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(4a*R**,8a*S**)-2,3-Diphenyl-4a,5,6,7,8,8a-hexahydroquinoxaline

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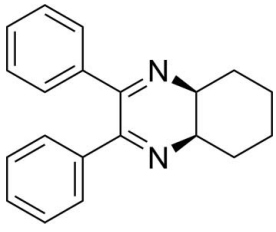
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.003 Å; R factor = 0.036; wR factor = 0.099; data-to-parameter ratio = 13.8.

In the title compound, $C_{20}H_{20}N_2$, the quinoxaline ring adopts a very distorted half-chair conformation [N=C–C=N = 22.7 (2)° for the nominally coplanar atoms] and the cyclohexane ring adopts a chair conformation. The quinoxaline and cyclohexane rings are *cis*-fused. The two phenyl rings form a dihedral angle of 63.88 (7)°.

Related literature

For background to dihydropyrazine derivatives, see: Raw *et al.* (2003). For related structures, see: Reich *et al.* (2004); Wang *et al.* (2008).



Experimental

Crystal data

$C_{20}H_{20}N_2$
M_r = 288.38
Orthorhombic, $P2_12_12_1$
a = 6.3546 (1) Å
b = 13.4894 (2) Å
c = 19.1921 (3) Å
V = 1645.14 (4) Å^3
Z = 4
Cu $K\alpha$ radiation
μ = 0.52 mm^{-1}
T = 293 K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.902, T_{max} = 0.949
4074 measured reflections
2739 independent reflections
2703 reflections with $I > 2\sigma(I)$
R_{int} = 0.010

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.05
2739 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); 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: HB6855).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
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supplementary materials

Acta Cryst. (2012). E**68**, o2212 [doi:10.1107/S1600536812028061]

(4a*R**,8a*S**)-2,3-Diphenyl-4a,5,6,7,8,8a-hexahydroquinoxaline

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Comment

Dihydropyrazine ring systems are found as a key unit in natural products and biochemical materials (Raw *et al.*, 2003). Therefore, the synthesis of dihydropyrazine derivatives attract much interest in organic chemistry. In this respect, we report herein the crystal structure of the title compound.

In the title compound, Fig. 1, the quinoxaline ring has a very distorted half-chair conformation and the cyclohexane ring has a chair conformation. The dihedral angle between the two benzene rings is 63.88 (7)°. The lengths of the C═N bonds [1.2678 (18)Å] are comparable to those in similar compounds (Wang *et al.*, 2008; Reich *et al.*, 2004).

Experimental

2-hydroxy-1,2-diphenylethanone (0.212 g, 1 mmol) and $YbCl_3$ (0.028 g, 0.1 mmol) were dissolved in 5 ml EtOH and stirred until the solid dissolved completely in refluxing, then (1*R*,2*S*)-cyclohexane-1,2-diamine (0.171 g, 1.5 mmol) and H_2O_2 (0.022 g, 0.2 mmol) were added into the mixture. After 30 min, TLC showed the reaction to be complete. The reaction mixture was cooled to room temperature. The solvent was evaporated in vacuum and the product purified by column chromatography on neutral alumina deactivated with H_2O (6 wt%) (PE-EtOAc = 5:1) to give the title compound. The compound was recrystallized from methanol to give yellow blocks.

Refinement

Hydrogen atoms were positioned geometrically and allowed to ride on their parent atoms, with C–H = 0.93–0.98 Å, and with U_{iso}(H) values set to 1.2U_{eq}(C).

Computing details

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008).

