

Space group (203) *Fd-3*203
cF160

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|-------------------------------|--------------|---------------------------|
| $\text{Rb}_3\text{AsSe}_{16}$ | <i>cF160</i> | (203) <i>Fd-3</i> – gecba |
|-------------------------------|--------------|---------------------------|

Rb₃AsSe₄·2Se₆ [1]; **K₃PSe₄·2Se₆** [2]Structural features: One AsSe₄ tetrahedron for two Se₆ rings in chair conformation.

Wachhold M., Sheldrick W.S. (1997) [1]

 $\text{AsRb}_3\text{Se}_{16}$ $a = 1.666 \text{ nm}$, $V = 4.6241 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|------|---|
| Se1 | 96g | 1 | 0.01201 | 0.111 | 0.42978 | | non-colinear Se ₂ |
| Se2 | 32e | .3. | 0.20516 | 0.20516 | 0.20516 | | single atom As |
| Rb3 | 16c | .-3. | 0 | 0 | 0 | | 14-vertex polyhedron Se ₁₂ As ₂ |
| Rb4 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | | icosahedron Se ₁₂ |
| As5 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | | tetrahedron Se ₄ |

Transformation from published data: -*y*, -*x*, -*z*Experimental: single crystal, diffractometer, X-rays, $R = 0.053$, $T = 294 \text{ K}$ References: [1] Wachhold M., Sheldrick W.S. (1997), *Z. Naturforsch. B* 52, 169-175. [2] Dickerson C.A., Fisher M.J., Sykora R.E., Albrecht Schmitt T.E., Cody J.A. (2002), *Inorg. Chem.* 41, 640-642.203
cF192

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|--|--------------|---|
| $\text{Cs}_{2.33}\text{As}_{1.67}\text{Se}_4(\text{Te}_{0.67}\text{Se}_{0.33})_{12}$ | <i>cF192</i> | (203) <i>Fd-3</i> – ge ² cba |
|--|--------------|---|

Cs₇As₅Se₁₂·6Te₄Se₂ [1]Structural features: AsSe₄ tetrahedra and As₂Se₄ units (two edge-linked :AsSe₃ ψ-tetrahedra, disorder where As and Se form defect (As, □)(As, □)₄Se₄ cubes); (Te, Se)₆ rings in chair conformation.

Wachhold M., Sheldrick W.S. (1997) [1]

 $\text{As}_{1.66}\text{Cs}_{2.33}\text{Se}_8\text{Te}_8$ $a = 1.7275 \text{ nm}$, $V = 5.1553 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|-------|-------------------------------------|
| M1 | 96g | 1 | 0.01121 | 0.11802 | 0.42882 | | non-colinear Te ₂ |
| As2 | 32e | .3. | 0.0636 | 0.0636 | 0.0636 | 0.333 | |
| Se3 | 32e | .3. | 0.2042 | 0.2042 | 0.2042 | | 4-vertex polyhedron As ₄ |
| Cs4 | 16c | .-3. | 0 | 0 | 0 | 0.667 | |
| Cs5 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | | icosahedron Te ₁₂ |
| As6 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.333 | tetrahedron As ₄ |

 $\text{M1} = 0.667\text{Te} + 0.333\text{Se}$ Transformation from published data: -*y*, -*x*, -*z*Experimental: single crystal, diffractometer, X-rays, $R = 0.057$, $T = 294 \text{ K}$ Remarks: Short interatomic distances for partly occupied site(s). In table II-2 of [1] the *x*-coordinate of former Se(2) is misprinted as 0.0485 instead of 0.0458 (identical to former Se(1)).References: [1] Wachhold M., Sheldrick W.S. (1997), *Z. Naturforsch. B* 52, 169-175.

203
cF208

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|--|--------------|------------------------------------|
| $\text{Na}_3\text{Mg}[\text{CO}_3]_2\text{Cl}$ | <i>cF208</i> | (203) <i>Fd-3</i> – g $\bar{f}edc$ |
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 $\text{Na}_3\text{Mg}(\text{CO}_3)_2\text{Cl}$ [2], northupite, Strukturbericht notation $G7_3$ Structural features: MgO_6 octahedra and planar CO_3 trigonal units share vertices to form a 3D-framework; Na and Cl in voids.

Negro A.D. et al. (1975) [1]

 $\text{C}_2\text{ClMgNa}_3\text{O}_6$ $a = 1.4069 \text{ nm}$, $V = 2.7848 \text{ nm}^3$, $Z = 16$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------------|------|---------------|---------------|---------------|------|------------------------------------|
| O1 | 96 <i>g</i> | 1 | 0.0127 | 0.10458 | 0.26989 | | single atom C |
| Na2 | 48 <i>f</i> | 2.. | 0.3977 | $\frac{1}{8}$ | $\frac{1}{8}$ | | 4-vertex polyhedron O_4 |
| C3 | 32 <i>e</i> | .3. | 0.21691 | 0.21691 | 0.21691 | | non-coplanar triangle O_3 |
| Cl4 | 16 <i>d</i> | .-3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | octahedron Na_6 |
| Mg5 | 16 <i>c</i> | .-3. | 0 | 0 | 0 | | octahedron O_6 |

Transformation from published data: $-y, -x, -z$; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.023$ Remarks: Natural specimen from Searles Lake. A structure proposal in space group (227) *Fd-3m* [3] is superseded (see [2]). Strukturbericht notation $G7_3$ was defined on the superseded structure proposal.

References: [1] Negro A.D., Giuseppetti G., Tadini C. (1975), TMPM, Tschermarks Mineral. Petrogr. Mitt. 22, 158-163. [2] Watanabe T. (1933), Sci. Pap. Phys. Chem. Res. Tokyo 21, 40-62. [3] Shiba H., Watanabe T. (1931), C. R. Hebd. Seances Acad. Sci. 193, 1421-1423.

203
cF224

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|---------------------------------------|--------------|-------------------------------------|
| $\text{Cd}_2[\text{BO}_3][\text{OH}]$ | <i>cF224</i> | (203) <i>Fd-3</i> – g $\bar{f}e^2c$ |
|---------------------------------------|--------------|-------------------------------------|

 $\text{Cd}_4(\text{BO}_3)_2(\text{OH})_2$ [1]Structural features: Distorted CdO_6 and $\text{Cd}(\text{O}_4[\text{OH}]_2)$ octahedra share edges and vertices to form a 3D-framework; B in voids (BO_3 trigonal units).

Kazanskaia E.V. et al. (1978) [1]

 BCd_2HO_4 $a = 1.4019 \text{ nm}$, $V = 2.7552 \text{ nm}^3$, $Z = 32$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|-------|-------------|------|----------|---------------|---------------|------|--------------------------------------|
| O1 | 96 <i>g</i> | 1 | 0.0195 | 0.093 | 0.2971 | | single atom B |
| Cd2 | 48 <i>f</i> | 2.. | 0.41898 | $\frac{1}{8}$ | $\frac{1}{8}$ | | octahedron $\text{O}_4(\text{OH})_2$ |
| B3 | 32 <i>e</i> | .3. | 0.2273 | 0.2273 | 0.2273 | | non-coplanar triangle O_3 |
| (OH)4 | 32 <i>e</i> | .3. | 0.4451 | 0.4451 | 0.4451 | | non-coplanar triangle Cd_3 |
| Cd5 | 16 <i>c</i> | .-3. | 0 | 0 | 0 | | octahedron O_6 |

Transformation from published data (origin choice 1): origin shift $\frac{5}{8} \frac{5}{8} \frac{5}{8}$ Experimental: single crystal, diffractometer, X-rays, $R = 0.058$

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kazanskaia E.V., Egorov Tismenko I.K., Simonov M.A., Belov N.V. (1978), Dokl. Akad. Nauk SSSR 240, 1100-1103.

203
cF232

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|---|--------------|---|
| $\text{Na}_6(\text{Mg}_{0.27}\text{Fe}_{0.73})_2[\text{CO}_3]_4[\text{SO}_4]$ | <i>cF232</i> | (203) <i>Fd-3</i> – gfe ² da |
|---|--------------|---|

$\text{Na}_6(\text{Fe,Mg})_2\text{SO}_4(\text{CO}_3)_4$ [1], ferrotychite; $\text{Na}_6\text{Mg}_2\text{SO}_4(\text{CO}_3)_4$ (see remark), tychite, Strukturbericht notation H5₆

Structural features: (Fe,Mg)O₆ octahedra and CO₃ trigonal units share vertices to form a 3D-framework; SO₄ tetrahedra and Na atoms in voids.

Malinovskii I.A. et al. (1979) [1]

$\text{C}_4\text{Fe}_{1.47}\text{Mg}_{0.53}\text{Na}_6\text{O}_{16}\text{S}$

$a = 1.3962 \text{ nm}$, $V = 2.7217 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|------|--------------------------------------|
| O1 | 96g | 1 | 0.22233 | 0.26721 | 0.35078 | | single atom C |
| Na2 | 48f | 2.. | 0.34178 | $\frac{1}{8}$ | $\frac{1}{8}$ | | octahedron O ₆ |
| O3 | 32e | .3. | 0.06369 | 0.06369 | 0.06369 | | single atom S |
| C4 | 32e | .3. | 0.28077 | 0.28077 | 0.28077 | | non-coplanar triangle O ₃ |
| M5 | 16d | -.3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | octahedron O ₆ |
| S6 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | | tetrahedron O ₄ |

$\text{M5} = 0.734\text{Fe} + 0.266\text{Mg}$

Experimental: single crystal, diffractometer, X-rays, R = 0.029

Remarks: Natural specimen from Kola Peninsula. Composition $\text{Na}_6(\text{Fe}_{1.241}\text{Mn}_{0.358}\text{Mg}_{0.401})[\text{SO}_4][\text{CO}_3]_4$ from electron microprobe analysis. A structure proposal for $\text{Na}_6\text{Mg}_2(\text{SO}_4)(\text{CO}_3)_4$ (tychite) in space group (227) *Fd-3m* [2] is superseded (see [3]). Strukturbericht notation H5₆ was defined on the superseded structure proposal for tychite.

References: [1] Malinovskii I.A., Baturin S.V., Belov N.V. (1979), Dokl. Akad. Nauk SSSR 249, 1365-1368. [2] Shiba H., Watanabe T. (1931), C. R. Hebd. Seances Acad. Sci. 193, 1421-1423. [3] Watanabe T. (1933), Sci. Pap. Phys. Chem. Res. Tokyo 21, 40-62.

203
cF280

| | | |
|---|--------------|--|
| $(\text{Ca}_{0.75}\text{Ce}_{0.25})_4\text{Al}_2[\text{SO}_4]\text{F}_{12}([\text{OH}]_{0.08}[\text{H}_2\text{O}]_{0.92})_{12}$ | <i>cF280</i> | (203) <i>Fd-3</i> – g ² e ² da |
|---|--------------|--|

$\text{Ca}_3\text{CeAl}_2(\text{SO}_4)(\text{OH})\text{F}_{12}\cdot 11\text{H}_2\text{O}$ [1], chukhrovite-(Ce)

Structural features: AlF₆ octahedra, SO₄ and empty (Ca,Ce)₄ tetrahedra, embedded in a (H₂O,OH) matrix.

Bokii G.B., Gorogotskaya L.I. (1965) [1]

$\text{Al}_2\text{Ca}_3\text{CeF}_{12}\text{H}_{23}\text{O}_{16}\text{S}$

$a = 1.68 \text{ nm}$, $V = 4.7416 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|------|--|
| M1 | 96g | 1 | 0.009 | 0.096 | 0.309 | | non-colinear CaO |
| F2 | 96g | 1 | 0.05 | 0.093 | 0.469 | | single atom Al |
| O3 | 32e | .3. | 0.174 | 0.174 | 0.174 | | single atom S |
| M4 | 32e | .3. | 0.292 | 0.292 | 0.292 | | octahedron F ₃ (OH) ₂) ₃ |
| Al5 | 16d | -.3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | octahedron F ₆ |

S6 8a 23. $\frac{1}{8}$ $\frac{1}{8}$ $\frac{1}{8}$ tetrahedron O₄

M1 = 0.917OH₂ + 0.083OH; M4 = 0.75Ca + 0.25Ce

Transformation from published data (origin choice 1): origin shift $\frac{1}{8} \frac{1}{8} \frac{1}{8}$

Experimental: single crystal, oscillation photographs, X-rays, R = 0.130

Remarks: Natural specimen from central Kazakhstan. Approximate composition, partial substitution by other rare-earth metals for Ce is ignored. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bokii G.B., Gorogotskaya L.I. (1965), Dokl. Akad. Nauk SSSR 163, 183-185.

203
cF288

Ca₄(Al_{0.5}Si_{0.5})₂[SO₄]F₁₃[H₂O]₁₂ cF288 (203) *Fd*-3 – g²e²cba

Ca₄AlSi(SO₄)F₁₃·12H₂O [1], chukhrovite-(Ca)

Structural features: (Al,Si)F₆ octahedra, SO₄ and FCa₄ tetrahedra, embedded in a H₂O matrix.

Mathew M. et al. (1981) [1]

AlCa₄F₁₃H₂₄O₁₆SSi

a = 1.671 nm, *V* = 4.6658 nm³, *Z* = 8

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|------|---|
| O1 | 96g | 1 | 0.02256 | 0.15481 | 0.44521 | | non-coplanar triangle CaOF |
| F2 | 96g | 1 | 0.0493 | 0.16351 | 0.27951 | | single atom Al |
| Ca3 | 32e | .3. | 0.20829 | 0.20829 | 0.20829 | | monocapped trigonal prism F ₄ O ₃ |
| O4 | 32e | .3. | 0.42604 | 0.42604 | 0.42604 | | single atom S |
| M5 | 16c | -.3. | 0 | 0 | 0 | | octahedron F ₆ |
| S6 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | | tetrahedron O ₄ |
| F7 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | | tetrahedron Ca ₄ |
| H8 | 96g | 1 | 0.019 | 0.135 | 0.405 | | |
| H9 | 96g | 1 | 0.028 | 0.126 | 0.479 | | |

M5 = 0.5Al + 0.5Si

Transformation from published data: -*y*, -*x*, -*z*; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.025

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Mathew M., Takagi S., Waerstad K.R., Frazier A.W. (1981), Am. Mineral. 66, 392-397.

203
cF320

K₃TlF₆ cF320 (203) *Fd*-3 – g²fedcba

K₃TlF₆ [1]

Structural features: TlF₆ octahedra and K atoms in a BiF₃-type arrangement.

Bode H., Voss E. (1957) [1]

F₆K₃Tl

a = 1.786 nm, *V* = 5.6970 nm³, *Z* = 32

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|------|--------------------|
| F1 | 96g | 1 | 0.015 | 0.02 | 0.11 | | single atom Tl |

| | | | | | | |
|-----|-----|------|---------------|---------------|---------------|-------------------------------|
| F2 | 96g | 1 | 0.02 | 0.11 | 0.485 | single atom Tl |
| K3 | 48f | 2.. | 0.375 | $\frac{1}{8}$ | $\frac{1}{8}$ | non-colinear F ₂ |
| K4 | 32e | .3. | 0.25 | 0.25 | 0.25 | octahedron F ₆ |
| Tl5 | 16d | .-3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | octahedron F ₆ |
| Tl6 | 16c | .-3. | 0 | 0 | 0 | octahedron F ₆ |
| K7 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | icosahedron F ₁₂ |
| K8 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | cuboctahedron F ₁₂ |

Transformation from published data: -y, -x, -z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: powder, film, X-rays, R = 0.142

References: [1] Bode H., Voss E. (1957), Z. Anorg. Allg. Chem. 290, 1-16.

203
cF320

[NH₄]_{0.5}CrNiCl_{5.5}[NH₃]₆[H₂O]₆ *cF*320 (203) *Fd-3* – g²fedcba

[Cr(NH₃)₆][Ni(H₂O)₆]Cl₅·0.5NH₄Cl [1]

Structural features: Cr(NH₃)₆ and Ni(OH₂)₆ octahedral units in an ordered Cu-type (c.c.p.) arrangement; Cl atoms and NH₄ tetrahedra in voids.

Moron M.C. et al. (1990) [1]

Cl_{5.50}CrH₃₂N_{6.50}NiO₆

a = 2.044 nm, *V* = 8.5397 nm³, *Z* = 16

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|------|--|
| N1 | 96g | 1 | 0.0005 | 0.0007 | 0.3987 | | single atom Cr |
| O2 | 96g | 1 | 0.0415 | 0.1633 | 0.2769 | | single atom Ni |
| Cl3 | 48f | 2.. | 0.3983 | $\frac{1}{8}$ | $\frac{1}{8}$ | | 8-vertex polyhedron O ₂ N ₆ |
| Cl4 | 32e | .3. | 0.2277 | 0.2277 | 0.2277 | | 7-vertex polyhedron O ₃ N ₄ |
| Cr5 | 16d | .-3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | octahedron N ₆ |
| Ni6 | 16c | .-3. | 0 | 0 | 0 | | octahedron O ₆ |
| Cl7 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | | cuboctahedron N ₁₂ |
| N8 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | | 16-vertex Frank-Kasper O ₁₂ Cl ₄ |
| H9 | 96g | 1 | 0.0183 | 0.0417 | 0.3786 | | |
| H10 | 96g | 1 | 0.035 | 0.1176 | 0.2594 | | |
| H11 | 96g | 1 | 0.0362 | 0.1199 | 0.4723 | | |
| H12 | 96g | 1 | 0.0447 | 0.5049 | 0.1197 | | |
| H13 | 96g | 1 | 0.0664 | 0.16 | 0.3183 | | |
| H14 | 32e | .3. | 0.1534 | 0.1534 | 0.1534 | | |

Experimental: single crystal, diffractometer, X-rays, R = 0.041, T = 293 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Moron M.C., Le Bail A., Pons J. (1990), J. Solid State Chem. 88, 498-504.

203
cF400

Cu₅Co₄Cl₁₇[NH₃]₂₄ *cF*400 (203) *Fd-3* – g³e²dcba

[Co(NH₃)₆]₄Cu₅Cl₁₇ [1]

Structural features: Single Co(NH₃)₆ octahedra and units of five vertex-linked CuCl₄ tetrahedra (a central tetrahedron sharing vertices with four others); additional Cl in voids.

Murray Rust P. (1973) [1]

$\text{Cl}_{16.62}\text{Co}_4\text{Cu}_5\text{H}_{72}\text{N}_{24}$

$a = 2.18 \text{ nm}$, $V = 10.3602 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|---------------|---------------|---------------|------|--|
| (NH ₃)1 | 96g | 1 | 0.0351 | 0.0776 | 0.4722 | | single atom Co |
| (NH ₃)2 | 96g | 1 | 0.0568 | 0.2805 | 0.1863 | | single atom Co |
| Cl3 | 96g | 1 | 0.1791 | 0.325 | 0.2782 | | single atom Cu |
| Cl4 | 32e | .3. | 0.1853 | 0.1853 | 0.1853 | | colinear Cu ₂ |
| Cu5 | 32e | .3. | 0.2515 | 0.2515 | 0.2515 | | tetrahedron Cl ₄ |
| Co6 | 16d | .-3. | $\frac{1}{2}$ | $\frac{1}{2}$ | $\frac{1}{2}$ | | octahedron (NH ₃) ₆ |
| Co7 | 16c | .-3. | 0 | 0 | 0 | | octahedron (NH ₃) ₆ |
| Cl8 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | 0.62 | icosahedron (NH ₃) ₁₂ |
| Cu9 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | | tetrahedron Cl ₄ |

Experimental: twinned crystal, diffractometer, X-rays, R = 0.085

Remarks: The same data are also reported in [2]. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Murray Rust P. (1973), Acta Crystallogr. B 29, 2559-2566. [2] Murray Rust P. (1975), Acta Crystallogr. B 31, 978-981.

203
cF432

$\text{Si}_{17}\text{O}_{34}[\text{CO}_2][\text{N}_2]_2$

cF432

(203) *Fd*-3 – g³fe²cba

Si₁₃₆O₂₇₂·16N₂·8CO₂ [1], zeolite MTN, dodecasil 3C

Structural features: SiO₄ tetrahedra share vertices to form a MTN-type zeolite framework with 12-face (pentagonal dodecahedra) and 16-face ([5¹²6⁴] hexaidecahedra) cages, centered by N₂ and CO₂, respectively.

Gies H. (1984) [1]

$\text{CN}_4\text{O}_{36}\text{Si}_{17}$

$a = 1.9402 \text{ nm}$, $V = 7.3036 \text{ nm}^3$, $Z = 8$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|---------------|---------------|---------------|------|--|
| O1 | 96g | 1 | 0.0001 | 0.0935 | 0.4068 | | non-colinear Si ₂ |
| O2 | 96g | 1 | 0.0495 | 0.0495 | 0.2933 | | non-colinear Si ₂ |
| Si3 | 96g | 1 | 0.0676 | 0.0676 | 0.37 | | tetrahedron O ₄ |
| O4 | 48f | 2.. | 0.3734 | $\frac{1}{8}$ | $\frac{1}{8}$ | | non-colinear Si ₂ |
| O5 | 32e | .3. | 0.1704 | 0.1704 | 0.1704 | | colinear Si ₂ |
| Si6 | 32e | .3. | 0.2164 | 0.2164 | 0.2164 | | tetrahedron O ₄ |
| (N ₂)7 | 16c | .-3. | 0 | 0 | 0 | | 26-vertex polyhedron O ₂₄ Si ₂ |
| (CO ₂)8 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | | 42-vertex polyhedron O ₄₂ |
| Si9 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | | tetrahedron O ₄ |

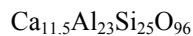
Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, wR = 0.064

Remarks: Substantial amounts of N₂, CO₂, and N(CH₃)₃, as well as smaller amounts of CH₄ and Ar, were detected by mass spectroscopy. Partial substitution of CH₄ for N₂ and N(CH₃)₃ for CO₂ is ignored here. The atom coordinates correspond to the positions of Si, C and framework O atoms and the centers of N₂ molecules. Space group (227) *Fd*-3*m* was tested and rejected (R = 0.213); dodecasil 3C was, however, refined in this space group in [2] and [3].

References: [1] Gies H. (1984), Z. Kristallogr. 167, 73-82. [2] Schlenker J.L., Dwyer F.G., Jenkins E.E., Rohrbaugh W.J., Kokotailo G.T., Meier W.M. (1981), Nature (London) 294, 340-342. [3] Könnecke M., Miehle G., Fuess H. (1992), Z. Kristallogr. 201, 147-155.

203
cF624



cF624

(203) $Fd\bar{3} - g^6ec$

Ca₄₆Al₉₂Si₁₀₀O₃₈₄ [2], zeolite FAU-Ca

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms and near the centers of single 6-rings. See Fig. II.57.

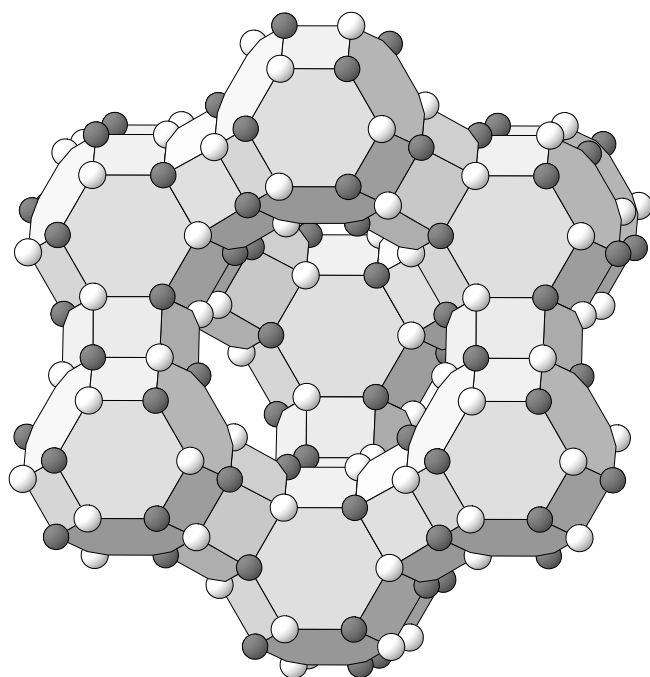
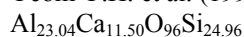


Fig. II.57. **Ca₄₆Al₉₂Si₁₀₀O₃₈₄**

FAU-type framework with an ordered arrangement of Al (light) and Si (dark) atoms.

Yeom Y.H. et al. (1997) [1]



$a = 2.5024 \text{ nm}$, $V = 15.6700 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0005 | 0.363 | 0.1431 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0335 | 0.127 | 0.304 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0366 | 0.3067 | 0.1285 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0611 | 0.1838 | 0.2861 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0766 | 0.0798 | 0.3095 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1429 | 0.2531 | 0.2537 | | non-colinear SiAl |
| Ca7 | 32e | .3. | 0.2234 | 0.2234 | 0.2234 | 0.938 | non-coplanar triangle O ₃ |
| Ca8 | 16c | .-3. | 0 | 0 | 0 | | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

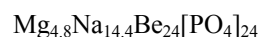
Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, $wR = 0.037$, $T = 294$ K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition.

References: [1] Yeom Y.H., Jang S.B., Kim Y. (1997), J. Phys. Chem. B 101, 6914-6920. [2] Jang S.B., Song S.H., Kim Y. (1995), J. Korean Phys. Soc. 39, 7-13.

203
cF624



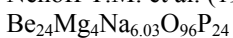
cF624

(203) $Fd-3 - g^6ec$

Na_{0.6}Mg_{0.2}BePO₄ [1], zeolite FAU(Be,P)-Na,Mg

Structural features: BeO₄ and PO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Mg at the centers of hexagonal prisms, Na above the centers of single 6-rings in supercages.

Nenoff T.M. et al. (1992) [1]



$a = 2.32422$ nm, $V = 12.5554$ nm³, $Z = 4$

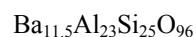
| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0065 | 0.1429 | 0.3624 | | non-colinear PBe |
| P2 | 96g | 1 | 0.0337 | 0.1277 | 0.3045 | | tetrahedron O ₄ |
| Be3 | 96g | 1 | 0.0363 | 0.3031 | 0.1272 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.061 | 0.2812 | 0.1888 | | non-colinear BeP |
| O5 | 96g | 1 | 0.0805 | 0.084 | 0.3185 | | non-colinear PBe |
| O6 | 96g | 1 | 0.1474 | 0.2575 | 0.2525 | | non-colinear PBe |
| Na7 | 32e | .3. | 0.238 | 0.238 | 0.238 | 0.754 | non-coplanar triangle O ₃ |
| Mg8 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

Experimental: powder, diffractometer, neutrons, $R_p = 0.064$, $T = 14$ K

Remarks: Refinement of the occupancy of site Mg8 showed no significant deviation from unity. Part of non framework cations not located.

References: [1] Nenoff T.M., Harrison W.T.A., Gier T.E., Nicol J.M., Stucky G.D. (1992), Zeolites 12, 770-775.

203
cF656



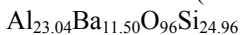
cF656

(203) $Fd-3 - g^6e^2c$

Ba₄₆Al₉₂Si₁₀₀O₃₈₄ [2], zeolite FAU-Ba; NaBePO₄ [3]

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ba at the centers of hexagonal prisms, above the centers of double 6-rings in β cages and single 6-rings in supercages (disorder).

Yeom Y.H. et al. (1997) [1]



$a = 2.5266$ nm, $V = 16.1291$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|--------------------|
| O1 | 96g | 1 | 0.0003 | 0.3618 | 0.1419 | | non-colinear SiAl |

| | | | | | | |
|-----|-----|------|--------|--------|--------|--|
| Si2 | 96g | 1 | 0.034 | 0.1247 | 0.3059 | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0363 | 0.3075 | 0.1254 | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0674 | 0.07 | 0.3129 | non-colinear SiAl |
| O5 | 96g | 1 | 0.0708 | 0.1757 | 0.2894 | non-colinear SiAl |
| O6 | 96g | 1 | 0.1371 | 0.2546 | 0.2543 | non-colinear SiAl |
| Ba7 | 32e | .3. | 0.053 | 0.053 | 0.053 | 0.047 4-vertex polyhedron BaO ₃ |
| Ba8 | 32e | .3. | 0.2409 | 0.2409 | 0.2409 | 0.938 non-coplanar triangle O ₃ |
| Ba9 | 16c | -.3. | 0 | 0 | 0 | 0.906 |

M3 = 0.96Al + 0.04Si

Transformation from published data: $-y, -x, -z$

Experimental: single crystal, diffractometer, X-rays, R = 0.046, T = 294 K

Remarks: Short interatomic distances for partly occupied site(s). We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Part of Na was not located in [3]. On page 6915 of [1] the cell parameter is misprinted as 2.2266 nm instead of 2.5266 nm (given in the abstract; checked on interatomic distances).

References: [1] Yeom Y.H., Jang S.B., Kim Y. (1997), J. Phys. Chem. B 101, 6914-6920. [2] Jang S.B., Kim Y. (1995), Bull. Korean Chem. Soc. 16, 248-251. [3] Harrison W.T.A., Gier T.E., Moran K.L., Nicol J.M., Eckert H., Stucky G.D. (1991), Chem. Mater. 3, 27-29.

203
cF664

Na₂₃Al₂₃Si₁₂₅O₉₆

cF664

(203) $Fd\bar{3} - g^6e^2ca$

Na₉₂Al₉₂Si₁₀₀O₃₈₄ [1], faujasite-(Na), zeolite FAU-Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of β cages and hexagonal prisms, above the centers of single 6-rings in supercages and double 6-rings in β cages. See Fig. II.58.

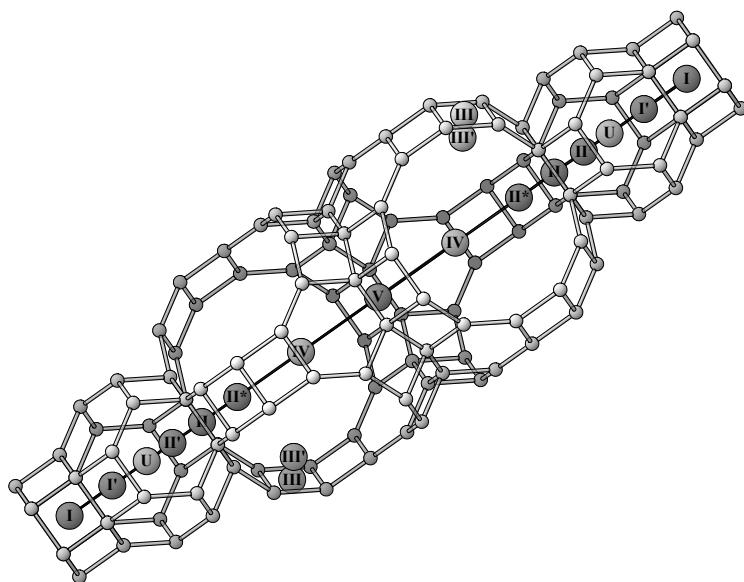


Fig. II.58. **Na₉₂Al₉₂Si₁₀₀O₃₈₄**

Commonly occupied interstitial sites in cages along $\langle 111 \rangle$ in FAU-type zeolites.

Ho K. et al. (1995) [1]

Al_{23.04}Na_{18.75}O₉₆Si_{24.96}

$a = 2.5052$ nm, $V = 15.7227$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0012 | 0.1412 | 0.3563 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0352 | 0.1248 | 0.3033 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0357 | 0.3044 | 0.1266 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.07 | 0.0731 | 0.3199 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0717 | 0.1741 | 0.2828 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1427 | 0.2538 | 0.2514 | | non-colinear SiAl |
| Na7 | 32e | .3. | 0.0574 | 0.0574 | 0.0574 | | non-coplanar triangle O ₃ |
| Na8 | 32e | .3. | 0.2305 | 0.2305 | 0.2305 | | non-coplanar triangle O ₃ |
| Na9 | 16c | -.3. | 0 | 0 | 0 | 0.188 | 8-vertex polyhedron Na ₂ O ₆ |
| Na10 | 8a | 23. | 1/8 | 1/8 | 1/8 | | tetrahedron Na ₄ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.126

Remarks: Part of Na not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances: d(Na7-Na9) = 0.249 nm.

References: [1] Ho K., Lee H.S., Leano B.C., Sun T., Seff K. (1995), Zeolites 15, 377-381.

203
cF688

| | | |
|---|-------|---|
| Mn ₁₂ Al ₂₄ [SiO ₄] ₂₄ [CO] _{7.5} | cF688 | (203) <i>Fd-3</i> – g ⁶ e ³ c |
|---|-------|---|

Mn₄₆Al₉₂Si₁₀₀O₃₈₄·30CO [1], zeolite FAU-Mn²⁺ (CO)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Mn at the centers of hexagonal prisms and near the centers of single 6-rings, CO deeper in supercages aligned along <111> (Mn-C-O).

Bae M.N. et al. (1998) [1]

Al₂₄C_{7.50}Mn_{11.50}O_{103.50}Si₂₄

a = 2.4715 nm, V = 15.0967 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0018 | 0.3606 | 0.146 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0336 | 0.1279 | 0.3021 | | tetrahedron O ₄ |
| Al3 | 96g | 1 | 0.0379 | 0.3043 | 0.1294 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0585 | 0.1863 | 0.2805 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0799 | 0.0841 | 0.3129 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1471 | 0.2517 | 0.2516 | | non-colinear SiAl |
| Mn7 | 32e | .3. | 0.2237 | 0.2237 | 0.2237 | 0.938 | non-coplanar triangle O ₃ |
| C8 | 32e | .3. | 0.2839 | 0.2839 | 0.2839 | 0.938 | single atom O |
| O9 | 32e | .3. | 0.3062 | 0.3062 | 0.3062 | 0.938 | single atom C |
| Mn10 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, wR = 0.049, T = 294 K

Remarks: In table 1 of [1] the y-coordinates of former O1 and O2 are misprinted as -0.0018 and -0.0001 instead of 0.0018 and -0.0017, respectively (checked on interatomic distances).

