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Disodium Zincosilicate, $\text{Na}_2\text{ZnSi}_3\text{O}_8$

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The structure of synthetic $\text{Na}_2\text{ZnSi}_3\text{O}_8$ [monoclinic $P2_1$; $a = 6.660$ (6), $b = 8.629$ (6), $c = 6.411$ (8) Å, $\beta = 103.70$ (7)°; $Z = 2$, $D_m = 2.94$, $D_x = 2.95$ g cm⁻³] has been refined to $R = 0.033$ for 1077 independent reflexions from Mo $K\alpha$ radiation. Corner-sharing $[\text{SiO}_4]$ tetrahedra form chains with three tetrahedra in the identity period of the chain. These *Dreierketten* form tetrahedral layers $\frac{2}{3}[\text{Si}_3\text{O}_8]$. Together with $[\text{ZnO}_4]$ tetrahedra the $[\text{SiO}_4]$ groups constitute a framework resembling that of paracelsian, $\text{BaAl}_2\text{Si}_2\text{O}_8$. The sodium ions occupy irregular cavities: Na(1) is seven-coordinated (mean bond length 2.718 Å) with two additional oxygens at 3.4 Å; Na(2) may be regarded as seven or eight-coordinated (mean bond lengths 2.529 or 2.600 Å). The structure of $\text{Na}_2\text{ZnSi}_3\text{O}_8$ shows remarkable similarities to the sodic plagioclase feldspars, $(\text{Na,Ca})\text{(Al,Si)}_4\text{O}_8$, and other framework aluminosilicates. The formula

$$\text{Si-O} = 1.571 - 0.068 \Delta Z_{\text{nr}} + 0.067[\Sigma 1/(\text{Na-O})^2] - 0.025/\cos(T-O-T),$$

whose constants were derived by multiple linear regression analysis for feldspars and modified to account for the substitution of Zn for Al, gives an excellent estimation of the 12 individual Si–O bond lengths in this compound.

Introduction

Disodium zincosilicate, $\text{Na}_2\text{ZnSi}_3\text{O}_8$, was first described by Litvin, Mel'nikov, Ilyukhin & Nikitin (1965). In the present study single crystals were synthesized by heating a mixture of 5.0 g gel of composition $\text{Na}_2\text{O} \cdot \text{ZnO} \cdot 3\text{SiO}_2 \cdot n\text{H}_2\text{O}$ [prepared by the method of Hamilton & Henderson (1968)] and 1.4 g pure SiO_2 (Riedel–de Haën) in sealed silver tubes for several days at 1 kbar and 450°C. Chemical, electron microprobe, and thermogravimetric analyses and IR spectra reveal a partial replacement of Na by H in agreement with the formula $\text{Na}_{2-x}\text{H}_x\text{ZnSi}_3\text{O}_8$ with $x \leq 0.25$.

The cell dimensions were obtained by a least-squares analysis of 19 peaks from a Guinier powder photograph (Cu $K\alpha$ radiation, $\lambda = 1.5418$ Å). Intensities of 1077 independent reflexions from a crystal of dimensions 0.08 × 0.17 × 0.22 mm were collected from θ – 2θ scans on a Siemens four-circle diffractometer with Mo $K\alpha$ radiation ($\mu = 40.3$ cm⁻¹). Lorentz, polarization and absorption corrections were applied. From systematic absences of $0k0$ reflexions with $k = 2n + 1$ and an $N(z)$ test (Howells, Phillips & Rogers, 1950) the space group $P2_1$ was deduced.

Approximate atomic coordinates were determined from a three-dimensional Patterson synthesis and were refined by least-squares and Fourier methods with scattering factors for half-ionized atoms. For the final coordinates in Table 1 the unweighted residual, using all

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Table 1. *Fractional atomic coordinates and thermal parameters with estimated standard deviations in parentheses*

Atomic coordinates and anisotropic thermal parameters have been multiplied by 10^4 . The origin is fixed by y for the zinc atom.
 $T = \exp[-(h^2B_{11} + k^2B_{22} + l^2B_{33} + 2hkB_{12} + 2hlB_{13} + 2klB_{23})]$.