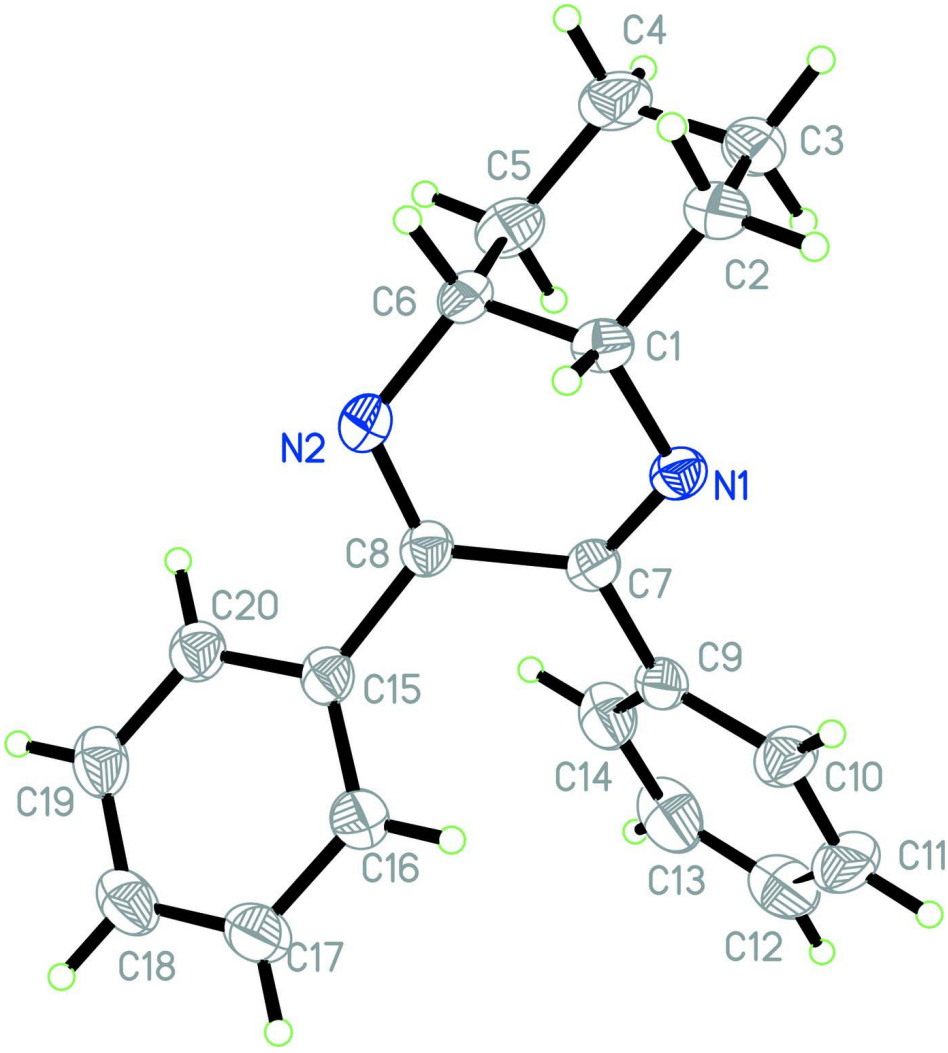

Figure 1

The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

(4a*R,8a*S**)-2,3-Diphenyl-4a,5,6,7,8,8a-hexahydroquinoxaline**

Crystal data

$C_{20}H_{20}N_2$
$M_r = 288.38$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 6.3546$ (1) Å
$b = 13.4894$ (2) Å
$c = 19.1921$ (3) Å
$V = 1645.14$ (4) Å^3
$Z = 4$

$F(000) = 616$
$D_x = 1.164$ Mg m^{-3}
Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Cell parameters from 2779 reflections
$\theta = 3.3$–72.4°
$\mu = 0.52$ mm^{-1}
$T = 293$ K
Block, yellow
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
phi and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.902, T_{max} = 0.949
4074 measured reflections
2739 independent reflections
2703 reflections with $I > 2\sigma(I)$
R_{int} = 0.010
θ_{max} = 72.6°, θ_{min} = 5.7°
$h = -7 \rightarrow 5$
$k = -15 \rightarrow 16$
$l = -17 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.099
S = 1.05
2739 reflections
199 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0617P)^2 + 0.1364P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.14 e Å^{-3}
Absolute structure: unk

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 $F^2 > \sigma(F^2)$ 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}
N1	0.18801 (18)	0.39372 (8)	0.62663 (6)	0.0410 (3)
N2	−0.0579 (2)	0.33893 (9)	0.50829 (6)	0.0492 (3)
C1	0.1165 (2)	0.29069 (10)	0.61739 (7)	0.0419 (3)
H1B	0.2255	0.2542	0.5920	0.050*
C2	0.0862 (3)	0.24167 (12)	0.68822 (8)	0.0544 (4)
H2B	0.0632	0.1712	0.6818	0.065*
H2C	0.2128	0.2501	0.7158	0.065*
C3	−0.0991 (3)	0.28592 (15)	0.72680 (8)	0.0654 (5)
H3A	−0.0700	0.3549	0.7372	0.079*
H3B	−0.1183	0.2512	0.7706	0.079*
C4	−0.2993 (3)	0.27893 (16)	0.68428 (11)	0.0674 (5)
H4A	−0.4138	0.3100	0.7096	0.081*
H4B	−0.3353	0.2098	0.6772	0.081*
C5	−0.2729 (2)	0.32958 (14)	0.61387 (10)	0.0605 (4)
H5A	−0.3992	0.3200	0.5863	0.073*
H5B	−0.2536	0.4002	0.6208	0.073*
C6	−0.0850 (2)	0.28777 (10)	0.57496 (7)	0.0453 (3)

