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# *N*-(2,6-Dimethylanilino)-5,6-dihydro-4*H*-1,3-thiazin-3-ium chloride monohydrate

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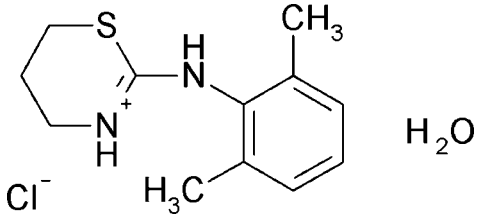
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.033; $wR$ factor = 0.089; data-to-parameter ratio = 16.3.

In the title compound, alternatively called xylazine hydrochloride monohydrate, $C_{12}H_{17}N_2S^+\cdot Cl^-\cdot H_2O$, the six-membered thiazine ring is in a half-chair conformation. In the crystal structure, six component centrosymmetric clusters are formed *via* intermolecular O—H···Cl, N—H···O and N—H···Cl hydrogen bonds involving xylazine cations, chloride anions and water molecules.

## Related literature

For related literature see: Carpy *et al.* (1979); Kalman *et al.* (1977).




## Experimental

### *Crystal data*

$C_{12}H_{17}N_2S^+\cdot Cl^-\cdot H_2O$
$M_r$ = 274.81
Monoclinic, $P2_1/c$
$a$ = 13.4546 (2) Å
$b$ = 8.6547 (1) Å
$c$ = 12.7732 (2) Å
$\beta$ = 109.210 (2)°
$V$ = 1404.56 (4) Å$^3$
$Z$ = 4
Cu $K\alpha$ radiation
$\mu$ = 3.69 mm$^{-1}$
$T$ = 100 K
0.44 × 0.25 × 0.14 mm

### *Data collection*

Oxford Diffraction Xcalibur diffractometer
Absorption correction: numerical (de Meulenaer & Tompa, 1965)
$T_{min}$ = 0.30, $T_{max}$ = 0.61
19046 measured reflections
2747 independent reflections
2509 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.029

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.088
$S$ = 1.01
2509 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.33 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N5—H5···O17 | 0.87 | 1.97 | 2.815 (2) | 163 |
| O17—H171···Cl16$^{i}$ | 0.82 | 2.36 | 3.158 (1) | 164 |
| N7—H7···Cl16$^{i}$ | 0.87 | 2.37 | 3.204 (1) | 162 |
| O17—H172···Cl16$^{ii}$ | 0.83 | 2.35 | 3.171 (1) | 173 |

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{1}{2}$; (ii) $x+1, -y+\frac{1}{2}, z-\frac{1}{2}$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CRYSTALS*.

We thank Oxford Diffraction Ltd for the low-temperature data collection and reduction. Cooperation of the University of Cincinnati Crystallography Centre and the Latvia Institute of Organic Synthesis is acknowledged. Financial aid was provided by Latvia Science Council grant 05.1737.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2620).

## References

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# supplementary materials

*Acta Cryst.* (2008). E**64**, o1062 [ **doi:10.1107/S160053680801372X** ]

# *N*-(2,6-Dimethylanilino)-5,6-dihydro-4*H*-1,3-thiazin-3-ium chloride monohydrate

**M. V. Veidis, L. Orola and R. Arajs**

## Comment

Xylazine hydrochloride monohydrate is a pharmaceutical used in veterinary medicine as an anesthetic. The substance is an alpha2-agonist with sedative, analgesic, and muscle relaxing properties.

The crystal structure of the title compound has been determined at 100 K. The structure is depicted in Fig. 1. The phenyl ring forms a dihedral angle of 83.24 (14)° with the plane defined by S1, C6 and N5 of the thiazine ring. The six-member thiazine ring assumes the half-chair conformation.

Hydrogen atoms are bonded to both nitrogen atoms forming a cation. Both hydrogen atoms participate in hydrogen bonding. The two xylazine moieties are held together through an extended H-bond network involving the nitrogen, oxygen, and chlorine anions. In the crystal structure, centrosymmetric clusters are formed by N—H···O—H···Cl···H—N hydrogen bond sequence between the two xylazine moieties.

