Table 3. *Valence-bond analysis of* $Na_2Ba_3Cr_4F_{20}$; *s values from Zachariasen's* (1978) *equation; valence-bond parameters from Ferey et al.* (1985)

	Na	Ba(1)	Ba(2)	Cr(1)	Cr(2)	$\sum s$
F(1)	0·149 (1)		0·193 (2) 0·209 (3)	0·503 (7)		1·054 (13)
F(2)	0·081 (1) 0·058 (1)	2 × 0·286 (1)		0·541 (8)		0·966 (12)
F(3)			0·026 (1) 0·156 (2) 0·250 (3)		0·551 (8)	0·983 (13)
F(4)	0·034 (1)	2 × 0·045 (1)		0·445 (6)	0·432 (6)	0·956 (14)
F(5)	0·188 (2)	2 × 0·093 (1) 2 × 0·104 (1)			0·541 (7)	0·926 (11)
F(6)	0·165 (1)	2 × 0·245 (3)	0·194 (2)		0·561 (8)	1·165 (14)
F(7)			0·026 (1) 0·177 (2) 0·218 (2)	0·539 (7)		0·960 (12)
F(8)	0·140 (1)			0·451 (6)	0·500 (7)	1·091 (14)
F(9)	0·167 (1)		0·098 (1) 0·214 (3)	0·575 (8)		1·054 (13)
F(10)	0·053 (1)	2 × 0·257 (3)	0·213 (3)		0·519 (7)	1·042 (14)
$\sum s$	1·03 (1)	2·06 (4)	1·97 (3)	3·05 (4)	3·10 (4)	
$\sum s$ (expected)	1	2	2	3	3	

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Structure of an Aluminosilicophosphate

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Abstract. $H_3O^+.Al_4SiP_3O^-_{16}.nH_2O$, $M_r = 503{\cdot}9 + (n \times 18)$, trigonal, $R3$, $a = 13{\cdot}781\ (1)$, $c = 14{\cdot}846\ (2)$ Å, $V = 2441{\cdot}7\ (5)$ Å^3, $Z = 4{\cdot}5$, $D_m = 1{\cdot}92\ (2)$, $D_x = 1{\cdot}54$ Mg m^{-3}, $\lambda(\text{Mo } K\alpha) = 0{\cdot}7107$ Å, $\mu(\text{Mo } K\alpha) = 0{\cdot}584$ mm^{-1}, $F(000) = 1125$, $T = 298\ (2)$ K, final $R = 0{\cdot}067$ for 1011 unique observed reflections. The structure is related to that of chabazite, and is formed by joining together four-, six- and eight-membered rings of AlO_4 and $(P,Si)O_4$ tetrahedra. There are large ellipsoidal cavities linked by 2 six-membered-, 6 eight-membered- and 12 four-membered-ring apertures.

Introduction. Several aluminosilicophosphate molecular sieves have been synthesized recently (Lok, Messina, Patton, Gajek, Cannan, & Flanigen, 1984); these possess important and unique properties suitable for adsorptive, catalytic and ion-exchange applications. However, there has been no report on the crystal structure of this new family of aluminosilicophosphate molecular sieves. In this paper, the crystal structure of $H_3O^+.Al_4SiP_3O_{16}^-.nH_2O$ (ZYT-6) is reported.

Experimental. The crystals were prepared hydrothermally from the gel composed of $P_2O_5/Al_2O_3/$morpholine$/SiO_2$ with molar ratio 1:1:2:1. The calculated density of the crystal is small in comparison with the measured density (flotation in aqueous ZnI_2); the discrepancy results from the presence of a large amount of zeolitic water in the cavities. Colorless prismatic crystals were obtained and used for the X-ray work. Atomic-absorption and ICP (inductively coupled plasma) spectrometry showed that the crystals contained P 15·1, Al 18, Si 4·12, Na 0·07 wt%, indicating that the composition of the crystal is $Al_{4.0}P_{2.92}Si_{0.88}O_{15.6}.nH_2O$. Small fragments from the chemical analysis are not reliable, and the composition was assumed to be $H_3O^+.Al_4SiP_3O_{16}^-.nH_2O$. Approximate dimensions of the crystal specimen 0·20 × 0·15 × 0·15 mm. Rigaku

