# Crystallographic analysis of dehydrated fully Tl$^+$-exchanged zeolite Y

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**Abstract :** The crystal structure of Tl$_{71}$-Y (Tl$_{71}$Si$_{121}$Al$_{71}$O$_{384}$), $a = 24.706(3)$ Å, dehydrated at 653 K and $8 \times 10^{-6}$ torr, has been determined by single-crystal X-ray diffraction techniques in the cubic space group $Fd\bar{3}m$ at 294(1) K. The structure was refined using all intensities to the final error indices (using only the 302 reflection for which $F_o > 4\sigma(F_o)$) $R_1 = 0.0602$ (based on $F$) and $R_w = 0.1744$ (based on $F_2$). The 71 Tl$^+$ ions per unit cell are found at four crystallographically distinct positions. Site I' position in the sodalite cavity opposite D6Rs are each occupied by eighteen Tl$^+$ ions per unit cell; these Tl$^+$ ions are recessed *ca.* 1.45 Å into the sodalite cavity from their O(3) plane (Tl-O = 2.701(15), 3.163(16) Å and O-Tl-O = 92.1(4)°). The 23 Tl$^+$ ions fill site II in the supercage; these Tl$^+$ ions are recessed *ca.* 1.58 Å into the supercage from their O(2) plane (Tl-O = 2.850(16), 3.156(16) Å and O-Tl-O = 85.1(5)°). The 19 Tl$^+$ ions lie at site III' in the supercage near a triple 4-ring (Tl-O = 3.10(7), 3.39(5) Å and O-Tl-O = 47.8(9), 95.3(18)°) and the remaining 11 ions occupy another site III' near a triple 4-ring in the supercage (Tl-O = 2.81(4), 2.71(4) Å and O-Tl-O = 57.3(8)°).

**Key words :** zeolite Y, thallium, single-crystal X-ray diffraction, crystal structure

## 1. Introduction

Although zeolites X and Y have the same framework structure (FAU), their chemical properties are quite different because of their differing Si/Al ratio.[1] Both are synthetic analogues of the naturally occurring mineral faujasite. The framework structure of the faujasite is characterized by the double 6-ring (D6R, hexagonal prism). The polyhedron with fourteen vertices known as the sodalite cavity (β-cage) is the principal building block of the aluminosilicate framework of the zeolite. These sodalite cavities are connected tetrahedrally at 6-rings by bridging oxygens to give D6Rs (hexagonal prisms) and concomitantly, an interconnected set of even larger cavities (supercages) accessible in three dimensions through 12-ring (24-membered) windows. These three cavities all lie on 3-fold axes (see *Fig.* 1). The Si and Al atoms occupy the vertices of polyhedra. The oxygen atoms lie approximately half-way between each pair of Si and Al atoms, but are displaced away from those points to give the near tetrahedral angles about Si and Al.[2]

The exchangeable cations, which balance the negative charge of the aluminosilicate framework, predominantly occupy the sites I, I', II, II', III, and III' in faujasite as shown

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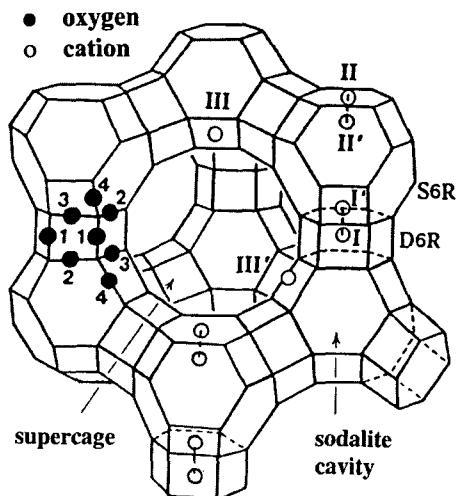E-mail: wtlim@andong.ac.kr

*Fig.* 1. Stylized drawing of the framework structure of zeolite Y. Near the center of the each line segment is an oxygen atom. The different oxygen atoms are indicated by the numbers 1 to 4. Silicon and aluminum atoms alternate at the tetrahedral intersections, with the exception that Si substitutes for Al at about 20% of the Al positions. Extraframework cation positions are labeled with Roman numerals.

in the *Fig.* 1. The nomenclature is as follows: site 1 is at the center of a D6R, site I' is in the sodalite cavity just on the other side of a D6R from site I, site II is on or on the supercage side of the single 6-ring (S6R) face of the sodalite cavity; site II' is in the sodalite unit opposite on S6R, site III is opposite the center of a triple 4-ring inside the supercage; and site III' at the opposite side of off center of the 4-ring ladder inside the supercage. Each unit cell has 8 sodalite units, 8 supercages, 16 D6Rs, 16 12-rings, and 32 S6Rs. The maximum occupancies at the cation sites I, I', II, II', III, and III' in faujasite are 16, 32, 32, 32, 48, and 96, respectively.

The zeolites X and Y are distinguished on the basis of chemical composition, details of structure smaller than topology, and their related physical and chemical properties. Differences are found in the cation composition and distribution, the Si/Al ratio and possible Si-Al ordering in tetrahedral sites.[1] Numerous investigations of the positions of the exchangeable cations in zeolites A and X (Si/Al ≈ 1) have been conducted by single-crystal X-ray diffraction due to their importance in adsorption and catalysis.[2-9]

Several Tl$^+$-exchanged faujasite-type zeolites have been studied for the structural investigation. Kim *et al.*[10] investigated a dehydrated Tl$^+$-exchanged zeolite X (Si/Al = 1.01) by single-crystal X-ray diffraction. Their single-crystal X-ray diffraction analysis of fully Tl$^+$-exchanged zeolite X showed that the ninety-two Tl$^+$ ions were located at four different crystallographic sites. Seff *et al.*[11] prepared dehydrated fully Tl$^+$-exchanged zeolite X using flowing aqueous 0.1 M TlNO$_3$ at room temperature.[11] Their structure of a single crystal of fully dehydrated Tl$^+$-exchanged zeolite X was determined by X-ray diffraction methods in the cubic space group $Fd\bar{3}$. They showed that the 74(4) and 83(1) of the 92 Na$^+$ ions per unit cell was replaced by Tl$^+$ for two single crystals.

Zeolite Y was first synthesized in its sodium form in 1964 by Union Carbide.[1] Intended for use as an adsorbent, zeolite Y eventually found use as the heterogeneous catalyst for the Fluidized Catalytic Cracking (FCC) of hydrocarbons. The chemical composition of zeolite Y can vary according to the silicon and aluminum content from a Si/Al ratio = 1.5 to 3.0.[1] Zeolite Y has a wide range of industrial applications due primarily to its excellent structural stability and its large and accessible pore volume. In addition to this pore volume, the adsorptive properties of zeolites depend heavily on the size (charge density) and distribution of the cations in the lattice.[1]

This work was initiated to determine the cation positions of the Tl$^+$ ions in dehydrated zeolite Y prepared by David Vaughan.[12] It was also done to investigate the bonding characteristics between the framework and cations and to reinvestigate the space group in the crystal structure of the dehydrated Tl$_{71}$Si$_{121}$Al$_{71}$O$_{384}$ (Si/Al ratio = 1.69). It was hoped that something more could be learned about the Si/Al ordering within this crystal.

