1,3-Dibenzyl-2-phenylimidazolidine

Crystal data

$C_{23}H_{24}N_2$	F_{000} = 704
M_r = 328.44	D_x = 1.150 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 6.0611 (12) Å	Cell parameters from 1633 reflections
b = 16.0637 (16) Å	θ = 2.7–20.4º
c = 19.494 (2) Å	μ = 0.07 mm^{-1}
β = 91.545 (2)º	T = 298 (2) K
V = 1897.3 (5) Å^3	Block, colourless
Z = 4	0.68 × 0.21 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	3344 independent reflections
Radiation source: fine-focus sealed tube	1682 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.073
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→7
T_{min} = 0.956, T_{max} = 0.993	k = −18→19
9261 measured reflections	l = −23→10

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.066	H-atom parameters constrained
$wR(F^2)$ = 0.161	$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.03	$(\Delta/\sigma)_{max} < 0.001$
3344 reflections	$\Delta\rho_{max}$ = 0.20 e Å^{-3}
226 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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	0.2099 (4)	0.13673 (13)	0.09252 (11)	0.0450 (6)
N2	0.2019 (4)	0.12748 (13)	0.20804 (12)	0.0441 (6)
C1	0.3331 (5)	0.06115 (17)	0.10993 (15)	0.0571 (9)
H1A	0.4870	0.0670	0.0984	0.068*
H1B	0.2714	0.0135	0.0856	0.068*
C2	0.3098 (6)	0.05136 (19)	0.18653 (15)	0.0633 (10)
H2A	0.2206	0.0030	0.1969	0.076*
H2B	0.4532	0.0454	0.2093	0.076*
C3	0.0643 (5)	0.15306 (16)	0.14996 (14)	0.0427 (7)
H3	−0.0676	0.1179	0.1462	0.051*
C4	−0.0006 (5)	0.24356 (17)	0.15271 (13)	0.0408 (7)
C5	0.1595 (5)	0.30273 (18)	0.16510 (16)	0.0564 (9)
H5	0.3046	0.2860	0.1736	0.068*
C6	0.1090 (6)	0.3857 (2)	0.16520 (17)	0.0644 (10)
H6	0.2194	0.4247	0.1743	0.077*
C7	−0.1020 (7)	0.4116 (2)	0.15209 (17)	0.0650 (10)
H7	−0.1354	0.4681	0.1514	0.078*
C8	−0.2628 (6)	0.3543 (2)	0.14001 (19)	0.0714 (11)
H8	−0.4072	0.3715	0.1311	0.086*
C9	−0.2119 (5)	0.2698 (2)	0.14094 (16)	0.0590 (9)
H9	−0.3234	0.2309	0.1335	0.071*
C10	0.0966 (5)	0.13572 (18)	0.02628 (14)	0.0542 (9)
H10A	−0.0059	0.1821	0.0238	0.065*
H10B	0.0113	0.0848	0.0221	0.065*
C11	0.2500 (5)	0.14128 (16)	−0.03344 (14)	0.0438 (8)
C12	0.4506 (5)	0.18111 (18)	−0.02765 (16)	0.0561 (9)
H12	0.4977	0.2021	0.0147	0.067*
C13	0.5840 (6)	0.1905 (2)	−0.08390 (19)	0.0673 (10)
H13	0.7194	0.2174	−0.0792	0.081*
C14	0.5152 (7)	0.1600 (2)	−0.14597 (19)	0.0749 (11)
H14	0.6038	0.1662	−0.1838	0.090*
C15	0.3185 (7)	0.1206 (2)	−0.15288 (18)	0.0757 (11)
H15	0.2724	0.1001	−0.1955	0.091*
C16	0.1852 (6)	0.11070 (19)	−0.09671 (16)	0.0637 (10)
H16	0.0508	0.0831	−0.1019	0.076*
C17	0.0859 (5)	0.12033 (18)	0.27187 (15)	0.0519 (8)
H17A	−0.0022	0.0699	0.2706	0.062*
H17B	−0.0141	0.1671	0.2758	0.062*

