# 4-(4-Methoxyphenyl)piperazin-1-ium chloride

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In the title compound, $C_{11}H_{17}N_2O^+\cdot Cl^-$, the dihedral angle between the benzene ring and the basal plane of piperazine ring is 39.20 (8)°. In the crystal, intermolecular N—H···Cl hydrogen bonds occur. There is also a C—H···$\pi$ interaction between the benzene rings.

## Related literature

The title compound was obtained as a by-product in a continuation of work on the synthesis of tin complexes containing piperazine, see: Zia-ur-Rahman *et al.* (2006, 2007). For related structures, see: Lu (2007); Sadiq-ur-Rehman *et al.* (2007).
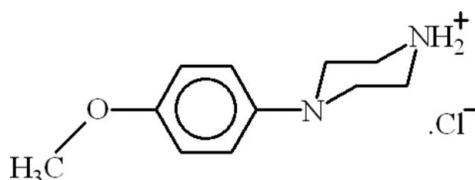


## Experimental

### Crystal data

| | |
|---|---|
| $C_{11}H_{17}N_2O^+\cdot Cl^-$ | $V$ = 2461.9 (3) Å$^3$ |
| $M_r$ = 228.72 | $Z$ = 8 |
| Orthorhombic, $Iba2$ | Mo $K\alpha$ radiation |
| $a$ = 10.2890 (7) Å | $\mu$ = 0.29 mm$^{-1}$ |
| $b$ = 31.5218 (18) Å | $T$ = 296 (2) K |
| $c$ = 7.5909 (5) Å | 0.28 × 0.22 × 0.15 mm |

### Data collection

| | |
|---|---|
| Bruker KAPPA APEXII CCD diffractometer | 7605 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Bruker, 2005) | 3073 independent reflections |
| $T_{min}$ = 0.922, $T_{max}$ = 0.950 | 2327 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.026 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | H-atom parameters constrained |
| $wR(F^2)$ = 0.139 | $\Delta\rho_{max}$ = 0.35 e Å$^{-3}$ |
| $S$ = 1.01 | $\Delta\rho_{min}$ = −0.29 e Å$^{-3}$ |
| 3073 reflections | Absolute structure: Flack (1983), 1076 Friedel pairs |
| 137 parameters | Flack parameter: 0.05 (9) |
| 1 restraint | |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2A···Cl1$^i$ | 0.90 | 2.20 | 3.082 (2) | 168 |
| N2—H2B···Cl1 | 0.90 | 2.24 | 3.134 (3) | 177 |
| C3—H3···CgA$^{ii}$ | 0.93 | 2.88 | 3.573 (2) | 133 |

Symmetry codes: (i) $x, -y, z + \frac{1}{2}$; (ii) $-x + \frac{1}{2}, -y + \frac{1}{2}, z - \frac{1}{2}$. CgA is the centroid of the benzene ring.

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* publication routines (Farrugia, 1999) and *PLATON*.

## References

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## organic compounds

# supporting information

# 4-(4-Methoxyphenyl)piperazin-1-ium chloride

## Zia-ur-Rehman, M. Nawaz Tahir, Muhammad Danish, Niaz Muhammad and Saqib Ali

### S1. Comment

In continuation to synthesizing the tin complexes containing piperazine (Zia-ur-Rahman *et al.*, 2006, 2007), the title compound (I), (Fig 1) has been obtained as a byproduct.

The crystal structures of (II) 4-nitrophenylpiperazinium chloride monohydrate (Lu, 2007) and 4-(2-pyridyl)piperazin-1-ium chloride (Sadiq-ur-Rehman *et al.*, 2007) has been reported. The title compound have a replacement of nitro group in (II) with methoxy at the same position. Due to this change it is observed that (I) does not contain water molecule although the aquas medium was present during crystallization. In the title compound the benzene ring A(C1—C6) is planar along with the methoxy group. The piperazinium is in chair form with the basal plane B(C8—C11) and the N–atoms are at a distance of 0.6680 (37) and -0.6620 (46) Å. The dihedral angle between the groups A and B is 39.20 (8)°. The molecules are linked each other through intra and intermolecular H–bonding (Table 1, Fig 2). There exists a $\pi$ interaction between the C3–H3 and the centroid of the benzene ring.

