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# Bis(2-ethyl-1*H*-imidazol-3-ium) tetrachloridomercurate(II)

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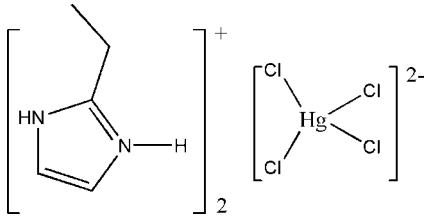
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.008 Å; disorder in main residue; $R$ factor = 0.036; $wR$ factor = 0.064; data-to-parameter ratio = 22.7.

The crystal structure of the title compound, $(C_5H_9N_2)_2[HgCl_4]$, consists of discrete tetrachloridomercurate dications and discrete 2-methylimidazolium cations. In the complex anion, the mercury cations are coordinated by four chloride anions with distances between 2.4568 (14) and 2.4936 (15) Å in a tetrahedral geometry. In the crystal, the cations and anions are connected by intermolecular N—H···Cl interactions. One C atom of the cations is disordered and was refined using a split model (occupancy ratio 0.75:0.25).

## Related literature

For a related structure and background to this study, see: Zhu (2011).




## Experimental

### Crystal data

$(C_5H_9N_2)_2[HgCl_4]$ $M_r$ = 536.67
Triclinic, $P\overline{1}$
$a$ = 7.5784 (15) Å
$b$ = 8.0972 (16) Å
$c$ = 14.661 (3) Å
$\alpha$ = 92.42 (3)°
$\beta$ = 97.88 (3)°
$\gamma$ = 98.17 (3)°
$V$ = 880.4 (3) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 9.34 mm$^{-1}$
$T$ = 293 K
0.33 × 0.28 × 0.20 mm

### Data collection

Rigaku SCXmini diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.216, $T_{max}$ = 0.459
9149 measured reflections
4032 independent reflections
3437 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.044

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.064
$S$ = 1.05
4032 reflections
178 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.80 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.72 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1*N*···Cl3$^{i}$ | 0.86 | 2.42 | 3.227 (4) | 157 |
| N2—H2*N*···Cl4$^{ii}$ | 0.86 | 2.37 | 3.188 (4) | 158 |
| N3—H3*N*···Cl2 | 0.86 | 2.37 | 3.220 (4) | 171 |
| N4—H4*N*···Cl2$^{iii}$ | 0.86 | 2.47 | 3.285 (4) | 159 |

Symmetry codes: (i) $x, y+1, z+1$; (ii) $-x+2, -y+1, -z+1$; (iii) $x, y+1, z$.

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *SHELXL97*.

This work was supported by Southeast University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2260).

## References

Brandenburg, K. & Putz, H. (2005). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Rigaku (2005). *CrystalClear*. Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Zhu, R.-Q. (2011). *Acta Cryst.* E**67**, m112.

# supporting information

*Acta Cryst.* (2012). E**68**, m148 [doi:10.1107/S1600536811055371]

## Bis(2-ethyl-1*H*-imidazol-3-ium) tetrachloridomercurate(II)

**Run-Qiang Zhu**

### S1. Experimental

A mixture of $HgCl_2$ (4.26 g, 25 mmol), hydrochloric acid (50 mmol, 36%, 8 ml), and 2 - ethyl imidazole (4.8 g, 50 mmol) in 30 ml water was stirred for 10 minutes at room temperature. On slow evaporation of solvent colourless crystals of the title compound grew within two weeks.

### S2. Refinement

Hydrogen atom positions were calculated and allowed to ride on their respective C atoms and N atoms with C–H distances of 0.93–0.97Å and N–H = 0.86 Å, and with $U_{iso}$(H)=1.2$U_{eq}$(C or N) or or 1.5 $U_{iso}$(C) for methy H atoms. One C atom is disordered and was refined using a split model and sof of 0.75:0.25. The atom of lower occupany was refined isotropic.

