and van der Waals interactions. These packing interactions apparently favor the less stable twist-boat conformation of the silacyclohexylidene ring.

Related literature. The title compound was prepared in 81% yield (m.p. 421–422 K) from the reaction of 1,1-dimethyl-1-silacyclohexan-4-one (Soderquist & Negron, 1989) with tosylhydrazine in acidic ethanol. Complete spectroscopic and analytical data were obtained for the tosylhydrazone which were in complete agreement with the structural data reported herein.

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Structure of *N,N'*-Dimethyl-4,4'-bipyridylium Dichloride Dihydrate

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Abstract. $C_{12}H_{14}N_2^{2+}.2Cl^-.2H_2O$, $M_r = 293$, triclinic, $P\bar{1}$, $a = 9.696$ (3), $b = 11.322$ (4), $c = 7.076$ (3) Å, $\alpha = 100.68$ (4), $\beta = 93.40$ (3), $\gamma = 107.04$ (4)°, $V = 724$ (6) Å^3, $Z = 2$, $D_x = 1.344$ Mg m^{-3}, λ(Cu $K\alpha$) = 1.5418 Å, $\mu = 4.4$ mm^{-1}, $F(000) = 308$, room temperature, $R = 0.052$ for 2201 independent reflections. *N,N'*-dimethyl-4,4'-bipyridylium dichloride (or paraquat, viologen) like mitoguazone (an anticancer drug), affects the polyamine uptake systems, a potential target in cancer chemotherapy. The description of the three-dimensional structure of this ion should allow a better assessment of the structure–activity relationship of these bioactive molecules.

Experimental. Crystals of the title compound were obtained in ethanol from commercial methyl viologen dichloride hydrate (Aldrich-Chemie). Pale yellow single crystal approximately 0.15 × 0.30 × 0.2 mm. The unit-cell dimensions (from 25 reflections, $13.8 < 2\theta < 26.5°$) and reflection intensities were measured with a Philips PW1100 diffractometer, graphite-monochromated radiation, scan type 'flying step scan', ω–2θ scan, scan range 1.8° θ, scan speed 0.02° θ s^{-1}, θ limits: 1–68°. $-11 \le h \le 11$, $-13 \le k \le 13$, $0 \le l \le 8$. 2866 reflections measured, 2633 unique ($R_{int} = 0.063$), three standard reflections, $\bar{1}5\bar{1}$, $\bar{3}20$ and $1\bar{5}1$, measured every hour (decomposition less than 3%), absorption correction by *DIFABS* (Walker & Stuart, 1983), $T_{min} = 0.743$, $T_{max} = 1.818$, average = 1.048. Structure solved using direct methods and successive Fourier maps [*SHELXS*86 and *CRYSTALS* from Sheldrick (1986) and Watkin, Carruthers & Betteridge (1985)]. H atoms found from difference series, complex atomic scattering factors from *International Tables for X-ray Crystallography* (1974, Vol. IV, pp. 99–101). All non-H atoms were given anisotropic thermal parameters,

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Table 1. *Atomic positional parameters and U_{eq} values for non-H atoms*

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U_{eq} (Å^2)
Cl(1)	0.2001 (1)	0.4241 (1)	0.2400 (1)	0.0406
Cl(2)	0.1747 (1)	0.9572 (1)	0.2353 (2)	0.0442
C(1)	−0.0671 (5)	0.6104 (4)	0.3027 (7)	0.0417
C(2)	−0.1680 (4)	0.3967 (4)	0.1060 (5)	0.0353
C(3)	−0.2813 (4)	0.2955 (4)	0.0098 (6)	0.0345
C(4)	−0.4231 (4)	0.2980 (3)	0.0176 (5)	0.0276
C(5)	−0.5478 (4)	0.1887 (3)	−0.0815 (5)	0.0278
C(6)	−0.5275 (4)	0.0810 (4)	−0.1914 (6)	0.0385
C(7)	−0.6448 (4)	−0.0206 (4)	−0.2746 (6)	0.0410
C(8)	−0.9040 (5)	−0.1320 (4)	−0.3309 (8)	0.0452
C(9)	−0.8035 (4)	0.0851 (4)	−0.1503 (6)	0.0355
C(10)	−0.6890 (4)	0.1887 (4)	−0.0668 (6)	0.0341
C(11)	−0.4434 (4)	0.4060 (3)	0.1268 (5)	0.0325
C(12)	−0.3268 (4)	0.5052 (4)	0.2194 (5)	0.0341
N(1)	−0.1915 (3)	0.4998 (3)	0.2079 (4)	0.0310
N(2)	−0.7792 (3)	−0.0177 (3)	−0.2511 (4)	0.0342
O(1)	0.3273 (4)	0.2422 (4)	0.4498 (5)	0.0616
O(2)	0.6359 (5)	0.2901 (4)	0.5168 (6)	0.0661

Table 2. *Intramolecular bond distances* (Å) *and angles* (°)