### S2. Experimental

$Me_2SnCl_2$ (0.24 g, 1.08 mmol) in methanol (30 ml) was added dropwise to 4-(4-methoxyphenyl)piperazinium 4-(4-methoxyphenyl)piperazine-1-carbodithioate (0.5 g, 1.08 mmol) in methanol (30 ml) and the mixture was refluxed for 3 h with constant stirring. The 4-(4-methoxyphenyl)piperazinium chloride thus formed, was filtered off and recrystallized from water-ethanol (1:4) to give colourless crystals.

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model, with N–H = 0.90Å and with $U_{iso}(H)$ = $1.2U_{eq}(C)$, and with C–H = 0.93–0.97Å and with $U_{iso}(H)$ = $1.2U_{eq}(C)$ [C–H = 0.96Å and $U_{iso}(H)$ = $1.5U_{eq}(C)$ for the methyl group].
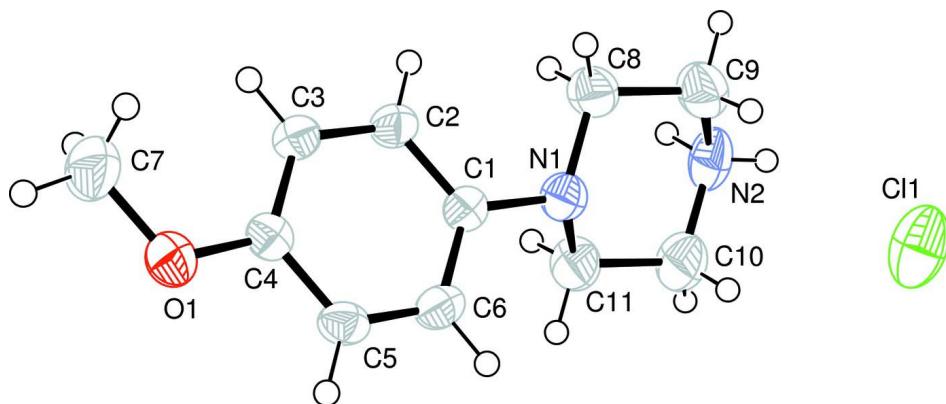
**Figure 1**

*ORTEP* drawing of the title compound, with the atom numbering scheme. The thermal ellipsoids are drawn at the 50% probability level. H-atoms are shown by small circles of arbitrary radii.
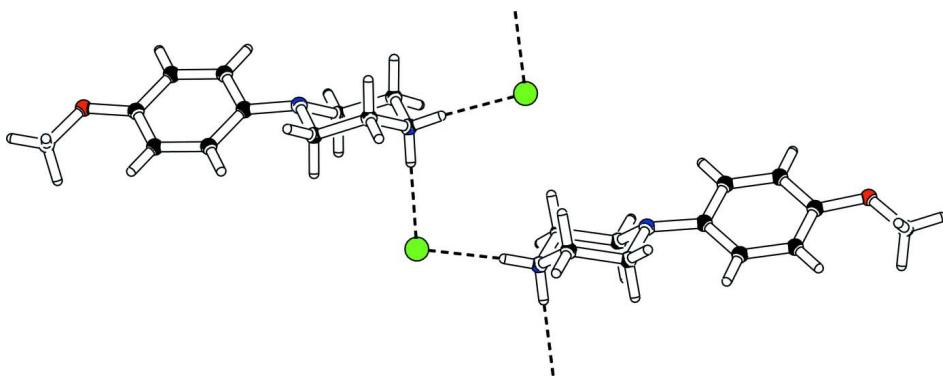


**Figure 2**

The partial packing figure (*PLATON*: Spek, 2009) which shows the dimeric nature of the compound.

### 4-(4-Methoxyphenyl)piperazin-1-ium chloride

*Crystal data*

| | |
|---|---|
| $C_{11}H_{17}N_2O^+ \cdot Cl^-$ | $F(000) = 976$ |
| $M_r = 228.72$ | $D_x = 1.234$ Mg m$^{-3}$ |
| Orthorhombic, *Iba*2 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| Hall symbol: I 2 -2c | Cell parameters from 3073 reflections |
| $a = 10.2890\,(7)$ Å | $\theta = 1.2$–30.5° |
| $b = 31.5218\,(18)$ Å | $\mu = 0.29$ mm$^{-1}$ |
| $c = 7.5909\,(5)$ Å | $T = 296$ K |
| $V = 2461.9\,(3)$ Å$^3$ | Prismatic, colourless |
| $Z = 8$ | $0.28 \times 0.22 \times 0.15$ mm |