## 2. Experimental Section

### 2.1. Synthesis of Tl$^+$-exchanged zeolite Y

Large colorless single crystals of sodium zeolite Y, stoichiometry Na$_{71}$Si$_{121}$Al$_{71}$O$_{384}$, were prepared by David Vaughan.[12] One of these, a colorless octahedron about 0.15 mm in cross-section was lodged in a fine Pyrex capillary.

Crystals of hydrated Tl$_{71}$-Y (or Tl-Y) were prepared by the dynamic (flow) ion-exchange of Na$_{71}$-Y with 0.1 M

aqueous thallous acetate (pH = 6.4, Aldrich Chemical Co., 99.99%).[10,13-15] The solution was allowed to flow past the crystal at a velocity of approximately 1.5 cm/s for 4 days at 294 K. The clear, colorless, hydrated $Tl^+$-exchanged Y was dehydrated at 653 K and $8 \times 10^{-6}$ torr for 2 days. While these conditions were maintained, the hot contiguous downstream lengths of the vacuum system, including a sequential U-tube of zeolite 5A beads fully activated in situ, were cooled to ambient temperature to prevent the movement of water molecules from more distant parts of the vacuum system to the crystal. Still under vacuum in its capillary, the crystal was then allowed to cool and was sealed in its capillary and removed from the vacuum line by torch. Microscopic examination showed that the crystal had become light red-brown.

The structure of the resultant crystal was determined by single-crystal X-ray diffraction techniques at 294(1) K. It was attached to the tip of a glass rod, transferred to a Bruker SMART diffractometer with a CCD area detector, and centered. The crystal evaluation and data collection were done using Mo Kα radiation employing 2-kw sealed-tube X-ray source operating at 1.5 kw and a detector-to-crystal distance of 4.8 cm.

Preliminary cell constants and an orientation matrix were determined from three series of scans at different starting angles. Each series consisted of 20 frames collected at intervals of 0.3° scan with an exposure time of 10 seconds per frame. The reflections were successfully indexed by the automated indexing routine of the SMART program. A total of 8,837 reflections were harvested by collecting four sets of frames with 0.3° scans with an exposure time of 10 seconds per frame. The highly redundant data sets were corrected for Lorentz and polarization effects, and a correction for crystal decay was also applied. The absorption correction was judged to be negligible for this crystal and was not applied. The space group $Fd\bar{3}m$ was determined by the program SAINT-plus.[16] A summary of the experimental and crystallographic data is presented in Table 1.

## 2.2. Structure determination

Full-matrix least-squares refinement (SHELXL97)[17] was done on $F_o^2$ using all data. Refinement was initiated with the atomic parameters of the framework atoms [(Si, Al),

Table 1. Experimental conditions and crystallographic data

| | |
|---|---|
| Crystal cross section (mm) | 0.15 |
| Ion exchange T (K) | 294 |
| Ion exchange for $Tl^+$ (days, mL) | 4, 12.0 |
| Data collection T (K) | 294(1) |
| Scan technique | ω-scan |
| Radiation (Mo Kα) $\lambda_1$ | 0.70930 |
| $\lambda_2$ | 0.71359 |
| Unit cell constant, $a$ (Å) | 24.706(3) |
| 2θ range in data collection (deg) | $2.82 < 2\theta < 56.6$ |
| No. of unique reflections, $m$ | 978 |
| No. of reflections with $F_o > 4\sigma(F_o)$ | 302 |
| No. of variables, $s$ | 47 |
| Data / parameter ratio, $m/s$ | 20.8 |
| Weighting parameters, $a/b$ | 0.110/853.7 |
| Final error indices | |
| $R_1/R_2$ ($F_o > 4\sigma(F_o))^a$ | 0.0602/0.1744 |
| $R_1/R_2$ (all intensities)$^b$ | 0.0626/0.1810 |
| Goodness-of-fit$^c$ | 1.153 |

$^aR_1 = \Sigma|F_o - |F_c||/\Sigma F_o$ and $R_2 = [\Sigma w(F_o^2 - F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$; $R_1$ and $R_2$ are calculated using only the 302 reflections for which $F_o > 4\sigma(F_o)$. $^bR_1$ and $R_2$ are calculated using all 978 unique reflections measured. $^c$Goodness-of-fit $= (\Sigma w(F_o^2 - F_c^2)^2/(m-s))^{1/2}$

O(1), O(2), O(3), and O(4)] in dehydrated $Tl_{92}$-X.[11] The initial refinement using anisotropic thermal parameters for all positions converged to the error indices (defined in footnotes to Table 1) $R_1 = 0.496$ and $R_2 = 0.869$.

Refinement including the Tl(1) position at a major peak (0.080, 0.080, 0.080, site I') from the initial difference Fourier function led to convergence with $R_1 = 0.452$ and $R_2 = 0.836$ and an occupancy of 2.3(6) $Tl^+$ ions per unit cell. The largest peak on the subsequent difference Fourier function (based on this model) revealed a peak at (0.259, 0.259, 0.259), at site II. Refinement including this peak as Tl(2) converged to $R_1 = 0.336$ and $R_2 = 0.660$, with occupancies of 22.2(26) and 36.7(5), respectively. A subsequent difference Fourier function based on this model revealed a peak in the supercage at (0.070, 0.070, 0.430) opposite a 4-ring. Refinement including this peak as Tl(3) converged to $R_1 = 0.278$ and $R_2 = 0.614$, with occupancies of 19.3(13), 34.8(29), and 14.2(27) for isotropically refined Tl(1), Tl(2), and Tl(3), respectively. A

*Table* 2. Positional, thermal, and occupancy parameters[a]

| Atom | Wyckoff Position | Cation site | x | y | z | $U_{11}$ or $U_{iso}$[b] | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ | Occupancy[c] fixed | Occupancy[c] varied |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| (Si,Al) | 192(i) | | -540(2) | 1257(2) | 362(2) | 485(31) | 431(31) | 441(32) | -58(24) | 8(25) | -12(22) | 192 | |
| O(1) | 96(h) | | -6065(5) | 0 | 6065(5) | 476(64) | 805(12) | 476(64) | -157(58) | -56(80) | -157(58) | 96 | |
| O(2) | 96(g) | | -24(4) | -24(4) | 1421(4) | 658(72) | 658(72) | 498(14) | -123(59) | -123(59) | 96(86) | 96 | |
| O(3) | 96(g) | | 9652(6) | -19235(4) | -19235(4) | 502(103) | 577(67) | 577(67) | 133(85) | -34(58) | -34(58) | 96 | |
| O(4) | 96(g) | | 703(4) | 703(4) | 3228(6) | 521(63) | 521(63) | 519(99) | 44(54) | 44(54) | -1(8) | 96 | |
| Tl(1) | 32(e) | I' | 745(4) | 745(4) | 745(4) | 652(17) | 652(17) | 652(17) | -19(9) | -19(9) | -19(9) | 18 | 18.1(3) |
| Tl(2) | 32(e) | II | 2572(10) | 2572(10) | 2572(10) | 735(16) | 735(16) | 735(16) | 10(8) | 10(8) | 10(8) | 23 | 23.0(4) |
| Tl(3) | 96(g) | III' | 903(21) | 903(21) | 4451(32) | 677(82) | | | | | | 19 | 18.8(5) |
| Tl(4) | 192(g) | III' | 256(15) | 637(14) | 4270(17) | 2343(17) | | | | | | 11 | 10.9(3) |

