parameters does indeed give a β phase (β') with the correct q value for the 'compressed' octahedron.

The super-reflections induced by the doubling of the c axis are difficult to find in the powder diffraction patterns. It is therefore possible that $CsCrCl_3$ (Crama et al., 1978) at 5 K also has a doubled c axis or all elongated octahedra, again on the basis of the magnitude of the distortion of the 'compressed' octahedron.

So it seems that the Cr^{2+} compounds, like the Cu^{2+} compounds, possess only elongated $CrCl_6$ octahedra. Unlike $CsCuCl_3$ (Schlueter, Jacobson & Rundle, 1966), however, the elongated axes do not form a screw-like configuration.

Details of the theoretical background of this type of ordering of 'D_{4h}' octahedra, in comparison with $CsCuCl_3$, will be published elsewhere.

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Structure of Scolecite from Poona, India

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Abstract. $CaAl_2Si_3O_{10}.3H_2O$, monoclinic, Cc, $a = 6.5174$ (4), $b = 18.956$ (2), $c = 9.7647$ (9) Å, $\beta = 108.860$ (8)°, $V = 1141.6$ Å^3, $Z = 4$, $D_m = 2.28$, $D_c = 2.28$ Mg m^{-3}, $R = 0.032$. The aluminosilicate framework of scolecite is isotypical with the framework of natrolite, except for a small monoclinic distortion. The Ca ion coordinates three water and four framework O atoms in a distorted pentagonal bipyramid.

Introduction. Scolecite is a widespread fibrous zeolite in the natrolite group and generally occurs in the cavities of basaltic rocks, in schists and in contact zones.

Proposals for the scolecite crystal structure have been made by Pauling (1930), Taylor, Meek & Jackson (1933) and Ivleva & Gabuda (1972). Our study was undertaken to determine the structure of scolecite and its relation to natrolite, since no study based on sufficient experimental data was found.

The material was taken from a specimen containing clear prismatic crystals of scolecite and some laumontite. The composition $Ca_{0.98}Al_{1.93}Si_{3.07}O_{10}.3.01H_2O$ (plus traces of Na) was obtained by AA spectrophotometry (Perkin–Elmer 306) and a determination of the water loss (300 mg zeolite, 1323 K for 1 h). The cell dimensions were refined by least squares from 42 single-indexed lines of a powder pattern obtained in a Guinier–Hägg focusing camera with Cu $K\alpha_1$ radiation. This powder pattern differed from published data (JCPDS Powder Diffraction File 26-1048) mainly in the indexing of the reflexions. The unit cell of Smith & Walls (1971) was redefined to give the conventional space group Cc.

Owing to extensive twinning the crystals were crushed and a thin plate ($0.110 \times 0.080 \times 0.020$ mm) was selected with the Weissenberg technique. Systematic absences were hkl: $h + k = 2n + 1$ and $h0l$: $l = 2n + 1$.

Information concerning the collection and reduction of the intensities and the refinement are given in Table 1. A CAD-4 four-circle diffractometer was used. A refinement of 49 accurately measured θ values confirmed the cell parameters.

During the data collection no systematic variation was observed in two standard reflexions which were checked every 2 h. I and $\sigma_c(I)$ (based on counting statistics) were corrected for Lorentz and polarization effects.

It was assumed that the aluminosilicate frameworks of scolecite and natrolite are identical and consequently the five independent positions of Al and Si in the $Fdd2$ cell of natrolite (Meier, 1960) were transformed into the scolecite cell. Full-matrix least-squares

refinement minimizing $\sum w(|F_o| - |F_c|)^2$ with weights $w^{-1} = \sigma_c^2(|F_o|) + (0\cdot031|F_o|)^2$ was then performed on these five atoms with scattering factors for Si. Repeated difference syntheses and refinements revealed the rest of the non-H atoms. Scattering factors for neutral atoms (Doyle & Turner, 1968) were used. An ordered (Al,Si) distribution was assigned because of significant differences in the (Al,Si)—O distances. The use of isotropic temperature factors gave $R = 0\cdot043$ and $R_w = 0\cdot054$. Anisotropic temperature factors and correction for absorption and isotropic extinction gave the final values. A final difference synthesis was featureless. The resulting atomic coordinates are given in Table 2 and some structural data in Table 3.*

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34430 (9 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Comparison of our model with experimental data was made by a δR plot (Abrahams & Keve, 1971) (Fig. 1). The plot is linear with a slope near unity and compatible with S (Table 1) and with an intercept near zero. This indicates that the systematic errors in $|F_o|$ are small, and that $\sigma(|F_o|) = w^{-1/2}$ is correct except for an average overestimation of about 15% and that the structure model is essentially correct.