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AFC-5 automated four-circle diffractometer, graphite monochromator. Cell parameters refined by least-squares methods on the basis of 24 2θ values, Mo $K\alpha$ radiation ($25° \le 2\theta \le 35°$). The only systematic-absence condition, hkl with $-h+k+l \neq 3n$, indicates the possible space groups $R3$ and $R\bar{3}$. Intensity measurement performed to $2\theta = 55°$. ω–2θ scan technique, scan speed 2 ° $\min^{-1}(\theta)$. Mean ratio of structure factors of five standard reflections $0{\cdot}93 \le \sum(|F_o|/|F_o|_{\rm init})/5 \le 1{\cdot}0$. 1510 reflections measured, 499 unobserved, 1011 unique [$|F_o| > 3\sigma(|F_o|)$]. Correction for Lp; no absorption or extinction corrections. Patterson maps revealed some of the heavy atoms in the framework. Remaining O atoms found by successive Fourier syntheses and refined by block-diagonal least squares using the *UNICS*III computation program system (Sakurai & Kobayashi, 1979); eight O atoms of ordered zeolitic water were found from difference density maps and refined isotropically. At an early stage of the refinement, all the heavy atoms were assumed to be Al and P. At a later stage, the population parameters of the Si atoms on the Al and P sites were refined, where the Si atoms were assumed to lie on the Al and P sites and the total population of the atoms on each tetrahedral site was constrained to 1·0. After a few cycles of refinement, the occupancy factors of the Si atoms on the Al sites and the P sites converged to 0·0 and 0·1 [for P(1)] or 0·2 [for P(2)], respectively, suggesting that the Si atoms are distributed on the P sites exclusively. The structure converged to the parameter values corresponding to the formula $Al_4SiP_3O_{16}$ in agreement with the result of the chemical analysis. The refinements have also been carried out both in the centrosymmetric space group $R\bar{3}$ and in the noncentrosymmetric $R3$. The former structure showed a significantly larger R factor, 8·0. Furthermore, some coordinates of the present structure are not within 10σ of the symmetrically related coordinates. $\sum w||F_o|-|F_c||^2$ minimized, $w^{-1} = \sigma^2(|F_o|) + (0{\cdot}015|F_o|)^2$; final $R = 0{\cdot}067$, $wR = 0{\cdot}110$, $S = 4{\cdot}0$ for 1011 observed reflections. In the final cycle $(\Delta/\sigma)_{\max} = 0{\cdot}3$ for a coordinate of O(6). No peaks higher than 0·2 e Å^{-3} in the final difference density map. Complex neutral-atom scattering factors from *International Tables for X-ray Crystallography* (1974). H atoms were not located.

Discussion. Atomic parameters are given in Table 1.* Interatomic distances and bond angles in the framework are listed in Table 2. The structure consists of a three-dimensional network formed by sharing corners of AlO_4 and $P(Si)O_4$ tetrahedra. The AlO_4 and $P(Si)O_4$ tetrahedra occur alternatively in the framework.

The average P—O and Al—O distances are 1·52 and 1·75 Å, respectively. These values and the bond angles around the P and Al atoms compare well with reported values (Bennett, Cohen, Flanigen, Pluth & Smith, 1983). The average P—O distance is significantly shorter than that of Al—O, clearly indicating the ordering of P and Al atoms in the structure.

The most important structural subunit of the framework is shown in Fig. 1 together with the numbering scheme. It is formed by linking together two six-membered rings of [P(Si),Al]O_4 tetrahedra, which form a double hexagonal ring around each corner of the rhombohedral cell. The double hexagonal ring possesses two P, two Al and eight O atoms (all crystallographically independent). It has approximate $3/m$ but

Table 1. *Positional parameters* ($\times 10^4$) *and equivalent isotropic temperature factors*

$$B_{\rm eq} = \tfrac{4}{3}\textstyle\sum_i\sum_j\beta_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	$B_{\rm eq}$(Å^2)
P(Si)(1)	38 (3)	2261 (3)	1082 (3)	1·5
P(Si)(2)	9973 (4)	7703 (4)	8921 (3)	1·5
Al(1)	2287 (4)	2266 (4)	1029 (3)	1·4
Al(2)	7709 (4)	7745 (4)	8957 (3)	1·5
O(1)	25 (10)	2638 (9)	72 (6)	2·1
O(2)	1139 (9)	2333 (11)	1318 (8)	2·8
O(3)	2005 (10)	908 (9)	1291 (9)	2·8
O(4)	3247 (9)	147 (10)	1706 (8)	2·8
O(5)	9950 (11)	7474 (13)	9904 (8)	3·6
O(6)	8814 (9)	7556 (10)	8617 (8)	2·5
O(7)	8095 (10)	9112 (9)	8779 (9)	3·0
O(8)	6757 (8)	9850 (9)	8358 (7)	2·4