[a]Positional parameters × $10^4$ and thermal parameters × $10^3$ are given. Numbers in parentheses are the estimated standard deviations in the units of the least significant figure given for the corresponding parameter. The anisotropic temperature factor is $\exp[-2\pi^2 a^{-2}(U_{11}h^2+U_{22}k^2+U_{33}l^2+2U_{12}hk+2U_{13}hl+2U_{23}kl)]$. [b]Isotropic thermal parameter in units of $Å^2$. [c]Occupancy factors are given as the number of atoms or ions per unit cell.

subsequent refinement including Tl(4), a peak found near 4-ring in the supercage at site III' (0.043, 0.071, 0.431), led to $R_1 = 0.080$ and $R_2 = 0.260$, with occupancies of 17.6(3), 22.4(5), 5.3(6), and 14.0(11), respectively.

Anisotropic refinement of all positions except Tl(3) and Tl(4), which were isotropically refined, converged with $R_1 = 0.074$ and $R_2 = 0.244$ with occupancies of 18.1(3), 23.0(4), 18.8(5), and 10.9(3) for Tl(1), Tl(2), Tl(3), and Tl(4), respectively. The final cycles of refinement with fixed occupancies of Tl(1), Tl(2), Tl(3), and Tl(4) as shown in *Table* 2 converged to $R_1 = 0.602$ and $R_2 = 0.174$. On the final difference Fourier function, the largest peak appeared at (0.0, 0.0, 0.5), a very special position, with height 0.67 $e^-/Å^3$. It was not included in the final model because it was too far from framework oxygen atoms to be a cation.

All shifts in the final cycles of refinement were less than 0.1% for the corresponding estimated standard deviations. The final structural parameters are given in *Table* 2. Selected interatomic distances and angles are given in *Table* 3.

Fixed weights were used initially; the final weights were assigned using the formula $w = 1/[\sigma^2(F_o)^2+(aP)^2+bP]$ where $P = [Max(F_o^2,0)+2F_c^2]/3$, with $a = 0.110$ and $b = 852.7$ as refined parameters (see *Table* 2). Atomic scattering factors for Tl⁺, O⁻, and (Si,Al)¹·⁸²⁺ were used.[18,19] The function describing (Si,Al)¹·⁸²⁺ is the weighted mean

*Table* 3. Selected interatomic distances (Å) and angles (deg)[a]

| Distance | | Angle | |
|---|---|---|---|
| (Si,Al)-O(1) | 1.646(7) | O(1)-(Si,Al)-O(2) | 111.5(6) |
| (Si,Al)-O(2) | 1.643(6) | O(1)-(Si,Al)-O(3) | 110.2(7) |
| (Si,Al)-O(3) | 1.640(6) | O(1)-(Si,Al)-O(4) | 106.7(7) |
| Mean (Si,Al) | 1.643 | O(2)-(Si,Al)-O(3) | 108.2(8) |
| | | O(2)-(Si,Al)-O(4) | 108.4(8) |
| Tl(1)-O(3) | 2.701(15) | O(3)-(Si,Al)-O(4) | 111.8(7) |
| Tl(1)-O(2) | 3.163(16) | | |
| Tl(2)-O(2) | 2.850(16) | (Si,Al)-O(1)-(Si,Al) | 138.5(11) |
| Tl(2)-O(4) | 3.156(16) | (Si,Al)-O(2)-(Si,Al) | 147.2(10) |
| Tl(3)-O(4) | 3.10(7) | (Si,Al)-O(3)-(Si,Al) | 144.7(10) |
| Tl(3)-O(1) | 3.39(5) | (Si,Al)-O(4)-(Si,Al) | 138.6(9) |
| Tl(4)-O(4) | 2.81(4) | | |
| Tl(4)-O(1) | 2.71(4) | O(3)-Tl(1)-O(3) | 92.1(4) |
| | | O(2)-Tl(2)-O(2) | 85.1(5) |
| | | O(1)-Tl(3)-O(4) | 47.8(9) |
| | | O(1)-Tl(3)-O(1) | 95.3(18) |
| | | O(1)-Tl(4)-O(4) | 57.3(8) |

[a]The numbers in parentheses are the estimated standard deviations in the units of the least significant digit given for the corresponding parameters.

of the Si⁴⁺, Si⁰, Al³⁺, and Al⁰ functions (Si/Al = 1.69). All scattering factors were modified to account for anomalous dispersion.[20,21]

# 3. Results and Discussion

## 3.1. Brief description of FAU

The framework structure of faujasite is characterized by the double 6-ring (D6R, hexagonal prism), the sodalite cavity (a cubooctahedron), and the supercage (see *Fig.* 1).

The exchangeable cations, which balance the negative charge of the faujasite framework, usually occupy some or all of the sites shown with Roman numerals in *Fig.* 1. Each unit cell has 8 supercages, 8 sodalite cavities, 16 D6Rs, 16 12-rings, and 32 S6Rs (single 6-rings). The maximum occupancies at the cation sites I, I', II, II', III, and III' in faujasite are 16, 32, 32, 32, 48, and 96 (192 is also possible in $Fd\bar{3}m$ but does not occur in this structure), respectively. Further description is available.

## 3.2. Space group consideration

If Si/Al = 1.00, the Si and Al atoms alternate in the zeolite FAU framework in obedience of Lowenstein's rule (-Al-O-Al- sequences are forbidden).[22] Then the space group is $Fd\bar{3}$; one 96(*g*) equipoint, Si, contains only Si atoms, another 96(*g*) equipoint, Al, contains only Al atoms, and Si-bond lengths are correctly seen crystallographically to be shorter than Al-O. This remains true even when about 4% of the Al sites are occupied by Si atoms to accomodate the excess Si atoms in $Na_{92}Si_{100}Al_{92}O_{384}$.[2] This ordering of Si and Al atoms is confirmed by the different average values of the Si-O and Al-O distances in $Na_{92}Si_{100}Al_{92}O_{384}$; enough long-range order is retained for the space group to remain $Fd\bar{3}$ with Si/Al disorder at the Al position and for the mean Si-O and Al-O distances to remain different.

In fully dehydrated $Tl_{71}$-Y, the X-ray diffraction intensities showed the obvious mirror planes at (110) in this work (see supporting material). This experimentally observed intensity equality between *hkl* and *khl* pairs of reflections indicates that the Si and Al positions are no longer distinguishable in the framework. When this crystal was refined using $Fd\bar{3}$, the average Si-O and Al-O distances, 1.654(2) and 1.657(4) Å, respectively, differ insignificantly, indicating that the Si and Al atoms are entirely or nearly entirely disordered in the long range. Furthermore, when $Fd\bar{3}$ was used, $R_1$ increased from 0.0602 to 0.070 and $R_2$ from 0.174 to 0.188. Accordingly, the crystal in this work was refined using space group $Fd\bar{3}m$.