	<i>x</i>	<i>y</i>	<i>z</i>	$B_{\text{iso}} (\text{Å}^2)$	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Na(1)	4673 (7)	8764 (6)	847 (7)	1.92 (7)	111 (7)	85 (5)	108 (8)	-29 (5)	12 (6)	12 (5)
Na(2)	2155 (6)	4337 (5)	3297 (6)	1.02 (6)	58 (6)	31 (3)	84 (7)	8 (4)	12 (5)	1 (4)
Zn	6070 (1)	2428 (1)	4646 (1)	0.50 (1)	25 (1)	17 (1)	48 (1)	3 (1)	8 (1)	3 (1)
Si(1)	2660 (3)	746 (3)	6440 (3)	0.40 (3)	18 (3)	13 (2)	44 (3)	2 (2)	5 (3)	0 (2)
Si(2)	-1038 (3)	568 (3)	-7508 (3)	0.40 (3)	25 (3)	12 (2)	35 (3)	2 (2)	5 (3)	0 (2)
Si(3)	127 (3)	2391 (4)	9067 (3)	0.39 (3)	22 (3)	14 (2)	35 (3)	0 (3)	3 (2)	-1 (3)
O(1)	5729 (9)	4352 (8)	2965 (9)	0.68 (9)	33 (9)	11 (5)	82 (11)	-7 (6)	8 (8)	7 (6)
O(2)	6691 (10)	830 (9)	2817 (10)	0.90 (9)	38 (9)	30 (6)	92 (11)	-2 (7)	18 (8)	-20 (7)
O(3)	3509 (8)	2297 (9)	5606 (9)	0.78 (8)	28 (8)	17 (5)	94 (10)	-4 (7)	19 (7)	10 (8)
O(4)	7935 (9)	2247 (9)	7478 (9)	0.81 (9)	41 (8)	31 (6)	66 (10)	-9 (7)	-8 (7)	-1 (7)
O(5)	8874 (9)	-862 (8)	798 (9)	0.71 (9)	50 (10)	15 (5)	55 (10)	9 (6)	4 (8)	-7 (7)
O(6)	546 (9)	109 (8)	4755 (10)	0.71 (9)	38 (9)	24 (6)	54 (10)	-12 (6)	-4 (8)	2 (6)
O(7)	1848 (10)	1173 (8)	8630 (10)	0.83 (9)	51 (10)	32 (6)	60 (11)	13 (6)	19 (8)	1 (7)
O(8)	-70 (9)	2075 (7)	-8476 (9)	0.68 (9)	49 (9)	17 (6)	52 (10)	6 (5)	17 (7)	4 (6)

Table 2. *Interatomic distances (Å) and valence angles (°) in $\text{Na}_2\text{ZnSi}_3\text{O}_8$*

O^b : oxygen atom bonded to two silicon atoms (bridging oxygen atom); all other oxygens are bonded to one silicon and one zinc atom.