*Data collection*

| | |
|---|---|
| Bruker KAPPA APEXII CCD diffractometer | Absorption correction: multi-scan (*SADABS*; Bruker, 2005) |
| Radiation source: fine-focus sealed tube | $T_{min} = 0.922$, $T_{max} = 0.950$ |
| Graphite monochromator | 7605 measured reflections |
| Detector resolution: 7.3 pixels mm$^{-1}$ | 3073 independent reflections |
| $\omega$ scans | 2327 reflections with $I > 2\sigma(I)$ |
| | $R_{int} = 0.026$ |

$\theta_{max} = 30.5°$, $\theta_{min} = 1.3°$

$h = -14 \rightarrow 12$

$k = -42 \rightarrow 44$

$l = -5 \rightarrow 10$

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | |
| $R[F^2 > 2\sigma(F^2)] = 0.044$ | H-atom parameters constrained |
| $wR(F^2) = 0.139$ | $w = 1/[\sigma^2(F_o^2) + (0.0883P)^2 + 0.0737P]$ |
| $S = 1.01$ | where $P = (F_o^2 + 2F_c^2)/3$ |
| 3073 reflections | $(\Delta/\sigma)_{max} < 0.001$ |
| 137 parameters | $\Delta\rho_{max} = 0.35$ e Å$^{-3}$ |
| 1 restraint | $\Delta\rho_{min} = -0.29$ e Å$^{-3}$ |
| Primary atom site location: structure-invariant direct methods | Extinction correction: *SHELXL*, Fc$^*$=kFc[1+0.001xFc$^2\lambda^3$/sin(2$\theta$)]$^{-1/4}$ |
| Secondary atom site location: difference Fourier map | Extinction coefficient: 0.0136 (13) |
| | Absolute structure: Flack (1983), 1076 Friedel pairs |
| | Absolute structure parameter: 0.05 (9) |

*Special details*

**Geometry**. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

**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$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.41690 (13) | 0.30736 (4) | 0.7357 (3) | 0.0454 (4) |
| N1 | 0.30676 (15) | 0.13295 (5) | 0.7320 (3) | 0.0407 (5) |
| N2 | 0.25384 (18) | 0.04631 (6) | 0.6512 (4) | 0.0561 (8) |
| C1 | 0.33328 (16) | 0.17757 (5) | 0.7214 (3) | 0.0334 (5) |
| C2 | 0.25085 (17) | 0.20603 (6) | 0.6364 (3) | 0.0368 (6) |
| C3 | 0.27578 (17) | 0.24960 (7) | 0.6389 (3) | 0.0362 (6) |
| C4 | 0.38456 (16) | 0.26505 (6) | 0.7235 (3) | 0.0329 (5) |
| C5 | 0.46885 (18) | 0.23669 (6) | 0.8075 (3) | 0.0371 (5) |
| C6 | 0.44271 (18) | 0.19397 (6) | 0.8060 (3) | 0.0386 (6) |
| C7 | 0.3309 (3) | 0.33675 (8) | 0.6540 (4) | 0.0641 (9) |
| C8 | 0.1772 (2) | 0.11964 (7) | 0.6751 (3) | 0.0486 (7) |
| C9 | 0.1533 (2) | 0.07386 (7) | 0.7291 (4) | 0.0563 (7) |
| C10 | 0.3855 (3) | 0.06000 (7) | 0.7054 (4) | 0.0617 (9) |
| C11 | 0.4071 (2) | 0.10588 (7) | 0.6540 (4) | 0.0513 (7) |
| Cl1 | 0.24567 (7) | 0.04913 (2) | 0.23863 (13) | 0.0710 (3) |
| H2 | 0.17815 | 0.19587 | 0.57701 | 0.0442* |
| H2A | 0.24059 | 0.01935 | 0.68585 | 0.0673* |
| H2B | 0.24770 | 0.04718 | 0.53299 | 0.0673* |
| H3 | 0.21888 | 0.26823 | 0.58342 | 0.0435* |
| H5 | 0.54265 | 0.24678 | 0.86451 | 0.0446* |