## 3.3. Framework and Tl⁺ ions

In this crystal structure, the 71 $Tl^+$ ions are located at the four different crystallographic sites. The 18 and 23 $Tl^+$ ions per unit cell are on 32-fold axes in the D6Rs, at site I' and II, respectively. The remaining 30 $Tl^+$ ions are distributed among two III' sites, the 19 at Tl(3) and the 11 at Tl(4). Site I, often a popular site, is empty. The total number of $Tl^+$ ions found per unit cell, 71, required to balance the negative charge of the zeolite framework.

About 18 $Tl^+$ ions are located at site I' positions of the 32-fold in the sodalite cavity opposite D6Rs (see *Fig.* 2). These $Tl^+$ ions at Tl(1) lie relatively far inside the sodalite cavity, *ca.* 1.45 Å from the (111) plane of three O(3) framework oxygens of the D6R to which it is bound, respectively. The 18 Tl(1) bond to three O(3)s at 2.701(15) Å (see *Fig.* 2). This distance of $Tl^+$ ions at Tl(1) with three O(3) are relatively same as the sum of the ionic radii of $Tl^+$ and $O^{2-}$, 2.79 Å,[22] when the esds are considered.

The Tl(2) position is at site II, far inside the supercage (see *Fig.* 3). Each Tl(2) ions lies relatively far inside the supercage, 1.58 Å, from the (111) plane of three O(2) framework oxygens of the S6R to which it is bound. The Tl(2)-O(2) distances are 2.850(16) Å, somewhat longer than the Tl(1)-O(3) distances. The Tl-O distances and $Tl^+$ displacements from 6-ring planes are also similar to those in dehydrated $Ag_{6.5}Tl_{5.5}$-A,[23] $Tl_{11}Na_1$-A,[24] and $Tl_{92}$-X[10] for the Tl(2) position.
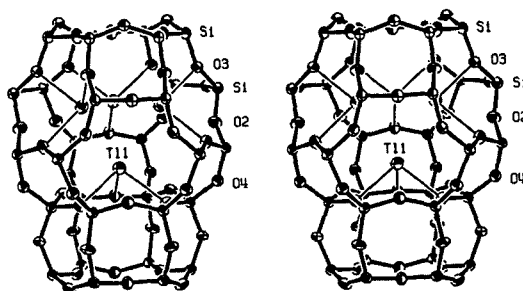
The remaining 19 and 11 $Tl^+$ ions at Tl(3) and Tl(4),



*Fig.* 2. Stereoview of a sodalite unit in $Tl_{71}$-Y. The zeolite framework is drawn with bonds of medium thickness. The coordination of $Tl^+$ ions to oxygens of the zeolite framework are indicated by the thinnest lines. Ellipsoids of 25% probability are shown.
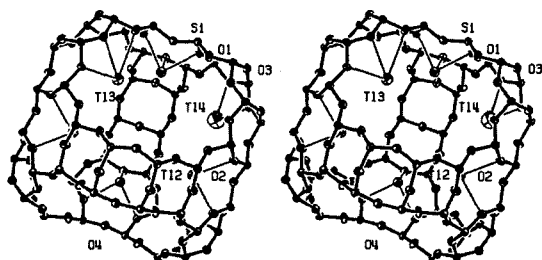
*Fig.* 3. A Stereoview of a supercage of dehydrated Tl$_{71}$-Y. See the caption to *Fig.* 2 for other details.

*Table* 4. Distribution of Tl⁺ ions over sites in Tl$_{92}$-X$^a$ and Tl$_{71}$-Y$^b$

| Site | I | I' | II | III | III' |
|---|---|---|---|---|---|
| Maximum occupancy | 16 | 32 | 32 | 48 | 96 |
| Position | - | Tl(1) | Tl(2) | - | Tl(3) Tl(4) |
| Structure | Occupancies | | | | |
| Tl$_{92}$-X$^a$ | - | 32 | 32 | - | 16    12 |
| Tl$_{71}$-Y$^b$ | - | 18 | 23 | - | 19    11 |

$^a$Ref. 10. $^b$This work.

*Table* 5. Comparison of the distances (Å) between Tl⁺ and its nearest framework oxygen atom in Tl$_{92}$-X$^a$ and Tl$_{71}$-Y$^b$

| | Tl$_{92}$-X$^a$ | Tl$_{71}$-Y$^b$ |
|---|---|---|
| Tl(1)-O(3) | 2.59(1) | 2.701(15) |
| Tl(2)-O(2) | 2.68(1) | 2.850(16) |
| Tl(3)-O(4) | 2.81(2) | 3.10(7) |
| Tl(4)-O(4) | 2.38(4) | 2.81(4) |

$^a$Ref. 10. $^b$This work.

respectively, occupy two site III' near a triple 4-ring in the supercage. Both positions are close to one O(4) and two O(1) framework oxygens. The site-III' cations, 19 and 11 Tl⁺ ions per unit cell are 3.39(5) Å and 3.10(7) Å at Tl(3) and 2.71(4) Å and 2.81(4) Å at Tl(4) from framework oxygens at O(1) and O(4), respectively (see *Table* 3 and *Fig.* 3). The occupation of two positions at sites III', rather than one of lowest energy, might be due to their closeness in energy, the asymmetric environment generated by the partial occupancy of Tl⁺ ions at site I', and the Si/Al disorder among the T atoms.

In this work, fully Tl⁺-exchanged zeolite Y was successfully synthesized and its structure was determined by X-ray diffraction methods. The 71 Tl⁺ ions are distributed in the four different crystallographic sites: 18 at site I', 23 at site II, 19 at a III' site, and the remaining 11 at another site III'.

### 3.4. Comparison of Tl$_{71}$-Y with Tl$_{92}$-X

Kim *et al.*[10] investigated a dehydrated zeolite X with unit-cell composition Tl$_{92}$Si$_{100}$Al$_{92}$O$_{384}$ (Si/Al = 1.09) by single crystal X-ray diffraction. In their structure, Tl⁺ ions were found four different crystallographic sites with the occupancies of 32, 32, 16, and 12 per unit cell at sites I', II, III', and another III', respectively (see *Table* 4). When the thermal parameters in Tl$_{92}$-Y[10] and Tl$_{71}$-X are compared, it can be seen that the thermal ellipsoids of all of the Tl⁺ ions in Tl$_{71}$-Y are more elongated than those in Tl$_{92}$-X[10] (*Table* 2). This is attributed to the greater 6-ring diversity to be expected in zeolite Y. For Tl$_{71}$-Y, 6-rings containing four Si and two Al atoms may predominate with the Al atoms in meta or in para positions. Six-ring with three Al atoms are expected to be second

in population, and 6-rings with one and perhaps zero Al atoms may be present. Tl⁺ ions should occupy different positions in these rings, and this disorder has been absorbed into the anisotropic thermal parameters of the Tl⁺ ions in least-squares refinement. These thermal ellipsoids, therefore, do not accurately indicate thermal motion.