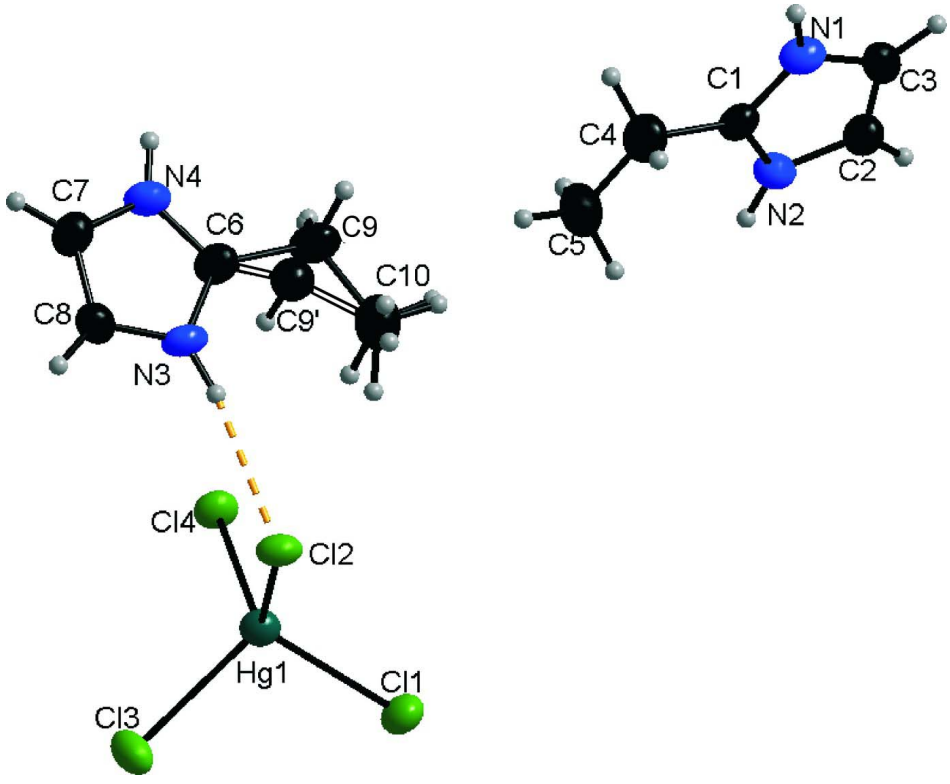



**Figure 1**

The molecular structure of the title compound, with labeling and displacement ellipsoids drawn at the 30% probability level. Intermolecular hydrogen bonding is shown as dashed lines and disordering as full and open bonds..

