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# 2,4-Bis(4-chlorophenyl)-3-azabicyclo-[3.3.1]nonan-9-one

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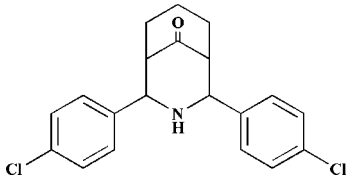
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.046; $wR$ factor = 0.135; data-to-parameter ratio = 22.6.

In the molecular structure of the title compound, $C_{20}H_{19}Cl_2NO$, the molecule exists in a twin-chair conformation with equatorial dispositions of the 4-chlorophenyl groups on both sides of the secondary amino group; the dihedral angle between the aromatic ring planes is 31.33 (3)°. The crystal structure is stabilized by N—H···O interactions, leading to chains of molecules.

## Related literature

For the biological activity of diterpenoid/norditerpenoid alkaloids, see: Hardick *et al.* (1996); Jeyaraman *et al.* (1981). For similiar structures, see: Parthiban *et al.* (2008*a*,*b*,*c*,*d*,*e*). For puckering parameters, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_{20}H_{19}Cl_2NO$
$M_r$ = 360.26
Monoclinic, $P2_1/n$
$a$ = 16.2589 (4) Å
$b$ = 6.8983 (2) Å
$c$ = 18.1291 (5) Å
$\beta$ = 116.149 (1)°
$V$ = 1825.23 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.36 mm$^{-1}$
$T$ = 298 K
0.42 × 0.38 × 0.25 mm

### Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1999)
$T_{min}$ = 0.863, $T_{max}$ = 0.915
15050 measured reflections
4997 independent reflections
3241 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.021

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.135
$S$ = 1.02
4997 reflections
221 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.42 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O1$^{i}$ | 0.85 (2) | 2.31 (2) | 3.1202 (18) | 160.2 (18) |

Symmetry code: (i) $x, y+1, z$.

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT-Plus* (Bruker, 2004); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); 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: BQ2124).

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# supplementary materials

*Acta Cryst.* (2009). E**65**, o609 [ **doi:10.1107/S160053680900590X** ]

# 2,4-Bis(4-chlorophenyl)-3-azabicyclo[3.3.1]nonan-9-one

**P. Parthiban, V. Ramkumar, M. S. Kim, S. Kabilan and Y. T. Jeong**

## Comment

The widespread diterpenoid/norditerpenoid alkaloids posses the 3-azabicyclo [3.3.1]nonane pharmacophore, and as a consequence, the above alkaloids having broad spectrum of biological activities (Jeyaraman *et al.*, 1981; Hardick *et al.*, 1996). Hence, the synthesis and stereochemistry of 3-azabicyclononan-9-ones are more important in recent days (Parthiban *et al.*, 2008a,b,c,d,e). A study of torsion angles, asymmetry parameters and least-squares plane calculation shows that the piperidine ring adopts near ideal chair conformation with the deviation of ring atoms N1 and C8 from the C1/C2/C6/C7 plane by -0.642 (3)Å and 0.712 (3)Å, respectively, $Q_T$=0.607 (2)Å, q(2)=0.044 (2)Å and q(3)=-0.606 (2)Å, θ=175.8 (2)°. whereas the cyclohexane ring deviate from the ideal chair conformation; the cyclohexane atoms C4 and C8 deviate from the C2/C3/C5/C6 plane by -0.557 (2)Å and 0.710 (3)Å, respectively, $Q_T$=0.560 (2) Å, q(2)=0.117 (2)Å and, q(3)=-0.548 (2)Å, θ=167.9 (2)°. (Cremer & Pople, 1975). Hence, the title compound $C_{20}H_{19}Cl_2NO$, exists in double chair conformation with equatorial dispositions of the *para* chlorophenyl groups with the torsion angles of C8—C2—C1—C9 and C8—C6—C7—C15 are 177.88 (4)° and -179.01 (4)°, respectively. The aryl groups are oriented at an angle of 31.33 (3)° to each other.

