Tilt and tetrahedra distortions in the zeolite A framework
W. Depmeier
Tilt and Tetrahedra Distortions in the Zeolite A Framework

by

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Abstract: A geometrical analysis of the zeolite A framework concerning the effects of the deviations from ideal geometry on the lattice parameter, the coordinates of the framework atoms and the T-O-T angles has been undertaken with the restriction of only one T atom present. The total deviation of the real framework from a hypothetical one, consisting of ideal TO₄ tetrahedra parallel to the unit cell edges, has been decomposed into three contributions: i) a cooperative rotation (tilt) of the tetrahedra about axes parallel to <100>; ii) distortions of the O-T-O angles of the TO₄ tetrahedra; iii) bond length distortions of the tetrahedra. The 0(1) atom has been used to differentiate i) from ii). The main results obtained are: i) the lattice parameter passes through a maximum on varying the tilt angle; θ(T-O(1)-T) increases, θ(T-O(2)-T)(beyond a maximum) and θ(T-O(3)-T) decrease with increasing tilt angle; ii) the angular tetrahedron distortion is explained as being composed of two contributions, one of which is determined by the framework composition, the other one depending essentially on the interchangeable cations. The mapping of 3D zeolite A species reveals that most of these scatter about a relaxed state with almost maximal lattice parameter and minimal deviations of the T-O-T angles from their mean value. Deviations from the relaxed state - by decreasing or increasing tilt angle- result in increasing structural strains, whereby limits are set to the stability field of the zeolite A framework. A clear correlation exists between tilt angle and bond length distortion of the TO₄ tetrahedra.
Annex 1

The Geometry of the Zeolite A Framework Being Tilted and Consisting of $T_4$
Tetrahedra with Angular and Bond Length Distortion.

Fig. A1 is a more detailed version of the corresponding figure in the main part
of this paper. In particular, it contains the designations for three tetrahedra,
viz. A, B, C. Their projection onto the horizontal edge of the unit cell define
the lattice parameter and the fractional coordinates of the framework atoms. The
appropriate designations are indicated on the top of the drawing. In addition to
the designations listed in Table 2, the following expressions have been used:
d$_{ij}$ and t$_{ij}$ are the tetrahedron edge formed by O(i) and O(j), t$_{ij}$ is the
projection of the corresponding edge onto the plane of the drawing; M is the pro-
jection of the atom O(3) onto the same plane and p is the distance M-T. The angles
M-T-O(1) and M-T-O(2) are designated $\alpha'$ and $\delta'$, respectively, whereas the angle
O(2)-M-T is named 42MT; other angles are designated correspondingly.

Each of the three tetrahedra marked A, B, C makes its contribution to the
lattice parameter $a$. We shall calculate the contributions of each of them to $a/2$
and call them also A, B, C.

A: The contribution of this tetrahedron is not affected by the tilt; it is, thus,
simply one half of the edge length d$_{33}$:

$$A = \frac{1}{2}d_{33} = \ell_3\sin\frac{1}{2}$$  \hspace{1cm} (1)

B: This tetrahedron contributes with the projection of t$_{23}$ onto the cell edge. We
consider first the effects of tetrahedron distortion and find

$$t_{23} = \left[p^2 + \ell_2^2 - 2p\ell_2\cos(360^\circ - \gamma - \alpha')\right]^{1/2}$$  \hspace{1cm} (2)

with

$$p = \ell_3\cos\frac{\gamma}{2}$$  \hspace{1cm} (3)

and

$$\alpha' = \arccos(\cos\alpha/\cos\frac{\gamma}{2})$$  \hspace{1cm} (4)

From the cosine law one obtains

$$42MT = \arccos\left(\frac{t_{23}^2 + p^2 - \ell_2^2}{2pt_{23}}\right)$$  \hspace{1cm} (5)
and, because $a'_{\text{ideal}} = 125.26^0$, the angle between $t_{23}$ and the parallel to the cell edge becomes

$$\varphi_B = \frac{\varphi_{12}}{2} - (a'_{\text{ideal}} - 125.26^0)$$

(6).

For the tilted framework this angle has to be decreased by the tilt angle $\varphi$ and the contribution of the tetrahedron $B$ becomes:

$$B = t_{23}\cos(\varphi_B - \varphi)$$

(7).

C: The contribution of tetrahedron $C$ is the projection of $d_{12}$ onto the cell edge.

$$d_{12} = (l_1^2 + l_2^2 - 2l_1l_2\cos\varphi_{23})^{1/2}$$

(8).

We note that the ideal value for $\varphi_{12}$ is $35.26^0$. For the distorted tetrahedron it becomes

$$\varphi_{12} = \arccos(\sin^2\varphi_{23})$$

(9).

Now, taking into account the tilt angle, one finds

$$C = d_{12}\cos\arccos(\sin^2\varphi_{23}) - 35.26^0 + \varphi$$

(10).

The expression for the lattice parameter is obtained by combining eqs. (1), (7), (10)

$$a = 2l_3\sin^2\varphi_{23} + t_{23}\cos(\varphi_B - \varphi) + \frac{d_{12}\cos\arccos(\sin^2\varphi_{23}) - 35.26^0 + \varphi}{\alpha}$$

(11).

$x_3$ and $x_2$ are then easily calculated from (1) and (11) and (1), (7) and (11), respectively:

$$x_3 = (l_3\sin^2\varphi_{23})/a$$

$$x_2 = (l_3\sin^2\varphi_{23} + t_{23}\cos(\varphi_B - \varphi))/a$$

(12).

(13).