The reduced aluminum content of zeolite Y as compared to zeolite X[10] should lead to a smaller negative charge density for the zeolite framework and, therefore, at each oxygen position. This in turn should lead to longer Tl-O distances. This can be seen in *Table* 5.

## Acknowledgement

## Supplementary Material Available

Calculated structure factors squared and observed structure factors squared with esds for Tl$_{71}$Si$_{121}$Al$_{71}$O$_{384}$.

## ∼∼ Supplementary Material ∼∼

### Table of calculated and observed structure factors squared

Values of $10 \times F_{obs}$ and $10 \times F_{calc}$

| h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ | h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ | h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ | h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 0 | 2 | 0 | 17.3 | 3.7 | 5 o | 0 | 18 | 12 | 57.6 | 31.4 | 35 o | 1 | 17 | 9 | 4017.0 | 39.3 | 36 o | 2 | 18 | 6 | 1909.1 | 31.2 | 42 o |
| 0 | 2 | 2 | 3101.0 | 52.3 | 17 o | 0 | 20 | 0 | 1782.6 | 100.1 | 16 o | 1 | 17 | 11 | 120.3 | 19.7 | 18 o | 2 | 18 | 8 | 46.3 | 18.4 | 15 o |
| 0 | 4 | 0 | 21260.2 | 548.1 | 23 o | 0 | 20 | 2 | 14.3 | 30.1 | 19 o | 1 | 17 | 13 | 2398.7 | 36.5 | 21 o | 2 | 18 | 10 | 2504.5 | 35.8 | 28 o |
| 0 | 4 | 2 | 17.6 | 5.1 | 24 o | 0 | 20 | 4 | 2346.5 | 54.0 | 24 o | 1 | 19 | 1 | 108.0 | 30.3 | 49 o | 2 | 18 | 12 | 1123.0 | 28.8 | 26 o |
| 0 | 4 | 4 | 13773.8 | 219.5 | 14 o | 0 | 20 | 6 | -1.7 | 29.0 | 41 o | 1 | 19 | 3 | 1742.6 | 31.7 | 48 o | 2 | 20 | 2 | 176.9 | 31.0 | 26 o |
| 0 | 6 | 0 | 378.2 | 22.1 | 17 o | 0 | 20 | 8 | 32942.0 | 451.4 | 42 o | 1 | 19 | 5 | 722.5 | 22.4 | 50 o | 2 | 20 | 4 | 53.5 | 20.6 | 21 o |
| 0 | 6 | 2 | 767.5 | 15.4 | 17 o | 0 | 20 | 10 | -2.3 | 34.6 | 24 o | 1 | 19 | 7 | 8041.1 | 71.1 | 23 o | 2 | 20 | 6 | 749.6 | 24.7 | 23 o |
| 0 | 6 | 4 | 28.6 | 9.2 | 21 o | 0 | 22 | 0 | 0.1 | 75.1 | 46 o | 1 | 19 | 9 | 9944.2 | 85.4 | 24 o | 2 | 20 | 8 | 343.9 | 21.9 | 31 o |
| 0 | 6 | 6 | 8603.0 | 133.3 | 25 o | 0 | 22 | 2 | 3370.8 | 75.0 | 18 o | 1 | 19 | 11 | 201.3 | 22.4 | 32 o | 2 | 20 | 10 | 4858.4 | 65.1 | 44 o |
| 0 | 8 | 0 | 76.3 | 18.7 | 26 o | 0 | 22 | 4 | 3.1 | 35.4 | 30 o | 1 | 21 | 1 | 8051.3 | 120.0 | 44 o | 2 | 22 | 2 | 2099.1 | 52.8 | 52 o |
| 0 | 8 | 2 | 587.9 | 15.4 | 42 o | 1 | 1 | 1 | 31281.6 | 839.4 | 35 o | 1 | 21 | 3 | 434.5 | 23.8 | 36 o | 2 | 22 | 4 | 117.2 | 25.5 | 58 o |
| 0 | 8 | 4 | 99626.6 | 1033.7 | 31 o | 1 | 3 | 1 | 822.6 | 12.8 | 44 o | 1 | 21 | 5 | 168.0 | 22.8 | 27 o | 3 | 3 | 3 | 9679.4 | 197.3 | 30 o |
| 0 | 8 | 6 | 13.9 | 12.1 | 11 o | 1 | 3 | 3 | 270.3 | 7.9 | 62 o | 1 | 21 | 7 | 108.6 | 22.0 | 30 o | 3 | 5 | 3 | 59741.5 | 733.0 | 36 o |
| 0 | 8 | 8 | 144566 | 2246 | 11 o | 1 | 5 | 1 | 7335.6 | 83.6 | 30 o | 2 | 2 | 2 | 31212.0 | 623.0 | 26 o | 3 | 5 | 5 | 5119.4 | 66.6 | 23 o |
| 0 | 10 | 0 | 51.8 | 23.3 | 29 o | 1 | 5 | 3 | 1974.7 | 18.6 | 32 o | 2 | 4 | 2 | 2038.8 | 28.8 | 39 o | 3 | 7 | 3 | 4387.6 | 56.1 | 19 o |
| 0 | 10 | 2 | 11619.9 | 132.8 | 12 o | 1 | 5 | 5 | 3351.9 | 44.0 | 34 o | 2 | 4 | 4 | 9690.3 | 119.2 | 41 o | 3 | 7 | 5 | 20236.6 | 155.9 | 39 o |
| 0 | 10 | 4 | 285.8 | 13.8 | 20 o | 1 | 7 | 1 | 1618.4 | 22.3 | 52 o | 2 | 6 | 2 | 106481 | 1255 | 43 o | 3 | 7 | 7 | 11281.8 | 126.4 | 28 o |
| 0 | 10 | 6 | 1420.7 | 27.7 | 17 o | 1 | 7 | 3 | 11046.4 | 84.9 | 35 o | 2 | 6 | 4 | 6134.5 | 51.9 | 33 o | 3 | 9 | 3 | 1018.3 | 22.0 | 44 o |
| 0 | 10 | 8 | 187.7 | 17.2 | 21 o | 1 | 7 | 5 | 5885.9 | 49.9 | 43 o | 2 | 6 | 6 | 11526.3 | 136.1 | 36 o | 3 | 9 | 5 | 9649.6 | 74.0 | 51 o |
| 0 | 10 | 10 | 77145.1 | 1203.9 | 38 o | 1 | 7 | 7 | 14333.6 | 174.1 | 52 o | 2 | 8 | 2 | 24735.3 | 275.6 | 56 o | 3 | 9 | 7 | 6498.3 | 54.7 | 39 o |
| 0 | 12 | 0 | 35298.1 | 701.7 | 30 o | 1 | 9 | 1 | 23848.0 | 250.5 | 43 o | 2 | 8 | 4 | 8364.9 | 63.1 | 38 o | 3 | 9 | 9 | 5983.7 | 73.3 | 22 o |
| 0 | 12 | 2 | 18.4 | 15.1 | 47 o | 1 | 9 | 3 | 8770.5 | 66.9 | 44 o | 2 | 8 | 6 | 3172.9 | 29.7 | 41 o | 3 | 11 | 3 | 144.0 | 14.8 | 30 o |
