Zeolitic Iron Cyanides: The Structure of $Na_2Zn_3[Fe(CN)_6]_2.xH_2O$*

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Abstract

$Na_2Zn_3[Fe(CN)_6]_2.9H_2O$, $M_r = 828 \cdot 14$, crystallizes in the space group $R\bar{3}c$ with $a = 13 \cdot 126$ (3) Å, $\alpha = 56 \cdot 71$ (2)°, $Z = 2$, $V = 1477 \cdot 8 \pm 0 \cdot 5$ Å^3 [hexagonal axes: $a_H = 12 \cdot 469$ (2), $c_H = 32 \cdot 92$ (2) Å; $Z = 6$; $V = 4433 \pm 2$ Å^3], $\rho_x = 1 \cdot 86$ Mg m^{-3}. The structure has been refined to $R = 0 \cdot 025$ ($R_w = 0 \cdot 029$) for 294 unique reflections [μ(Mo $K\alpha$) $= 3 \cdot 5$ mm^{-1}]. The results confirm with greater accuracy the new structural type found for $K_2Zn_3[Fe(CN)_6]_2.xH_2O$. FeC_6 octahedra and ZnN_4 tetrahedra are held together by the CN^- ions making up a three-dimensional frame with large cavities in which Na^+ ions and water molecules are randomly distributed. This rhombic framework proves to be characteristic of a larger series of zinc iron cyanides showing ion-exchange behaviour and zeolitic properties.

Introduction

The X-ray characterization and crystal structure determination of $Na_2Zn_3[Fe(CN)_6]_2.xH_2O$ are within the scope of our study of the relations between physicochemical properties and structures of zeolitic iron cyanides (Renaud, Gravereau, Garnier & Cartraud, 1979).

The new type of structure determined for $K_2Zn_3[Fe(CN)_6]_2.xH_2O$ (Gravereau, Garnier & Hardy, 1979) appears to be representative of a larger series but is not accurately defined since available single crystals are difficult to obtain. Better preparation results with the sodium compound have allowed us to establish more precisely this model and the three-dimensional framework in particular. This structural determination will also be useful in confirming the accuracy of the unindexed X-ray powder pattern given by Kawamura, Kuraku & Kurotaki (1970), and in explaining the ion-exchange properties of these compounds (Vlasselaer, D'Olieslager & D'Hont, 1976).

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* Disodium trizinc hexacyanoferrate(II) hydrate.

Powder characterization

Preparation of sodium zinc hexacyanoferrate(II) powder

$Na_2Zn_3[Fe(CN)_6]_2.xH_2O$ was prepared by the dropwise and simultaneous addition while stirring of $0 \cdot 1$ M sodium hexacyanoferrate(II) and $0 \cdot 1$ M zinc nitrate in a ratio of 2 to 3. The white slurry obtained was heated in boiling water for 2 h and left for six days at room temperature. It was washed with distilled water, and centrifuged, then left to dry for three days at 313 K. Before analysis and X-ray diffraction it was allowed to stand one week in air at room temperature (Kawamura *et al.*, 1970).

Analysis

The iron, carbon, nitrogen, sodium and zinc contents were determined by the CNRS Service Central de Microanalyse (France). The mean values of a threefold analysis are summarized in Table 1. The values of the molar ratios were calculated by taking the atomic weight of C as 12. They indicate the composition $Na_2Zn_3[Fe(CN)_6]_2.9H_2O$.

The thermal behaviour of this compound in air was studied by differential thermal analysis and thermogravimetric analysis. The loss of water occurs in two steps: 7·6 molecules are released near 458 K and a total number of 9·0 by 503 K. The decomposition of this solid takes place soon after the loss of the last molecules of water.