[SiO₄] tetrahedra

	Si—O distances			$\Delta Z n_{\text{br}}$		O...O distances	O—Si—O angles
	Observed	Predicted					
Si(1)—O(1)	1.597 (7)	1.607	0.5	O(1)—O(3)	2.708 (10)	116.2 (4)	
Si(1)—O(3)	1.594 (8)	1.603	0.5	O(1)—O(6) ^b	2.646 (9)	109.0 (4)	
Si(1)—O(6) ^b	1.653 (7)	1.648	-0.5	O(1)—O(7) ^b	2.627 (10)	107.5 (4)	
Si(1)—O(7) ^b	1.661 (8)	1.650	-0.5	O(3)—O(6) ^b	2.693 (10)	112.0 (4)	
Mean	1.626	1.629		O(3)—O(7) ^b	2.634 (10)	108.0 (4)	
				O(6) ^b —O(7) ^b	2.598 (9)	103.2 (3)	
				Mean	2.651	109.3	
Si(2)—O(2)	1.591 (7)	1.587	0.75	O(2)—O(5) ^b	2.610 (10)	108.0 (4)	
Si(2)—O(5) ^b	1.636 (7)	1.642	-0.25	O(2)—O(6) ^b	2.648 (9)	110.7 (4)	
Si(2)—O(6) ^b	1.628 (7)	1.631	-0.25	O(2)—O(8) ^b	2.709 (10)	114.1 (4)	
Si(2)—O(8) ^b	1.637 (7)	1.638	-0.25	O(5) ^b —O(6) ^b	2.653 (9)	108.8 (4)	
Mean	1.623	1.624		O(5) ^b —O(8) ^b	2.642 (9)	107.6 (4)	
				O(6) ^b —O(8) ^b	2.634 (9)	107.6 (4)	
				Mean	2.649	109.5	
Si(3)—O(4)	1.575 (6)	1.568	0.75	O(4)—O(5) ^b	2.700 (9)	114.1 (4)	
Si(3)—O(5) ^b	1.642 (8)	1.642	-0.25	O(4)—O(7) ^b	2.699 (9)	114.9 (4)	
Si(3)—O(7) ^b	1.627 (7)	1.633	-0.25	O(4)—O(8) ^b	2.627 (9)	109.7 (4)	
Si(3)—O(8) ^b	1.634 (8)	1.638	-0.25	O(5) ^b —O(7) ^b	2.645 (10)	108.0 (4)	
Mean	1.620	1.622		O(5) ^b —O(8) ^b	2.525 (9)	103.1 (3)	
				O(7) ^b —O(8) ^b	2.611 (10)	106.2 (4)	
				Mean	2.635	109.3	

[ZnO₄] tetrahedron

	Zn—O distances			$\Delta Z n_{\text{br}}$		O...O distances	O—Zn—O angles
	Observed	Predicted					
Zn—O(1)	1.963 (7)	1.963	0	O(1)—O(2)	3.112 (10)	106.6 (3)	
Zn—O(2)	1.918 (7)	1.961	0	O(1)—O(3)	3.063 (10)	103.1 (3)	
Zn—O(3)	1.949 (6)	1.960	0	O(1)—O(4)	3.437 (10)	123.0 (3)	
Zn—O(4)	1.948 (6)	1.941	0	O(2)—O(3)	3.329 (10)	118.9 (3)	
Mean	1.945	1.95		O(2)—O(4)	3.153 (10)	109.3 (3)	
				O(3)—O(4)	2.908 (8)	96.5 (3)	
				Mean	3.167	109.6	

Table 2. (cont.)

T-O-T angles		Summary of mean angles and distances	
Si(1)—O(6)—Si(2)	140.6 (5)	Mean Si—O ^b	1.640
Si(1)—O(7)—Si(3)	132.2 (4)	Mean Si—O	1.589
Si(2)—O(5)—Si(3)	135.0 (4)	Grand mean Si—O	1.623
Si(2)—O(8)—Si(3)	128.8 (4)	Grand mean Zn—O	1.945
Mean	134.2	Grand mean O...O	
Zn—O(1)—Si(1)	121.5 (3)	Si tetrahedra	2.645
Zn—O(2)—Si(2)	122.1 (4)	Zn tetrahedron	3.167
Zn—O(3)—Si(1)	124.1 (4)	Mean O—Si—O	116.2
Zn—O(4)—Si(3)	152.3 (4)	Mean O—Si—O ^b	110.9
Mean	130.0	Mean O ^b —Si—O ^b	106.4
		Grand mean O—T—O	
		Si tetrahedra	109.4
		Zn tetrahedron	109.6

Na polyhedra		Na—O distances	
Na(1)—O(2)	2.403 (9)	Na(2)—O(3)	2.339 (8)
—O(1)	2.448 (8)	—O(1)	2.440 (8)
—O(4)	2.602 (9)	—O(6)	2.510 (9)
—O(3)	2.634 (8)	—O(8)	2.550 (7)
—O(5)	2.824 (8)	—O(5)	2.557 (8)
—O(7)	2.934 (8)	—O(4)	2.558 (9)
—O(7')	3.180 (8)	—O(2)	2.748 (8)
—O(8)	3.410 (8)	—O(7)	3.096 (7)
—O(2')	3.427 (8)	Mean (CN = 7)	2.529
Mean (CN = 7)	2.718	Mean (CN = 8)	2.600
Mean (CN = 9)	2.874		

reflexions, is $R = 0.048$ for the isotropic refinement and 0.033 for the anisotropic (Hesse, 1972).^{*} Bond lengths and valence angles are listed in Table 2.