C18	0.2370 (5)	0.11810 (16)	0.33424 (15)	0.0456 (8)
C19	0.4406 (6)	0.15655 (18)	0.33508 (16)	0.0561 (9)
H19	0.4898	0.1816	0.2953	0.067*
C20	0.5717 (6)	0.1585 (2)	0.3935 (2)	0.0708 (11)
H20	0.7088	0.1844	0.3929	0.085*
C21	0.5023 (8)	0.1225 (2)	0.4528 (2)	0.0810 (13)
H21	0.5905	0.1244	0.4926	0.097*
C22	0.3011 (8)	0.0835 (2)	0.45296 (18)	0.0785 (12)
H22	0.2534	0.0583	0.4929	0.094*
C23	0.1690 (6)	0.08140 (18)	0.39426 (16)	0.0599 (9)
H23	0.0326	0.0550	0.3950	0.072*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0580 (15)	0.0464 (14)	0.0308 (14)	0.0057 (12)	0.0030 (13)	−0.0005 (11)
N2	0.0589 (15)	0.0428 (14)	0.0309 (13)	0.0073 (12)	0.0075 (13)	0.0023 (11)
C1	0.071 (2)	0.0498 (18)	0.051 (2)	0.0065 (17)	0.0090 (18)	−0.0026 (16)
C2	0.092 (3)	0.056 (2)	0.042 (2)	0.0182 (19)	0.0050 (19)	0.0006 (16)
C3	0.0479 (17)	0.0439 (17)	0.0365 (17)	−0.0035 (14)	0.0062 (15)	−0.0038 (14)
C4	0.0469 (18)	0.0426 (17)	0.0333 (17)	0.0022 (15)	0.0066 (15)	0.0023 (13)
C5	0.0519 (19)	0.0468 (19)	0.071 (2)	−0.0017 (17)	0.0048 (18)	−0.0011 (17)
C6	0.073 (2)	0.046 (2)	0.074 (3)	−0.0089 (19)	0.014 (2)	−0.0027 (18)
C7	0.083 (3)	0.048 (2)	0.065 (2)	0.012 (2)	0.021 (2)	0.0062 (17)
C8	0.059 (2)	0.066 (2)	0.090 (3)	0.016 (2)	0.011 (2)	0.013 (2)
C9	0.053 (2)	0.056 (2)	0.068 (2)	−0.0021 (17)	0.0016 (18)	0.0022 (17)
C10	0.057 (2)	0.065 (2)	0.0404 (19)	−0.0023 (16)	0.0040 (17)	−0.0043 (16)
C11	0.0579 (19)	0.0406 (16)	0.0332 (18)	0.0039 (15)	0.0031 (16)	0.0006 (14)
C12	0.069 (2)	0.062 (2)	0.0376 (19)	−0.0042 (18)	−0.0005 (18)	0.0058 (16)
C13	0.070 (2)	0.070 (2)	0.063 (2)	−0.0016 (19)	0.016 (2)	0.023 (2)
C14	0.094 (3)	0.079 (3)	0.053 (3)	0.020 (2)	0.028 (2)	0.012 (2)
C15	0.107 (3)	0.081 (3)	0.039 (2)	0.008 (3)	0.009 (2)	−0.0122 (19)
C16	0.083 (2)	0.065 (2)	0.044 (2)	−0.0012 (19)	0.003 (2)	−0.0088 (18)
C17	0.062 (2)	0.0514 (19)	0.0423 (18)	−0.0030 (16)	0.0094 (17)	0.0040 (15)
C18	0.063 (2)	0.0355 (16)	0.0381 (18)	0.0062 (16)	0.0047 (16)	−0.0026 (14)
C19	0.070 (2)	0.0514 (19)	0.047 (2)	0.0022 (18)	0.0057 (19)	−0.0057 (15)
C20	0.074 (3)	0.070 (2)	0.067 (3)	0.0099 (19)	−0.010 (2)	−0.018 (2)
C21	0.109 (3)	0.080 (3)	0.052 (3)	0.019 (3)	−0.024 (3)	−0.012 (2)
C22	0.120 (3)	0.071 (3)	0.044 (2)	0.014 (3)	0.005 (2)	0.0061 (18)
C23	0.083 (2)	0.055 (2)	0.042 (2)	0.0034 (18)	0.006 (2)	0.0068 (17)

