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# 1,3-Bis(2,6-diisopropylphenyl)-1*H*-imidazol-3-ium bromide dichloromethane disolvate

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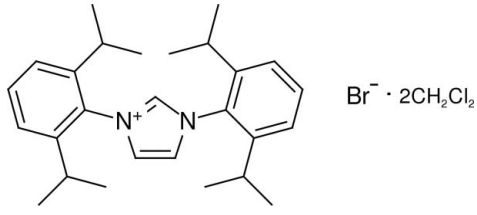
Key indicators: single-crystal X-ray study; $T$ = 173 K; mean $\sigma$(C–C) = 0.004 Å; disorder in solvent or counterion; $R$ factor = 0.038; $wR$ factor = 0.090; data-to-parameter ratio = 16.2.

In the title compound, $C_{27}H_{37}N_2^+\cdot Br^-\cdot 2CH_2Cl_2$, both the cation and the anion are located on a crystallographic mirror plane. Both of the dichloromethane solvent molecules show a disorder across a mirror plane over two equally occupied positions. In the crystal, the cations are connnected to the bromide ions *via* C—H···Br hydrogen bonds.

## Related literature

For the preparation of imidazolium salts, see: Arduengo *et al.* (1995, 1999); Hintermann (2007). For structures with the same cation but different anions, see: Stasch *et al.* (2004); Blue *et al.* (2006); Berger *et al.* (2012). For compounds with the 1,3-bis-(2,6-diisopropylphenyl)imidazolium unit, see: Ikhile *et al.* (2010); Giffin *et al.* (2010).




## Experimental

### Crystal data

$C_{27}H_{37}N_2^+\cdot Br^-\cdot 2CH_2Cl_2$ $M_r$ = 639.35
Monoclinic, $P2_1/m$
$a$ = 9.1874 (8) Å
$b$ = 16.5165 (12) Å
$c$ = 11.030 (1) Å
$\beta$ = 102.332 (7)°
$V$ = 1635.1 (2) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 1.60 mm$^{-1}$
$T$ = 173 K
0.52 × 0.28 × 0.24 mm

### Data collection

Stoe IPDS II two-circle diffractometer
Absorption correction: multi-scan (*MULABS*; Spek, 2009; Blessing, 1995)
$T_{min}$ = 0.489, $T_{max}$ = 0.700
20988 measured reflections
3200 independent reflections
2867 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.084

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.090
$S$ = 1.03
3200 reflections
197 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.36 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···Br1 | 0.95 | 2.59 | 3.538 (3) | 175 |

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-AREA*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97* .

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5272).

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# supporting information

*Acta Cryst.* (2012). E**68**, o1845 [doi:10.1107/S1600536812022246]

# 1,3-Bis(2,6-diisopropylphenyl)-1*H*-imidazol-3-ium bromide dichloromethane disolvate

**Matthias Berger, Norbert Auner, Tanja Sinke and Michael Bolte**

## S1. Comment

Imidazolium salts are precursors for the synthesis of N-heterocyclic carbenes (NHC) and can be prepared according to Arduengo *et al.* (1995, 1999) and Hintermann (2007). Deprotonation by strong bases gives the free stable NHC, which is widely used as ligands.

The title compound crystallizes with discrete cations, anions and solvent dichloromethane molecules. Both cations and anions are located on a crystallographic mirror plane. Both dichloromethane molecules show a disorder across a mirror plane over two equally occupied positions. The Br anions are connnected to the cations *via* C—H···Br hydrogen bonds. Structures with the same cation, but with different anions and solvent molecules, have been determined by Stasch *et al.* (2004), Blue *et al.* (2006) and Berger *et al.* (2012). For compounds with 1,3-bis-(2,6-diisopropylphenyl)imidazolium unit, see: Ikhile *et al.* (2010) and Giffin *et al.* (2010).