| 0 | 12 | 4 | 10232.1 | 109.9 | 57 o | 1 | 9 | 5 | 13530.8 | 102.9 | 38 o | 2 | 8 | 8 | 501.3 | 17.0 | 26 o | 3 | 11 | 5 | 5433.5 | 46.0 | 51 o |
| 0 | 12 | 6 | 15.4 | 16.3 | 12 o | 1 | 9 | 7 | 3079.8 | 31.1 | 44 o | 2 | 10 | 2 | 39192.7 | 398.6 | 16 o | 3 | 11 | 7 | 8783.7 | 69.1 | 30 o |
| 0 | 12 | 8 | 2484.3 | 39.0 | 24 o | 1 | 9 | 9 | 1407.6 | 29.6 | 29 o | 2 | 10 | 4 | 1885.1 | 20.6 | 13 o | 3 | 11 | 9 | 2006.2 | 25.3 | 42 o |
| 0 | 12 | 10 | 5.7 | 20.6 | 14 o | 1 | 11 | 1 | 8146.7 | 93.1 | 48 o | 2 | 10 | 6 | 30589.6 | 221.3 | 16 o | 3 | 11 | 11 | 1452.4 | 32.8 | 40 o |
| 0 | 12 | 12 | 90540.2 | 1413.1 | 22 o | 1 | 11 | 3 | 1540.8 | 19.0 | 53 o | 2 | 10 | 8 | 968.7 | 17.5 | 18 o | 3 | 13 | 3 | 3393.0 | 45.2 | 43 o |
| 0 | 14 | 0 | 60.6 | 37.8 | 18 o | 1 | 11 | 5 | 2848.0 | 27.9 | 20 o | 2 | 10 | 10 | 17113.5 | 195.6 | 24 o | 3 | 13 | 5 | 12977.4 | 99.5 | 43 o |
| 0 | 14 | 2 | 8138.7 | 99.2 | 19 o | 1 | 11 | 7 | 805.6 | 15.9 | 11 o | 2 | 12 | 2 | 4519.6 | 56.3 | 33 o | 3 | 13 | 7 | 447.9 | 14.3 | 36 o |
| 0 | 14 | 4 | 29.1 | 17.5 | 42 o | 1 | 11 | 9 | 8199.1 | 65.9 | 16 o | 2 | 12 | 4 | 6569.4 | 52.8 | 28 o | 3 | 13 | 9 | 1061.8 | 20.0 | 36 o |
| 0 | 14 | 6 | 864.4 | 24.9 | 26 o | 1 | 11 | 11 | 60786.1 | 617.7 | 19 o | 2 | 12 | 6 | 3528.5 | 32.1 | 30 o | 3 | 13 | 11 | 500.1 | 16.1 | 36 o |
| 0 | 14 | 8 | 13.7 | 19.5 | 14 o | 1 | 13 | 1 | 326.2 | 19.3 | 19 o | 2 | 12 | 8 | 672.1 | 15.4 | 47 o | 3 | 13 | 13 | 917.2 | 29.6 | 24 o |
| 0 | 14 | 10 | 200.8 | 23.7 | 19 o | 1 | 13 | 3 | 6386.5 | 53.9 | 40 o | 2 | 12 | 10 | 3920.3 | 39.0 | 14 o | 3 | 15 | 3 | 20074.2 | 210.3 | 43 o |
| 0 | 14 | 12 | 5.4 | 26.4 | 21 o | 1 | 13 | 5 | 2760.2 | 28.1 | 42 o | 2 | 12 | 12 | 345.2 | 24.3 | 26 o | 3 | 15 | 5 | 564.9 | 16.8 | 50 o |
| 0 | 14 | 14 | 74.1 | 41.5 | 35 o | 1 | 13 | 7 | 3356.1 | 32.2 | 47 o | 2 | 14 | 2 | 4639.7 | 61.8 | 24 o | 3 | 15 | 7 | 37.0 | 14.7 | 46 o |
| 0 | 16 | 0 | 57397.2 | 1272.1 | 23 o | 1 | 13 | 9 | 3622.4 | 35.5 | 46 o | 2 | 14 | 4 | 402.6 | 14.2 | 44 o | 3 | 15 | 9 | 746.3 | 20.2 | 54 o |
| 0 | 16 | 2 | -1.4 | 22.3 | 34 o | 1 | 13 | 11 | 2347.2 | 31.3 | 13 o | 2 | 14 | 6 | 17496.8 | 128.8 | 28 o | 3 | 15 | 11 | 172.8 | 20.8 | 49 o |
| 0 | 16 | 4 | 12176.7 | 140.1 | 25 o | 1 | 13 | 13 | 3028.1 | 52.5 | 13 o | 2 | 14 | 8 | 20.7 | 13.6 | 24 o | 3 | 15 | 13 | 1999.0 | 35.0 | 54 o |
| 0 | 16 | 6 | 6.4 | 21.4 | 25 o | 1 | 15 | 1 | 1545.5 | 35.9 | 16 o | 2 | 14 | 10 | 9740.6 | 78.1 | 23 o | 3 | 15 | 15 | 2833.1 | 62.9 | 25 o |
| 0 | 16 | 8 | 585.1 | 24.9 | 32 o | 1 | 15 | 3 | 7696.3 | 66.0 | 18 o | 2 | 14 | 12 | 1321.6 | 25.0 | 27 o | 3 | 17 | 3 | 4411.8 | 61.7 | 18 o |
| 0 | 16 | 10 | 109.2 | 24.6 | 46 o | 1 | 15 | 5 | 449.6 | 15.7 | 26 o | 2 | 14 | 14 | 131.9 | 27.7 | 31 o | 3 | 17 | 5 | 211.3 | 17.2 | 38 o |
| 0 | 16 | 12 | 2848.5 | 53.7 | 55 o | 1 | 15 | 7 | 511.8 | 16.1 | 29 o | 2 | 16 | 2 | 1411.4 | 36.2 | 52 o | 3 | 17 | 7 | 321.2 | 17.9 | 22 o |
| 0 | 16 | 14 | 14.6 | 33.0 | 13 o | 1 | 15 | 9 | 75.9 | 16.1 | 36 o | 2 | 16 | 4 | 2598.7 | 31.3 | 33 o | 3 | 17 | 9 | 7632.7 | 68.2 | 20 o |
| 0 | 16 | 16 | 308.3 | 53.3 | 16 o | 1 | 15 | 11 | 2040.7 | 31.0 | 47 o | 2 | 16 | 6 | 93.8 | 15.8 | 38 o | 3 | 17 | 11 | 313.7 | 23.8 | 23 o |
| 0 | 18 | 0 | 302.6 | 56.1 | 20 o | 1 | 15 | 13 | 710.5 | 23.9 | 14 o | 2 | 16 | 8 | 6885.7 | 58.4 | 39 o | 3 | 17 | 13 | 2229.1 | 43.8 | 38 o |
| 0 | 18 | 2 | 3240.6 | 58.1 | 23 o | 1 | 15 | 15 | 1159.6 | 40.5 | 15 o | 2 | 16 | 10 | 110.4 | 17.8 | 26 o | 3 | 19 | 3 | 17.9 | 25.9 | 29 o |
| 0 | 18 | 4 | 9.8 | 24.8 | 36 o | 1 | 17 | 1 | 1017.8 | 34.4 | 28 o | 2 | 16 | 12 | 2540.8 | 34.9 | 32 o | 3 | 19 | 5 | 477.0 | 20.9 | 48 o |
| 0 | 18 | 6 | 5255.3 | 73.5 | 25 o | 1 | 17 | 3 | 7118.4 | 63.8 | 29 o | 2 | 16 | 14 | 378.4 | 21.4 | 36 o | 3 | 19 | 7 | 4023.7 | 44.7 | 23 o |
| 0 | 18 | 8 | -2.6 | 24.9 | 33 o | 1 | 17 | 5 | 199.5 | 17.2 | 29 o | 2 | 18 | 2 | 11801.5 | 138.8 | 35 o | 3 | 19 | 9 | 53.8 | 19.3 | 36 o |
| 0 | 18 | 10 | 669.6 | 30.8 | 36 o | 1 | 17 | 7 | 996.2 | 21.9 | 28 o | 2 | 18 | 4 | 1080.6 | 25.0 | 28 o | 3 | 19 | 11 | 4328.2 | 57.2 | 30 o |

