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## Structure Reports

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# 1,2,3-Triphenyl-1,2-dihydroquinoxaline

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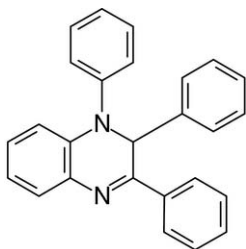
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 Key indicators: single-crystal X-ray study;  $T = 143$  K; mean  $\sigma(\text{C}-\text{C}) = 0.003$  Å;  $R$  factor = 0.053;  $wR$  factor = 0.120; data-to-parameter ratio = 13.5.

The title compound,  $\text{C}_{26}\text{H}_{20}\text{N}_2$ , first reported in 1891, was obtained as a by-product in the preparation of benzildianil from benzil and excess aniline. The dihedral angles between the fused benzene ring and the pendant phenyl rings are 17.93 (11), 53.18 (10) and 89.08 (12)°.

## Related literature

For related literature, see: Bodforss (1960); Kehrmann & Messinger (1891); Sannicolò (1983); Lorenz *et al.* (1994); Siegfeld (1892).



## Experimental

### Crystal data

$\text{C}_{26}\text{H}_{20}\text{N}_2$	$V = 1937.4$ (7) Å <sup>3</sup>
$M_r = 360.44$	$Z = 4$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
$a = 10.121$ (2) Å	$\mu = 0.07$ mm <sup>-1</sup>
$b = 10.374$ (2) Å	$T = 143$ (2) K
$c = 18.572$ (4) Å	$0.40 \times 0.25 \times 0.20$ mm
$\beta = 96.49$ (3)°	

### Data collection

Stoe STADI4 diffractometer	$R_{\text{int}} = 0.038$
Absorption correction: none	3 standard reflections
5587 measured reflections	frequency: 90 min
3413 independent reflections	intensity decay: none
2249 reflections with $I > 2\sigma(I)$	

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.053$	253 parameters
$wR(F^2) = 0.120$	H-atom parameters constrained
$S = 1.06$	$\Delta\rho_{\text{max}} = 0.17$ e Å <sup>-3</sup>
3413 reflections	$\Delta\rho_{\text{min}} = -0.20$ e Å <sup>-3</sup>

Data collection: *DIF4* (Stoe & Cie, 1992); cell refinement: *DIF4*; data reduction: *REDU4* (Stoe & Cie, 1992); program(s) used to solve structure: *SHELXS86* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP5* in *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: BT2784).

## References

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**supplementary materials**

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## 1,2,3-Triphenyl-1,2-dihydroquinoxaline

F. T. Edelmann, S. Blaurock, V. Lorenz and A. Fischer

### Comment

The title compound, 1,2,4-triphenyl-1,2-dihydroquinoxaline (**1**), was first reported as early as 1891 by Kehrmann & Messinger. In the original paper the compound was named 'quinoxaline base from benzoin and phenylphenylenediamine' and was already assigned the correct structure. It was described as 'magnificent uranium-yellow crystals' showing a bright blue–green fluorescence in solution (alcohols, ether, benzene) (Kehrmann & Messinger, 1891). In 1960, Bodforss used **1** and substituted derivatives thereof to prepare cationic quinoxalinium salts which in many respects resembled the well known triphenylmethane dyes (Bodforss, 1960). For example, the dimethylamino derivatives were found to give blue solutions, while the dihydroxyphenyl derivative was orange–red. The only other report on **1** found in the literature is a paper by Sannicolò entitled 'New Heterocyclic Syntheses from Benzil Dianils' (Sannicolò, 1983). In this paper it was reported that **1** is formed as a by-product in the preparation of benzildianil from benzil and excess aniline in the presence of 4-toluenesulfonic acid as catalyst. Under suitable reaction conditions the isolated yield of **1** can be as high as 31% (Sannicolò, 1983). We obtained the beautiful yellow crystals of the title compound by chance in minor amounts as a by-product in the preparation of benzildianil according to the literature procedure (Siegfried *et al.*, 1892; Lorenz *et al.*, 1994). A crystal structure determination revealed the presence of 1,2,4-triphenyl-1,2-dihydroquinoxaline (**1**) containing three adjacent phenyl substituents attached to the 1,2-dihydroquinoxaline core. With a short distance of 1.282 (3) Å the C2—N2 bond is clearly a double bond. Thus this study confirmed that Kehrmann & Messinger had assigned the correct structure of the title compound almost 120 years ago (Kehrmann & Messinger, 1891).

