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# The Crystal Structure of a New Ferroelectric Compound, $NaTh_2(PO_4)_3$**

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*The crystal structure of ferroelectric $NaTh_2(PO_4)_3$ has been determined using X-ray diffraction techniques. The crystals are monoclinic with dimensions $a = 17.37(2)$, $b = 6.81(1)$, $c = 8.13(1)$ Å, $\beta = 101.03(10)°$ and belong to the space group Cc. The density calculated for $Z = 4$ is 5.435 g . $cm^{-3}$; that determined by a picnometer is 5.41 g . $cm^{-3}$. The structure was solvend from 913 observed, independent reflections. The atomic coordinates and temperature factors were refined by full-matrix least squares. The discrepancy indices had final values of 7.1% (including unobserved reflections) and 6.2% (omitting unobserved reflections). The compound may be designated as sodium trisphosphatodithorate. The thorium atom is nine coordinated and thorium-oxygen distances are from 2.27 to 2.58 Å, and phosphorus-oxygen distances vary from 1.52 to 1.59 Å. The atomic arrangement is isostructural with that of $KTh_2(PO_4)_3$. The main difference in the structures of $NaTh_2(PO_4)_3$ and $KTh_2(PO_4)_3$ is the position of the alkali metal atom. The potassium atom in $KTh_2(PO_4)_3$ is on the special position 0, y, ¼ on the twofold axis in the space group C2/c, and the sodium atom in $NaTh_2(PO_4)_3$ is out of twofold axis for 0.8 Å.*

## Introduction

X-ray diffraction data,[1] the preparation of single crystals and crystallographic data of $NaTh_2(PO_4)_3$ [2] have been published already. Crystallographic data for other alkaline metal salts of thorium phosphates have been also reported.[3] These compounds are monoclinic, space groups C2/c or Cc, $Z = 4$. Similar values of lattice constants and the same space group extinctions between all alkaline metal salts of thorium phosphates suggest close structural relationship among them. The crystal structure of $KTh_2(PO_4)_3$ has been solved in centrosymmetric space group C2/c and published recently.[4] $NaTh_2(PO_4)_3$ [5] and $NaU_2(PO_4)_3$ [6] are piezoelectric, ferroelectric and therefore noncentrosymmetric, space group Cc.

## Experimental Section

To obtain single crystals of $NaTh_2(PO_4)_3$ previously described preparations were followed.[2,3,4]

The crystals are monoclinic, space group Cc (No 9), with unit cell dimensions:

$a = 17.37 \pm .02$ Å
$b = 6.81 \pm .01$
$c = 8.13 \pm .01$
$\beta = 101°3' \pm 10'$
$Dm = 5.41$; $Dx = 5.435$ g/cm³
$Z = 4$

The unit cell parameters were determined from oscillation and Weissenberg photographs with CuKα radiation. The density (Dm) was determined by a picnometer with decalin as liquid.

The three-dimensional intensity data were collected on multiple equi-inclination Weissenberg photographs using CuKα radiation. Three crystals were made spherical by grinding for absorption corrections ($\mu = 1133.4$ cm$^{-1}$). On such ground specimens (with the radius of sphere r = 0.081 mm, $\mu r = 9.2$; r = 0.082 mm, $\mu r = 9.3$ and r = 0.065 mm, $\mu r = 7.4$) following zones of reflections were collected: 0kl; h0l to h3l and hk0 to hk4. The relative intensities were determined from the optical densities of each spot by means of a microdensitometer. The corrections for absorption, polarization and Lorentz factors were made in the usual way and the structure amplitudes derived. The scale factors among the various hkl levels of data were improved in the course of structure determination. At the later stages of refinement the observed structure factors were transformed into absolute scale and the mean values were calculated for reflections whose intensities were determined several times. Weights were assigned using the method described by Wiesner and Lingafelter.[7]

*Solution and Refinement of the Structure.* The initial atomic coordinates, corresponding to those found in $KTh_2(PO_4)_3$,[4] were assumed. The least squares refinement cycles were continued in C2/c space group and resulted in a high isotropic temperature factor