C(1)	N(1)		1.476 (5)	C(6)	C(7)		1.366 (5)
C(2)	C(3)		1.366 (5)	C(7)	N(2)		1.333 (5)
C(2)	N(1)		1.341 (5)	C(8)	N(2)		1.479 (5)
C(3)	C(4)		1.388 (5)	C(9)	C(10)		1.364 (5)
C(4)	C(5)		1.478 (5)	C(9)	N(2)		1.339 (5)
C(4)	C(11)		1.392 (5)	C(11)	C(12)		1.366 (5)
C(5)	C(6)		1.392 (5)	C(12)	N(1)		1.338 (5)
C(5)	C(10)		1.380 (5)				
N(1)	C(2)	C(3)	120.9 (3)	N(2)	C(9)	C(10)	119.7 (4)
C(4)	C(3)	C(2)	120.1 (4)	C(9)	C(10)	C(5)	121.0 (4)
C(5)	C(4)	C(3)	121.2 (3)	C(12)	C(11)	C(4)	120.5 (3)
C(11)	C(4)	C(3)	117.4 (3)	N(1)	C(12)	C(11)	120.5 (4)
C(11)	C(4)	C(5)	121.4 (3)	C(2)	N(1)	C(1)	119.9 (3)
C(6)	C(5)	C(4)	121.4 (3)	C(12)	N(1)	C(1)	119.5 (3)
C(10)	C(5)	C(4)	121.3 (3)	C(12)	N(1)	C(2)	120.6 (3)
C(10)	C(5)	C(6)	117.3 (3)	C(8)	N(2)	C(7)	119.5 (4)
C(7)	C(6)	C(5)	120.1 (4)	C(9)	N(2)	C(7)	121.4 (3)
N(2)	C(7)	C(6)	120.4 (4)	C(9)	N(2)	C(8)	119.1 (3)

isotropic thermal parameter for H atoms. Full-matrix least-squares refinement on F. Final $R = 0.052$ and $wR = 0.057$ (unit weights) for 2201 reflections ($I > 3\sigma I$). $S = 2.3$ and $(\Delta/\sigma)_{max} = 0.1$. Max. height in final difference Fourier synthesis 0.2 e Å^{-3}, min. height −0.4 e Å^{-3}. Computer used: VAX 6310. The final atomic parameters are given in Table 1.* The principal distances and angles are given in Table 2. Fig. 1 is a view of the paraquat ion and Fig. 2 a view of the packing (figures drawn using *ORTEP*; Johnson, 1965).

Related literature. The crystal structures of *N,N'*-dimethyl-4,4'-bipyridylium dichloride, dibromide and diiodide have already been determined (Russell & Wallwork, 1972). The main difference from this previous study concerns the symmetry and chlorine–paraquat interactions. As in the other compounds, one of the Cl atoms is bound to an N atom of the paraquat ion [Cl(1)···N(1) 3.437 (3) Å] while the second Cl atom is bound to a methyl and two C atoms of two different paraquat ions but not to an N atom (Table 2). Both Cl(1) and Cl(2) are bound to water molecules which are close to each other [O(1)···O(2) 2.874 (6) Å]. There are a number of intermolecular C···C and C···N close approaches.

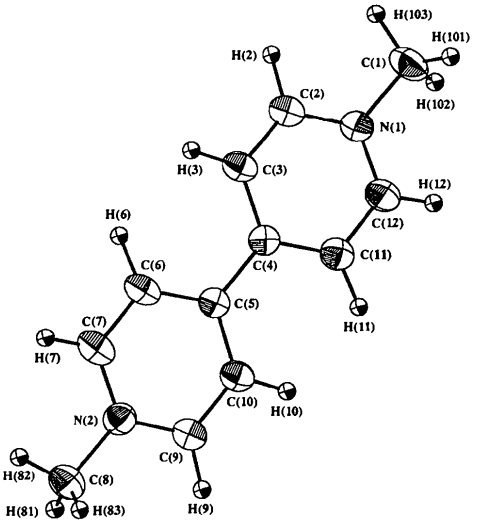

Fig. 1. Molecular structure of $C_{12}H_{14}N_2^{2+}$.

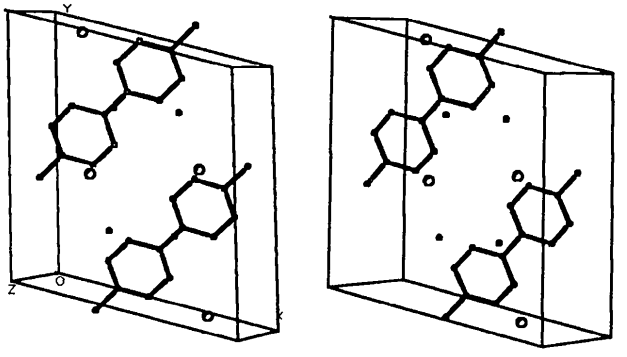

Fig. 2. Stereoscopic view of $C_{12}H_{14}N_2^{2+}.2Cl^-.2H_2O$.

* Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55774 (23 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: PA0264]

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