## Experimental

In a warm solution of ammonium acetate (0.075 mol) in 50 ml of absolute ethanol, a mixture of cyclohexanone (0.05 mol) and *para* chlorobenzaldehyde (0.1 mol) was added and gently warmed with stirring on a hot plate till the yellow color was formed during the mixing of the reactants and cooled to room temperature. Then 50 ml of ether was added and allowed to stir over night at room temperature. Thus the obtained crude azabicyclic ketone was separated by filtration and washed with 1:5 ethanol-ether mixture till the solid became colorless. Recrystallization of the compound from ethanol gave X-ray diffraction quality crystals of 2,4-bis(4-chlorophenyl)-3-azabicyclo[3.3.1]nonan-9-one.

## Refinement

Nitrogen H atoms were located in a difference Fourier map and refined isotropically. Other hydrogen atoms were fixed geometrically and allowed to ride on the parent carbon atoms, with aromatic C—H =0.93Å, aliphatic C—H =0.98Å and methylene C—H=0.97Å. The displacement parameters were set for phenyl, methylene and aliphatic H atoms at $U_{iso}$(H)=1.2$U_{eq}$(C).

## Figures

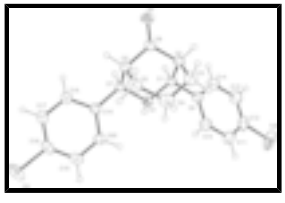


Fig. 1. *ORTEP* of the molecule with atoms represented as 30% probability ellipsoids.

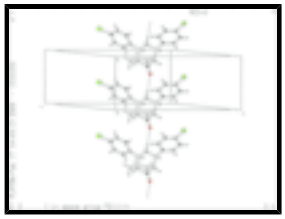


Fig. 2. Packing of molecules via N-H..O bond.

**2,4-Bis(4-chlorophenyl)-3-azabicyclo[3.3.1]nonan-9-one**

*Crystal data*

| | |
|---|---|
| $C_{20}H_{19}Cl_2NO$ | $F_{000}$ = 752 |
| $M_r$ = 360.26 | $D_x$ = 1.311 Mg m$^{-3}$ |
| Monoclinic, $P2_1/n$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -P 2yn | Cell parameters from 4308 reflections |
| $a$ = 16.2589 (4) Å | θ = 2.8–26.3º |
| $b$ = 6.8983 (2) Å | μ = 0.36 mm$^{-1}$ |
| $c$ = 18.1291 (5) Å | $T$ = 298 K |
| β = 116.149 (1)º | Rectangular, colourless |
| $V$ = 1825.23 (9) Å$^3$ | 0.42 × 0.38 × 0.25 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Bruker APEXII CCD area-detector diffractometer | 4997 independent reflections |
| Radiation source: fine-focus sealed tube | 3241 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.021 |
| $T$ = 298 K | $\theta_{max}$ = 29.8º |
| φ and ω scans | $\theta_{min}$ = 2.3º |
| Absorption correction: multi-scan (SADABS; Bruker, 1999) | $h$ = −21→20 |
| $T_{min}$ = 0.863, $T_{max}$ = 0.915 | $k$ = −9→9 |
| 15050 measured reflections | $l$ = −15→25 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.046 | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2)$ = 0.135 | $w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.4485P]$<br>where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.02 | $(\Delta/\sigma)_{max} < 0.001$ |
| 4997 reflections | $\Delta\rho_{max}$ = 0.38 e Å$^{-3}$ |