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(2) B. Matković and M. Šljukić, *Croat. Chem. Acta, 37,* 115 (1965).
(3) B. Matković, B. Prodić, and M. Šljukić, *Bull. Soc. Chim. France,* 1777 (1968).
(4) B. Matković, B. Prodić, M. Šljukić, and S. W. Peterson, *Croat. Chem. Acta, 40,* 147 (1968).
(5) M. Topić, B. Prodić, and M. Šljukić, *Czech. J. Phys., B19,* 1295 (1969).
(6) M. Topić and B. Prodić, *J. Appl. Cryst., 2,* 230 (1969).
(7) J. R. Wiesner and E. C. Lingafelter, *Inorg. Chem., 5,* 1170 (1966).

for the sodium atom. In the three-dimensional Fourier map the sodium atom peak was split, and suggested that the sodium atoms were disordered. The correct space group for $NaTh_2(PO_4)_3$ must be Cc because the crystals are piezoelectric.[2] When a non centric model was refined by least squares in the space group Cc with all the atoms in general positions, some of the isotropic temperature factors were negative and the coordinates of phosphorus and oxygen atoms were shifted so that P–O bond distances varied from 1.35 to 1.65 Å. Also some oxygen-oxygen distances between different $PO_4$ groupings were also too short, the shortest one was 2.48 Å. Since these irregularities in distances between the atoms could not have a physico-chemical explanation, a further refinement of the structure was attempted in the centric space group C2/c with the sodium atoms disordered about the twofold axis. The atomic coordinates and temperature factors obtained after several full-matrix least squares refinement cycles are listed in Table I and the observed and calculated structure factors in Table II. The atomic scattering factors used were from International Tables for X-ray Crystallography.[8] Both, the real and imaginary, anomalous dispersion corrections were applied in the atomic scattering factor of Th atom. Isotropic thermal parameters for Th and P atoms, listed in Table I, are those

**Table I.** Fractional Coordinates for $NaTh_2(PO_4)_3$. Standard errors are given in parentheses

| | x | y | z | B(Å²) |
|---|---|---|---|---|
| Th(1) | 0.1530(1) | 0.0924(1) | 0.0365(1) | 0.59(3) |
| Na(2) | 0.0184(31) | 0.3883(83) | 0.3482(64) | 7.5 (1.4) |
| P(3) | 0.3120(4) | 0.0828(10) | 0.3130(8) | 0.7 (1) |
| P(4) | 0 | −0.1041(14) | 1/4 | 1.1 (2) |
| O(5) | 0.0752(11) | 0.0297(31) | 0.2530(26) | 1.5 (4) |
| O(6) | −0.0240(13) | −0.2231(38) | 0.0889(30) | 2.2 (4) |
| O(7) | 0.2270(10) | 0.0517(26) | 0.3310(21) | 0.6 (2) |
| O(8) | 0.3619(10) | −0.1017(28) | 0.3392(23) | 0.9 (3) |
| O(9) | 0.2998(9) | 0.1502(26) | 0.1249(20) | 0.5 (3) |
| O(10) | 0.3486(11) | 0.2644(34) | 0.4127(26) | 1.7 (4) |

The anisotropic thermal parameters of Th and P atoms are of the form $T=\exp-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}\ell^2+2\beta_{12}hk+2\beta_{13}h\ell+2\beta_{23}k\ell)$. Each thermal parameter is multiplied by $10^4$. $\beta_{12}$ and $\beta_{23}$ for P(4) are required to be zero by symmetry.

| | $\beta_{11}$ | $\beta_{22}$ | $\beta_{33}$ | $\beta_{12}$ | $\beta_{13}$ | $\beta_{23}$ |
|---|---|---|---|---|---|---|
| Th(1) | 5(1) | 26(2) | 32(1) | 0(0) | 7(1) | 1(1) |
| P(3) | 10(2) | 30(12) | 22(8) | −7(4) | 7(3) | 3(9) |
| P(4) | 7(3) | 37(18) | 80(15) | 0 | 8(5) | 0 |

$R_1 = \sum_{hk\ell} ||F_o|-|F_c|| / \sum_{hk\ell} |F_o| = 0.071$ (including unobserved reflections)