### Experimental

Well formed, bright yellow single crystals of the title compound were obtained as a minor by-product (less than 5% isolated yield) during a preparation of benzildianil from benzil and excess aniline according to the literature (Lorenz *et al.*, 1994).

### Refinement

H atoms were refined using a riding model, with aromatic C—H = 0.95 Å, tertiary C—H = 0.99 Å and  $U_{iso}(H) = 1.2U_{eq}(C)$ .

### Figures

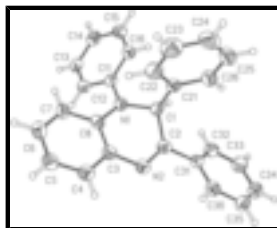


Fig. 1. The molecule of the title compound in the crystal. Displacement ellipsoids represent 50% probability levels. H-Atom radii are arbitrary.

## 1,2,3-Triphenyl-1,2-dihydroquinoxaline

### Crystal data

$C_{26}H_{20}N_2$	$F_{000} = 760$
$M_r = 360.44$	$D_x = 1.236 \text{ Mg m}^{-3}$
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation
Hall symbol: -P2yn	$\lambda = 0.71073 \text{ \AA}$
$a = 10.121 (2) \text{ \AA}$	Cell parameters from 58 reflections
$b = 10.374 (2) \text{ \AA}$	$\theta = 10\text{--}11.5^\circ$
$c = 18.572 (4) \text{ \AA}$	$\mu = 0.07 \text{ mm}^{-1}$
$\beta = 96.49 (3)^\circ$	$T = 143 (2) \text{ K}$
$V = 1937.4 (7) \text{ \AA}^3$	Prism, yellow
$Z = 4$	$0.40 \times 0.25 \times 0.20 \text{ mm}$

### Data collection

Stoe STADI4 diffractometer	$R_{\text{int}} = 0.038$
Radiation source: fine-focus sealed tube	$\theta_{\text{max}} = 25.0^\circ$
Monochromator: graphite	$\theta_{\text{min}} = 3.1^\circ$
$T = 143(2) \text{ K}$	$h = -11 \rightarrow 12$
$\omega/\theta$ scans	$k = -12 \rightarrow 6$
Absorption correction: none	$l = -22 \rightarrow 0$
5587 measured reflections	3 standard reflections
3413 independent reflections	every 90 min
2249 reflections with $I > 2\sigma(I)$	intensity decay: none

