Table 2. *Intramolecular distances in* 6-*azathymine* (6*AT*) *thymine* (*T*), *and* 6-*azauracil* (6*AU*), *in* Å

	6AT	T[a]	6AU[b]
N(1) -C(2)	1·354 (5)	1·31 (2)	1·366 (3)
C(2)—N(3)	1·383 (5)	1·35 (2)	1·378 (2)
N(3) -C(4)	1·365 (4)	1·41 (2)	1·359 (2)
C(4)—C(5)	1·470 (5)	1·48 (2)	1·456 (2)
C(5)—N(6)[c]	1·271 (5)	1·37 (2)	1·291 (2)
N(6)[c]-N(1)	1·365 (5)	1·41 (2)	1·351 (3)
C(5)—C(7)	1·479 (6)	1·52 (2)	—
C(2)—O(2)	1·213 (5)	1·25 (2)	1·224 (2)
C(4)—O(4)	1·242 (5)	1·19 (1)	1·224 (2)
N(1) -H(1)	0·83 (4)	*d*	1·02 (3)
N(3) -H(3)	0·88 (5)	*d*	0·92 (3)
C(7)—H(71)	0·84 (6)	*d*	—
C(7)—H(72)	0·88 (4)	*d*	—

(*a*) Data from Ozeki *et al.* (1969). (*b*) Data from Singh & Hodgson (1974*c*). (*c*) C(6) in thymine. (*d*) H atoms were not located.

Table 3. *Probable intermolecular A*–H···*B hydrogen bonds*

A	H	*B*	*A*···*B* (Å)	H···*B* (Å)	*A*–H···*B* (°)
N(1)	H(1)	O(4)	2·791 (5)	1·97 (4)	170 (3)
N(3)	H(3)	O(2)	2·790 (4)	1·93 (5)	166 (4)

sheet-like structure which is perpendicular to the *c* axis; neighboring sheets are separated by 3·17 Å, or one-half of the *c* axis length. The shortest interatomic distances between molecules in adjacent sheets are N(1)-N(6) and C(4)-O(4) separations of 3·20 and 3·23 Å, respectively. As can be seen in Fig. 2, there is evidently very little overlap between the individual molecules in the adjacent sheets.

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Vanadium Oxychloride

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Abstract. VOCl, orthorhombic, *Pmmn*, $a=3{\cdot}780$ (5), $b=3{\cdot}300$ (5), $c=7{\cdot}91$ (1) Å, $V=98{\cdot}67$ Å^3, $Z=2$, $D_c=3{\cdot}45$ g cm^{-3}. Final *R* 0·091 for 491 reflexions. VOCl is isotypic with FeOCl and TiOCl.

Introduction. VOCl was prepared by the reaction of VCl_3 with V_2O_3. Single crystals were obtained by transport over the vapour phase in a temperature gradient using the method of Schäfer & Wartenpfuhl (1961). X-ray diffraction diagrams of VOCl powder are known from the work of Ehrlich & Seifert (1959) and have been indexed on the assumption that VOCl is isomorphous with TiOCl (Schäfer, Wartenpfuhl & Weise, 1958) and FeOCl (Goldsztaub, 1935). The indexing was based on the structure suggested by Goldsztaub.

In order to determine the structure of VOCl a plate-like single crystal with dimensions 0·20 × 0·06 × 0·005 mm was mounted in air with the rotation axis parallel to the plane of the plate. This direction proved to be that of the *b* axis. The unit-cell parameters $a=3{\cdot}78$, $b=3{\cdot}30$, $c=7{\cdot}91$ Å, $Z=2$ and the space group *Pmmn* were known from previous work by Schäfer & Wartenpfuhl (1961) and by Ehrlich & Seifert (1959) and were confirmed by our own X-ray investigation with photographic methods.

A Nonius CAD-4 four-circle automatic diffractometer and graphite-monochromated Mo $K\alpha$ radiation

Table 1. *Final fractional coordinates and thermal parameters with e.s.d.'s in parentheses*

Thermal parameters are in the form $\exp[-2\pi^2(U_{11}h^2a^{*2}+\ldots+2U_{12}hka^*b^*+\ldots)\times10^{-3}]$.