X-ray powder diffraction pattern

The X-ray powder diffraction pattern was obtained with a Philips diffractometer at room temperature using

Table 1. *Powder analysis*

	Fe	C	N	Na	Zn	H₂O
Wt %	14·23	17·42	20·27	5·12	24·11	18·85
Molar ratio	2·11	12	11·97	1·84	3·05	8·66

Table 2. *X-ray powder diffraction data and line-by-line figure-of-merit calculation for* $Na_2Zn_3[Fe(CN)_6]_2 \cdot 9H_2O$

d_{obs} (Å)	$100 \frac{I}{I_o}$	h k l in obverse rhombo-hedral lattice	$2\theta_{obs}$ (°)	$\Delta 2\theta$ (°) $(2\theta_o - 2\theta_c)$	$F_N(\overline{\lvert\Delta 2\theta\rvert}, N_{poss})$
9·039	5	1 1 0	11·366	−0·0055	182 (0·0055, 1)
6·547	7	2 1 1	15·716	+0·0017	278 (0·0036, 2)
6·243	8	1 1̄ 0	16·486	−0·0053	240 (0·0042, 3)
5·479	9	2 2 2	18·806	+0·0258	104 (0·0096, 4)
5·425	100	2 1 0	18·996	+0·0023	123 (0·0081, 5)
5·133	1	2 0 0	20·086	+0·0099	119 (0·0084, 6)
4·518	33	2 2 0	22·855	+0·0005	137 (0·0073, 7)
4·124	71	3 2 1	25·075	−0·0166	118 (0·0085, 8)
4·055	22	2 1̄ 0	25·505	−0·0005	132 (0·0076, 9)
3·846	2	3 3 2	26·915	−0·0038	126 (0·0072, 11)
3·658	9	3 1 0	28·325	+0·0114	121 (0·0076, 12)
3·6037	35	2 1̄ 1̄	28·765	+0·0004	132 (0·0070, 13)
3·4715	13	3 2 0	29·885	+0·0035	138 (0·0067, 14)
3·1550	27	4 3 2	32·965	+0·0096	127 (0·0069, 16)
3·1210	8	2 2̄ 0	33·334	−0·0006	128 (0·0065, 18)
3·0851	4	4 2 1	33·734	−0·0055	131 (0·0064, 19)
3·0123	8	4 1 1	34·574	−0·0020	131 (0·0062, 21)
3·0009	<1	3 1 1̄	34·709	+0·0115	127 (0·0065, 22)
2·9905	1	2 2̄ 1̄	34·834	−0·0524	93 (0·0089, 23)
2·9495	2	3 1̄ 0	35·334	+0·0057	96 (0·0087, 24)
2·8995	1	4 3 1	35·964	+0·0006	101 (0·0083, 25)
2·8134	<1	3 2 1̄	37·104	+0·0539	81 (0·0104, 26)
		4 4 2		−0·0237	78 (0·0110, 27)
2·7436	<1	4 4 4	38·084	−0·0033	80 (0·0107, 28)
2·7284	1	4 1 0	38·304	+0·0064	82 (0·0105, 29)
2·7134	11	4 2 0	38·524	−0·0092	83 (0·0104, 30)
2·6675	5	2 2̄ 2̄	39·214	−0·0059	85 (0·0103, 31)
2·5641	8	4 0 0	40·864	+0·0628	72 (0·0122, 32)
		5 3 2		−0·0088	73 (0·0120, 33)
2·5281	10	4 3 0	41·473	+0·0042	75 (0·0118, 34)
2·5108	2	5 4 3	41·773	+0·0132	75 (0·0118, 35)
2·4735	<1	3 2̄ 0	42·433	−0·0029	77 (0·0115, 36)
2·4525	<1	3 2̄ 1̄	42·813	+0·0018	79 (0·0112, 37)
2·4229	2	5 2 1	43·363	+0·0100	80 (0·0112, 38)
2·4155	1	5 4 2	43·503	−0·0186	79 (0·0114, 39)
2·3745	12	4 1 1̄	44·293	+0·0063	80 (0·0113, 40)
		5 3 1̄		−0·0054	81 (0·0111, 41)
2·3588	<1	3 2̄ 1̄	44·603	+0·0085	82 (0·0111, 42)
2·3209	3	4 2 1̄	45·373	+0·0048	83 (0·0109, 43)
2·3069	5	3 2̄ 2̄	45·663	−0·0073	84 (0·0108, 44)
2·3069		4 1̄ 0	45·663	−0·0073	85 (0·0107, 45)
2·2979	1	5 5 4	45·853	+0·0019	87 (0·0105, 46)
2·2597	3	4 4 0	46·673	−0·0118	87 (0·0105, 47)
2·2172	8	5 4 1	47·622	−0·0084	87 (0·0105, 48)
2·1938	5	5 2 0	48·162	+0·0028	89 (0·0103, 49)
2·1832	4	5 5 2	48·412	−0·0061	90 (0·0102, 50)
2·1832		6 3 3	48·412	−0·0061	91 (0·0101, 51)
2·1676	3	4 3 1̄	48·782	−0·0046	92 (0·0100, 52)
2·1676		5 1̄ 0	48·782	−0·0046	93 (0·0099, 53)
2·1560	2	6 4 4	49·062	+0·0082	94 (0·0099, 54)

