Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

4-Methoxyphenylguanidinium chloride

Hong Ren, Chao Cai, Jun-Zhi Liu and Jian-Wu Wang*

School of Chemistry and Chemical Engineering, Shandong University, Jinan 250100, People's Republic of China

Correspondence e-mail: yugp2005@yahoo.com.cn

Key indicators

Single-crystal X-ray study
T = 298 K
Mean σ(C–C) = 0.003 Å
R factor = 0.039
wR factor = 0.101
Data-to-parameter ratio = 14.9

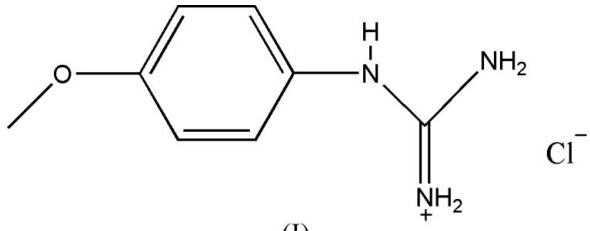
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 12 November 2006
Accepted 8 December 2006

In the title compound, $C_8H_{12}N_3O^+\cdot Cl^-$, all bond lengths and angles show normal values. The crystal packing is stabilized by intermolecular N—H···Cl and N—H···O hydrogen bonds, which link the molecules into infinite ribbons running along the *b* axis.

Comment

Guanidine-containing compounds have been employed as antimicrobials and fungicides on a considerable scale (Yonehara & Otake, 1966). Drugs containing the guanidine framework are not only easy to transport (Berlinck, 1995; Gao & Xie, 2006), but also make the functions of absorption and osmosis more selective due to the good solubility of their various acid salts in aqueous solution (Gobbi & Frenking, 1993; Riordan, 1979). We report here the crystal structure of the title guanidine-containing compound, (I).



(I)

In (I) (Fig. 1), all bond lengths and angles are normal (Allen *et al.*, 1987). The dihedral angle between the guanidine (atoms N1–N3/C8) mean plane and benzene ring C2–C7 is 74.76 (2)°. Intermolecular N—H···Cl and N—H···O hydrogen bonds (Table 1) link the molecules into infinite ribbons running along the *b* axis (Fig. 2).

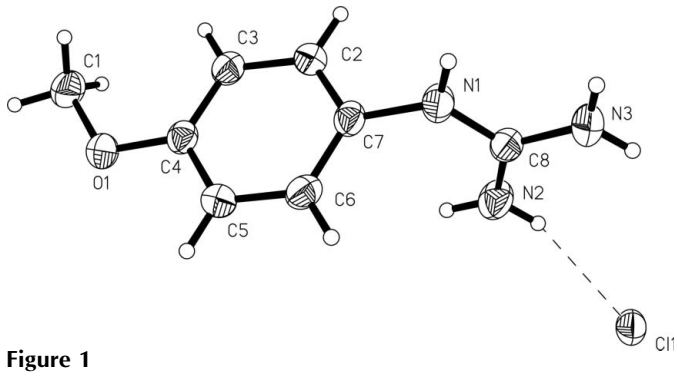


Figure 1
The molecular structure of the title compound (I), with displacement ellipsoids drawn at the 40% probability level. The dashed line indicates a hydrogen bond.

Experimental

The title compound was prepared according to the method of Maryanoff *et al.* (1986). Aminoiminomethanesulfonic acid (0.01 mol) was added to a solution of 4-methoxybenzenamine (0.01 mol) in acetonitrile (20 ml) and stirred at room temperature. The reaction process was monitored by thin-layer chromatography until the starting material had disappeared. The reaction mixture was adjusted to pH 2–3 with concentrated hydrochloric acid, and the desired product then precipitated and was collected by filtration. Single crystals suitable for X-ray measurements were obtained by recrystallization from methanol at room temperature.

Crystal data

$C_8H_{12}N_3O^+\cdot Cl^-$
M_r = 201.66
Triclinic, $P\overline{1}$
a = 6.605 (4) Å
b = 7.618 (5) Å
c = 10.497 (7) Å
α = 70.778 (8)°
β = 78.696 (9)°
γ = 89.888 (9)°
V = 487.9 (5) Å^3
Z = 2
D_x = 1.373 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 298 (2) K
Block, colourless
0.49 × 0.46 × 0.38 mm

Data collection

Bruker SMART CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.845, T_{max} = 0.877
2626 measured reflections
1778 independent reflections
1519 reflections with $I > 2\sigma(I)$
R_{int} = 0.016
θ_{max} = 25.5°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.08
1778 reflections
119 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.1401P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.072 (8)

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl1	0.86	2.44	3.270 (2)	161
N1—H1A···Cl1^{i}	0.86	2.38	3.202 (2)	161
N3—H3B···Cl1^{ii}	0.86	2.56	3.244 (3)	137
N3—H3C···Cl1^{i}	0.86	2.65	3.397 (3)	146
N2—H2B···O1^{iii}	0.86	2.36	3.093 (3)	144

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

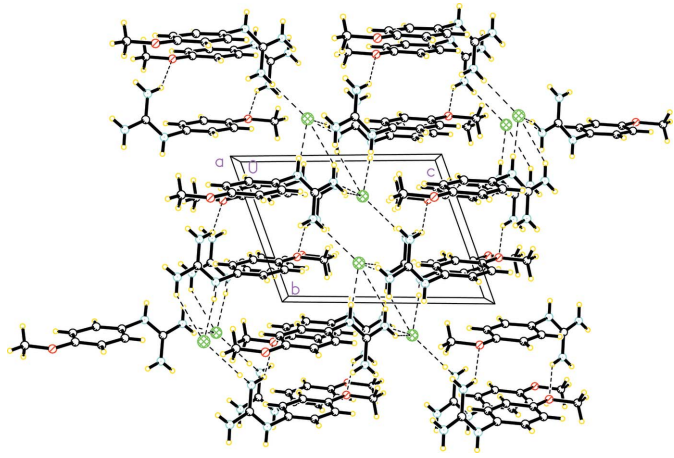


Figure 2
A packing diagram of the title compound, viewed down the *a* axis. The dashed lines indicate hydrogen bonds.

All H atoms were placed in calculated positions, with C—H = 0.93 or 0.96 Å and N—H = 0.86 Å, and refined using a riding model, with U_{iso}(H) = 1.2U_{eq} (1.5U_{eq} for the methyl group) of the parent atom.

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

References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Berlinck, R. G. S. (1995). *Prog. Chem. Org. Nat. Prod.* **66**, 119–295.
Bruker (1998). *SMART*. Version 5.054. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (1999). *SAINT* (Version 6.36a) and *SHELXTL* (Version 5.1). Bruker AXS Inc., Madison, Wisconsin, USA.
Gao, R. J. & Xie, G. Q. (2006). *Chem. Res. Chin. Univ.* **2**, 56–59.
Gobbi, M. & Frenking, G. (1993). *J. Am. Chem. Soc.* **115**, 2362–2372.
Maryanoff, C. A., Stanzione, R. C., Plampin, J. N. & Mills, J. E. (1986). *J. Org. Chem.* **51**, 1882–1884.
Riordan, J. F. (1979). *Mol. Cell. Biochem.* **26**, 71–92.
Sheldrick, G. M. (1996). *SADABS*. Version 2.0. University of Göttingen, Germany.
Yonehara, H. & Otake, N. (1966). *Tetrahedron Lett.* **32**, 3785–3791.