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# 1-{2-[(2-hydroxybenzylidene)-amino]-ethyl}-3-methyl-3*H*-imidazolium hexafluorophosphate

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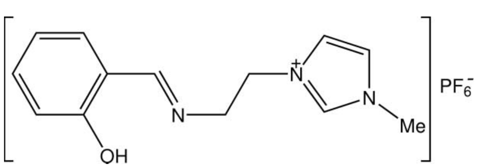
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.009 Å; $R$ factor = 0.066; $wR$ factor = 0.215; data-to-parameter ratio = 13.4.

The title Schiff base compound, $C_{13}H_{16}N_3O^+\cdot PF_6^-$, was derived from the condensation of 2-hydroxybenaldehyde with the ionic liquid 1-(2-aminoethyl)-3-methylimidazolium hexafluorophosphate in an ethanol solution. The asymmetric unit comprises one cation and two $PF_6^-$ anions. The dihedral angle between the aromatic and imidazole rings is 15.2 (2)°. An intramolecular O—H···N hydrogen bond is found which generates an $S$(6) ring motif.

## Related literature

For the synthesis of Schiff bases, see: Pradeep (2005); Butcher *et al.* (2005). For background on ionic liquids and their applications, see: Cai *et al.* (2006); Peng & Song (2006).




## Experimental

### Crystal data

$C_{13}H_{16}N_3O^+\cdot PF_6^-$
$M_r$ = 375.26
Monoclinic, $C2/c$
$a$ = 28.239 (15) Å
$b$ = 7.134 (4) Å
$c$ = 18.017 (9) Å
$\beta$ = 118.342 (6)°
$V$ = 3194 (3) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.24 mm$^{-1}$
$T$ = 298 (2) K
0.32 × 0.25 × 0.15 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.926, $T_{max}$ = 0.965
8091 measured reflections
2969 independent reflections
1965 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.043

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.215
$S$ = 1.01
2969 reflections
221 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.72 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.29 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.85 | 2.572 (5) | 147 |

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2322).

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o2365 [ doi:10.1107/S1600536808037124 ]

# 1-{2-[(2-hydroxybenzylidene)-amino]-ethyl}-3-methyl-3*H*-imidazolium hexafluorophosphate

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## Comment

The use of functionalized ionic liquids continues to receive attention in chemical synthesis and engineering, including as catalysts in organic synthesis (Cai *et al.*, 2006; Peng & Song, 2006). Schiff base compounds are one of most prevalent mixed-donor ligands in the field of coordination chemistry (Pradeep, 2005; Butcher *et al.*, 2005). Herein, we report the crystal structure of the title salt, (I).

Compound (I) is a Schiff base formed from the reaciton of 2-hydroxybenaldehyde and ionic liquid 1-(2-aminoethyl)-3-methylimidazolium hexafluorophosphate. The molecular structure of the cation is shown in Fig. 1. The aromatic and imidazole rings form a dihedral angle of 15.2 (2)°. In the cation, an intramolecular O1—H1···N1 hydrogen bond leads to a six-membered ring S(6) motif, Table 1.

## Experimental

A mixture of the ionic liquid 1-(2-aminoethyl)-3-methylimidazolium hexafluorophosphate (5 mmol) and 2-hydroxybenzaldehyde (5 mmol) in ethanol was stirred for 4 h. After the completion of the reaction, the excess ethanol was removed by distillation. The colorless solid obtained was filtered and washed with ethanol. Single crystals suitable for X-ray diffraction were obtained by slow evaporation of an ethyl acetate solution of (I) at room temperature.

## Refinement

The H atom bound to O1 was located from a difference Fourier map and refined as riding, with O—H = 0.82 Å, and with $U_{iso}$(H) = 1.5 $U_{eq}$(O). The remaining H atoms were located in a difference syntheses and refined with C—H = 0.93–0.97 Å, and with $U_{iso}$(H) = 1.2 - 1.5$U_{eq}$(C)].

## Figures

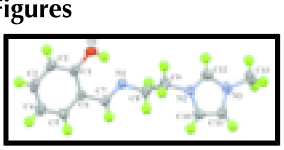

Fig. 1. The molecular structure of the cation in (I) showing the atom numbering Scheme. Displacement ellipsoids are drawn at the 50% probability level.