| | |
|---|---|
| 221 parameters | $\Delta\rho_{min} = -0.42$ 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 $F^2 > \sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.33305 (11) | 0.1260 (2) | 0.01759 (10) | 0.0384 (3) |
| H1 | 0.3907 | 0.1019 | 0.0665 | 0.046* |
| C2 | 0.29289 (11) | −0.0738 (2) | −0.02171 (10) | 0.0410 (4) |
| H2 | 0.3380 | −0.1414 | −0.0345 | 0.049* |
| C3 | 0.20110 (12) | −0.0678 (3) | −0.09929 (11) | 0.0533 (4) |
| H3A | 0.2079 | 0.0135 | −0.1399 | 0.064* |
| H3B | 0.1864 | −0.1977 | −0.1219 | 0.064* |
| C4 | 0.12129 (12) | 0.0082 (3) | −0.08496 (12) | 0.0581 (5) |
| H4A | 0.1268 | 0.1478 | −0.0779 | 0.070* |
| H4B | 0.0643 | −0.0190 | −0.1330 | 0.070* |
| C5 | 0.11811 (12) | −0.0827 (3) | −0.00979 (12) | 0.0534 (5) |
| H5A | 0.0944 | −0.2136 | −0.0235 | 0.064* |
| H5B | 0.0756 | −0.0096 | 0.0037 | 0.064* |
| C6 | 0.21147 (11) | −0.0905 (2) | 0.06658 (11) | 0.0418 (4) |
| H6 | 0.2052 | −0.1688 | 0.1090 | 0.050* |
| C7 | 0.25223 (11) | 0.1109 (2) | 0.10384 (10) | 0.0375 (3) |
| H7 | 0.3106 | 0.0893 | 0.1524 | 0.045* |
| C8 | 0.27891 (11) | −0.1870 (2) | 0.04285 (10) | 0.0390 (4) |
| C9 | 0.35398 (11) | 0.2533 (2) | −0.03978 (10) | 0.0414 (4) |
| C10 | 0.29057 (13) | 0.3777 (3) | −0.09592 (12) | 0.0544 (5) |
| H10 | 0.2316 | 0.3836 | −0.1000 | 0.065* |