There are H-bonds which do not join the xylazine moities between oxygen and chlorine (Fig. 2). These may impart additional rigidity in the cluster. As a result of Cl···H—O hydrogen bonding a parallelogram is formed by the Cl—O—Cl—O atoms.

The hydrogen bond lengths are given in the Table 1.

## Experimental

The title compound was supplied by Grindeks Company. For crystal structure determination suitable crystals were grown by slow evaporation of an ethanol (96%) solution at room temperature.

## Refinement

The hydrogen atoms were located by difference Fourier method. During refinement hydrogen atoms were costrained to the riding mode. $U_{iso}$(H)=$xU_{eq}$(C,*N*,*O*), where the average values of *x* are 1.15 for H atoms bonded to the thiazine ring, 1.48 for methyl H atoms, 1.16 for benzene ring H atoms, 1.17 fot the H atoms bonded to the nitrogen atoms and 1.44 for the H atoms of the water molecule.

## Figures

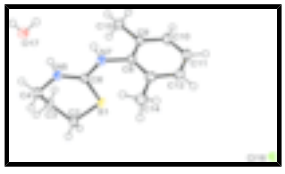

Fig. 1. The molecular structure of the title compound with thermal ellipsoids drawn at the 50% probability level.

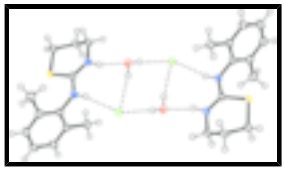

Fig. 2. Intermolecular hydrogen bond formation (dashed lines) in the title compound.

### *N*-(2,6-Dimethylanilino)-5,6-dihydro-4*H*-1,3-thiazin-3-ium chloride monohydrate

*Crystal data*

| | |
|---|---|
| $C_{12}H_{17}N_2S^+\cdot Cl^-\cdot H_2O$ | $F_{000}$ = 584 |
| $M_r$ = 274.81 | $D_x$ = 1.300 Mg m$^{-3}$ |
| Monoclinic, $P2_1/c$ | Cu $K\alpha$ radiation<br>λ = 1.5418 Å |
| Hall symbol: -P 2ybc | Cell parameters from 19046 reflections |
| $a$ = 13.4546 (2) Å | θ = 3.5–74.6º |
| $b$ = 8.6547 (1) Å | μ = 3.69 mm$^{-1}$ |
| $c$ = 12.7732 (2) Å | $T$ = 100 K |
| β = 109.210 (2)º | Prism, white |
| $V$ = 1404.56 (4) Å$^3$ | 0.44 × 0.25 × 0.14 mm |
| $Z$ = 4 | |

