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# Melitracenium chloride

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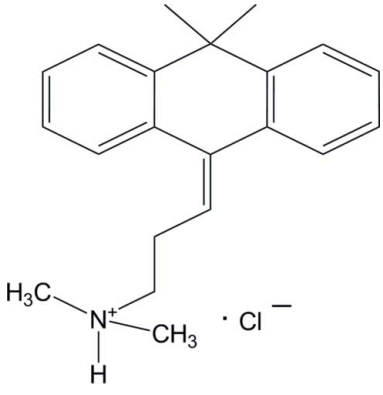
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.063; $wR$ factor = 0.212; data-to-parameter ratio = 24.8.

In the title compound [systematic name: 3-(10,10-dimethylanthracen-9-ylidene)-*N*,*N*,*N*-trimethylpropanaminium chloride], $C_{21}H_{26}N^+\cdot Cl^-$, the cyclohexane ring adopts a chair conformation. The dihedral angle between the terminal benzene rings is 40.43 (12)°. In the crystal, ions are linked through intermolecular N—H···Cl and C—H···Cl hydrogen bonds, forming supramolecular layers parallel to the *bc* plane.

## Related literature

For the pharmaceutical properties of the title compound, see: Van Moffaert *et al.* (1983). For ring conformations, see: Cremer & Pople (1975).




## Experimental

### Crystal data

$C_{21}H_{26}N^+\cdot Cl^-$
$M_r$ = 327.88
Monoclinic, $P2_1/c$
$a$ = 15.0129 (18) Å
$b$ = 8.8092 (11) Å
$c$ = 14.0135 (17) Å
$\beta$ = 91.506 (2)°
$V$ = 1852.7 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 296 K
0.43 × 0.32 × 0.16 mm

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.917, $T_{max}$ = 0.967
19785 measured reflections
5366 independent reflections
3587 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.039

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.063
$wR(F^2)$ = 0.212
$S$ = 1.05
5366 reflections
216 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.30 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*1···Cl1 | 0.98 (3) | 2.03 (3) | 3.0024 (19) | 176 (3) |
| C17—H17*A*···Cl1$^{i}$ | 0.97 | 2.81 | 3.710 (2) | 155 |
| C17—H17*B*···Cl1$^{ii}$ | 0.97 | 2.77 | 3.717 (3) | 164 |
| C18—H18*B*···Cl1$^{iii}$ | 0.96 | 2.68 | 3.625 (3) | 169 |

Symmetry codes: (i) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (ii) $-x, y+\frac{1}{2}, -z+\frac{1}{2}$; (iii) $-x, y-\frac{1}{2}, -z+\frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2608).

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‡ Thomson Reuters ResearcherID: A-3561-2009.

# supplementary materials

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# Melitracenium chloride

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## Comment

Melitracen (systematic IUPAC name: 3-(10,10-dimethylanthracen-9(10*H*)-ylidene)-N,N-dimethylpropan-1-amine) is a tricyclic antidepressant (TCA) for the treatment of depression and anxiety. Its hydrochloride derivative has actions and effects similar to amitriptyline and is administered orally in the treatment of depression. Melitracen, a bipolar thymoleptic with activating properties in low dose, is usually coadministered with flupentixol in order to decrease the side effects. This combination has none serious side effects due to low drug dosage (Van Moffaert *et al.*, 1983). In view of the importance of the title compound, herein we report its crystal structure.

The asymmetric unit of the title compound (Fig 1) contains a melitracenium cation and a chloride anion. The central cyclohexane ring (C1/C6–C8/C13–C14) adopts a chair conformation with puckering parameters Q = 0.521 (2) Å, θ = 92.7 (2)° and φ = 298.8 (3)° (Cremer & Pople, 1975). The dihedral angle between the terminal benzene (C8–C13, C1–C6) rings is 40.43 (12)°. In the crystal structure (Fig. 2), the ions are linked through intermolecular N1—H1N1···Cl1, C17—H17A···Cl1, C17—H17B···Cl1 and C18—H18B···Cl1 (Table 1) hydrogen bonds, forming two-dimensional supramolecular layers parallel to the *bc* plane.