### Refinement

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.053$	H-atom parameters constrained
$wR(F^2) = 0.120$	$w = 1/[\sigma^2(F_o^2) + (0.0357P)^2 + 0.6314P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
3413 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
253 parameters	$\Delta\rho_{\text{max}} = 0.17 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{\text{min}} = -0.20 \text{ e \AA}^{-3}$
	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. Weighted  $R$ -factors  $wR$  and all goodnesses 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 observed criterion of  $F^2 > \sigma(F^2)$  is used only for calculating `_R_factor_obs` 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 ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.03731 (18)	0.21070 (18)	0.24908 (10)	0.0289 (5)
C1	-0.0288 (2)	0.3104 (2)	0.28694 (12)	0.0288 (5)
H1	-0.0601	0.3783	0.2508	0.035*
C2	0.0724 (2)	0.3722 (2)	0.34379 (12)	0.0284 (5)
N2	0.16822 (18)	0.30815 (19)	0.37782 (10)	0.0330 (5)
C3	0.1878 (2)	0.1800 (2)	0.35655 (13)	0.0314 (6)
C4	0.2750 (2)	0.1022 (2)	0.40081 (14)	0.0403 (6)
H4	0.3131	0.1338	0.4465	0.048*
C5	0.3068 (2)	-0.0197 (3)	0.37920 (14)	0.0429 (7)
H5	0.3662	-0.0722	0.4097	0.052*
C6	0.2513 (2)	-0.0648 (3)	0.31256 (13)	0.0389 (6)
H6	0.2745	-0.1483	0.2971	0.047*
C7	0.1631 (2)	0.0087 (2)	0.26827 (13)	0.0339 (6)
H7	0.1251	-0.0246	0.2229	0.041*
C8	0.1293 (2)	0.1322 (2)	0.28974 (12)	0.0290 (5)
C11	-0.0053 (2)	0.1892 (2)	0.17475 (12)	0.0275 (5)
C12	0.0861 (2)	0.1544 (2)	0.12738 (12)	0.0311 (5)
H12	0.1769	0.1423	0.1452	0.037*
C13	0.0448 (2)	0.1374 (2)	0.05486 (12)	0.0325 (6)
H13	0.1078	0.1140	0.0229	0.039*
C14	-0.0871 (2)	0.1540 (2)	0.02785 (13)	0.0378 (6)
H14	-0.1151	0.1413	-0.0222	0.045*
C15	-0.1772 (2)	0.1891 (2)	0.07428 (13)	0.0375 (6)
H15	-0.2677	0.2017	0.0560	0.045*
C16	-0.1375 (2)	0.2062 (2)	0.14755 (13)	0.0333 (6)
H16	-0.2010	0.2297	0.1792	0.040*
C21	-0.1490 (2)	0.2648 (2)	0.32301 (12)	0.0325 (6)
C22	-0.1641 (3)	0.1378 (3)	0.34323 (14)	0.0440 (7)
H22	-0.0993	0.0756	0.3338	0.053*
C23	-0.2732 (3)	0.1008 (3)	0.37709 (16)	0.0583 (8)
H23	-0.2823	0.0136	0.3914	0.070*
C24	-0.3685 (3)	0.1902 (4)	0.39001 (15)	0.0589 (9)
H24	-0.4438	0.1644	0.4128	0.071*
C25	-0.3549 (3)	0.3163 (3)	0.37011 (14)	0.0514 (8)
H25	-0.4202	0.3781	0.3793	0.062*
C26	-0.2458 (2)	0.3532 (3)	0.33650 (13)	0.0405 (6)
H26	-0.2370	0.4406	0.3225	0.049*
C31	0.0561 (2)	0.5091 (2)	0.36335 (12)	0.0288 (5)

## supplementary materials

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C32	0.0050 (2)	0.6012 (2)	0.31318 (14)	0.0368 (6)
H32	-0.0229	0.5759	0.2647	0.044*
C34	0.0335 (2)	0.7668 (3)	0.40346 (15)	0.0429 (7)
H34	0.0259	0.8544	0.4171	0.052*
C35	0.0839 (2)	0.6766 (3)	0.45398 (14)	0.0403 (6)
H35	0.1106	0.7023	0.5025	0.048*
C36	0.0956 (2)	0.5495 (2)	0.43407 (13)	0.0339 (6)
H36	0.1312	0.4884	0.4691	0.041*
C33	-0.0058 (3)	0.7291 (2)	0.33302 (15)	0.0426 (7)
H33	-0.0402	0.7910	0.2981	0.051*