*Data collection*

| | |
|---|---|
| Oxford Diffraction Xcalibur diffractometer | 2747 independent reflections |
| Radiation source: Enhance (Cu) X-ray Source | 2509 reflections with $I > 2.0\sigma(I)$ |
| Monochromator: graphite | $R_{int}$ = 0.029 |
| $T$ = 100 K | $\theta_{max}$ = 74.6º |
| φ and ω scans | $\theta_{min}$ = 3.5º |
| Absorption correction: numerical (de Meulenaer & Tompa, 1965) | $h$ = −16→16 |
| $T_{min}$ = 0.30, $T_{max}$ = 0.61 | $k$ = −10→10 |
| 19046 measured reflections | $l$ = −15→15 |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | H-atom parameters constrained |
| Least-squares matrix: full | W = [*w*eight][1-(δ$F$/6σ$F$)$^2$]$^2$ |
| $R[F^2 > 2\sigma(F^2)]$ = 0.033 | $(\Delta/\sigma)_{max}$ = 0.0003 |
| $wR(F^2)$ = 0.088 | $\Delta\rho_{max}$ = 0.43 e Å$^{-3}$ |
| $S$ = 1.02 | $\Delta\rho_{min}$ = −0.33 e Å$^{-3}$ |
| 2509 reflections | Extinction correction: none |
| 154 parameters | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.72343 (3) | 0.06408 (5) | 0.19253 (3) | 0.0234 |
| C2 | 0.79732 (14) | −0.11421 (19) | 0.19970 (14) | 0.0244 |
| C3 | 0.90751 (14) | −0.0827 (2) | 0.19854 (14) | 0.0252 |
| C4 | 0.90283 (13) | −0.0099 (2) | 0.08935 (14) | 0.0244 |
| N5 | 0.84522 (11) | 0.13793 (17) | 0.06888 (12) | 0.0225 |
| C6 | 0.76970 (12) | 0.17936 (19) | 0.10687 (13) | 0.0199 |
| N7 | 0.72435 (11) | 0.31807 (16) | 0.08222 (11) | 0.0217 |
| C8 | 0.65460 (13) | 0.37922 (18) | 0.13689 (14) | 0.0210 |
| C9 | 0.69975 (13) | 0.4718 (2) | 0.23077 (14) | 0.0224 |
| C10 | 0.63438 (14) | 0.5346 (2) | 0.28445 (15) | 0.0278 |
| C11 | 0.52719 (15) | 0.5046 (2) | 0.24466 (17) | 0.0319 |
| C12 | 0.48404 (14) | 0.4128 (2) | 0.15214 (17) | 0.0300 |
| C13 | 0.54694 (13) | 0.3482 (2) | 0.09525 (15) | 0.0255 |
| C14 | 0.49879 (15) | 0.2481 (2) | −0.00495 (16) | 0.0319 |
| C15 | 0.81647 (13) | 0.4980 (2) | 0.27462 (14) | 0.0249 |
| Cl16 | 0.18401 (3) | 0.10294 (5) | 0.51765 (3) | 0.0238 |
| O17 | 0.94136 (9) | 0.31268 (14) | −0.05720 (10) | 0.0272 |
| H21 | 0.8012 | −0.1644 | 0.2678 | 0.0280* |
| H31 | 0.9450 | −0.1803 | 0.2067 | 0.0276* |
| H32 | 0.9432 | −0.0145 | 0.2573 | 0.0277* |
| H41 | 0.9748 | 0.0101 | 0.0908 | 0.0289* |
| H42 | 0.8694 | −0.0804 | 0.0300 | 0.0289* |
| H141 | 0.4312 | 0.2885 | −0.0488 | 0.0475* |
| H142 | 0.5426 | 0.2414 | −0.0510 | 0.0467* |
| H143 | 0.4889 | 0.1450 | 0.0189 | 0.0475* |
| H151 | 0.8332 | 0.5724 | 0.3339 | 0.0357* |
| H152 | 0.8415 | 0.5357 | 0.2174 | 0.0356* |
| H153 | 0.8515 | 0.4017 | 0.3030 | 0.0359* |
| H171 | 0.9124 | 0.3966 | −0.0570 | 0.0391* |
| H172 | 1.0056 | 0.3286 | −0.0335 | 0.0395* |
| H22 | 0.7604 | −0.1794 | 0.1379 | 0.0278* |
| H5 | 0.8667 | 0.2066 | 0.0318 | 0.0267* |
| H7 | 0.7466 | 0.3812 | 0.0417 | 0.0250* |
| H10 | 0.6635 | 0.5960 | 0.3474 | 0.0320* |
| H11 | 0.4838 | 0.5483 | 0.2825 | 0.0362* |
| H12 | 0.4111 | 0.3933 | 0.1255 | 0.0341* |