^{*} A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32226 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Discussion of the structure

A short description of this structure was given at the 1973 Annual Meeting of the Deutsche Mineralogische Gesellschaft in Frankfurt/Main (Hesse & Liebau, 1974). It is in fair agreement with the result of an independent structure analysis of $\text{Na}_2\text{ZnSi}_3\text{O}_8$ by Plakhov, Simonov & Belov (1974).

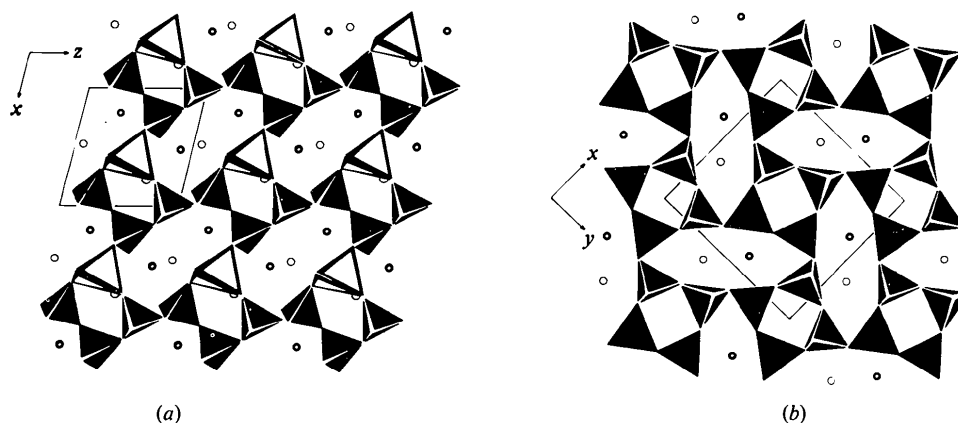


Fig. 1. Comparison between the structures of (a) $\text{Na}_2\text{ZnSi}_3\text{O}_8$ and (b) paracelsian $\text{BaAl}_2\text{Si}_2\text{O}_8$. Only one of the two tetrahedral layers per unit cell has been shown for each structure. $[\text{SiO}_4]$ and $[(\text{Si,Al})\text{O}_4]$ tetrahedra are shown black, $[\text{ZnO}_4]$ tetrahedra white. Heavy circles are sodium and barium ions above the layers, light circles are those below.

In Na₂ZnSi₃O₈ the [SiO₄] tetrahedra are corner-shared to form chains parallel to [001] containing three tetrahedra in their repeat unit (*Dreiereinfachketten*: Liebau, 1972). These chains are linked to *Dreiereinfachschichten* of composition 2[Si₃O₈] parallel to (100) (Fig. 1 of Plakhov, Simonov & Belov, 1974). The non-bridging O atoms of the silicate layers are bonded to tetrahedral Zn oxyanions so that [SiO₄] and [ZnO₄] tetrahedra form a three-dimensional framework. Na₂ZnSi₃O₈ is an ordered tektozincosilicate, as evidenced by the mean Si—O bond lengths (Table 1) which are similar to those found in ordered paracelsian-type structures [1.623 and 1.624 Å in SrAl₂Si₂O₈ (Griffen, Ribbe & Gibbs, 1977) and 1.616 and 1.622 Å in BaAl₂Si₂O₈ (Craig, Louisnathan & Gibbs, 1973)]. The topology of this framework is similar to that in paracelsian, BaAl₂Si₂O₈, (Smith, 1953) with the sodium zincosilicate-to-paracelsian transformation matrix 101/101/010 (Fig. 1). The Na⁺ ions fill cavities within the framework resulting in irregular coordination polyhedra of seven O atoms at less than 3.19 Å and two more at 3.4 Å for Na(1) and eight at less than 3.10 Å for Na(2). It is interesting that the isotropic temperature factors of 1.9 and 1.0 Å² correspond to mean ^[VII]Na—O bond lengths of 2.718 and 2.529 Å, respectively, for Na(1) and Na(2); the larger temperature factor may be due in part to H replacing Na in the Na(1) site.