$R_2 = \sum_{hk\ell} ||F_o|-|F_c|| / \sum_{hk\ell} |F_o| = 0.062$ (omitting unobserved reflections)

obtained at $R_2=0.067$ (omitting unobserved reflections) before anisotropic temperature factors were adopted. Anisotropic temperature factors for Th and P were refined in the final stages of refinement. The refinement cycles[9,10] and the calculation of bond lengths and angles[11,12] were carried out on the IBM 360-67 computer at the Washington State University Computing Center[9,11] and on the CAE 90-40 computer at the Institute of Mathematics Computing Center (University of Zagreb).[10,12] Table III gives the interatomic distances and angles obtained from the atomic coordinates in Table I. At this time it was found that the crystals of $NaTh_2(PO_4)_3$ possess ferroelectric properties.[5] The samples investigated were thought to be polydomain crystals, and the observed structure an average. Several attempts were made to distinguish the positions of the sodium atoms in the domains assuming that the samples investigated were two-domain crystals and that all atoms except sodium met the symmetry requirements of C2/c. None of these models was significantly better on Hamilton's test[13] than the disordered model.

## Description and Discussion of the Structure

The main features of the structure of $KTh_2(PO_4)_3$ are repeated in $NaTh_2(PO_4)_3$. All $PO_4$ tetrahedra are discrete groups with no oxygen atom common to two phosphorus atoms, as is obvious from the formula of compound. Each oxygen atom, in addition to being bonded to a phosphorus atom, is also attached to the thorium atom. The packing of thorium atoms and

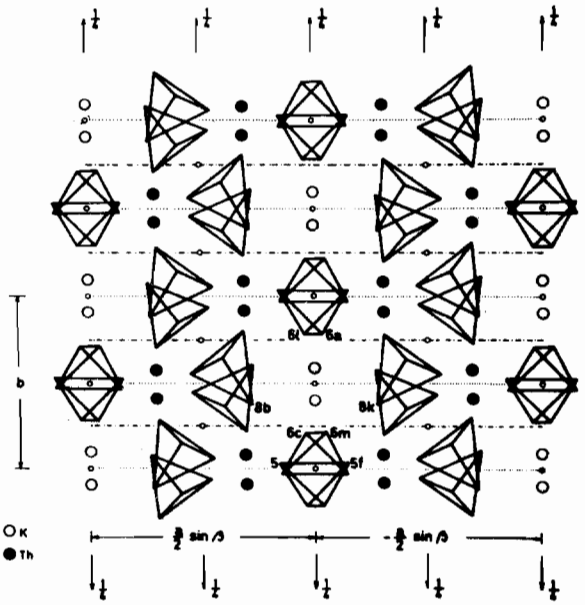


Figure 1. The structure of $KTh_2(PO_4)_3$ and symmetry elements projected down the c-axis. Oxygen atoms from the phosphate groups are connected by full lines. Oxygen atoms O(6c) and O(6m) belong to two different phosphate groups related by symmetry operation of twofold axis.

(8) International Tables for X-ray Crystallography, Vol. III, Birmingham: Kynoch Press (1962).

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**Table II.** Observed, FO, and calculated, FC, structure factors