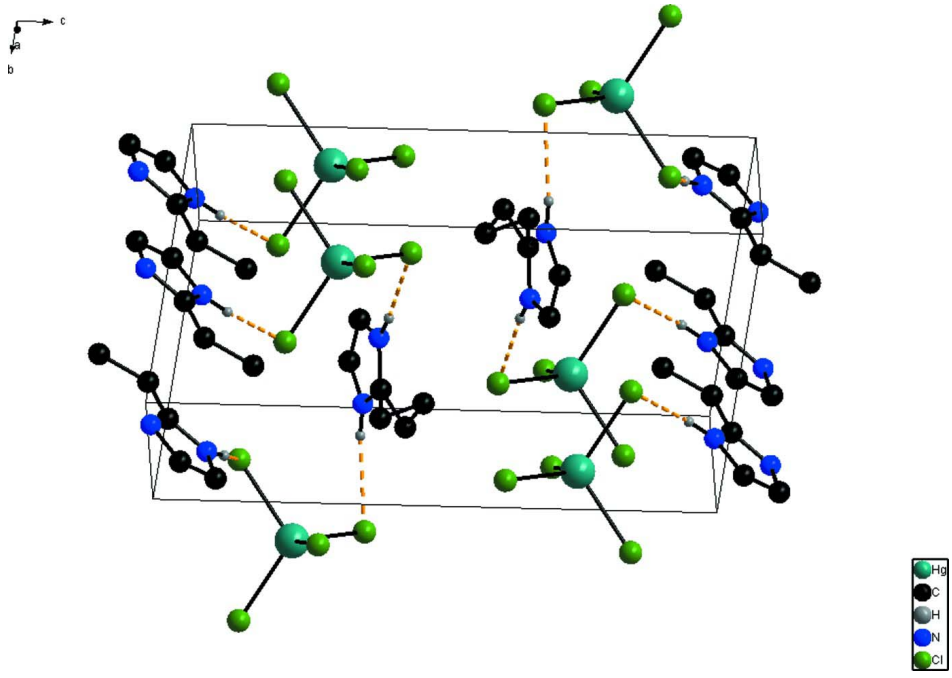



**Figure 2**

Crystal structure of the title compound with intermolecular hydrogen bonding shown as dashed lines. A-atoms not involved in hydrogen bonding are omitted for clarity.

### Bis(2-ethyl-1*H*-imidazol-3-ium) tetrachloridomercurate(II)

*Crystal data*

$(C_5H_9N_2)_2[HgCl_4]$
$M_r = 536.67$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.5784\ (15)$ Å
$b = 8.0972\ (16)$ Å
$c = 14.661\ (3)$ Å
$\alpha = 92.42\ (3)°$
$\beta = 97.88\ (3)°$
$\gamma = 98.17\ (3)°$
$V = 880.4\ (3)$ Å$^3$
$Z = 2$
$F(000) = 508$
$D_x = 2.025$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4032 reflections
$\theta = 2.3–27.5°$
$\mu = 9.34$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.33 × 0.28 × 0.20 mm

*Data collection*

Rigaku SCXmini diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min} = 0.216$, $T_{max} = 0.459$
9149 measured reflections
4032 independent reflections
3437 reflections with $I > 2\sigma(I)$
$R_{int} = 0.044$
$\theta_{max} = 27.5°$, $\theta_{min} = 3.3°$
$h = -9\rightarrow9$
$k = -10\rightarrow10$
$l = -19\rightarrow19$
2 standard reflections every 150 reflections
intensity decay: none

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.036$
$wR(F^2) = 0.064$
$S = 1.05$
4032 reflections
178 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
$w = 1/[\sigma^2(F_o^2) + (0.0134P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.80$ e Å$^{-3}$
$\Delta\rho_{min} = -0.72$ e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0113 (4)

*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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| Hg1 | 0.79183 (2) | 0.20862 (2) | 0.266500 (12) | 0.05040 (10) | |
| C1 | 0.8846 (6) | 0.7508 (6) | 1.0072 (3) | 0.0491 (11) | |
| C2 | 1.1813 (6) | 0.8008 (6) | 1.0293 (3) | 0.0573 (13) | |
| H2 | 1.3004 | 0.8002 | 1.0206 | 0.069* | |
| C3 | 1.1239 (7) | 0.8776 (7) | 1.0993 (3) | 0.0585 (13) | |
| H3 | 1.1950 | 0.9403 | 1.1492 | 0.070* | |
| C4 | 0.6932 (6) | 0.6871 (7) | 0.9695 (4) | 0.0713 (16) | |
| H4A | 0.6255 | 0.7802 | 0.9668 | 0.086* | |
| H4B | 0.6434 | 0.6101 | 1.0116 | 0.086* | |
| C5 | 0.6688 (8) | 0.6002 (8) | 0.8757 (4) | 0.0884 (19) | |
| H5A | 0.7108 | 0.6775 | 0.8327 | 0.133* | |
| H5B | 0.5434 | 0.5589 | 0.8567 | 0.133* | |
| H5C | 0.7365 | 0.5085 | 0.8775 | 0.133* | |
| C6 | 0.5651 (7) | 0.7388 (7) | 0.3880 (4) | 0.0593 (13) | |
| C7 | 0.2790 (7) | 0.7388 (7) | 0.3359 (3) | 0.0616 (14) | |
| H7 | 0.1715 | 0.7778 | 0.3157 | 0.074* | |
| C8 | 0.3024 (7) | 0.5809 (7) | 0.3409 (3) | 0.0594 (13) | |
| H8 | 0.2153 | 0.4872 | 0.3255 | 0.071* | |
| C9 | 0.7550 (11) | 0.8057 (10) | 0.4345 (7) | 0.079 (3) | 0.75 |
| H9A | 0.8126 | 0.8820 | 0.3945 | 0.095* | 0.75 |
| H9B | 0.7478 | 0.8690 | 0.4912 | 0.095* | 0.75 |
| C9′ | 0.771 (4) | 0.770 (4) | 0.3870 (18) | 0.066 (8)* | 0.25 |
| H9C | 0.7969 | 0.7341 | 0.3268 | 0.080* | 0.25 |

