cott, 1977) presented very interesting graphic relationships between the two independent metal—oxygen bond distances and atomic numbers as well as crystal radii. Also plotted were O—O lengths *versus* atomic numbers and crystal radii. When the Ce—O(1,2) and the O—O distances are interpolated from the graphic structural trend presentations, it is found that all the bond distances experimentally determined in this study are within one standard deviation of the projected values. The apical Ce—O(2) bond distance of 2·567 (4) Å has significant meaning when the recent finding of Beall *et al.* (1977) is considered. These investigators found the radius of the hydroxyl group to be 1·487 (3) Å which compares well with the values found by Christensen (1965) and Hall & Britton (1972) of 1·51 (2) and 1·50 (2) Å, respectively. If one assumes the hydroxyl-ion radius to be 1·487 (3) Å, it is found that the crystal radius of Ce^{III} is 1·080 (7) Å. This value is within 1σ of the determined crystal radius proposed by Templeton & Dauben (1954) after correction to nine-coordination [1·073 (5) Å]. The results of the present study lend support to the work of Beall, Milligan & Wolcott (1977) and help to broaden and strengthen the possible parallel between the actinide and lanthanide series. One of the main objectives of this laboratory is to be able to predict readily the structural properties of the actinide trihydroxides. This will only be possible after all the related lanthanide structural studies have been completely and properly analyzed.

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Zinc(II) Chlorite Dihydrate

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Abstract. $Zn(ClO_2)_2.2H_2O$, monoclinic, $P2_1/n$, a = 6·425 (3), b = 6·892 (2), c = 6·454 (3) Å, β = 94·70 (4)° (at 295 K), V = 284·7 (2) Å^3, Z = 2, M_r = 236·30, D_c = 2·756 Mg m^{-3}, $F(000)$ = 232, λ(Mo $K\alpha$) = 0·71069 Å, μ(Mo $K\alpha$) = 5·316 mm^{-1}. R = 0·031 for 1158 diffractometer-measured reflections. The O atoms of ClO_2^- bridge octahedrally coordinated Zn^{2+}. Water molecules are also coordinated to Zn and are involved in hydrogen bonding with chlorite O atoms. Cl—O distances are 1·580 (3) and 1·590 (3) Å; the O—Cl—O angle is 111·4 (1)°; Zn—O distances range between 2·050 (2) and 2·133 (3) Å.

Introduction. The crystal chemistry of chlorites has not been studied very extensively. In an effort to correlate the structure and bonding of different metal chlorites, an X-ray analysis of zinc chlorite has been undertaken. The unit cell of the compound has been reported earlier (with no other structural information) (Levi & Scherillo, 1931). The compound was prepared by

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Table 1. *Final atomic coordinates* ($\times 10^4$) *and isotropic temperature factors*

Standard deviations are given in parentheses.

	x	y	z	B (Å^2)
Zn(1)	0	0	0	1·0
Cl(1)	2383 (1)	1130 (1)	5948 (1)	1·3
O(1)	4411 (4)	2382 (4)	6612 (4)	1·6
O(2)	526 (4)	1657 (4)	7304 (4)	1·7
O(3)	3063 (4)	215 (4)	1135 (4)	1·6
H(1)	1565 (105)	3855 (101)	3551 (100)	7·1
H(2)	3827 (100)	1111 (96)	1128 (96)	5·1

mixing 1 mol dm^{-3} zinc nitrate and 4 mol dm^{-3} sodium chlorite solutions. A white precipitate was filtered and dissolved in hot water; white crystals formed upon cooling. A preliminary photographic X-ray investigation indicated that the crystals were monoclinic, belonging to the space group $P2_1/n$ (according to the systematic absences in the diffraction pattern). The unit-cell parameters were determined at 295 K from least-squares refinement of the angular settings of 21 reflections with a Syntex $P2_1$ diffractometer. The intensity data were collected on the same diffractometer with graphite-monochromatized Mo $K\alpha$ radiation by the θ–2θ method and at a fixed scan rate of 2° min^{-1}. All 1436 reflections up to $2\theta = 70°$ were measured and, according to the criterion $I > 3\sigma(I)$, 1158 were considered observed and used in the subsequent calculations. The net intensities were corrected for Lorentz, polarization and absorption effects. An empirical absorption correction was made from φ-scan data; transmission factors varied from 0·52 to 1·00.