## S2. Experimental

1,3-Bis(2,6-di-isopropylphenyl)1*H*-imidazol-3-ium bromide chloroform disolvate was prepared by reacting 167 mg of 1,3-bis(2,6-diisopropylphenyl)-1,3-dihydro-2*H*-imidazol-2-ylidene with 115 mg of $Si_2Br_6$ in deuterated dichloromethane. After two weeks at 253 K colorless needles of the title compound crystallized in the NMR-Tube.

## S3. Refinement

H atoms were refined using a riding model, with C—H ranging from 0.95 Å to 1.00 Å and with $U_{iso}$(H) = 1.2$U_{eq}$(C) or $U_{iso}$(H) = 1.5$U_{eq}$($C_{methyl}$).

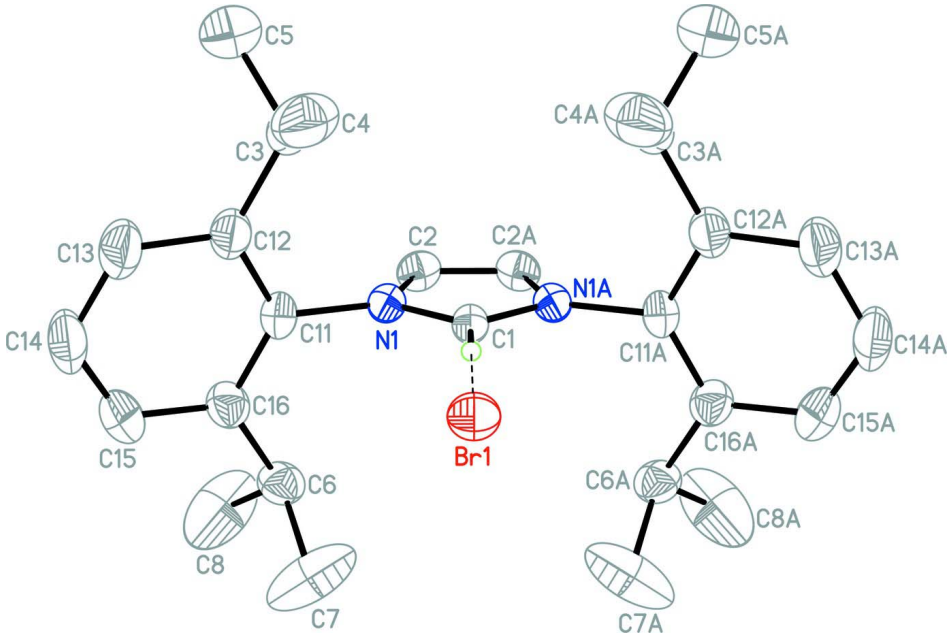


**Figure 1**

A perspective view of the title compound, showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bonds are shown as dashed lines. H atoms not involved in hydrogen bonding and dichloromethane molecules are omitted for clarity. Atoms labelled with suffix A were generated by the symmetry operator $x, -y + 1/2, z$.

### 1,3-Bis(2,6-diisopropylphenyl)-1*H*-imidazol-3-ium bromide dichloromethane disolvate

*Crystal data*

$C_{27}H_{37}N_2^+\cdot Br^-\cdot 2CH_2Cl_2$
$M_r = 639.35$
Monoclinic, $P2_1/m$
Hall symbol: -P 2yb
$a = 9.1874\ (8)$ Å
$b = 16.5165\ (12)$ Å
$c = 11.030\ (1)$ Å
$\beta = 102.332\ (7)°$
$V = 1635.1\ (2)$ Å$^3$
$Z = 2$
$F(000) = 664$
$D_x = 1.299$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 19135 reflections
$\theta = 3.4–26.0°$
$\mu = 1.60$ mm$^{-1}$
$T = 173$ K
Plate, colourless
0.52 × 0.28 × 0.24 mm