| | | | | | |
|---|---|---|---|---|---|
| H9D | 0.8152 | 0.8883 | 0.3977 | 0.080* | 0.25 |
| C10 | 0.8631 (8) | 0.6817 (9) | 0.4553 (5) | 0.099 (2) | |
| H10A | 0.9809 | 0.7330 | 0.4838 | 0.149* | 0.75 |
| H10B | 0.8729 | 0.6193 | 0.3995 | 0.149* | 0.75 |
| H10C | 0.8097 | 0.6078 | 0.4968 | 0.149* | 0.75 |
| H10D | 0.9795 | 0.7445 | 0.4775 | 0.149* | 0.25 |
| H10E | 0.8776 | 0.5746 | 0.4291 | 0.149* | 0.25 |
| H10F | 0.7946 | 0.6664 | 0.5055 | 0.149* | 0.25 |
| N1 | 0.9390 (5) | 0.8458 (5) | 1.0834 (3) | 0.0551 (10) | |
| H1N | 0.8690 | 0.8828 | 1.1183 | 0.066* | |
| N2 | 1.0314 (5) | 0.7232 (5) | 0.9728 (3) | 0.0530 (10) | |
| H2N | 1.0323 | 0.6648 | 0.9225 | 0.064* | |
| N3 | 0.4807 (6) | 0.5828 (5) | 0.3731 (3) | 0.0577 (11) | |
| H3N | 0.5303 | 0.4948 | 0.3828 | 0.069* | |
| N4 | 0.4401 (6) | 0.8336 (5) | 0.3658 (3) | 0.0570 (11) | |
| H4N | 0.4583 | 0.9411 | 0.3696 | 0.068* | |
| Cl1 | 1.08854 (17) | 0.11817 (17) | 0.30103 (10) | 0.0661 (4) | |
| Cl2 | 0.62204 (16) | 0.22853 (13) | 0.39872 (8) | 0.0516 (3) | |
| Cl3 | 0.60382 (15) | −0.01229 (18) | 0.15686 (8) | 0.0652 (4) | |
| Cl4 | 0.84770 (16) | 0.47931 (15) | 0.19336 (8) | 0.0567 (3) | |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Hg1 | 0.05255 (14) | 0.04618 (14) | 0.05352 (14) | 0.00583 (9) | 0.01238 (9) | 0.00504 (9) |
| C1 | 0.048 (3) | 0.043 (3) | 0.060 (3) | 0.010 (2) | 0.014 (2) | 0.014 (2) |
| C2 | 0.048 (3) | 0.058 (3) | 0.066 (3) | 0.006 (2) | 0.010 (3) | 0.007 (3) |
| C3 | 0.065 (3) | 0.051 (3) | 0.055 (3) | 0.002 (3) | −0.002 (3) | 0.009 (3) |
| C4 | 0.053 (3) | 0.076 (4) | 0.083 (4) | 0.001 (3) | 0.012 (3) | 0.011 (3) |
| C5 | 0.068 (4) | 0.101 (5) | 0.088 (4) | 0.004 (4) | −0.006 (3) | −0.003 (4) |
| C6 | 0.052 (3) | 0.051 (3) | 0.076 (4) | 0.004 (3) | 0.016 (3) | 0.012 (3) |
| C7 | 0.058 (3) | 0.065 (4) | 0.064 (3) | 0.012 (3) | 0.011 (3) | 0.016 (3) |
| C8 | 0.061 (3) | 0.055 (3) | 0.058 (3) | 0.001 (3) | 0.001 (3) | 0.002 (3) |
| C9 | 0.075 (6) | 0.044 (5) | 0.118 (8) | 0.006 (4) | 0.013 (6) | 0.011 (5) |
| C10 | 0.077 (4) | 0.105 (6) | 0.108 (5) | 0.011 (4) | −0.007 (4) | 0.002 (4) |
| N1 | 0.063 (3) | 0.052 (3) | 0.057 (3) | 0.013 (2) | 0.027 (2) | 0.010 (2) |
| N2 | 0.063 (2) | 0.050 (2) | 0.048 (2) | 0.009 (2) | 0.015 (2) | 0.0008 (19) |
| N3 | 0.074 (3) | 0.037 (2) | 0.068 (3) | 0.019 (2) | 0.017 (2) | 0.008 (2) |
| N4 | 0.071 (3) | 0.036 (2) | 0.067 (3) | 0.007 (2) | 0.020 (2) | 0.010 (2) |
| Cl1 | 0.0564 (7) | 0.0618 (8) | 0.0825 (9) | 0.0211 (6) | 0.0061 (7) | 0.0030 (7) |
| Cl2 | 0.0655 (7) | 0.0368 (6) | 0.0575 (7) | 0.0104 (5) | 0.0234 (6) | 0.0046 (5) |
| Cl3 | 0.0490 (6) | 0.0764 (9) | 0.0646 (8) | −0.0031 (6) | 0.0088 (6) | −0.0196 (7) |
| Cl4 | 0.0670 (7) | 0.0450 (7) | 0.0610 (7) | 0.0097 (6) | 0.0157 (6) | 0.0124 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Hg1—Cl1 | 2.4568 (14) | C7—C8 | 1.320 (7) |
| Hg1—Cl2 | 2.4811 (13) | C7—N4 | 1.353 (6) |