References: [1] Bae M.N., Kim Y., Seff K. (1998), Microporous Mesoporous Mater. 26, 101-107.

203
cF704

| | | |
|--|--------------|------------------------|
| $\text{Al}_{23}\text{Pb}_{16}\text{Si}_{25}\text{O}_{104}$ | <i>cF704</i> | $(203) Fd-3 - g^6 e^4$ |
|--|--------------|------------------------|

Pb₆₄Al₉₂Si₁₀₀O₄₁₆ [1], zeolite FAU-Pb²⁺, Pb⁴⁺ (PbO)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Pb²⁺₄O₄ cubes in β cages, additional Pb²⁺ and Pb⁴⁺ above the centers of single 6-rings in supercages (distinct positions, disorder).

Yeom Y.H., Kim Y. (1997) [1]

 $\text{Al}_{23.04}\text{O}_{104}\text{Pb}_{16}\text{Si}_{24.96}$ $a = 2.5238 \text{ nm}$, $V = 16.0755 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|-----------------------|-------|------|----------|----------|----------|-------|---|
| O1 | 96g | 1 | 0.0001 | 0.3574 | 0.1453 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0003 | 0.1092 | 0.2532 | | non-colinear SiAl |
| Si3 | 96g | 1 | 0.0353 | 0.1243 | 0.3046 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0367 | 0.3069 | 0.1251 | | tetrahedron O ₄ |
| O5 | 96g | 1 | 0.0666 | 0.0678 | 0.3164 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0764 | 0.1704 | 0.285 | | non-colinear SiAl |
| (Pb ²⁺)7 | 32e | .3. | 0.07051 | 0.07051 | 0.07051 | | octahedron O ₆ |
| O8 | 32e | .3. | 0.1721 | 0.1721 | 0.1721 | | tetrahedron (Pb ⁴⁺)(Pb ²⁺) ₃ |
| (Pb ⁴⁺)9 | 32e | .3. | 0.2237 | 0.2237 | 0.2237 | 0.438 | |
| (Pb ²⁺)10 | 32e | .3. | 0.23989 | 0.23989 | 0.23989 | 0.562 | |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, wR = 0.070, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Yeom Y.H., Kim Y. (1997), J. Phys. Chem. B 101, 5314-5318.

203
cF704

| | | |
|--|--------------|---------------------------|
| $\text{K}_7\text{Ca}_8\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | <i>cF704</i> | $(203) Fd-3 - g^6 fe^2 c$ |
|--|--------------|---------------------------|

K₂₈Ca₃₂Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ca,K

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms, additional Ca and K opposite single 6-rings in supercages (distinct positions, split site), additional K opposite 4-rings in supercages.

Jang S.B. et al. (1995) [1]

 $\text{Al}_{23.04}\text{Ca}_8\text{K}_7\text{O}_{96}\text{Si}_{24.96}$ $a = 2.5002 \text{ nm}$, $V = 15.6288 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|------|----------------------------|
| O1 | 96g | 1 | 0.003 | 0.1375 | 0.3576 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0329 | 0.128 | 0.3026 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.037 | 0.3065 | 0.1282 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0609 | 0.1857 | 0.2866 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.078 | 0.0823 | 0.3112 | | non-colinear SiAl |

| | | | | | | | |
|------|-----|------|--------|---------------|---------------|------|-----------------------------|
| O6 | 96g | 1 | 0.1435 | 0.255 | 0.2552 | | non-colinear SiAl |
| K7 | 48f | 2.. | 0.418 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.25 | non-colinear O ₂ |
| Ca8 | 32e | .3. | 0.2239 | 0.2239 | 0.2239 | 0.5 | |
| K9 | 32e | .3. | 0.2465 | 0.2465 | 0.2465 | 0.5 | |
| Ca10 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, wR = 0.057, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Jang S.B., Song S.H., Kim Y. (1995), J. Korean Phys. Soc. 39, 7-13.

203
cF720

| | | |
|---|-------|---|
| Ca _{5,9} Mg _{5,6} Al ₂₃ Si ₂₅ O ₉₆ | cF720 | (203) <i>Fd-3</i> – g ⁶ e ⁴ c |
|---|-------|---|

Ca_{23,6}Mg_{22,4}Al₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ca,Mg

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms, above the centers of double and single 6-rings (in supercages for the latter), Mg at and near the centers of single 6-rings (split site).

Anderson A.A. et al. (1990) [1]

Al_{23,04}Ca_{5,80}Mg_{5,60}O₉₆Si_{24,96}

$a = 2.493$ nm, $V = 15.4941$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|--|
| O1 | 96g | 1 | 0.0009 | 0.3591 | 0.1466 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0353 | 0.1262 | 0.3018 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0377 | 0.3045 | 0.1276 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0645 | 0.1819 | 0.2818 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0778 | 0.0807 | 0.3144 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1459 | 0.2521 | 0.2515 | | non-colinear SiAl |
| Ca7 | 32e | .3. | 0.062 | 0.062 | 0.062 | 0.12 | non-coplanar triangle O ₃ |
| Mg8 | 32e | .3. | 0.2 | 0.2 | 0.2 | 0.25 | |
| Mg9 | 32e | .3. | 0.218 | 0.218 | 0.218 | 0.45 | |
| Ca10 | 32e | .3. | 0.231 | 0.231 | 0.231 | 0.22 | |
| Ca11 | 16c | -.3. | 0 | 0 | 0 | 0.77 | 8-vertex polyhedron O ₆ Ca ₂ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.057, T = 673 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Anderson A.A., Shepelev Y.F., Smolin Y.I. (1990), Zeolites 10, 32-37.

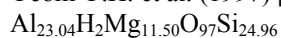
203
cF720

| | | |
|---|-------|---|
| Mg _{11,5} Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] | cF720 | (203) <i>Fd-3</i> – g ⁶ e ⁴ c |
|---|-------|---|

Mg₄₆Al₉₂Si₁₀₀O₃₈₄·4H₂O [1], zeolite FAU-Mg residual water

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Mg at the centers of hexagonal prisms, near the centers of single 6-rings, above the centers of single (in supercages) and double 6-rings, H_2O deeper in β cages (disorder).

Yeom Y.H. et al. (1997) [1]



$$a = 2.4671 \text{ nm}, V = 15.0162 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|-------|---|
| O1 | 96g | 1 | 0.002 | 0.3615 | 0.1437 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0339 | 0.1273 | 0.302 | | tetrahedron O_4 |
| M3 | 96g | 1 | 0.0377 | 0.3039 | 0.1289 | | tetrahedron O_4 |
| O4 | 96g | 1 | 0.0583 | 0.1865 | 0.2813 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0806 | 0.0843 | 0.3155 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1471 | 0.2527 | 0.2529 | | non-colinear SiAl |
| Mg7 | 32e | .3. | 0.0585 | 0.0585 | 0.0585 | 0.125 | non-coplanar triangle O_3 |
| (OH ₂)8 | 32e | .3. | 0.145 | 0.145 | 0.145 | 0.125 | |
| Mg9 | 32e | .3. | 0.2026 | 0.2026 | 0.2026 | 0.125 | |
| Mg10 | 32e | .3. | 0.2288 | 0.2288 | 0.2288 | 0.75 | |
| Mg11 | 16c | -.3. | 0 | 0 | 0 | 0.875 | 8-vertex polyhedron O_6Mg_2 |

$$\text{M3} = 0.96\text{Al} + 0.04\text{Si}$$

Transformation from published data: $-y, -x, -z$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.046$, $T = 294 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Yeom Y.H., Jang S.B., Kim Y. (1997), J. Phys. Chem. B 101, 6914-6920.

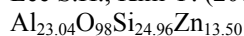
203
cF720

| | | |
|---|-------|------------------------|
| $\text{Zn}_{13.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF720 | (203) $Fd-3 - g^6e^4c$ |
|---|-------|------------------------|

$\text{Zn}_{46}\text{Al}_{92}\text{Si}_{100}\text{O}_{384} \cdot 8\text{ZnO}$ [1], zeolite FAU-Zn (ZnO)

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; ZnO in β cages, additional Zn at the centers of hexagonal prisms, at and near the centers of single 6-rings (partial disorder).

Lee S.H., Kim Y. (2000) [1]



$$a = 2.471 \text{ nm}, V = 15.0875 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|------------------------------------|
| O1 | 96g | 1 | 0.0007 | 0.0011 | 0.1507 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0011 | 0.3519 | 0.1544 | | non-colinear AlSi |
| Si3 | 96g | 1 | 0.0364 | 0.2996 | 0.1255 | | tetrahedron O_4 |
| M4 | 96g | 1 | 0.0382 | 0.1274 | 0.3022 | | tetrahedron O_4 |
| O5 | 96g | 1 | 0.0704 | 0.1751 | 0.2691 | | non-coplanar triangle AlSiZn |
| O6 | 96g | 1 | 0.0777 | 0.0813 | 0.3207 | | non-colinear AlSi |
| Zn7 | 32e | .3. | 0.0586 | 0.0586 | 0.0586 | 0.875 | non-coplanar triangle O_3 |
| O8 | 32e | .3. | 0.1488 | 0.1488 | 0.1488 | 0.25 | non-coplanar triangle O_3 |

| | | | | | | | |
|------|-----|------|--------|--------|--------|-------|--|
| Zn9 | 32e | .3. | 0.1996 | 0.1996 | 0.1996 | 0.25 | |
| Zn10 | 32e | .3. | 0.2186 | 0.2186 | 0.2186 | 0.5 | |
| Zn11 | 16c | -.3. | 0 | 0 | 0 | 0.125 | 8-vertex polyhedron Zn ₂ O ₆ |

M4 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, wR = 0.047, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Lee S.H., Kim Y. (2000), Bull. Korean Chem. Soc. 21, 180-186.

203
cF728

Cd_{13.9}Al₂₃Si₂₅O₉₆[OH]_{4.75}

cF728

(203) *Fd*-3 – g⁶e⁴ca

Cd_{55.1}Al₉₂Si₁₀₀O₃₈₄(OH)₁₉ [1], zeolite FAU-Cd

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cd at the centers of hexagonal prisms, β cages and single 6-rings, above the centers of single (in supercages) and double 6-rings, OH deeper in β cages.

Smolin Y.I. et al. (1998) [1]

Al_{23.04}Cd_{13.18}H_{4.75}O_{100.75}Si_{24.96}

a = 2.504 nm, *V* = 15.7001 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|-------|-------|------|----------|----------|----------|-------|--|
| O1 | 96g | 1 | 0.0 | 0.1047 | 0.251 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0008 | 0.1489 | 0.3575 | | non-colinear SiAl |
| Si3 | 96g | 1 | 0.03507 | 0.30204 | 0.12612 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.03762 | 0.12775 | 0.30456 | | tetrahedron O ₄ |
| O5 | 96g | 1 | 0.0664 | 0.2781 | 0.1791 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0766 | 0.3159 | 0.0804 | | non-colinear SiAl |
| Cd7 | 32e | .3. | 0.06356 | 0.06356 | 0.06356 | 0.497 | non-coplanar triangle O ₃ |
| (OH)8 | 32e | .3. | 0.1605 | 0.1605 | 0.1605 | 0.594 | single atom Cd |
| Cd9 | 32e | .3. | 0.20896 | 0.20896 | 0.20896 | 0.447 | |
| Cd10 | 32e | .3. | 0.2291 | 0.2291 | 0.2291 | 0.472 | |
| Cd11 | 16c | -.3. | 0 | 0 | 0 | 0.431 | 8-vertex polyhedron O ₆ Cd ₂ |
| Cd12 | 8a | 23. | 1/8 | 1/8 | 1/8 | 0.063 | tetrahedron (OH) ₄ |

M4 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.047, T = 523 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (1998), Kristallografiya 43, 421-424.

203
cF736

Ag₂₃Al₂₃Si₂₅O₉₆

cF736

(203) *Fd*-3 – g⁶fe³c

Ag₉₂Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ag

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms and near the centers of single 6-rings, above double 6-rings in β , above single 6- and 4-rings in supercages. Bulky clusters of four or more Ag in β cages.

Butikova I.K. et al. (1989) [1]

$\text{Ag}_{20.60}\text{Al}_{23.04}\text{O}_{96}\text{Si}_{24.96}$

$a = 2.502 \text{ nm}$, $V = 15.6625 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|------|------------------------------------|
| O1 | 96g | 1 | 0.001 | 0.3567 | 0.1481 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0348 | 0.126 | 0.3014 | | tetrahedron O_4 |
| M3 | 96g | 1 | 0.0361 | 0.3035 | 0.1262 | | tetrahedron O_4 |
| O4 | 96g | 1 | 0.0706 | 0.176 | 0.2762 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0745 | 0.0781 | 0.3222 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1426 | 0.2522 | 0.2501 | | non-colinear SiAl |
| Ag7 | 48f | 2.. | 0.389 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.13 | non-colinear O_2 |
| Ag8 | 32e | .3. | 0.0805 | 0.0805 | 0.0805 | 0.88 | octahedron O_3Ag_3 |
| Ag9 | 32e | .3. | 0.1924 | 0.1924 | 0.1924 | 0.43 | single atom Ag |
| Ag10 | 32e | .3. | 0.2336 | 0.2336 | 0.2336 | 0.57 | single atom Ag |
| Ag11 | 16c | -.3. | 0 | 0 | 0 | | octahedron O_6 |

$\text{M3} = 0.96\text{Al} + 0.04\text{Si}$

Transformation from published data: $-y, -x, -z$

Experimental: single crystal, precession photographs, X-rays, $R = 0.040$, $T = 673 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Butikova I.K., Shepelev Y.F., Smolin Y.I. (1989), Sov. Phys. Crystallogr. (Engl. Transl.) 34, 684-687.

203
cF736

| | | |
|--|-------|---------------------------------------|
| $\text{Cs}_{5.5}\text{Ca}_{8.75}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF736 | (203) $Fd-3 - g^6\text{fe}^3\text{c}$ |
|--|-------|---------------------------------------|

$\text{Cs}_{22}\text{Ca}_{35}\text{Al}_{92}\text{Si}_{100}\text{O}_{384}$ [1], zeolite FAU-Ca,Cs

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms and near the centers of single 6-rings, Cs opposite single 6-rings in β cages, 6- and 4-rings in supercages (disorder).

Jang S.B. et al. (1996) [1]

$\text{Al}_{23.04}\text{Ca}_{8.75}\text{Cs}_{5.51}\text{O}_{96}\text{Si}_{24.96}$

$a = 2.5071 \text{ nm}$, $V = 15.7585 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|-------|---------------------------|
| O1 | 96g | 1 | 0.0014 | 0.3631 | 0.1429 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0336 | 0.127 | 0.304 | | tetrahedron O_4 |
| M3 | 96g | 1 | 0.0363 | 0.3063 | 0.1281 | | tetrahedron O_4 |
| O4 | 96g | 1 | 0.0605 | 0.1842 | 0.2858 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.077 | 0.0801 | 0.313 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1429 | 0.2542 | 0.2541 | | non-colinear SiAl |
| Cs7 | 48f | 2.. | 0.425 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.188 | non-colinear O_2 |

| | | | | | | |
|------|-----|------|--------|--------|--------|---------------------------|
| Cs8 | 32e | .3. | 0.1642 | 0.1642 | 0.1642 | 0.094 |
| Ca9 | 32e | .3. | 0.2231 | 0.2231 | 0.2231 | 0.594 |
| Cs10 | 32e | .3. | 0.262 | 0.262 | 0.262 | 0.313 |
| Ca11 | 16c | -.3. | 0 | 0 | 0 | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, wR = 0.044, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Jang S.B., Song S.H., Kim Y. (1996), J. Korean Phys. Soc. 40, 427-435.

203
cF736

| | | |
|---|-------|--|
| Tl _{10.75} Cd _{6.125} Al ₂₃ Si ₂₅ O ₉₆ | cF736 | (203) <i>Fd-3</i> – g ⁶ fe ³ c |
|---|-------|--|

Tl₄₃Cd_{24.5}Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Cd,Tl

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cd at the centers of hexagonal prisms and near the centers of single 6-rings, Tl opposite double 6-rings in β cages and 6- and 4-rings in supercages (disorder).

Kwon J.H. et al. (1996) [1]

Al_{23.04}Cd_{6.13}O₉₆Si_{24.96}Tl_{10.76}

a = 2.4858 nm, *V* = 15.3603 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|-----------------------------|-----------------------------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0 | 0.143 | 0.3556 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0352 | 0.1277 | 0.3031 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0353 | 0.3032 | 0.1276 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0647 | 0.1849 | 0.2803 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0793 | 0.0822 | 0.3165 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1476 | 0.2542 | 0.253 | | non-coplanar triangle SiAlCd |
| Tl7 | 48f | 2.. | 0.4099 | ¹ / ₈ | ¹ / ₈ | 0.375 | non-colinear O ₂ |
| Tl8 | 32e | .3. | 0.0711 | 0.0711 | 0.0711 | 0.094 | non-coplanar triangle O ₃ |
| Cd9 | 32e | .3. | 0.215 | 0.215 | 0.215 | 0.313 | single atom Tl |
| Tl10 | 32e | .3. | 0.2534 | 0.2534 | 0.2534 | 0.688 | single atom Cd |
| Cd11 | 16c | -.3. | 0 | 0 | 0 | 0.906 | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, wR = 0.051, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Kwon J.H., Jang S.B., Kim Y., Seff K. (1996), J. Phys. Chem. 100, 13720-13724.

203
cF736

| | | |
|---|-------|---|
| Na _{21.75} Al _{21.75} Si _{26.25} O ₉₆ | cF736 | (203) <i>Fd-3</i> – g ⁷ e ² |
|---|-------|---|

Na₈₇Al₈₇Si₁₀₅O₃₈₄ [1], zeolite FAU-Na; Li₉₆Al₉₆Si₉₆O₃₈₄ [2], zeolite FAU-Li

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages

sharing 12-rings; Na above the centers of double 6-rings in β cages, single 6-rings in supercages and in 12-rings.

Vitale G. et al. (1997) [1]

$\text{Al}_{21.84}\text{Na}_{22}\text{O}_{96}\text{Si}_{26.16}$

$a = 2.50328 \text{ nm}$, $V = 15.6866 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0026 | 0.141 | 0.3564 | | non-colinear SiAl |
| Na2 | 96g | 1 | 0.03 | 0.422 | 0.068 | 0.25 | 4-vertex polyhedron O_2Na_2 |
| Si3 | 96g | 1 | 0.0344 | 0.1258 | 0.3021 | | tetrahedron O_4 |
| M4 | 96g | 1 | 0.0371 | 0.3065 | 0.1256 | | tetrahedron O_4 |
| O5 | 96g | 1 | 0.0691 | 0.0737 | 0.32 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0722 | 0.1747 | 0.2845 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.142 | 0.2512 | 0.2521 | | non-colinear SiAl |
| Na8 | 32e | .3. | 0.0459 | 0.0459 | 0.0459 | | non-coplanar triangle O_3 |
| Na9 | 32e | .3. | 0.2324 | 0.2324 | 0.2324 | | non-coplanar triangle O_3 |

$\text{M4} = 0.91\text{Al} + 0.09\text{Si}$

Experimental: powder, diffractometer, neutrons, $R_B = 0.033$, $T = 5 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition.

References: [1] Vitale G., Mellot C.F., Bull L.M., Cheetham A.K. (1997), J. Phys. Chem. B 101, 4559-4564. [2] Feuerstein M., Lobo R.F. (1998), Chem. Mater. 10, 2197-2204.

203
cF752

| | | |
|--|--------------|------------------------|
| $\text{Na}_{7.5}\text{Mg}_{7.75}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | <i>cF752</i> | $(203) Fd-3 - g^6e^5c$ |
|--|--------------|------------------------|

$\text{Na}_{30}\text{Mg}_{31}\text{Al}_{92}\text{Si}_{100}\text{O}_{382}$ [1], zeolite FAU-Mg,Na

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms and above the centers of single 6-rings in supercages, double 6-rings in β cages, Mg near the centers of single 6-rings, opposite double 6-rings in β cages.

Anderson A.A. et al. (1990) [1]

$\text{Al}_{23.04}\text{Mg}_{6.32}\text{Na}_{7.84}\text{O}_{96}\text{Si}_{24.96}$

$a = 2.478 \text{ nm}$, $V = 15.2161 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|--------------------------|
| O1 | 96g | 1 | 0.001 | 0.3597 | 0.1469 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0346 | 0.1268 | 0.3013 | | tetrahedron O_4 |
| M3 | 96g | 1 | 0.0381 | 0.3034 | 0.1287 | | tetrahedron O_4 |
| O4 | 96g | 1 | 0.0577 | 0.1852 | 0.2806 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0797 | 0.0838 | 0.315 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1466 | 0.2522 | 0.2528 | | non-colinear SiAl |
| Mg7 | 32e | .3. | 0.054 | 0.054 | 0.054 | 0.29 | |
| Na8 | 32e | .3. | 0.072 | 0.072 | 0.072 | 0.18 | |
| Mg9 | 32e | .3. | 0.2 | 0.2 | 0.2 | 0.18 | |
| Mg10 | 32e | .3. | 0.218 | 0.218 | 0.218 | 0.32 | |
| Na11 | 32e | .3. | 0.237 | 0.237 | 0.237 | 0.46 | |

Na12 16c .-3. 0 0 0 0.68 8-vertex polyhedron O₆Mg₂

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.046, T = 673 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Anderson A.A., Shepelev Y.F., Smolin Y.I. (1990), Zeolites 10, 32-37.

203
cF752

Ca_{11.5}Al₂₃Si₂₅O₉₆

cF752

(203) *Fd-3* – g⁷e²c

Ca₄₆Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ca

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca mainly at the centers of hexagonal prisms and single 6-rings, small amounts above 4-rings and single 6-rings in β cages.

Smolin Y.I. et al. (1989) [1]

Al_{23.04}Ca_{12.28}O₉₆Si_{24.96}

a = 2.506 nm, *V* = 15.7378 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|------|--------------------------------------|
| O1 | 96g | 1 | 0.0007 | 0.3609 | 0.1425 | | non-colinear SiAl |
| Ca2 | 96g | 1 | 0.027 | 0.034 | 0.372 | 0.03 | single atom O |
| Si3 | 96g | 1 | 0.0345 | 0.127 | 0.3045 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0366 | 0.306 | 0.1284 | | tetrahedron O ₄ |
| O5 | 96g | 1 | 0.0636 | 0.1845 | 0.2854 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.077 | 0.0785 | 0.3096 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1424 | 0.2531 | 0.254 | | non-colinear SiAl |
| Ca8 | 32e | .3. | 0.07 | 0.07 | 0.07 | 0.08 | non-coplanar triangle O ₃ |
| Ca9 | 32e | .3. | 0.2238 | 0.2238 | 0.2238 | 0.91 | non-coplanar triangle O ₃ |
| Ca10 | 16c | .-3. | 0 | 0 | 0 | 0.91 | octahedron O ₆ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.042, T = 673 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Smolin Y.I., Shepelev Y.F., Anderson A.A. (1989), Acta Crystallogr. B 45, 124-128.

203
cF752

Na_{26.5}Al₂₃Si₂₅O₉₆

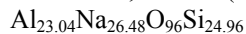
cF752

(203) *Fd-3* – g⁷e²d

Na₁₀₆Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Na (Na)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; linear (Na₃)²⁺ clusters in 12-rings, additional Na⁺ above the centers of single 6-rings in supercages, double 6-rings in β cages.

Shibata W., Seff K. (1997) [1]



$$a = 2.51 \text{ nm}, V = 15.8133 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|--------------------------------------|
| O1 | 96g | 1 | 0.0002 | 0.1438 | 0.3611 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0348 | 0.3045 | 0.1242 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0363 | 0.1259 | 0.3056 | | tetrahedron O ₄ |
| Na4 | 96g | 1 | 0.0421 | 0.0493 | 0.4076 | 0.29 | single atom O |
| O5 | 96g | 1 | 0.0695 | 0.3194 | 0.0721 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0706 | 0.2856 | 0.1752 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1407 | 0.2513 | 0.2526 | | non-colinear SiAl |
| Na8 | 32e | .3. | 0.048 | 0.048 | 0.048 | | non-coplanar triangle O ₃ |
| Na9 | 32e | .3. | 0.2292 | 0.2292 | 0.2292 | | non-coplanar triangle O ₃ |
| Na10 | 16d | -.3. | 1/2 | 1/2 | 1/2 | 0.88 | coplanar hexagon Na ₆ |

$$\text{M3} = 0.96\text{Al} + 0.04\text{Si}$$

Experimental: single crystal, diffractometer, X-rays, R = 0.071, T = 295 K

Remarks: Refinement of the occupancies of sites Na8 and Na9 showed no significant deviation from unity. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition.

References: [1] Shibata W., Seff K. (1997), J. Phys. Chem. B 101, 9022-9026.

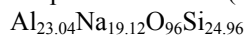
203
cF768

| | | |
|---|-------|----------------------------|
| $\text{Na}_{23}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF768 | (203) $Fd\bar{3} - g^7e^3$ |
|---|-------|----------------------------|

Na₉₂Al₉₂Si₁₀₀O₃₈₄ [2], zeolite FAU-Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na near the centers of hexagonal prisms, above the centers of double 6-rings in β cages and single 6-rings in supercages and in 12-rings.

Shepelev Y.F. et al. (1988) [1]



$$a = 2.506 \text{ nm}, V = 15.7378 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|---------------------------------------|
| O1 | 96g | 1 | 0.0002 | 0.3575 | 0.1459 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0355 | 0.124 | 0.303 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0365 | 0.304 | 0.1256 | | tetrahedron O ₄ |
| Na4 | 96g | 1 | 0.052 | 0.059 | 0.41 | 0.16 | single atom O |
| O5 | 96g | 1 | 0.0707 | 0.0735 | 0.3223 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0727 | 0.173 | 0.2815 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1448 | 0.2528 | 0.2511 | | non-colinear SiAl |
| Na8 | 32e | .3. | 0.005 | 0.005 | 0.005 | 0.14 | |
| Na9 | 32e | .3. | 0.0633 | 0.0633 | 0.0633 | 0.85 | 4-vertex polyhedron O ₃ Na |
| Na10 | 32e | .3. | 0.2356 | 0.2356 | 0.2356 | 0.92 | non-coplanar triangle O ₃ |

$$\text{M3} = 0.96\text{Al} + 0.04\text{Si}$$

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, T = 108 K

Remarks: The atom coordinates were refined for a phase with sorbed benzene; the authors state that the refinement of the benzene-free phase led to the same positions both for the framework atoms and the cations. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Shepelev Y.F., Anderson A.A., Smolin Y.I. (1988), Sov. Phys. Crystallogr. (Engl. Transl.) 33, 211-214. [2] Smolin Y.I., Shepelev Y.F., Butikova I.K., Petranovskii V.P. (1983), Sov. Phys. Crystallogr. (Engl. Transl.) 28, 36-39.

203
cF784

| | | |
|---|--------------|---|
| $\text{Ag}_{23}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | <i>cF784</i> | (203) <i>Fd-3 - g⁷e³c</i> |
|---|--------------|---|

Ag₉₂Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ag

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms, opposite double and single 6-rings in β cages, opposite 6-rings in supercages and in 12-rings (partial disorder). Ag_x clusters in β cages.

Jang S.B. et al. (1996) [1]

$\text{Ag}_{23}\text{Al}_{23.04}\text{O}_{96}\text{Si}_{24.96}$

$a = 2.4922 \text{ nm}$, $V = 15.4792 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0 | 0.105 | 0.252 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.002 | 0.152 | 0.352 | | non-colinear AlSi |
| Ag3 | 96g | 1 | 0.005 | 0.071 | 0.42 | 0.125 | non-coplanar triangle OAg ₂ |
| Si4 | 96g | 1 | 0.0363 | 0.126 | 0.3016 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.037 | 0.3009 | 0.127 | | tetrahedron O ₄ |
| O6 | 96g | 1 | 0.067 | 0.178 | 0.277 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.078 | 0.079 | 0.323 | | non-colinear SiAl |
| Ag8 | 32e | .3. | 0.0821 | 0.0821 | 0.0821 | | octahedron Ag ₃ O ₃ |
| Ag9 | 32e | .3. | 0.1849 | 0.1849 | 0.1849 | 0.531 | 7-vertex polyhedron Ag ₄ O ₃ |
| Ag10 | 32e | .3. | 0.2337 | 0.2337 | 0.2337 | 0.469 | 4-vertex polyhedron AgO ₃ |
| Ag11 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

$\text{M5} = 0.96\text{Al} + 0.04\text{Si}$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.091$, $T = 294 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Jang S.B., Park S.Y., Song S.H., Jeong M.S., Kim Y. (1996), J. Korean Phys. Soc. 40, 474-482.

203
cF784

| | | |
|---|--------------|---|
| $\text{Ca}_{11.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_5$ | <i>cF784</i> | (203) <i>Fd-3 - g⁷e³c</i> |
|---|--------------|---|

Ca₄₆Al₉₂Si₁₀₀O₃₈₄·xH₂O [1], zeolite FAU-Ca partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms, above the centers of 6-rings in supercages, double 6-rings in β cages and in 12-rings, H₂O opposite single 6-rings in β cages (disorder).

Smolin Y.I. et al. (1989) [1]

 $\text{Al}_{23.04}\text{Ca}_{11.52}\text{H}_{5.44}\text{O}_{98.72}\text{Si}_{24.96}$ $a = 2.506 \text{ nm}$, $V = 15.7378 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0016 | 0.3626 | 0.1442 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0342 | 0.1268 | 0.3043 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0379 | 0.3062 | 0.1284 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0604 | 0.1832 | 0.2855 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0762 | 0.0793 | 0.315 | | non-colinear SiAl |
| Ca6 | 96g | 1 | 0.09 | 0.093 | 0.399 | 0.06 | non-colinear OCa |
| O7 | 96g | 1 | 0.1433 | 0.2533 | 0.2532 | | non-colinear SiAl |
| Ca8 | 32e | .3. | 0.063 | 0.063 | 0.063 | 0.18 | 7-vertex polyhedron O ₃ (OH ₂) ₃ Ca |
| (OH ₂)9 | 32e | .3. | 0.164 | 0.164 | 0.164 | 0.34 | non-coplanar triangle Ca ₃ |
| Ca10 | 32e | .3. | 0.2331 | 0.2331 | 0.2331 | 0.64 | non-coplanar triangle O ₃ |
| Ca11 | 16c | -.3. | 0 | 0 | 0 | 0.88 | 8-vertex polyhedron O ₆ Ca ₂ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.057, T = 423 K

Remarks: The cell parameter was determined on a fully hydrated sample at 298 K. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Anderson A.A. (1989), Acta Crystallogr. B 45, 124-128.

203
cF784

| | | |
|---|--------------|-------------------------------|
| $\text{Li}_{24}\text{Al}_{24}\text{Si}_{24}\text{O}_{96}$ | <i>cF784</i> | $(203) Fd-3 - g^7\text{fe}^2$ |
|---|--------------|-------------------------------|

NaLi₉₅Al₉₆Si₉₆O₃₈₄ rt [1], zeolite FAU-Li rt

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Li above the centers of 6- and 4-rings in supercages, double 6-rings in β cages and in 12-rings (partial disorder).

Plévert J. et al. (1997) [1]

 $\text{Al}_{24}\text{Li}_{23.92}\text{O}_{96}\text{Si}_{24}$ $a = 2.46665 \text{ nm}$, $V = 15.0080 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|------|---|
| O1 | 96g | 1 | 0.0004 | 0.0976 | 0.2515 | | non-coplanar triangle AlSiLi |
| O2 | 96g | 1 | 0.0027 | 0.1514 | 0.3543 | | non-coplanar triangle SiAlLi |
| Al3 | 96g | 1 | 0.0371 | 0.1268 | 0.2999 | | tetrahedron O ₄ |
| Si4 | 96g | 1 | 0.0372 | 0.3003 | 0.1254 | | tetrahedron O ₄ |
| Li5 | 96g | 1 | 0.0589 | 0.108 | 0.39 | 0.17 | non-coplanar triangle LiO ₂ |
| O6 | 96g | 1 | 0.0688 | 0.2716 | 0.1766 | | non-coplanar triangle SiAlLi |
| O7 | 96g | 1 | 0.0785 | 0.3238 | 0.0824 | | 4-vertex polyhedron SiAlLi ₂ |
| Li8 | 48f | 2.. | 0.3756 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.32 | |
| Li9 | 32e | .3. | 0.0457 | 0.0457 | 0.0457 | | non-coplanar triangle O ₃ |
| Li10 | 32e | .3. | 0.2226 | 0.2226 | 0.2226 | | non-coplanar triangle O ₃ |

Experimental: powder, diffractometer, neutrons, $wR_p = 0.029$, $T = 300$ K

Remarks: Short interatomic distances for partly occupied site(s).

References: [1] Plévert J., Di Renzo F., Fajula F., Chiari G. (1997), J. Phys. Chem. B 101, 10340-10346.

203
cF800

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|--|-------|-----------------------|
| $\text{Al}_{22}\text{Pb}_{13.5}\text{Si}_{26}\text{O}_{96}[\text{OH}]_5$ | cF800 | (203) $Fd-3 - g^7e^4$ |
|--|-------|-----------------------|

Pb₅₄Al₈₈Si₁₀₄O₃₈₄(OH)₂₀ [1], zeolite FAU-Pb²⁺

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; defect [Pb(OH)]_{4-x} cubane-like clusters in β cages, additional Pb above the centers of 6-rings in supercages (split site) and in 12-rings (disorder).