Discussion. The aluminosilicate framework of scolecite is isotypical with that of natrolite (Meier, 1960), except for a small monoclinic distortion. The main distortion is a slight rotation of the center Si tetrahedron of the chains around the chain axis. This results in a shorter chain axis and the channel along a becomes asymmetric in order to accommodate $W(2)$ (see Fig. 2 which gives a projection of the structure).

Table 1. Collection and reduction of the intensity data, and the least-squares refinement

Radiation	Mo $K\alpha$ (Zr filter)
Take-off angle (°)	6
θ interval (°)	3–30
ω–2θ scan width $\Delta\omega$ (°)	$0\cdot5 + 0\cdot8 \tan \theta$
Maximum recording time (min)	5
Measured reflexions	[3, 25°] all; [25, 30°] $I > 2\sigma_c(I)$
μ (mm^{-1})	1·06
Range of transmission factors	0·93–0·98
Number of reflexions measured	1702
Number of reflexions with zero weight	396 [$I < 3\sigma_c(I)$]
Number of reflexions used in final refinement, m	1306
Number of parameters refined, n	171
$R = \sum||F_o| - |F_c||/\sum|F_o|$	0·032
$R_w = [\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2]^{1/2}$	0·040
$S = [\sum w(|F_o| - |F_c|)^2/(m - n)]^{1/2}$	0·94
g ($\times 10^{-4}$) (extinction)	0·73 (9)

Table 2. Atomic coordinates with e.s.d.'s

	x	y	z
Ca	0·1102 (3)	0·39328 (6)	0·4479 (2)
Al(1)	0·9217 (3)	0·46661 (7)	0·0664 (2)
Al(2)	0·3344 (3)	0·21209 (8)	0·4002 (2)
Si(1)	0·5	0·37937 (7)	0·0
Si(2)	0·2088 (3)	0·33245 (7)	0·1690 (2)
Si(3)	0·5296 (3)	0·08187 (7)	0·2998 (2)
O(1)	0·4966 (7)	0·0213 (2)	0·4091 (4)
O(2)	0·4956 (6)	0·0495 (2)	0·1421 (4)
O(3)	0·3622 (7)	0·1457 (2)	0·2853 (4)
O(4)	0·1247 (7)	0·1867 (2)	0·4658 (5)
O(5)	0·2717 (6)	0·2960 (2)	0·3260 (4)
O(6)	0·0810 (7)	0·2816 (2)	0·0400 (4)
O(7)	0·4316 (7)	0·3600 (2)	0·1430 (4)
O(8)	0·0661 (6)	0·4016 (2)	0·1845 (4)
O(9)	0·7799 (7)	0·1087 (2)	0·3653 (4)
O(10)	0·6477 (6)	0·4497 (2)	0·0319 (4)
W(1)	0·9685 (8)	0·0760 (3)	0·0587 (7)
W(2)	0·7044 (8)	0·1953 (2)	0·1263 (4)
W(3)	0·7821 (8)	0·3302 (3)	0·3918 (6)

Table 3. Structural data

Symmetry code: superscripts: none x,y,z; (i) $\frac{1}{2} + x, \frac{1}{2} + y, z$; (ii) $\frac{1}{2} + x, \frac{1}{2} - y, \frac{1}{2} + z$.

(a) TO_4 tetrahedra

T	Range of distance T–O (Å)	Range of angle O–T–O (°)
Al(1)	1·736 (4)–1·770 (4)	97·8 (2)–115·1 (2)
Al(2)	1·734 (4)–1·753 (5)	107·1 (2)–117·0 (2)
Si(1)	1·587 (4)–1·639 (4)	107·6 (2)–112·3 (2)
Si(2)	1·591 (4)–1·642 (4)	103·4 (2)–113·6 (2)
Si(3)	1·605 (4)–1·629 (4)	106·9 (2)–111·5 (2)

Mean Al–O = 1·745 (4) Å; mean Si–O = 1·617 (5) Å

(b) CaO$_7$ polyhedron

Distances (Å)		Deviations (Å) from the least-squares plane through the five equatorial O atoms, $\sigma = 0\cdot203$ Å	
Ca–W(1^{ii})	2·308 (5)	W(2^{ii})	0·012
Ca–W(2^{ii})	2·353 (4)	O(2^{ii})	0·157
Ca–W(3)	2·355 (5)	O(1^i)	−0·257
Ca–O(2^{ii})	2·499 (4)	O(8)	0·279
Ca–O(8)	2·499 (4)	O(5)	−0·191
Ca–O(1^i)	2·530 (4)	W(1^{ii})	−2·291
Ca–O(5)	2·595 (4)	W(3)	2·304
		Ca	−0·012

Axial angle (°)

W(1^{ii})–Ca–W(3)   160·4 (2)