The coordinates of the Zn and Cl atoms were obtained from a three-dimensional Patterson map and all other atoms were located from successive difference Fourier maps. The atomic parameters were refined by full-matrix least-squares techniques using anisotropic temperature factors for nonhydrogen atoms and isotropic ones for H. The final R index was 0·031. The weighted R was 0·041 using the weighting scheme $w = 1/\sigma^2(F_o^2)$. The final positional parameters are given in Table 1.[*]

Discussion. Fig. 1 shows the numbering of the atoms and the coordination sphere of the Zn atom. Table 2 gives selected interatomic distances and angles. Four chlorite and two water O atoms are octahedrally coordinated to Zn. The O—Zn—O angles are very close to 90° and the Zn—O(water) distance of 2·050 Å is slightly shorter than the virtually equal Zn—O(chlorite) distances of 2·133 and 2·132 Å.

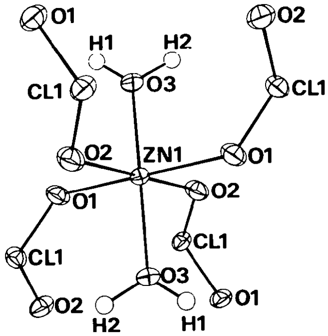

Fig. 1. A perspective view of the coordination sphere of Zn with the atomic numbering. The thermal ellipsoids are scaled to include 70% probability.

Table 2. *Interatomic distances* (Å) *and angles* (°)

Estimated standard deviations are given in parentheses.

Environment of zinc			
Zn(1)—O(1)$^{\text{i}}$	2·133 (3)	O(1)$^{\text{i}}$—Zn(1)—O(2)$^{\text{ii}}$	89·5 (1)
Zn(1)—O(2)$^{\text{ii}}$	2·132 (3)	O(1)$^{\text{i}}$—Zn(1)—O(3)	88·3 (1)
Zn(1)—O(3)	2·050 (2)	O(2)$^{\text{i}}$—Zn(1)—O(3)	92·4 (1)
Chlorite ion		Symmetry code	
Cl(1)—O(1)	1·590 (3)	(i)	$x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$
Cl(1)—O(2)	1·580 (3)	(ii)	$x, y, z-1$
O(1)—Cl(1)—O(2)	111·4 (1)	(iii)	$-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$
		(iv)	$-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$
Water and possible hydrogen bonds		(v)	$x+\frac{1}{2}, \frac{1}{2}-y, z+\frac{1}{2}$
O(3)—H(1)$^{\text{iii}}$	0·99 (7)		
O(3)—H(2)	0·79 (7)		
H(1)$^{\text{iii}}$—O(3)—H(2)	127 (6)		
O(1)$^{\text{i}}$—O(3)$^{\text{iv}}$	2·751 (3)		
O(2)$^{\text{v}}$—O(3)	2·744 (3)		

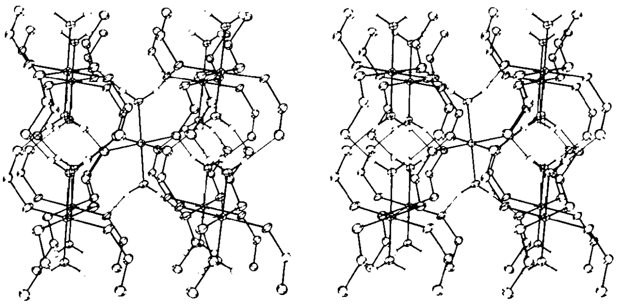

Fig. 2. A stereoview of the unit-cell contents. The a axis points out from the page and the c axis up the page.