Nardin G. et al. (1995) [1]

$\text{Al}_{22.01}\text{H}_{4.72}\text{O}_{100.72}\text{Pb}_{13.25}\text{Si}_{25.99}$

$a = 2.5078$ nm, $V = 15.7717$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|-------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.001 | 0.359 | 0.142 | | non-colinear SiAl |
| M2 | 96g | 1 | 0.0354 | 0.1245 | 0.3058 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.036 | 0.3072 | 0.1254 | | tetrahedron O ₄ |
| Pb4 | 96g | 1 | 0.0468 | 0.048 | 0.4153 | 0.104 | non-coplanar triangle OPb ₂ |
| O5 | 96g | 1 | 0.067 | 0.32 | 0.068 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.078 | 0.168 | 0.287 | | non-colinear AlSi |
| O7 | 96g | 1 | 0.141 | 0.253 | 0.251 | | non-colinear AlSi |
| Pb8 | 32e | .3. | 0.0699 | 0.0699 | 0.0699 | 0.719 | 9-vertex polyhedron (OH) ₃ O ₆ |
| (OH)9 | 32e | .3. | 0.167 | 0.167 | 0.167 | 0.59 | non-coplanar triangle Pb ₃ |
| Pb10 | 32e | .3. | 0.2303 | 0.2303 | 0.2303 | 0.437 | |
| Pb11 | 32e | .3. | 0.2492 | 0.2492 | 0.2492 | 0.188 | |

$M2 = 0.917\text{Al} + 0.083\text{Si}$

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, $R = 0.071$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Nardin G., Randaccio L., Zangrando E. (1995), Zeolites 15, 684-688.

203
cF800

| | | |
|--|-------|-------------------------|
| $\text{K}_{23}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF800 | (203) $Fd-3 - g^7fe^2c$ |
|--|-------|-------------------------|

K₉₂Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-K

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; K at the centers of hexagonal prisms, above the centers of single 6- and 4-rings in supercages, double 6-rings in β cages and in 12-rings (disorder).

Jang S.B., Kim Y. (1995) [1]

$\text{Al}_{23.04}\text{K}_{22.99}\text{O}_{96}\text{Si}_{24.96}$

$a = 2.5128$ nm, $V = 15.8662$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.001 | 0.141 | 0.36 | | non-colinear AlSi |
| Si2 | 96g | 1 | 0.0349 | 0.3033 | 0.126 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0354 | 0.1256 | 0.3055 | | tetrahedron O ₄ |
| K4 | 96g | 1 | 0.056 | 0.068 | 0.427 | 0.104 | single atom K |
| O5 | 96g | 1 | 0.0693 | 0.2876 | 0.1797 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0726 | 0.3179 | 0.0735 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1394 | 0.2543 | 0.2538 | | non-colinear SiAl |
| K8 | 48f | 2.. | 0.406 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.458 | non-colinear K ₂ |
| K9 | 32e | .3. | 0.071 | 0.071 | 0.071 | 0.375 | non-coplanar triangle O ₃ |
| K10 | 32e | .3. | 0.2435 | 0.2435 | 0.2435 | | non-coplanar triangle O ₃ |
| K11 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, wR = 0.039, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Jang S.B., Kim Y. (1995), Bull. Korean Chem. Soc. 16, 539-542.

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cF816

| | | |
|---|-------|---|
| Na _{7.5} Li _{15.5} Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₅₀ | cF816 | (203) <i>Fd-3</i> – g ⁷ e ⁴ c |
|---|-------|---|

Na₃₀Li₆₂Al₉₆Si₁₀₀O₃₈₂·200H₂O [1], zeolite FAU-Li,Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Li above the centers of double 6-rings in β cages, Na opposite single 6-rings in supercages, H₂O at the centers of hexagonal prisms, in β cages and supercages (disorder).

Shepelev Y.F. et al. (1990) [1]

Al_{23.04}H_{27.12}Li_{4.32}Na_{7.68}O_{109.56}Si_{24.96}

a = 2.482 nm, V = 15.2899 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0006 | 0.1433 | 0.3526 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0358 | 0.1256 | 0.3016 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.037 | 0.3024 | 0.1266 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0704 | 0.1762 | 0.2778 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0742 | 0.0775 | 0.3225 | | non-colinear SiAl |
| (OH ₂)6 | 96g | 1 | 0.079 | 0.083 | 0.439 | 0.24 | 4-vertex polyhedron O ₃ (OH ₂) |
| O7 | 96g | 1 | 0.1482 | 0.2528 | 0.2512 | | non-colinear SiAl |
| Li8 | 32e | .3. | 0.054 | 0.054 | 0.054 | 0.54 | |
| (OH ₂)9 | 32e | .3. | 0.074 | 0.074 | 0.074 | 0.61 | |
| (OH ₂)10 | 32e | .3. | 0.165 | 0.165 | 0.165 | 0.21 | non-coplanar triangle (OH ₂) ₃ |
| Na11 | 32e | .3. | 0.2589 | 0.2589 | 0.2589 | 0.96 | non-coplanar triangle O ₃ |
| (OH ₂)12 | 16c | -.3. | 0 | 0 | 0 | 0.31 | colinear Li ₂ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.067, T = 298 K

Remarks: Part of Li and H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s); impossibly short distances occur for the refined occupancies. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Shepelev Y.F., Anderson A.A., Smolin Y.I. (1990), Zeolites 10, 61-63.

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cF816

| | | |
|---|-------|-----------------------------|
| $\text{Na}_{7.5}\text{Li}_{15.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_{2.25}$ | cF816 | (203) $Fd\bar{3} - g^7e^4c$ |
|---|-------|-----------------------------|

$\text{Na}_{30}\text{Li}_{62}\text{Al}_{96}\text{Si}_{100}\text{O}_{382} \cdot 10\text{H}_2\text{O}$ [1], zeolite FAU-Li,Na residual water

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Li and Na opposite double 6-rings in β cages, near and above the centers of single 6-rings in supercages (split sites), additional Na in supercages, H₂O at the centers of hexagonal prisms.

Shepelev Y.F. et al. (1990) [1]

$\text{Al}_{23.04}\text{H}_{4.32}\text{Li}_{10.32}\text{Na}_{6.08}\text{O}_{98.16}\text{Si}_{24.96}$

$a = 2.475 \text{ nm}$, $V = 15.1609 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|------------------------------|
| O1 | 96g | 1 | 0.0007 | 0.353 | 0.15 | | non-collinear SiAl |
| Si2 | 96g | 1 | 0.0367 | 0.1244 | 0.3005 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0375 | 0.301 | 0.1255 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0696 | 0.1793 | 0.2735 | | non-coplanar triangle SiAlLi |
| O5 | 96g | 1 | 0.0769 | 0.0786 | 0.3206 | | non-collinear SiAl |
| Na6 | 96g | 1 | 0.102 | 0.104 | 0.42 | 0.09 | |
| O7 | 96g | 1 | 0.1507 | 0.251 | 0.2508 | | non-coplanar triangle SiAlLi |
| Li8 | 32e | .3. | 0.053 | 0.053 | 0.053 | 0.78 | |
| Na9 | 32e | .3. | 0.073 | 0.073 | 0.073 | 0.15 | |
| Li10 | 32e | .3. | 0.21 | 0.21 | 0.21 | 0.51 | |
| Na11 | 32e | .3. | 0.25 | 0.25 | 0.25 | 0.34 | |
| (OH ₂)12 | 16c | -.3. | 0 | 0 | 0 | 0.54 | collinear Li ₂ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.065, T = 548 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Shepelev Y.F., Anderson A.A., Smolin Y.I. (1990), Zeolites 10, 61-63.

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cF816

| | | |
|--|-------|-----------------------------|
| $\text{Ca}_{11.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_{15}$ | cF816 | (203) $Fd\bar{3} - g^7e^4c$ |
|--|-------|-----------------------------|

$\text{Ca}_{46}\text{Al}_{92}\text{Si}_{100}\text{O}_{384} \cdot 60\text{H}_2\text{O}$ [1], zeolite FAU-Ca partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms, above the centers of double 6-rings in β cages, single 6-rings in supercages (split site) and in 12-rings, H₂O opposite single 6-rings in β cages.

Smolin Y.I. et al. (1989) [1]



$a = 2.506 \text{ nm}, V = 15.7378 \text{ nm}^3, Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0022 | 0.3605 | 0.1462 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0346 | 0.1262 | 0.3039 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0369 | 0.3053 | 0.1284 | | tetrahedron O ₄ |
| Ca4 | 96g | 1 | 0.048 | 0.049 | 0.405 | 0.04 | single atom O |
| O5 | 96g | 1 | 0.0622 | 0.1831 | 0.2839 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0755 | 0.0784 | 0.3173 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1433 | 0.2538 | 0.2535 | | non-colinear SiAl |
| Ca8 | 32e | .3. | 0.072 | 0.072 | 0.072 | 0.27 | octahedron (OH ₂) ₃ O ₃ |
| (OH ₂)9 | 32e | .3. | 0.167 | 0.167 | 0.167 | | tetrahedron Ca ₄ |
| Ca10 | 32e | .3. | 0.223 | 0.223 | 0.223 | 0.16 | |
| Ca11 | 32e | .3. | 0.242 | 0.242 | 0.242 | 0.37 | |
| Ca12 | 16c | -.3. | 0 | 0 | 0 | 0.68 | octahedron O ₆ |

$M3 = 0.96\text{Al} + 0.04\text{Si}$

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.048, T = 348 K

Remarks: The cell parameter was determined on a fully hydrated sample at 298 K. The authors state that ~40 H₂O per unit cell are delocalized in supercages. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Anderson A.A. (1989), Acta Crystallogr. B 45, 124-128.

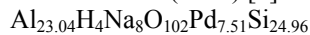
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cF816

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|--|-------|--------------------------|
| $\text{Na}_8\text{Pd}_{7.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{98}[\text{OH}]_4$ | cF816 | (203) $Fd-3 - g^7 e^4 c$ |
|--|-------|--------------------------|

Na₃₂Pd₃₀Al₉₂Si₁₀₀O₃₉₂(OH)₁₆ [1], zeolite FAU-Pd²⁺, Pd⁴⁺, Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; HO-Pd⁴⁺-O-Pd⁴⁺-OH linear clusters, Pd²⁺ at the centers of hexagonal prisms, above the centers of double 6-rings in β cages and in supercages (disorder), Na above 6-rings in supercages.

Lee S.H. et al. (2000) [1]



$a = 2.4982 \text{ nm}, V = 15.5913 \text{ nm}^3, Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|-------|----------------------------|
| O1 | 96g | 1 | 0.0007 | 0.1404 | 0.356 | | non-colinear SiAl |
| (Pd ²⁺)2 | 96g | 1 | 0.0185 | 0.0791 | 0.4141 | 0.042 | single atom O |
| Si3 | 96g | 1 | 0.0354 | 0.1251 | 0.3018 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0374 | 0.3043 | 0.126 | | tetrahedron O ₄ |
| O5 | 96g | 1 | 0.068 | 0.1794 | 0.2834 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0698 | 0.0762 | 0.3143 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1465 | 0.2562 | 0.2533 | | non-colinear SiAl |
| (Pd ⁴⁺)8 | 32e | .3. | 0.0387 | 0.0387 | 0.0387 | 0.5 | |
| (Pd ²⁺)9 | 32e | .3. | 0.0607 | 0.0607 | 0.0607 | 0.063 | |

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|--------|-----|------|--------|--------|--------|-----|--------------------------------------|
| (OH)10 | 32e | .3. | 0.0866 | 0.0866 | 0.0866 | 0.5 | |
| Na11 | 32e | .3. | 0.2296 | 0.2296 | 0.2296 | | non-coplanar triangle O ₃ |
| M12 | 16c | -.3. | 0 | 0 | 0 | | colinear Pd ₂ |

M4 = 0.96Al + 0.04Si; M12 = 0.5O + 0.5Pd²⁺

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, wR = 0.051, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee S.H., Kim Y., Seff K. (2000), J. Phys. Chem. B 104, 2490-2494.

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| Ca _{11.5} Al ₂₃ Si ₂₅ S ₁₄₉ [H ₂ S] _{37.2} | cF816 | (203) <i>Fd</i> -3 – g ⁸ ec |
|--|-------|--|

Ca₄₆Al₉₂Si₁₀₀O₃₈₄·149H₂S [1], zeolite FAU-Ca (H₂S); Ca₄₆Al₉₂Si₁₀₀O₃₈₄·135NH₃ [2], zeolite FAU-Ca (NH₃)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; H₂S in 12-rings and supercages, Ca at the centers of hexagonal prisms and above the centers of single 6-rings in supercages.

Jang S.B. et al. (1998) [1]

Al_{23.04}Ca_{11.50}H_{74.54}O₉₆S_{37.27}Si_{24.96}
a = 2.4864 nm, V = 15.3714 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0012 | 0.3619 | 0.1427 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0336 | 0.1265 | 0.3038 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0369 | 0.3049 | 0.1281 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0617 | 0.1878 | 0.2844 | | non-colinear AlSi |
| (SH ₂)5 | 96g | 1 | 0.072 | 0.0792 | 0.4491 | 0.615 | single atom SH ₂ |
| O6 | 96g | 1 | 0.0775 | 0.0817 | 0.3155 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1448 | 0.255 | 0.2535 | | non-colinear SiAl |
| (SH ₂)8 | 96g | 1 | 0.2547 | 0.2741 | 0.3558 | 0.938 | single atom SH ₂ |
| Ca9 | 32e | .3. | 0.2372 | 0.2372 | 0.2372 | 0.938 | non-coplanar triangle O ₃ |
| Ca10 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, wR = 0.067, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Jang S.B., Jeong M.S., Kim Y., Han Y.W., Seff K. (1998), Microporous Mesoporous Mater. 23, 33-44. [2] Jang S.B., Jeong M.S., Kim Y., Song S.H., Seff K. (1999), Microporous Mesoporous Mater. 28, 173-183.

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cF832

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| $\text{K}_{16.5}\text{Na}_{5.5}\text{Al}_{22}\text{Si}_{26}\text{O}_{96}[\text{H}_2\text{O}]_{1.75}$ | <i>cF832</i> | (203) <i>Fd-3</i> – $\text{g}^6\text{fe}^6\text{c}$ |
|--|--------------|---|

K₆₆Na₂₂Al₈₈Si₁₀₄O₃₈₄·7H₂O [1], zeolite FAU-K,Na residual water

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; K at the centers of hexagonal prisms, opposite double and single 6-rings in β cages, 4- and 6-rings in supercages, Na above 6-rings in supercages, H₂O deep in supercages (disorder).

Kirschhock C.E.A. et al. (2000) [1]

$\text{Al}_{22.08}\text{H}_{3.57}\text{K}_{16.64}\text{Na}_{5.42}\text{O}_{97.78}\text{Si}_{25.92}$
 $a = 2.51042 \text{ nm}$, $V = 15.8212 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------------|---------------|-------|---|
| O1 | 96g | 1 | 0.0019 | 0.1453 | 0.3574 | | non-colinear SiAl |
| M2 | 96g | 1 | 0.0352 | 0.12484 | 0.30391 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.03615 | 0.3051 | 0.12601 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0742 | 0.3206 | 0.0751 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0754 | 0.1732 | 0.28849 | | non-colinear AlSi |
| O6 | 96g | 1 | 0.1411 | 0.253 | 0.2538 | | non-colinear AlSi |
| K7 | 48f | 2.. | 0.4281 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.601 | non-colinear O ₂ |
| K8 | 32e | .3. | 0.0686 | 0.0686 | 0.0686 | 0.352 | octahedron O ₃ K ₃ |
| K9 | 32e | .3. | 0.1781 | 0.1781 | 0.1781 | 0.24 | single atom Na |
| Na10 | 32e | .3. | 0.2317 | 0.2317 | 0.2317 | 0.43 | |
| K11 | 32e | .3. | 0.2451 | 0.2451 | 0.2451 | 0.32 | |
| Na12 | 32e | .3. | 0.25 | 0.25 | 0.25 | 0.247 | |
| (OH ₂)13 | 32e | .3. | 0.3098 | 0.3098 | 0.3098 | 0.223 | |
| K14 | 16c | -.3. | 0 | 0 | 0 | 0.533 | 8-vertex polyhedron O ₆ K ₂ |

M2 = 0.92Al + 0.08Si

Experimental: powder, diffractometer, X-rays, R_p = 0.044, T = 673 K

Remarks: We placed Si in former site T1 and assigned an approximate value to the Al/Si ratio of former site T2 based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 (KNaX) of [1] the occupation factor of site SII(Na) is misprinted as 0.667 instead of 0.430 (13.76 atoms per cell given in the same table).

References: [1] Kirschhock C.E.A., Hunger B., Martens J., Jacobs P.A. (2000), J. Phys. Chem. B 104, 439-448.

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cF832

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|--|--------------|--|
| $\text{Tl}_{4.5}\text{Al}_{23}\text{Pb}_{12.25}\text{Si}_{25}\text{O}_{100.5}$ | <i>cF832</i> | (203) <i>Fd-3</i> – g^7e^5 |
|--|--------------|--|

Tl₁₈Pb₄₉Al₉₂Si₁₀₀O₄₀₁ [1], zeolite FAU-Pb,Tl⁺ (PbO_x)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Pb²⁺₄O₄(Pb²⁺,Pb⁴⁺)₄ cubane-like units in β cages (distinct positions for Pb²⁺ and Pb⁴⁺), Tl above 6-rings in supercages and in 12-rings (partial disorder).

Yeom Y.H. et al. (1999) [1]

$\text{Al}_{23.04}\text{O}_{100.25}\text{Pb}_{11.91}\text{Si}_{24.96}\text{Tl}_{4.50}$
 $a = 2.5119 \text{ nm}$, $V = 15.8492 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|-----------------------|-------|------|---------|---------|---------|-------|---------------------------------|
| O1 | 96g | 1 | 0.0001 | 0.1454 | 0.3502 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0358 | 0.1245 | 0.3033 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0366 | 0.305 | 0.126 | | tetrahedron O ₄ |
| Tl4 | 96g | 1 | 0.0582 | 0.4189 | 0.0611 | 0.031 | single atom O |
| O5 | 96g | 1 | 0.0693 | 0.0713 | 0.3199 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0744 | 0.1723 | 0.2809 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1439 | 0.2512 | 0.2504 | | non-colinear SiAl |
| (Pb ²⁺)8 | 32e | .3. | 0.07216 | 0.07216 | 0.07216 | | octahedron O ₆ |
| O9 | 32e | .3. | 0.1763 | 0.1763 | 0.1763 | 0.531 | single atom (Pb ⁴⁺) |
| (Pb ⁴⁺)10 | 32e | .3. | 0.22511 | 0.22511 | 0.22511 | 0.156 | |
| (Pb ²⁺)11 | 32e | .3. | 0.24033 | 0.24033 | 0.24033 | 0.333 | |
| Tl12 | 32e | .3. | 0.2514 | 0.2514 | 0.2514 | 0.469 | |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, wR = 0.055, T = 294 K

Remarks: Pb²⁺₄₄Pb⁴⁺₅Tl⁺₁₈O²⁻₁₇Al₉₂Si₁₀₀O₃₈₄. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Yeom Y.H., Kim Y., Seff K. (1999), Microporous Mesoporous Mater. 28, 103-112.

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cF832

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|--|-------|--|
| Ag ₂₃ Al ₂₃ Si ₂₅ O ₉₆ | cF832 | (203) <i>Fd-3</i> – g ⁷ fe ³ c |
|--|-------|--|

Ag₉₂Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ag

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms, near the centers of single 6-rings, opposite double 6-rings in β cages, 6- and 4-rings in supercages and in 12-rings. Ag_x clusters in β cages.

Jang S.B. et al. (1996) [1]

Ag_{22.99}Al_{23.04}O₉₆Si_{24.96}

a = 2.4901 nm, V = 15.4401 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0003 | 0.1022 | 0.2517 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.001 | 0.3517 | 0.1503 | | non-colinear SiAl |
| Ag3 | 96g | 1 | 0.012 | 0.07 | 0.415 | 0.062 | single atom O |
| M4 | 96g | 1 | 0.036 | 0.3003 | 0.1259 | | tetrahedron O ₄ |
| Si5 | 96g | 1 | 0.037 | 0.126 | 0.3028 | | tetrahedron O ₄ |
| O6 | 96g | 1 | 0.0677 | 0.1801 | 0.2772 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0784 | 0.0791 | 0.3215 | | non-colinear SiAl |
| Ag8 | 48f | 2.. | 0.396 | 1/8 | 1/8 | 0.125 | non-colinear O ₂ |
| Ag9 | 32e | .3. | 0.0813 | 0.0813 | 0.0813 | | octahedron Ag ₃ O ₃ |
| Ag10 | 32e | .3. | 0.1862 | 0.1862 | 0.1862 | 0.5 | 7-vertex polyhedron Ag ₄ O ₃ |
| Ag11 | 32e | .3. | 0.232 | 0.232 | 0.232 | 0.5 | 4-vertex polyhedron AgO ₃ |
| Ag12 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, wR = 0.085, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Jang S.B., Park S.Y., Song S.H., Jeong M.S., Kim Y. (1996), J. Korean Phys. Soc. 40, 474-482.

203
cF832

| | | |
|---|--------------|---------------------------------------|
| $\text{Na}_{13.5}[\text{H}_3\text{O}]_{10.5}\text{Al}_{24}\text{Si}_{24}\text{O}_{96}[\text{H}_2\text{O}]_{20}$ | <i>cF832</i> | $(203) Fd-3 - g^7\text{fe}^3\text{c}$ |
|---|--------------|---------------------------------------|

$\text{Na}_{54}(\text{H}_3\text{O})_{42}\text{Al}_{96}\text{Si}_{96}\text{O}_{384} \sim 80\text{H}_2\text{O}$ [1], zeolite FAU-Na,H partly hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na above 6-rings in supercages and at the centers of hexagonal prisms, H_3O^+ opposite double 6-rings in β cages, H_2O in β cages and supercages.

Zhu L. et al. (1999) [1]

$\text{Al}_{24}\text{D}_{38.94}\text{Na}_{9.16}\text{O}_{113.24}\text{Si}_{24}$

$a = 2.50523 \text{ nm}$, $V = 15.7233 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------|-------|------|----------|---------------|---------------|-------|----------------------------------|
| O1 | 96g | 1 | 0.0003 | 0.1422 | 0.3549 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0344 | 0.1252 | 0.3026 | | tetrahedron O_4 |
| Al3 | 96g | 1 | 0.0386 | 0.3047 | 0.1233 | | tetrahedron O_4 |
| O4 | 96g | 1 | 0.0678 | 0.0747 | 0.3249 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0745 | 0.1717 | 0.2841 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1435 | 0.2527 | 0.252 | | non-colinear SiAl |
| (OD ₂)7 | 96g | 1 | 0.2769 | 0.3027 | 0.2895 | 0.333 | |
| (OD ₂)8 | 48f | 2.. | 0.098 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.167 | |
| O9 | 32e | .3. | 0.0703 | 0.0703 | 0.0703 | 0.556 | |
| (OD ₂)10 | 32e | .3. | 0.1847 | 0.1847 | 0.1847 | 0.35 | |
| Na11 | 32e | .3. | 0.2374 | 0.2374 | 0.2374 | | |
| Na12 | 16c | -.3. | 0 | 0 | 0 | 0.29 | 8-vertex polyhedron O_8 |
| D13 | 96g | 1 | 0.026 | 0.0636 | 0.0748 | 0.556 | |

Transformation from published data: -*y*, -*x*, -*z*

Experimental: powder, diffractometer, neutrons, time-of-flight, $wR_p = 0.032$, $T = 10 \text{ K}$

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Occupation of the non framework site type II', (OD₂)10, could not be assigned with certainty, interatomic distances 0.261 nm to site O6.

References: [1] Zhu L., Seff K., Olson D.H., Cohen B.J., Von Dreele R.B. (1999), J. Phys. Chem. B 103, 10365-10372.

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cF832

| | | |
|---|--------------|------------------------------|
| $\text{Tl}_{23}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | <i>cF832</i> | $(203) Fd-3 - g^8\text{e}^2$ |
|---|--------------|------------------------------|

$\text{Tl}_{92}\text{Al}_{92}\text{Si}_{100}\text{O}_{384}$ [1], zeolite FAU-Tl

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Tl opposite double 6-rings in β cages, opposite single 6-rings and near 4-rings in supercages.

Kim Y. et al. (1997) [1]

$\text{Al}_{23.04}\text{O}_9\text{Si}_{24.96}\text{Ti}_{23.01}$

$a = 2.5043 \text{ nm}$, $V = 15.7058 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.001 | 0.3529 | 0.1439 | | non-colinear SiAl |
| M2 | 96g | 1 | 0.036 | 0.126 | 0.3036 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.036 | 0.303 | 0.1242 | | tetrahedron O ₄ |
| Tl4 | 96g | 1 | 0.0696 | 0.0749 | 0.4168 | 0.125 | |
| O5 | 96g | 1 | 0.073 | 0.322 | 0.0741 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0732 | 0.2805 | 0.1726 | | non-colinear SiAl |
| Tl7 | 96g | 1 | 0.1113 | 0.1358 | 0.4073 | 0.167 | |
| O8 | 96g | 1 | 0.1453 | 0.2515 | 0.2525 | | non-colinear SiAl |
| Tl9 | 32e | .3. | 0.073 | 0.073 | 0.073 | | non-coplanar triangle O ₃ |
| Tl10 | 32e | .3. | 0.2522 | 0.2522 | 0.2522 | | non-coplanar triangle O ₃ |

$\text{M2} = 0.96\text{Al} + 0.04\text{Si}$

Transformation from published data: $-y, -x, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.047$, $T = 295 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Kim Y., Han Y.W., Seff K. (1997), Zeolites 18, 325-333.

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cF840

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|---|-------|---|
| $\text{Rb}_{35}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF840 | (203) $Fd\bar{3} - g^7\text{fe}^3\text{cb}$ |
|---|-------|---|

Rb₁₄₀Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Rb (Rb)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Rb⁺ at the centers of hexagonal prisms, additional Rb and Rb⁺ form a 3D-framework with Rb₁₄ tetrahedral clusters in supercages.

Lee S.H. et al. (2000) [1]

$\text{Al}_{23.04}\text{O}_9\text{Rb}_{34.45}\text{Si}_{24.96}$

$a = 2.52 \text{ nm}$, $V = 16.0030 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|---------------|---------------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0007 | 0.3617 | 0.1394 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0356 | 0.1234 | 0.3064 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0355 | 0.3061 | 0.1237 | | tetrahedron O ₄ |
| Rb4 | 96g | 1 | 0.0581 | 0.0594 | 0.4295 | 0.477 | |
| O5 | 96g | 1 | 0.068 | 0.3216 | 0.0705 | | non-colinear AlSi |
| O6 | 96g | 1 | 0.0765 | 0.1721 | 0.2863 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1385 | 0.2541 | 0.2551 | | non-colinear AlSi |
| Rb8 | 48f | 2.. | 0.4158 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.5 | |
| Rb9 | 32e | .3. | 0.0758 | 0.0758 | 0.0758 | 0.25 | |
| Rb10 | 32e | .3. | 0.1705 | 0.1705 | 0.1705 | 0.25 | |
| Rb11 | 32e | .3. | 0.2546 | 0.2546 | 0.2546 | | non-coplanar triangle O ₃ |
| Rb12 | 16c | -.3. | 0 | 0 | 0 | 0.75 | octahedron O ₆ |

Rb13 8b 23. $\frac{5}{8}$ $\frac{5}{8}$ $\frac{5}{8}$ 22-vertex polyhedron Rb₂₂

M3 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.054, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Lee S.H., Kim Y., Seff K. (2000), J. Phys. Chem. B 104, 11162-11167.

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cF848

Na_{2.25}Tl_{20.75}Al₂₃Si₂₅O₉₆

cF848

(203) *Fd-3* – g⁸e²c

Na₉Tl₈₃Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Tl,Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, Tl opposite double 6-rings in β cages, single 6-rings in supercages and in 12-rings.

Zhu L., Seff K. (2000) [1]

Al_{23.04}Na_{0.90}O₉₆Si_{24.96}Tl_{20.74}

a = 2.5071 nm, *V* = 15.7585 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0007 | 0.1465 | 0.3569 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0019 | 0.0027 | 0.144 | | non-colinear SiAl |
| M3 | 96g | 1 | 0.036 | 0.1257 | 0.3037 | | tetrahedron O ₄ |
| Si4 | 96g | 1 | 0.036 | 0.3027 | 0.1246 | | tetrahedron O ₄ |
| Tl5 | 96g | 1 | 0.0691 | 0.0699 | 0.4192 | 0.168 | |
| O6 | 96g | 1 | 0.0718 | 0.2782 | 0.1757 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0732 | 0.3228 | 0.0738 | | non-colinear SiAl |
| Tl8 | 96g | 1 | 0.111 | 0.1353 | 0.4073 | 0.169 | |
| Tl9 | 32e | .3. | 0.073 | 0.073 | 0.073 | 0.775 | non-coplanar triangle O ₃ |
| Tl10 | 32e | .3. | 0.2524 | 0.2524 | 0.2524 | 0.806 | non-coplanar triangle O ₃ |
| Na11 | 16c | -.3. | 0 | 0 | 0 | 0.225 | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.049, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Zhu L., Seff K. (2000), Microporous Mesoporous Mater. 39, 187-193.

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cF848

Sr_{11.5}Al₂₃Si₂₅O₉₆[NH₃]_{25.5}

cF848

(203) *Fd-3* – g⁸e²c

Sr₄₆Al₉₂Si₁₀₀O₃₈₄·102NH₃ [1], zeolite FAU-Sr (NH₃)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Sr at the centers of hexagonal prisms, above the centers of double 6-rings in β cages and single 6-rings in supercages, NH₃ in β cages and supercages.

Kim M.J. et al. (1999) [1]

$\text{Al}_{23.04}\text{H}_{76.46}\text{N}_{25.49}\text{O}_9\text{Si}_{24.96}\text{Sr}_{11.50}$
 $a = 2.5127 \text{ nm}$, $V = 15.8643 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0008 | 0.3618 | 0.1426 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0338 | 0.1252 | 0.3049 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0366 | 0.3062 | 0.1264 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0679 | 0.1782 | 0.2871 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0699 | 0.0728 | 0.3148 | | non-colinear SiAl |
| (NH ₃)6 | 96g | 1 | 0.077 | 0.1563 | 0.0917 | 0.125 | |
| O7 | 96g | 1 | 0.1405 | 0.2543 | 0.2536 | | non-colinear SiAl |
| (NH ₃)8 | 96g | 1 | 0.2204 | 0.3166 | 0.3203 | 0.937 | non-colinear SrO |
| Sr9 | 32e | .3. | 0.0685 | 0.0685 | 0.0685 | 0.125 | |
| Sr10 | 32e | .3. | 0.2419 | 0.2419 | 0.2419 | 0.937 | 9-vertex polyhedron O ₆ (NH ₃) ₃ |
| Sr11 | 16c | -.3. | 0 | 0 | 0 | 0.75 | 8-vertex polyhedron O ₆ Sr ₂ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, wR = 0.045, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kim M.J., Jeong M.S., Kim Y., Seff K. (1999), Microporous Mesoporous Mater. 30, 233-241.

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cF856

| | | |
|--|-------|------------------------------|
| $\text{Rb}_7\text{Na}_{19.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF856 | (203) $Fd\bar{3} - g^8e^2ca$ |
|--|-------|------------------------------|

Rb₂₈Na₇₈Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Na,Rb (Na)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; (NaNa₄)⁴⁺ tetrahedra in β cages, additional Na at the centers of hexagonal prisms and above the centers of single 6-rings in supercages, Rb in supercages.

Kim Y. et al. (1994) [1]

$\text{Al}_{23.04}\text{Na}_{19.50}\text{O}_9\text{Rb}_{7.01}\text{Si}_{24.96}$
 $a = 2.5045 \text{ nm}$, $V = 15.7095 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0008 | 0.3548 | 0.1403 | | non-colinear SiAl |
| M2 | 96g | 1 | 0.0354 | 0.1266 | 0.3047 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.0353 | 0.3036 | 0.1255 | | tetrahedron O ₄ |
| Rb4 | 96g | 1 | 0.0572 | 0.0597 | 0.4245 | 0.063 | |
| O5 | 96g | 1 | 0.0697 | 0.2823 | 0.1762 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0722 | 0.3209 | 0.0763 | | non-colinear SiAl |
| Rb7 | 96g | 1 | 0.1137 | 0.1333 | 0.4226 | 0.229 | |
| O8 | 96g | 1 | 0.1443 | 0.2507 | 0.2541 | | non-colinear SiAl |
| Na9 | 32e | .3. | 0.0604 | 0.0604 | 0.0604 | | non-coplanar triangle O ₃ |

| | | | | | | |
|------|-----|------|---------------|---------------|---------------|--|
| Na10 | 32e | .3. | 0.2288 | 0.2288 | 0.2288 | non-coplanar triangle O ₃ |
| Na11 | 16c | .-3. | 0 | 0 | 0 | 0.375 8-vertex polyhedron Na ₂ O ₆ |
| Na12 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | tetrahedron Na ₄ |

M2 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.082, T = 295 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Kim Y., Han Y.W., Seff K. (1994), Stud. Surf. Sci. Catal. 84, 629-636.

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| | | |
|--|-------|--|
| Na ₂₂ Al ₂₂ Si ₂₆ O ₉₆ [H ₂ O] _{8.1} | cF864 | (203) <i>Fd-3</i> – g ⁷ fe ⁴ c |
|--|-------|--|

Na₈₈Al₈₈Si₁₀₄O₃₈₄·32.5H₂O [1], zeolite FAU-Na residual water

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, above the centers of single and double 6-rings in β cages, 6-rings and 4-rings in supercages, H₂O in supercages.