(c) Possible hydrogen bonds

W(1)–O(10^i)	2·712 (6) Å	O(3)–W(1)–O(10^i)	99·4 (2)°
W(1)–O(3)	3·092 (7)	O(4^{ii})–W(2)–O(9)	159·4 (2)
W(2)–O(4^{ii})	2·684 (6)	O(2)–W(2)–O(5^{ii})	106·9 (2)
W(2)–O(9)	2·764 (6)	O(6^{ii})–W(3)–O(7)	101·2 (9)
W(2)–O(2)	3·107 (6)	W(1)–W(2)–W(3^{ii})	99·1 (1)
W(2)–O(5)	3·107 (6)		
W(3)–O(7)	2·802 (6)		
W(3)–O(6^{ii})	3·086 (6)		
W(1)–W(2)	3·041 (7)		
W(2)–W(3^{ii})	2·996 (7)		

The Ca ions are coordinated by three water and four framework O atoms in distorted pentagonal bipyramids which are distributed in the channels along **a** (Fig. 3).

If the hydrogen-bond system of scolecite were analogous to that in natrolite (Torrie, Brown & Petch,
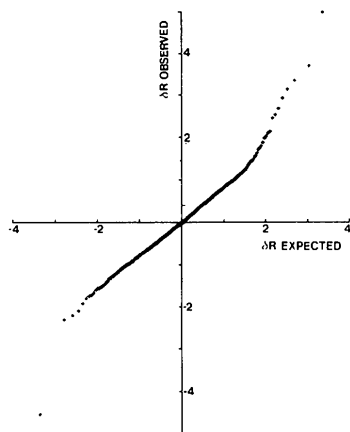

Fig. 1. A δR plot comparing model and experiment: slope 0·87, intercept 0·03.
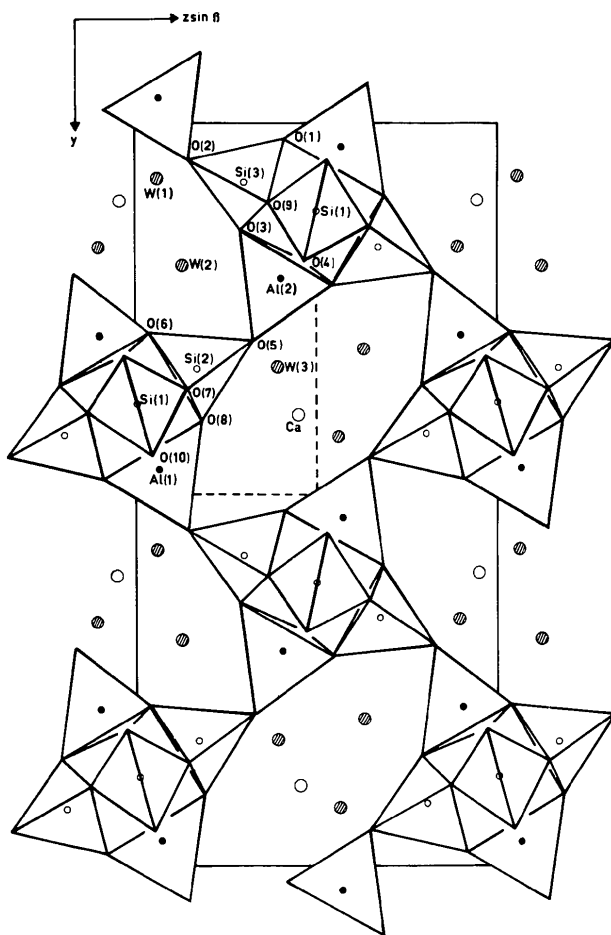

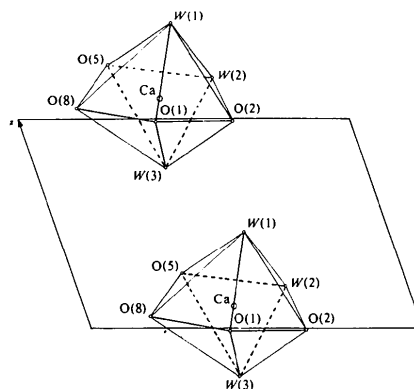Fig. 2. Projection of the structure along **a**.

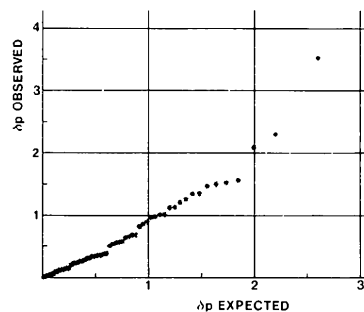Fig. 3. Projection along **b** of the CaO_7 polyhedra in one of the channels.

Fig. 4. A δp plot of the positional parameters from the two independent determinations of the structure: slope 0·94, intercept −0·06.