H6A	−0.1155	0.2181	0.5647	0.054*
C7	0.1606 (2)	0.45124 (10)	0.57517 (7)	0.0388 (3)
C8	0.0606 (2)	0.41514 (9)	0.50853 (7)	0.0414 (3)
C9	0.2231 (3)	0.55791 (10)	0.58259 (7)	0.0442 (3)
C10	0.4058 (3)	0.58177 (13)	0.61799 (9)	0.0591 (4)
H10A	0.4885	0.5318	0.6371	0.071*
C11	0.4658 (4)	0.68056 (16)	0.62502 (11)	0.0769 (6)
H11A	0.5903	0.6965	0.6479	0.092*
C12	0.3419 (5)	0.75417 (13)	0.59834 (10)	0.0843 (8)
H12A	0.3823	0.8201	0.6031	0.101*
C13	0.1589 (5)	0.73123 (13)	0.56464 (10)	0.0803 (7)
H13A	0.0740	0.7816	0.5472	0.096*
C14	0.0993 (4)	0.63297 (11)	0.55626 (9)	0.0614 (4)
H14A	−0.0247	0.6177	0.5328	0.074*
C15	0.1024 (3)	0.46329 (10)	0.43996 (7)	0.0444 (3)
C16	0.2983 (3)	0.50275 (13)	0.42434 (8)	0.0535 (4)
H16A	0.4023	0.5054	0.4584	0.064*
C17	0.3394 (3)	0.53842 (14)	0.35770 (9)	0.0631 (4)
H17A	0.4713	0.5644	0.3473	0.076*
C18	0.1862 (4)	0.53548 (13)	0.30698 (9)	0.0634 (5)
H18A	0.2147	0.5590	0.2624	0.076*
C19	−0.0101 (3)	0.49741 (13)	0.32258 (8)	0.0605 (4)
H19A	−0.1142	0.4958	0.2886	0.073*
C20	−0.0522 (3)	0.46158 (11)	0.38877 (8)	0.0514 (4)
H20A	−0.1848	0.4362	0.3990	0.062*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0362 (5)	0.0423 (6)	0.0445 (6)	−0.0035 (5)	0.0028 (5)	−0.0021 (5)
N2	0.0577 (7)	0.0453 (6)	0.0446 (6)	−0.0099 (6)	−0.0039 (6)	−0.0055 (5)
C1	0.0413 (7)	0.0367 (6)	0.0476 (7)	0.0000 (6)	0.0081 (6)	−0.0014 (6)
C2	0.0568 (9)	0.0541 (8)	0.0523 (8)	−0.0089 (7)	0.0006 (7)	0.0092 (7)
C3	0.0728 (11)	0.0777 (11)	0.0458 (8)	−0.0250 (10)	0.0162 (8)	−0.0067 (8)
C4	0.0529 (9)	0.0777 (11)	0.0716 (10)	−0.0188 (9)	0.0248 (8)	−0.0114 (10)
C5	0.0380 (7)	0.0664 (10)	0.0771 (11)	−0.0071 (7)	0.0026 (7)	−0.0018 (9)
C6	0.0510 (7)	0.0387 (6)	0.0462 (7)	−0.0117 (6)	0.0013 (6)	−0.0057 (6)
C7	0.0368 (6)	0.0378 (6)	0.0419 (6)	−0.0007 (5)	0.0043 (5)	−0.0047 (5)
C8	0.0455 (7)	0.0360 (6)	0.0427 (6)	0.0001 (6)	0.0007 (6)	−0.0060 (5)
C9	0.0560 (8)	0.0390 (7)	0.0376 (6)	−0.0067 (6)	0.0075 (6)	−0.0065 (5)
C10	0.0606 (9)	0.0534 (8)	0.0632 (9)	−0.0126 (8)	0.0026 (8)	−0.0113 (7)
C11	0.0866 (13)	0.0702 (12)	0.0738 (12)	−0.0356 (11)	0.0105 (11)	−0.0232 (10)
C12	0.148 (2)	0.0435 (9)	0.0617 (10)	−0.0306 (12)	0.0243 (14)	−0.0141 (8)
C13	0.142 (2)	0.0406 (8)	0.0581 (9)	0.0044 (11)	0.0039 (13)	−0.0052 (7)
C14	0.0894 (12)	0.0426 (7)	0.0522 (8)	0.0040 (8)	−0.0030 (9)	−0.0040 (6)
C15	0.0567 (8)	0.0340 (6)	0.0425 (7)	0.0010 (6)	0.0005 (6)	−0.0050 (5)
C16	0.0607 (9)	0.0529 (8)	0.0469 (7)	−0.0056 (8)	0.0019 (7)	−0.0016 (7)
C17	0.0737 (11)	0.0616 (9)	0.0539 (8)	−0.0074 (9)	0.0126 (8)	0.0062 (7)
C18	0.0919 (13)	0.0539 (8)	0.0443 (8)	0.0018 (9)	0.0072 (8)	0.0071 (7)
C19	0.0833 (12)	0.0513 (8)	0.0469 (8)	0.0057 (9)	−0.0121 (8)	0.0012 (7)