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0282 (10)	0.0312 (12)	0.0270 (10)	0.0036 (9)	0.0016 (8)	-0.0023 (9)
C1	0.0295 (12)	0.0277 (13)	0.0289 (12)	0.0019 (10)	0.0021 (10)	-0.0023 (11)
C2	0.0275 (12)	0.0320 (14)	0.0261 (12)	-0.0033 (11)	0.0044 (9)	0.0001 (11)
N2	0.0305 (11)	0.0336 (12)	0.0338 (11)	0.0007 (9)	-0.0008 (9)	-0.0005 (9)
C3	0.0278 (12)	0.0299 (14)	0.0354 (13)	-0.0002 (10)	-0.0006 (10)	0.0024 (11)
C4	0.0389 (14)	0.0384 (16)	0.0410 (15)	0.0018 (12)	-0.0073 (12)	-0.0018 (12)
C5	0.0398 (15)	0.0372 (16)	0.0492 (16)	0.0059 (12)	-0.0068 (12)	0.0047 (13)
C6	0.0391 (14)	0.0346 (15)	0.0436 (15)	0.0050 (12)	0.0079 (12)	0.0024 (12)
C7	0.0338 (13)	0.0328 (15)	0.0356 (13)	0.0022 (11)	0.0066 (11)	-0.0026 (11)
C8	0.0247 (12)	0.0319 (14)	0.0308 (12)	0.0004 (10)	0.0051 (10)	0.0036 (11)
C11	0.0306 (12)	0.0236 (13)	0.0281 (12)	-0.0026 (10)	0.0028 (10)	-0.0018 (10)
C12	0.0299 (12)	0.0309 (14)	0.0321 (13)	-0.0014 (11)	0.0017 (10)	-0.0013 (11)
C13	0.0397 (14)	0.0280 (14)	0.0306 (13)	0.0011 (11)	0.0069 (11)	-0.0031 (11)
C14	0.0478 (15)	0.0353 (15)	0.0289 (13)	0.0001 (12)	-0.0009 (11)	-0.0026 (11)
C15	0.0337 (14)	0.0410 (16)	0.0355 (14)	0.0014 (12)	-0.0058 (11)	-0.0034 (12)
C16	0.0288 (13)	0.0361 (15)	0.0353 (13)	0.0014 (11)	0.0054 (10)	-0.0035 (11)
C21	0.0271 (12)	0.0416 (16)	0.0282 (13)	-0.0030 (11)	0.0011 (10)	-0.0096 (11)
C22	0.0421 (15)	0.0428 (17)	0.0489 (16)	-0.0065 (13)	0.0137 (13)	-0.0051 (14)
C23	0.0592 (19)	0.058 (2)	0.0613 (19)	-0.0188 (16)	0.0202 (16)	-0.0030 (16)
C24	0.0383 (16)	0.089 (3)	0.0526 (18)	-0.0173 (17)	0.0193 (14)	-0.0163 (18)
C25	0.0333 (15)	0.076 (2)	0.0463 (17)	0.0024 (15)	0.0094 (12)	-0.0148 (16)
C26	0.0342 (14)	0.0492 (18)	0.0378 (14)	0.0043 (12)	0.0031 (11)	-0.0073 (13)
C31	0.0245 (12)	0.0293 (14)	0.0326 (13)	-0.0010 (10)	0.0033 (10)	-0.0023 (11)
C32	0.0372 (14)	0.0348 (15)	0.0374 (14)	-0.0026 (11)	-0.0008 (11)	-0.0002 (12)
C34	0.0413 (16)	0.0297 (15)	0.0584 (18)	-0.0026 (12)	0.0084 (13)	-0.0072 (13)
C35	0.0400 (14)	0.0418 (17)	0.0399 (15)	-0.0037 (12)	0.0080 (11)	-0.0116 (13)
C36	0.0315 (13)	0.0366 (15)	0.0338 (13)	0.0006 (11)	0.0043 (11)	-0.0009 (12)
C33	0.0441 (16)	0.0301 (15)	0.0523 (17)	0.0003 (12)	-0.0003 (13)	0.0049 (13)

### Geometric parameters ( $\text{\AA}$ , $^\circ$ )

N1—C8	1.394 (3)	C14—H14	0.9500
N1—C11	1.417 (3)	C15—C16	1.386 (3)
N1—C1	1.455 (3)	C15—H15	0.9500
C1—C2	1.527 (3)	C16—H16	0.9500