*Data collection*

Stoe IPDS II two-circle diffractometer
Radiation source: Genix 3D I$\mu$S microfocus X-ray source
Genix 3D multilayer optics monochromator
$\omega$ scans
Absorption correction: multi-scan (*MULABS*; Spek, 2009; Blessing, 1995)
$T_{min} = 0.489$, $T_{max} = 0.700$
20988 measured reflections
3200 independent reflections
2867 reflections with $I > 2\sigma(I)$
$R_{int} = 0.084$
$\theta_{max} = 25.7°$, $\theta_{min} = 3.4°$
$h = -11\rightarrow11$
$k = -19\rightarrow20$
$l = -13\rightarrow13$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.090$
$S = 1.03$
3200 reflections
197 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.041P)^2 + 0.9357P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.43$ e Å$^{-3}$
$\Delta\rho_{min} = -0.36$ e Å$^{-3}$

*Special details*

**Experimental**. ;
**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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| N1 | 0.29660 (18) | 0.18481 (10) | 0.41051 (15) | 0.0255 (4) | |
| C1 | 0.2134 (3) | 0.2500 | 0.4158 (3) | 0.0241 (6) | |
| H1 | 0.1119 | 0.2500 | 0.4222 | 0.029* | |
| C2 | 0.4378 (2) | 0.20927 (14) | 0.4033 (2) | 0.0313 (5) | |
| H2 | 0.5197 | 0.1751 | 0.3992 | 0.038* | |
| C3 | 0.1307 (3) | 0.11525 (15) | 0.1796 (2) | 0.0440 (6) | |
| H3 | 0.1846 | 0.1682 | 0.1925 | 0.053* | |
| C4 | −0.0359 (4) | 0.1327 (2) | 0.1415 (3) | 0.0594 (8) | |
| H4A | −0.0567 | 0.1626 | 0.0629 | 0.089* | |
| H4B | −0.0669 | 0.1652 | 0.2059 | 0.089* | |
| H4C | −0.0911 | 0.0815 | 0.1311 | 0.089* | |
| C5 | 0.1838 (3) | 0.0696 (2) | 0.0773 (3) | 0.0545 (7) | |
| H5A | 0.1607 | 0.1012 | 0.0004 | 0.082* | |
| H5B | 0.1333 | 0.0171 | 0.0640 | 0.082* | |
| H5C | 0.2917 | 0.0611 | 0.1017 | 0.082* | |
| C6 | 0.3631 (3) | 0.09778 (16) | 0.6435 (2) | 0.0394 (5) | |
| H6 | 0.4138 | 0.1470 | 0.6197 | 0.047* | |
| C7 | 0.2619 (4) | 0.1250 (3) | 0.7253 (4) | 0.0934 (15) | |
| H7A | 0.1868 | 0.1621 | 0.6791 | 0.140* | |
| H7B | 0.3203 | 0.1529 | 0.7980 | 0.140* | |
| H7C | 0.2123 | 0.0779 | 0.7523 | 0.140* | |
| C8 | 0.4824 (5) | 0.0423 (3) | 0.7119 (4) | 0.1023 (17) | |
| H8A | 0.5472 | 0.0256 | 0.6565 | 0.153* | |
| H8B | 0.4361 | −0.0057 | 0.7401 | 0.153* | |