## 1-{2-[(2-hydroxybenzylidene)-amino]-ethyl}-3-methyl-3H-imidazolium hexafluorophosphate

*Crystal data*

| | |
|---|---|
| $C_{13}H_{16}N_3O^+ \cdot PF_6^-$ | $F_{000}$ = 1536 |
| $M_r$ = 375.26 | $D_x$ = 1.561 Mg m$^{-3}$ |
| Monoclinic, *C*2/*c* | Mo *K*α radiation |

| | |
|---|---|
| | $\lambda$ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 2060 reflections |
| $a$ = 28.239 (15) Å | $\theta$ = 2.9–22.9° |
| $b$ = 7.134 (4) Å | $\mu$ = 0.24 mm$^{-1}$ |
| $c$ = 18.017 (9) Å | $T$ = 298 (2) K |
| $\beta$ = 118.342 (6)° | Prism, yellow |
| $V$ = 3194 (3) Å$^3$ | 0.32 × 0.25 × 0.15 mm |
| $Z$ = 8 | |

*Data collection*

| | |
|---|---|
| Bruker SMART CCD area-detector diffractometer | 2969 independent reflections |
| Radiation source: fine-focus sealed tube | 1965 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.043 |
| $T$ = 298(2) K | $\theta_{max}$ = 25.5° |
| $\varphi$ and $\omega$ scans | $\theta_{min}$ = 2.3° |
| Absorption correction: multi-scan (SADABS; Sheldrick, 1996) | $h = -19 \rightarrow 34$ |
| $T_{min}$ = 0.926, $T_{max}$ = 0.965 | $k = -8 \rightarrow 8$ |
| 8091 measured reflections | $l = -21 \rightarrow 19$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)]$ = 0.066 | H-atom parameters constrained |
| $wR(F^2)$ = 0.215 | $w = 1/[\sigma^2(F_o^2) + (0.095P)^2 + 15.5678P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S$ = 1.01 | $(\Delta/\sigma)_{max} < 0.001$ |
| 2969 reflections | $\Delta\rho_{max}$ = 0.72 e Å$^{-3}$ |
| 221 parameters | $\Delta\rho_{min}$ = −0.29 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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| P1 | 0.7500 | 0.7500 | 0.0000 | 0.0501 (5) |
| P2 | 1.0000 | 0.6525 (3) | 0.2500 | 0.0583 (5) |
| F1 | 0.81350 (11) | 0.7434 (5) | 0.05733 (18) | 0.0696 (9) |
| F2 | 0.74441 (13) | 0.5737 (5) | 0.04985 (19) | 0.0742 (9) |
| F3 | 0.74598 (13) | 0.8887 (5) | 0.06617 (18) | 0.0737 (9) |
| F4 | 1.0089 (2) | 0.5007 (9) | 0.3170 (3) | 0.159 (2) |
| F5 | 0.93929 (17) | 0.6504 (10) | 0.2199 (4) | 0.162 (2) |
| F6 | 1.0081 (3) | 0.8057 (8) | 0.3156 (3) | 0.156 (2) |
| O1 | 0.80570 (15) | 0.2094 (7) | 0.2303 (3) | 0.0801 (12) |
| H1 | 0.8137 | 0.1973 | 0.1923 | 0.120* |
| N1 | 0.86812 (17) | 0.1728 (6) | 0.1638 (3) | 0.0551 (10) |
| N2 | 0.86519 (16) | 0.3299 (5) | −0.0349 (2) | 0.0513 (10) |
| N3 | 0.85173 (18) | 0.3101 (6) | −0.1622 (3) | 0.0591 (11) |
| C1 | 0.8504 (2) | 0.1958 (7) | 0.3054 (3) | 0.0566 (12) |
| C2 | 0.8461 (3) | 0.2063 (8) | 0.3792 (4) | 0.0671 (15) |
| H2 | 0.8126 | 0.2218 | 0.3762 | 0.081* |
| C3 | 0.8914 (3) | 0.1938 (8) | 0.4566 (4) | 0.0722 (16) |
| H3 | 0.8882 | 0.2028 | 0.5055 | 0.087* |
| C4 | 0.9408 (3) | 0.1686 (8) | 0.4625 (4) | 0.0719 (16) |
| H4 | 0.9710 | 0.1597 | 0.5152 | 0.086* |
| C5 | 0.9460 (2) | 0.1563 (7) | 0.3911 (3) | 0.0626 (13) |
| H5 | 0.9799 | 0.1381 | 0.3956 | 0.075* |
| C6 | 0.90111 (19) | 0.1708 (6) | 0.3114 (3) | 0.0491 (11) |
| C7 | 0.9077 (2) | 0.1593 (7) | 0.2363 (3) | 0.0536 (12) |
| H7 | 0.9419 | 0.1416 | 0.2420 | 0.064* |
| C8 | 0.8777 (2) | 0.1599 (7) | 0.0908 (3) | 0.0600 (13) |
| H8A | 0.8596 | 0.0508 | 0.0571 | 0.072* |
| H8B | 0.9160 | 0.1475 | 0.1095 | 0.072* |
| C9 | 0.8567 (2) | 0.3333 (8) | 0.0397 (3) | 0.0634 (14) |
| H9A | 0.8185 | 0.3450 | 0.0217 | 0.076* |
| H9B | 0.8748 | 0.4416 | 0.0741 | 0.076* |