| | | | |
|---|---|---|---|
| H6 | 0.49937 | 0.17549 | 0.86277 | 0.0464* |
| H7A | 0.36281 | 0.36507 | 0.67113 | 0.0962* |
| H7B | 0.32577 | 0.33080 | 0.53014 | 0.0962* |
| H7C | 0.24605 | 0.33421 | 0.70556 | 0.0962* |
| H8A | 0.11208 | 0.13783 | 0.72828 | 0.0583* |
| H8B | 0.17019 | 0.12226 | 0.54811 | 0.0583* |
| H9A | 0.06804 | 0.06493 | 0.68906 | 0.0675* |
| H9B | 0.15557 | 0.07151 | 0.85649 | 0.0675* |
| H10A | 0.39486 | 0.05691 | 0.83195 | 0.0742* |
| H10B | 0.45021 | 0.04222 | 0.64893 | 0.0742* |
| H11A | 0.40474 | 0.10852 | 0.52670 | 0.0615* |
| H11B | 0.49212 | 0.11503 | 0.69420 | 0.0615* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0468 (7) | 0.0384 (7) | 0.0510 (9) | −0.0060 (5) | −0.0035 (8) | 0.0000 (8) |
| N1 | 0.0415 (8) | 0.0359 (7) | 0.0447 (9) | 0.0009 (6) | 0.0001 (9) | 0.0004 (8) |
| N2 | 0.0814 (15) | 0.0327 (10) | 0.0542 (14) | −0.0018 (8) | −0.0042 (10) | 0.0048 (9) |
| C1 | 0.0351 (8) | 0.0346 (8) | 0.0306 (9) | 0.0019 (6) | 0.0006 (9) | −0.0009 (8) |
| C2 | 0.0353 (9) | 0.0401 (10) | 0.0351 (11) | −0.0007 (7) | −0.0065 (8) | 0.0002 (8) |
| C3 | 0.0345 (9) | 0.0382 (10) | 0.0359 (10) | 0.0024 (7) | −0.0041 (8) | 0.0011 (8) |
| C4 | 0.0340 (8) | 0.0373 (8) | 0.0273 (8) | −0.0021 (6) | 0.0038 (8) | −0.0019 (8) |
| C5 | 0.0320 (8) | 0.0467 (10) | 0.0327 (9) | −0.0036 (8) | −0.0052 (8) | −0.0020 (8) |
| C6 | 0.0352 (9) | 0.0458 (10) | 0.0349 (10) | 0.0064 (8) | −0.0030 (8) | 0.0038 (8) |
| C7 | 0.0701 (16) | 0.0391 (12) | 0.083 (2) | −0.0030 (11) | −0.0173 (15) | 0.0059 (12) |
| C8 | 0.0468 (11) | 0.0391 (11) | 0.0599 (16) | −0.0038 (9) | −0.0042 (10) | −0.0035 (9) |
| C9 | 0.0571 (12) | 0.0463 (11) | 0.0654 (15) | −0.0088 (9) | 0.0005 (14) | 0.0007 (13) |
| C10 | 0.0658 (14) | 0.0392 (11) | 0.080 (2) | 0.0088 (10) | 0.0024 (14) | 0.0063 (12) |
| C11 | 0.0502 (12) | 0.0381 (10) | 0.0655 (15) | 0.0066 (9) | 0.0077 (11) | 0.0001 (10) |
| Cl1 | 0.1167 (6) | 0.0368 (3) | 0.0596 (4) | 0.0072 (3) | −0.0038 (4) | −0.0031 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.378 (2) | C10—C11 | 1.514 (3) |
| O1—C7 | 1.423 (3) | C2—H2 | 0.9300 |
| N1—C1 | 1.435 (2) | C3—H3 | 0.9300 |
| N1—C8 | 1.463 (3) | C5—H5 | 0.9300 |
| N1—C11 | 1.464 (3) | C6—H6 | 0.9300 |
| N2—C9 | 1.474 (3) | C7—H7A | 0.9600 |
| N2—C10 | 1.480 (4) | C7—H7B | 0.9600 |
| N2—H2A | 0.9000 | C7—H7C | 0.9600 |
| N2—H2B | 0.9000 | C8—H8A | 0.9700 |
| C1—C2 | 1.393 (3) | C8—H8B | 0.9700 |
| C1—C6 | 1.396 (3) | C9—H9A | 0.9700 |
| C2—C3 | 1.397 (3) | C9—H9B | 0.9700 |
| C3—C4 | 1.379 (3) | C10—H10A | 0.9700 |
| C4—C5 | 1.399 (3) | C10—H10B | 0.9700 |