| | | | | | |
|---|---|---|---|---|---|
| H8C | 0.5415 | 0.0707 | 0.7838 | 0.153* | |
| C11 | 0.2443 (2) | 0.10184 (13) | 0.4124 (2) | 0.0317 (5) | |
| C12 | 0.1641 (3) | 0.06934 (14) | 0.3013 (2) | 0.0382 (5) | |
| C13 | 0.1118 (4) | −0.00958 (16) | 0.3072 (3) | 0.0531 (7) | |
| H13 | 0.0559 | −0.0343 | 0.2342 | 0.064* | |
| C14 | 0.1396 (4) | −0.05222 (16) | 0.4166 (3) | 0.0578 (8) | |
| H14 | 0.1019 | −0.1057 | 0.4183 | 0.069* | |
| C15 | 0.2209 (3) | −0.01857 (16) | 0.5234 (3) | 0.0500 (7) | |
| H15 | 0.2401 | −0.0494 | 0.5978 | 0.060* | |
| C16 | 0.2761 (3) | 0.06008 (14) | 0.5248 (2) | 0.0366 (5) | |
| Br1 | −0.17082 (3) | 0.2500 | 0.41902 (3) | 0.03239 (11) | |
| C9 | 0.6207 (8) | 0.2781 (5) | 0.1008 (6) | 0.083 (4) | 0.50 |
| H9A | 0.6687 | 0.2735 | 0.1899 | 0.100* | 0.309 (13) |
| H9B | 0.6987 | 0.2657 | 0.0540 | 0.100* | 0.309 (13) |
| H9C | 0.6825 | 0.2561 | 0.0452 | 0.100* | 0.191 (13) |
| H9D | 0.6666 | 0.2661 | 0.1886 | 0.100* | 0.191 (13) |
| Cl1 | 0.5757 (3) | 0.3808 (3) | 0.0739 (3) | 0.1306 (12) | 0.50 |
| Cl2 | 0.4398 (9) | 0.2500 | 0.0600 (7) | 0.091 (3) | 0.38 (3) |
| Cl2′ | 0.4863 (16) | 0.1966 (13) | 0.0681 (6) | 0.129 (7) | 0.309 (13) |
| C10 | 0.7893 (8) | 0.2231 (4) | 0.7366 (6) | 0.0643 (18) | 0.50 |
| H10A | 0.7776 | 0.2363 | 0.6475 | 0.077* | 0.50 |
| H10B | 0.7760 | 0.1639 | 0.7438 | 0.077* | 0.50 |
| Cl3 | 0.96814 (15) | 0.2500 | 0.81560 (13) | 0.0802 (4) | |
| Cl4 | 0.6535 (2) | 0.27308 (11) | 0.79502 (16) | 0.0803 (7) | 0.50 |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0245 (9) | 0.0254 (8) | 0.0255 (8) | 0.0012 (7) | 0.0030 (7) | −0.0009 (7) |
| C1 | 0.0239 (14) | 0.0225 (14) | 0.0246 (14) | 0.000 | 0.0022 (11) | 0.000 |
| C2 | 0.0247 (10) | 0.0374 (11) | 0.0322 (11) | 0.0053 (9) | 0.0074 (8) | −0.0019 (9) |
| C3 | 0.0606 (16) | 0.0333 (12) | 0.0331 (12) | −0.0058 (12) | −0.0012 (11) | −0.0042 (10) |
| C4 | 0.074 (2) | 0.0622 (19) | 0.0383 (14) | 0.0213 (16) | 0.0033 (13) | −0.0042 (13) |
| C5 | 0.0549 (17) | 0.0630 (18) | 0.0446 (15) | 0.0006 (15) | 0.0085 (13) | −0.0039 (14) |
| C6 | 0.0428 (13) | 0.0418 (13) | 0.0325 (12) | 0.0040 (11) | 0.0055 (10) | 0.0051 (10) |
| C7 | 0.057 (2) | 0.142 (4) | 0.081 (3) | 0.000 (2) | 0.0153 (19) | −0.065 (3) |
| C8 | 0.100 (3) | 0.100 (3) | 0.080 (3) | 0.056 (3) | −0.042 (2) | −0.025 (2) |
| C11 | 0.0341 (12) | 0.0226 (10) | 0.0381 (12) | 0.0013 (9) | 0.0073 (9) | −0.0009 (9) |
| C12 | 0.0456 (14) | 0.0276 (11) | 0.0384 (12) | −0.0020 (10) | 0.0025 (10) | −0.0018 (10) |
| C13 | 0.071 (2) | 0.0321 (13) | 0.0501 (16) | −0.0120 (13) | 0.0003 (14) | −0.0050 (12) |
| C14 | 0.081 (2) | 0.0268 (13) | 0.0620 (18) | −0.0124 (13) | 0.0074 (16) | 0.0036 (12) |
| C15 | 0.0673 (19) | 0.0345 (13) | 0.0484 (15) | −0.0004 (13) | 0.0128 (14) | 0.0118 (11) |
| C16 | 0.0396 (13) | 0.0321 (12) | 0.0381 (12) | 0.0050 (10) | 0.0082 (10) | 0.0048 (10) |
| Br1 | 0.02843 (17) | 0.03733 (18) | 0.03321 (18) | 0.000 | 0.01058 (12) | 0.000 |
| C9 | 0.056 (3) | 0.148 (12) | 0.041 (3) | −0.028 (4) | −0.003 (2) | −0.009 (4) |
| Cl1 | 0.0784 (17) | 0.170 (3) | 0.129 (2) | 0.0489 (19) | −0.0110 (16) | −0.020 (2) |
| Cl2 | 0.068 (3) | 0.144 (9) | 0.063 (3) | 0.000 | 0.019 (2) | 0.000 |
| Cl2′ | 0.094 (7) | 0.234 (17) | 0.063 (2) | −0.100 (10) | 0.024 (3) | −0.035 (5) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.084 (4) | 0.064 (4) | 0.056 (3) | −0.011 (3) | 0.039 (3) | −0.015 (3) |
| Cl3 | 0.0666 (8) | 0.1076 (11) | 0.0723 (8) | 0.000 | 0.0278 (6) | 0.000 |
| Cl4 | 0.0721 (10) | 0.099 (2) | 0.0690 (9) | 0.0362 (10) | 0.0134 (8) | −0.0046 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.329 (2) | C11—C12 | 1.395 (3) |
| N1—C2 | 1.377 (3) | C12—C13 | 1.396 (4) |
| N1—C11 | 1.454 (3) | C13—C14 | 1.373 (4) |
| C1—N1$^{i}$ | 1.329 (2) | C13—H13 | 0.9500 |
| C1—H1 | 0.9500 | C14—C15 | 1.371 (4) |
| C2—C2$^{i}$ | 1.346 (5) | C14—H14 | 0.9500 |
| C2—H2 | 0.9500 | C15—C16 | 1.393 (4) |
| C3—C12 | 1.515 (3) | C15—H15 | 0.9500 |
| C3—C5 | 1.521 (4) | C9—Cl2 | 1.691 (10) |
| C3—C4 | 1.525 (4) | C9—Cl1 | 1.757 (10) |
| C3—H3 | 1.0000 | C9—Cl2′ | 1.810 (11) |
| C4—H4A | 0.9800 | C9—H9A | 0.9900 |
| C4—H4B | 0.9800 | C9—H9B | 0.9900 |
| C4—H4C | 0.9800 | C9—H9C | 0.9900 |
| C5—H5A | 0.9800 | C9—H9D | 0.9900 |
| C5—H5B | 0.9800 | Cl1—Cl2′$^{i}$ | 1.51 (3) |
| C5—H5C | 0.9800 | Cl2—C9$^{i}$ | 1.691 (10) |
| C6—C7 | 1.496 (4) | Cl2′—C9$^{i}$ | 1.280 (11) |
| C6—C8 | 1.503 (4) | Cl2′—Cl1$^{i}$ | 1.51 (3) |
| C6—C16 | 1.514 (3) | Cl2′—Cl2′$^{i}$ | 1.76 (4) |
| C6—H6 | 1.0000 | C10—Cl4 | 1.731 (6) |
| C7—H7A | 0.9800 | C10—Cl3 | 1.745 (7) |
| C7—H7B | 0.9800 | C10—H10A | 0.9900 |
| C7—H7C | 0.9800 | C10—H10B | 0.9900 |
| C8—H8A | 0.9800 | Cl3—C10$^{i}$ | 1.745 (7) |
| C8—H8B | 0.9800 | Cl4—Cl4$^{i}$ | 0.763 (4) |
| C8—H8C | 0.9800 | Cl4—C10$^{i}$ | 1.523 (6) |
| C11—C16 | 1.394 (3) | | |