Kirschhock C.E.A. et al. (2000) [1]

Al_{22.08}H_{16.32}Na_{21.82}O_{104.16}Si_{25.92}

a = 2.49443 nm, *V* = 15.5208 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|---------------------|-------|------|----------|---------------|---------------|-------|--|
| O1 | 96g | 1 | 0.0007 | 0.145 | 0.356 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.03501 | 0.12406 | 0.30497 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.03627 | 0.30376 | 0.12417 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0707 | 0.0716 | 0.3213 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0784 | 0.1696 | 0.2849 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.1418 | 0.2519 | 0.2518 | | non-colinear AlSi |
| (OH ₂)7 | 96g | 1 | 0.2364 | 0.3244 | 0.3245 | 0.34 | non-colinear Na ₂ |
| Na8 | 48f | 2.. | 0.4117 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.418 | tetrahedron (OH ₂) ₂ O ₂ |
| Na9 | 32e | .3. | 0.0624 | 0.0624 | 0.0624 | 0.49 | non-coplanar triangle O ₃ |
| Na10 | 32e | .3. | 0.1819 | 0.1819 | 0.1819 | 0.401 | |
| Na11 | 32e | .3. | 0.2317 | 0.2317 | 0.2317 | 0.602 | |
| Na12 | 32e | .3. | 0.2591 | 0.2591 | 0.2591 | 0.345 | |
| Na13 | 16c | .-3. | 0 | 0 | 0 | 0.526 | 8-vertex polyhedron Na ₂ O ₆ |

M3 = 0.92Al + 0.08Si

Transformation from published data: -y,-x,-z

Experimental: powder, diffractometer, X-rays, R_p = 0.030, T = 673 K

Remarks: We placed Si in former site T1 and assigned an approximate value to the Al/Si ratio of former site T2 based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kirschhock C.E.A., Hunger B., Martens J., Jacobs P.A. (2000), J. Phys. Chem. B 104, 439-448.

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|---|--------------|--|
| $\text{Cs}_{1.1}\text{Na}_{20.9}\text{Al}_{22}\text{Si}_{26}\text{O}_{96}[\text{H}_2\text{O}]_{8.75}$ | <i>cF864</i> | (203) <i>Fd-3 - g⁷fe⁴c</i> |
|---|--------------|--|

Cs_{4.5}Na_{83.5}Al₈₈Si₁₀₄O₃₈₄·35H₂O [1], zeolite FAU-Cs,Na partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, above the centers of double 6-rings in β cages, 6- (split site) and 4-rings in supercages, Cs opposite double 6-rings in β cages, H₂O in supercages.

Kirschhock C.E.A. et al. (2000) [1]

$\text{Al}_{22.08}\text{Cs}_{1.13}\text{H}_{17.42}\text{Na}_{20.94}\text{O}_{104.71}\text{Si}_{25.92}$
 $a = 2.5064 \text{ nm}$, $V = 15.7453 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|---------|---------------|---------------|-------|--|
| O1 | 96g | 1 | 0.0047 | 0.3643 | 0.1418 | | non-colinear AlSi |
| M2 | 96g | 1 | 0.0308 | 0.12412 | 0.30435 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.03655 | 0.30723 | 0.12369 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0685 | 0.0711 | 0.3191 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0755 | 0.1733 | 0.2917 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.142 | 0.2501 | 0.2551 | | non-colinear SiAl |
| (OH ₂)7 | 96g | 1 | 0.2302 | 0.3187 | 0.319 | 0.363 | non-colinear Na ₂ |
| Na8 | 48f | 2.. | 0.4126 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.74 | non-colinear (OH ₂) ₂ |
| Na9 | 32e | .3. | 0.0621 | 0.0621 | 0.0621 | 0.284 | |
| Cs10 | 32e | .3. | 0.0882 | 0.0882 | 0.0882 | 0.141 | |
| Na11 | 32e | .3. | 0.2293 | 0.2293 | 0.2293 | 0.657 | |
| Na12 | 32e | .3. | 0.2469 | 0.2469 | 0.2469 | 0.363 | |
| Na13 | 16c | -.3. | 0 | 0 | 0 | 0.406 | 8-vertex polyhedron Na ₂ O ₆ |

M2 = 0.92Al + 0.08Si

Experimental: powder, diffractometer, X-rays, $R_p = 0.048$, $T = 673 \text{ K}$

Remarks: We placed Si in former site T1 and assigned an approximate value to the Al/Si ratio of former site T2 based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kirschhock C.E.A., Hunger B., Martens J., Jacobs P.A. (2000), J. Phys. Chem. B 104, 439-448.

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| | | |
|--|--------------|--|
| $\text{Rb}_{17.75}\text{Na}_{3.25}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | <i>cF864</i> | (203) <i>Fd-3 - g⁷fe⁴c</i> |
|--|--------------|--|

Rb₇₁Na₂₁Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Rb,Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; (Na,Rb) at the centers of hexagonal prisms, Rb opposite double and single 6-rings in β cages, opposite 6- and 4- and near 12-rings in supercages, Na above the centers of 6-rings in supercages.

Lee S.H. et al. (1998) [1]

$\text{Al}_{23.04}\text{Na}_{5.26}\text{O}_{96}\text{Rb}_{17.75}\text{Si}_{24.96}$
 $a = 2.5007 \text{ nm}$, $V = 15.6381 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|----------------------------|
| O1 | 96g | 1 | 0.0009 | 0.1385 | 0.358 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0343 | 0.1261 | 0.304 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.036 | 0.3047 | 0.1271 | | tetrahedron O ₄ |
| Rb4 | 96g | 1 | 0.051 | 0.0556 | 0.432 | 0.052 | |
| O5 | 96g | 1 | 0.0667 | 0.1796 | 0.2851 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0753 | 0.0778 | 0.3183 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1424 | 0.2563 | 0.2556 | | non-colinear SiAl |
| Rb8 | 48f | 2.. | 0.4127 | 1/8 | 1/8 | 0.667 | |
| Rb9 | 32e | .3. | 0.0801 | 0.0801 | 0.0801 | 0.281 | |
| Rb10 | 32e | .3. | 0.1704 | 0.1704 | 0.1704 | 0.078 | |
| Na11 | 32e | .3. | 0.2268 | 0.2268 | 0.2268 | 0.438 | |
| Rb12 | 32e | .3. | 0.2539 | 0.2539 | 0.2539 | 0.563 | |
| M13 | 16c | .-3. | 0 | 0 | 0 | 0.719 | octahedron O ₆ |

M3 = 0.96Al + 0.04Si; M13 = 0.609Na + 0.391Rb

Experimental: single crystal, diffractometer, X-rays, wR = 0.040, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). In table 2 of [1] the Wyckoff position of former Rb(5) is misprinted as 48g instead of 48f and the x-coordinate of former O(2) as 0.0063 instead of -0.0063 (checked on interatomic distances).

References: [1] Lee S.H., Kim Y., Kim D.S., Seff K. (1998), Bull. Korean Chem. Soc. 19, 98-103.

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| | | |
|--|-------|---|
| Ca _{4.5} Tl ₁₄ Al ₂₃ Si ₂₅ O ₉₆ | cF880 | (203) <i>Fd-3</i> – g ⁸ c ³ c |
|--|-------|---|

Tl₅₆Ca₁₈Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Ca,Tl

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca at the centers of hexagonal prisms and above the centers of single 6-rings in supercages, Tl opposite single 6-rings in β cages and distributed over several sites in supercages.

Choi E.Y., Kim Y. (1999) [1]

Al_{23.04}Ca_{4.50}O₉₆Si_{24.96}Tl_{14.01}

a = 2.4883 nm, V = 15.4067 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|----------------------------|
| O1 | 96g | 1 | 0.0002 | 0.3605 | 0.1424 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0342 | 0.127 | 0.3038 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.036 | 0.3043 | 0.1276 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0622 | 0.1845 | 0.2859 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0795 | 0.0824 | 0.3164 | | non-colinear SiAl |
| Tl6 | 96g | 1 | 0.083 | 0.0865 | 0.4182 | 0.042 | |
| Tl7 | 96g | 1 | 0.1109 | 0.1353 | 0.4114 | 0.229 | |
| O8 | 96g | 1 | 0.1437 | 0.2547 | 0.254 | | non-colinear SiAl |
| Tl9 | 32e | .3. | 0.1781 | 0.1781 | 0.1781 | 0.125 | single atom Ca |
| Ca10 | 32e | .3. | 0.2336 | 0.2336 | 0.2336 | 0.063 | |
| Tl11 | 32e | .3. | 0.2521 | 0.2521 | 0.2521 | 0.813 | |
| Ca12 | 16c | .-3. | 0 | 0 | 0 | | octahedron O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, $wR = 0.036$, $T = 294$ K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). In table 1 of [1] the cell parameter is misprinted as 2.5200 nm instead of 2.4883 nm (given elsewhere).

References: [1] Choi E.Y., Kim Y. (1999), J. Korean Phys. Soc. 43, 384-392.

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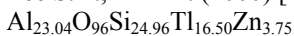
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(203) $Fd-3 - g^8 e^4$

Tl₆₆Zn₁₃Al₉₂Si₁₀₀O₃₈₄·2ZnO [1], zeolite FAU-Tl,Zn (ZnO)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Zn above the centers of double 6-rings in β cages and near the centers of single 6-rings, Tl opposite double 6-rings in β cages and on several sites in supercages.

Lee S.H., Kim Y. (2000) [1]



$$a = 2.4984 \text{ nm}, V = 15.5950 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|---------------------------------------|
| O1 | 96g | 1 | 0.0004 | 0.3523 | 0.1458 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0357 | 0.3024 | 0.1253 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0369 | 0.1261 | 0.3033 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0706 | 0.2766 | 0.177 | | non-coplanar triangle SiAlZn |
| O5 | 96g | 1 | 0.0756 | 0.3215 | 0.0773 | | non-colinear SiAl |
| Tl6 | 96g | 1 | 0.0824 | 0.0873 | 0.4165 | 0.031 | |
| Tl7 | 96g | 1 | 0.1115 | 0.1377 | 0.41 | 0.146 | |
| O8 | 96g | 1 | 0.1459 | 0.2514 | 0.2513 | | non-colinear SiAl |
| Zn9 | 32e | .3. | 0.0409 | 0.0409 | 0.0409 | 0.406 | |
| Tl10 | 32e | .3. | 0.0736 | 0.0736 | 0.0736 | 0.594 | |
| Zn11 | 32e | .3. | 0.199 | 0.199 | 0.199 | 0.063 | 4-vertex polyhedron O ₃ Tl |
| Tl12 | 32e | .3. | 0.2532 | 0.2532 | 0.2532 | 0.938 | single atom Zn |

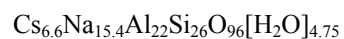
$$\text{M3} = 0.96\text{Al} + 0.04\text{Si}$$

Experimental: single crystal, diffractometer, X-rays, $wR = 0.034$, $T = 294$ K

Remarks: Non framework O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). In table 2b of [1] the Wyckoff position of former Tl(3) is misprinted as 48f instead of 96g.

References: [1] Lee S.H., Kim Y. (2000), Bull. Korean Chem. Soc. 21, 180-186.

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cF912

(203) $Fd-3 - g^7 f^2 e^4 c$

Cs_{26.5}Na_{61.5}Al₈₈Si₁₀₄O₃₈₄·19H₂O [1], zeolite FAU-Cs,Na partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cs opposite double 6-rings in β cages and 4-rings in supercages, Na in hexagonal prisms, above the centers of single 6-rings in β cages and supercages and 4-rings in supercages, H₂O in supercages.

Kirschhock C.E.A. et al. (2000) [1]

 $\text{Al}_{22.08}\text{Cs}_{6.87}\text{H}_{9.36}\text{Na}_{15.22}\text{O}_{100.68}\text{Si}_{25.92}$
 $a = 2.5073 \text{ nm}$, $V = 15.7623 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|---------|---------------|---------------|-------|---|
| O1 | 96g | 1 | 0.0006 | 0.3557 | 0.1488 | | non-colinear AlSi |
| M2 | 96g | 1 | 0.03603 | 0.12425 | 0.30136 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.03687 | 0.30649 | 0.12287 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0684 | 0.0721 | 0.3249 | | non-colinear AlSi |
| O5 | 96g | 1 | 0.0785 | 0.2823 | 0.1701 | | non-colinear AlSi |
| (OH ₂)6 | 96g | 1 | 0.088 | 0.16 | 0.491 | 0.195 | single atom Cs |
| O7 | 96g | 1 | 0.1446 | 0.255 | 0.2582 | | non-colinear SiAl |
| Na8 | 48f | 2.. | 0.3974 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.335 | |
| Cs9 | 48f | 2.. | 0.4188 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.46 | |
| Cs10 | 32e | .3. | 0.0867 | 0.0867 | 0.0867 | 0.169 | 6-vertex polyhedron Na ₃ Cs ₃ |
| Na11 | 32e | .3. | 0.1859 | 0.1859 | 0.1859 | 0.287 | |
| Na12 | 32e | .3. | 0.2294 | 0.2294 | 0.2294 | 0.59 | |
| Na13 | 32e | .3. | 0.267 | 0.267 | 0.267 | 0.208 | |
| Na14 | 16c | -.3. | 0 | 0 | 0 | 0.63 | octahedron O ₆ |

M2 = 0.92Al + 0.08Si

Experimental: powder, diffractometer, X-rays, $R_p = 0.051$, $T = 673 \text{ K}$

Remarks: We placed Si in former site T1 and assigned an approximate value to the Al/Si ratio of former site T2 based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Kirschhock C.E.A., Hunger B., Martens J., Jacobs P.A. (2000), J. Phys. Chem. B 104, 439-448.

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cF912

| | | |
|--|-------|--------------------------|
| $\text{Zn}_5\text{Cd}_{11.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF912 | (203) $Fd-3 - g^8 e^4 c$ |
|--|-------|--------------------------|

Cd₄₆Al₉₂Si₁₀₀O₃₈₄·20Zn [1], zeolite FAU-Cd (Zn)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; (Zn₄)⁰ tetrahedra in β cages, additional Zn above 6-rings in supercages, Cd at the centers of hexagonal prisms, near the centers of single 6-rings (Zn⁰-Cd²⁺-Zn⁰ units) and in supercages.

Zhen S., Seff K. (1999) [1]

 $\text{Al}_{23.04}\text{Cd}_{11.50}\text{O}_{96}\text{Si}_{24.96}\text{Zn}_5$
 $a = 2.4895 \text{ nm}$, $V = 15.4290 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|----------------------------|
| O1 | 96g | 1 | 0.0004 | 0.1407 | 0.3576 | | non-colinear SiAl |
| Cd2 | 96g | 1 | 0.0061 | 0.4183 | 0.0763 | 0.083 | |
| Cd3 | 96g | 1 | 0.0311 | 0.0818 | 0.4303 | 0.063 | |
| Si4 | 96g | 1 | 0.0355 | 0.1267 | 0.3032 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0363 | 0.3035 | 0.1271 | | tetrahedron O ₄ |
| O6 | 96g | 1 | 0.0643 | 0.1838 | 0.2818 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0795 | 0.0804 | 0.3176 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.1444 | 0.2536 | 0.2531 | | non-colinear SiAl |

| | | | | | | | |
|------|-----|------|--------|--------|--------|-------|---|
| Cd9 | 32e | .3. | 0.0709 | 0.0709 | 0.0709 | 0.25 | octahedron Zn ₃ O ₃ |
| Zn10 | 32e | .3. | 0.1659 | 0.1659 | 0.1659 | 0.375 | tetrahedron Cd ₄ |
| Cd11 | 32e | .3. | 0.2217 | 0.2217 | 0.2217 | 0.375 | trigonal bipyramid Zn ₂ O ₃ |
| Zn12 | 32e | .3. | 0.2674 | 0.2674 | 0.2674 | 0.25 | single atom Cd |
| Cd13 | 16c | -.3. | 0 | 0 | 0 | 0.75 | octahedron O ₆ |

M5 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.081, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Zhen S., Seff K. (1999), J. Phys. Chem. B 103, 6493-6497.

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|--|-------|--|
| Na _{4.5} Tl _{18.5} Al ₂₃ Si ₂₅ O ₉₆ | cF928 | (203) <i>Fd-3</i> - g ⁸ fe ³ c |
|--|-------|--|

Na₁₈Tl₇₄Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Tl,Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms and near the centers of single 6-rings, Tl opposite double 6-rings in β cages, opposite 6- and 4-rings in supercages.

Zhu L., Seff K. (2000) [1]

Al_{23.04}Na_{4.44}O₉₆Si_{24.96}Tl₁₈

$a = 2.5054$ nm, $V = 15.7265$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|-----------------------------|-----------------------------|------|--------------------------------------|
| O1 | 96g | 1 | 0.0 | 0.142 | 0.353 | | non-collinear SiAl |
| O2 | 96g | 1 | 0.0009 | 0.1065 | 0.2542 | | non-collinear SiAl |
| Si3 | 96g | 1 | 0.036 | 0.124 | 0.3044 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0366 | 0.3038 | 0.1253 | | tetrahedron O ₄ |
| Tl5 | 96g | 1 | 0.0686 | 0.0687 | 0.4196 | 0.19 | |
| O6 | 96g | 1 | 0.0712 | 0.1735 | 0.277 | | non-collinear SiAl |
| O7 | 96g | 1 | 0.0757 | 0.0783 | 0.3207 | | non-collinear SiAl |
| Tl8 | 96g | 1 | 0.107 | 0.4106 | 0.1426 | 0.08 | |
| Tl9 | 48f | 2.. | 0.4077 | ¹ / ₈ | ¹ / ₈ | 0.12 | |
| Tl10 | 32e | .3. | 0.0729 | 0.0729 | 0.0729 | 0.64 | non-coplanar triangle O ₃ |
| Na11 | 32e | .3. | 0.2351 | 0.2351 | 0.2351 | 0.37 | |
| Tl12 | 32e | .3. | 0.2527 | 0.2527 | 0.2527 | 0.62 | |
| Na13 | 16c | -.3. | 0 | 0 | 0 | 0.37 | octahedron O ₆ |

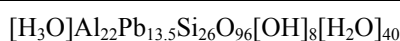
M4 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.074, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Zhu L., Seff K. (2000), Microporous Mesoporous Mater. 39, 187-193.

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(203) $Fd-3 - g^9 e^3$

(H₃O)₁₂Pb₅₄Al₈₈Si₁₀₄O₃₈₄(OH)₃₂·xH₂O [1], zeolite FAU-Pb²⁺ hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Pb₄(OH)₄ cubane-like clusters in β cages, additional Pb opposite 6- and near 12-rings in supercages, H₂O in supercages.

Nardin G. et al. (1995) [1]

Al_{23.04}H_{34.50}O_{117.25}Pb_{13.50}Si_{24.96}
 $a = 2.5059 \text{ nm}$, $V = 15.7359 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|-------|---|
| O1 | 96g | 1 | 0.003 | 0.139 | 0.358 | | non-colinear AlSi |
| (OH ₂)2 | 96g | 1 | 0.025 | 0.505 | 0.13 | 0.427 | single atom (OH ₂) |
| M3 | 96g | 1 | 0.0345 | 0.123 | 0.3063 | | tetrahedron O ₄ |
| Si4 | 96g | 1 | 0.0356 | 0.3064 | 0.123 | | tetrahedron O ₄ |
| Pb5 | 96g | 1 | 0.0501 | 0.0526 | 0.4199 | 0.146 | square antiprism O ₃ (OH ₂) ₃ Pb ₂ |
| (OH ₂)6 | 96g | 1 | 0.06 | 0.45 | 0.17 | 0.125 | single atom (OH ₂) |
| O7 | 96g | 1 | 0.07 | 0.07 | 0.321 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.079 | 0.17 | 0.288 | | non-colinear AlSi |
| O9 | 96g | 1 | 0.139 | 0.252 | 0.253 | | non-colinear SiAl |
| Pb10 | 32e | .3. | 0.0706 | 0.0706 | 0.0706 | | 9-vertex polyhedron (OH) ₃ O ₆ |
| (OH)11 | 32e | .3. | 0.168 | 0.168 | 0.168 | | non-coplanar triangle Pb ₃ |
| Pb12 | 32e | .3. | 0.2543 | 0.2543 | 0.2543 | 0.25 | icosahedron (OH ₂) ₆ O ₆ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.077

Remarks: H₃O⁺ and part of H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. Short interatomic distances for partly occupied site(s).

References: [1] Nardin G., Randaccio L., Zangrando E. (1995), Zeolites 15, 684-688.

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(203) $Fd-3 - g^7 e^9 c$

Cd_{57.2}Al₉₂Si₁₀₀O₃₈₄(OH)_{44.8}·xH₂O [1], zeolite FAU-Cd residual water

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cd and H₂O distributed over several sites along <111> in β cages and supercages, additional Cd near 12-rings in supercages (high degree of disorder).

Smolin Y.I. et al. (1998) [1]

Al_{23.04}Cd_{14.33}H_{12.99}O_{102.50}Si_{24.96}
 $a = 2.499 \text{ nm}$, $V = 15.6063 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|--------------------|
| O1 | 96g | 1 | 0.0001 | 0.1458 | 0.3493 | | non-colinear SiAl |

| | | | | | | | |
|----------------------|-----|------|---------|---------|---------|-------|--|
| Si2 | 96g | 1 | 0.0364 | 0.1256 | 0.3013 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0376 | 0.3035 | 0.1271 | | tetrahedron O ₄ |
| Cd4 | 96g | 1 | 0.049 | 0.11 | 0.427 | 0.023 | single atom O |
| O5 | 96g | 1 | 0.0719 | 0.1747 | 0.2737 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0749 | 0.0782 | 0.3187 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.1472 | 0.2516 | 0.2503 | | non-colinear SiAl |
| Cd8 | 32e | .3. | 0.0578 | 0.0578 | 0.0578 | 0.175 | |
| Cd9 | 32e | .3. | 0.06857 | 0.06857 | 0.06857 | 0.553 | |
| Cd10 | 32e | .3. | 0.0804 | 0.0804 | 0.0804 | 0.138 | |
| (OH ₂)11 | 32e | .3. | 0.1631 | 0.1631 | 0.1631 | 0.656 | single atom Cd |
| Cd12 | 32e | .3. | 0.194 | 0.194 | 0.194 | 0.031 | |
| Cd13 | 32e | .3. | 0.2096 | 0.2096 | 0.2096 | 0.428 | |
| Cd14 | 32e | .3. | 0.2225 | 0.2225 | 0.2225 | 0.169 | |
| Cd15 | 32e | .3. | 0.242 | 0.242 | 0.242 | 0.163 | |
| (OH ₂)16 | 32e | .3. | 0.259 | 0.259 | 0.259 | 0.156 | |
| Cd17 | 16c | -.3. | 0 | 0 | 0 | 0.131 | 8-vertex polyhedron Cd ₂ O ₆ |

M3 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.044, T = 413 K

Remarks: CdX zeolite (Si/Al = 1.09) treated with Na₂S, then Cd(NO₃)₂ aqueous solutions and dehydrated at 413 K. Composition not specified, we took the Cd content from the refinement and adjusted the charge balance assuming that part of the residual water molecules are OH (the authors state that partial substitution of OH for H₂O cannot be excluded). We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (1998), Crystallogr. Rep. 43, 387-394 (Kristallografiya 43, 425-432).

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|--|-------|---|
| Na ₂₂ Al ₂₂ Si ₂₆ O ₉₆ | cF976 | (203) <i>Fd-3</i> – g ⁹ e ³ c |
|--|-------|---|

Na₈₈Al₈₈Si₁₀₄O₃₈₄ [1], zeolite FAU-Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, above the centers of double 6-rings in β cages (split site) and distributed over several sites in supercages.

Olson D.H. (1995) [1]

Al_{22.08}Na_{23.20}O₉₆Si_{25.92}

a = 2.5099 nm, *V* = 15.8114 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|------|----------------------------|
| O1 | 96g | 1 | 0.0003 | 0.3599 | 0.1444 | | non-colinear SiAl |
| Na2 | 96g | 1 | 0.03 | 0.068 | 0.414 | 0.11 | |
| Si3 | 96g | 1 | 0.03508 | 0.12435 | 0.30381 | | tetrahedron O ₄ |
| Na4 | 96g | 1 | 0.035 | 0.408 | 0.067 | 0.09 | |
| M5 | 96g | 1 | 0.03639 | 0.30524 | 0.12582 | | tetrahedron O ₄ |
| O6 | 96g | 1 | 0.07 | 0.0726 | 0.3193 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0711 | 0.1742 | 0.2846 | | non-colinear SiAl |
| Na8 | 96g | 1 | 0.076 | 0.077 | 0.408 | 0.11 | |

| | | | | | | | |
|------|-----|------|--------|--------|--------|------|--------------------------------------|
| O9 | 96g | 1 | 0.1416 | 0.2528 | 0.2511 | | non-colinear SiAl |
| Na10 | 32e | .3. | 0.0454 | 0.0454 | 0.0454 | 0.66 | |
| Na11 | 32e | .3. | 0.056 | 0.056 | 0.056 | 0.25 | |
| Na12 | 32e | .3. | 0.2292 | 0.2292 | 0.2292 | 0.97 | non-coplanar triangle O ₃ |
| Na13 | 16c | -.3. | 0 | 0 | 0 | 0.18 | |

M5 = 0.92Al + 0.08Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.046

Remarks: Short interatomic distances for partly occupied site(s). The authors state that the results indicate substantial ordering of Al and Si. We placed Si on former site T1 and assigned an approximate value to the Al/Si ratio of former site T2 based on the nominal composition.

References: [1] Olson D.H. (1995), Zeolites 15, 439-443.

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|---|--------|--|
| Ca _{11.5} Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₅₀ | cF1008 | (203) <i>Fd-3</i> – g ⁹ fe ³ |
|---|--------|--|

Ca₄₆Al₉₂Si₁₀₀O₃₈₄·200H₂O [1], zeolite FAU-Ca hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca opposite double 6-rings in β cages, opposite 6- and near 12-rings in supercages, H₂O opposite single 6-rings in β cages, opposite 4- and near 12-rings in supercages.

Smolin Y.I. et al. (1989) [1]

Al_{23.04}Ca_{9.84}H_{30.32}O_{111.16}Si_{24.96}

$a = 2.508$ nm, $V = 15.7755$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|--|
| O1 | 96g | 1 | 0.0005 | 0.1459 | 0.3532 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.001 | 0.365 | 0.002 | 0.16 | single atom Ca |
| Si3 | 96g | 1 | 0.0365 | 0.1248 | 0.3029 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0367 | 0.3036 | 0.125 | | tetrahedron O ₄ |
| Ca5 | 96g | 1 | 0.042 | 0.046 | 0.416 | 0.1 | |
| (OH ₂)6 | 96g | 1 | 0.064 | 0.065 | 0.422 | 0.1 | |
| O7 | 96g | 1 | 0.0695 | 0.0709 | 0.3223 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0762 | 0.1719 | 0.2832 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.1454 | 0.2528 | 0.2517 | | non-colinear SiAl |
| (OH ₂)10 | 48f | 2.. | 0.415 | 1/8 | 1/8 | 0.13 | non-colinear (OH ₂) ₂ |
| Ca11 | 32e | .3. | 0.0687 | 0.0687 | 0.0687 | 0.61 | octahedron (OH ₂) ₃ O ₃ |
| (OH ₂)12 | 32e | .3. | 0.167 | 0.167 | 0.167 | 0.92 | non-coplanar triangle Ca ₃ |
| Ca13 | 32e | .3. | 0.251 | 0.251 | 0.251 | 0.32 | 9-vertex polyhedron O ₆ (OH ₂) ₃ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.064, T = 298 K

Remarks: Part of H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 (298 K, rehydrated) of [1] the y-coordinate of former O(3) is misprinted as -0.0781 instead of 0.0781 (checked on interatomic distances).

References: [1] Smolin Y.I., Shepelev Y.F., Anderson A.A. (1989), Acta Crystallogr. B 45, 124-128.

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|---|--------|---|
| $\text{Na}_{15}[\text{H}_3\text{O}]_8\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_6$ | cF1008 | (203) <i>Fd-3</i> – g^9fe^3 |
|---|--------|---|

$\text{Na}_{60}(\text{H}_3\text{O})_{32}\text{Al}_{92}\text{Si}_{100}\text{O}_{384}\cdot 24\text{H}_2\text{O}$ [1], zeolite FAU-Na, H_3O partly hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; $(\text{H}_2\text{O})(\text{Na}_2[\text{H}_3\text{O}]^{+}_2)$ tetrahedral clusters in β cages, $\text{Na-H}_2\text{O-(H}_3\text{O)}^{+}$ clusters in supercages, additional Na above the centers of single 6-rings in supercages.

Zhu L. et al. (1999) [1]

$\text{Al}_{23.04}\text{H}_{36.05}\text{Na}_{15.61}\text{O}_{110.02}\text{Si}_{24.96}$
 $a = 2.5128 \text{ nm}$, $V = 15.8662 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|---------------|---------------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0001 | 0.1425 | 0.3551 | | non-colinear SiAl |
| (OH ₃)2 | 96g | 1 | 0.0137 | 0.058 | 0.4166 | 0.167 | |
| Si3 | 96g | 1 | 0.0355 | 0.1242 | 0.3037 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0363 | 0.3044 | 0.125 | | tetrahedron O ₄ |
| Na5 | 96g | 1 | 0.065 | 0.0743 | 0.4179 | 0.167 | |
| O6 | 96g | 1 | 0.0691 | 0.0711 | 0.3214 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0749 | 0.1728 | 0.2827 | | non-colinear SiAl |
| (OH ₂)8 | 96g | 1 | 0.0917 | 0.4485 | 0.1427 | 0.167 | single atom (OH ₂) |
| O9 | 96g | 1 | 0.143 | 0.2523 | 0.251 | | non-colinear SiAl |
| (OH ₂)10 | 48f | 2.. | 0.098 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.167 | |
| Na11 | 32e | .3. | 0.0547 | 0.0547 | 0.0547 | 0.5 | |
| (OH ₃)12 | 32e | .3. | 0.0676 | 0.0676 | 0.0676 | 0.5 | |
| Na13 | 32e | .3. | 0.233 | 0.233 | 0.233 | 0.95 | non-coplanar triangle O ₃ |

$\text{M4} = 0.96\text{Al} + 0.04\text{Si}$

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.056, T = 293 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Zhu L., Seff K., Olson D.H., Cohen B.J., Von Dreele R.B. (1999), J. Phys. Chem. B 103, 10365-10372.

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cF1024

| | | |
|---|--------|---|
| $\text{Ag}_{23}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}$ | cF1024 | (203) <i>Fd-3</i> – $\text{g}^9\text{fe}^3\text{c}$ |
|---|--------|---|

$\text{Ag}_{92}\text{Al}_{92}\text{Si}_{100}\text{O}_{384}$ [1], zeolite FAU-Ag

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms, opposite double 6-rings in β cages and distributed over several sites in supercages (Ag₃ clusters, high degree of disorder).

Lee S.H. et al. (2000) [1]

$\text{Ag}_{23.02}\text{Al}_{23.04}\text{O}_{96}\text{Si}_{24.96}$
 $a = 2.52 \text{ nm}$, $V = 16.0030 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|-----------------------------|-----------------------------|-------|---|
| O1 | 96g | 1 | 0.0004 | 0.1417 | 0.3549 | | non-colinear AlSi |
| Ag2 | 96g | 1 | 0.0115 | 0.0679 | 0.4161 | 0.031 | |
| M3 | 96g | 1 | 0.0351 | 0.1252 | 0.3043 | | tetrahedron O ₄ |
| Si4 | 96g | 1 | 0.036 | 0.3051 | 0.1258 | | tetrahedron O ₄ |
| Ag5 | 96g | 1 | 0.0492 | 0.4032 | 0.0517 | 0.042 | |
| O6 | 96g | 1 | 0.0712 | 0.1757 | 0.2848 | | non-colinear AlSi |
| O7 | 96g | 1 | 0.0732 | 0.0766 | 0.3201 | | non-colinear AlSi |
| Ag8 | 96g | 1 | 0.1004 | 0.3943 | 0.1492 | 0.167 | single atom Ag |
| O9 | 96g | 1 | 0.1421 | 0.2528 | 0.2514 | | non-colinear AlSi |
| Ag10 | 48f | 2.. | 0.0492 | ¹ / ₈ | ¹ / ₈ | 0.042 | non-colinear Ag ₂ |
| Ag11 | 32e | .3. | 0.037 | 0.037 | 0.037 | 0.813 | trigonal bipyramid Ag ₂ O ₃ |
| Ag12 | 32e | .3. | 0.0744 | 0.0744 | 0.0744 | 0.188 | tetrahedron Ag ₄ |
| Ag13 | 32e | .3. | 0.2219 | 0.2219 | 0.2219 | | non-coplanar triangle O ₃ |
| Ag14 | 16c | .-3. | 0 | 0 | 0 | 0.188 | colinear Ag ₂ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, wR = 0.041, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Lee S.H., Kim Y., Seff K. (2000), Microporous Mesoporous Mater. 41, 49-59.

203
cF1040

| | | |
|---|--------|---|
| Ag ₂₃ Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₃₀ | cF1040 | (203) <i>Fd-3</i> – g ⁹ e ⁵ c |
|---|--------|---|

Ag₉₂Al₉₂Si₁₀₀O₃₈₄·xH₂O [1], zeolite FAU-Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms, opposite double 6-rings in β cages, single 6-rings in β and supercages and near 4-rings in supercages, H₂O in β cages and supercages.