C1—C21	1.529 (3)	C21—C22	1.383 (3)
C1—H1	1.0000	C21—C26	1.385 (3)
C2—N2	1.282 (3)	C22—C23	1.385 (4)
C2—C31	1.480 (3)	C22—H22	0.9500
N2—C3	1.408 (3)	C23—C24	1.379 (4)
C3—C4	1.394 (3)	C23—H23	0.9500
C3—C8	1.404 (3)	C24—C25	1.370 (4)
C4—C5	1.376 (3)	C24—H24	0.9500
C4—H4	0.9500	C25—C26	1.383 (4)
C5—C6	1.382 (3)	C25—H25	0.9500
C5—H5	0.9500	C26—H26	0.9500
C6—C7	1.375 (3)	C31—C32	1.392 (3)
C6—H6	0.9500	C31—C36	1.393 (3)
C7—C8	1.395 (3)	C32—C33	1.385 (3)
C7—H7	0.9500	C32—H32	0.9500
C11—C16	1.387 (3)	C34—C33	1.380 (4)
C11—C12	1.394 (3)	C34—C35	1.381 (4)
C12—C13	1.376 (3)	C34—H34	0.9500
C12—H12	0.9500	C35—C36	1.379 (3)
C13—C14	1.383 (3)	C35—H35	0.9500
C13—H13	0.9500	C36—H36	0.9500
C14—C15	1.372 (3)	C33—H33	0.9500
C8—N1—C11	123.18 (19)	C14—C15—C16	120.8 (2)
C8—N1—C1	117.98 (18)	C14—C15—H15	119.6
C11—N1—C1	118.46 (18)	C16—C15—H15	119.6
N1—C1—C2	108.88 (18)	C15—C16—C11	120.1 (2)
N1—C1—C21	115.09 (19)	C15—C16—H16	119.9
C2—C1—C21	109.38 (18)	C11—C16—H16	119.9
N1—C1—H1	107.7	C22—C21—C26	118.7 (2)
C2—C1—H1	107.7	C22—C21—C1	122.1 (2)
C21—C1—H1	107.7	C26—C21—C1	119.2 (2)
N2—C2—C31	118.4 (2)	C21—C22—C23	120.4 (3)
N2—C2—C1	122.3 (2)	C21—C22—H22	119.8
C31—C2—C1	119.24 (19)	C23—C22—H22	119.8
C2—N2—C3	118.30 (19)	C24—C23—C22	120.1 (3)
C4—C3—C8	119.5 (2)	C24—C23—H23	119.9
C4—C3—N2	118.8 (2)	C22—C23—H23	119.9
C8—C3—N2	121.5 (2)	C25—C24—C23	120.1 (3)
C5—C4—C3	120.9 (2)	C25—C24—H24	119.9
C5—C4—H4	119.6	C23—C24—H24	119.9
C3—C4—H4	119.6	C24—C25—C26	119.7 (3)
C4—C5—C6	119.2 (2)	C24—C25—H25	120.1
C4—C5—H5	120.4	C26—C25—H25	120.1
C6—C5—H5	120.4	C25—C26—C21	121.0 (3)
C7—C6—C5	121.3 (2)	C25—C26—H26	119.5
C7—C6—H6	119.4	C21—C26—H26	119.5
C5—C6—H6	119.4	C32—C31—C36	118.0 (2)
C6—C7—C8	120.1 (2)	C32—C31—C2	122.5 (2)
C6—C7—H7	119.9	C36—C31—C2	119.5 (2)