The calculation of $x_1$ requires the knowledge of

$$t_{13} = (p^2 + l_1^2 - 2pl_1\cos\varphi_{13})^{1/2}$$

(14).

and of

$$\frac{\varphi_{13}}{2} = \arccos(-\frac{l_1^2 - t_{13}^2 - p^2}{2pt_{13}})$$

(15).

Because of $a'_{\text{ideal}} = 125.26^0$, the angle between $t_{13}$ and the horizontal cell edge is

$$\frac{\varphi_{13}}{2} + a'_{\text{ideal}} = 125.26^0$$

(16).

for the effects of tetrahedron distortion alone. For the tilted framework this angle has to be increased by $\varphi$. Thus, we obtain

$$x_1 = \frac{(l_3\sin^2\varphi_{23} + t_{13}\cos(\frac{\varphi_{13}}{2} + a'_{\text{ideal}} - 125.26^0 + \varphi))}{a}$$

(17).

$z_3$ is the projection of $t_{13}$ of tetrahedron $C$ onto $d_{12}$ of the undistorted, zero-tilt structure. For the calculation $\frac{\varphi_{13}}{2}$ is necessary which is, in fact,
that of ideal tetrahedra: \( \phi_{12} = \phi_{12,\text{ideal}} = 35.26^\circ \) \( \tag{18} \)

Furthermore, the knowledge of \( \phi_{MT} \) is required:

\[
\phi_{MT} = \arccos\left(\frac{1 - \cos\alpha}{1 + \cos^2\gamma - 2\cos\gamma}\right)
\] \( \tag{19} \)

The sum of these angles has to be decreased by \( \phi \) and \( z_3 \) becomes

\[
z_3 = \frac{1}{3} \left( \frac{\phi_{MT} + 35.26^\circ - \phi}{a} \right)
\] \( \tag{20} \)

\( y_T \) and \( z_T \) are obtained similarly:

\[
y_T = 1 - \left( \frac{\ell_1 \cos(35.26^\circ - \phi)}{a} \right)
\] \( \tag{21} \)

\[
z_T = \frac{1}{3} \left( \frac{\ell_3 \sin^2 \gamma + p \cos(a' - 125.26^\circ + \phi)}{a} \right)
\] \( \tag{22} \)

The angles T-O-T are

\[
\gamma = 109.47^\circ + 2 \phi, \text{ by definition,}
\] \( \tag{23} \)

and

\[
\alpha = 180^\circ - \left( 100^\circ - 1100^\circ - 160.53^\circ - 2(109.47^\circ - \phi) - 2\phi \right)
\] \( \tag{24} \)

and

\[
\gamma = \arccos\left( 1 - \frac{\alpha^2}{\ell_3^2} \right)
\] \( \tag{25} \)

with

\[
\alpha = a' - 125.26^\circ + \phi.
\]

If \( a, \phi, \) and \( \gamma \) are given, \( \gamma \) can be calculated from

\[
\gamma = \cos^2\alpha \cos(360^\circ - \arccos(\cos \alpha / \cos \gamma)) - \phi
\] \( \tag{26} \)

The \( a = f(\phi) \) curve has a maximum at

\[
\phi_{\text{max}} = \arctan\left( \frac{\frac{t_23 \sin B}{t_23 \cos B} + d_1 \sin(\arccos(\sin^2 \gamma - 35.26^\circ))}{\frac{t_23 \sin B}{t_23 \cos B} - d_1 \cos(\arccos(\sin^2 \gamma) - 35.26^\circ)} \right)
\] \( \tag{27} \)

The size of the aperture of the O-rings is limited by the shorter of the distances between opposite O(1) or O(2) atoms, respectively, across the B-rings:

\[
D_{11} = (1 - 2x_1)a
\] \( \tag{28} \)

\[
D_{22} = \sqrt{2}(1 - 2x_2)a
\] \( \tag{29} \)

where \( D_{11} \) and \( D_{22} \) correspond to O(1) and O(2) atoms, respectively.
Observed structural data for zeolite A frameworks, arranged according to increasing tilt angle. The various species can be identified by the symbol in the first column; this is usually the chemical symbol of the principal exchangeable cation, preceded by d or h (for dehydrated or hydrated); p stands for partially. The same symbols have been used in Fig.3. The second column contains the lattice parameters; those observed are given above the corresponding value normalized to the average T-O bond length (1.6636 Å) for the zeolites in this table. The following column contains individual and mean T-O bond distances with the standard deviation of the latter as a measure for the bond-length distortion of the T0₄ tetrahedron. The fourth and fifth column contain information on O-T-O, T-O-T and tilt angles. The last column gives the references; these should be consulted for any further information desired. The structural data in this table refer to the pseudosymmetric 12 R unit cell, space group Pm3m, with no distinction between different T cations. Where in the literature only the ordered structure is given, the distances and angles reported are those calculated from the averaged atomic positions.
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**Table 1, page 2**

*References:
Pluth & Smith, J. Am. Chem. Soc. 102, 4704 (1980)
Kim et al., ACS Symp. Ser. 135, 137 (1980)
Gramlich & Meier, Z. Kristalllogr. 133, 134 (1971)
Cheng et al., Zeolites 3, 343 (1983)
Riley et al., J. Phys. Chem. 76, 2593 (1972)*
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<td>McCusker &amp; Seff., J. Phys. Chem. 95, 405 (1991)</td>
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<td>(\Delta Cd)</td>
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Roney & Seff, J. Am. Chem. Soc. 100, 5052 (1978)
McCusker & Seff, J. Am. Chem. Soc. 100, 5052 (1978)
Jirak et al., Zeolites 3, 255 (1983)
Jirak et al., Zeolites 3, 255 (1983)