Values of 10×Fobs and 10×Fcalc

| h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ | h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ | h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ | h | k | l | $F_c^2$ | $F_o^2$ | $\sigma(F_o^2)$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 3 | 21 | 3 | 494.0 | 32.5 | 42 o | 5 | 13 | 9 | 3240.3 | 38.1 | 42 o | 7 | 13 | 7 | 807.6 | 28.6 | 36 o | 11 | 13 | 11 | 25.4 | 43.6 | 35 o |
| 3 | 21 | 5 | 276.1 | 22.0 | 42 o | 5 | 13 | 11 | 23.3 | 20.7 | 15 o | 7 | 13 | 9 | 899.4 | 25.2 | 18 o | 11 | 13 | 13 | 156.1 | 47.7 | 16 o |
| 3 | 21 | 7 | 80.5 | 22.5 | 44 o | 5 | 13 | 13 | 7795.9 | 109.8 | 28 o | 7 | 13 | 11 | 18.7 | 21.0 | 21 o | 11 | 15 | 11 | 2597.4 | 93.5 | 19 o |
| 4 | 4 | 4 | 34963.0 | 775.5 | 32 o | 5 | 15 | 5 | 2341.6 | 39.7 | 26 o | 7 | 13 | 13 | 1972.1 | 51.6 | 49 o | 12 | 12 | 12 | 262.5 | 79.1 | 24 o |
| 4 | 6 | 4 | 28500.7 | 340.1 | 39 o | 5 | 15 | 7 | 9704.2 | 85.1 | 26 o | 7 | 15 | 7 | 13651.9 | 154.5 | 48 o | 12 | 14 | 12 | 102.1 | 52.3 | 41 o |
| 4 | 6 | 6 | 15530.9 | 188.5 | 44 o | 5 | 15 | 9 | 1440.1 | 28.5 | 21 o | 7 | 15 | 9 | 705.3 | 23.2 | 50 o | 13 | 13 | 13 | 64.8 | 100.4 | 42 o |
| 4 | 8 | 4 | 49447.5 | 565.1 | 35 o | 5 | 15 | 11 | 1389.1 | 31.3 | 23 o | 7 | 15 | 11 | 9143.0 | 101.7 | 23 o | | | | | | |
| 4 | 8 | 6 | 9361.4 | 76.6 | 52 o | 5 | 15 | 13 | 84.6 | 26.2 | 31 o | 7 | 15 | 13 | 756.0 | 28.9 | 24 o | | | | | | |
| 4 | 8 | 8 | 3867.0 | 56.5 | 37 o | 5 | 15 | 15 | 47.3 | 42.2 | 44 o | 7 | 15 | 15 | 563.2 | 43.7 | 32 o | | | | | | |
| 4 | 10 | 4 | 865.6 | 21.2 | 34 o | 5 | 17 | 5 | 39030.7 | 391.8 | 52 o | 7 | 17 | 7 | 1875.3 | 46.0 | 44 o | | | | | | |
| 4 | 10 | 6 | 1489.8 | 21.0 | 50 o | 5 | 17 | 7 | 144.9 | 20.1 | 58 o | 7 | 17 | 9 | 758.8 | 26.1 | 36 o | | | | | | |
| 4 | 10 | 8 | 29.1 | 12.3 | 58 o | 5 | 17 | 9 | 1867.9 | 33.8 | 30 o | 7 | 17 | 11 | 227.6 | 29.0 | 27 o | | | | | | |
| 4 | 10 | 10 | 65.3 | 21.0 | 51 o | 5 | 17 | 11 | 6968.8 | 71.5 | 36 o | 7 | 17 | 13 | 78.1 | 31.3 | 30 o | | | | | | |
| 4 | 12 | 4 | 23420.7 | 255.6 | 23 o | 5 | 17 | 13 | 32.0 | 29.1 | 23 o | 7 | 19 | 7 | 45.7 | 31.8 | 26 o | | | | | | |
| 4 | 12 | 6 | 4328.7 | 42.1 | 22 o | 5 | 19 | 5 | 383.1 | 27.5 | 39 o | 7 | 19 | 9 | 497.8 | 28.3 | 39 o | | | | | | |
| 4 | 12 | 8 | 6653.4 | 60.5 | 23 o | 5 | 19 | 7 | 475.9 | 24.1 | 39 o | 8 | 8 | 8 | 14141.1 | 330.9 | 41 o | | | | | | |
| 4 | 12 | 10 | 93.2 | 15.9 | 38 o | 5 | 19 | 9 | 440.6 | 25.5 | 28 o | 8 | 10 | 8 | 1436.5 | 43.0 | 43 o | | | | | | |
| 4 | 12 | 12 | 3509.3 | 63.6 | 36 o | 5 | 19 | 11 | 651.1 | 32.6 | 44 o | 8 | 10 | 10 | 12665.3 | 169.6 | 33 o | | | | | | |
| 4 | 14 | 4 | 6453.8 | 74.0 | 50 o | 5 | 21 | 5 | 1233.9 | 46.7 | 51 o | 8 | 12 | 8 | 51128.7 | 631.9 | 36 o | | | | | | |
| 4 | 14 | 6 | 614.1 | 16.0 | 30 o | 6 | 6 | 6 | 28626.6 | 639.6 | 39 o | 8 | 12 | 10 | 416.0 | 26.7 | 56 o | | | | | | |
| 4 | 14 | 8 | 3753.2 | 41.1 | 30 o | 6 | 8 | 6 | 618.0 | 24.1 | 22 o | 8 | 12 | 12 | 32.5 | 37.6 | 38 o | | | | | | |
| 4 | 14 | 10 | 243.8 | 19.0 | 59 o | 6 | 8 | 8 | 11859.3 | 143.8 | 30 o | 8 | 14 | 8 | 610.1 | 29.0 | 41 o | | | | | | |
| 4 | 14 | 12 | 4034.5 | 47.9 | 44 o | 6 | 10 | 6 | 21074.6 | 231.7 | 42 o | 8 | 14 | 10 | 6077.9 | 74.9 | 26 o | | | | | | |