| | | | |
|---|---|---|---|
| Hg1—Cl4 | 2.4885 (14) | C7—H7 | 0.9300 |
| Hg1—Cl3 | 2.4936 (15) | C8—N3 | 1.366 (6) |
| C1—N1 | 1.312 (6) | C8—H8 | 0.9300 |
| C1—N2 | 1.325 (5) | C9—C10 | 1.402 (10) |
| C1—C4 | 1.490 (6) | C9—H9A | 0.9700 |
| C2—C3 | 1.332 (6) | C9—H9B | 0.9700 |
| C2—N2 | 1.366 (6) | C9′—C10 | 1.41 (3) |
| C2—H2 | 0.9300 | C9′—H9C | 0.9700 |
| C3—N1 | 1.373 (6) | C9′—H9D | 0.9700 |
| C3—H3 | 0.9300 | C10—H10A | 0.9600 |
| C4—C5 | 1.494 (7) | C10—H10B | 0.9600 |
| C4—H4A | 0.9700 | C10—H10C | 0.9600 |
| C4—H4B | 0.9700 | C10—H10D | 0.9600 |
| C5—H5A | 0.9600 | C10—H10E | 0.9601 |
| C5—H5B | 0.9600 | C10—H10F | 0.9600 |
| C5—H5C | 0.9600 | N1—H1N | 0.8602 |
| C6—N4 | 1.317 (6) | N2—H2N | 0.8606 |
| C6—N3 | 1.327 (6) | N3—H3N | 0.8598 |
| C6—C9 | 1.519 (10) | N4—H4N | 0.8599 |
| C6—C9′ | 1.55 (3) | | |