## Experimental

The title compound was obtained as a gift sample from R. L. Fine Chem. Ltd., Bangalore, India. The compound was recrystallized from methanol (m. p.: 512–514 K).

## Refinement

Atom H1N1 was located from a difference Fourier maps and refined freely [N–H = 0.97 (3) Å]. The remaining H atoms were positioned geometrically [C–H = 0.93–0.97 Å] and were refined using a riding model, with $U_{iso}$(H) = 1.2 $U_{eq}$(C). A rotating group model was applied to the methyl groups.

## Figures

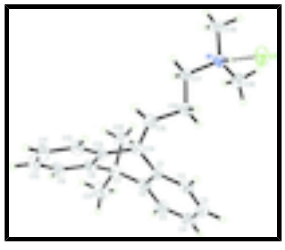

Fig. 1. The asymmetric unit of the title compound, showing 50% probability displacement ellipsoids. The intramolecular N—H···Cl hydrogen bond is shown as a dashed line.

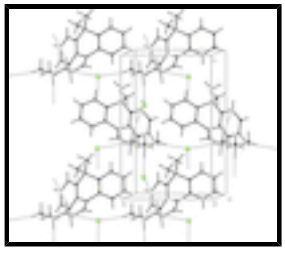

Fig. 2. The crystal packing of the title compound. Hydrogen bonds are shown as dashed lines.

### 3-(10,10-dimethylanthracen-9-ylidene)-*N*,*N*,*N*- trimethylpropanaminium chloride

*Crystal data*

| | |
|---|---|
| $C_{21}H_{26}N^+ \cdot Cl^-$ | $F(000) = 704$ |
| $M_r = 327.88$ | $D_x = 1.176$ Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: -P 2ybc | Cell parameters from 4582 reflections |
| $a = 15.0129$ (18) Å | $\theta = 2.7$–$29.4°$ |
| $b = 8.8092$ (11) Å | $\mu = 0.21$ mm$^{-1}$ |
| $c = 14.0135$ (17) Å | $T = 296$ K |
| $\beta = 91.506$ (2)° | Block, colourless |
| $V = 1852.7$ (4) Å$^3$ | 0.43 × 0.32 × 0.16 mm |
| $Z = 4$ | |

*Data collection*

| | |
|---|---|
| Bruker APEXII DUO CCD area-detector diffractometer | 5366 independent reflections |
| Radiation source: fine-focus sealed tube | 3587 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.039$ |
| φ and ω scans | $\theta_{max} = 30.0°$, $\theta_{min} = 2.7°$ |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2009) | $h = -20 \rightarrow 21$ |
| $T_{min} = 0.917$, $T_{max} = 0.967$ | $k = -12 \rightarrow 12$ |
| 19785 measured reflections | $l = -19 \rightarrow 19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.063$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.212$ | H atoms treated by a mixture of independent and constrained refinement |
| $S = 1.05$ | $w = 1/[\sigma^2(F_o^2) + (0.0919P)^2 + 0.9294P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 5366 reflections | $(\Delta/\sigma)_{max} < 0.001$ |

| | |
|---|---|
| 216 parameters | $\Delta\rho_{max} = 0.43$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.30$ e Å$^{-3}$ |