Discussion of the bonding

There are a number of Na-containing compounds — NaAlSi₃O₈ (the plagioclase feldspar mineral albite), NaAlSi₂O₆·H₂O (the zeolite analcime), and Na₂(OH)AlSi₃O₈ (ussingite) — which share structural

similarities with Na₂ZnSi₃O₈. Albite and analcime are like Na₂ZnSi₃O₈ in that every O atom (excluding water molecules) is bonded to two tetrahedrally coordinated (*T*) cations, forming an infinite three-dimensional framework, but ussingite has an 'interrupted' framework (Rossi, Tazzoli & Ungaretti, 1974).

Phillips & Ribbe (1973) applied multiple linear regression analysis to the geometric and chemical variables in sodic plagioclase feldspars (Na_x-Ca_{1-x}Al_{2-x}Si_{2+x}O₈; 0 ≤ *x* ≤ 0.3) in order to determine their relative effects on individual *T*—O bond lengths. They showed that *T*—O bond lengths in all the aforementioned compounds could be predicted with correlation coefficients of 0.99. Thus, to determine if the bonding effects observed in these Na-rich aluminosilicates are similar to those in Na₂ZnSi₃O₈, we have slightly modified Phillips & Ribbe's (1973, p. 337) regression equation to account for the substitution of tetrahedral Zn for Al in the structural framework. We have estimated the 12 individual Si—O bond lengths using this equation:

$$\text{Si-O} = 1.571 - 0.068\Delta Z_{n_{br}} + 0.067[\Sigma 1/(\text{Na-O})^2] - 0.025/\cos(T\text{-O-T}),$$

where $\Delta Z_{n_{br}} \equiv Z_{n_{br}} - \langle Z_{n_{br}} \rangle$, and the term $Z_{n_{br}}$ represents the Zn content of the tetrahedron adjoining the individual Si—O distance under consideration, and $\langle Z_{n_{br}} \rangle$ is the mean content of all four tetrahedra adjacent to the tetrahedron under consideration. Values of $\Delta Z_{n_{br}}$ are listed in Table 2; those which are positive and non-zero are associated with bonds to Si from O atoms which are also bonded to Zn.

The $\Delta Z_{n_{br}}$ term in the equation accounts for what might be called a 'linkage effect'. In Na₂ZnSi₃O₈ the Si—O(→Zn) bonds (given in italics in Table 2) are 0.051 Å shorter on average than the Si—O(→Si) bonds. The second term in the equation accounts for the Coulombic interaction of the Na cation(s) with the O in an individual Si—O bond. Coordination-number effects are considered by summing over all Na—O bonds to that oxygen. Note that Si—O bonds to three coordination O atoms in this structure are 0.034 Å longer on average than those of four-coordinated O atoms. As documented in many previous studies of compounds containing polymerized tetrahedra (*e.g.* Louisnathan & Gibbs, 1972*a,b*), the *T*—O distances involved in wide *T*—O—*T* angles tend to be shorter than those involved in narrow *T*—O—*T* angles, regardless of the chemical identity of the *T* atoms or the degree of polymerization. The last term in the equation accounts for this effect, and it is expressed as the inverse cosine of the *T*—O—*T* angle in order to best linearize the relation to *T*—O distances (Gibbs, Hamil, Louisnathan, Bartell & Yow, 1972). Values predicted from this equation are listed in Table 2 and plotted in Fig. 2. The correlation coefficient for the estimated and observed Si—O distances, which range from 1.575 to 1.661 Å, is *r* = 0.97. The least-