Butikova I.K. et al. (1989) [1]

Ag_{18.48}Al_{23.04}H_{57.12}O_{124.56}Si_{24.96}
a = 2.502 nm, V = 15.6625 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|--|
| O1 | 96g | 1 | 0.0003 | 0.3552 | 0.1484 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0012 | 0.1039 | 0.253 | | non-colinear SiAl |
| Ag3 | 96g | 1 | 0.01 | 0.063 | 0.409 | 0.04 | single atom (OH ₂) |
| Si4 | 96g | 1 | 0.0358 | 0.1246 | 0.301 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.037 | 0.3025 | 0.1262 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.062 | 0.076 | 0.426 | 0.57 | single atom Ag |
| O7 | 96g | 1 | 0.0707 | 0.1745 | 0.2755 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0755 | 0.0784 | 0.3237 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.283 | 0.283 | 0.355 | 0.37 | non-colinear (OH ₂) ₂ |
| Ag10 | 32e | .3. | 0.0609 | 0.0609 | 0.0609 | 0.13 | |
| Ag11 | 32e | .3. | 0.0802 | 0.0802 | 0.0802 | 0.76 | |
| (OH ₂)12 | 32e | .3. | 0.177 | 0.177 | 0.177 | 0.75 | |
| Ag13 | 32e | .3. | 0.1824 | 0.1824 | 0.1824 | 0.24 | |
| Ag14 | 32e | .3. | 0.2467 | 0.2467 | 0.2467 | 0.69 | non-coplanar triangle O ₃ |

Ag15 16c .-3. 0 0 0 0.74 8-vertex polyhedron Ag₂O₆

M5 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, precession photographs, X-rays, R = 0.050, T = 293 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Butikova I.K., Shepelev Y.F., Smolin Y.I. (1989), Sov. Phys. Crystallogr. (Engl. Transl.) 34, 684-687.

203
cF1056

Cs₁₁Na₁₂Al₂₃Si₂₅O₉₆ cF1056 (203) *Fd*-3 - g⁹fe⁴c

Cs₄₄Na₄₈Al₉₂Si₁₀₀O₃₈₂ [1], zeolite FAU-Cs,Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na in hexagonal prisms, above the centers of single 6-rings in supercages and double 6-rings in β cages, Cs opposite single and double 6-rings in β cages and on several sites in supercages.

Shepelev Y.F. et al. (1991) [1]

Al_{23.04}Cs_{11.20}Na_{13.28}O₉₆Si_{24.96}

a = 2.498 nm, *V* = 15.5875 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|----------|----------|------|--|
| O1 | 96g | 1 | 0.001 | 0.3611 | 0.1437 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0346 | 0.1256 | 0.3037 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0362 | 0.3039 | 0.1275 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0646 | 0.1814 | 0.2852 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0762 | 0.0789 | 0.3177 | | non-colinear SiAl |
| Cs6 | 96g | 1 | 0.077 | 0.078 | 0.442 | 0.03 | |
| Cs7 | 96g | 1 | 0.1067 | 0.1422 | 0.4255 | 0.09 | |
| Cs8 | 96g | 1 | 0.1101 | 0.1113 | 0.427 | 0.13 | |
| O9 | 96g | 1 | 0.1452 | 0.2551 | 0.2531 | | non-colinear SiAl |
| Cs10 | 48f | 2.. | 0.4195 | 1/8 | 1/8 | 0.28 | |
| Na11 | 32e | .3. | 0.053 | 0.053 | 0.053 | 0.16 | |
| Cs12 | 32e | .3. | 0.0905 | 0.0905 | 0.0905 | 0.18 | |
| Cs13 | 32e | .3. | 0.157 | 0.157 | 0.157 | 0.05 | |
| Na14 | 32e | .3. | 0.2283 | 0.2283 | 0.2283 | | non-coplanar triangle O ₃ |
| Na15 | 16c | .-3. | 0 | 0 | 0 | | 8-vertex polyhedron Na ₂ O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.058, T = 673 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. The occupancy of site Na15 was set to unity for standardized data, refined value 1.08(5). Short interatomic distances for partly occupied site(s).

References: [1] Shepelev Y.F., Butikova I.K., Smolin Y.I. (1991), Zeolites 11, 287-292.

203
cF1064 $\text{Al}_{23}\text{In}_{22}\text{Si}_{25}\text{O}_{96}$

cF1064

(203) $Fd\bar{3} - g^{10}e^3a$ **In₈₈Al₉₂Si₁₀₀O₃₈₄** [1], zeolite FAU-In

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; $\text{In}^0(\text{In}^{2+})_4$ tetrahedra in β cages, In^+ opposite single 6-rings and on several other sites in supercages (disorder).

Heo N.H. et al. (2000) [1]

 $\text{Al}_{23.04}\text{In}_{22.01}\text{O}_{96}\text{Si}_{24.96}$ $a = 2.4913 \text{ nm}$, $V = 15.4624 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|---------------|---------------|---------------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0002 | 0.3552 | 0.1491 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0358 | 0.1247 | 0.3013 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.037 | 0.3026 | 0.1264 | | tetrahedron O ₄ |
| In4 | 96g | 1 | 0.038 | 0.4171 | 0.0686 | 0.063 | |
| In5 | 96g | 1 | 0.0435 | 0.0715 | 0.4186 | 0.115 | |
| In6 | 96g | 1 | 0.0634 | 0.4213 | 0.0821 | 0.052 | |
| In7 | 96g | 1 | 0.0701 | 0.0984 | 0.4232 | 0.031 | |
| O8 | 96g | 1 | 0.071 | 0.1744 | 0.2762 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.074 | 0.0762 | 0.323 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.1485 | 0.2519 | 0.2505 | | non-colinear SiAl |
| In11 | 32e | .3. | 0.063 | 0.063 | 0.063 | 0.25 | |
| In12 | 32e | .3. | 0.0751 | 0.0751 | 0.0751 | 0.75 | |
| In13 | 32e | .3. | 0.2518 | 0.2518 | 0.2518 | 0.906 | non-coplanar triangle O ₃ |
| In14 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.25 | tetrahedron In ₄ |

 $\text{M3} = 0.96\text{Al} + 0.04\text{Si}$ Transformation from published data: $-y, -x, -z$ Experimental: single crystal, diffractometer, X-rays, $R = 0.058$, $T = 294 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Heo N.H., Jung S.W., Park S.W., Park M., Lim W.T., Seff K. (2000), J. Phys. Chem. B 104, 8372-8381.

203
cF1072 $\text{Ca}_{11.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_{50}$

cF1072

(203) $Fd\bar{3} - g^{10}e^3c$ **Ca₄₆Al₉₂Si₁₀₀O₃₈₄·200H₂O** [1], faujasite-(Ca), zeolite FAU-Ca hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca opposite double 6-rings in β cages, opposite 6- and near 12-rings in supercages, H_2O at the centers of hexagonal prisms, opposite single 6-rings in β cages and on several sites in supercages.

Smolin Y.I. et al. (1989) [1]

 $\text{Al}_{23.04}\text{Ca}_{11.76}\text{H}_{54.32}\text{O}_{123.16}\text{Si}_{24.96}$ $a = 2.506 \text{ nm}$, $V = 15.7378 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0004 | 0.1438 | 0.3544 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.003 | 0.379 | 0.004 | 0.31 | |
| (OH ₂)3 | 96g | 1 | 0.02 | 0.027 | 0.405 | 0.14 | |
| Si4 | 96g | 1 | 0.0364 | 0.1246 | 0.3029 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0366 | 0.3034 | 0.1253 | | tetrahedron O ₄ |
| Ca6 | 96g | 1 | 0.053 | 0.063 | 0.423 | 0.17 | |
| O7 | 96g | 1 | 0.0726 | 0.0741 | 0.324 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0752 | 0.173 | 0.28 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.11 | 0.424 | 0.137 | 0.26 | |
| O10 | 96g | 1 | 0.1441 | 0.2522 | 0.2512 | | non-colinear SiAl |
| Ca11 | 32e | .3. | 0.0692 | 0.0692 | 0.0692 | 0.63 | octahedron O ₃ (OH ₂) ₃ |
| (OH ₂)12 | 32e | .3. | 0.1681 | 0.1681 | 0.1681 | | non-coplanar triangle Ca ₃ |
| Ca13 | 32e | .3. | 0.254 | 0.254 | 0.254 | 0.33 | non-coplanar triangle O ₃ |
| (OH ₂)14 | 16c | -.3. | 0 | 0 | 0 | 0.53 | 8-vertex polyhedron O ₆ Ca ₂ |

M5 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.063, T = 298 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Anderson A.A. (1989), Acta Crystallogr. B 45, 124-128.

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cF1072

| | | |
|--|--------|--|
| Ca _{5.75} Mg _{5.75} Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₂₈ | cF1072 | (203) <i>Fd</i> -3 – g ⁹ e ⁶ c |
|--|--------|--|

Ca₂₃Mg₂₃Al₉₆Si₉₆O₃₈₄·xH₂O [1], zeolite FAU-Ca,Mg hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ca and Mg near the centers of single 6-rings and above double 6-rings in β cages (distinct positions), H₂O in hexagonal prisms, β cages and supercages (disorder).

Anderson A.A. et al. (1990) [1]

Al_{23.04}Ca_{4.64}H_{54.72}Mg_{2.16}O_{123.36}Si_{24.96}

a = 2.506 nm, *V* = 15.7378 nm³, *Z* = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|--|
| O1 | 96g | 1 | 0.0007 | 0.1433 | 0.3534 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.024 | 0.403 | 0.025 | 0.17 | single atom (OH ₂) |
| Si3 | 96g | 1 | 0.0362 | 0.1239 | 0.3028 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0369 | 0.3037 | 0.1253 | | tetrahedron O ₄ |
| (OH ₂)5 | 96g | 1 | 0.054 | 0.059 | 0.422 | 0.15 | single atom (OH ₂) |
| O6 | 96g | 1 | 0.0714 | 0.0736 | 0.3222 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0753 | 0.1713 | 0.28 | | non-colinear SiAl |
| (OH ₂)8 | 96g | 1 | 0.088 | 0.154 | 0.444 | 0.24 | non-colinear (OH ₂) ₂ |
| O9 | 96g | 1 | 0.1425 | 0.2536 | 0.2518 | | non-colinear SiAl |
| Mg10 | 32e | .3. | 0.05 | 0.05 | 0.05 | 0.09 | |
| Ca11 | 32e | .3. | 0.069 | 0.069 | 0.069 | 0.52 | |
| (OH ₂)12 | 32e | .3. | 0.1693 | 0.1693 | 0.1693 | 0.77 | |
| Ca13 | 32e | .3. | 0.196 | 0.196 | 0.196 | 0.06 | |

| | | | | | | | |
|----------------------|-----|------|--------|--------|--------|------|--------------------------|
| Mg14 | 32e | .3. | 0.216 | 0.216 | 0.216 | 0.18 | |
| (OH ₂)15 | 32e | .3. | 0.2622 | 0.2622 | 0.2622 | 0.71 | single atom Mg |
| (OH ₂)16 | 16c | -.3. | 0 | 0 | 0 | 0.52 | colinear Mg ₂ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.062, T = 298 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Anderson A.A., Shepelev Y.F., Smolin Y.I. (1990), Zeolites 10, 32-37.

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cF1072

| | | |
|---|--------|---|
| Na ₂ Co _{11.5} Al ₂₃ Si ₂₅ O ₉₆ [OH] ₂ [H ₂ O] ₁₂ | cF1072 | (203) <i>Fd-3</i> – g ⁹ e ⁶ c |
|---|--------|---|

Na₈Co₄₆Al₉₂Si₁₀₀O₃₈₄(OH)₈·xH₂O [1], zeolite FAU-Co²⁺,Na partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Co near the centers of single 6-rings, opposite double 6-rings in β cages and near 12-rings in supercages, Na at the centers of hexagonal prisms, OH near the centers of β cages, H₂O in supercages.

Bae D., Seff K. (1999) [1]

Al_{23.04}Co_{11.59}H_{21.87}Na₂O_{107.94}Si_{24.96}

$a = 2.4905$ nm, $V = 15.4476$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0003 | 0.1002 | 0.2517 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0004 | 0.1448 | 0.3514 | | non-colinear SiAl |
| Si3 | 96g | 1 | 0.0356 | 0.1254 | 0.3011 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0371 | 0.3023 | 0.1274 | | tetrahedron O ₄ |
| Co5 | 96g | 1 | 0.0469 | 0.1001 | 0.4103 | 0.108 | 4-vertex polyhedron (OH ₂) ₂ O ₂ |
| (OH ₂)6 | 96g | 1 | 0.0504 | 0.0962 | 0.4891 | 0.108 | non-colinear Co(OH ₂) |
| O7 | 96g | 1 | 0.0704 | 0.1761 | 0.276 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0736 | 0.0788 | 0.3208 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.0838 | 0.4395 | 0.163 | 0.108 | non-colinear Co(OH ₂) |
| Co10 | 32e | .3. | 0.0579 | 0.0579 | 0.0579 | 0.25 | |
| Co11 | 32e | .3. | 0.067 | 0.067 | 0.067 | 0.25 | |
| (OH)12 | 32e | .3. | 0.1057 | 0.1057 | 0.1057 | 0.25 | |
| Co13 | 32e | .3. | 0.1917 | 0.1917 | 0.1917 | 0.031 | single atom Co |
| Co14 | 32e | .3. | 0.2302 | 0.2302 | 0.2302 | 0.594 | trigonal bipyramid Co(OH ₂)O ₃ |
| (OH ₂)15 | 32e | .3. | 0.2756 | 0.2756 | 0.2756 | 0.594 | single atom Co |
| Na16 | 16c | -.3. | 0 | 0 | 0 | 0.5 | 8-vertex polyhedron Co ₂ O ₆ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.131, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 4(c) of [1] the Wyckoff position of former Co(II') is misprinted as 96g instead of 32e.

References: [1] Bae D., Seff K. (1999), Microporous Mesoporous Mater. 33, 265-280.

203
cF1080

| Ca ₁₂ [UO ₂] ₄ [CO ₃] ₁₂ Cl ₈ [H ₂ O] ₄₇ cF1080 (203) <i>Fd-3</i> – g⁹f²e³ca | | | | | | | |
|--|-------|------|-----------------------------|-----------------------------|-----------------------------|-------|---|
| Ca₁₂[(UO₂)(CO₃)₃]₄Cl₈·47H₂O [1] | | | | | | | |
| Structural features: U([CO ₃] ₃ O ₂) units (UO ₈ hexagonal bipyramid sharing edges with three equatorial CO ₃ trigonal units) share atoms with rings of six edge-linked Ca(O ₃ [OH ₂] ₅) square antiprisms to form a 3D-framework; Cl and additional H ₂ O in channels. | | | | | | | |
| Li Y., Burns P.C. (2002) [1] | | | | | | | |
| C ₁₂ Ca ₁₂ Cl ₈ H ₉₄ O ₉₁ U ₄ | | | | | | | |
| $a = 2.7489 \text{ nm}$, $V = 20.7719 \text{ nm}^3$, $Z = 8$ | | | | | | | |
| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
| Ca1 | 96g | 1 | 0.0235 | 0.0707 | 0.3764 | 0.667 | square antiprism O ₃ (OH ₂) ₅ |
| Cl2 | 96g | 1 | 0.0336 | 0.2699 | 0.1531 | | trigonal bipyramid (OH ₂) ₅ |
| (OH ₂)3 | 96g | 1 | 0.0419 | 0.4702 | 0.0615 | | single atom Ca |
| (OH ₂)4 | 96g | 1 | 0.044 | 0.1125 | 0.3014 | | single atom Ca |
| C5 | 96g | 1 | 0.0467 | 0.1697 | 0.4394 | | coplanar triangle O ₃ |
| (OH ₂)6 | 96g | 1 | 0.0496 | 0.3699 | 0.1132 | 0.333 | non-colinear Ca ₂ |
| O7 | 96g | 1 | 0.0601 | 0.1434 | 0.4051 | | single atom C |
| O8 | 96g | 1 | 0.2016 | 0.3194 | 0.2911 | | single atom C |
| O9 | 96g | 1 | 0.2165 | 0.2587 | 0.3402 | | single atom C |
| (OH ₂)10 | 48f | 2.. | 0.044 | ¹ / ₈ | ¹ / ₈ | | single atom (OH ₂) |
| (OH ₂)11 | 48f | 2.. | 0.5085 | ¹ / ₈ | ¹ / ₈ | | non-colinear O ₂ |
| O12 | 32e | .3. | 0.2333 | 0.2333 | 0.2333 | | single atom U |
| U13 | 32e | .3. | 0.2704 | 0.2704 | 0.2704 | | colinear O ₂ |
| O14 | 32e | .3. | 0.309 | 0.309 | 0.309 | | single atom U |
| (OH ₂)15 | 16c | .-3. | 0 | 0 | 0 | | octahedron Cl ₆ |
| (OH ₂)16 | 8a | 23. | ¹ / ₈ | ¹ / ₈ | ¹ / ₈ | | octahedron (OH ₂) ₆ |

Transformation from published data: -y,-x,-z; origin shift ¹/₂ ¹/₂ ¹/₂

Experimental: single crystal, diffractometer, X-rays, R = 0.037, T = 293 K

Remarks: Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Li Y., Burns P.C. (2002), J. Solid State Chem. 166, 219-228.

203
cF1088

| Na ₂₃ Al ₂₃ Si ₂₅ Te _{9.5} O ₉₆ cF1088 (203) <i>Fd-3</i> – g⁹fe⁵c | | | | | | | |
|---|--|--|--|--|--|--|--|
| Na₉₂Al₉₂Si₁₀₀O₃₈₄·xTe [1], zeolite FAU-Na (Te) | | | | | | | |
| Structural features: SiO ₄ and AlO ₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Te ₄ rings in β cages, Te ₈ rings or finite Te ₁₆ chains in supercages, Na at the centers of hexagonal prisms and near the centers of single 6-rings. | | | | | | | |
| Smolin Y.I. et al. (2000) [1] | | | | | | | |
| Al ₂₄ Na _{8.76} O ₉₆ Si ₂₄ Te _{9.54} | | | | | | | |
| $a = 2.514 \text{ nm}$, $V = 15.8890 \text{ nm}^3$, $Z = 4$ | | | | | | | |

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|-----------------------------|-----------------------------|-------|---|
| O1 | 96g | 1 | 0.001 | 0.145 | 0.357 | | non-colinear SiAl |
| Te2 | 96g | 1 | 0.01 | 0.114 | 0.509 | 0.106 | |
| Te3 | 96g | 1 | 0.029 | 0.102 | 0.474 | 0.052 | |
| Si4 | 96g | 1 | 0.0349 | 0.3024 | 0.1266 | | tetrahedron O ₄ |
| Al5 | 96g | 1 | 0.0368 | 0.1277 | 0.3044 | | tetrahedron O ₄ |
| Te6 | 96g | 1 | 0.046 | 0.438 | 0.067 | 0.042 | single atom Te |
| O7 | 96g | 1 | 0.069 | 0.284 | 0.178 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.074 | 0.321 | 0.076 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.144 | 0.254 | 0.255 | | non-colinear SiAl |
| Te10 | 48f | 2.. | 0.433 | ¹ / ₈ | ¹ / ₈ | 0.081 | non-colinear Te ₂ |
| Te11 | 32e | .3. | 0.079 | 0.079 | 0.079 | 0.128 | octahedron Te ₃ O ₃ |
| Te12 | 32e | .3. | 0.186 | 0.186 | 0.186 | 0.14 | single atom Na |
| Na13 | 32e | .3. | 0.232 | 0.232 | 0.232 | | single atom Te |
| Te14 | 32e | .3. | 0.403 | 0.403 | 0.403 | 0.106 | |
| Te15 | 32e | .3. | 0.436 | 0.436 | 0.436 | 0.097 | |
| Na16 | 16c | -.3. | 0 | 0 | 0 | 0.19 | octahedron O ₆ |

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.097

Remarks: Part of Na not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (2000), Kristallografiya 45, 27-31.

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cF1104

| | | |
|---|--------|---|
| Na ₂₃ Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] _{53.3} | cF1104 | (203) <i>Fd</i> -3 - g ¹⁰ e ⁴ c |
|---|--------|---|

Na₉₂Al₉₂Si₁₀₀O₃₈₄·213H₂O [1], faujasite-(Na), zeolite FAU-Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na opposite double 6-rings in β cages and above the centers of single 6-rings in supercages, (H₂O,Na) at the centers of hexagonal prisms and near 12-rings, additional H₂O in β cages and supercages.

Smolin Y.I. et al. (1983) [1]

Al_{22.56}H_{74.27}Na_{16.22}O_{133.14}Si_{25.44}

a = 2.501 nm, *V* = 15.6438 nm³, *Z* = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0008 | 0.3603 | 0.1445 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.008 | 0.012 | 0.397 | 0.32 | non-coplanar triangle (OH ₂) ₃ |
| Si3 | 96g | 1 | 0.0353 | 0.1246 | 0.303 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0369 | 0.3039 | 0.1265 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.04 | 0.071 | 0.418 | 0.24 | non-colinear (OH ₂) ₂ |
| (OH ₂)6 | 96g | 1 | 0.05 | 0.137 | 0.451 | 0.06 | non-coplanar triangle (OH ₂) ₃ |
| O7 | 96g | 1 | 0.0694 | 0.1754 | 0.2821 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0725 | 0.075 | 0.3212 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.092 | 0.443 | 0.153 | 0.61 | single atom (OH ₂) |
| O10 | 96g | 1 | 0.1441 | 0.2541 | 0.2522 | | non-colinear SiAl |
| Na11 | 32e | .3. | 0.0604 | 0.0604 | 0.0604 | 0.68 | non-coplanar triangle O ₃ |

| | | | | | | | |
|----------------------------------|-----|------|--------|--------|--------|------|--|
| (OH ₂) ₁₂ | 32e | .3. | 0.172 | 0.172 | 0.172 | 0.71 | 7-vertex polyhedron Na ₄ O ₃ |
| Na ₁₃ | 32e | .3. | 0.2363 | 0.2363 | 0.2363 | 0.94 | non-coplanar triangle O ₃ |
| (OH ₂) ₁₄ | 32e | .3. | 0.298 | 0.298 | 0.298 | 0.41 | single atom Na |
| M15 | 16c | -.3. | 0 | 0 | 0 | 0.48 | 8-vertex polyhedron Na ₂ O ₆ |

M4 = 0.94Al + 0.06Si; M5 = 0.56OH₂ + 0.44Na; M15 = 0.62OH₂ + 0.38Na

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.059, T = 298 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Butikova I.K., Petranovskii V.P. (1983), Sov. Phys. Crystallogr. (Engl. Transl.) 28, 36-39.

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| | | |
|---|--------|---|
| Ag ₂₃ Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₅₀ | cF1104 | (203) <i>Fd</i> -3 - g ¹⁰ e ⁴ c |
|---|--------|---|

Ag₉₂Al₉₂Si₁₀₀O₃₈₄·xH₂O [1], zeolite FAU-Ag hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms, above the centers of double 6-rings in β cages, near 6- and 12-rings in supercages, H₂O opposite single 6-rings in β cages and supercages.

Lee S.H. et al. (2000) [1]

Ag_{23.03}Al_{23.04}H₂₄O₁₀₈Si_{24.96}

a = 2.4996 nm, *V* = 15.6175 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------------------|-------|------|----------|----------|----------|-------|---|
| Ag1 | 96g | 1 | 0.0037 | 0.4315 | 0.0777 | 0.094 | non-collinear SiAl |
| O2 | 96g | 1 | 0.0063 | 0.1429 | 0.3558 | | |
| Ag3 | 96g | 1 | 0.0267 | 0.092 | 0.4452 | 0.073 | |
| Si4 | 96g | 1 | 0.0358 | 0.1259 | 0.3033 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0361 | 0.3034 | 0.1259 | | tetrahedron O ₄ |
| Ag6 | 96g | 1 | 0.0497 | 0.4416 | 0.098 | 0.063 | non-collinear SiAl |
| Ag7 | 96g | 1 | 0.06663 | 0.1139 | 0.4301 | 0.063 | |
| O8 | 96g | 1 | 0.0687 | 0.18 | 0.2821 | | |
| O9 | 96g | 1 | 0.0758 | 0.0777 | 0.3226 | | non-collinear SiAl |
| O10 | 96g | 1 | 0.1451 | 0.2527 | 0.2524 | | non-collinear SiAl |
| Ag11 | 32e | .3. | 0.0703 | 0.0703 | 0.0703 | 0.5 | octahedron (OH ₂) ₃ O ₃ |
| (OH ₂) ₁₂ | 32e | .3. | 0.1587 | 0.1587 | 0.1587 | 0.5 | 6-vertex polyhedron Ag ₃ (OH ₂) ₃ |
| Ag13 | 32e | .3. | 0.2406 | 0.2406 | 0.2406 | | tetrahedron (OH ₂)O ₃ |
| (OH ₂) ₁₄ | 32e | .3. | 0.2947 | 0.2947 | 0.2947 | | single atom Ag |
| Ag15 | 16c | -.3. | 0 | 0 | 0 | | octahedron O ₆ |

M5 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.088, T = 294 K

Remarks: Part of H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee S.H., Kim Y., Seff K. (2000), Microporous Mesoporous Mater. 41, 49-59.

| | | |
|-------------------------------------|---------------|--------------------------------|
| $K_{13}Na_{10}Al_{23}Si_{25}O_{96}$ | <i>cF1120</i> | (203) <i>Fd-3</i> – g^9fe^6c |
|-------------------------------------|---------------|--------------------------------|

$K_{52}Na_{40}Al_{92}Si_{100}O_{382}$ [1], zeolite FAU-K,Na

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, near the centers of single 6-rings and above double 6-rings in β cages, K opposite single and double 6-rings in β cages and on several sites in supercages.

Shepelev Y.F. et al. (1991) [1]

$Al_{23.04}K_{14.36}Na_{10.72}O_{96}Si_{24.96}$

$a = 2.486$ nm, $V = 15.3640$ nm³, $Z = 4$

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|------|-------|------|----------|---------------|---------------|------|----------------------------|
| O1 | 96g | 1 | 0.0014 | 0.3613 | 0.1438 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0345 | 0.1258 | 0.3043 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0369 | 0.3044 | 0.1268 | | tetrahedron O ₄ |
| Na4 | 96g | 1 | 0.044 | 0.429 | 0.081 | 0.11 | |
| K5 | 96g | 1 | 0.051 | 0.061 | 0.426 | 0.16 | |
| K6 | 96g | 1 | 0.06 | 0.104 | 0.454 | 0.06 | |
| O7 | 96g | 1 | 0.0633 | 0.1792 | 0.2825 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0741 | 0.0779 | 0.3213 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.1449 | 0.2535 | 0.2528 | | non-colinear SiAl |
| K10 | 48f | 2.. | 0.414 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.05 | |
| Na11 | 32e | .3. | 0.063 | 0.063 | 0.063 | 0.32 | |
| K12 | 32e | .3. | 0.07 | 0.07 | 0.07 | 0.19 | |
| K13 | 32e | .3. | 0.156 | 0.156 | 0.156 | 0.13 | |
| K14 | 32e | .3. | 0.171 | 0.171 | 0.171 | 0.16 | |
| Na15 | 32e | .3. | 0.231 | 0.231 | 0.231 | 0.35 | |
| K16 | 32e | .3. | 0.2567 | 0.2567 | 0.2567 | 0.58 | |
| Na17 | 16c | -.3. | 0 | 0 | 0 | 0.68 | octahedron O ₆ |

$M3 = 0.96Al + 0.04Si$

Experimental: single crystal, diffractometer, X-rays, $R = 0.078$, $T = 673$ K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). In table 2 (d-KNaX) of [1] the occupation factors of former Na(I) and Na(I') are misprinted as 1.68 and 1.32 instead of 0.68 and 0.32, respectively (agreement with the number of atoms per site).

References: [1] Shepelev Y.F., Butikova I.K., Smolin Y.I. (1991), Zeolites 11, 287-292.

| | | |
|--|---------------|----------------------------------|
| $Na_6Co_{9.5}Al_{23}Si_{25}O_{96}[OH]_2[H_2O]_5$ | <i>cF1136</i> | (203) <i>Fd-3</i> – $g^{10}e^5c$ |
|--|---------------|----------------------------------|

$Na_{24}Co_{38}Al_{92}Si_{100}O_{384}(OH)_8 \cdot xH_2O$ [1], zeolite FAU- Co^{2+} ,Na partly hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Co opposite double 6-rings in β cages, near 6- and 12-rings in supercages, Na at the centers of hexagonal prisms, above double 6-rings in β and single 6-rings in supercages, Co-OH-Na bridges.

Bae D., Seff K. (1999) [1]

$\text{Al}_{23.04}\text{Co}_{9.59}\text{H}_{22.36}\text{Na}_6\text{O}_{108.18}\text{Si}_{24.96}$
 $a = 2.492 \text{ nm}$, $V = 15.4755 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0001 | 0.3545 | 0.1505 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0008 | 0.1005 | 0.2517 | | non-colinear SiAl |
| (OH ₂)3 | 96g | 1 | 0.0332 | 0.4441 | 0.0782 | 0.108 | non-colinear Co ₂ |
| Si4 | 96g | 1 | 0.0362 | 0.1243 | 0.3011 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0375 | 0.3026 | 0.1263 | | tetrahedron O ₄ |
| Co6 | 96g | 1 | 0.0422 | 0.0888 | 0.4083 | 0.108 | single atom (OH ₂) |
| O7 | 96g | 1 | 0.0719 | 0.0757 | 0.3232 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.073 | 0.1724 | 0.2759 | | non-colinear SiAl |
| (OH)9 | 96g | 1 | 0.0919 | 0.1208 | 0.1044 | 0.083 | |
| (OH ₂)10 | 96g | 1 | 0.1136 | 0.1361 | 0.4463 | 0.108 | |
| Co11 | 32e | .3. | 0.0584 | 0.0584 | 0.0584 | 0.25 | |
| Na12 | 32e | .3. | 0.0724 | 0.0724 | 0.0724 | 0.5 | |
| Co13 | 32e | .3. | 0.231 | 0.231 | 0.231 | 0.625 | |
| Na14 | 32e | .3. | 0.2483 | 0.2483 | 0.2483 | 0.156 | |
| (OH ₂)15 | 32e | .3. | 0.2811 | 0.2811 | 0.2811 | 0.625 | |
| Na16 | 16c | -.3. | 0 | 0 | 0 | 0.188 | 8-vertex polyhedron Co ₂ O ₆ |

$M5 = 0.96\text{Al} + 0.04\text{Si}$

Transformation from published data: $-y, -x, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.083$, $T = 296 \text{ K}$

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 4a of [1] the Wyckoff positions of former O(7) and O(8) are misprinted as 48f instead of 96g.

References: [1] Bae D., Seff K. (1999), Microporous Mesoporous Mater. 33, 265-280.

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| | | |
|--|--------|----------------------------------|
| $\text{H}_{18.5}\text{Cd}_{8.1}\text{Al}_{23}\text{Si}_{25}\text{S}_{5.85}\text{O}_{96}[\text{H}_2\text{O}]_{1.4}$ | cF1152 | (203) $Fd\bar{3} - g^{10}e^5cba$ |
|--|--------|----------------------------------|

H₇₄Cd_{32.4}Al₉₂Si₁₀₀S_{23.4}O₃₈₄·5.6H₂O [1], zeolite FAU-Cd (H₂S) ht residual water

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; $[\text{Cd}_{20}\text{S}_{13}]^{14+}$ tetrahedral clusters in supercages, additional Cd at the centers of hexagonal prisms and β cages and opposite double 6-rings in β cages, H₂O opposite single 6-rings in β cages.

Smolin Y.I. et al. (1998) [1]

$\text{Al}_{23.04}\text{Cd}_{8.12}\text{H}_{2.75}\text{O}_{97.38}\text{S}_{5.83}\text{Si}_{24.96}$
 $a = 2.479 \text{ nm}$, $V = 15.2345 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|------------------------------|
| O1 | 96g | 1 | 0.0018 | 0.3636 | 0.1422 | | non-colinear SiAl |
| S2 | 96g | 1 | 0.003 | 0.012 | 0.475 | 0.079 | |
| Cd3 | 96g | 1 | 0.019 | 0.07 | 0.418 | 0.029 | |
| Cd4 | 96g | 1 | 0.028 | 0.456 | 0.103 | 0.027 | |
| S5 | 96g | 1 | 0.032 | 0.109 | 0.485 | 0.136 | non-colinear Cd ₂ |
| Si6 | 96g | 1 | 0.0343 | 0.1266 | 0.3032 | | tetrahedron O ₄ |

| | | | | | | | |
|----------------------|-----|------|-----------------------------|-----------------------------|-----------------------------|-------|--|
| M7 | 96g | 1 | 0.0375 | 0.3039 | 0.1278 | | tetrahedron O ₄ |
| O8 | 96g | 1 | 0.0607 | 0.1849 | 0.2846 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.0788 | 0.0832 | 0.3177 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.145 | 0.2556 | 0.255 | | non-colinear SiAl |
| Cd11 | 32e | .3. | 0.066 | 0.066 | 0.066 | 0.056 | 8-vertex polyhedron (OH ₂) ₃ O ₃ Cd ₂ |
| (OH ₂)12 | 32e | .3. | 0.16 | 0.16 | 0.16 | 0.172 | single atom Cd |
| Cd13 | 32e | .3. | 0.2351 | 0.2351 | 0.2351 | 0.247 | |
| Cd14 | 32e | .3. | 0.254 | 0.254 | 0.254 | 0.066 | |
| Cd15 | 32e | .3. | 0.432 | 0.432 | 0.432 | 0.05 | tetrahedron S ₄ |
| Cd16 | 16c | -.3. | 0 | 0 | 0 | 0.825 | 8-vertex polyhedron O ₆ Cd ₂ |
| S17 | 8b | 23. | ⁵ / ₈ | ⁵ / ₈ | ⁵ / ₈ | 0.335 | tetrahedron Cd ₄ |
| Cd18 | 8a | 23. | ¹ / ₈ | ¹ / ₈ | ¹ / ₈ | 0.063 | tetrahedron (OH ₂) ₄ |

M7 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.063, T = 373 K

Remarks: Approximate composition, we took the amounts of Cd and S from the refinement and adjusted the charge balance in the formula given above by adding H. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 2 (ht-CdX(H₂S)) of [1] the occupancy of former Cd(I) is misprinted as 3.2/16 instead of 13.2/16 (from the description of the structure).

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (1998), Crystallogr. Rep. 43, 387-394 (Kristallografiya 43, 425-432).

