There are three zeolites whose nominal compositions can be represented by the general formula \( \text{CaAl}_2\text{Si}_4\text{O}_{12} \cdot n\text{H}_2\text{O} \): chabazite \((n = 6)\), laumontite \((n = 4)\), and wairakite \((n = 2)\). The name chabazite is derived from Greek \( \text{chabazios} \), an ancient name of a stone celebrated in a poem ascribed to Orpheus. The mineral was discovered in 1792 \[1\]. The exact date of the discovery of laumontite is unknown. It was first named lomonite by Jameson \[2\] in 1805 and laumonite by Haüy \[3\] in 1809. The current name was given by von Leonhard \[4\] in 1821. It is named for Gillet de Lau-mont (1747–1834), who discovered the mineral and transmitted specimens to Haüy in 1801 \[5\]. Wairakite was originally found in 1955 in the Wairakei geothermal zone, New Zealand, about 6 km north-northwest of Lake Taupo (North Island) \[6, 7\].

Yet another mineral with this cation stoichiometry, \( \text{CaAl}_2\text{Si}_4\text{O}_{12} \cdot 3.5\text{H}_2\text{O} \) \((n = 3.5)\), was called leonhardtite before the International Commission on New Minerals and Minerals Names qualified it as a partially dehydrated laumontite rather than as an individual species \[8\].

In the Strunz classification, chabazite, laumontite, and wairakite belong to different series: willhenderso-nite–chabazite–perlialite, ferrierite–laumontite, and analcime–paulingite.

These zeolites are close in density: chabazite, 2.05–2.15; laumontite, 2.25–2.35; wairakite, 2.26 g/cm³. Mohs’ hardness decreases in going from wairakite (5.5–6) to chabazite (4) and to laumontite (3–4).

The three-dimensional framework of zeolites is made up of corner-shared \( \text{Si}_4\text{O}_{12} \) and \( \text{Al}_4\text{O}_{12} \) tetrahedra. The zeolites under consideration are identical in Si and Al contents. It is, therefore, of interest to examine the effect of water content on the structural framework of these zeolites and to reveal similar and dissimilar features of their structures. This issue is addressed in this paper.

In contrast to the general formula above, the three zeolites typically contain alkali metals on the calcium site and have broad solid-solution ranges. Chabazite crystallizes in rhombohedral symmetry \[9\], whereas laumontite and wairakite have monoclinic structures \[10–13\] (Table 1).

<table>
<thead>
<tr>
<th>Structure</th>
<th>Framework Type</th>
<th>Similar/Unique Features</th>
</tr>
</thead>
<tbody>
<tr>
<td>Chabazite</td>
<td>4- and 6-membered rings</td>
<td>Network of oxygen–hydrogen bonds between intraframework oxygens and water molecules</td>
</tr>
<tr>
<td>Laumontite</td>
<td>Alternating aluminum and silicon layers</td>
<td>Ordered arrangement of silicon and aluminum sites</td>
</tr>
<tr>
<td>Wairakite</td>
<td></td>
<td>No oxygen–hydrogen bonds between water molecules</td>
</tr>
</tbody>
</table>

The transition from the chabazite framework to the laumontite framework can be interpreted in terms of the ordering and displacement of aluminum and silicon atoms. In addition to the differences between the frameworks of laumontite and wairakite, which are attributable to the fact that these zeolites were formed at different temperatures and pressures, they differ in the relative arrangement of the water molecules and calcium atoms, which cannot be accounted for by different formation conditions.
CRYSTAL STRUCTURES OF ZEOLITES WITH THE GENERAL FORMULA CaAl$_2$Si$_4$O$_{12}$ · nH$_2$O

Table 1. Nominal and empirical compositions and lattice parameters of chabazite, laumontite, and wairakite

VIII/J.26-30, chabazite, CaAl$_2$Si$_4$O$_{12}$ · 6H$_2$O

Rhombohedral symmetry, R$\bar{3}$m (166)

Ca$_{1.95}$Al$_{0.9}$Si$_{0.1}$O$_{1.24}$ · 13H$_2$O [9]

$\alpha = 9.42$ Å, $b = 9.42$ Å, $c = 9.42$ Å, $\alpha = 94.47^\circ$, $\beta = 94.47^\circ$, $\gamma = 94.47^\circ$, $V = 827.85$ Å$^3$

(in a hexagonal setting: $a = 13.675$ Å, $c = 14.767$ Å)

VIII/J.22-50, laumontite, CaAl$_2$Si$_4$O$_{12}$ · 4H$_2$O

Monoclinic symmetry, C$_2$/m (12)

Ca$_{4.2}$Al$_{2}$Si$_{4}$O$_{12}$ · 13.2H$_2$O [10]

$\alpha = 14.724$ Å, $b = 13.075$ Å, $c = 7.559$ Å, $\beta = 112.01^\circ$, $V = 1349.17$ Å$^3$

Ca$_4$Al$_2$Si$_4$O$_{16}$ · 16H$_2$O [11]

$\alpha = 14.863$ Å, $b = 13.169$ Å, $c = 7.537$ Å, $\beta = 110.18^\circ$, $V = 1384.66$ Å$^3$

Ca$_{3.88}$Na$_{0.15}$K$_{0.03}$Al$_{0.00}$Si$_{16.00}$O$_{48}$ · nH$_2$O [12]

$n = 12.50(4)$

$n = 12.70(4)$

$n = 12.89(5)$

$n = 14.04(6)$

$n = 14.09(7)$

$n = 17.16(5)$

$n = 14.8494(2)$ Å, $b = 13.1792(1)$ Å, $c = 7.53672(9)$ Å, $\beta = 110.50(1)^\circ$, $V = 1381.52$ Å$^3$

$n = 17.29(5)$

VIII/J.27-30, wairakite, CaAl$_2$Si$_4$O$_{12}$ · 2H$_2$O

Monoclinic symmetry, I2/a (15)

Ca$_{7.19}$Na$_{0.01}$Al$_{15.38}$Si$_{32.50}$O$_{96}$ · 16H$_2$O [13]

$a = 13.692$ Å, $b = 13.643$ Å, $c = 13.550$ Å, $\beta = 90.5^\circ$, $V = 2532.91$ Å$^3$

Cules, and chabazite should contain 12 water molecules per unit cell.

Figure 1 illustrates the key features of the structural framework of chabazite. A salient feature of the framework is that it has identical projections along the three axes (as an example, Fig. 1 shows the ab projection). The aluminum and silicon atoms form a 12-membered ring; stacking of unit cells along one of the axis gives an eight-membered ring. The eight-membered rings are linked along the other two axes by four-membered rings and along the diagonal by a polyhedron produced by rotation of a right hexagonal prism. The example of eight unit cells demonstrates that the 12-membered rings are linked in the [111] direction so as to form regular hexagons separated by quadrangles. When viewed along [101], the structure is clearly seen to contain eight-membered rings separated by two types of four-membered rings.