*Special details*

**Geometry**. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.03811 (5) | 0.75554 (7) | 0.14829 (4) | 0.0618 (2) |
| N1 | 0.03401 (12) | 0.7409 (2) | 0.36218 (13) | 0.0440 (4) |
| C1 | 0.34015 (14) | 0.9607 (2) | 0.49383 (15) | 0.0431 (5) |
| C2 | 0.37422 (16) | 0.8711 (3) | 0.42136 (19) | 0.0564 (6) |
| H2A | 0.3513 | 0.8806 | 0.3593 | 0.068* |
| C3 | 0.44190 (18) | 0.7681 (3) | 0.4410 (3) | 0.0686 (8) |
| H3A | 0.4640 | 0.7085 | 0.3922 | 0.082* |
| C4 | 0.4763 (2) | 0.7535 (3) | 0.5316 (3) | 0.0738 (9) |
| H4A | 0.5213 | 0.6832 | 0.5446 | 0.089* |
| C5 | 0.44455 (18) | 0.8427 (3) | 0.6034 (2) | 0.0631 (7) |
| H5A | 0.4688 | 0.8324 | 0.6648 | 0.076* |
| C6 | 0.37647 (14) | 0.9487 (3) | 0.58655 (17) | 0.0466 (5) |
| C7 | 0.33971 (16) | 1.0491 (3) | 0.66438 (16) | 0.0505 (5) |
| C8 | 0.32016 (14) | 1.2066 (3) | 0.62347 (15) | 0.0434 (5) |
| C9 | 0.33233 (19) | 1.3385 (3) | 0.67659 (19) | 0.0610 (7) |
| H9A | 0.3545 | 1.3321 | 0.7390 | 0.073* |
| C10 | 0.3118 (2) | 1.4800 (3) | 0.6378 (2) | 0.0711 (8) |
| H10A | 0.3204 | 1.5671 | 0.6744 | 0.085* |
| C11 | 0.2791 (2) | 1.4919 (3) | 0.5461 (2) | 0.0672 (7) |
| H11A | 0.2661 | 1.5867 | 0.5200 | 0.081* |
| C12 | 0.26541 (17) | 1.3617 (3) | 0.49243 (18) | 0.0530 (6) |
| H12A | 0.2427 | 1.3697 | 0.4303 | 0.064* |
| C13 | 0.28522 (14) | 1.2188 (2) | 0.53003 (15) | 0.0412 (4) |
| C14 | 0.27061 (14) | 1.0775 (3) | 0.47466 (14) | 0.0416 (4) |
| C15 | 0.19768 (16) | 1.0598 (3) | 0.41783 (15) | 0.0480 (5) |
| H15A | 0.1633 | 1.1461 | 0.4068 | 0.058* |
| C16 | 0.16583 (16) | 0.9172 (3) | 0.37049 (17) | 0.0521 (6) |
| H16A | 0.2048 | 0.8334 | 0.3882 | 0.063* |
| H16B | 0.1662 | 0.9288 | 0.3017 | 0.063* |
| C17 | 0.07204 (15) | 0.8853 (3) | 0.40238 (14) | 0.0437 (5) |