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

P(1)—O(1)	1·58 (1)	P(2)—O(5)	1·48 (1)
P(1)—O(2)	1·51 (1)	P(2)—O(6)	1·57 (1)
P(1)—O(3)	1·51 (1)	P(2)—O(7)	1·58 (1)
P(1)—O(4)	1·59 (1)	P(2)—O(8)	1·49 (1)
Al(1)—O(2)	1·68 (1)	Al(2)—O(1)	1·72 (1)
Al(1)—O(3)	1·75 (1)	Al(2)—O(4)	1·68 (1)
Al(1)—O(5)	1·69 (1)	Al(2)—O(6)	1·74 (1)
Al(1)—O(8)	1·74 (1)	Al(2)—O(7)	1·70 (1)
O(1)—P(1)—O(2)	111·8 (7)	O(5)—P(2)—O(6)	110·0 (8)
O(1)—P(1)—O(3)	113·4 (6)	O(5)—P(2)—O(7)	106·7 (8)
O(1)—P(1)—O(4)	106·2 (8)	O(5)—P(2)—O(8)	112·7 (7)
O(2)—P(1)—O(3)	109·1 (8)	O(6)—P(2)—O(7)	107·3 (8)
O(2)—P(1)—O(4)	109·6 (7)	O(6)—P(2)—O(8)	105·8 (8)
O(3)—P(1)—O(4)	106·5 (8)	O(7)—P(2)—O(8)	114·2 (6)
O(2)—Al(1)—O(3)	106·8 (7)	O(1)—Al(2)—O(4)	110·0 (8)
O(2)—Al(1)—O(5)	110·4 (8)	O(1)—Al(2)—O(6)	111·9 (7)
O(2)—Al(1)—O(8)	110·2 (8)	O(1)—Al(2)—O(7)	110·8 (8)
O(3)—Al(1)—O(5)	108·7 (8)	O(4)—Al(2)—O(6)	106·3 (7)
O(3)—Al(1)—O(8)	106·7 (8)	O(4)—Al(2)—O(7)	115·0 (8)
O(5)—Al(1)—O(8)	113·8 (6)	O(6)—Al(2)—O(7)	107·9 (7)
P(1)—O(1)—Al(2)	144·2 (8)	P(2)—O(5)—Al(1)	157·8 (9)
P(1)—O(2)—Al(1)	151·2 (9)	P(2)—O(6)—Al(2)	143·5 (8)
P(1)—O(3)—Al(1)	147·4 (9)	P(2)—O(7)—Al(2)	144·1 (8)
P(1)—O(4)—Al(2)	145·8 (8)	P(2)—O(8)—Al(1)	147·3 (8)

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* Lists of structure factors, anisotropic thermal parameters for non-H atoms and parameters for ordered water molecules have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42421 (14 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

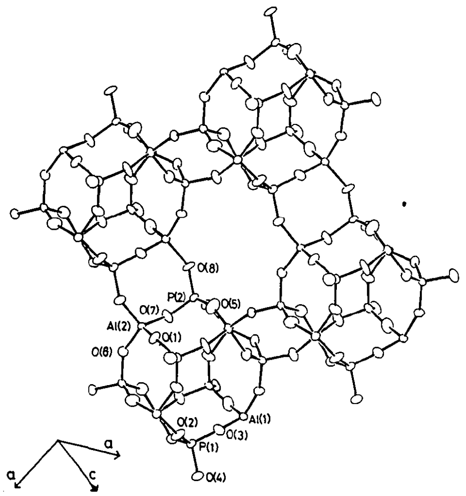

Fig. 1. *ORTEP* drawing (Johnson, 1965) of the four double hexagonal ring units. Thermal ellipsoids are at the 50% probability level. Only the unique atoms have been labeled.

strict 3 symmetry. Si substitution for the P sites results in an excess charge of −1 e per framework Si atom, which may be compensated by protonated water located near the center of the hexagonal ring. The distances between these protonated water O atoms and the O atoms of the hexagonal ring range from 2·75 to 3·10 Å.

The four double hexagonal ring units are interconnected to form circular 12-membered-ring pore openings. There are large ellipsoidal cavities linked by these apertures. These structural features are closely related to the natural zeolite chabazite (Smith, 1962).

Table 3. *Comparison of the pore-size values for ZYT-6 with those of chabazite*

	ZYT-6	Chabazite
Cavity size (Å) (long and short axes)	11·69 (4) 10·63 (5)	11·7 10·6
Diameter of the eight-membered ring (Å)	6·31 (1)	6·34
Diameter of the six-membered ring (Å)	4·15 (1)	4·41

Table 3 compares the pore-size values for ZYT-6 with those of chabazite. The dimensions of the cavity along its long and short axes are 11·69 (4) and 10·63 (5) Å, respectively. The shape of the eight-membered ring is almost circular but non-planar with diameter 6·31 (1) Å. The largest deviations from the best plane of the ring are for O(4) and O(8) at 0·51 (1), 0·53 (1) Å, respectively.

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The Sr^{2+} Distribution in Sr^{2+} β''-Alumina

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Abstract. Idealized formula: $Sr_xMg_{2x-1}Al_{12-2x}O_{17}$, $M_r = 640{\cdot}02$ for $x = \frac{5}{6}$, rhombohedral, $R\bar{3}m$. In hexagonal cell: $a = 5{\cdot}610\ (1)$, $c = 33{\cdot}720\ (5)$ Å, $V = 919{\cdot}1\ (5)$ Å^3, $Z = 3$, $D_x = 3{\cdot}469\ (2)$ Mg m^{-3}, Mo $K\bar{\alpha}$, $\lambda = 0{\cdot}71069$ Å, $\mu = 4{\cdot}96$ mm^{-1}, $F(000) = 930$, $T = 295$ K, final $R = 0{\cdot}073$, $R(F^2) = 0{\cdot}130$, $wR(F^2) = 0{\cdot}178$ for refinement on 1874 F^2. The Sr^{2+} ions ($r = 1{\cdot}18$ Å) lie distributed along edge-linked hexagonal

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