| | | | |
|---|---|---|---|
| C5—C6 | 1.373 (3) | C11—H11A | 0.9700 |
| C8—C9 | 1.520 (3) | C11—H11B | 0.9700 |
| | | | |
| Cl1···N2 | 3.134 (3) | H2···H8A | 2.2600 |
| Cl1···N2ⁱ | 3.082 (2) | H2···H8B | 2.3300 |
| Cl1···H2Aⁱ | 2.2000 | H2A···Cl1�vⁱ | 2.2000 |
| Cl1···H9Bⁱⁱ | 3.1300 | H2B···H11A | 2.5200 |
| Cl1···H2B | 2.2400 | H2B···Cl1 | 2.2400 |
| Cl1···H7Aⁱⁱⁱ | 2.9700 | H2B···H8B | 2.5000 |
| O1···H2ⁱv | 2.7700 | H3···C5ⁱⁱⁱ | 2.8500 |
| O1···H8Av | 2.6500 | H3···C7 | 2.5100 |
| N1···N2 | 2.852 (3) | H3···H7B | 2.2900 |
| N2···N1 | 2.852 (3) | H3···H7C | 2.2900 |
| N2···Cl1 | 3.134 (3) | H3···C6ⁱⁱⁱ | 2.9400 |
| N2···Cl1vⁱ | 3.082 (2) | H3···C5vⁱⁱ | 3.0900 |
| N1···H7Bⁱv | 2.8800 | H5···C3ⁱx | 2.8000 |
| C2···C4ⁱⁱⁱ | 3.549 (3) | H5···C3v | 2.9500 |
| C3···C5vⁱⁱ | 3.435 (3) | H5···C4ⁱx | 2.8800 |
| C3···C5ⁱⁱⁱ | 3.585 (3) | H6···C11 | 2.8700 |
| C3···C4ⁱⁱⁱ | 3.589 (3) | H6···H11B | 2.3000 |
| C4···C2ⁱv | 3.549 (3) | H7A···Cl1ⁱv | 2.9700 |
| C4···C3ⁱv | 3.589 (3) | H7B···C3 | 2.7400 |
| C5···C3v | 3.435 (3) | H7B···C1ⁱⁱⁱ | 2.8700 |
| C5···C3ⁱv | 3.585 (3) | H7B···H3 | 2.2900 |
| C1···H7Bⁱv | 2.8700 | H7B···N1ⁱⁱⁱ | 2.8800 |
| C2···H8A | 2.6700 | H7B···H8Aⁱⁱⁱ | 2.5800 |
| C2···H8B | 2.8500 | H7C···H3 | 2.2900 |
| C3···H5vⁱⁱⁱ | 2.8000 | H7C···C3 | 2.7300 |
| C3···H5vⁱⁱ | 2.9500 | H8A···C2 | 2.6700 |
| C3···H7C | 2.7300 | H8A···H7Bⁱv | 2.5800 |
| C3···H7B | 2.7400 | H8A···O1vⁱⁱ | 2.6500 |
| C4···H2ⁱv | 3.0200 | H8A···H2 | 2.2600 |
| C4···H5vⁱⁱⁱ | 2.8800 | H8A···C7vⁱⁱ | 3.0500 |
| C5···H3v | 3.0900 | H8B···H2B | 2.5000 |
| C5···H3ⁱv | 2.8500 | H8B···H11A | 2.4600 |
| C6···H11B | 2.6800 | H8B···C2 | 2.8500 |
| C6···H3ⁱv | 2.9400 | H8B···H2 | 2.3300 |
| C7···H8Av | 3.0500 | H9B···Cl1x | 3.1300 |
| C7···H3 | 2.5100 | H9B···H10A | 2.5100 |
| C8···H2 | 2.5200 | H10A···H9B | 2.5100 |
| C11···H6 | 2.8700 | H11A···H2B | 2.5200 |
| H2···C8 | 2.5200 | H11A···H8B | 2.4600 |
| H2···C4ⁱⁱⁱ | 3.0200 | H11B···H6 | 2.3000 |
| H2···O1ⁱⁱⁱ | 2.7700 | H11B···C6 | 2.6800 |
| | | | |
| C4—O1—C7 | 116.79 (18) | C6—C5—H5 | 120.00 |
| C1—N1—C8 | 115.97 (16) | C1—C6—H6 | 119.00 |
| C1—N1—C11 | 114.48 (16) | C5—C6—H6 | 119.00 |