| | | | | |
|---|---|---|---|---|
| H17A | 0.0723 | 0.8797 | 0.4715 | 0.052* |
| H17B | 0.0338 | 0.9691 | 0.3830 | 0.052* |
| C18 | 0.0842 (2) | 0.6043 (3) | 0.39637 (19) | 0.0593 (6) |
| H18A | 0.1430 | 0.6057 | 0.3712 | 0.089* |
| H18B | 0.0536 | 0.5143 | 0.3751 | 0.089* |
| H18C | 0.0882 | 0.6050 | 0.4648 | 0.089* |
| C19 | −0.06121 (18) | 0.7248 (4) | 0.3865 (2) | 0.0726 (8) |
| H19A | −0.0846 | 0.6328 | 0.3591 | 0.109* |
| H19B | −0.0943 | 0.8099 | 0.3616 | 0.109* |
| H19C | −0.0663 | 0.7214 | 0.4546 | 0.109* |
| C20 | 0.2502 (2) | 0.9793 (4) | 0.6960 (2) | 0.0701 (8) |
| H20A | 0.2115 | 0.9649 | 0.6411 | 0.105* |
| H20B | 0.2224 | 1.0466 | 0.7401 | 0.105* |
| H20C | 0.2613 | 0.8832 | 0.7264 | 0.105* |
| C21 | 0.4023 (2) | 1.0579 (4) | 0.7525 (2) | 0.0798 (9) |
| H21A | 0.4602 | 1.0903 | 0.7336 | 0.120* |
| H21B | 0.4067 | 0.9596 | 0.7818 | 0.120* |
| H21C | 0.3790 | 1.1292 | 0.7972 | 0.120* |
| H1N1 | 0.0369 (17) | 0.750 (3) | 0.293 (2) | 0.048 (7)* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0908 (5) | 0.0586 (4) | 0.0356 (3) | 0.0045 (3) | −0.0033 (3) | −0.0024 (2) |
| N1 | 0.0412 (9) | 0.0561 (11) | 0.0347 (8) | −0.0039 (8) | 0.0010 (7) | −0.0039 (7) |
| C1 | 0.0384 (10) | 0.0438 (11) | 0.0471 (11) | −0.0067 (8) | 0.0035 (8) | −0.0010 (8) |
| C2 | 0.0449 (13) | 0.0620 (15) | 0.0626 (14) | −0.0067 (11) | 0.0066 (10) | −0.0133 (12) |
| C3 | 0.0469 (14) | 0.0614 (17) | 0.098 (2) | −0.0064 (12) | 0.0139 (14) | −0.0238 (15) |
| C4 | 0.0483 (15) | 0.0596 (17) | 0.113 (3) | 0.0060 (12) | −0.0039 (15) | −0.0030 (16) |
| C5 | 0.0510 (14) | 0.0561 (15) | 0.0815 (19) | −0.0003 (11) | −0.0097 (12) | 0.0124 (13) |
| C6 | 0.0398 (11) | 0.0457 (12) | 0.0540 (12) | −0.0053 (9) | −0.0018 (9) | 0.0084 (9) |
| C7 | 0.0543 (13) | 0.0566 (14) | 0.0406 (10) | −0.0045 (10) | −0.0013 (9) | 0.0086 (9) |
| C8 | 0.0409 (11) | 0.0497 (12) | 0.0398 (10) | −0.0068 (9) | 0.0022 (8) | −0.0004 (8) |
| C9 | 0.0677 (17) | 0.0622 (16) | 0.0528 (13) | −0.0090 (13) | −0.0024 (11) | −0.0129 (12) |
| C10 | 0.081 (2) | 0.0486 (15) | 0.084 (2) | −0.0099 (14) | −0.0014 (15) | −0.0177 (14) |
| C11 | 0.0720 (18) | 0.0422 (13) | 0.087 (2) | −0.0061 (12) | 0.0023 (14) | 0.0035 (13) |
| C12 | 0.0541 (14) | 0.0474 (13) | 0.0573 (13) | −0.0015 (10) | −0.0014 (10) | 0.0073 (10) |
| C13 | 0.0395 (10) | 0.0422 (11) | 0.0419 (10) | −0.0059 (8) | 0.0038 (8) | 0.0012 (8) |
| C14 | 0.0452 (11) | 0.0449 (11) | 0.0346 (9) | −0.0042 (9) | 0.0016 (8) | 0.0016 (8) |
| C15 | 0.0508 (12) | 0.0497 (12) | 0.0431 (11) | −0.0040 (10) | −0.0045 (9) | −0.0006 (9) |
| C16 | 0.0478 (12) | 0.0626 (15) | 0.0458 (11) | −0.0053 (11) | −0.0017 (9) | −0.0115 (10) |