| | | | |
|---|---|---|---|
| Cl1—Hg1—Cl2 | 115.95 (5) | C10—C9′—H9C | 109.3 |
| Cl1—Hg1—Cl4 | 105.47 (5) | C6—C9′—H9C | 109.3 |
| Cl2—Hg1—Cl4 | 112.40 (4) | C10—C9′—H9D | 109.3 |
| Cl1—Hg1—Cl3 | 106.12 (5) | C6—C9′—H9D | 109.3 |
| Cl2—Hg1—Cl3 | 105.11 (4) | H9C—C9′—H9D | 108.0 |
| Cl4—Hg1—Cl3 | 111.73 (5) | C9—C10—C9′ | 32.0 (9) |
| N1—C1—N2 | 106.7 (4) | C9—C10—H10A | 109.5 |
| N1—C1—C4 | 125.2 (4) | C9′—C10—H10A | 117.4 |
| N2—C1—C4 | 128.1 (5) | C9—C10—H10B | 109.5 |
| C3—C2—N2 | 106.8 (4) | C9′—C10—H10B | 77.9 |
| C3—C2—H2 | 126.6 | H10A—C10—H10B | 109.5 |
| N2—C2—H2 | 126.6 | C9—C10—H10C | 109.5 |
| C2—C3—N1 | 106.4 (4) | C9′—C10—H10C | 126.8 |
| C2—C3—H3 | 126.8 | H10A—C10—H10C | 109.5 |
| N1—C3—H3 | 126.8 | H10B—C10—H10C | 109.5 |
| C1—C4—C5 | 113.8 (5) | C9—C10—H10D | 103.4 |
| C1—C4—H4A | 108.8 | C9′—C10—H10D | 109.5 |
| C5—C4—H4A | 108.8 | H10A—C10—H10D | 8.0 |
| C1—C4—H4B | 108.8 | H10B—C10—H10D | 107.7 |
| C5—C4—H4B | 108.8 | H10C—C10—H10D | 117.0 |
| H4A—C4—H4B | 107.7 | C9—C10—H10E | 137.6 |
| C4—C5—H5A | 109.5 | C9′—C10—H10E | 109.5 |
| C4—C5—H5B | 109.5 | H10A—C10—H10E | 106.2 |
| H5A—C5—H5B | 109.5 | H10B—C10—H10E | 35.0 |
| C4—C5—H5C | 109.5 | H10C—C10—H10E | 78.5 |
| H5A—C5—H5C | 109.5 | H10D—C10—H10E | 109.5 |
| H5B—C5—H5C | 109.5 | C9—C10—H10F | 83.0 |

| | | | |
|---|---|---|---|
| N4—C6—N3 | 105.3 (4) | C9′—C10—H10F | 109.5 |
| N4—C6—C9 | 123.8 (5) | H10A—C10—H10F | 104.5 |
| N3—C6—C9 | 130.2 (6) | H10B—C10—H10F | 136.5 |
| N4—C6—C9′ | 131.4 (12) | H10C—C10—H10F | 31.4 |
| N3—C6—C9′ | 117.9 (11) | H10D—C10—H10F | 109.5 |
| C9—C6—C9′ | 29.3 (9) | H10E—C10—H10F | 109.5 |
| C8—C7—N4 | 107.3 (5) | C1—N1—C3 | 110.2 (4) |
| C8—C7—H7 | 126.3 | C1—N1—H1N | 124.9 |
| N4—C7—H7 | 126.3 | C3—N1—H1N | 124.9 |
| C7—C8—N3 | 106.1 (5) | C1—N2—C2 | 109.9 (4) |
| C7—C8—H8 | 126.9 | C1—N2—H2N | 125.1 |
| N3—C8—H8 | 126.9 | C2—N2—H2N | 125.0 |
| C10—C9—C6 | 114.1 (6) | C6—N3—C8 | 110.5 (4) |
| C10—C9—H9A | 108.7 | C6—N3—H3N | 125.1 |
| C6—C9—H9A | 108.7 | C8—N3—H3N | 124.4 |
| C10—C9—H9B | 108.7 | C6—N4—C7 | 110.8 (4) |
| C6—C9—H9B | 108.7 | C6—N4—H4N | 124.7 |
| H9A—C9—H9B | 107.6 | C7—N4—H4N | 124.5 |
| C10—C9′—C6 | 111.5 (18) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*N*···Cl3$^{i}$ | 0.86 | 2.42 | 3.227 (4) | 157 |
| N2—H2*N*···Cl4$^{ii}$ | 0.86 | 2.37 | 3.188 (4) | 158 |
| N3—H3*N*···Cl2 | 0.86 | 2.37 | 3.220 (4) | 171 |
| N4—H4*N*···Cl2$^{iii}$ | 0.86 | 2.47 | 3.285 (4) | 159 |

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