The geometry of the ClO_2^- groups has been determined for a few other chlorites. The following Cl—O distances and O—Cl—O angles have been reported: 1·57 (3) Å and 110·5° for ammonium chlorite (Gillespie, Sparks & Trueblood, 1959); 1·55 (5) Å and

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[*] Lists of structure factors and thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34594 (21 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

111 (3)° for silver chlorite (Cooper & Marsh, 1961); 1·54 (4) Å and 109·7 (2·5)° for lanthanum chlorite trihydrate (Coda, Giuseppetti & Tadini, 1965); 1·557 (1), 1·564 (1) Å and 108·23 (6)° for sodium chlorite trihydrate (Tarimci, Schempp & Chang, 1975; Tazzoli, Riganti, Giuseppetti & Coda, 1975); and for anhydrous sodium chlorite 1·564 (3) Å and 108·6 (1)° (Tarimci, Rosenstein & Schempp, 1976). In the present structure the bond lengths are slightly longer [1·580 (3) and 1·590 (3) Å] than in the other structures, but the O—Cl—O angle agrees well with the earlier determinations.

A stereoview of the unit-cell contents is shown in Fig. 2. The chlorite ions bridge the Zn octahedra in three dimensions. Additional strength is given to the structure by hydrogen bonds from the water molecules to the chlorite O atoms.

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Structure du Pentasulfure de Disamarium et d'Etain

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Abstract. Sm_2SnS_5, orthorhombic, *Pbam*, a = 11·276 (8), b = 7·773 (5), c = 3·895 (3) Å, Z = 2. The structure has been refined by a least-squares procedure to a final R value of 0·047 for 418 reflections. The Sm atoms are eight-coordinated and the Sn atom has a sixfold coordination.

Introduction. La combinaison du sulfure stannique SnS_2 avec les sulfures de terres rares Ln_2S_3 donne une série unique de composés intermédiaires, de formule Ln_2SnS_5 (Ln = La à Dy). Les diagrammes de Guinier de l'ensemble de ces composés, bien que très semblables, présentent une nette discontinuité entre le néodyme et le samarium (Guittard, Julien-Pouzol, Jaulmes & Lavenant, 1976). De plus l'évolution des paramètres montre, elle aussi, une discontinuité au même niveau. Tandis que le paramètre c décroît régulièrement, parallèlement à la contraction lanthanidique, les paramètres a et b décroissent tout d'abord jusqu'au niveau du néodyme, et restent ensuite sensiblement constants (Tableau 1). Il en résulte que les volumes des mailles ne diminuent pas uniformément en fonction de la contraction lanthanidique, et qu'une cassure se produit dans la courbe au niveau du samarium. Nous avons été conduites à penser que des modifications appréciables devaient se produire à l'intérieur de la structure, notamment au voisinage de l'atome de samarium, et nous avons effectué sur un cristal l'étude de la structure de Sm_2SnS_5 après celle de La_2SnS_5 (Jaulmes, 1974).

Tableau 1. *Paramètres cristallins des composés* Ln_2SnS_5 (*d'après Guittard, Julien-Pouzol, Jaulmes & Lavenant*, 1976)

	a (Å) (±0,05 Å)	b (Å) (±0,03 Å)	c (Å) (±0,01 Å)
Type La_2SnS_5			
La_2SnS_5	11,26	7,89	3,99
Ce_2SnS_5	11,24	7,86	3,95
Pr_2SnS_5	11,17	7,83	3,93
Nd_2SnS_5	11,15	7,78	3,92
Type Sm_2SnS_5			
Sm_2SnS_5	11,18	7,76	3,90
Gd_2SnS_5	11,16	7,75	3,88
Tb_2SnS_5	11,15	7,75	3,87
Dy_2SnS_5	11,14	7,75	3,86

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