| C17 | 0.0483 (12) | 0.0447 (11) | 0.0382 (10) | 0.0017 (9) | 0.0014 (8) | −0.0039 (8) |
| C18 | 0.0683 (16) | 0.0472 (13) | 0.0628 (15) | 0.0032 (12) | 0.0074 (12) | −0.0010 (11) |
| C19 | 0.0431 (14) | 0.095 (2) | 0.0795 (19) | −0.0131 (14) | 0.0083 (13) | −0.0070 (16) |
| C20 | 0.0776 (19) | 0.0710 (18) | 0.0628 (16) | −0.0100 (15) | 0.0214 (13) | 0.0165 (14) |
| C21 | 0.097 (2) | 0.093 (2) | 0.0487 (14) | 0.0018 (19) | −0.0208 (14) | 0.0090 (15) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N1—C19 | 1.485 (3) | C11—C12 | 1.384 (4) |
| N1—C18 | 1.492 (3) | C11—H11A | 0.9300 |
| N1—C17 | 1.498 (3) | C12—C13 | 1.394 (3) |
| N1—H1N1 | 0.97 (3) | C12—H12A | 0.9300 |
| C1—C2 | 1.394 (3) | C13—C14 | 1.481 (3) |
| C1—C6 | 1.400 (3) | C14—C15 | 1.346 (3) |
| C1—C14 | 1.485 (3) | C15—C16 | 1.494 (3) |
| C2—C3 | 1.385 (4) | C15—H15A | 0.9300 |
| C2—H2A | 0.9300 | C16—C17 | 1.515 (3) |
| C3—C4 | 1.364 (5) | C16—H16A | 0.9700 |
| C3—H3A | 0.9300 | C16—H16B | 0.9700 |
| C4—C5 | 1.372 (5) | C17—H17A | 0.9700 |
| C4—H4A | 0.9300 | C17—H17B | 0.9700 |
| C5—C6 | 1.400 (4) | C18—H18A | 0.9600 |
| C5—H5A | 0.9300 | C18—H18B | 0.9600 |
| C6—C7 | 1.519 (4) | C18—H18C | 0.9600 |
| C7—C8 | 1.527 (3) | C19—H19A | 0.9600 |
| C7—C21 | 1.533 (3) | C19—H19B | 0.9600 |
| C7—C20 | 1.553 (4) | C19—H19C | 0.9600 |
| C8—C9 | 1.389 (3) | C20—H20A | 0.9600 |
| C8—C13 | 1.402 (3) | C20—H20B | 0.9600 |
| C9—C10 | 1.392 (4) | C20—H20C | 0.9600 |
| C9—H9A | 0.9300 | C21—H21A | 0.9600 |
| C10—C11 | 1.368 (5) | C21—H21B | 0.9600 |
| C10—H10A | 0.9300 | C21—H21C | 0.9600 |
| C19—N1—C18 | 109.3 (2) | C12—C13—C8 | 119.6 (2) |
| C19—N1—C17 | 110.8 (2) | C12—C13—C14 | 122.3 (2) |
| C18—N1—C17 | 112.33 (19) | C8—C13—C14 | 118.12 (19) |
| C19—N1—H1N1 | 107.7 (16) | C15—C14—C13 | 120.9 (2) |
| C18—N1—H1N1 | 110.5 (15) | C15—C14—C1 | 125.7 (2) |
| C17—N1—H1N1 | 106.2 (15) | C13—C14—C1 | 113.21 (18) |
| C2—C1—C6 | 119.5 (2) | C14—C15—C16 | 127.3 (2) |
| C2—C1—C14 | 122.0 (2) | C14—C15—H15A | 116.4 |
| C6—C1—C14 | 118.36 (19) | C16—C15—H15A | 116.4 |
| C3—C2—C1 | 120.5 (3) | C15—C16—C17 | 108.3 (2) |
| C3—C2—H2A | 119.8 | C15—C16—H16A | 110.0 |
| C1—C2—H2A | 119.8 | C17—C16—H16A | 110.0 |
| C4—C3—C2 | 120.4 (3) | C15—C16—H16B | 110.0 |
| C4—C3—H3A | 119.8 | C17—C16—H16B | 110.0 |
| C2—C3—H3A | 119.8 | H16A—C16—H16B | 108.4 |
| C3—C4—C5 | 119.9 (3) | N1—C17—C16 | 113.25 (18) |
| C3—C4—H4A | 120.1 | N1—C17—H17A | 108.9 |
| C5—C4—H4A | 120.1 | C16—C17—H17A | 108.9 |
| C4—C5—C6 | 121.6 (3) | N1—C17—H17B | 108.9 |
| C4—C5—H5A | 119.2 | C16—C17—H17B | 108.9 |
| C6—C5—H5A | 119.2 | H17A—C17—H17B | 107.7 |