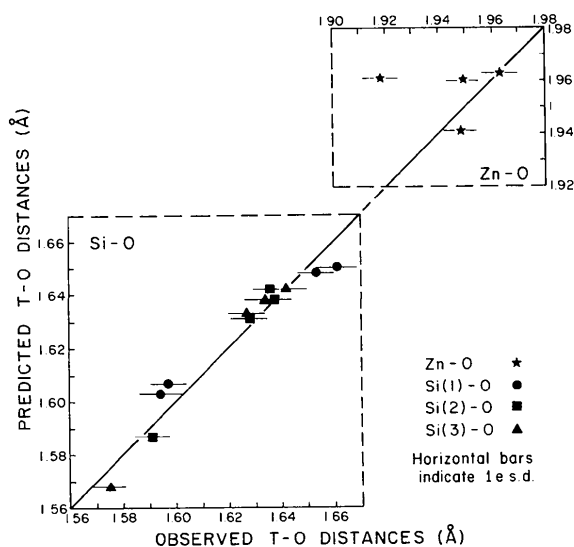


Fig. 2. A plot of the observed *T*—O distances *versus* those calculated from the regression equation for Na₂ZnSi₃O₈.

squares line of best fit $(\text{Si}-\text{O})_{\text{est}} = 0.94(\text{Si}-\text{O})_{\text{obs}} + 0.09$ is statistically the same as the expected 45° line. We regard this as evidence of the correctness of the bonding model proposed for $\text{Na}_2\text{ZnSi}_3\text{O}_8$.^{*} Zn—O bonds may be predicted reasonably well by adding to the intercept the difference between the mean Zn—O and Si—O distances ($1.945 - 1.623 = 0.322 \text{ \AA}$).

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^{*} A reviewer has pointed out that the equation $\text{Si}-\text{O} = 1.623 - 0.055\Delta Z_{\text{nbr}}$ estimates Si—O slightly better than the more general equation derived and used successfully by Phillips & Ribbe (1973) and Ribbe (1974) for the aluminosilicates. This indicates that ΔZ_{nbr} can be considered to be the preponderant factor in the analysis of bonding effects in $\text{Na}_2\text{ZnSi}_3\text{O}_8$, although this may not be the case in other framework structures. For example, in $\text{Na}_2\text{ZnSiO}_4$ (Plakhov, Simonov, Egorov-Tismenko & Belov, 1976) $[\text{ZnO}_4]$ and $[\text{SiO}_4]$ tetrahedra alternate in the framework, and therefore ΔZ_{nbr} is zero for all Si—O bonds. Our model predicts Si—O bond lengths of 1.645, 1.636, 1.645, 1.634 Å corresponding to observed values 1.640, 1.625, 1.648, 1.626 Å. The longer Si—O bond lengths are those to O atoms coordinated by three Na atoms, the shorter to those coordinated by only two Na.

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A Neutron Diffraction Study of Anhydrous Ethylenediamine D-Tartrate

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$\text{C}_6\text{H}_{14}\text{N}_2\text{O}_6$, monoclinic, $P2_1$, $a = 8.974(5)$, $b = 8.797(5)$, $c = 5.984(4)$ Å, $\beta = 105.40(10)^\circ$, $Z = 2$, $\rho_{\text{obs}} = 1.52(1)$, $\rho_{\text{calc}} = 1.533(3)$ g cm⁻³. Neutron diffraction was used to locate precisely all the H atoms. The structure consists of diprotonated ethylenediamine cations and tartrate anions with extensive interionic hydrogen bonding and a weak intraionic hydrogen bond between a tartrate —OH and —COO⁻ group [$\text{O}-\text{H} = 0.956(6)$ Å and $\text{H}\cdots\text{O} = 2.138(8)$ Å]. The shortest hydrogen bonds are from amine H atoms to carboxyl O atoms [$\text{H}(21)\cdots\text{O}(2) = 1.74(1)$ and $\text{H}(20)\cdots\text{O}(1) = 1.74(1)$ Å]. A comparison with D-tartaric acid is presented.

Experimental

The crystal was provided by G. K. Johnson and was prepared by slow evaporation at room temperature of a one-to-one aqueous mixture of ethylenediamine and D-tartaric acid. Only the anhydrous form was obtained. The crystal used for this study was bounded by ten faces and had axial dimensions of

about $0.30 \times 0.40 \times 0.15$ cm. The neutron data were collected on a Mitsubishi Diffractometer equipped with a full circle, designed and built by the Department of Physics, University of Missouri—Columbia, machine shop, and interfaced to a PDP-11 computer at the University of Missouri Research Reactor. The data were collected by the θ - 2θ step-scan technique. With 25 carefully centered reflections, for