1964), the hydrogen bonds would be: $O(9)\cdots W(1)\cdots O(10^i)$ and $O(4^{ii})\cdots W(3)\cdots O(7)$, but this is impossible since $W(1)\cdots O(9) = 3\cdot638\ (8)$ Å and $W(3)\cdots O(4^{ii}) = 3\cdot444\ (6)$ Å are too long. Table 3(c) lists some possible hydrogen bonds.

Since the completion of our work a thesis (Adiwidjaja, 1972; hereafter A) dealing with the same subject has come to our attention. The structural details of the two investigations are in good agreement. A reports $R = 0\cdot059$ based on $m = 1067$ intensities with the monoclinic space group Fd. In order to compare the two models the atomic coordinates with e.s.d.'s in the Fd setting were transformed to Cc. A δp plot (Abrahams & Keve, 1971) was prepared with 54 positional parameters from each of the two independent determinations (Fig. 4). The greatest differences are in the x,y parameters of $O(4)$ and correspond to $<0\cdot03$ Å. The e.s.d.'s of A are approximately twice our values and so the δp plot depends mainly (80%) on the e.s.d.'s of A. The characteristics of the δp plot indicate the absence of systematic differences in the two models and a small average overestimation in the e.s.d.'s of A. However, since the slope of our δR plot indicated that on average $\sigma(|F_o|)$ was correct, we expect the e.s.d.'s of our derived parameters to be mainly correct.

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Structure of Phuralumite

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Abstract. $Al_2[(OH)_2(PO_4)_2(UO_2)_3].(OH)_4.10H_2O$ (a mineral from Kobokobo, Kivu, Zaïre), monoclinic, $P2_1/a$, $a = 13.836$ (6), $b = 20.918$ (6), $c = 9.428$ (3) Å, $\beta = 112.44$ (3)°, $Z = 4$, $V = 2522$ Å^3, $D_m = 3.5$, $D_c = 3.52$ Mg m^{-3}. Structure type: phosphuranylite. The $[(OH)_2(PO_4)_2(UO_2)_3]_n^{2n-}$ layers are connected principally by Al_4O_{14} groups, composed of two octahedra and two trigonal bipyramids sharing edges.

Introduction. Phuralumite is a mineral recently described by Deliens & Piret (1979). The results are here completed with the structure determination. The space group was determined from Weissenberg and precession photographs (systematic absences, *hkl*: none; *h0l*: $h = 2n + 1$; *0k0*: $k = 2n + 1$). Final cell dimensions and intensities were measured on a Syntex $P2_1$ four-circle diffractometer with the experimental conditions given in Table 1. Intensities were corrected for absorption by an experimental method (Syntex, 1976). Scattering factors were those given by Cromer & Mann (1968) for neutral atoms; that for U was corrected for anomalous scattering (Cromer, 1965). The structure was solved by the use of the Patterson function. Refinement by Fourier methods and least squares (block-diagonal) gave a final residual R of 0.070 for all observed reflexions.* Calculations were performed with the XRAY system (1972). The final coordinates and temperature factors are given in Table 2.

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 34417 (19 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. The structure consists of $[(OH)_2(PO_4)_2(UO_2)_3]_n^{2n-}$ layers similar to those in phosphuranylite (Shashkin & Sidorenko, 1974), dumontite (Piret-Meunier, Léonard & Van Meerssche,
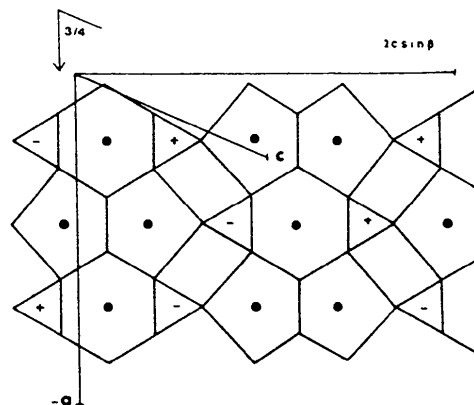

Fig. 1. Idealized $[(OH)_2(PO_4)_2(UO_2)_3]_n^{2n-}$ layer, with symmetry elements of the real layer. Full circles are UO_2, plus signs P–O, and minus signs O–P.

Table 1. *Experimental conditions*

Radiation: Mo $K\alpha$, $\lambda = 0.71069$ Å
Graphite monochromator
ω scan: $-0.7°$ to $+0.7°$ (65 s) (background 2 × 16 s)
$2\theta_{max} = 47°$
Total number of independent reflexions: 3730
Total observed $|I \geq 2.5\,\sigma(I)|$: 2971
Crystal dimensions along **a**, **b**, **c**: 0.08 and 0.25, 0.18, 0.07 mm (rectangular trapezohedron)
μ(Mo $K\alpha$) = 18.68 mm^{-1}