

$\text{HCs}_3[\text{H}_3\text{O}]\text{Cl}_5$
 $hP20$
 $(176) P6_3/m - h^2fe$
CsCl·0.33H₃OHCl₂ [1]

Structural features: Cl-H-Cl linear units arranged in infinite chains and directly superposed :O(-H··Cl)₃ ψ-tetrahedra (split O site).

Schroeder L.W., Ibers J.A. (1968) [1]

 $\text{Cl}_5\text{Cs}_3\text{H}_3\text{O}$

$a = 1.028$, $c = 0.678$ nm, $c/a = 0.660$, $V = 0.6205$ nm³, $Z = 2$

site	Wyck.	sym.	x	y	z	occ.	atomic environment
Cl1	6h	$m..$	0.2654	0.2727	$\frac{1}{4}$		non-colinear (OH ₃) ₂
Cs2	6h	$m..$	0.3855	0.0151	$\frac{1}{4}$		tricapped trigonal prism Cl ₉
Cl3	4f	3..	$\frac{1}{3}$	$\frac{2}{3}$	0.0181		single atom Cl
(OH ₃)4	4e	3..	0	0	0.1104	0.5	colinear (OH ₃) ₂

Transformation from published data: $y, x, -z$

Experimental: single crystal, Weissenberg photographs, X-rays, $R = 0.093$

Remarks: H not belonging to H₃O was not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Space group (173) $P6_3$ was tested and rejected.

References: [1] Schroeder L.W., Ibers J.A. (1968), Inorg. Chem. 7, 594-599.