unfiltered Co $K\bar{\alpha}$ radiation ($\lambda = 1 \cdot 79026$ Å). The conditions were: 40 kV and 40 mA, time constant 4 s, scan speed $\frac{1}{4}°$ (2θ) min^{-1}, paper speed 1 cm min^{-1}, counting scale 10^4 counts s^{-1}. 2θ values were corrected for eccentricity and scan speed. The relative intensities were simply estimated by the peak-to-background intensity. The results are summarized in Table 2, using the quantitative figure of merit $F_N = (1/\overline{\lvert\Delta 2\theta\rvert})N/N_{poss}$, where N_{poss} is the number of possible diffraction lines up to the Nth observed line and $\overline{\lvert\Delta 2\theta\rvert}$ is the average absolute discrepancy between the observed and calculated 2θ values (Smith & Snyder, 1979).

All the lines were attributed to the rhombohedral system. Parameters a and α were refined with 50 2θ

values using Tournarie's program *SPSRM* 379 (No. 77 in *World List of Crystallographic Computer Programs*, 1973): $a = 13 \cdot 130$ (2) Å, $\alpha = 56 \cdot 776$ (5)°, $V = 1481 \cdot 3 \pm 0 \cdot 5$ Å^3. It should be noted that these parameters relate to nine molecules of water (Table 1).

Single crystals

Single crystals were grown in silica gel obtained by mixing a sodium metasilicate and sodium chloride solution (60 g of $Na_2SiO_3 \cdot 9H_2O$ and 7·3 g of NaCl in 500 cm^3 of water) and 3 M hydrochloric acid to a pH of approximately 6·1.

The solution was poured into U-tubes of 40 mm diameter and permitted to gel at 313 K. After six days, the solution of 5×10^{-3} M zinc chloride acidified to a pH of 4 was carefully added to one end of the U-tube while the solution of 5×10^{-3} M sodium hexacyanoferrate(II) acidified to a pH of 5 was added to the other end (all reagents were Baker-analysed reagents). After three months a few colourless single crystals with nearly rhombic habit and an edge size of approximately 0·050 mm had grown which were suitable for an X-ray structure determination. Many different experiments were carried out with variations in the concentrations of the reactants, initial pH of the reactants, pH of the gel, gel density and temperature.

A quantitative electron probe analysis was carried out. The atomic concentration ratio found for Zn/Fe: 1·50 (2) was in close agreement with the theoretical value (1·5) but Na/Fe values were low and variable due to the decomposition of the solid by the electron beam.

Crystallographic study and data collection

Precession and retigram photographs reveal that $Na_2Zn_3[Fe(CN)_6]_2 \cdot 9H_2O$ belongs to the $\bar{3}m$ Laue group. The cell parameters were refined by Tournarie's program from the diffractometer settings for 15 reflections. With graphite-monochromatized Mo $K\alpha$ radiation, data were collected in the hexagonal cell in the range $0° < \theta < 20°$ with $-12 \leq h \leq 12, -12 \leq k \leq 12$ and $0 \leq l \leq 31$ by the $\omega-2\theta$ scan technique with an angular width of $1 \cdot 5° + 0 \cdot 45°$ tg θ, a horizontal aperture of 3 mm and 60 s as the maximum time for the final scan. The take-off angle optimized with four reflections was equal to 4°. Crystal orientation was monitored and the intensities of three standard reflections were checked every 100 reflections throughout the data collection, with no significant fluctuations and a maximum relative deviation of 5%.