| | | | |
|---|---|---|---|
| C1—N1—C2 | 108.82 (18) | H8A—C8—H8C | 109.5 |
| C1—N1—C11 | 124.62 (18) | H8B—C8—H8C | 109.5 |
| C2—N1—C11 | 126.56 (18) | C16—C11—C12 | 124.2 (2) |
| N1$^{i}$—C1—N1 | 108.2 (3) | C16—C11—N1 | 118.2 (2) |
| N1$^{i}$—C1—H1 | 125.9 | C12—C11—N1 | 117.7 (2) |
| N1—C1—H1 | 125.9 | C11—C12—C13 | 116.2 (2) |
| C2$^{i}$—C2—N1 | 107.06 (12) | C11—C12—C3 | 123.7 (2) |
| C2$^{i}$—C2—H2 | 126.5 | C13—C12—C3 | 120.1 (2) |
| N1—C2—H2 | 126.5 | C14—C13—C12 | 121.2 (3) |
| C12—C3—C5 | 111.9 (2) | C14—C13—H13 | 119.4 |
| C12—C3—C4 | 109.9 (2) | C12—C13—H13 | 119.4 |
| C5—C3—C4 | 110.6 (2) | C15—C14—C13 | 120.8 (2) |
| C12—C3—H3 | 108.1 | C15—C14—H14 | 119.6 |