| | | | |
|---|---|---|---|
| C1—C6—C5 | 118.1 (2) | N1—C18—H18A | 109.5 |
| C1—C6—C7 | 118.8 (2) | N1—C18—H18B | 109.5 |
| C5—C6—C7 | 123.0 (2) | H18A—C18—H18B | 109.5 |
| C6—C7—C8 | 109.23 (18) | N1—C18—H18C | 109.5 |
| C6—C7—C21 | 112.4 (2) | H18A—C18—H18C | 109.5 |
| C8—C7—C21 | 111.4 (2) | H18B—C18—H18C | 109.5 |
| C6—C7—C20 | 107.9 (2) | N1—C19—H19A | 109.5 |
| C8—C7—C20 | 107.9 (2) | N1—C19—H19B | 109.5 |
| C21—C7—C20 | 107.8 (2) | H19A—C19—H19B | 109.5 |
| C9—C8—C13 | 118.5 (2) | N1—C19—H19C | 109.5 |
| C9—C8—C7 | 122.5 (2) | H19A—C19—H19C | 109.5 |
| C13—C8—C7 | 119.0 (2) | H19B—C19—H19C | 109.5 |
| C8—C9—C10 | 121.0 (2) | C7—C20—H20A | 109.5 |
| C8—C9—H9A | 119.5 | C7—C20—H20B | 109.5 |
| C10—C9—H9A | 119.5 | H20A—C20—H20B | 109.5 |
| C11—C10—C9 | 120.4 (3) | C7—C20—H20C | 109.5 |
| C11—C10—H10A | 119.8 | H20A—C20—H20C | 109.5 |
| C9—C10—H10A | 119.8 | H20B—C20—H20C | 109.5 |
| C10—C11—C12 | 119.4 (3) | C7—C21—H21A | 109.5 |
| C10—C11—H11A | 120.3 | C7—C21—H21B | 109.5 |
| C12—C11—H11A | 120.3 | H21A—C21—H21B | 109.5 |
| C11—C12—C13 | 121.1 (2) | C7—C21—H21C | 109.5 |
| C11—C12—H12A | 119.5 | H21A—C21—H21C | 109.5 |
| C13—C12—H12A | 119.5 | H21B—C21—H21C | 109.5 |
| C6—C1—C2—C3 | 1.6 (4) | C7—C8—C9—C10 | −178.4 (3) |
| C14—C1—C2—C3 | 177.0 (2) | C8—C9—C10—C11 | 0.0 (5) |
| C1—C2—C3—C4 | −0.3 (4) | C9—C10—C11—C12 | 0.8 (5) |
| C2—C3—C4—C5 | −0.8 (5) | C10—C11—C12—C13 | −0.6 (4) |
| C3—C4—C5—C6 | 0.5 (5) | C11—C12—C13—C8 | −0.5 (4) |
| C2—C1—C6—C5 | −1.9 (3) | C11—C12—C13—C14 | 179.5 (2) |
| C14—C1—C6—C5 | −177.4 (2) | C9—C8—C13—C12 | 1.3 (3) |
| C2—C1—C6—C7 | 178.9 (2) | C7—C8—C13—C12 | 178.7 (2) |
| C14—C1—C6—C7 | 3.4 (3) | C9—C8—C13—C14 | −178.7 (2) |
| C4—C5—C6—C1 | 0.8 (4) | C7—C8—C13—C14 | −1.2 (3) |
| C4—C5—C6—C7 | 180.0 (3) | C12—C13—C14—C15 | −39.9 (3) |
| C1—C6—C7—C8 | −39.0 (3) | C8—C13—C14—C15 | 140.1 (2) |
| C5—C6—C7—C8 | 141.8 (2) | C12—C13—C14—C1 | 143.6 (2) |
| C1—C6—C7—C21 | −163.2 (2) | C8—C13—C14—C1 | −36.4 (3) |
| C5—C6—C7—C21 | 17.7 (3) | C2—C1—C14—C15 | 43.7 (3) |
| C1—C6—C7—C20 | 78.1 (3) | C6—C1—C14—C15 | −140.9 (2) |
| C5—C6—C7—C20 | −101.1 (3) | C2—C1—C14—C13 | −140.0 (2) |
| C6—C7—C8—C9 | −144.6 (2) | C6—C1—C14—C13 | 35.5 (3) |
| C21—C7—C8—C9 | −19.9 (3) | C13—C14—C15—C16 | −169.1 (2) |
| C20—C7—C8—C9 | 98.3 (3) | C1—C14—C15—C16 | 6.9 (4) |
| C6—C7—C8—C13 | 38.0 (3) | C14—C15—C16—C17 | 122.4 (3) |
| C21—C7—C8—C13 | 162.7 (2) | C19—N1—C17—C16 | −173.4 (2) |
| C20—C7—C8—C13 | −79.1 (3) | C18—N1—C17—C16 | 64.1 (2) |
| C13—C8—C9—C10 | −1.0 (4) | C15—C16—C17—N1 | −177.84 (18) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1N1···Cl1 | 0.98 (3) | 2.03 (3) | 3.0024 (19) | 176 (3) |
| C17—H17A···Cl1$^{i}$ | 0.97 | 2.81 | 3.710 (2) | 155 |
| C17—H17B···Cl1$^{ii}$ | 0.97 | 2.77 | 3.717 (3) | 164 |
| C18—H18B···Cl1$^{iii}$ | 0.96 | 2.68 | 3.625 (3) | 169 |