| | | | |
|---|---|---|---|
| C8—N1—C11 | 110.85 (17) | O1—C7—H7A | 109.00 |
| C9—N2—C10 | 111.0 (2) | O1—C7—H7B | 109.00 |
| C9—N2—H2B | 109.00 | O1—C7—H7C | 109.00 |
| C10—N2—H2A | 109.00 | H7A—C7—H7B | 109.00 |
| C10—N2—H2B | 109.00 | H7A—C7—H7C | 109.00 |
| H2A—N2—H2B | 108.00 | H7B—C7—H7C | 109.00 |
| C9—N2—H2A | 109.00 | N1—C8—H8A | 110.00 |
| N1—C1—C2 | 122.78 (16) | N1—C8—H8B | 110.00 |
| N1—C1—C6 | 119.39 (17) | C9—C8—H8A | 110.00 |
| C2—C1—C6 | 117.76 (16) | C9—C8—H8B | 110.00 |
| C1—C2—C3 | 120.99 (17) | H8A—C8—H8B | 108.00 |
| C2—C3—C4 | 120.16 (18) | N2—C9—H9A | 110.00 |
| O1—C4—C5 | 115.99 (17) | N2—C9—H9B | 110.00 |
| O1—C4—C3 | 124.69 (18) | C8—C9—H9A | 110.00 |
| C3—C4—C5 | 119.31 (18) | C8—C9—H9B | 110.00 |
| C4—C5—C6 | 120.09 (18) | H9A—C9—H9B | 108.00 |
| C1—C6—C5 | 121.68 (18) | N2—C10—H10A | 110.00 |
| N1—C8—C9 | 109.88 (17) | N2—C10—H10B | 110.00 |
| N2—C9—C8 | 109.72 (19) | C11—C10—H10A | 110.00 |
| N2—C10—C11 | 110.0 (2) | C11—C10—H10B | 110.00 |
| N1—C11—C10 | 110.4 (2) | H10A—C10—H10B | 108.00 |
| C1—C2—H2 | 119.00 | N1—C11—H11A | 110.00 |
| C3—C2—H2 | 120.00 | N1—C11—H11B | 110.00 |
| C2—C3—H3 | 120.00 | C10—C11—H11A | 110.00 |
| C4—C3—H3 | 120.00 | C10—C11—H11B | 110.00 |
| C4—C5—H5 | 120.00 | H11A—C11—H11B | 108.00 |
| | | | |
| C7—O1—C4—C3 | −0.2 (3) | N1—C1—C2—C3 | 175.8 (2) |
| C7—O1—C4—C5 | −178.8 (2) | C6—C1—C2—C3 | −1.2 (3) |
| C8—N1—C1—C2 | −10.2 (3) | N1—C1—C6—C5 | −176.6 (2) |
| C8—N1—C1—C6 | 166.8 (2) | C2—C1—C6—C5 | 0.5 (3) |
| C11—N1—C1—C2 | 120.9 (2) | C1—C2—C3—C4 | 1.2 (3) |
| C11—N1—C1—C6 | −62.2 (3) | C2—C3—C4—O1 | −179.0 (2) |
| C1—N1—C8—C9 | −168.1 (2) | C2—C3—C4—C5 | −0.4 (3) |
| C11—N1—C8—C9 | 59.1 (3) | O1—C4—C5—C6 | 178.4 (2) |
| C1—N1—C11—C10 | 167.9 (2) | C3—C4—C5—C6 | −0.3 (3) |
| C8—N1—C11—C10 | −58.6 (3) | C4—C5—C6—C1 | 0.3 (3) |
| C10—N2—C9—C8 | 57.6 (3) | N1—C8—C9—N2 | −58.2 (3) |
| C9—N2—C10—C11 | −56.9 (3) | N2—C10—C11—N1 | 56.8 (3) |

Symmetry codes: (i) $x$, $-y$, $z-1/2$; (ii) $x$, $y$, $z-1$; (iii) $-x+1/2$, $-y+1/2$, $z-1/2$; (iv) $-x+1/2$, $-y+1/2$, $z+1/2$; (v) $x+1/2$, $-y+1/2$, $z$; (vi) $x$, $-y$, $z+1/2$; (vii) $x-1/2$, $-y+1/2$, $z$; (viii) $-x+1$, $y$, $z-1/2$; (ix) $-x+1$, $y$, $z+1/2$; (x) $x$, $y$, $z+1$.

*Hydrogen-bond geometry (Å, º)*

| D—H···A | D—H | H···A | D···A | D—H···A |
|---|---|---|---|---|
| N2—H2A···Cl1[vi] | 0.90 | 2.20 | 3.082 (2) | 168 |

| | | | | |
|---|---|---|---|---|
| N2—H2*B*···Cl1 | 0.90 | 2.24 | 3.134 (3) | 177 |
| C3—H3···CgA[iii] | 0.93 | 2.88 | 3.573 (2) | 133 |

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