C20	0.0616 (9)	0.0428 (7)	0.0496 (8)	−0.0009 (7)	−0.0029 (7)	−0.0028 (6)

Geometric parameters (Å, º)

N1—C7	1.2680 (18)	C9—C14	1.378 (2)
N1—C1	1.4728 (17)	C9—C10	1.383 (2)
N2—C8	1.2745 (19)	C10—C11	1.393 (3)
N2—C6	1.4638 (19)	C10—H10A	0.9300
C1—C6	1.518 (2)	C11—C12	1.367 (4)
C1—C2	1.524 (2)	C11—H11A	0.9300
C1—H1B	0.9800	C12—C13	1.366 (4)
C2—C3	1.513 (2)	C12—H12A	0.9300
C2—H2B	0.9700	C13—C14	1.388 (3)
C2—H2C	0.9700	C13—H13A	0.9300
C3—C4	1.515 (3)	C14—H14A	0.9300
C3—H3A	0.9700	C15—C16	1.387 (2)
C3—H3B	0.9700	C15—C20	1.390 (2)
C4—C5	1.523 (3)	C16—C17	1.391 (2)
C4—H4A	0.9700	C16—H16A	0.9300
C4—H4B	0.9700	C17—C18	1.377 (3)
C5—C6	1.517 (2)	C17—H17A	0.9300
C5—H5A	0.9700	C18—C19	1.381 (3)
C5—H5B	0.9700	C18—H18A	0.9300
C6—H6A	0.9800	C19—C20	1.385 (2)
C7—C9	1.4996 (18)	C19—H19A	0.9300
C7—C8	1.5087 (18)	C20—H20A	0.9300
C8—C15	1.4914 (19)		
C7—N1—C1	116.18 (11)	C9—C7—C8	120.12 (12)
C8—N2—C6	116.52 (12)	N2—C8—C15	116.95 (12)
N1—C1—C6	110.45 (11)	N2—C8—C7	120.82 (12)
N1—C1—C2	109.94 (12)	C15—C8—C7	122.18 (11)
C6—C1—C2	111.15 (12)	C14—C9—C10	119.24 (15)
N1—C1—H1B	108.4	C14—C9—C7	121.25 (14)
C6—C1—H1B	108.4	C10—C9—C7	119.49 (14)
C2—C1—H1B	108.4	C9—C10—C11	120.01 (19)
C3—C2—C1	111.32 (14)	C9—C10—H10A	120.0
C3—C2—H2B	109.4	C11—C10—H10A	120.0
C1—C2—H2B	109.4	C12—C11—C10	120.1 (2)
C3—C2—H2C	109.4	C12—C11—H11A	120.0
C1—C2—H2C	109.4	C10—C11—H11A	120.0
H2B—C2—H2C	108.0	C13—C12—C11	120.20 (17)
C2—C3—C4	111.43 (13)	C13—C12—H12A	119.9
C2—C3—H3A	109.3	C11—C12—H12A	119.9
C4—C3—H3A	109.3	C12—C13—C14	120.2 (2)
C2—C3—H3B	109.3	C12—C13—H13A	119.9
C4—C3—H3B	109.3	C14—C13—H13A	119.9
H3A—C3—H3B	108.0	C9—C14—C13	120.2 (2)
C3—C4—C5	110.93 (13)	C9—C14—H14A	119.9
C3—C4—H4A	109.5	C13—C14—H14A	119.9

C5—C4—H4A	109.5	C16—C15—C20	119.22 (14)
C3—C4—H4B	109.5	C16—C15—C8	121.16 (14)
C5—C4—H4B	109.5	C20—C15—C8	119.41 (14)
H4A—C4—H4B	108.0	C15—C16—C17	119.99 (16)
C6—C5—C4	110.90 (15)	C15—C16—H16A	120.0
C6—C5—H5A	109.5	C17—C16—H16A	120.0
C4—C5—H5A	109.5	C18—C17—C16	120.46 (18)
C6—C5—H5B	109.5	C18—C17—H17A	119.8
C4—C5—H5B	109.5	C16—C17—H17A	119.8
H5A—C5—H5B	108.0	C17—C18—C19	119.72 (15)
N2—C6—C5	110.33 (13)	C17—C18—H18A	120.1
N2—C6—C1	110.95 (11)	C19—C18—H18A	120.1
C5—C6—C1	112.96 (12)	C18—C19—C20	120.20 (17)
N2—C6—H6A	107.4	C18—C19—H19A	119.9
C5—C6—H6A	107.4	C20—C19—H19A	119.9
C1—C6—H6A	107.4	C19—C20—C15	120.39 (17)
N1—C7—C9	118.48 (12)	C19—C20—H20A	119.8
N1—C7—C8	121.37 (12)	C15—C20—H20A	119.8