After correction by the Lorentz–polarization factor, the 8407 reflections recorded were averaged and reduced to 294 independent observations with $\sigma(I)/I <$

0·5. No absorption corrections were made ($\mu = 3·5$ mm^{-1}, extremal sizes of the crystal are equal to 20 μm and 50 μm and azimuthal scans collected for 10 reflections show a relative deviation of less than 6% for intensity values). The $hh(0)l$ absences with $l = 2n + 1$ lead to two possible space groups $R\bar{3}c$ and $R3c$.

Structure determination and refinement

The atomic positions of Zn, Fe, C and N found in the space group $R3c$ for the potassium compound were used as the starting model. All calculations were performed with *SHELX* (Sheldrick, 1976). Scattering factors for Zn^{2+}, Fe^{2+}, C, N, Na^+ and O^- were taken from *International Tables for X-ray Crystallography* (1974) and corrected for anomalous dispersion. Na^+ ions and water molecules were located with several difference Fourier syntheses, and their relative occupancy factors were introduced as variable parameters during the refinement. As there is a slight difference in the scattering factors of O^- and Na^+, several hypotheses were tried. Five independent water molecules were thus found. Because of the strong correlation observed for these atoms between thermal parameters and occupancy factors we have introduced an overall Debye–Waller factor for water molecules. The structure was refined with isotropic temperature factors to $R = 0·029$ ($R_w = 0·029$). Anisotropic values introduced for Zn and Fe did not improve the model ($R = 0·025$). The residual difference Fourier synthesis was featureless and its maximum electron density was less than 0·4 e Å^{-3}. Table 3 gives the final atomic parameters.*

* Tables of structure factors and anisotropic thermal parameters for Zn and Fe have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36585 (5 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Description of the structure and discussion

The new type of structure found for the potassium compound is thus confirmed and established more precisely here. The structure is a three-dimensional framework made up of FeC_6 octahedra and ZnN_4 tetrahedra linked together by the CN groups. In such a framework, large cavities occur, each of which communicates with six others by means of six 'windows'. Na^+ ions and water molecules are located inside these cavities.

The three-dimensional framework

The basic element $[(ZnN_4)_3(FeC_6)_2]^{2-}$ of this framework may be seen in Fig. 1. Principal bond lengths and angles in the coordination polyhedra are listed in Table 4. The FeC_6 octahedron is very slightly deformed with a mean Fe–C bond length of 1·88 Å. Angular distortions around the ideal value (109·47°) are somewhat greater in the ZnN_4 tetrahedron. This observation may be correlated with angular Fe–C–N values ($\simeq180°$) which indicate that CN^- ions are aligned with Fe atoms. The mean C–N distance (1·164 Å) is consistent with previously reported values (Buser, Schwarzenbach, Petter & Ludi, 1977).

In this framework all the centres of symmetry on the threefold axis are centres of large cavities (Fig. 2). In Table 5 we have indicated some characteristic cavity dimensions which may be useful in studying zeolitic properties and the molecular-sieving effect of this compound. Distances for unoccupied space have been calculated considering the CN^- ions as cylinders with a mean radius $r_{CN} \simeq 1·4$ Å.

Table 3. Atomic parameters in the hexagonal lattice

For each atom the relative occupancy of the site, the fractional coordinates and isotropic thermal parameters (equivalent values for Zn and Fe) are given.