| | | | | |
|---|---|---|---|---|
| C11 | 0.31400 (15) | 0.4943 (3) | −0.14645 (12) | 0.0615 (5) |
| H11 | 0.2710 | 0.5776 | −0.1841 | 0.074* |
| C12 | 0.40091 (16) | 0.4852 (3) | −0.14022 (12) | 0.0584 (5) |
| C13 | 0.46439 (15) | 0.3618 (3) | −0.08633 (14) | 0.0654 (6) |
| H13 | 0.5228 | 0.3545 | −0.0835 | 0.078* |
| C14 | 0.44093 (13) | 0.2474 (3) | −0.03588 (13) | 0.0555 (5) |
| H14 | 0.4845 | 0.1646 | 0.0015 | 0.067* |
| C15 | 0.18866 (11) | 0.2164 (2) | 0.13081 (10) | 0.0385 (3) |
| C16 | 0.17785 (12) | 0.1464 (3) | 0.19803 (11) | 0.0473 (4) |
| H16 | 0.2125 | 0.0407 | 0.2271 | 0.057* |
| C17 | 0.11692 (13) | 0.2301 (3) | 0.22247 (11) | 0.0528 (4) |
| H17 | 0.1097 | 0.1804 | 0.2670 | 0.063* |
| C18 | 0.06701 (12) | 0.3877 (3) | 0.18023 (12) | 0.0509 (4) |
| C19 | 0.07748 (13) | 0.4646 (3) | 0.11480 (12) | 0.0540 (5) |
| H19 | 0.0446 | 0.5740 | 0.0877 | 0.065* |
| C20 | 0.13769 (12) | 0.3765 (2) | 0.08997 (11) | 0.0471 (4) |
| H20 | 0.1440 | 0.4259 | 0.0450 | 0.057* |
| Cl1 | −0.01108 (4) | 0.49239 (10) | 0.21027 (4) | 0.0838 (2) |
| Cl2 | 0.43337 (5) | 0.64178 (11) | −0.19813 (4) | 0.0956 (3) |
| N1 | 0.27045 (9) | 0.2229 (2) | 0.04419 (9) | 0.0401 (3) |
| O1 | 0.31840 (9) | −0.33704 (16) | 0.07301 (8) | 0.0515 (3) |
| H1A | 0.2917 (13) | 0.334 (3) | 0.0645 (12) | 0.058 (6)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0379 (8) | 0.0331 (8) | 0.0479 (9) | −0.0024 (6) | 0.0223 (7) | 0.0015 (7) |
| C2 | 0.0440 (9) | 0.0329 (8) | 0.0532 (9) | −0.0007 (7) | 0.0278 (8) | −0.0020 (7) |
| C3 | 0.0591 (11) | 0.0489 (10) | 0.0498 (10) | −0.0103 (9) | 0.0221 (9) | −0.0051 (8) |
| C4 | 0.0413 (10) | 0.0552 (12) | 0.0634 (12) | −0.0046 (8) | 0.0100 (9) | −0.0021 (10) |
| C5 | 0.0407 (9) | 0.0473 (10) | 0.0750 (13) | −0.0100 (8) | 0.0279 (9) | −0.0112 (9) |
| C6 | 0.0462 (9) | 0.0304 (8) | 0.0578 (10) | −0.0030 (7) | 0.0312 (8) | 0.0018 (7) |
| C7 | 0.0387 (8) | 0.0317 (7) | 0.0458 (9) | 0.0003 (6) | 0.0218 (7) | 0.0016 (7) |
| C8 | 0.0401 (8) | 0.0273 (7) | 0.0514 (9) | −0.0059 (6) | 0.0219 (7) | −0.0053 (7) |
| C9 | 0.0470 (9) | 0.0327 (8) | 0.0530 (9) | −0.0049 (7) | 0.0298 (8) | −0.0023 (7) |
| C10 | 0.0526 (11) | 0.0557 (11) | 0.0635 (11) | 0.0042 (9) | 0.0334 (9) | 0.0110 (9) |
| C11 | 0.0770 (14) | 0.0560 (12) | 0.0556 (11) | 0.0002 (10) | 0.0331 (11) | 0.0112 (9) |
| C12 | 0.0821 (14) | 0.0544 (11) | 0.0527 (10) | −0.0244 (10) | 0.0424 (10) | −0.0081 (9) |
| C13 | 0.0637 (13) | 0.0668 (13) | 0.0862 (15) | −0.0121 (11) | 0.0517 (12) | 0.0008 (12) |
| C14 | 0.0514 (11) | 0.0483 (10) | 0.0781 (13) | −0.0017 (8) | 0.0387 (10) | 0.0053 (9) |
| C15 | 0.0397 (8) | 0.0334 (8) | 0.0445 (8) | −0.0023 (6) | 0.0205 (7) | −0.0035 (7) |
| C16 | 0.0531 (10) | 0.0452 (10) | 0.0471 (9) | 0.0052 (8) | 0.0254 (8) | 0.0035 (8) |