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

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0236 (2) | 0.0216 (2) | 0.0306 (2) | 0.00450 (15) | 0.01642 (17) | 0.00271 (14) |
| C2 | 0.0292 (9) | 0.0208 (8) | 0.0269 (8) | 0.0023 (6) | 0.0143 (7) | 0.0055 (6) |
| C3 | 0.0257 (8) | 0.0265 (8) | 0.0251 (8) | −0.0001 (7) | 0.0109 (7) | 0.0059 (7) |
| C4 | 0.0227 (8) | 0.0262 (9) | 0.0274 (8) | −0.0012 (7) | 0.0127 (7) | 0.0037 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N5 | 0.0227 (7) | 0.0222 (7) | 0.0268 (7) | 0.0015 (5) | 0.0137 (5) | 0.0004 (5) |
| C6 | 0.0186 (7) | 0.0218 (8) | 0.0203 (7) | −0.0012 (6) | 0.0076 (6) | −0.0019 (6) |
| N7 | 0.0237 (7) | 0.0206 (7) | 0.0245 (7) | 0.0018 (5) | 0.0130 (6) | 0.0002 (5) |
| C8 | 0.0203 (7) | 0.0193 (8) | 0.0258 (8) | 0.0046 (6) | 0.0107 (6) | 0.0032 (6) |
| C9 | 0.0225 (8) | 0.0204 (8) | 0.0258 (8) | 0.0035 (6) | 0.0103 (7) | 0.0035 (6) |
| C10 | 0.0297 (9) | 0.0274 (8) | 0.0296 (9) | −0.0003 (7) | 0.0140 (7) | 0.0043 (7) |
| C11 | 0.0274 (9) | 0.0319 (10) | 0.0432 (10) | 0.0024 (8) | 0.0209 (8) | 0.0065 (7) |
| C12 | 0.0181 (8) | 0.0290 (9) | 0.0442 (11) | 0.0072 (8) | 0.0121 (7) | 0.0020 (7) |
| C13 | 0.0221 (8) | 0.0218 (8) | 0.0319 (9) | 0.0052 (7) | 0.0078 (7) | 0.0008 (6) |
| C14 | 0.0264 (8) | 0.0263 (9) | 0.0382 (10) | 0.0001 (8) | 0.0042 (7) | −0.0029 (7) |
| C15 | 0.0224 (8) | 0.0254 (9) | 0.0259 (8) | 0.0012 (7) | 0.0065 (7) | 0.0007 (6) |
| Cl16 | 0.0232 (2) | 0.0239 (2) | 0.0266 (2) | 0.00033 (14) | 0.01150 (16) | 0.00127 (14) |
| O17 | 0.0244 (6) | 0.0248 (6) | 0.0351 (7) | −0.0025 (5) | 0.0135 (5) | −0.0028 (5) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| S1—C2 | 1.8215 (17) | C9—C10 | 1.391 (2) |
| S1—C6 | 1.7403 (16) | C9—C15 | 1.501 (2) |
| C2—C3 | 1.512 (2) | C10—C11 | 1.387 (3) |
| C2—H21 | 0.959 | C10—H10 | 0.936 |
| C2—H22 | 0.964 | C11—C12 | 1.383 (3) |
| C3—C4 | 1.513 (2) | C11—H11 | 0.950 |
| C3—H31 | 0.971 | C12—C13 | 1.401 (3) |
| C3—H32 | 0.952 | C12—H12 | 0.942 |
| C4—N5 | 1.474 (2) | C13—C14 | 1.504 (3) |
| C4—H41 | 0.977 | C14—H141 | 0.964 |
| C4—H42 | 0.961 | C14—H142 | 0.961 |
| N5—C6 | 1.312 (2) | C14—H143 | 0.966 |
| N5—H5 | 0.866 | C15—H151 | 0.963 |
| C6—N7 | 1.336 (2) | C15—H152 | 0.957 |
| N7—C8 | 1.442 (2) | C15—H153 | 0.967 |
| N7—H7 | 0.870 | O17—H171 | 0.825 |
| C8—C9 | 1.404 (2) | O17—H172 | 0.829 |
| C8—C13 | 1.395 (2) | | |
| C2—S1—C6 | 102.42 (8) | C9—C8—C13 | 122.61 (15) |
| S1—C2—C3 | 111.57 (12) | C8—C9—C10 | 118.55 (16) |
| S1—C2—H21 | 107.2 | C8—C9—C15 | 120.71 (15) |
| C3—C2—H21 | 109.3 | C10—C9—C15 | 120.71 (16) |
| S1—C2—H22 | 109.2 | C9—C10—C11 | 119.76 (17) |
| C3—C2—H22 | 109.9 | C9—C10—H10 | 119.4 |
| H21—C2—H22 | 109.7 | C11—C10—H10 | 120.8 |
| C2—C3—C4 | 109.91 (14) | C10—C11—C12 | 120.93 (16) |
| C2—C3—H31 | 108.6 | C10—C11—H11 | 118.6 |
| C4—C3—H31 | 108.9 | C12—C11—H11 | 120.5 |
| C2—C3—H32 | 110.3 | C11—C12—C13 | 121.14 (16) |
| C4—C3—H32 | 109.0 | C11—C12—H12 | 120.4 |
| H31—C3—H32 | 110.2 | C13—C12—H12 | 118.5 |
| C3—C4—N5 | 112.65 (13) | C12—C13—C8 | 117.01 (16) |
| C3—C4—H41 | 108.4 | C12—C13—C14 | 120.45 (16) |