	Site	Relative occupancy	x	y	z	B_{eq} or B_{iso} (Å^2)
Zn	18(e)	1	0·2896 (1)	0	¼	1·57 (5)
Fe	12(c)	1	0	0	0·1474 (1)	1·12 (6)
C(1)	36(f)	1	0·1137 (9)	−0·0146 (9)	0·1811 (3)	1·7 (2)
C(2)	36(f)	1	0·5341 (9)	0·2162 (8)	0·2177 (2)	1·6 (2)
N(1)	36(f)	1	0·1825 (8)	−0·0248 (8)	0·2028 (2)	2·7 (2)
N(2)	36(f)	1	0·4520 (7)	0·1442 (7)	0·2370 (2)	2·2 (2)
Na	36(f)	0·30 (5)	0·579 (4)	0·356 (4)	0·303 (1)	11 (2)
O(1)	36(f)	0·17 (3)	0·511 (9)	0·254 (11)	0·316 (3)	⎫
O(2)	36(f)	0·15 (3)	0·455 (12)	0·314 (12)	0·322 (3)	⎪
O(3)	36(f)	0·28 (5)	0·542 (7)	0·398 (8)	0·313 (2)	⎬ 11·1 (7)
O(4)	36(f)	0·56 (4)	0·404 (4)	0·351 (3)	0·296 (1)	⎪
O(5)	36(f)	0·40 (4)	0·330 (5)	0·320 (4)	0·283 (1)	⎭

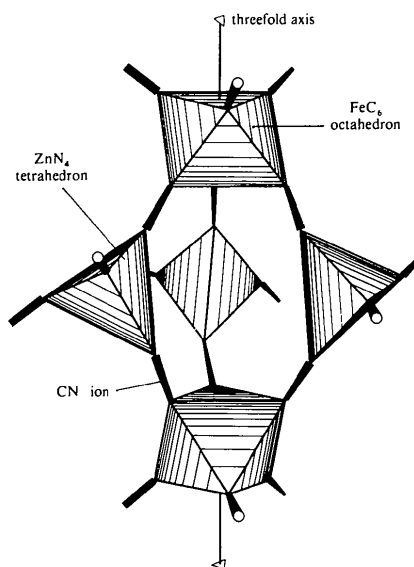

Fig. 1. Polyhedron grouping in ${Zn_3[Fe(CN)_6]_2}^{2-}$.

Table 4. *Interatomic distances (Å) and angles (°) with e.s.d.'s in parentheses*

Symmetry code: (i) $-y, x - y, z$; (ii) $-x + \frac{2}{3}, -y + \frac{1}{3}, -z + \frac{1}{3}$; (iii) $y - \frac{1}{3}, y - x + \frac{1}{3}, -z + \frac{1}{3}$; (iv) $x - y - \frac{1}{3}, x - \frac{2}{3}, -z + \frac{1}{3}$; (v) $x - y, -y, \frac{1}{2} - z$.
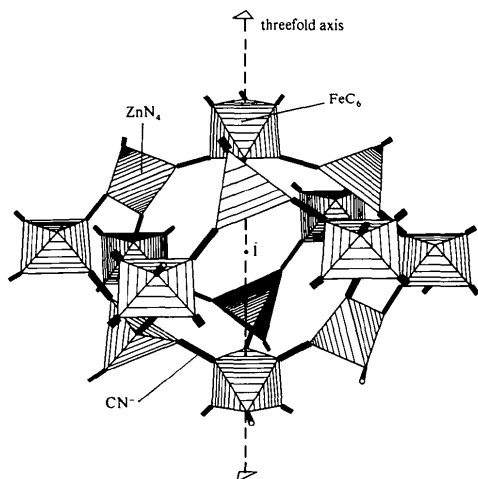
Fe octahedron

		C(1)–Fe–C(1ⁱ)	88·8 (4)
		C(1)–Fe–C(2ⁱⁱ)	89·5 (4)
Fe–C(1)	1·878 (9)	C(1)–Fe–C(2ⁱⁱⁱ)	177·6 (5)
Fe–C(2ⁱⁱ)	1·884 (9)	C(1)–Fe–C(2ⁱᵛ)	89·7 (4)
		C(2ⁱⁱ)–Fe–C(2ⁱⁱⁱ)	92·1 (4)