| C17 | 0.0584 (11) | 0.0601 (12) | 0.0475 (10) | −0.0022 (9) | 0.0305 (9) | −0.0062 (9) |
| C18 | 0.0442 (10) | 0.0534 (11) | 0.0576 (11) | −0.0012 (8) | 0.0249 (9) | −0.0186 (9) |
| C19 | 0.0515 (11) | 0.0435 (10) | 0.0654 (12) | 0.0096 (8) | 0.0243 (9) | −0.0027 (9) |
| C20 | 0.0534 (10) | 0.0394 (9) | 0.0528 (10) | 0.0025 (8) | 0.0274 (8) | 0.0022 (8) |
| Cl1 | 0.0721 (4) | 0.0962 (5) | 0.0986 (5) | 0.0135 (3) | 0.0519 (3) | −0.0262 (4) |
| Cl2 | 0.1246 (6) | 0.1079 (5) | 0.0667 (4) | −0.0502 (4) | 0.0535 (4) | 0.0061 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N1 | 0.0490 (8) | 0.0274 (6) | 0.0524 (8) | −0.0046 (6) | 0.0302 (7) | −0.0020 (6) |
| O1 | 0.0613 (8) | 0.0313 (6) | 0.0686 (8) | 0.0042 (5) | 0.0347 (7) | 0.0037 (6) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| C1—N1 | 1.466 (2) | C9—C10 | 1.382 (3) |
| C1—C9 | 1.511 (2) | C9—C14 | 1.385 (2) |
| C1—C2 | 1.557 (2) | C10—C11 | 1.393 (3) |
| C1—H1 | 0.9800 | C10—H10 | 0.9300 |
| C2—C8 | 1.505 (2) | C11—C12 | 1.368 (3) |
| C2—C3 | 1.535 (2) | C11—H11 | 0.9300 |
| C2—H2 | 0.9800 | C12—C13 | 1.363 (3) |
| C3—C4 | 1.524 (3) | C12—Cl2 | 1.7422 (18) |
| C3—H3A | 0.9700 | C13—C14 | 1.383 (3) |
| C3—H3B | 0.9700 | C13—H13 | 0.9300 |
| C4—C5 | 1.522 (3) | C14—H14 | 0.9300 |
| C4—H4A | 0.9700 | C15—C20 | 1.383 (2) |
| C4—H4B | 0.9700 | C15—C16 | 1.392 (2) |
| C5—C6 | 1.540 (3) | C16—C17 | 1.378 (2) |
| C5—H5A | 0.9700 | C16—H16 | 0.9300 |
| C5—H5B | 0.9700 | C17—C18 | 1.371 (3) |
| C6—C8 | 1.499 (2) | C17—H17 | 0.9300 |
| C6—C7 | 1.559 (2) | C18—C19 | 1.377 (3) |
| C6—H6 | 0.9800 | C18—Cl1 | 1.7433 (17) |
| C7—N1 | 1.462 (2) | C19—C20 | 1.385 (2) |
| C7—C15 | 1.511 (2) | C19—H19 | 0.9300 |
| C7—H7 | 0.9800 | C20—H20 | 0.9300 |
| C8—O1 | 1.2137 (19) | N1—H1A | 0.85 (2) |
| N1—C1—C9 | 111.16 (13) | O1—C8—C6 | 123.91 (15) |
| N1—C1—C2 | 110.05 (12) | O1—C8—C2 | 124.16 (15) |
| C9—C1—C2 | 112.08 (13) | C6—C8—C2 | 111.92 (13) |
| N1—C1—H1 | 107.8 | C10—C9—C14 | 118.01 (16) |
| C9—C1—H1 | 107.8 | C10—C9—C1 | 123.14 (15) |
| C2—C1—H1 | 107.8 | C14—C9—C1 | 118.85 (16) |
| C8—C2—C3 | 107.89 (13) | C9—C10—C11 | 120.76 (18) |
| C8—C2—C1 | 106.25 (13) | C9—C10—H10 | 119.6 |
| C3—C2—C1 | 115.97 (14) | C11—C10—H10 | 119.6 |
| C8—C2—H2 | 108.8 | C12—C11—C10 | 119.42 (19) |
| C3—C2—H2 | 108.8 | C12—C11—H11 | 120.3 |
| C1—C2—H2 | 108.8 | C10—C11—H11 | 120.3 |
| C4—C3—C2 | 114.21 (15) | C13—C12—C11 | 121.07 (17) |
| C4—C3—H3A | 108.7 | C13—C12—Cl2 | 118.99 (16) |
| C2—C3—H3A | 108.7 | C11—C12—Cl2 | 119.86 (18) |
| C4—C3—H3B | 108.7 | C12—C13—C14 | 119.24 (19) |
| C2—C3—H3B | 108.7 | C12—C13—H13 | 120.4 |
| H3A—C3—H3B | 107.6 | C14—C13—H13 | 120.4 |
| C5—C4—C3 | 112.21 (16) | C13—C14—C9 | 121.49 (19) |
| C5—C4—H4A | 109.2 | C13—C14—H14 | 119.3 |
| C3—C4—H4A | 109.2 | C9—C14—H14 | 119.3 |