| | | | |
|---|---|---|---|
| N5—C4—H41 | 108.0 | C8—C13—C14 | 122.53 (16) |
| C3—C4—H42 | 109.2 | C13—C14—H141 | 110.2 |
| N5—C4—H42 | 109.1 | C13—C14—H142 | 112.1 |
| H41—C4—H42 | 109.3 | H141—C14—H142 | 108.5 |
| C4—N5—C6 | 126.70 (14) | C13—C14—H143 | 109.2 |
| C4—N5—H5 | 116.2 | H141—C14—H143 | 108.5 |
| C6—N5—H5 | 116.9 | H142—C14—H143 | 108.3 |
| S1—C6—N5 | 123.83 (13) | C9—C15—H151 | 109.9 |
| S1—C6—N7 | 115.66 (12) | C9—C15—H152 | 110.8 |
| N5—C6—N7 | 120.50 (15) | H151—C15—H152 | 108.8 |
| C6—N7—C8 | 122.35 (13) | C9—C15—H153 | 109.3 |
| C6—N7—H7 | 118.9 | H151—C15—H153 | 108.8 |
| C8—N7—H7 | 117.6 | H152—C15—H153 | 109.3 |
| N7—C8—C9 | 117.10 (14) | H171—O17—H172 | 106.9 |
| N7—C8—C13 | 120.28 (15) | | |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N5—H5···O17 | 0.87 | 1.97 | 2.815 (2) | 163 |
| O17—H171···Cl16$^{i}$ | 0.82 | 2.36 | 3.158 (1) | 164 |
| N7—H7···Cl16$^{i}$ | 0.87 | 2.37 | 3.204 (1) | 162 |
| O17—H172···Cl16$^{ii}$ | 0.83 | 2.35 | 3.171 (1) | 173 |

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

**Fig. 1**

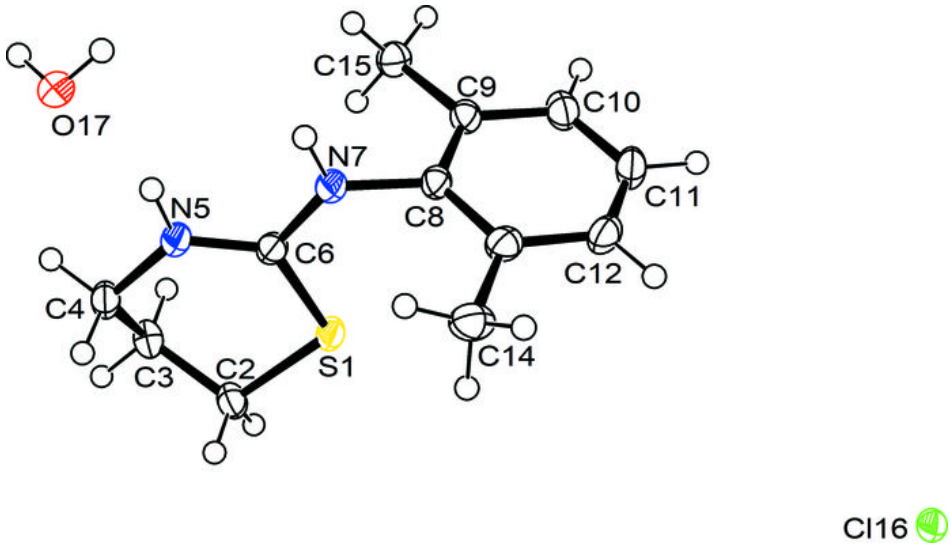

**Fig. 2**