Geometric parameters (Å, °)

N1—C10	1.446 (3)	C10—H10B	0.9700
N1—C1	1.460 (3)	C11—C16	1.375 (4)
N1—C3	1.468 (3)	C11—C12	1.376 (4)
N2—C3	1.448 (3)	C12—C13	1.388 (4)
N2—C17	1.450 (4)	C12—H12	0.9300
N2—C2	1.454 (3)	C13—C14	1.360 (4)

C1—C2	1.512 (4)	C13—H13	0.9300
C1—H1A	0.9700	C14—C15	1.353 (5)
C1—H1B	0.9700	C14—H14	0.9300
C2—H2A	0.9700	C15—C16	1.387 (5)
C2—H2B	0.9700	C15—H15	0.9300
C3—C4	1.507 (4)	C16—H16	0.9300
C3—H3	0.9800	C17—C18	1.503 (4)
C4—C9	1.362 (4)	C17—H17A	0.9700
C4—C5	1.375 (4)	C17—H17B	0.9700
C5—C6	1.368 (4)	C18—C19	1.380 (4)
C5—H5	0.9300	C18—C23	1.383 (4)
C6—C7	1.362 (4)	C19—C20	1.372 (4)
C6—H6	0.9300	C19—H19	0.9300
C7—C8	1.357 (4)	C20—C21	1.369 (5)
C7—H7	0.9300	C20—H20	0.9300
C8—C9	1.392 (4)	C21—C22	1.371 (5)
C8—H8	0.9300	C21—H21	0.9300
C9—H9	0.9300	C22—C23	1.379 (4)
C10—C11	1.512 (4)	C22—H22	0.9300
C10—H10A	0.9700	C23—H23	0.9300
C10—N1—C1	115.2 (2)	N1—C10—H10B	108.9
C10—N1—C3	113.7 (2)	C11—C10—H10B	108.9
C1—N1—C3	106.6 (2)	H10A—C10—H10B	107.7
C3—N2—C17	114.3 (2)	C16—C11—C12	118.1 (3)
C3—N2—C2	105.5 (2)	C16—C11—C10	120.2 (3)
C17—N2—C2	114.4 (2)	C12—C11—C10	121.6 (3)
N1—C1—C2	104.8 (2)	C11—C12—C13	121.2 (3)
N1—C1—H1A	110.8	C11—C12—H12	119.4
C2—C1—H1A	110.8	C13—C12—H12	119.4
N1—C1—H1B	110.8	C14—C13—C12	119.5 (3)
C2—C1—H1B	110.8	C14—C13—H13	120.2
H1A—C1—H1B	108.9	C12—C13—H13	120.2
N2—C2—C1	104.6 (2)	C15—C14—C13	120.3 (4)
N2—C2—H2A	110.8	C15—C14—H14	119.8
C1—C2—H2A	110.8	C13—C14—H14	119.8
N2—C2—H2B	110.8	C14—C15—C16	120.4 (3)
C1—C2—H2B	110.8	C14—C15—H15	119.8
H2A—C2—H2B	108.9	C16—C15—H15	119.8
N2—C3—N1	101.5 (2)	C11—C16—C15	120.6 (3)
N2—C3—C4	113.0 (2)	C11—C16—H16	119.7
N1—C3—C4	111.2 (2)	C15—C16—H16	119.7
N2—C3—H3	110.2	N2—C17—C18	113.4 (2)
N1—C3—H3	110.2	N2—C17—H17A	108.9
C4—C3—H3	110.2	C18—C17—H17A	108.9
C9—C4—C5	118.1 (3)	N2—C17—H17B	108.9
C9—C4—C3	122.5 (3)	C18—C17—H17B	108.9
C5—C4—C3	119.3 (2)	H17A—C17—H17B	107.7
C6—C5—C4	121.1 (3)	C19—C18—C23	117.9 (3)
C6—C5—H5	119.4	C19—C18—C17	121.6 (3)