| | | | |
|---|---|---|---|
| C5—C4—H4B | 109.2 | C20—C15—C16 | 117.94 (15) |
| C3—C4—H4B | 109.2 | C20—C15—C7 | 123.06 (14) |
| H4A—C4—H4B | 107.9 | C16—C15—C7 | 118.96 (14) |
| C4—C5—C6 | 114.24 (14) | C17—C16—C15 | 121.48 (17) |
| C4—C5—H5A | 108.7 | C17—C16—H16 | 119.3 |
| C6—C5—H5A | 108.7 | C15—C16—H16 | 119.3 |
| C4—C5—H5B | 108.7 | C18—C17—C16 | 119.03 (17) |
| C6—C5—H5B | 108.7 | C18—C17—H17 | 120.5 |
| H5A—C5—H5B | 107.6 | C16—C17—H17 | 120.5 |
| C8—C6—C5 | 108.27 (14) | C17—C18—C19 | 121.29 (16) |
| C8—C6—C7 | 107.15 (12) | C17—C18—Cl1 | 119.16 (15) |
| C5—C6—C7 | 114.88 (14) | C19—C18—Cl1 | 119.55 (15) |
| C8—C6—H6 | 108.8 | C18—C19—C20 | 118.97 (17) |
| C5—C6—H6 | 108.8 | C18—C19—H19 | 120.5 |
| C7—C6—H6 | 108.8 | C20—C19—H19 | 120.5 |
| N1—C7—C15 | 112.03 (12) | C15—C20—C19 | 121.25 (17) |
| N1—C7—C6 | 109.68 (13) | C15—C20—H20 | 119.4 |
| C15—C7—C6 | 110.42 (12) | C19—C20—H20 | 119.4 |
| N1—C7—H7 | 108.2 | C7—N1—C1 | 113.48 (12) |
| C15—C7—H7 | 108.2 | C7—N1—H1A | 109.2 (14) |
| C6—C7—H7 | 108.2 | C1—N1—H1A | 110.1 (13) |
| N1—C1—C2—C8 | −57.87 (16) | C1—C9—C10—C11 | 178.93 (17) |
| C9—C1—C2—C8 | 177.89 (13) | C9—C10—C11—C12 | 0.0 (3) |
| N1—C1—C2—C3 | 61.99 (18) | C10—C11—C12—C13 | 1.1 (3) |
| C9—C1—C2—C3 | −62.25 (18) | C10—C11—C12—Cl2 | −175.72 (16) |
| C8—C2—C3—C4 | 53.9 (2) | C11—C12—C13—C14 | −1.5 (3) |
| C1—C2—C3—C4 | −65.1 (2) | Cl2—C12—C13—C14 | 175.27 (16) |
| C2—C3—C4—C5 | −46.3 (2) | C12—C13—C14—C9 | 1.0 (3) |
| C3—C4—C5—C6 | 45.7 (2) | C10—C9—C14—C13 | 0.0 (3) |
| C4—C5—C6—C8 | −53.0 (2) | C1—C9—C14—C13 | −179.45 (18) |
| C4—C5—C6—C7 | 66.6 (2) | N1—C7—C15—C20 | 14.1 (2) |
| C8—C6—C7—N1 | 57.05 (17) | C6—C7—C15—C20 | −108.49 (17) |
| C5—C6—C7—N1 | −63.26 (17) | N1—C7—C15—C16 | −168.34 (15) |
| C8—C6—C7—C15 | −179.02 (13) | C6—C7—C15—C16 | 69.09 (19) |
| C5—C6—C7—C15 | 60.67 (18) | C20—C15—C16—C17 | 1.5 (3) |
| C5—C6—C8—O1 | −118.50 (18) | C7—C15—C16—C17 | −176.24 (16) |
| C7—C6—C8—O1 | 117.07 (17) | C15—C16—C17—C18 | −1.0 (3) |
| C5—C6—C8—C2 | 62.45 (17) | C16—C17—C18—C19 | −0.8 (3) |
| C7—C6—C8—C2 | −61.98 (17) | C16—C17—C18—Cl1 | 179.30 (14) |
| C3—C2—C8—O1 | 118.08 (18) | C17—C18—C19—C20 | 2.0 (3) |
| C1—C2—C8—O1 | −116.94 (17) | Cl1—C18—C19—C20 | −178.05 (14) |
| C3—C2—C8—C6 | −62.87 (17) | C16—C15—C20—C19 | −0.2 (3) |
| C1—C2—C8—C6 | 62.11 (17) | C7—C15—C20—C19 | 177.44 (16) |
| N1—C1—C9—C10 | −35.0 (2) | C18—C19—C20—C15 | −1.5 (3) |
| C2—C1—C9—C10 | 88.57 (19) | C15—C7—N1—C1 | 179.14 (13) |
| N1—C1—C9—C14 | 144.36 (16) | C6—C7—N1—C1 | −57.87 (17) |
| C2—C1—C9—C14 | −92.02 (19) | C9—C1—N1—C7 | −176.47 (13) |
| C14—C9—C10—C11 | −0.5 (3) | C2—C1—N1—C7 | 58.76 (17) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1A···O1$^{i}$ | 0.85 (2) | 2.31 (2) | 3.1202 (18) | 160.2 (18) |