| C10 | 0.9137 (2) | 0.3503 (8) | −0.0329 (3) | 0.0612 (13) |
| H10 | 0.9466 | 0.3686 | 0.0150 | 0.073* |
| C11 | 0.9053 (2) | 0.3392 (8) | −0.1120 (3) | 0.0627 (13) |
| H11 | 0.9312 | 0.3494 | −0.1297 | 0.075* |
| C12 | 0.8285 (2) | 0.3056 (7) | −0.1133 (3) | 0.0612 (13) |
| H12 | 0.7920 | 0.2881 | −0.1319 | 0.073* |
| C13 | 0.8247 (3) | 0.2925 (10) | −0.2541 (3) | 0.087 (2) |
| H13A | 0.7873 | 0.2649 | −0.2742 | 0.131* |
| H13B | 0.8410 | 0.1930 | −0.2699 | 0.131* |
| H13C | 0.8280 | 0.4080 | −0.2786 | 0.131* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| P1 | 0.0469 (10) | 0.0621 (11) | 0.0450 (9) | 0.0109 (8) | 0.0248 (8) | 0.0034 (8) |
| P2 | 0.0526 (11) | 0.0736 (13) | 0.0541 (10) | 0.000 | 0.0296 (9) | 0.000 |
| F1 | 0.0422 (16) | 0.088 (2) | 0.0708 (19) | 0.0081 (15) | 0.0202 (14) | −0.0014 (16) |
| F2 | 0.084 (2) | 0.075 (2) | 0.0696 (19) | 0.0024 (17) | 0.0408 (17) | 0.0159 (16) |
| F3 | 0.084 (2) | 0.082 (2) | 0.0611 (18) | 0.0150 (17) | 0.0393 (17) | −0.0107 (15) |
| F4 | 0.181 (5) | 0.157 (5) | 0.135 (4) | −0.002 (4) | 0.073 (4) | 0.072 (4) |
| F5 | 0.063 (3) | 0.243 (7) | 0.174 (5) | −0.004 (3) | 0.051 (3) | −0.033 (5) |
| F6 | 0.209 (6) | 0.150 (5) | 0.108 (4) | −0.003 (4) | 0.076 (4) | −0.052 (3) |
| O1 | 0.055 (2) | 0.116 (3) | 0.080 (3) | −0.006 (2) | 0.040 (2) | −0.018 (2) |
| N1 | 0.058 (3) | 0.061 (2) | 0.057 (2) | 0.001 (2) | 0.035 (2) | −0.002 (2) |
| N2 | 0.056 (2) | 0.051 (2) | 0.046 (2) | 0.0114 (18) | 0.0238 (19) | 0.0029 (17) |
| N3 | 0.069 (3) | 0.056 (2) | 0.051 (2) | 0.004 (2) | 0.027 (2) | 0.0005 (19) |
| C1 | 0.062 (3) | 0.053 (3) | 0.070 (3) | −0.009 (2) | 0.043 (3) | −0.004 (2) |
| C2 | 0.078 (4) | 0.063 (3) | 0.089 (4) | −0.009 (3) | 0.062 (4) | −0.006 (3) |
| C3 | 0.111 (5) | 0.056 (3) | 0.077 (4) | −0.003 (3) | 0.067 (4) | 0.005 (3) |
| C4 | 0.092 (4) | 0.068 (4) | 0.060 (3) | 0.007 (3) | 0.040 (3) | 0.009 (3) |
| C5 | 0.064 (3) | 0.063 (3) | 0.063 (3) | 0.011 (3) | 0.033 (3) | 0.010 (3) |
| C6 | 0.056 (3) | 0.046 (2) | 0.053 (3) | 0.002 (2) | 0.031 (2) | 0.003 (2) |
| C7 | 0.057 (3) | 0.050 (3) | 0.069 (3) | 0.005 (2) | 0.042 (3) | 0.005 (2) |
| C8 | 0.072 (3) | 0.061 (3) | 0.062 (3) | 0.003 (3) | 0.044 (3) | −0.006 (2) |
| C9 | 0.079 (4) | 0.065 (3) | 0.057 (3) | 0.016 (3) | 0.042 (3) | 0.003 (2) |
| C10 | 0.049 (3) | 0.068 (3) | 0.063 (3) | 0.003 (2) | 0.024 (2) | 0.003 (3) |
| C11 | 0.065 (3) | 0.067 (3) | 0.067 (3) | 0.006 (3) | 0.040 (3) | 0.008 (3) |
| C12 | 0.056 (3) | 0.062 (3) | 0.066 (3) | −0.001 (2) | 0.029 (3) | −0.005 (3) |
| C13 | 0.105 (5) | 0.101 (5) | 0.047 (3) | 0.002 (4) | 0.029 (3) | −0.005 (3) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| P1—F1$^{i}$ | 1.589 (3) | C1—C6 | 1.396 (7) |
| P1—F1 | 1.589 (3) | C2—C3 | 1.377 (8) |
| P1—F3 | 1.594 (3) | C2—H2 | 0.9300 |
| P1—F3$^{i}$ | 1.594 (3) | C3—C4 | 1.359 (8) |
| P1—F2$^{i}$ | 1.596 (3) | C3—H3 | 0.9300 |
| P1—F2 | 1.596 (3) | C4—C5 | 1.366 (7) |
| P2—F5$^{ii}$ | 1.533 (4) | C4—H4 | 0.9300 |
| P2—F5 | 1.533 (4) | C5—C6 | 1.398 (7) |
| P2—F6 | 1.544 (5) | C5—H5 | 0.9300 |
| P2—F6$^{ii}$ | 1.544 (5) | C6—C7 | 1.454 (6) |
| P2—F4$^{ii}$ | 1.550 (5) | C7—H7 | 0.9300 |
| P2—F4 | 1.550 (5) | C8—C9 | 1.487 (7) |
| O1—C1 | 1.346 (6) | C8—H8A | 0.9700 |
| O1—H1 | 0.8200 | C8—H8B | 0.9700 |
| N1—C7 | 1.256 (6) | C9—H9A | 0.9700 |