C4—C5—H5	119.4	C23—C18—C17	120.4 (3)
C7—C6—C5	120.5 (3)	C20—C19—C18	121.2 (3)
C7—C6—H6	119.8	C20—C19—H19	119.4
C5—C6—H6	119.8	C18—C19—H19	119.4
C8—C7—C6	119.4 (3)	C21—C20—C19	120.5 (4)
C8—C7—H7	120.3	C21—C20—H20	119.7
C6—C7—H7	120.3	C19—C20—H20	119.7
C7—C8—C9	120.1 (3)	C20—C21—C22	119.2 (4)
C7—C8—H8	119.9	C20—C21—H21	120.4
C9—C8—H8	119.9	C22—C21—H21	120.4
C4—C9—C8	120.8 (3)	C21—C22—C23	120.4 (4)
C4—C9—H9	119.6	C21—C22—H22	119.8
C8—C9—H9	119.6	C23—C22—H22	119.8
N1—C10—C11	113.6 (2)	C22—C23—C18	120.8 (3)
N1—C10—H10A	108.9	C22—C23—H23	119.6
C11—C10—H10A	108.9	C18—C23—H23	119.6
C10—N1—C1—C2	−145.1 (3)	C1—N1—C10—C11	−71.5 (3)
C3—N1—C1—C2	−17.9 (3)	C3—N1—C10—C11	165.1 (2)
C3—N2—C2—C1	30.7 (3)	N1—C10—C11—C16	155.5 (3)
C17—N2—C2—C1	157.1 (2)	N1—C10—C11—C12	−28.5 (4)
N1—C1—C2—N2	−7.5 (3)	C16—C11—C12—C13	0.2 (4)
C17—N2—C3—N1	−167.9 (2)	C10—C11—C12—C13	−175.9 (3)
C2—N2—C3—N1	−41.4 (3)	C11—C12—C13—C14	0.2 (5)
C17—N2—C3—C4	72.8 (3)	C12—C13—C14—C15	−0.2 (5)
C2—N2—C3—C4	−160.7 (2)	C13—C14—C15—C16	−0.2 (5)
C10—N1—C3—N2	164.5 (2)	C12—C11—C16—C15	−0.5 (4)
C1—N1—C3—N2	36.5 (3)	C10—C11—C16—C15	175.5 (3)
C10—N1—C3—C4	−75.0 (3)	C14—C15—C16—C11	0.6 (5)
C1—N1—C3—C4	157.0 (2)	C3—N2—C17—C18	−163.5 (2)
N2—C3—C4—C9	−132.9 (3)	C2—N2—C17—C18	74.8 (3)
N1—C3—C4—C9	113.6 (3)	N2—C17—C18—C19	28.4 (4)
N2—C3—C4—C5	49.4 (4)	N2—C17—C18—C23	−155.7 (3)
N1—C3—C4—C5	−64.1 (3)	C23—C18—C19—C20	0.0 (4)
C9—C4—C5—C6	−0.4 (5)	C17—C18—C19—C20	176.0 (3)
C3—C4—C5—C6	177.3 (3)	C18—C19—C20—C21	−0.4 (5)
C4—C5—C6—C7	−0.8 (5)	C19—C20—C21—C22	0.8 (5)
C5—C6—C7—C8	1.1 (5)	C20—C21—C22—C23	−0.8 (5)
C6—C7—C8—C9	−0.1 (5)	C21—C22—C23—C18	0.3 (5)
C5—C4—C9—C8	1.4 (5)	C19—C18—C23—C22	0.1 (4)
C3—C4—C9—C8	−176.2 (3)	C17—C18—C23—C22	−176.0 (3)
C7—C8—C9—C4	−1.2 (5)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···Cg1^{i}	0.93	3.07	3.76 (2)	132
C20—H20···Cg2^{ii}	0.93	2.85	3.59 (2)	137