Symmetry codes: (i) *x*, −*y*+3/2, *z*+1/2; (ii) −*x*, *y*+1/2, −*z*+1/2; (iii) −*x*, *y*−1/2, −*z*+1/2.

**Fig. 1**

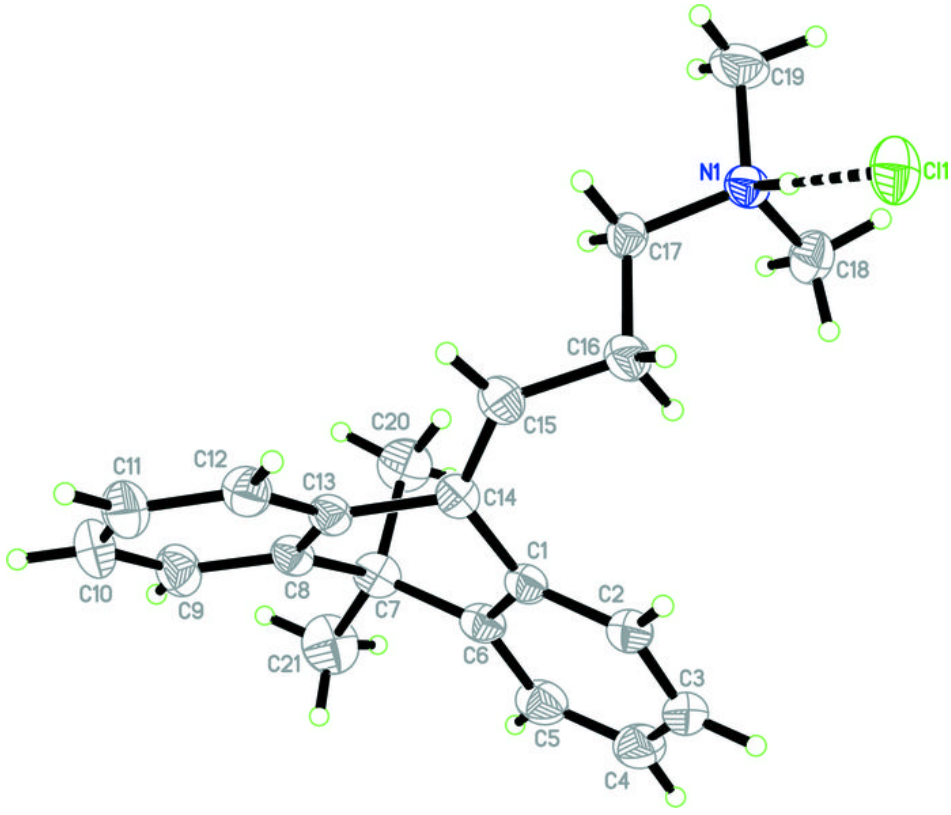
C19
N1
Cl1
C17
C18
C16
C15
C20
C11
C12
C13
C14
C1
C10
C9
C8
C7
C2
C21
C6
C3
C5
C4

**Fig. 2**