| | | | |
|---|---|---|---|
| N1—C8 | 1.467 (6) | C9—H9B | 0.9700 |
| N2—C12 | 1.308 (6) | C10—C11 | 1.333 (7) |
| N2—C10 | 1.360 (6) | C10—H10 | 0.9300 |
| N2—C9 | 1.474 (6) | C11—H11 | 0.9300 |
| N3—C12 | 1.324 (6) | C12—H12 | 0.9300 |
| N3—C11 | 1.360 (7) | C13—H13A | 0.9600 |
| N3—C13 | 1.464 (6) | C13—H13B | 0.9600 |
| C1—C2 | 1.392 (7) | C13—H13C | 0.9600 |

| | | | |
|---|---|---|---|
| $F1^{i}$—P1—F1 | 180.00 (12) | C1—C2—H2 | 119.9 |
| $F1^{i}$—P1—F3 | 90.50 (16) | C4—C3—C2 | 120.9 (5) |
| F1—P1—F3 | 89.50 (16) | C4—C3—H3 | 119.6 |
| $F1^{i}$—P1—$F3^{i}$ | 89.50 (16) | C2—C3—H3 | 119.6 |
| F1—P1—$F3^{i}$ | 90.50 (16) | C3—C4—C5 | 120.1 (6) |
| F3—P1—$F3^{i}$ | 180.0 (2) | C3—C4—H4 | 120.0 |
| $F1^{i}$—P1—$F2^{i}$ | 89.62 (17) | C5—C4—H4 | 120.0 |
| F1—P1—$F2^{i}$ | 90.38 (17) | C4—C5—C6 | 120.8 (5) |
| F3—P1—$F2^{i}$ | 89.60 (17) | C4—C5—H5 | 119.6 |
| $F3^{i}$—P1—$F2^{i}$ | 90.40 (17) | C6—C5—H5 | 119.6 |
| $F1^{i}$—P1—F2 | 90.38 (17) | C1—C6—C5 | 119.1 (4) |
| F1—P1—F2 | 89.62 (17) | C1—C6—C7 | 121.1 (5) |
| F3—P1—F2 | 90.40 (17) | C5—C6—C7 | 119.8 (4) |
| $F3^{i}$—P1—F2 | 89.60 (17) | N1—C7—C6 | 121.3 (4) |
| $F2^{i}$—P1—F2 | 180.0 (2) | N1—C7—H7 | 119.4 |
| $F5^{ii}$—P2—F5 | 178.9 (5) | C6—C7—H7 | 119.4 |
| $F5^{ii}$—P2—F6 | 90.1 (4) | N1—C8—C9 | 108.2 (4) |
| F5—P2—F6 | 90.7 (3) | N1—C8—H8A | 110.1 |
| $F5^{ii}$—P2—$F6^{ii}$ | 90.7 (3) | C9—C8—H8A | 110.1 |
| F5—P2—$F6^{ii}$ | 90.1 (3) | N1—C8—H8B | 110.1 |
| F6—P2—$F6^{ii}$ | 89.9 (5) | C9—C8—H8B | 110.1 |
| $F5^{ii}$—P2—$F4^{ii}$ | 90.6 (3) | H8A—C8—H8B | 108.4 |
| F5—P2—$F4^{ii}$ | 88.6 (3) | N2—C9—C8 | 111.1 (4) |
| F6—P2—$F4^{ii}$ | 179.0 (4) | N2—C9—H9A | 109.4 |
| $F6^{ii}$—P2—$F4^{ii}$ | 89.3 (3) | C8—C9—H9A | 109.4 |
| $F5^{ii}$—P2—F4 | 88.6 (3) | N2—C9—H9B | 109.4 |