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cF1152

| | | |
|---|--------|--|
| Cs _{11.25} Na _{11.75} Al ₂₃ Si ₂₅ SiO ₉₆ | cF1152 | (203) <i>Fd</i> -3 - g ¹⁰ fe ⁴ c |
|---|--------|--|

Cs₄₅Na₄₇Al₉₂Si₁₀₀O₃₈₄ [1], zeolite FAU-Cs,Na

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, opposite double 6-rings in β cages and near the centers of single 6-rings, Cs opposite single and double 6-rings in β cages, and in supercages.

Butikova I.K. et al. (1989) [1]

Al_{23.04}Cs_{11.44}Na_{13.28}O₉₆Si_{24.96}

$a = 2.496$ nm, $V = 15.5501$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|-----------------------------|-----------------------------|------|----------------------------|
| O1 | 96g | 1 | 0.001 | 0.3611 | 0.1437 | | non-colinear SiAl |
| Si2 | 96g | 1 | 0.0346 | 0.1256 | 0.3037 | | tetrahedron O ₄ |
| M3 | 96g | 1 | 0.0362 | 0.3039 | 0.1275 | | tetrahedron O ₄ |
| Cs4 | 96g | 1 | 0.046 | 0.438 | 0.049 | 0.01 | |
| O5 | 96g | 1 | 0.0646 | 0.1814 | 0.2852 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0762 | 0.0789 | 0.3177 | | non-colinear SiAl |
| Cs7 | 96g | 1 | 0.077 | 0.078 | 0.442 | 0.03 | |
| Cs8 | 96g | 1 | 0.1067 | 0.1422 | 0.4255 | 0.09 | |
| Cs9 | 96g | 1 | 0.1101 | 0.1113 | 0.427 | 0.13 | |
| O10 | 96g | 1 | 0.1452 | 0.2551 | 0.2531 | | non-colinear SiAl |
| Cs11 | 48f | 2.. | 0.4195 | ¹ / ₈ | ¹ / ₈ | 0.28 | |
| Na12 | 32e | .3. | 0.053 | 0.053 | 0.053 | 0.16 | |
| Cs13 | 32e | .3. | 0.0905 | 0.0905 | 0.0905 | 0.18 | |
| Cs14 | 32e | .3. | 0.157 | 0.157 | 0.157 | 0.05 | |

| | | | | | | |
|------|-----|------|--------|--------|--------|--|
| Na15 | 32e | .3. | 0.2283 | 0.2283 | 0.2283 | non-coplanar triangle O ₃ |
| Na16 | 16c | -.3. | 0 | 0 | 0 | 8-vertex polyhedron Na ₂ O ₆ |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.058, T = 673 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). On page 687 of [1] the chemical formula is misprinted as Cs₄₅Na₄₇Al₉₂Si₁₀O₃₈₄ instead of Cs₄₅Na₄₇Al₉₂Si₁₀₀O₃₈₄.

References: [1] Butikova I.K., Shepelev Y.F., Smolin Y.I. (1989), Sov. Phys. Crystallogr. (Engl. Transl.) 34, 687-690.

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cF1168

| | | |
|---|--------|---|
| Ag ₂₃ Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₅₀ | cF1168 | (203) <i>Fd</i> -3 - g ¹¹ e ³ c |
|---|--------|---|

Ag₉₂Al₉₂Si₁₀₀O₃₈₄·xH₂O [1], zeolite FAU-Ag hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Ag at the centers of hexagonal prisms, opposite double 6-rings in β cages (linear Ag₃ clusters), near the centers of single 6-rings and in supercages, H₂O in supercages.

Butikova I.K. et al. (1989) [1]

Ag_{18.56}Al_{23.04}H_{39.36}O_{115.68}Si_{24.96}
a = 2.502 nm, V = 15.6625 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|--|
| O1 | 96g | 1 | 0.0002 | 0.3597 | 0.1453 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0044 | 0.2527 | 0.1057 | | non-colinear AlSi |
| Ag3 | 96g | 1 | 0.013 | 0.443 | 0.094 | 0.05 | |
| Ag4 | 96g | 1 | 0.023 | 0.081 | 0.426 | 0.05 | |
| (OH ₂)5 | 96g | 1 | 0.032 | 0.111 | 0.46 | 0.23 | |
| Si6 | 96g | 1 | 0.0349 | 0.1253 | 0.3033 | | tetrahedron O ₄ |
| M7 | 96g | 1 | 0.0369 | 0.3039 | 0.1265 | | tetrahedron O ₄ |
| (OH ₂)8 | 96g | 1 | 0.06 | 0.111 | 0.429 | 0.2 | |
| O9 | 96g | 1 | 0.067 | 0.1777 | 0.2825 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.0749 | 0.0786 | 0.3207 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.088 | 0.157 | 0.429 | 0.39 | single atom (OH ₂) |
| Ag12 | 32e | .3. | 0.0679 | 0.0679 | 0.0679 | 0.62 | non-coplanar triangle O ₃ |
| Ag13 | 32e | .3. | 0.202 | 0.202 | 0.202 | 0.1 | single atom Ag |
| Ag14 | 32e | .3. | 0.2394 | 0.2394 | 0.2394 | 0.87 | single atom Ag |
| Ag15 | 16c | -.3. | 0 | 0 | 0 | 0.86 | 8-vertex polyhedron O ₆ Ag ₂ |

M7 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, precession photographs, X-rays, R = 0.047, T = 293 K

Remarks: Part of Ag and H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Butikova I.K., Shepelev Y.F., Smolin Y.I. (1989), Sov. Phys. Crystallogr. (Engl. Transl.) 34, 684-687.

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cF1184

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|---|---------------|--|
| $\text{Na}_{23}\text{Al}_{23}\text{Si}_{25}\text{Se}_{11.5}\text{O}_{96}$ | <i>cF1184</i> | (203) <i>Fd-3</i> – $\text{g}^{10}\text{fe}^5\text{c}$ |
|---|---------------|--|

Na₉₂Al₉₂Si₁₀₀O₃₈₄·xSe [1], zeolite FAU-Na (Se)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Se₄ and Se₆ rings in β cages, Se₂ dumbbells in supercages, Na at the centers of hexagonal prisms and near the centers of single 6-rings.

Smolin Y.I. et al. (2000) [1]

 $\text{Al}_{23.04}\text{Na}_{1.84}\text{O}_{96}\text{Se}_{11.51}\text{Si}_{24.96}$ $a = 2.506 \text{ nm}$, $V = 15.7378 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0009 | 0.3603 | 0.144 | | non-colinear SiAl |
| Se2 | 96g | 1 | 0.009 | 0.012 | 0.394 | 0.034 | single atom Se |
| Si3 | 96g | 1 | 0.035 | 0.1252 | 0.303 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0367 | 0.304 | 0.1263 | | tetrahedron O ₄ |
| Se5 | 96g | 1 | 0.056 | 0.082 | 0.535 | 0.03 | |
| O6 | 96g | 1 | 0.0694 | 0.1753 | 0.2811 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0725 | 0.0748 | 0.3232 | | non-colinear SiAl |
| Se8 | 96g | 1 | 0.092 | 0.155 | 0.448 | 0.074 | single atom Se |
| O9 | 96g | 1 | 0.1441 | 0.2526 | 0.2506 | | non-colinear SiAl |
| Se10 | 96g | 1 | 0.274 | 0.303 | 0.279 | 0.072 | |
| Se11 | 48f | 2.. | 0.037 | 1/8 | 1/8 | 0.079 | non-colinear Se ₂ |
| Se12 | 32e | .3. | 0.0574 | 0.0574 | 0.0574 | 0.184 | |
| Se13 | 32e | .3. | 0.072 | 0.072 | 0.072 | 0.125 | |
| Se14 | 32e | .3. | 0.166 | 0.166 | 0.166 | 0.125 | non-coplanar triangle Se ₃ |
| Na15 | 32e | .3. | 0.231 | 0.231 | 0.231 | 0.09 | |
| Se16 | 32e | .3. | 0.2363 | 0.2363 | 0.2363 | 0.256 | |
| Na17 | 16c | -.3. | 0 | 0 | 0 | 0.28 | 8-vertex polyhedron Se ₂ O ₆ |

M4 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.051

Remarks: Part of Na not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s).

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (2000), Kristallografiya 45, 27-31.

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|---|---------------|---|
| $\text{Cs}_{11.5}\text{Al}_{22}\text{Pb}_{9.25}\text{Si}_{26}\text{O}_{96}[\text{OH}]_8[\text{H}_2\text{O}]_{50}$ | <i>cF1192</i> | (203) <i>Fd-3</i> – $\text{g}^{11}\text{e}^4\text{b}$ |
|---|---------------|---|

Cs₄₆Pb₃₇Al₈₈Si₁₀₄O₃₈₄(OH)₃₂·xH₂O [1], zeolite FAU-Pb²⁺, Cs hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; cubane-like Pb₄(OH)₄ clusters in β cages, additional Pb opposite 6-rings in supercages, Cs and H₂O in supercages.

Nardin G. et al. (1995) [1]

 $\text{Al}_{23.04}\text{Cs}_{11.49}\text{H}_{32.08}\text{O}_{116.04}\text{Pb}_{9.25}\text{Si}_{24.96}$ $a = 2.5143 \text{ nm}$, $V = 15.8947 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------------|---------------|---------------|-------|--|
| O1 | 96g | 1 | 0.0001 | 0.1431 | 0.358 | | non-colinear AlSi |
| (OH ₂)2 | 96g | 1 | 0.02 | 0.04 | 0.42 | 0.12 | |
| M3 | 96g | 1 | 0.0355 | 0.3053 | 0.1236 | | tetrahedron O ₄ |
| Si4 | 96g | 1 | 0.0357 | 0.1234 | 0.3049 | | trigonal bipyramid O ₄ (OH ₂) |
| Cs5 | 96g | 1 | 0.0432 | 0.0639 | 0.4229 | 0.125 | |
| Cs6 | 96g | 1 | 0.0474 | 0.4216 | 0.0611 | 0.135 | |
| O7 | 96g | 1 | 0.0681 | 0.0681 | 0.3218 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0784 | 0.1716 | 0.2872 | | non-coplanar triangle SiAl(OH ₂) |
| (OH ₂)9 | 96g | 1 | 0.087 | 0.157 | 0.362 | 0.14 | single atom O |
| (OH ₂)10 | 96g | 1 | 0.093 | 0.157 | 0.446 | 0.21 | non-colinear (OH ₂) ₂ |
| O11 | 96g | 1 | 0.1383 | 0.2525 | 0.2543 | | non-colinear AlSi |
| Pb12 | 32e | .3. | 0.0707 | 0.0707 | 0.0707 | | 9-vertex polyhedron (OH) ₃ O ₆ |
| (OH)13 | 32e | .3. | 0.1659 | 0.1659 | 0.1659 | | non-coplanar triangle Pb ₃ |
| Pb14 | 32e | .3. | 0.2568 | 0.2568 | 0.2568 | 0.156 | |
| Cs15 | 32e | .3. | 0.2689 | 0.2689 | 0.2689 | 0.656 | |
| (OH ₂)16 | 8b | 23. | $\frac{5}{8}$ | $\frac{5}{8}$ | $\frac{5}{8}$ | 0.38 | |

M3 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.050

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Nardin G., Randaccio L., Zangrando E. (1995), Zeolites 15, 684-688.

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Na₂₂Al₂₂Si₂₆O₉₆[H₂O]₅₅

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(203) *Fd*-3 - g¹¹e⁴c

Na₈₈Al₈₈Si₁₀₄O₃₈₆·220H₂O [1], faujasite-(Na), zeolite FAU-Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, above the centers of double 6-rings in β cages and single 6-rings in supercages and on a second site in supercages, mainly coordinated by H₂O.

Calestani G. et al. (1987) [1]

Al_{22.01}H_{81.12}Na_{20.83}O_{136.56}Si_{25.99}

a = 2.5031 nm, *V* = 15.6832 nm³, *Z* = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0007 | 0.3605 | 0.1445 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.0081 | 0.403 | 0.0221 | 0.22 | non-colinear (OH ₂) ₂ |
| (OH ₂)3 | 96g | 1 | 0.0241 | 0.4516 | 0.0965 | 0.31 | non-coplanar triangle (OH ₂) ₂ Na |
| Si4 | 96g | 1 | 0.0351 | 0.1251 | 0.3028 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.037 | 0.3036 | 0.1271 | | tetrahedron O ₄ |
| Na6 | 96g | 1 | 0.0385 | 0.0792 | 0.4206 | 0.24 | non-coplanar triangle (OH ₂) ₃ |
| O7 | 96g | 1 | 0.068 | 0.1775 | 0.2823 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0741 | 0.0773 | 0.3208 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.0961 | 0.152 | 0.4394 | 0.5 | single atom (OH ₂) |
| O10 | 96g | 1 | 0.1438 | 0.2543 | 0.2528 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.251 | 0.2573 | 0.3604 | 0.29 | single atom (OH ₂) |
| Na12 | 32e | .3. | 0.0661 | 0.0661 | 0.0661 | 0.63 | octahedron O ₃ (OH ₂) ₃ |

| | | | | | | |
|--------------------------|------|--------|--------|--------|-------|---|
| (OH ₂)13 32e | .3. | 0.1631 | 0.1631 | 0.1631 | 0.6 | 6-vertex polyhedron Na ₃ (OH ₂) ₃ |
| Na14 32e | .3. | 0.2363 | 0.2363 | 0.2363 | 0.96 | tetrahedron (OH ₂)O ₃ |
| (OH ₂)15 32e | .3. | 0.284 | 0.284 | 0.284 | 0.51 | tetrahedron Na(OH ₂) ₃ |
| Na16 16c | -.3. | 0 | 0 | 0 | 0.588 | 8-vertex polyhedron O ₆ Na ₂ |

M5 = 0.917Al + 0.083Si

Experimental: single crystal, diffractometer, X-rays, R = 0.061

Remarks: Part of H₂O not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Calestani G., Bacca G., Andreotti G.D. (1987), Zeolites 7, 54-58.

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|--|--------|--|
| Na _{2.75} [H ₃ O] _{4.5} Co _{9.5} Al ₂₃ Si ₂₅ O ₉₆ [OH] _{3.25} [H ₂ O] ₁₅ | cF1216 | (203) <i>Fd</i> -3 - g ¹⁰ fe ⁶ c |
|--|--------|--|

Na₁₁(H₃O)₁₈Co₃₈Al₉₂Si₁₀₀O₃₈₄(OH)₁₃·xH₂O [1], zeolite FAU-Co²⁺, Na, H₃O⁺

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms and above the centers of single 6-rings, [H₃O⁺]₂H₂O(Co²⁺)₂ clusters in β cages, additional Co near the centers of single 6-rings and near 12-rings.

Bae D., Seff K. (1999) [1]

Al_{23.04}Co_{9.50}H_{47.25}Na_{2.75}O_{118.99}Si_{24.96}
a = 2.495 nm, V = 15.5314 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|-------|--|
| O1 | 96g | 1 | 0.0004 | 0.1431 | 0.3518 | | non-collinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.0183 | 0.4169 | 0.049 | 0.271 | non-coplanar triangle Co ₂ (OH ₂) |
| Si3 | 96g | 1 | 0.0357 | 0.1245 | 0.3016 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0371 | 0.303 | 0.1263 | | tetrahedron O ₄ |
| (OH ₂)5 | 96g | 1 | 0.0464 | 0.1281 | 0.4642 | 0.156 | non-collinear (OH)Co |
| Co6 | 96g | 1 | 0.0472 | 0.0911 | 0.4095 | 0.135 | single atom (OH ₂) |
| O7 | 96g | 1 | 0.0718 | 0.1732 | 0.2782 | | non-collinear SiAl |
| O8 | 96g | 1 | 0.0733 | 0.075 | 0.3232 | | non-collinear SiAl |
| (OH)9 | 96g | 1 | 0.0911 | 0.1571 | 0.4376 | 0.135 | single atom (OH ₂) |
| O10 | 96g | 1 | 0.1479 | 0.2515 | 0.2506 | | non-collinear SiAl |
| (OH ₂)11 | 48f | 2.. | 0.0882 | 1/8 | 1/8 | 0.104 | |
| Co12 | 32e | .3. | 0.0594 | 0.0594 | 0.0594 | 0.313 | |
| (OH ₃)13 | 32e | .3. | 0.0859 | 0.0859 | 0.0859 | 0.313 | |
| (OH ₃)14 | 32e | .3. | 0.1678 | 0.1678 | 0.1678 | 0.25 | |
| Co15 | 32e | .3. | 0.2282 | 0.2282 | 0.2282 | 0.469 | |
| Na16 | 32e | .3. | 0.2414 | 0.2414 | 0.2414 | 0.281 | |
| (OH ₂)17 | 32e | .3. | 0.2765 | 0.2765 | 0.2765 | 0.469 | single atom Na |
| Na18 | 16c | -.3. | 0 | 0 | 0 | 0.125 | 8-vertex polyhedron Co ₂ O ₆ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.125, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Bae D., Seff K. (1999), Microporous Mesoporous Mater. 33, 265-280.

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|---|---------------|---|
| $\text{Zn}_{13.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{OH}]_4[\text{H}_2\text{O}]_{14.5}$ | <i>cF1224</i> | (203) <i>Fd-3</i> – $\text{g}^{11}\text{e}^5\text{a}$ |
|---|---------------|---|

Zn₅₄Na₉₂Al₉₂Si₁₀₀O₃₈₄(OH)₁₆·xH₂O [1], zeolite FAU-Zn (Zn[OH]₂) partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Zn(OH)₂ in supercages, Zn(OH)₂(H₂O)₂ clusters in β cages, additional Zn above double 6-rings in β cages, near the centers of single 6-rings and near 12-rings.

Bae D., Seff K. (2000) [1]

 $\text{Al}_{23.04}\text{H}_{32.27}\text{O}_{108.21}\text{Si}_{24.96}\text{Zn}_{13.66}$ $a = 2.475 \text{ nm}$, $V = 15.1609 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------------|---------------|---------------|-------|---------------------------------------|
| O1 | 96g | 1 | 0.0006 | 0.1428 | 0.3525 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0011 | 0.102 | 0.2532 | | non-colinear SiAl |
| Zn3 | 96g | 1 | 0.0306 | 0.0746 | 0.4068 | 0.123 | single atom Zn |
| Si4 | 96g | 1 | 0.0358 | 0.1245 | 0.3024 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0368 | 0.303 | 0.1264 | | tetrahedron O ₄ |
| Zn6 | 96g | 1 | 0.0473 | 0.1142 | 0.4597 | 0.062 | |
| M7 | 96g | 1 | 0.0598 | 0.0788 | 0.1553 | 0.121 | |
| O8 | 96g | 1 | 0.0709 | 0.1732 | 0.2785 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.0714 | 0.0756 | 0.323 | | non-colinear SiAl |
| Zn10 | 96g | 1 | 0.0758 | 0.0787 | 0.4911 | 0.066 | |
| Zn11 | 96g | 1 | 0.2138 | 0.2893 | 0.2916 | 0.031 | single atom (OH ₃) |
| Zn12 | 32e | .3. | 0.0544 | 0.0544 | 0.0544 | 0.3 | |
| (OH ₃)13 | 32e | .3. | 0.0806 | 0.0806 | 0.0806 | 0.638 | |
| Zn14 | 32e | .3. | 0.2276 | 0.2276 | 0.2276 | 0.381 | single atom (OH ₃) |
| (OH ₃)15 | 32e | .3. | 0.27 | 0.27 | 0.27 | 0.525 | 4-vertex polyhedron Zn ₄ |
| Zn16 | 32e | .3. | 0.4613 | 0.4613 | 0.4613 | 0.088 | non-coplanar triangle Zn ₃ |
| Zn17 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.37 | |

M5 = 0.96Al + 0.04Si; M7 = 0.5OH + 0.5OH₂

Transformation from published data: -y, -x, -z

Experimental: single crystal, diffractometer, X-rays, R = 0.126, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3a of [1] the Wyckoff position of former ZnE is misprinted as 96g instead of 32e.

References: [1] Bae D., Seff K. (2000), Microporous Mesoporous Mater. 40, 233-245.

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|---|---------------|---|
| $\text{Zn}_{13.5}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{OH}]_4[\text{H}_2\text{O}]_{60}$ | <i>cF1232</i> | (203) <i>Fd-3</i> – $\text{g}^{10}\text{e}^8\text{c}$ |
|---|---------------|---|

Zn₅₄Al₉₂Si₁₀₀O₃₈₄(OH)₁₆·xH₂O [1], zeolite FAU-Zn (Zn[OH]₂) hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; cubane-like Zn₄(OH)₄ clusters in β cages, additional Zn at the centers of prisms, near the centers of single 6-rings and on several sites in supercages, H₃O⁺ opposite 6-rings in β and supercages.

Bae D., Seff K. (2000) [1]

 $\text{Al}_{23.04}\text{H}_{35.65}\text{O}_{109.86}\text{Si}_{24.96}\text{Zn}_{12.84}$
 $a = 2.4872 \text{ nm}$, $V = 15.3862 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|-------|---------------------------------------|
| O1 | 96g | 1 | 0.001 | 0.1422 | 0.3544 | | non-colinear SiAl |
| Zn2 | 96g | 1 | 0.0307 | 0.079 | 0.4084 | 0.104 | single atom Zn |
| Si3 | 96g | 1 | 0.036 | 0.1249 | 0.3031 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0368 | 0.3032 | 0.1259 | | tetrahedron O ₄ |
| Zn5 | 96g | 1 | 0.0547 | 0.1311 | 0.4501 | 0.062 | non-coplanar triangle Zn ₃ |
| O6 | 96g | 1 | 0.0715 | 0.1745 | 0.281 | | non-colinear SiAl |
| O7 | 96g | 1 | 0.0723 | 0.0761 | 0.3229 | | non-colinear SiAl |
| Zn8 | 96g | 1 | 0.0781 | 0.0794 | 0.4889 | 0.084 | non-coplanar triangle Zn ₃ |
| O9 | 96g | 1 | 0.1455 | 0.2532 | 0.2509 | | non-colinear SiAl |
| Zn10 | 96g | 1 | 0.2158 | 0.2932 | 0.2946 | 0.031 | non-colinear (OH ₃)Zn |
| Zn11 | 32e | .3. | 0.0448 | 0.0448 | 0.0448 | 0.188 | |
| Zn12 | 32e | .3. | 0.0712 | 0.0712 | 0.0712 | 0.25 | |
| (OH)13 | 32e | .3. | 0.1653 | 0.1653 | 0.1653 | 0.26 | |
| (OH ₃)14 | 32e | .3. | 0.1677 | 0.1677 | 0.1677 | 0.562 | |
| Zn15 | 32e | .3. | 0.2221 | 0.2221 | 0.2221 | 0.219 | single atom (OH ₃) |
| (OH ₃)16 | 32e | .3. | 0.2627 | 0.2627 | 0.2627 | 0.69 | tetrahedron Zn ₄ |
| (OH ₂)17 | 32e | .3. | 0.3284 | 0.3284 | 0.3284 | 0.22 | single atom (OH ₃) |
| Zn18 | 32e | .3. | 0.4565 | 0.4565 | 0.4565 | 0.042 | non-coplanar triangle Zn ₃ |
| Zn19 | 16c | -.3. | 0 | 0 | 0 | 0.125 | colinear Zn ₂ |

M4 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.115, T = 296 K

Remarks: Part of H₂O not located. Site occupancies corresponding to 54 Zn per unit cell are reported here. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3b of [1] the Wyckoff position of former ZnE and O(6) is misprinted as 96g instead of 32e.

References: [1] Bae D., Seff K. (2000), Microporous Mesoporous Mater. 40, 233-245.

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| | | |
|---|---------------|---|
| $\text{H}_9\text{Cd}_{10.5}\text{Al}_{23}\text{Si}_{25}\text{S}_{3.5}\text{O}_{96}[\text{H}_2\text{O}]_5$ | <i>cF1232</i> | (203) <i>Fd-3</i> – g ¹⁰ fe ⁶ cba |
|---|---------------|---|

H₃₆Cd₄₂Al₉₂Si₁₀₀S₁₄O₃₈₄·20H₂O [1], zeolite FAU-Cd (H₂S) lt residual water

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; [Cd₂₀S₁₃]¹⁴⁺ tetrahedral clusters in supercages, additional Cd at the centers of β cages and hexagonal prisms and opposite double 6-rings in β cages, H₂O opposite single 6-rings in β cages.

Smolin Y.I. et al. (1998) [1]

 $\text{Al}_{23.04}\text{Cd}_{10.48}\text{H}_{9.50}\text{O}_{100.75}\text{S}_{3.56}\text{Si}_{24.96}$
 $a = 2.484 \text{ nm}$, $V = 15.3269 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|-------|--------|-------|---------------------------------------|
| O1 | 96g | 1 | 0.0008 | 0.361 | 0.1435 | | non-colinear SiAl |
| S2 | 96g | 1 | 0.013 | 0.117 | 0.505 | 0.115 | non-coplanar triangle Cd ₃ |

| | | | | | | | |
|----------------------|-----|------|-----------------------------|-----------------------------|-----------------------------|-------|--|
| Si3 | 96g | 1 | 0.0346 | 0.1264 | 0.3033 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.037 | 0.3037 | 0.1274 | | tetrahedron O ₄ |
| Cd5 | 96g | 1 | 0.042 | 0.081 | 0.42 | 0.067 | |
| Cd6 | 96g | 1 | 0.042 | 0.422 | 0.082 | 0.049 | |
| O7 | 96g | 1 | 0.0614 | 0.1836 | 0.2838 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.0794 | 0.0828 | 0.3197 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.1455 | 0.2557 | 0.2541 | | non-colinear SiAl |
| Cd10 | 96g | 1 | 0.22 | 0.306 | 0.304 | 0.024 | non-colinear Cd ₂ |
| Cd11 | 48f | 2.. | 0.388 | ¹ / ₈ | ¹ / ₈ | 0.027 | non-colinear O ₂ |
| Cd12 | 32e | .3. | 0.07 | 0.07 | 0.07 | 0.134 | 7-vertex polyhedron Cd(OH ₂) ₃ O ₃ |
| (OH ₂)13 | 32e | .3. | 0.1662 | 0.1662 | 0.1662 | 0.594 | single atom Cd |
| Cd14 | 32e | .3. | 0.2439 | 0.2439 | 0.2439 | 0.1 | |
| Cd15 | 32e | .3. | 0.2627 | 0.2627 | 0.2627 | 0.119 | |
| Cd16 | 32e | .3. | 0.295 | 0.295 | 0.295 | 0.025 | |
| Cd17 | 32e | .3. | 0.4326 | 0.4326 | 0.4326 | 0.134 | tetrahedron S ₄ |
| Cd18 | 16c | .-3. | 0 | 0 | 0 | 0.649 | octahedron O ₆ |
| S19 | 8b | 23. | ⁵ / ₈ | ⁵ / ₈ | ⁵ / ₈ | 0.4 | tetrahedron Cd ₄ |
| Cd20 | 8a | 23. | ¹ / ₈ | ¹ / ₈ | ¹ / ₈ | 0.05 | tetrahedron (OH ₂) ₄ |

M4 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.057, T = 173 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (1998), Crystallogr. Rep. 43, 387-394 (Kristallografiya 43, 425-432).

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cF1248

| | | |
|--|--------|---|
| [H ₃ O] ₄ La _{8.3} Al ₂₃ Si ₂₅ O ₉₆ [OH] ₆ [H ₂ O] ₃₈ | cF1248 | (203) <i>Fd</i> -3 – g ¹¹ e ⁶ |
|--|--------|---|

(H₃O)₁₆La₃₃Al₉₂Si₁₀₀O₃₈₄(OH)₂₄·152H₂O [1], zeolite FAU-La³⁺ hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; La near the centers of single 6- and 12-rings and opposite double 6-rings in β cages, OH and H₃O opposite single 6-rings in β cages, additional H₃O and H₂O in supercages.

Park H.S., Seff K. (2000) [1]

Al_{23.04}H_{94.03}La_{8.25}O_{144.02}Si_{124.96}

a = 2.5154 nm, *V* = 15.9155 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------|-------|------|----------|----------|----------|-------|---|
| O1 | 96g | 1 | 0.00009 | 0.36087 | 0.14057 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.01844 | 0.44669 | 0.07639 | 0.25 | |
| (OH ₂)3 | 96g | 1 | 0.0262 | 0.08734 | 0.44868 | 0.25 | single atom (OH ₂) |
| Si4 | 96g | 1 | 0.0354 | 0.1239 | 0.30587 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.03578 | 0.30595 | 0.12493 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.0384 | 0.45651 | 0.11042 | 0.167 | |
| O7 | 96g | 1 | 0.06555 | 0.06661 | 0.31512 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.07604 | 0.17151 | 0.29077 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.11678 | 0.1179 | 0.42087 | 0.167 | |
| O10 | 96g | 1 | 0.13806 | 0.25487 | 0.25465 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.22758 | 0.31154 | 0.31118 | 0.75 | non-colinear (OH ₃)(OH ₂) |

| | | | | | | | |
|----------------------|-----|-----|---------|---------|---------|-------|---|
| La12 | 32e | .3. | 0.06894 | 0.06894 | 0.06894 | 0.25 | |
| (OH ₃)13 | 32e | .3. | 0.1443 | 0.1443 | 0.1443 | 0.25 | |
| (OH)14 | 32e | .3. | 0.17971 | 0.17971 | 0.17971 | 0.75 | single atom (OH ₃) |
| La15 | 32e | .3. | 0.23844 | 0.23844 | 0.23844 | 0.75 | |
| (OH ₃)16 | 32e | .3. | 0.25612 | 0.25612 | 0.25612 | 0.25 | |
| La17 | 32e | .3. | 0.46145 | 0.46145 | 0.46145 | 0.031 | 6-vertex polyhedron (OH ₂) ₆ |

M5 = 0.96Al + 0.04Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.077, T = 294 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Park H.S., Seff K. (2000), J. Phys. Chem. B 104, 2224-2236.

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cF1248

| | | |
|---|--------|--|
| Cd ₁₁ Al ₂₂ Si ₂₆ O ₉₆ [H ₂ O] _{34.5} | cF1248 | (203) <i>Fd</i> -3 - g ¹¹ fe ⁴ c |
|---|--------|--|

Cd₄₄Al₈₈Si₁₀₄O₃₈₄·138H₂O [1], zeolite FAU-Cd partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cd at the centers of hexagonal prisms, opposite double 6-rings in β cages, near the centers of single 6-rings and near 12-rings in supercages, H₂O distributed over six sites.

Calligaris M. et al. (1986) [1]

Al_{22.01}Cd_{12.96}H_{68.80}O_{130.40}Si_{25.99}

$a = 2.4818$ nm, $V = 15.2862$ nm³, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|-----------------------------|-----------------------------|------|---|
| O1 | 96g | 1 | 0.001 | 0.3521 | 0.1473 | | non-colinear AlSi |
| (OH ₂)2 | 96g | 1 | 0.02 | 0.03 | 0.424 | 0.18 | |
| Si3 | 96g | 1 | 0.0365 | 0.1253 | 0.3011 | | tetrahedron O ₄ |
| M4 | 96g | 1 | 0.0365 | 0.3025 | 0.1268 | | tetrahedron O ₄ |
| Cd5 | 96g | 1 | 0.04 | 0.087 | 0.416 | 0.06 | |
| (OH ₂)6 | 96g | 1 | 0.045 | 0.421 | 0.084 | 0.31 | non-colinear Cd(OH ₂) |
| (OH ₂)7 | 96g | 1 | 0.048 | 0.097 | 0.51 | 0.17 | non-coplanar triangle (OH ₂) ₂ Cd |
| O8 | 96g | 1 | 0.0714 | 0.274 | 0.1761 | | non-colinear AlSi |
| O9 | 96g | 1 | 0.0751 | 0.076 | 0.3237 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.1487 | 0.2521 | 0.2519 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.268 | 0.275 | 0.312 | 0.38 | non-colinear (OH ₂) ₂ |
| (OH ₂)12 | 48f | 2.. | 0.43 | ¹ / ₈ | ¹ / ₈ | 0.12 | coplanar square (OH ₂) ₂ Cd ₂ |
| Cd13 | 32e | .3. | 0.0726 | 0.0726 | 0.0726 | 0.72 | octahedron (OH ₂) ₃ O ₃ |
| (OH ₂)14 | 32e | .3. | 0.1665 | 0.1665 | 0.1665 | | tetrahedron Cd ₄ |
| Cd15 | 32e | .3. | 0.2248 | 0.2248 | 0.2248 | 0.36 | |
| Cd16 | 32e | .3. | 0.2469 | 0.2469 | 0.2469 | 0.27 | |
| Cd17 | 16c | -.3. | 0 | 0 | 0 | 0.18 | octahedron O ₆ |

M4 = 0.917Al + 0.083Si

Experimental: single crystal, diffractometer, X-rays, R = 0.088

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Calligaris M., Nardin G., Randaccio L., Zangrando E. (1986), *Zeolites* 6, 439-444.

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cF1264

| | | |
|---|--------|---------------------------|
| $\text{Na}_{7.5}\text{Mg}_{7.75}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_{50}$ | cF1264 | (203) $Fd-3 - g^{11}e^6c$ |
|---|--------|---------------------------|

$\text{Na}_{30}\text{Mg}_{31}\text{Al}_{92}\text{Si}_{100}\text{O}_{382}\cdot 200\text{H}_2\text{O}$ [1], zeolite FAU-Mg,Na hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, (Na,Mg) opposite double 6-rings in β cages and near the centers of single 6-rings in supercages, additional Mg in supercages, H_2O distributed over six sites.