| | | | |
|---|---|---|---|
| C5—C3—H3 | 108.1 | C13—C14—H14 | 119.6 |
| C4—C3—H3 | 108.1 | C14—C15—C16 | 121.2 (2) |
| C3—C4—H4A | 109.5 | C14—C15—H15 | 119.4 |
| C3—C4—H4B | 109.5 | C16—C15—H15 | 119.4 |
| H4A—C4—H4B | 109.5 | C15—C16—C11 | 116.4 (2) |
| C3—C4—H4C | 109.5 | C15—C16—C6 | 121.1 (2) |
| H4A—C4—H4C | 109.5 | C11—C16—C6 | 122.5 (2) |
| H4B—C4—H4C | 109.5 | Cl2—C9—Cl1 | 92.2 (4) |
| C3—C5—H5A | 109.5 | Cl2—C9—H9A | 116.6 |
| C3—C5—H5B | 109.5 | Cl1—C9—H9A | 106.3 |
| H5A—C5—H5B | 109.5 | Cl2′—C9—H9A | 106.3 |
| C3—C5—H5C | 109.5 | Cl2—C9—H9B | 125.7 |
| H5A—C5—H5C | 109.5 | Cl1—C9—H9B | 106.3 |
| H5B—C5—H5C | 109.5 | Cl2′—C9—H9B | 106.3 |
| C7—C6—C8 | 111.2 (3) | H9A—C9—H9B | 106.4 |
| C7—C6—C16 | 111.3 (2) | Cl2—C9—H9C | 113.3 |
| C8—C6—C16 | 112.1 (2) | Cl1—C9—H9C | 113.3 |
| C7—C6—H6 | 107.3 | Cl2—C9—H9D | 113.3 |
| C8—C6—H6 | 107.3 | Cl1—C9—H9D | 113.3 |
| C16—C6—H6 | 107.3 | Cl2′—C9—H9D | 100.2 |
| C6—C7—H7A | 109.5 | H9C—C9—H9D | 110.6 |
| C6—C7—H7B | 109.5 | Cl2′$^{i}$—Cl1—C9 | 45.3 (3) |
| H7A—C7—H7B | 109.5 | Cl1$^{i}$—Cl2′—C9 | 106.2 (9) |
| C6—C7—H7C | 109.5 | Cl4—C10—Cl3 | 111.7 (3) |
| H7A—C7—H7C | 109.5 | Cl4—C10—H10A | 109.3 |
| H7B—C7—H7C | 109.5 | Cl3—C10—H10A | 109.3 |
| C6—C8—H8A | 109.5 | Cl4—C10—H10B | 109.3 |
| C6—C8—H8B | 109.5 | Cl3—C10—H10B | 109.3 |
| H8A—C8—H8B | 109.5 | H10A—C10—H10B | 107.9 |
| C6—C8—H8C | 109.5 | | |