## supplementary materials

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C8—C7—H7	119.9	C33—C32—C31	120.9 (2)
N1—C8—C7	123.5 (2)	C33—C32—H32	119.6
N1—C8—C3	117.5 (2)	C31—C32—H32	119.6
C7—C8—C3	119.0 (2)	C33—C34—C35	119.8 (2)
C16—C11—C12	119.0 (2)	C33—C34—H34	120.1
C16—C11—N1	120.7 (2)	C35—C34—H34	120.1
C12—C11—N1	120.3 (2)	C36—C35—C34	120.1 (2)
C13—C12—C11	120.1 (2)	C36—C35—H35	119.9
C13—C12—H12	120.0	C34—C35—H35	119.9
C11—C12—H12	120.0	C35—C36—C31	121.1 (2)
C12—C13—C14	120.8 (2)	C35—C36—H36	119.5
C12—C13—H13	119.6	C31—C36—H36	119.5
C14—C13—H13	119.6	C34—C33—C32	120.0 (2)
C15—C14—C13	119.2 (2)	C34—C33—H33	120.0
C15—C14—H14	120.4	C32—C33—H33	120.0
C13—C14—H14	120.4		
C8—N1—C1—C2	40.5 (3)	N1—C11—C12—C13	-178.0 (2)
C11—N1—C1—C2	-146.37 (19)	C11—C12—C13—C14	-0.2 (4)
C8—N1—C1—C21	-82.7 (2)	C12—C13—C14—C15	0.6 (4)
C11—N1—C1—C21	90.5 (2)	C13—C14—C15—C16	-0.8 (4)
N1—C1—C2—N2	-33.5 (3)	C14—C15—C16—C11	0.6 (4)
C21—C1—C2—N2	93.0 (3)	C12—C11—C16—C15	-0.2 (4)
N1—C1—C2—C31	149.66 (19)	N1—C11—C16—C15	177.9 (2)
C21—C1—C2—C31	-83.8 (2)	N1—C1—C21—C22	24.1 (3)
C31—C2—N2—C3	-176.7 (2)	C2—C1—C21—C22	-98.8 (3)
C1—C2—N2—C3	6.5 (3)	N1—C1—C21—C26	-156.4 (2)
C2—N2—C3—C4	-168.5 (2)	C2—C1—C21—C26	80.7 (3)
C2—N2—C3—C8	16.2 (3)	C26—C21—C22—C23	-0.8 (4)
C8—C3—C4—C5	1.4 (4)	C1—C21—C22—C23	178.7 (2)
N2—C3—C4—C5	-174.0 (2)	C21—C22—C23—C24	0.9 (4)
C3—C4—C5—C6	0.1 (4)	C22—C23—C24—C25	-0.7 (4)
C4—C5—C6—C7	-1.3 (4)	C23—C24—C25—C26	0.5 (4)
C5—C6—C7—C8	0.9 (4)	C24—C25—C26—C21	-0.5 (4)
C11—N1—C8—C7	-16.9 (3)	C22—C21—C26—C25	0.6 (4)
C1—N1—C8—C7	155.9 (2)	C1—C21—C26—C25	-178.9 (2)
C11—N1—C8—C3	164.7 (2)	N2—C2—C31—C32	148.6 (2)
C1—N1—C8—C3	-22.5 (3)	C1—C2—C31—C32	-34.5 (3)
C6—C7—C8—N1	-177.7 (2)	N2—C2—C31—C36	-30.0 (3)
C6—C7—C8—C3	0.7 (3)	C1—C2—C31—C36	146.9 (2)
C4—C3—C8—N1	176.6 (2)	C36—C31—C32—C33	0.2 (3)
N2—C3—C8—N1	-8.1 (3)	C2—C31—C32—C33	-178.4 (2)
C4—C3—C8—C7	-1.8 (3)	C33—C34—C35—C36	0.3 (4)
N2—C3—C8—C7	173.5 (2)	C34—C35—C36—C31	-0.6 (4)
C8—N1—C11—C16	139.9 (2)	C32—C31—C36—C35	0.3 (3)
C1—N1—C11—C16	-32.9 (3)	C2—C31—C36—C35	179.0 (2)
C8—N1—C11—C12	-42.1 (3)	C35—C34—C33—C32	0.2 (4)
C1—N1—C11—C12	145.1 (2)	C31—C32—C33—C34	-0.5 (4)
C16—C11—C12—C13	0.0 (3)		

Fig. 1