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

Fig. 1

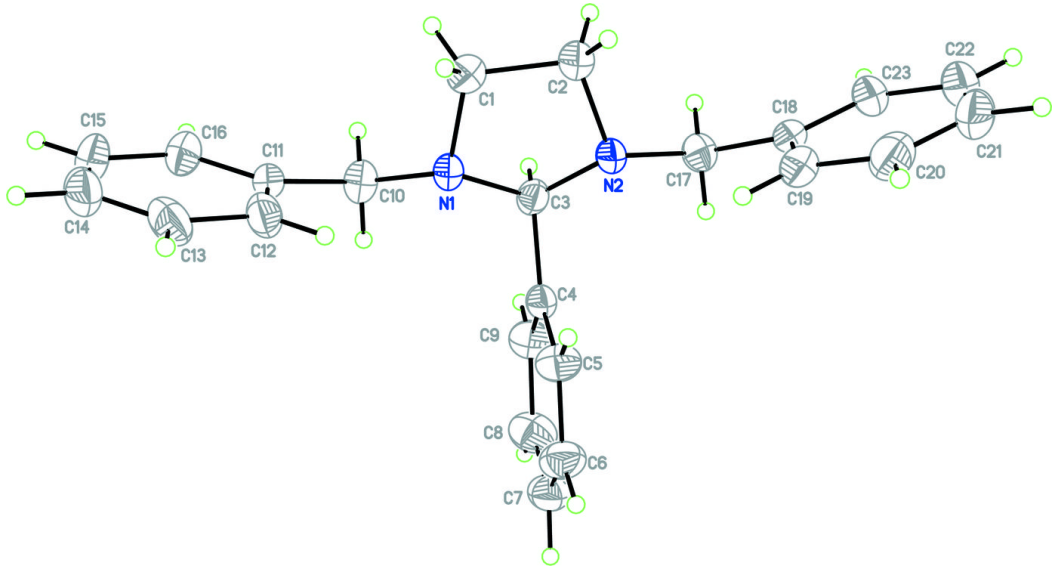
C15
C16
C11
C14
C13
C12
C10
N1
C1
C2
C3
N2
C17
C18
C19
C20
C21
C22
C23
C4
C9
C5
C8
C6
C7

Fig. 2

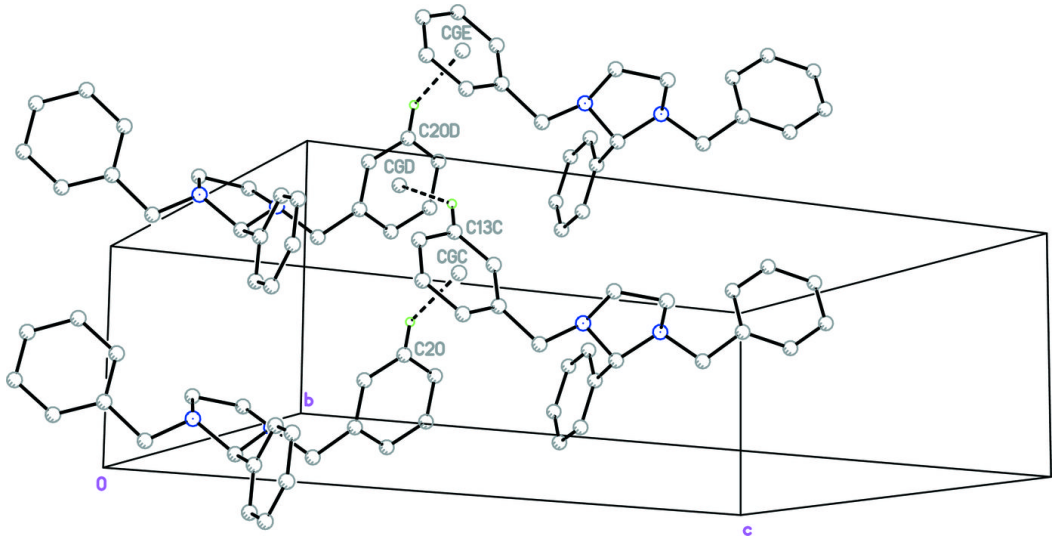

Fig. 3