| | | | |
|---|---|---|---|
| C2—N1—C1—N1$^{i}$ | 0.8 (3) | C12—C11—C16—C15 | −0.9 (4) |
| C11—N1—C1—N1$^{i}$ | −179.28 (14) | N1—C11—C16—C15 | 178.5 (2) |
| C1—N1—C2—C2$^{i}$ | −0.50 (18) | C12—C11—C16—C6 | −179.8 (2) |
| C11—N1—C2—C2$^{i}$ | 179.60 (16) | N1—C11—C16—C6 | −0.4 (3) |
| C1—N1—C11—C16 | −98.5 (3) | C7—C6—C16—C15 | −77.5 (4) |
| C2—N1—C11—C16 | 81.4 (3) | C8—C6—C16—C15 | 47.7 (4) |
| C1—N1—C11—C12 | 81.0 (3) | C7—C6—C16—C11 | 101.3 (3) |
| C2—N1—C11—C12 | −99.1 (3) | C8—C6—C16—C11 | −133.5 (3) |
| C16—C11—C12—C13 | 1.2 (4) | Cl2—C9—Cl1—Cl2′$^{i}$ | 2.7 (5) |
| N1—C11—C12—C13 | −178.1 (2) | Cl2′—C9—Cl1—Cl2′$^{i}$ | 7.6 (4) |
| C16—C11—C12—C3 | −179.8 (2) | Cl1—C9—Cl2—C9$^{i}$ | 174.0 (2) |
| N1—C11—C12—C3 | 0.8 (4) | Cl2′—C9—Cl2—C9$^{i}$ | 1.6 (6) |
| C5—C3—C12—C11 | 124.9 (3) | Cl2—C9—Cl2′—C9$^{i}$ | −177.7 (8) |
| C4—C3—C12—C11 | −111.8 (3) | Cl1—C9—Cl2′—C9$^{i}$ | 173.1 (2) |
| C5—C3—C12—C13 | −56.2 (4) | Cl2—C9—Cl2′—Cl1$^{i}$ | 175.3 (9) |
| C4—C3—C12—C13 | 67.1 (3) | Cl1—C9—Cl2′—Cl1$^{i}$ | 166.1 (5) |
| C11—C12—C13—C14 | −0.5 (4) | Cl2—C9—Cl2′—Cl2′$^{i}$ | 2.3 (8) |

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|---|---|---|---|
| C3—C12—C13—C14 | −179.5 (3) | Cl1—C9—Cl2′—Cl2″$^{i}$ | −6.9 (2) |
| C12—C13—C14—C15 | −0.6 (5) | Cl4—C10—Cl3—C10$^{i}$ | −50.6 (3) |
| C13—C14—C15—C16 | 0.9 (5) | Cl3—C10—Cl4—Cl4$^{i}$ | −121.8 (4) |
| C14—C15—C16—C11 | −0.2 (4) | Cl3—C10—Cl4—C10$^{i}$ | 58.2 (4) |
| C14—C15—C16—C6 | 178.7 (3) | | |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···Br1 | 0.95 | 2.59 | 3.538 (3) | 175 |