Anderson A.A. et al. (1990) [1]

$\text{Al}_{23.04}\text{H}_{53.12}\text{Mg}_{4.80}\text{Na}_{6.80}\text{O}_{122.56}\text{Si}_{24.96}$

$a = 2.506 \text{ nm}$, $V = 15.7378 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|--|
| O1 | 96g | 1 | 0.0 | 0.1401 | 0.3554 | | non-coplanar triangle SiAlMg |
| (OH ₂)2 | 96g | 1 | 0.003 | 0.01 | 0.386 | 0.17 | |
| (OH ₂)3 | 96g | 1 | 0.023 | 0.404 | 0.028 | 0.13 | |
| Mg4 | 96g | 1 | 0.033 | 0.081 | 0.404 | 0.08 | |
| Si5 | 96g | 1 | 0.0354 | 0.1248 | 0.3031 | | tetrahedron O ₄ |
| M6 | 96g | 1 | 0.037 | 0.3036 | 0.1264 | | tetrahedron O ₄ |
| O7 | 96g | 1 | 0.0705 | 0.1748 | 0.2823 | | non-collinear SiAl |
| O8 | 96g | 1 | 0.0726 | 0.0751 | 0.3219 | | non-collinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.08 | 0.145 | 0.442 | 0.31 | |
| (OH ₂)10 | 96g | 1 | 0.104 | 0.42 | 0.141 | 0.09 | |
| O11 | 96g | 1 | 0.1447 | 0.2549 | 0.2526 | | non-collinear SiAl |
| Mg12 | 32e | .3. | 0.06 | 0.06 | 0.06 | 0.23 | |
| Na13 | 32e | .3. | 0.0706 | 0.0706 | 0.0706 | 0.29 | |
| (OH ₂)14 | 32e | .3. | 0.1689 | 0.1689 | 0.1689 | 0.7 | single atom Mg |
| Mg15 | 32e | .3. | 0.213 | 0.213 | 0.213 | 0.13 | |
| Na16 | 32e | .3. | 0.232 | 0.232 | 0.232 | 0.22 | |
| (OH ₂)17 | 32e | .3. | 0.2631 | 0.2631 | 0.2631 | 0.52 | |
| Na18 | 16c | -.3. | 0 | 0 | 0 | 0.68 | 8-vertex polyhedron Mg ₂ O ₆ |

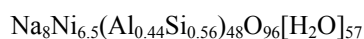
$\text{M6} = 0.96\text{Al} + 0.04\text{Si}$

Transformation from published data: $-y, -x, -z$

Experimental: single crystal, diffractometer, X-rays, $R = 0.056$, $T = 298 \text{ K}$

Remarks: Part of non framework cations and H_2O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Anderson A.A., Shepelev Y.F., Smolin Y.I. (1990), *Zeolites* 10, 32-37.



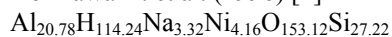
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(203) $Fd\bar{3} - g^{12}e^3c$

Na₃₃Ni₂₅Al₈₃Si₁₀₉O₃₈₄·xH₂O [1], zeolite FAU-Ni²⁺, Na hydrated

Structural features: (Si,Al)O₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms and opposite single 6-rings in supercages, Ni opposite double 6-rings in β cages and single 6-rings in supercages, H₂O distributed over six sites.

Horikawa Y. et al. (1996) [1]



$a = 2.4946 \text{ nm}$, $V = 15.5240 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.001 | 0.353 | 0.14 | | non-colinear Si ₂ |
| (OH ₂)2 | 96g | 1 | 0.017 | 0.406 | 0.056 | 0.59 | single atom (OH ₂) |
| (OH ₂)3 | 96g | 1 | 0.029 | 0.48 | 0.12 | 0.29 | single atom (OH ₂) |
| M4 | 96g | 1 | 0.035 | 0.2993 | 0.126 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0359 | 0.1238 | 0.3041 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.056 | 0.09 | 0.55 | 0.18 | non-colinear (OH ₂) ₂ |
| (OH ₂)7 | 96g | 1 | 0.059 | 0.082 | 0.427 | 0.3 | single atom (OH ₂) |
| (OH ₂)8 | 96g | 1 | 0.068 | 0.077 | 0.14 | 0.57 | non-colinear (OH ₂) ₂ |
| O9 | 96g | 1 | 0.071 | 0.076 | 0.321 | | non-colinear Si ₂ |
| O10 | 96g | 1 | 0.072 | 0.176 | 0.2822 | | non-colinear Si ₂ |
| (OH ₂)11 | 96g | 1 | 0.088 | 0.444 | 0.144 | 0.45 | single atom (OH ₂) |
| O12 | 96g | 1 | 0.1458 | 0.251 | 0.256 | | non-colinear Si ₂ |
| Ni13 | 32e | .3. | 0.0626 | 0.0626 | 0.0626 | 0.3 | non-coplanar triangle (OH ₂) ₃ |
| Na14 | 32e | .3. | 0.2403 | 0.2403 | 0.2403 | 0.3 | |
| Ni15 | 32e | .3. | 0.274 | 0.274 | 0.274 | 0.22 | |
| Na16 | 16c | -.3. | 0 | 0 | 0 | 0.23 | 8-vertex polyhedron O ₆ Ni ₂ |

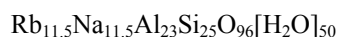
M4 = 0.567Si + 0.433Al; M5 = 0.567Si + 0.433Al

Transformation from published data: -y, -x, -z

Experimental: powder, diffractometer, X-rays, R = 0.026

Remarks: Approximate composition, Na_{29.8}Ni_{24.8}Al_{83.2}Si₁₀₉O₃₈₄·xH₂O from chemical analysis. We assigned approximate values to the Al/Si ratio of former sites AlSi1 and AlSi2 based on the chemical analysis. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. A disordered arrangement of Si and Al, assumed by the authors, is unusual for space group (203) $Fd\bar{3}$.

References: [1] Horikawa Y., Ohnishi N., Hiraga K. (1996), Mater. Sci. & Eng., A 217/218, 139-141.



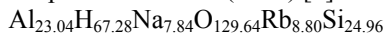
cF1328

(203) $Fd\bar{3} - g^{12}e^5c$

Rb₄₆Na₄₆Al₉₂Si₁₀₀O₃₈₂·xH₂O [1], zeolite FAU-Rb, Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na opposite double 6-rings in β cages and near the centers of single 6-rings, Rb opposite double 6-rings in β cages, 6- and 4-rings in supercages, H₂O distributed over seven sites.

Shepelev Y.F. et al. (1991) [1]



$$a = 2.512 \text{ nm}, V = 15.8511 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|---|
| O1 | 96g | 1 | 0.0003 | 0.3574 | 0.1469 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.008 | 0.496 | 0.117 | 0.23 | non-coplanar triangle (OH ₂) ₃ |
| (OH ₂)3 | 96g | 1 | 0.024 | 0.029 | 0.413 | 0.2 | non-colinear (OH ₂) ₂ |
| Si4 | 96g | 1 | 0.0356 | 0.1235 | 0.3036 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.0365 | 0.3043 | 0.1251 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.038 | 0.125 | 0.47 | 0.11 | |
| (OH ₂)7 | 96g | 1 | 0.044 | 0.469 | 0.133 | 0.11 | |
| (OH ₂)8 | 96g | 1 | 0.056 | 0.067 | 0.422 | 0.34 | single atom (OH ₂) |
| O9 | 96g | 1 | 0.07 | 0.0711 | 0.3213 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.0749 | 0.1704 | 0.2837 | | non-colinear SiAl |
| Rb11 | 96g | 1 | 0.088 | 0.158 | 0.447 | 0.1 | |
| O12 | 96g | 1 | 0.1411 | 0.2543 | 0.2516 | | non-colinear SiAl |
| Na13 | 32e | .3. | 0.0607 | 0.0607 | 0.0607 | 0.7 | |
| Rb14 | 32e | .3. | 0.072 | 0.072 | 0.072 | 0.09 | |
| (OH ₂)15 | 32e | .3. | 0.1672 | 0.1672 | 0.1672 | 0.77 | tetrahedron NaRb ₃ |
| Na16 | 32e | .3. | 0.2186 | 0.2186 | 0.2186 | 0.28 | |
| Rb17 | 32e | .3. | 0.2613 | 0.2613 | 0.2613 | 0.71 | |
| (OH ₂)18 | 16c | -.3. | 0 | 0 | 0 | 0.93 | colinear Na ₂ |

$$\text{M5} = 0.96\text{Al} + 0.04\text{Si}$$

Experimental: single crystal, diffractometer, X-rays, R = 0.045, T = 298 K

Remarks: Part of non framework cations and H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Shepelev Y.F., Butikova I.K., Smolin Y.I. (1991), Zeolites 11, 287-292.

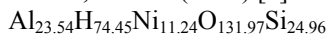
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cF1400



(H₃O)₄₆Ni₂(NiOH)₃₅(Ni₄AlO₄)₂Al₉₁Si₁₀₁O₃₈₄ [1], zeolite FAU-Ni²⁺, H partly hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Al(Ni₄O₄) clusters or four H₃O⁺ in β cages (disorder), additional Ni at the centers of hexagonal prisms and in supercages, the latter causing hydrolysis (NiOH + H₃O).

Bae D., Seff K. (2000) [1]



$$a = 2.4788 \text{ nm}, V = 15.2309 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|-------|---|
| O1 | 96g | 1 | 0.0005 | 0.1422 | 0.3552 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.0112 | 0.4904 | 0.1329 | 0.208 | non-colinear (OH ₂) ₂ |
| (OH ₂)3 | 96g | 1 | 0.0134 | 0.4004 | 0.0283 | 0.208 | single atom (OH ₂) |
| (OH ₂)4 | 96g | 1 | 0.0236 | 0.4579 | 0.0864 | 0.208 | non-coplanar triangle Ni(OH ₂) ₂ |
| Ni5 | 96g | 1 | 0.0339 | 0.4025 | 0.0818 | 0.104 | non-colinear (OH ₂) ₂ |

| | | | | | | | |
|----------------------|-----|------|---------------|---------------|---------------|-------|--|
| Ni6 | 96g | 1 | 0.0357 | 0.0803 | 0.4064 | 0.208 | non-colinear Ni(OH ₂) |
| Si7 | 96g | 1 | 0.0361 | 0.1253 | 0.3032 | | tetrahedron O ₄ |
| M8 | 96g | 1 | 0.0371 | 0.3031 | 0.1261 | | tetrahedron O ₄ |
| (OH ₂)9 | 96g | 1 | 0.0403 | 0.1305 | 0.4638 | 0.104 | single atom (OH ₂) |
| O10 | 96g | 1 | 0.0709 | 0.1761 | 0.2813 | | non-colinear SiAl |
| O11 | 96g | 1 | 0.0737 | 0.0739 | 0.3228 | | non-colinear SiAl |
| (OH)12 | 96g | 1 | 0.1041 | 0.1383 | 0.4398 | 0.208 | single atom (OH) |
| O13 | 96g | 1 | 0.1452 | 0.2545 | 0.2537 | | non-colinear SiAl |
| Ni14 | 32e | .3. | 0.0672 | 0.0672 | 0.0672 | 0.25 | 7-vertex polyhedron O ₃ Al(OH ₃) ₃ |
| M15 | 32e | .3. | 0.1658 | 0.1658 | 0.1658 | | single atom Al |
| Ni16 | 32e | .3. | 0.2387 | 0.2387 | 0.2387 | 0.156 | |
| (OH ₃)17 | 32e | .3. | 0.264 | 0.264 | 0.264 | 0.688 | |
| Ni18 | 16c | -.3. | 0 | 0 | 0 | 0.125 | 8-vertex polyhedron O ₆ Ni ₂ |
| Al19 | 8a | 23. | $\frac{1}{8}$ | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.25 | tetrahedron (OH ₃) ₄ |

M8 = 0.96Al + 0.04Si; M15 = 0.75OH₃ + 0.25O

Transformation from published data: -y,-x,-z

Experimental: single crystal, diffractometer, X-rays, R = 0.080, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Space group (227) *Fd-3m* was tested and rejected. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. In table 3 of [1] the Wyckoff position of former O(8) and O(9) is misprinted as 192i instead of 96g.

References: [1] Bae D., Seff K. (2000), Microporous Mesoporous Mater. 40, 219-232.

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| | | |
|---|--------|--|
| Cd _{13.9} Al ₂₃ Si ₂₅ O ₉₆ [OH] _{4.8} [H ₂ O] ₅₀ | cF1424 | (203) <i>Fd-3</i> – g ¹³ e ⁵ c |
|---|--------|--|

Cd_{55.1}Al₉₂Si₁₀₀O₃₈₄(OH)₁₉·xH₂O [1], zeolite FAU-Cd hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cd near the centers of single 6-rings, above the centers of double 6-rings in β cages and on several sites in supercages; (OH,H₂O) above the centers of single 6-rings in β cages.

Smolin Y.I. et al. (1998) [1]

Al_{23.04}Cd_{13.76}H_{61.27}O_{129.02}Si_{24.96}

a = 2.4858 nm, *V* = 15.3603 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------|-------|------|----------|----------|----------|-------|-----------------------------------|
| O1 | 96g | 1 | 0.0012 | 0.1451 | 0.3505 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.005 | 0.4 | 0.016 | 0.094 | |
| (OH ₂)3 | 96g | 1 | 0.022 | 0.066 | 0.41 | 0.448 | |
| Cd4 | 96g | 1 | 0.023 | 0.0665 | 0.4098 | 0.057 | |
| Si5 | 96g | 1 | 0.03647 | 0.12478 | 0.30116 | | tetrahedron O ₄ |
| M6 | 96g | 1 | 0.03725 | 0.30222 | 0.12663 | | tetrahedron O ₄ |
| Cd7 | 96g | 1 | 0.0449 | 0.0824 | 0.4155 | 0.077 | |
| Cd8 | 96g | 1 | 0.052 | 0.42 | 0.079 | 0.031 | |
| O9 | 96g | 1 | 0.0725 | 0.1733 | 0.2741 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.0743 | 0.0771 | 0.3237 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.091 | 0.155 | 0.442 | 0.156 | non-colinear Cd(OH ₂) |
| O12 | 96g | 1 | 0.1492 | 0.253 | 0.2511 | | non-colinear SiAl |
| (OH ₂)13 | 96g | 1 | 0.2512 | 0.264 | 0.347 | 0.156 | single atom (OH ₂) |

| | | | | | | | |
|----------------------|-----|------|---------|---------|---------|-------|---|
| Cd14 | 32e | .3. | 0.07299 | 0.07299 | 0.07299 | 0.766 | octahedron (OH) ₃ O ₃ |
| M15 | 32e | .3. | 0.1667 | 0.1667 | 0.1667 | 0.903 | tetrahedron Cd ₄ |
| Cd16 | 32e | .3. | 0.22432 | 0.22432 | 0.22432 | 0.253 | |
| Cd17 | 32e | .3. | 0.2472 | 0.2472 | 0.2472 | 0.206 | |
| (OH ₂)18 | 32e | .3. | 0.2718 | 0.2718 | 0.2718 | 0.406 | |
| (OH ₂)19 | 16c | -.3. | 0 | 0 | 0 | 0.513 | octahedron O ₆ |

M6 = 0.96Al + 0.04Si; M15 = 0.66OH + 0.34OH₂

Experimental: single crystal, diffractometer, X-rays, R = 0.046, T = 293 K

Remarks: Part of H₂O not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (1998), Kristallografiya 43, 421-424.

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[NH₄]₁₇Hg₁₁Al₂₃Si₂₅Cl₁₆O₉₆

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(203) *Fd*-3 - g¹³e⁵d

(NH₄)₆₈Hg₄₄Al₉₂Si₁₀₀O₃₈₄Cl₆₄ [1], zeolite FAU-Hg²⁺ (NH₄Cl)

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; cationic (HgCl₂)_m(NH₄⁺)_n clusters in supercages, additional Hg at the centers of hexagonal prisms (6-coordinated) and above the centers of single 6-rings (3-coordinated).

Zhen S., Seff K. (1999) [1]

Al_{23.04}Cl_{16.01}Hg_{68.03}N_{17.01}O₉₆Si_{24.96}

a = 2.5094 nm, *V* = 15.8019 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------|-------|------|----------|----------|----------|-------|--------------------------------------|
| O1 | 96g | 1 | 0.0014 | 0.1104 | 0.3909 | | non-colinear SiAl |
| Hg2 | 96g | 1 | 0.0043 | 0.3196 | 0.1788 | 0.125 | |
| Cl3 | 96g | 1 | 0.0052 | 0.2756 | 0.1531 | 0.208 | |
| O4 | 96g | 1 | 0.0062 | 0.3569 | 0.0073 | | non-colinear SiAl |
| Cl5 | 96g | 1 | 0.0103 | 0.1413 | 0.2583 | 0.292 | |
| Hg6 | 96g | 1 | 0.0301 | 0.1722 | 0.3198 | 0.083 | |
| Si7 | 96g | 1 | 0.0361 | 0.1239 | 0.447 | | tetrahedron O ₄ |
| M8 | 96g | 1 | 0.0365 | 0.4465 | 0.1244 | | tetrahedron O ₄ |
| Hg9 | 96g | 1 | 0.0448 | 0.3236 | 0.1693 | 0.083 | |
| Hg10 | 96g | 1 | 0.0596 | 0.179 | 0.3282 | 0.083 | |
| O11 | 96g | 1 | 0.067 | 0.0695 | 0.4623 | | non-colinear SiAl |
| O12 | 96g | 1 | 0.0773 | 0.1717 | 0.4314 | | non-colinear SiAl |
| Cl13 | 96g | 1 | 0.1097 | 0.2989 | 0.1101 | 0.167 | |
| Hg14 | 32e | .3. | 0.051 | 0.051 | 0.051 | 0.063 | |
| (NH ₄)15 | 32e | .3. | 0.0802 | 0.0802 | 0.0802 | 0.938 | |
| (NH ₄)16 | 32e | .3. | 0.2417 | 0.2417 | 0.2417 | 0.938 | |
| Hg17 | 32e | .3. | 0.2552 | 0.2552 | 0.2552 | 0.063 | |
| (NH ₄)18 | 32e | .3. | 0.4201 | 0.4201 | 0.4201 | 0.25 | non-coplanar triangle O ₃ |
| Hg19 | 16d | -.3. | 1/2 | 1/2 | 1/2 | 0.25 | octahedron O ₆ |

M8 = 0.96Al + 0.04Si

Transformation from published data: -*y*, -*x*, -*z*; origin shift 1/2 1/2 1/2

Experimental: single crystal, diffractometer, X-rays, R = 0.121, T = 296 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Zhen S., Seff K. (1999), J. Phys. Chem. B 103, 10409-10416.

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| | | |
|---|--------|-----------------------------|
| $\text{Cd}_{11}\text{Al}_{22}\text{Si}_{26}\text{O}_{96}[\text{H}_2\text{O}]_{58.25}$ | cF1440 | (203) $Fd-3 - g^{13}f^2e^3$ |
|---|--------|-----------------------------|

$\text{Cd}_{44}\text{Al}_{88}\text{Si}_{104}\text{O}_{384} \cdot 233\text{H}_2\text{O}$ [1], zeolite FAU-Cd hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Cd opposite double 6-rings in β cages, opposite 6- and 4-rings in supercages, H_2O distributed over nine sites (high degree of disorder).

Calligaris M. et al. (1986) [1]

$\text{Al}_{22.01}\text{Cd}_{12.24}\text{H}_{116.32}\text{O}_{154.16}\text{Si}_{25.99}$

$a = 2.4797 \text{ nm}$, $V = 15.2475 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------------|---------------|------|---|
| O1 | 96g | 1 | 0.0014 | 0.1032 | 0.4014 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.0013 | 0.3491 | 0.003 | | non-colinear SiAl |
| (OH ₂)3 | 96g | 1 | 0.003 | 0.02 | 0.148 | 0.53 | non-colinear (OH ₂) ₂ |
| (OH ₂)4 | 96g | 1 | 0.007 | 0.204 | 0.336 | 0.29 | |
| Cd5 | 96g | 1 | 0.033 | 0.171 | 0.338 | 0.08 | |
| Si6 | 96g | 1 | 0.0371 | 0.1255 | 0.4502 | | tetrahedron O ₄ |
| M7 | 96g | 1 | 0.0375 | 0.4495 | 0.1234 | | tetrahedron O ₄ |
| (OH ₂)8 | 96g | 1 | 0.049 | 0.326 | 0.166 | 0.29 | |
| (OH ₂)9 | 96g | 1 | 0.055 | 0.16 | 0.324 | 0.37 | |
| (OH ₂)10 | 96g | 1 | 0.059 | 0.098 | 0.097 | 0.21 | |
| O11 | 96g | 1 | 0.0722 | 0.0781 | 0.4788 | | non-colinear SiAl |
| O12 | 96g | 1 | 0.0751 | 0.171 | 0.4259 | | non-colinear SiAl |
| (OH ₂)13 | 96g | 1 | 0.087 | 0.087 | 0.301 | 0.2 | single atom (OH ₂) |
| (OH ₂)14 | 48f | 2.. | 0.092 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.14 | |
| (OH ₂)15 | 48f | 2.. | 0.325 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.26 | non-colinear (OH ₂) ₂ |
| Cd16 | 32e | .3. | 0.2501 | 0.2501 | 0.2501 | 0.36 | octahedron O ₃ (OH ₂) ₃ |
| (OH ₂)17 | 32e | .3. | 0.3343 | 0.3343 | 0.3343 | | non-coplanar triangle Cd ₃ |
| Cd18 | 32e | .3. | 0.42543 | 0.42543 | 0.42543 | 0.93 | octahedron (OH ₂) ₃ O ₃ |

$M7 = 0.917\text{Al} + 0.083\text{Si}$

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.082

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Calligaris M., Nardin G., Randaccio L., Zangrando E. (1986), Zeolites 6, 439-444.

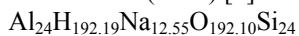
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| | | |
|--|--------|---------------------------|
| $\text{Na}_{24}\text{Al}_{24}\text{Si}_{24}\text{O}_{96}[\text{H}_2\text{O}]_{96}$ | cF1456 | (203) $Fd-3 - g^{14}e^3c$ |
|--|--------|---------------------------|

$\text{Na}_{96}\text{Al}_{96}\text{Si}_{96}\text{O}_{384} \cdot x\text{H}_2\text{O}$ [1], faujasite-(Na), zeolite FAU-Na hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, opposite double 6-rings in β cages and opposite single 6-rings in supercages, H_2O distributed over nine sites (high degree of disorder).

Lee Y. et al. (1998) [1]



$$a = 2.50491 \text{ nm}, V = 15.7172 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------|---------|-------|---|
| O1 | 96g | 1 | 0.0007 | 0.3594 | 0.1456 | | non-collinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.016 | 0.1 | 0.498 | 0.512 | single atom (OH ₂) |
| (OH ₂)3 | 96g | 1 | 0.021 | 0.056 | 0.421 | 0.582 | non-coplanar triangle (OH ₂) ₃ |
| Si4 | 96g | 1 | 0.03443 | 0.12544 | 0.30223 | | tetrahedron O ₄ |
| Al5 | 96g | 1 | 0.03738 | 0.30411 | 0.12669 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.046 | 0.133 | 0.463 | 0.372 | non-collinear (OH ₂) ₂ |
| (OH ₂)7 | 96g | 1 | 0.052 | 0.432 | 0.085 | 0.594 | non-collinear (OH ₂) ₂ |
| O8 | 96g | 1 | 0.0681 | 0.1771 | 0.2826 | | non-collinear SiAl |
| O9 | 96g | 1 | 0.0741 | 0.0783 | 0.322 | | non-collinear SiAl |
| (OH ₂)10 | 96g | 1 | 0.077 | 0.544 | 0.109 | 0.488 | non-coplanar triangle (OH ₂) ₃ |
| (OH ₂)11 | 96g | 1 | 0.078 | 0.093 | 0.154 | 0.27 | |
| (OH ₂)12 | 96g | 1 | 0.088 | 0.158 | 0.442 | 0.653 | single atom (OH ₂) |
| O13 | 96g | 1 | 0.145 | 0.2533 | 0.2527 | | non-collinear SiAl |
| (OH ₂)14 | 96g | 1 | 0.273 | 0.283 | 0.304 | 0.387 | |
| Na15 | 32e | .3. | 0.0612 | 0.0612 | 0.0612 | 0.291 | |
| (OH ₂)16 | 32e | .3. | 0.072 | 0.072 | 0.072 | 0.438 | |
| Na17 | 32e | .3. | 0.2354 | 0.2354 | 0.2354 | 0.925 | |
| Na18 | 16c | -.3. | 0 | 0 | 0 | 0.706 | 8-vertex polyhedron O ₆ Na ₂ |

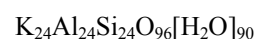
Transformation from published data: -y, -x, -z

Experimental: powder, diffractometer, X-rays, $R_B = 0.059$

Remarks: Part of Na not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee Y., Carr S.W., Parise J.B. (1998), Chem. Mater. 10, 2561-2570.

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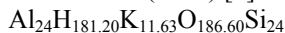
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(203) $Fd\bar{3} - g^{14}e^3c$

K₉₅NaAl₉₆Si₉₆O₃₈₄·xH₂O [1], zeolite FAU-K hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; K at the centers of hexagonal prisms and opposite single 6-rings in supercages, H_2O distributed over ten sites (high degree of disorder).

Lee Y. et al. (1998) [1]



$$a = 2.52486 \text{ nm}, V = 16.0958 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|-------|--------------------------------|
| O1 | 96g | 1 | 0.0001 | 0.3598 | 0.1429 | | non-collinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.015 | 0.11 | 0.515 | 0.345 | single atom (OH ₂) |
| (OH ₂)3 | 96g | 1 | 0.017 | 0.045 | 0.416 | 0.566 | single atom (OH ₂) |

| | | | | | | | |
|----------------------|-----|------|---------|---------|---------|-------|--|
| Si4 | 96g | 1 | 0.0336 | 0.12545 | 0.3043 | | tetrahedron O ₄ |
| (OH ₂)5 | 96g | 1 | 0.037 | 0.107 | 0.463 | 0.318 | non-colinear (OH ₂) ₂ |
| Al6 | 96g | 1 | 0.03763 | 0.30506 | 0.12495 | | tetrahedron O ₄ |
| (OH ₂)7 | 96g | 1 | 0.059 | 0.433 | 0.077 | 0.504 | non-colinear (OH ₂) ₂ |
| (OH ₂)8 | 96g | 1 | 0.066 | 0.156 | 0.464 | 0.39 | non-colinear (OH ₂) ₂ |
| O9 | 96g | 1 | 0.0687 | 0.0739 | 0.3196 | | non-colinear SiAl |
| (OH ₂)10 | 96g | 1 | 0.07 | 0.09 | 0.16 | 0.503 | |
| O11 | 96g | 1 | 0.0713 | 0.1742 | 0.2861 | | non-colinear SiAl |
| (OH ₂)12 | 96g | 1 | 0.082 | 0.437 | 0.159 | 0.52 | |
| (OH ₂)13 | 96g | 1 | 0.085 | 0.104 | 0.552 | 0.279 | non-colinear (OH ₂) ₂ |
| O14 | 96g | 1 | 0.1408 | 0.2547 | 0.2535 | | non-colinear SiAl |
| (OH ₂)15 | 32e | .3. | 0.0748 | 0.0748 | 0.0748 | 0.731 | |
| K16 | 32e | .3. | 0.2514 | 0.2514 | 0.2514 | 0.969 | bicapped square prism (OH ₂) ₄ O ₆ |
| (OH ₂)17 | 32e | .3. | 0.314 | 0.314 | 0.314 | 0.319 | non-coplanar triangle (OH ₂) ₃ |
| K18 | 16c | -.3. | 0 | 0 | 0 | 0.969 | octahedron O ₆ |

Transformation from published data: -y,-x,-z

Experimental: powder, diffractometer, X-rays, R_B = 0.063

Remarks: Small amounts of Na ignored, part of K not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee Y., Carr S.W., Parise J.B. (1998), Chem. Mater. 10, 2561-2570.

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| | | |
|--|--------|---|
| Na ₂₄ Al ₂₄ Ge ₂₄ O ₉₆ [H ₂ O] ₁₂₀ | cF1456 | (203) <i>Fd</i> -3 - g ¹⁴ e ³ c |
|--|--------|---|

Na₉₆Al₉₆Ge₉₆O₃₈₄·xH₂O [1], zeolite FAU(Ge)-Na hydrated

Structural features: GeO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, opposite double 6-rings in β cages and opposite single 6-rings in supercages, H₂O distributed over nine sites (high degree of disorder).

Johnson G.M. et al. (1999) [1]

Al₂₄Ge₂₄H_{233.44}Na_{12.76}O_{212.72}

a = 2.5589 nm, *V* = 16.7556 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------|-------|------|----------|----------|----------|------|---|
| O1 | 96g | 1 | 0.0026 | 0.1434 | 0.3577 | | non-colinear AlGe |
| (OH ₂)2 | 96g | 1 | 0.019 | 0.035 | 0.416 | 0.8 | non-colinear (OH ₂) ₂ |
| (OH ₂)3 | 96g | 1 | 0.03 | 0.491 | 0.123 | 0.53 | single atom (OH ₂) |
| Ge4 | 96g | 1 | 0.03562 | 0.30237 | 0.12646 | | tetrahedron O ₄ |
| Al5 | 96g | 1 | 0.03697 | 0.12739 | 0.30188 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.061 | 0.095 | 0.436 | 0.92 | non-coplanar triangle (OH ₂) ₃ |
| (OH ₂)7 | 96g | 1 | 0.062 | 0.07 | 0.552 | 0.35 | |
| O8 | 96g | 1 | 0.0672 | 0.2789 | 0.1821 | | non-colinear AlGe |
| O9 | 96g | 1 | 0.0791 | 0.0795 | 0.3244 | | non-colinear AlGe |
| (OH ₂)10 | 96g | 1 | 0.082 | 0.083 | 0.167 | 0.45 | |
| (OH ₂)11 | 96g | 1 | 0.092 | 0.435 | 0.146 | 0.71 | non-coplanar triangle (OH ₂) ₃ |
| O12 | 96g | 1 | 0.1488 | 0.2535 | 0.2522 | | non-colinear AlGe |
| (OH ₂)13 | 96g | 1 | 0.241 | 0.307 | 0.322 | 0.53 | single atom (OH ₂) |
| (OH ₂)14 | 96g | 1 | 0.305 | 0.352 | 0.349 | 0.48 | non-coplanar triangle (OH ₂) ₃ |
| Na15 | 32e | .3. | 0.0715 | 0.0715 | 0.0715 | 0.4 | |

| | | | | | | | |
|----------------------|-----|------|--------|--------|--------|------|---|
| Na16 | 32e | .3. | 0.2431 | 0.2431 | 0.2431 | 0.72 | |
| (OH ₂)17 | 32e | .3. | 0.273 | 0.273 | 0.273 | 0.28 | tetrahedron Na(OH ₂) ₃ |
| Na18 | 16c | -.3. | 0 | 0 | 0 | 0.95 | octahedron O ₆ |

Experimental: powder, diffractometer, X-rays, $wR_p = 0.023$

Remarks: Part of Na not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Johnson G.M., Lee Y., Tripathi A., Parise J.B. (1999), Microporous Mesoporous Mater. 31, 195-204.

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| | | |
|---|--------|---------------------------|
| $K_{21}Na_3Al_{24}Si_{24}O_{96}[H_2O]_{96}$ | cF1488 | (203) $Fd-3 - g^{14}e^4c$ |
|---|--------|---------------------------|

K₇₇Na₁₉Al₉₆Si₉₆O₃₈₄·xH₂O [1], zeolite FAU-K,Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; K at the centers of hexagonal prisms and above the centers of double 6-rings in β cages, additional K and Na above single 6-rings in supercages, H₂O distributed over nine sites.

Lee Y. et al. (1998) [1]

$Al_{24}H_{192.83}K_{11.54}Na_{1.20}O_{192.42}Si_{24}$
 $a = 2.52086$ nm, $V = 16.0194$ nm³, $Z = 4$

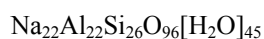
| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------|---------|-------|---|
| O1 | 96g | 1 | 0.0003 | 0.1429 | 0.3544 | | non-collinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.01 | 0.032 | 0.414 | 0.39 | non-coplanar triangle (OH ₂) ₃ |
| (OH ₂)3 | 96g | 1 | 0.022 | 0.114 | 0.474 | 0.37 | non-coplanar triangle (OH ₂) ₃ |
| Si4 | 96g | 1 | 0.03548 | 0.12563 | 0.30343 | | tetrahedron O ₄ |
| Al5 | 96g | 1 | 0.03727 | 0.3048 | 0.12208 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.038 | 0.101 | 0.528 | 0.355 | non-collinear (OH ₂) ₂ |
| (OH ₂)7 | 96g | 1 | 0.05 | 0.436 | 0.07 | 0.768 | non-collinear (OH ₂) ₂ |
| O8 | 96g | 1 | 0.0667 | 0.0732 | 0.3237 | | non-collinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.069 | 0.161 | 0.088 | 0.435 | |
| (OH ₂)10 | 96g | 1 | 0.072 | 0.442 | 0.163 | 0.76 | single atom (OH ₂) |
| O11 | 96g | 1 | 0.0764 | 0.1718 | 0.2855 | | non-collinear SiAl |
| (OH ₂)12 | 96g | 1 | 0.078 | 0.127 | 0.45 | 0.4 | non-collinear (OH ₂) ₂ |
| (OH ₂)13 | 96g | 1 | 0.097 | 0.114 | 0.551 | 0.259 | non-collinear (OH ₂) ₂ |
| O14 | 96g | 1 | 0.1423 | 0.2548 | 0.2525 | | non-collinear SiAl |
| K15 | 32e | .3. | 0.0729 | 0.0729 | 0.0729 | 0.287 | |
| Na16 | 32e | .3. | 0.2303 | 0.2303 | 0.2303 | 0.15 | |
| K17 | 32e | .3. | 0.2524 | 0.2524 | 0.2524 | 0.8 | |
| (OH ₂)18 | 32e | .3. | 0.311 | 0.311 | 0.311 | 0.841 | non-coplanar triangle (OH ₂) ₃ |
| K19 | 16c | -.3. | 0 | 0 | 0 | 0.712 | 8-vertex polyhedron O ₆ K ₂ |

Transformation from published data: -y,-x,-z

Experimental: powder, diffractometer, X-rays, $R_B = 0.086$

Remarks: Part of K and Na not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee Y., Carr S.W., Parise J.B. (1998), Chem. Mater. 10, 2561-2570.



cF1520

(203) $Fd\bar{3} - g^{14}e^5c$

Na₈₈Al₈₈Si₁₀₄O₃₈₄·220H₂O [1], faujasite-(Na), zeolite FAU-Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, opposite double 6-rings in β cages and opposite single 6-rings in supercages (split site), H₂O distributed over ten sites (high degree of disorder).