Zn tetrahedron

		N(1)–Zn–N(1ᵛ)	106·3 (5)
Zn–N(1)	1·968 (8)	N(1)–Zn–N(2)	106·2 (3)
Zn–N(2)	1·969 (8)	N(1)–Zn–N(2ᵛ)	114·0 (3)
		N(2)–Zn–N(2ᵛ)	110·2 (5)

CN⁻ ions

		Fe–C(1)–N(1)	178·3 (8)
C(1)–N(1)	1·172 (10)	Fe–C(2ⁱⁱ)–N(2ⁱⁱ)	179·4 (8)
C(2)–N(2)	1·156 (10)	Zn–N(1)–C(1)	160·1 (8)
		Zn–N(2)–C(2)	159·3 (7)

Fig. 2. Constitution of a framework cavity with its $\bar{3}$ symmetry.

Table 5. *Distances in zeolitic cavities of the framework $n\{Zn_3[Fe(CN)_6]_2\}^{2-}$*

		CN–CN distances d (Å)	Distances for unoccupied space $d-2r_{CN}$ (Å)
Ellipsoidal cavities	Height ~ parallel to c_H	8·10 (3)	5·3
	Range of variation in plane $\simeq (a_H, b_H)$	11·02 (3)–15·43 (3)	8·2–12·6
'Window'	Upper limit	8·00 (3)	5·2
	Lower limit	6·85 (3)	4·0

Sodium ions and water molecules

The large dimensions of the cavities and the statistical occupancy of sites account for the relative lack of accuracy of the atomic parameters obtained for Na^+ ions and water molecules. In spite of a strong correlation with thermal parameters the following comments can be made about the occupancy factors:

(1) For sodium the theoretical value is $\frac{1}{3}$ (two Na^+ randomly distributed among the six equivalent positions of a $\bar{3}$ site in each cavity). The value obtained is slightly lower and this trend has also been observed for all our powder analyses (Table 1).
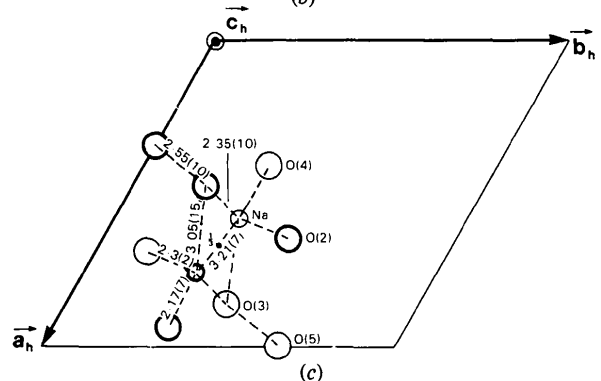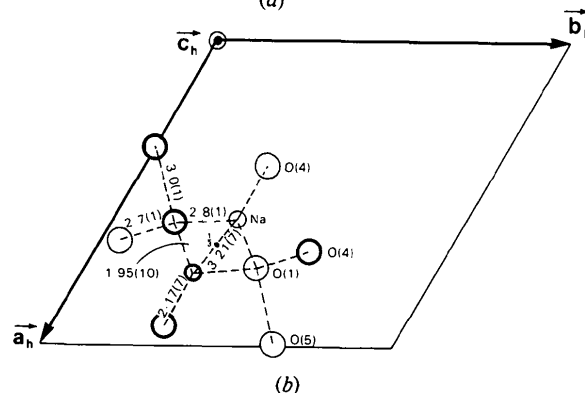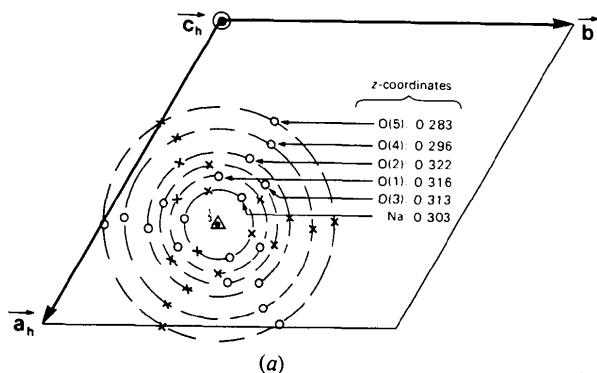

(a)

(b)

(c)

Fig. 3. Na^+ ions and water molecules inside cavity centred at $\frac{2}{3},\frac{1}{3},\frac{1}{3}$. (a) All statistical sites with $\bar{3}$ symmetry. (b), (c) Two hypotheses of ordered positions with only 1 symmetry.