| 4 | 14 | 14 | 31.6 | 37.5 | 39 o | 6 | 10 | 8 | 1031.7 | 21.9 | 40 o | 8 | 14 | 12 | 632.7 | 32.6 | 16 o | | | | | | |
| 4 | 16 | 4 | 6661.2 | 76.9 | 38 o | 6 | 10 | 10 | 16466.5 | 186.0 | 43 o | 8 | 14 | 14 | 691.1 | 53.1 | 18 o | | | | | | |
| 4 | 16 | 6 | 7682.2 | 65.2 | 51 o | 6 | 12 | 6 | 3046.6 | 47.3 | 43 o | 8 | 16 | 8 | 21177.1 | 253.2 | 24 o | | | | | | |
| 4 | 16 | 8 | 1647.6 | 29.6 | 45 o | 6 | 12 | 8 | 4769.5 | 49.0 | 36 o | 8 | 16 | 10 | 372.0 | 26.0 | 33 o | | | | | | |
| 4 | 16 | 10 | 204.4 | 21.4 | 29 o | 6 | 12 | 10 | 2267.6 | 34.9 | 36 o | 8 | 16 | 12 | 1295.2 | 43.6 | 28 o | | | | | | |
| 4 | 16 | 12 | 648.0 | 25.4 | 42 o | 6 | 12 | 12 | 6195.1 | 87.4 | 36 o | 8 | 18 | 8 | 756.1 | 38.3 | 30 o | | | | | | |
| 4 | 16 | 14 | 2122.8 | 44.7 | 50 o | 6 | 14 | 6 | 36.7 | 22.5 | 24 o | 8 | 18 | 10 | 3463.8 | 55.1 | 47 o | | | | | | |
| 4 | 18 | 4 | 1563.5 | 38.5 | 38 o | 6 | 14 | 8 | 5992.7 | 57.3 | 43 o | 9 | 9 | 9 | 41007.1 | 916.9 | 14 o | | | | | | |
| 4 | 18 | 6 | 344.0 | 18.0 | 48 o | 6 | 14 | 10 | 5901.9 | 64.3 | 50 o | 9 | 11 | 9 | 7405.5 | 109.9 | 26 o | | | | | | |
| 4 | 18 | 8 | 683.7 | 24.0 | 28 o | 6 | 14 | 12 | 50.7 | 23.5 | 46 o | 9 | 11 | 11 | 269.8 | 38.2 | 24 o | | | | | | |
| 4 | 18 | 10 | 2417.9 | 40.7 | 28 o | 6 | 14 | 14 | 1656.7 | 53.5 | 54 o | 9 | 13 | 9 | 347.1 | 38.6 | 44 o | | | | | | |
| 4 | 18 | 12 | 164.1 | 25.6 | 37 o | 6 | 16 | 8 | 355.6 | 21.1 | 49 o | 9 | 13 | 11 | 5977.3 | 73.0 | 28 o | | | | | | |
| 4 | 20 | 4 | 92.9 | 27.8 | 43 o | 6 | 16 | 10 | 656.6 | 25.6 | 54 o | 9 | 13 | 13 | 4983.5 | 105.0 | 24 o | | | | | | |
| 4 | 20 | 6 | 417.7 | 21.7 | 49 o | 6 | 16 | 12 | 781.9 | 29.8 | 49 o | 9 | 15 | 9 | 281.8 | 41.9 | 44 o | | | | | | |
| 4 | 20 | 8 | 2076.7 | 37.7 | 40 o | 6 | 16 | 14 | 357.0 | 30.3 | 54 o | 9 | 15 | 11 | 340.6 | 33.3 | 24 o | | | | | | |
| 5 | 5 | 5 | 3791.6 | 100.5 | 39 o | 6 | 18 | 6 | 8219.0 | 107.2 | 25 o | 9 | 15 | 13 | 215.6 | 35.6 | 23 o | | | | | | |
| 5 | 7 | 5 | 17668.8 | 206.7 | 52 o | 6 | 18 | 8 | 16.3 | 21.1 | 18 o | 9 | 17 | 9 | 35.8 | 43.7 | 27 o | | | | | | |
| 5 | 7 | 7 | 266.3 | 18.9 | 57 o | 6 | 18 | 10 | 3009.5 | 44.2 | 38 o | 9 | 17 | 11 | 1470.9 | 48.8 | 31 o | | | | | | |
| 5 | 9 | 5 | 2454.6 | 38.9 | 54 o | 6 | 18 | 12 | 77.5 | 33.2 | 22 o | 10 | 10 | 10 | 7833.3 | 208.0 | 52 o | | | | | | |
| 5 | 9 | 7 | 818.2 | 17.2 | 44 o | 6 | 20 | 6 | 40.4 | 33.3 | 20 o | 10 | 12 | 10 | 1680.8 | 56.8 | 33 o | | | | | | |
| 5 | 9 | 9 | 24940.2 | 290.8 | 55 o | 6 | 20 | 8 | 21.8 | 23.8 | 23 o | 10 | 12 | 12 | 959.9 | 48.7 | 38 o | | | | | | |
| 5 | 11 | 5 | 541.9 | 20.7 | 56 o | 7 | 7 | 7 | 512.8 | 45.1 | 38 o | 10 | 14 | 10 | 5706.0 | 105.7 | 39 o | | | | | | |
| 5 | 11 | 7 | 1083.8 | 20.6 | 48 o | 7 | 9 | 7 | 2607.3 | 50.0 | 29 o | 10 | 14 | 12 | 212.0 | 33.7 | 26 o | | | | | | |
| 5 | 11 | 9 | 291.7 | 17.2 | 50 o | 7 | 9 | 9 | 4537.6 | 71.6 | 48 o | 10 | 14 | 14 | 1197.9 | 63.3 | 32 o | | | | | | |
| 5 | 11 | 11 | 3002.8 | 52.6 | 48 o | 7 | 11 | 7 | 14930.3 | 173.5 | 23 o | 10 | 16 | 10 | 1685.6 | 69.7 | 36 o | | | | | | |
| 5 | 13 | 5 | 232.2 | 20.8 | 53 o | 7 | 11 | 9 | 11168.6 | 102.9 | 36 o | 10 | 16 | 12 | 116.6 | 37.9 | 35 o | | | | | | |
| 5 | 13 | 7 | 2443.1 | 30.1 | 58 o | 7 | 11 | 11 | 1633.0 | 50.6 | 30 o | 11 | 11 | 11 | 1875.3 | 98.9 | 28 o | | | | | | |

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