| F5—P2—F4 | 90.6 (3) | C8—C9—H9B | 109.4 |
| F6—P2—F4 | 89.3 (3) | H9A—C9—H9B | 108.0 |
| $F6^{ii}$—P2—F4 | 179.0 (4) | C11—C10—N2 | 107.4 (5) |
| $F4^{ii}$—P2—F4 | 91.4 (5) | C11—C10—H10 | 126.3 |
| C1—O1—H1 | 109.5 | N2—C10—H10 | 126.3 |
| C7—N1—C8 | 118.3 (4) | C10—C11—N3 | 107.3 (5) |
| C12—N2—C10 | 108.3 (4) | C10—C11—H11 | 126.4 |
| C12—N2—C9 | 126.8 (5) | N3—C11—H11 | 126.4 |
| C10—N2—C9 | 124.9 (4) | N2—C12—N3 | 109.1 (5) |
| C12—N3—C11 | 107.9 (4) | N2—C12—H12 | 125.5 |

| | | | |
|---|---|---|---|
| C12—N3—C13 | 126.4 (5) | N3—C12—H12 | 125.5 |
| C11—N3—C13 | 125.7 (5) | N3—C13—H13A | 109.5 |
| O1—C1—C2 | 119.5 (5) | N3—C13—H13B | 109.5 |
| O1—C1—C6 | 121.6 (4) | H13A—C13—H13B | 109.5 |
| C2—C1—C6 | 118.9 (5) | N3—C13—H13C | 109.5 |
| C3—C2—C1 | 120.3 (5) | H13A—C13—H13C | 109.5 |
| C3—C2—H2 | 119.9 | H13B—C13—H13C | 109.5 |

| | | | |
|---|---|---|---|
| O1—C1—C2—C3 | −179.6 (5) | C7—N1—C8—C9 | −123.0 (5) |
| C6—C1—C2—C3 | 0.6 (8) | C12—N2—C9—C8 | 107.3 (6) |
| C1—C2—C3—C4 | −0.9 (8) | C10—N2—C9—C8 | −72.1 (7) |
| C2—C3—C4—C5 | 0.4 (9) | N1—C8—C9—N2 | 179.9 (4) |
| C3—C4—C5—C6 | 0.5 (9) | C12—N2—C10—C11 | 0.5 (6) |
| O1—C1—C6—C5 | −179.6 (5) | C9—N2—C10—C11 | 180.0 (5) |
| C2—C1—C6—C5 | 0.3 (7) | N2—C10—C11—N3 | −0.6 (6) |
| O1—C1—C6—C7 | 0.3 (7) | C12—N3—C11—C10 | 0.5 (6) |
| C2—C1—C6—C7 | −179.9 (5) | C13—N3—C11—C10 | 178.9 (5) |
| C4—C5—C6—C1 | −0.8 (8) | C10—N2—C12—N3 | −0.1 (6) |
| C4—C5—C6—C7 | 179.3 (5) | C9—N2—C12—N3 | −179.6 (4) |
| C8—N1—C7—C6 | −180.0 (4) | C11—N3—C12—N2 | −0.2 (6) |
| C1—C6—C7—N1 | 0.5 (7) | C13—N3—C12—N2 | −178.6 (5) |
| C5—C6—C7—N1 | −179.7 (5) | | |

Symmetry codes: (i) $-x+3/2$, $-y+3/2$, $-z$; (ii) $-x+2$, $y$, $-z+1/2$.

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1 | 0.82 | 1.85 | 2.572 (5) | 147 |

**Fig. 1**