Olson D.H. (1970) [1]

Al_{22.08}H_{86.08}Na_{10.24}O_{139.04}Si_{25.92}
 $a = 2.5028 \text{ nm}$, $V = 15.6776 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------|---------|------|---|
| O1 | 96g | 1 | 0.0002 | 0.3599 | 0.1446 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.008 | 0.454 | 0.088 | 0.14 | single atom (OH ₂) |
| (OH ₂)3 | 96g | 1 | 0.01 | 0.011 | 0.392 | 0.29 | single atom (OH ₂) |
| Si4 | 96g | 1 | 0.03509 | 0.12543 | 0.30291 | | tetrahedron O ₄ |
| M5 | 96g | 1 | 0.03671 | 0.30352 | 0.12691 | | tetrahedron O ₄ |
| (OH ₂)6 | 96g | 1 | 0.038 | 0.113 | 0.462 | 0.17 | non-coplanar triangle (OH ₂) ₃ |
| (OH ₂)7 | 96g | 1 | 0.046 | 0.076 | 0.422 | 0.18 | non-colinear (OH ₂) ₂ |
| (OH ₂)8 | 96g | 1 | 0.062 | 0.45 | 0.119 | 0.1 | non-colinear (OH ₂) ₂ |
| O9 | 96g | 1 | 0.068 | 0.177 | 0.2821 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.0739 | 0.0772 | 0.3206 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.074 | 0.086 | 0.157 | 0.27 | |
| (OH ₂)12 | 96g | 1 | 0.095 | 0.147 | 0.436 | 0.31 | single atom (OH ₂) |
| O13 | 96g | 1 | 0.1445 | 0.2541 | 0.2525 | | non-colinear SiAl |
| (OH ₂)14 | 96g | 1 | 0.275 | 0.298 | 0.281 | 0.13 | |
| Na15 | 32e | .3. | 0.06 | 0.06 | 0.06 | 0.25 | |
| (OH ₂)16 | 32e | .3. | 0.074 | 0.074 | 0.074 | 0.36 | |
| Na17 | 32e | .3. | 0.23 | 0.23 | 0.23 | 0.38 | |
| Na18 | 32e | .3. | 0.238 | 0.238 | 0.238 | 0.37 | |
| (OH ₂)19 | 32e | .3. | 0.245 | 0.245 | 0.245 | 0.25 | |
| Na20 | 16c | -.3. | 0 | 0 | 0 | 0.56 | 8-vertex polyhedron Na ₂ O ₆ |

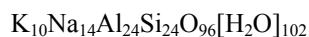
M5 = 0.92Al + 0.08Si

Transformation from published data: -y,-x,-z

Experimental: single crystal, photographs, X-rays, R = 0.088

Remarks: Part of Na not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Olson D.H. (1970), J. Phys. Chem. 74, 2758-2764.



cF1520

(203) $Fd\bar{3} - g^{14}e^5c$

K₄₀Na₅₆Al₉₆Si₉₆O₃₈₄·xH₂O [1], zeolite FAU-K,Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, K and additional Na above the centers of double 6-rings in β cages and single 6-rings in supercages, H₂O distributed over nine sites (high degree of disorder).

Lee Y. et al. (1998) [1]



$$a = 2.50385 \text{ nm}, V = 15.6973 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------|---------|-------|--|
| O1 | 96g | 1 | 0.0011 | 0.3593 | 0.1449 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.015 | 0.054 | 0.419 | 0.66 | non-colinear (OH ₂) ₂ |
| (OH ₂)3 | 96g | 1 | 0.028 | 0.12 | 0.469 | 0.48 | single atom (OH ₂) |
| (OH ₂)4 | 96g | 1 | 0.034 | 0.088 | 0.514 | 0.36 | single atom (OH ₂) |
| Si5 | 96g | 1 | 0.03402 | 0.12534 | 0.30289 | | tetrahedron O ₄ |
| Al6 | 96g | 1 | 0.03765 | 0.30337 | 0.1271 | | tetrahedron O ₄ |
| (OH ₂)7 | 96g | 1 | 0.058 | 0.438 | 0.085 | 0.69 | non-colinear (OH ₂) ₂ |
| O8 | 96g | 1 | 0.0669 | 0.1774 | 0.283 | | non-colinear SiAl |
| (OH ₂)9 | 96g | 1 | 0.07 | 0.091 | 0.157 | 0.39 | |
| O10 | 96g | 1 | 0.0749 | 0.0789 | 0.3218 | | non-colinear SiAl |
| (OH ₂)11 | 96g | 1 | 0.079 | 0.546 | 0.102 | 0.41 | square pyramid (OH ₂) ₅ |
| (OH ₂)12 | 96g | 1 | 0.083 | 0.156 | 0.443 | 0.95 | single atom (OH ₂) |
| O13 | 96g | 1 | 0.1448 | 0.2532 | 0.2522 | | non-colinear SiAl |
| (OH ₂)14 | 96g | 1 | 0.269 | 0.296 | 0.302 | 0.153 | |
| Na15 | 32e | .3. | 0.0612 | 0.0612 | 0.0612 | 0.04 | |
| K16 | 32e | .3. | 0.0738 | 0.0738 | 0.0738 | 0.29 | |
| Na17 | 32e | .3. | 0.2352 | 0.2352 | 0.2352 | 0.36 | |
| K18 | 32e | .3. | 0.2561 | 0.2561 | 0.2561 | 0.54 | |
| (OH ₂)19 | 32e | .3. | 0.32 | 0.32 | 0.32 | 0.49 | |
| Na20 | 16c | -.3. | 0 | 0 | 0 | 0.96 | 8-vertex polyhedron O ₆ Na ₂ |

Transformation from published data: -y,-x,-z

Experimental: powder, diffractometer, X-rays, R_B = 0.061

Remarks: Part of non framework cations not located. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Lee Y., Carr S.W., Parise J.B. (1998), Chem. Mater. 10, 2561-2570.

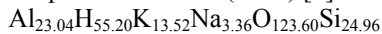
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cF1584

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|---|--------|--|
| $\text{K}_{13}\text{Na}_{10}\text{Al}_{23}\text{Si}_{25}\text{O}_{96}[\text{H}_2\text{O}]_{29.5}$ | cF1584 | (203) <i>Fd-3</i> – g ¹⁵ e ⁴ c |
|---|--------|--|

K₅₂Na₄₀Al₉₂Si₁₀₀O₃₈₂·xH₂O [1], zeolite FAU-K,Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; K at the centers of hexagonal prisms and opposite single 6-rings in supercages, Na and additional K opposite double 6-rings in β cages and on several sites in supercages, H₂O distributed over six sites.

Shepelev Y.F. et al. (1991) [1]



$$a = 2.507 \text{ nm}, V = 15.7566 \text{ nm}^3, Z = 4$$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|---------------------|-------|------|--------|--------|--------|------|----------------------------|
| O1 | 96g | 1 | 0.0005 | 0.3579 | 0.1457 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.026 | 0.459 | 0.11 | 0.08 | |
| Si3 | 96g | 1 | 0.0351 | 0.1231 | 0.3027 | | tetrahedron O ₄ |

| | | | | | | | |
|----------------------|-----|------|--------|--------|--------|------|--|
| M4 | 96g | 1 | 0.0366 | 0.3041 | 0.1258 | | tetrahedron O ₄ |
| Na5 | 96g | 1 | 0.048 | 0.062 | 0.406 | 0.06 | |
| K6 | 96g | 1 | 0.053 | 0.13 | 0.457 | 0.04 | |
| (OH ₂)7 | 96g | 1 | 0.053 | 0.464 | 0.144 | 0.17 | |
| (OH ₂)8 | 96g | 1 | 0.063 | 0.451 | 0.133 | 0.05 | |
| Na9 | 96g | 1 | 0.065 | 0.067 | 0.424 | 0.02 | |
| O10 | 96g | 1 | 0.0703 | 0.0737 | 0.3238 | | non-colinear SiAl |
| O11 | 96g | 1 | 0.0735 | 0.1736 | 0.2831 | | non-colinear SiAl |
| (OH ₂)12 | 96g | 1 | 0.077 | 0.085 | 0.437 | 0.26 | |
| K13 | 96g | 1 | 0.081 | 0.446 | 0.102 | 0.03 | |
| O14 | 96g | 1 | 0.1448 | 0.2541 | 0.2508 | | non-colinear SiAl |
| (OH ₂)15 | 96g | 1 | 0.253 | 0.256 | 0.365 | 0.32 | |
| Na16 | 32e | .3. | 0.053 | 0.053 | 0.053 | 0.18 | |
| K17 | 32e | .3. | 0.0687 | 0.0687 | 0.0687 | 0.42 | |
| (OH ₂)18 | 32e | .3. | 0.167 | 0.167 | 0.167 | 0.81 | non-coplanar triangle K ₃ |
| K19 | 32e | .3. | 0.2572 | 0.2572 | 0.2572 | 0.77 | 9-vertex polyhedron (OH ₂) ₆ O ₃ |
| K20 | 16c | -.3. | 0 | 0 | 0 | 0.58 | colinear Na ₂ |

M4 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.031, T = 298 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Shepelev Y.F., Butikova I.K., Smolin Y.I. (1991), Zeolites 11, 287-292.

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cF1728

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|--|--------|--|
| Cs ₁₁ Na ₁₂ Al ₂₃ Si ₂₅ O ₉₆ [H ₂ O] ₅₅ | cF1728 | (203) <i>Fd</i> -3 - g ¹⁶ fe ⁴ c |
|--|--------|--|

Cs₄₅Na₄₇Al₉₂Si₁₀₀O₃₈₄·220H₂O [1], zeolite FAU-Cs,Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, opposite double 6-rings in β cages and single 6-rings in supercages, Cs opposite 6- and 4-rings in supercages, H₂O distributed over eight sites (disorder).

Butikova I.K. et al. (1989) [1]

Al_{23.04}Cs_{9.84}H_{82.24}Na_{10.20}O_{137.12}Si_{24.96}

a = 2.511 nm, *V* = 15.8322 nm³, *Z* = 4

| site | Wyck. | sym. | <i>x</i> | <i>y</i> | <i>z</i> | occ. | atomic environment |
|----------------------|-------|------|----------|----------|----------|------|--|
| O1 | 96g | 1 | 0.0002 | 0.36 | 0.1442 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.001 | 0.06 | 0.435 | 0.25 | single atom (OH ₂) |
| (OH ₂)3 | 96g | 1 | 0.023 | 0.459 | 0.101 | 0.32 | non-colinear (OH ₂) ₂ |
| (OH ₂)4 | 96g | 1 | 0.025 | 0.125 | 0.45 | 0.28 | |
| Si5 | 96g | 1 | 0.0352 | 0.1257 | 0.303 | | tetrahedron O ₄ |
| M6 | 96g | 1 | 0.0368 | 0.3034 | 0.1271 | | tetrahedron O ₄ |
| (OH ₂)7 | 96g | 1 | 0.051 | 0.127 | 0.454 | 0.14 | |
| O8 | 96g | 1 | 0.0633 | 0.1787 | 0.2819 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.0753 | 0.0786 | 0.3199 | | non-colinear SiAl |
| (OH ₂)10 | 96g | 1 | 0.08 | 0.445 | 0.141 | 0.11 | |
| Cs11 | 96g | 1 | 0.084 | 0.108 | 0.441 | 0.03 | |
| Cs12 | 96g | 1 | 0.1055 | 0.4328 | 0.1095 | 0.07 | |
| Cs13 | 96g | 1 | 0.1062 | 0.1394 | 0.4428 | 0.08 | |

| | | | | | | | |
|----------------------|-----|------|--------|-----------------------------|-----------------------------|------|---|
| O14 | 96g | 1 | 0.1445 | 0.2545 | 0.2527 | | non-colinear SiAl |
| (OH ₂)15 | 96g | 1 | 0.245 | 0.371 | 0.251 | 0.13 | non-colinear (OH ₂) ₂ |
| (OH ₂)16 | 96g | 1 | 0.257 | 0.287 | 0.279 | 0.21 | |
| Cs17 | 48f | 2.. | 0.4293 | ¹ / ₈ | ¹ / ₈ | 0.2 | |
| Na18 | 32e | .3. | 0.07 | 0.07 | 0.07 | 0.53 | octahedron (OH ₂) ₃ O ₃ |
| (OH ₂)19 | 32e | .3. | 0.166 | 0.166 | 0.166 | 0.82 | non-coplanar triangle Na ₃ |
| Na20 | 32e | .3. | 0.236 | 0.236 | 0.236 | 0.37 | |
| Cs21 | 32e | .3. | 0.267 | 0.267 | 0.267 | 0.39 | |
| Na22 | 16c | -.3. | 0 | 0 | 0 | 0.75 | octahedron O ₆ |

M6 = 0.96Al + 0.04Si

Experimental: single crystal, diffractometer, X-rays, R = 0.063, T = 293 K

Remarks: We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments. The same data are also reported in [2]. On page 687 of [1] the chemical formula is misprinted as Cs₄₅Na₄₇Al₉₂Si₁₀O₃₈₄·~220H₂O instead of Cs₄₅Na₄₇Al₉₂Si₁₀₀O₃₈₄·~220H₂O.

References: [1] Butikova I.K., Shepelev Y.F., Smolin Y.I. (1989), Sov. Phys. Crystallogr. (Engl. Transl.) 34, 687-690. [2] Shepelev Y.F., Butikova I.K., Smolin Y.I. (1991), Zeolites 11, 287-292.

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cF1792

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| Na ₁₇ Fe _{2.33} Al ₂₄ Si ₂₄ O ₉₆ [H ₂ O] ₅₀ | cF1792 | (203) <i>Fd</i> -3 – g ¹⁶ fe ⁶ c |
|--|--------|--|

Na₆₈Fe_{9.3}Al₉₆Si₉₆O₃₈₄·xH₂O [1], zeolite FAU-Fe³⁺, Na hydrated

Structural features: SiO₄ and AlO₄ tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; Na at the centers of hexagonal prisms, opposite double 6-rings in β cages and single 6-rings in supercages, H₂O and small amounts of Fe distributed over several sites (high degree of disorder).

Evmerides N.P. et al. (1976) [1]

Al₂₄Fe_{2.31}H_{86.08}Na_{10.24}O_{139.04}Si₂₄
a = 2.5 nm, V = 15.6250 nm³, Z = 4

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|-----------------------------|-----------------------------|-------|---|
| O1 | 96g | 1 | 0.0002 | 0.3599 | 0.1446 | | non-colinear SiAl |
| (OH ₂)2 | 96g | 1 | 0.008 | 0.454 | 0.088 | 0.14 | tetrahedron (OH ₂) ₃ Fe |
| (OH ₂)3 | 96g | 1 | 0.01 | 0.011 | 0.392 | 0.29 | non-colinear (OH ₂) ₂ |
| Fe4 | 96g | 1 | 0.017 | 0.217 | 0.308 | 0.034 | 4-vertex polyhedron NaFe ₂ O |
| Si5 | 96g | 1 | 0.03509 | 0.12543 | 0.30291 | | tetrahedron O ₄ |
| Al6 | 96g | 1 | 0.03671 | 0.30352 | 0.12691 | | tetrahedron O ₄ |
| (OH ₂)7 | 96g | 1 | 0.038 | 0.113 | 0.462 | 0.17 | tetrahedron (OH ₂) ₃ Fe |
| (OH ₂)8 | 96g | 1 | 0.046 | 0.076 | 0.422 | 0.18 | non-coplanar triangle Fe(OH ₂) ₂ |
| Fe9 | 96g | 1 | 0.058 | 0.458 | 0.067 | 0.034 | 4-vertex polyhedron (OH ₂) ₄ |
| (OH ₂)10 | 96g | 1 | 0.062 | 0.45 | 0.119 | 0.1 | non-coplanar triangle Fe(OH ₂) ₂ |
| O11 | 96g | 1 | 0.068 | 0.177 | 0.2821 | | non-coplanar triangle SiAlFe |
| O12 | 96g | 1 | 0.0739 | 0.0772 | 0.3206 | | non-coplanar triangle SiAlFe |
| (OH ₂)13 | 96g | 1 | 0.074 | 0.086 | 0.157 | 0.27 | |
| (OH ₂)14 | 96g | 1 | 0.095 | 0.147 | 0.436 | 0.31 | single atom (OH ₂) |
| O15 | 96g | 1 | 0.1445 | 0.2541 | 0.2525 | | non-colinear SiAl |
| (OH ₂)16 | 96g | 1 | 0.275 | 0.298 | 0.281 | 0.13 | |
| Fe17 | 48f | 2.. | 0.301 | ¹ / ₈ | ¹ / ₈ | 0.034 | tetrahedron O ₄ |
| Fe18 | 32e | .3. | 0.05 | 0.05 | 0.05 | 0.034 | |

| | | | | | | |
|----------------------|-----|------|-------|-------|-------|------|
| Na19 | 32e | .3. | 0.06 | 0.06 | 0.06 | 0.25 |
| (OH ₂)20 | 32e | .3. | 0.074 | 0.074 | 0.074 | 0.36 |
| Na21 | 32e | .3. | 0.23 | 0.23 | 0.23 | 0.38 |
| Na22 | 32e | .3. | 0.238 | 0.238 | 0.238 | 0.37 |
| (OH ₂)23 | 32e | .3. | 0.245 | 0.245 | 0.245 | 0.25 |
| Na24 | 16c | -.3. | 0 | 0 | 0 | 0.56 |

Transformation from published data: -y,-x,-z

Experimental: powder, diffractometer, X-rays

Remarks: Approximate composition, Si/Al ratio not known. Difference Fourier analysis applied after a refinement considering positions for zeolite NaX from [2]; peaks attributed to Fe according to model 2 are included here. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Evmerides N.P., Beagley B., Dwyer J. (1976), Inorg. Chim. Acta 20, 243-250. [2] Olson D.H. (1970), J. Phys. Chem. 74, 2758-2764.

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cF2000

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|---|--------|--|
| $\text{Cd}_{14.8}\text{Al}_{23}\text{Si}_{25}\text{S}_{1.2}\text{O}_{96}[\text{OH}]_{4.2}[\text{H}_2\text{O}]_{20}$ | cF2000 | (203) <i>Fd-3</i> – g^{18}fe^7 |
|---|--------|--|

$\text{Cd}_{59.2}\text{Al}_{92}\text{Si}_{100}\text{S}_{4.8}\text{O}_{384}(\text{OH})_{16.8}\cdot 80\text{H}_2\text{O}$ [1], zeolite FAU-Cd (CdS) hydrated

Structural features: SiO_4 and AlO_4 tetrahedra share vertices to form a FAU-type zeolite framework with β cages (14-face truncated octahedra) interconnected tetrahedrally via hexagonal prisms, and supercages sharing 12-rings; CdS units in supercages, additional Cd opposite double 6-rings in β cages and opposite 6- and 4-rings in supercages, H_2O distributed over ten sites (high degree of disorder).

Smolin Y.I. et al. (1998) [1]

$\text{Al}_{23.04}\text{Cd}_{14.80}\text{H}_{49.94}\text{O}_{120.97}\text{S}_{1.18}\text{Si}_{24.96}$

$a = 2.4847 \text{ nm}$, $V = 15.3399 \text{ nm}^3$, $Z = 4$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|---------|---------------|---------------|-------|--|
| O1 | 96g | 1 | 0.0 | 0.3489 | 0.002 | | non-colinear SiAl |
| O2 | 96g | 1 | 0.001 | 0.1023 | 0.4008 | | non-colinear SiAl |
| (OH ₂)3 | 96g | 1 | 0.003 | 0.014 | 0.161 | 0.115 | non-colinear (OH ₂) ₂ |
| (OH ₂)4 | 96g | 1 | 0.003 | 0.316 | 0.18 | 0.094 | |
| Cd5 | 96g | 1 | 0.009 | 0.051 | 0.056 | 0.017 | |
| (OH ₂)6 | 96g | 1 | 0.027 | 0.035 | 0.127 | 0.055 | single atom (OH ₂) |
| Cd7 | 96g | 1 | 0.028 | 0.183 | 0.339 | 0.03 | |
| Si8 | 96g | 1 | 0.0369 | 0.12528 | 0.44977 | | tetrahedron O ₄ |
| Cd9 | 96g | 1 | 0.0373 | 0.065 | 0.1832 | 0.033 | |
| M10 | 96g | 1 | 0.03727 | 0.44915 | 0.12396 | | tetrahedron O ₄ |
| Cd11 | 96g | 1 | 0.038 | 0.334 | 0.201 | 0.027 | |
| Cd12 | 96g | 1 | 0.0527 | 0.16 | 0.3296 | 0.098 | |
| (OH ₂)13 | 96g | 1 | 0.053 | 0.061 | 0.274 | 0.125 | single atom (OH ₂) |
| Cd14 | 96g | 1 | 0.0561 | 0.3284 | 0.1569 | 0.045 | |
| O15 | 96g | 1 | 0.0733 | 0.0769 | 0.4782 | | non-colinear SiAl |
| O16 | 96g | 1 | 0.0752 | 0.1718 | 0.4251 | | non-colinear SiAl |
| (OH ₂)17 | 96g | 1 | 0.096 | 0.097 | 0.252 | 0.073 | non-colinear Cd(OH ₂) |
| (OH ₂)18 | 96g | 1 | 0.101 | 0.267 | 0.271 | 0.063 | |
| (OH ₂)19 | 48f | 2.. | 0.328 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.104 | non-colinear Cd ₂ |
| (OH ₂)20 | 32e | .3. | 0.053 | 0.053 | 0.053 | 0.134 | |
| S21 | 32e | .3. | 0.089 | 0.089 | 0.089 | 0.056 | |
| S22 | 32e | .3. | 0.142 | 0.142 | 0.142 | 0.091 | |

| | | | | | | | |
|----------------------|-----|-----|---------|---------|---------|-------|---|
| (OH ₂)23 | 32e | .3. | 0.239 | 0.239 | 0.239 | 0.34 | |
| Cd24 | 32e | .3. | 0.25179 | 0.25179 | 0.25179 | 0.25 | |
| (OH ₂)25 | 32e | .3. | 0.3358 | 0.3358 | 0.3358 | 0.916 | non-coplanar triangle Cd ₃ |
| Cd26 | 32e | .3. | 0.4263 | 0.4263 | 0.4263 | 0.85 | octahedron (OH ₂) ₃ O ₃ |

M10 = 0.96Al + 0.04Si

Transformation from published data: -y, -x, -z; origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.052, T = 298 K

Remarks: OH not located. We assigned an approximate value to the Al/Si ratio of former site Al based on the nominal composition. Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Smolin Y.I., Shepelev Y.F., Lapshin A.E., Vasil'eva E.A. (1998), Crystallogr. Rep. 43, 387-394 (Kristallografiya 43, 425-432).

203
cF2304

| | | |
|---|--------|--------------------------------------|
| NaAl[SiO ₄][H ₂ O] _{1.35} | cF2304 | (203) <i>Fd</i> -3 - g ²⁴ |
|---|--------|--------------------------------------|

NaAlSiO₄·1.35H₂O [1], zeolite LTN

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a zeolite framework with α (26-face truncated cuboctahedra), β (14-face truncated octahedra) and other cages.

Fälth L., Andersson S. (1982) [1]

AlO₄Si

$a = 3.693$ nm, $V = 50.3661$ nm³, $Z = 384$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|------|-------|------|--------|--------|--------|------|----------------------------|
| Al1 | 96g | 1 | 0.0013 | 0.128 | 0.3068 | | tetrahedron O ₄ |
| Al2 | 96g | 1 | 0.0017 | 0.1247 | 0.0639 | | tetrahedron O ₄ |
| Si3 | 96g | 1 | 0.0022 | 0.063 | 0.1246 | | tetrahedron O ₄ |
| O4 | 96g | 1 | 0.0026 | 0.3445 | 0.1552 | | non-colinear SiAl |
| O5 | 96g | 1 | 0.0031 | 0.0714 | 0.4292 | | non-colinear SiAl |
| O6 | 96g | 1 | 0.0037 | 0.0849 | 0.324 | | non-colinear SiAl |
| Si7 | 96g | 1 | 0.0042 | 0.3106 | 0.1284 | | tetrahedron O ₄ |
| O8 | 96g | 1 | 0.0048 | 0.3264 | 0.0874 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.0057 | 0.0764 | 0.501 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.0137 | 0.0157 | 0.3186 | | non-colinear SiAl |
| O11 | 96g | 1 | 0.0143 | 0.0882 | 0.0907 | | non-colinear SiAl |
| Al12 | 96g | 1 | 0.0224 | 0.4646 | 0.0852 | | tetrahedron O ₄ |
| Si13 | 96g | 1 | 0.0264 | 0.0851 | 0.4643 | | tetrahedron O ₄ |
| O14 | 96g | 1 | 0.0315 | 0.4566 | 0.1306 | | non-colinear SiAl |
| O15 | 96g | 1 | 0.0338 | 0.128 | 0.4592 | | non-colinear SiAl |
| O16 | 96g | 1 | 0.0347 | 0.0362 | 0.136 | | non-colinear SiAl |
| O17 | 96g | 1 | 0.041 | 0.2882 | 0.1362 | | non-colinear SiAl |
| O18 | 96g | 1 | 0.0417 | 0.1376 | 0.2836 | | non-colinear SiAl |
| O19 | 96g | 1 | 0.0649 | 0.4656 | 0.0652 | | non-colinear SiAl |
| O20 | 96g | 1 | 0.0873 | 0.0902 | 0.2584 | | non-colinear SiAl |
| O21 | 96g | 1 | 0.1138 | 0.2805 | 0.2867 | | non-colinear SiAl |
| Al22 | 96g | 1 | 0.2037 | 0.2662 | 0.3296 | | tetrahedron O ₄ |
| Si23 | 96g | 1 | 0.2041 | 0.3286 | 0.2661 | | tetrahedron O ₄ |
| O24 | 96g | 1 | 0.2096 | 0.3015 | 0.2996 | | non-colinear SiAl |

Transformation from published data (origin choice 1): origin shift $\frac{1}{8} \frac{1}{8} \frac{1}{8}$

Experimental: single crystal, diffractometer, X-rays, $R = 0.124$

Remarks: Na and H₂O not located. Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Fäth L., Andersson S. (1982), Z. Kristallogr. 160, 313-316.

203
cF4080

| | | |
|--|--------|---------------------------|
| NaAl[SiO ₄][H ₂ O] _{1.1} | cF4080 | (203) $Fd-3 - g^{39}fe^9$ |
|--|--------|---------------------------|

NaAlSiO₄·1.1H₂O [1], zeolite LTN

Structural features: AlO₄ and SiO₄ tetrahedra share vertices to form a zeolite framework with α (26-face truncated cuboctahedra), β cages (14-face truncated octahedra) and other cages; Na and H₂O distributed over several sites (high degree of disorder).

Shepelev I.F. et al. (1983) [1]

AlH_{2.05}Na_{1.02}O_{5.03}Si

$a = 3.695$ nm, $V = 50.4479$ nm³, $Z = 384$

| site | Wyck. | sym. | x | y | z | occ. | atomic environment |
|----------------------|-------|------|--------|--------|--------|------|----------------------------|
| Al1 | 96g | 1 | 0.0016 | 0.1279 | 0.3066 | | tetrahedron O ₄ |
| Si2 | 96g | 1 | 0.0019 | 0.0633 | 0.1248 | | tetrahedron O ₄ |
| O3 | 96g | 1 | 0.0029 | 0.3444 | 0.1556 | | non-colinear SiAl |
| O4 | 96g | 1 | 0.0037 | 0.0709 | 0.4302 | | non-colinear SiAl |
| Na5 | 96g | 1 | 0.0041 | 0.389 | 0.1115 | 0.25 | |
| Si6 | 96g | 1 | 0.0044 | 0.3103 | 0.1287 | | tetrahedron O ₄ |
| O7 | 96g | 1 | 0.0046 | 0.0844 | 0.3233 | | non-colinear SiAl |
| O8 | 96g | 1 | 0.006 | 0.3261 | 0.0877 | | non-colinear SiAl |
| O9 | 96g | 1 | 0.0067 | 0.0777 | 0.5018 | | non-colinear SiAl |
| O10 | 96g | 1 | 0.0139 | 0.0152 | 0.3186 | | non-colinear SiAl |
| O11 | 96g | 1 | 0.0143 | 0.0887 | 0.0917 | | non-colinear SiAl |
| Na12 | 96g | 1 | 0.0189 | 0.1084 | 0.386 | 0.15 | |
| Na13 | 96g | 1 | 0.0223 | 0.3889 | 0.1121 | 0.6 | |
| Al14 | 96g | 1 | 0.0227 | 0.465 | 0.0853 | | tetrahedron O ₄ |
| Si15 | 96g | 1 | 0.027 | 0.0852 | 0.4642 | | tetrahedron O ₄ |
| O16 | 96g | 1 | 0.0303 | 0.4564 | 0.1307 | | non-colinear SiAl |
| O17 | 96g | 1 | 0.034 | 0.1272 | 0.4583 | | non-colinear SiAl |
| O18 | 96g | 1 | 0.0349 | 0.0365 | 0.1355 | | non-colinear SiAl |
| O19 | 96g | 1 | 0.0417 | 0.1374 | 0.2846 | | non-colinear SiAl |
| O20 | 96g | 1 | 0.0417 | 0.2884 | 0.1365 | | non-colinear SiAl |
| Na21 | 96g | 1 | 0.0494 | 0.1999 | 0.2983 | 0.23 | |
| Na22 | 96g | 1 | 0.0605 | 0.1879 | 0.3156 | 0.24 | |
| Al23 | 96g | 1 | 0.0641 | 0.2516 | 0.1251 | | tetrahedron O ₄ |
| O24 | 96g | 1 | 0.0648 | 0.4661 | 0.0653 | | non-colinear SiAl |
| (OH ₂)25 | 96g | 1 | 0.0672 | 0.3821 | 0.0911 | 0.2 | |
| (OH ₂)26 | 96g | 1 | 0.0673 | 0.0841 | 0.3801 | 0.17 | |
| Na27 | 96g | 1 | 0.0695 | 0.0705 | 0.3177 | | |
| Na28 | 96g | 1 | 0.073 | 0.1758 | 0.3278 | 0.46 | |
| (OH ₂)29 | 96g | 1 | 0.0752 | 0.3807 | 0.0758 | 0.63 | |
| (OH ₂)30 | 96g | 1 | 0.0849 | 0.388 | 0.1558 | 0.6 | |
| O31 | 96g | 1 | 0.0866 | 0.0894 | 0.258 | | non-colinear SiAl |
| (OH ₂)32 | 96g | 1 | 0.0996 | 0.4529 | 0.1487 | 0.61 | |
| (OH ₂)33 | 96g | 1 | 0.1029 | 0.1434 | 0.3896 | 0.36 | |
| (OH ₂)34 | 96g | 1 | 0.1053 | 0.4724 | 0.1412 | 0.38 | |

| | | | | | | | |
|----------------------|-----|-----|--------|---------------|---------------|------|--|
| O35 | 96g | 1 | 0.1143 | 0.2808 | 0.286 | | non-colinear SiAl |
| Al36 | 96g | 1 | 0.2035 | 0.2664 | 0.3294 | | tetrahedron O ₄ |
| Si37 | 96g | 1 | 0.204 | 0.3283 | 0.2654 | | tetrahedron O ₄ |
| O38 | 96g | 1 | 0.2083 | 0.3018 | 0.2995 | | non-colinear SiAl |
| (OH ₂)39 | 96g | 1 | 0.2937 | 0.2949 | 0.3543 | 0.29 | single atom Na |
| (OH ₂)40 | 48f | 2.. | 0.3268 | $\frac{1}{8}$ | $\frac{1}{8}$ | 0.86 | |
| Na41 | 32e | .3. | 0.0436 | 0.0436 | 0.0436 | 0.09 | |
| Na42 | 32e | .3. | 0.0678 | 0.0678 | 0.0678 | 0.21 | |
| Na43 | 32e | .3. | 0.0816 | 0.0816 | 0.0816 | 0.53 | |
| Na44 | 32e | .3. | 0.1964 | 0.1964 | 0.1964 | 0.77 | tetrahedron (OH ₂)O ₃ |
| (OH ₂)45 | 32e | .3. | 0.2315 | 0.2315 | 0.2315 | 0.89 | colinear Na ₂ |
| Na46 | 32e | .3. | 0.2663 | 0.2663 | 0.2663 | 0.26 | |
| Na47 | 32e | .3. | 0.2868 | 0.2868 | 0.2868 | 0.56 | |
| (OH ₂)48 | 32e | .3. | 0.4246 | 0.4246 | 0.4246 | 0.4 | single atom Na |
| Na49 | 32e | .3. | 0.458 | 0.458 | 0.458 | | tetrahedron (OH ₂)O ₃ |

Transformation from published data: origin shift $\frac{1}{2} \frac{1}{2} \frac{1}{2}$

Experimental: single crystal, diffractometer, X-rays, R = 0.051

Remarks: Short interatomic distances for partly occupied site(s). Hydrogen atoms are not taken into consideration for Pearson symbol, Wyckoff sequence and atomic environments.

References: [1] Shepelev I.F., Smolin I.I., Butikova I.K., Tarasov V.I. (1983), Dokl. Akad. Nauk SSSR 272, 1133-1137.