(2) The total number of water molecules in a cavity is 9·4 (1·2). This is in close agreement with the values found for powder in room conditions by classical analysis (Table 1), or by thermogravimetric analysis.

To discuss the environments of Na^+ ions and water molecules, a hypothesis of the distribution inside a cavity is necessary. The solution obtained is likely to be an averaged value of a large number of possibilities. Fig. 3(a) shows all possible sites inside the cavity centred at $(\frac{2}{3},\frac{1}{3},\frac{1}{3})$. Fig. 3(b) and (c) are two hypotheses of ordered positions for which only $\bar{1}$ centres of symmetry are retained. Equal probabilities for these two distributions would lead to a formula unit with eight water molecules [one (1), one (2), one (3), three (4), two (5)]. The main purpose of such a hypothesis is to indicate some interatomic distances and to characterize two kinds of water molecules: some of them surround the Na^+ ions and others [one (4) and two (5) in the considered hypothesis] are mostly zeolitic ones. This could explain why the removal of water molecules occurs in two steps as observed with differential thermal analysis and thermogravimetric analysis.

It is impossible to establish the existence of hydrogen bonds from these results and we now intend to carry out a spectroscopic study of the series $M_2^I Zn_3$-$[Fe(CN)_6]_2.xH_2O$ with M^I = Na, K, Cs to complete our crystallographic investigation.

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Structure of Lithium Sodium Yttrium Silicate Na2LiYSi6O15

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Abstract

$Na_2LiYSi_6O_{15}$ is orthorhombic, space group *Cmca*, with cell dimensions $a = 14\cdot505$ (1), $b = 17\cdot596$ (1) and $c = 10\cdot375$ (1) Å; $Z = 8$. The structure was refined by the block-diagonal least-squares method to $R = 0\cdot082$ for 1501 independent reflections. The crystal structure consists of corrugated double silicate chains which have a six-tetrahedral repeat (*Sechser-Doppelkette*) in the c direction. Na(2) polyhedral chains and tetrahedral–octahedral chains composed of (LiO_4) and (YO_6) units link the silicate chains to form a three-dimensional structure. $Na_2LiYSi_6O_{15}$ is isostructural with synthetic $Na_2Mg_2Si_6O_{15}$ and the minerals zektzerite and emeleusite. The variation in the silicate component of these structures appears to be very small. Distortion of the tetrahedral site permits this structure type to accommodate a wide range of cations in the octahedral sites.

Introduction

Glasser & Marr (1979) reported the synthesis of $Na_2LiYSi_6O_{15}$, which from powder data was believed to be isostructural with $Na_2Mg_2Si_6O_{15}$ and with zektzerite, $NaLiZrSi_6O_{15}$ (Cradwick & Taylor, 1972; Ghose & Wang, 1978); both contain double silicate chains having a characteristic six-tetrahedral repeat known as *Sechser-Doppelkette*. The same anion is found to occur in the minerals tuhualite, $(Na,K)Fe^{2+}$-$Fe^{3+}Si_6O_{15}.0\cdot5H_2O$, and emeleusite, $Na_2LiFeSi_6O_{15}$, whose structures were determined by Merlino (1969) and Neilsen & Søtofte (1978). In this work the crystal structure of $Na_2LiYSi_6O_{15}$ has been determined and its structure is compared with other isostructural phases.

Experimental

Single crystals were grown from a melt having the bulk composition (in mol%), $Na_2O = 12\cdot6$, $Li_2O = 6\cdot2$,