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
V(1)	0	$\frac{1}{2}$	0·1148 (4)	9 (1)	6 (1)	12 (1)	0	0	0
Cl(1)	0	0	0·3279 (5)	23 (2)	6 (2)	14 (1)	0	0	0
O(1)	0	0	−0·0458 (15)	1 (3)	6 (4)	18 (4)	0	0	0

were used in conjunction with a scintillation detector and pulse-height discrimination. 885 unique reflexions were collected in the range $2°\le\theta\le45°$. Only the 491 reflexions with $I>2\sigma(I)$ were used for making absorption corrections ($\mu=61\cdot44$ cm^{-1}) with the program *ORABS*-2 (Schwarzenbach, Busing & Levy, 1972). Lorentz and polarization corrections were also made. Starting with the positional parameters given for FeOCl, the refinement of these parameters, the isotropic temperature factors and the overall scale factor, with the full-matrix least-squares program *CRYLSQ* and unit weights, led to an R value of 0·114 [$R=(\sum||F_o|-|F_c||)/\sum|F_o|$]. The scattering factors used were those for neutral atoms (Hanson, Herman, Lea & Skillman, 1964). The anomalous dispersion corrections, $\Delta f'=0\cdot1$ and $\Delta f''=0\cdot2$ for Cl and $\Delta f'=0\cdot3$ and $\Delta f''=0\cdot7$ for V, were taken from *International Tables for X-ray Crystallography* (1962). Further refinement, varying the temperature factors of the atoms anisotropically, reduced R to 0·091.* The programs used in this structure determination were those of the X-RAY 70 System (Stewart, Kundell & Baldwin, 1970) running on the 1106-2 Univac computer of the University of Freiburg, Germany.

The final positional and thermal parameters are listed in Table 1. Interatomic distances and several valence angles around the vanadium atom, calculated by the program *BONDLA*, are listed in Table 2.

Table 2. *Interatomic distances* (Å) *of* VOCl *and several bond angles* (°) *of vanadium*

E.s.d.'s are in parentheses.

V(1)–V(1)	3·300 (5)	O(1')–V(1)–O(1)	104·8 (4)
V(1)–V(2)	3·097 (3)	O(2')–V(1)–O(2)	147·8 (5)
V(1)–O(1)	2·082 (8)	O(1)—V(1)–O(2)	80·3 (2)
V(1)–O(2)	1·967 (4)	Cl(1)–V(1)–O(2)	101·4 (2)
V(1)–Cl(1)	2·359 (5)	Cl(1)–V(1)–O(1)	83·2 (3)
O(1)–O(2)	2·611 (5)	Cl(1')–V(1)–Cl(1)	88·8 (2)
O(1)–Cl(1)	2·956 (13)		
Cl(1)–Cl(2)	3·702 (6)		

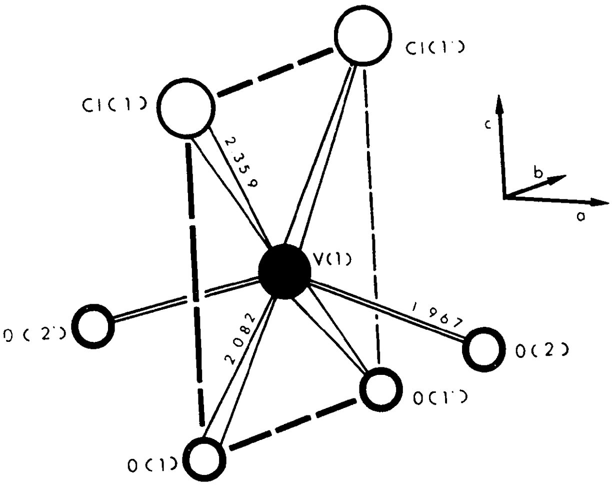

Fig. 1. Arrangement of oxygen and chlorine atoms around vanadium in VOCl. The bond lengths are given in Å.

Discussion. The structure of VOCl, which corresponds to the model given by Goldsztaub for FeOCl, consists of layers perpendicular to the c axis. The layers are obviously constructed by areas of closely packed V and O atoms. These areas are connected by layers of Cl atoms. The contact distance between these Cl atoms [Cl(1)–Cl(2) = 3·70 Å] corresponds to the distance expected for touching Cl ions.

Each O atom is surrounded by a tetrahedron of V atoms. Each V atom is surrounded by four O and two Cl atoms forming a distorted octahedron, as shown in Fig. 1.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31109 (3 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.