Symmetry codes: (i) *x*, *y*+1, *z*.

**Fig. 1**

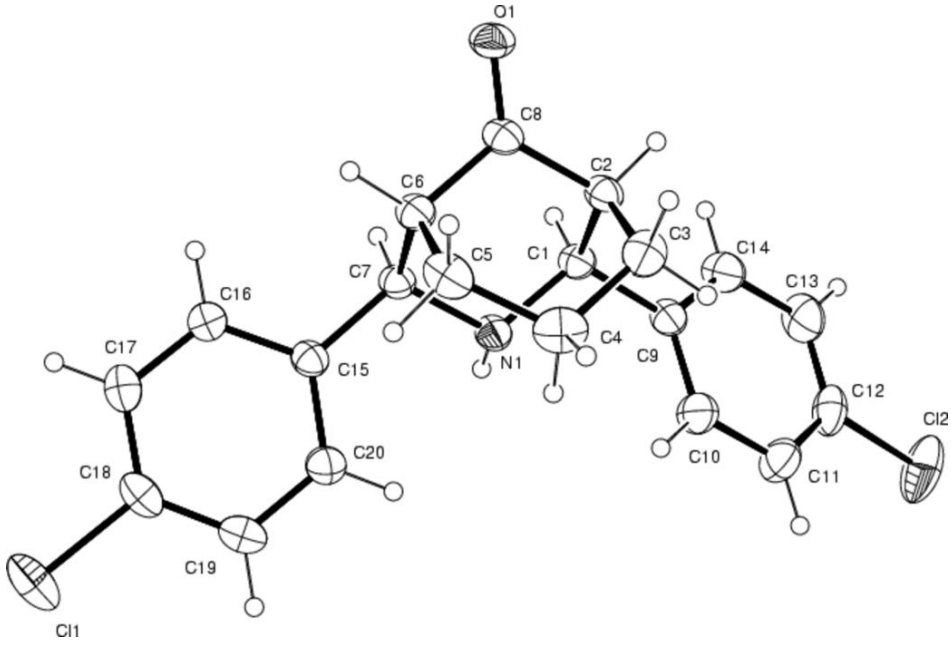
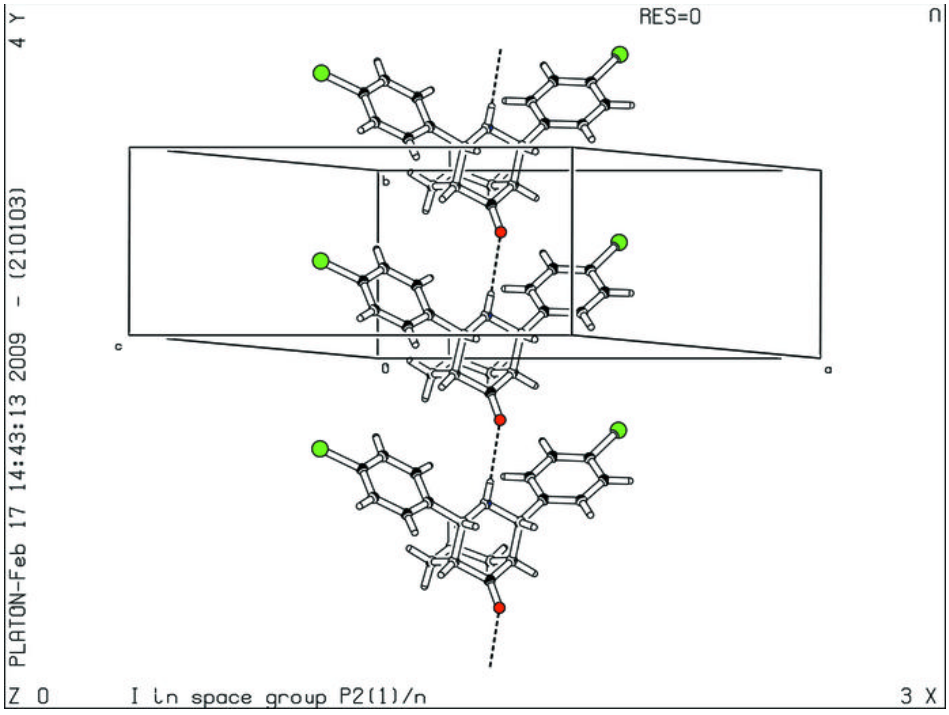

O1
C8
C2
C6
C3
C14
C5
C1
C7
C13
C16
C4
C17
C15
N1
C9
C12
Cl2
C20
C10
C18
C11
C19
Cl1

**Fig. 2**


RES=0
PLATON-Feb 17 14:43:13 2009 - (210103)
4 Y
Z 0
I In space group P2(1)/n
3 X