| H | K | L | 10F0 | 10FC |
|---|---|---|---|---|
| 0 | 0 | 2 | 3665 | 3837 |
| 0 | 0 | 4 | 2458 | 2551 |
| 0 | 0 | 6 | 948 | 932 |
| 0 | 0 | 8 | 1155 | -1077 |
| 0 | 0 | 10 | 1355 | -1664 |
| 0 | 2 | 0 | 3266 | 3009 |
| 0 | 2 | 1 | 1732 | -1558 |
| 0 | 2 | 2 | 789 | 716 |
| 0 | 2 | 3 | 3024 | -3075 |
| 0 | 2 | 4 | 1736 | 1785 |
| 0 | 2 | 5 | 3123 | -3357 |
| 0 | 2 | 6 | 892 | 851 |
| 0 | 2 | 7 | 3624 | -3747 |
| 0 | 2 | 8 | 548 | -480 |
| 0 | 2 | 9 | 1939 | -1986 |
| 0 | 2 | 10 | 670 | -769 |
| 0 | 4 | 0 | 3837 | -3903 |
| 0 | 4 | 1 | 1575 | -1471 |
| 0 | 4 | 2 | 2531 | -2366 |
| 0 | 4 | 3 | 2067 | -1968 |
| 0 | 4 | 4 | 1809 | -1703 |
| 0 | 4 | 5 | 2533 | -2536 |
| 0 | 4 | 6 | 1017 | -895 |
| 0 | 4 | 7 | 2840 | -2829 |
| 0 | 4 | 8 | 537 | 528 |
| 0 | 4 | 9 | 1385 | -1268 |
| 0 | 6 | 0 | 4557 | -4669 |
| 0 | 6 | 1 | 0 | -163 |
| 0 | 6 | 2 | 2889 | -2816 |
| 0 | 6 | 3 | 1368 | 1312 |
| 0 | 6 | 4 | 2124 | -2052 |
| 0 | 6 | 5 | 1059 | 980 |
| 0 | 6 | 6 | 834 | -801 |
| 0 | 6 | 7 | 904 | 836 |
| 0 | 8 | 0 | 241 | -254 |
| 0 | 8 | 1 | 569 | 475 |
| 0 | 8 | 2 | 230 | -85 |
| 0 | 8 | 3 | 1599 | 1778 |
| 0 | 8 | 4 | 257 | -106 |
| 1 | 1 | 0 | 3351 | 3302 |
| 1 | 1 | 1 | 2815 | -2595 |
| 1 | 1 | -1 | 2457 | -2820 |
| 1 | 1 | 2 | 1413 | 1272 |
| 1 | 1 | -2 | 2902 | 3266 |
| 1 | 1 | 3 | 2623 | -2738 |
| 1 | 1 | -3 | 1206 | -1365 |
| 1 | 1 | 4 | 1444 | -1561 |
| 1 | 1 | -4 | 6250 | 6177 |
| 1 | 1 | 5 | 1612 | -1556 |
| 1 | 1 | -5 | 0 | 405 |
| 1 | 1 | 6 | 2538 | -2580 |
| 1 | 1 | -6 | 2117 | 2145 |
| 1 | 1 | 7 | 1588 | -1619 |
| 1 | 1 | -7 | 1121 | 1204 |
| 1 | 1 | 8 | 2178 | -2043 |
| 1 | 1 | -8 | 2018 | 1963 |
| 1 | 1 | 9 | 494 | -432 |
| 1 | 1 | -9 | 1478 | 1464 |
| 1 | 1 | 10 | 2559 | -2642 |
| 1 | 1 | -10 | 571 | 742 |
| 1 | 3 | 0 | 0 | -299 |
| 1 | 3 | 1 | 4837 | -5196 |
| 1 | 3 | -1 | 3272 | -3426 |
| 1 | 3 | 2 | 0 | 68 |
| 1 | 3 | -2 | 1623 | -1571 |
| 1 | 3 | 3 | 5720 | -6056 |
| 1 | 3 | -3 | 1337 | -1208 |
| 1 | 3 | 4 | 0 | 171 |
| 1 | 3 | -4 | 836 | -731 |
| 1 | 3 | 5 | 2710 | -2717 |
| 1 | 3 | -5 | 1365 | 1343 |
| 1 | 3 | 6 | 278 | 428 |
| 1 | 3 | -6 | 282 | -341 |
| 1 | 3 | 7 | 1970 | -1911 |
| 1 | 3 | -7 | 2138 | 1863 |
| 1 | 3 | 8 | 698 | 565 |
| 1 | 3 | -8 | 355 | -273 |
| 1 | 3 | 9 | 462 | -486 |
| 1 | 3 | -9 | 2253 | 2222 |
| 1 | 5 | 0 | 2113 | -2064 |
| 1 | 5 | 1 | 0 | -509 |
| 1 | 5 | -1 | 0 | -247 |
| 1 | 5 | 2 | 1329 | -1099 |
| 1 | 5 | -2 | 3206 | -3155 |
| 1 | 5 | 3 | 1513 | -1292 |
| 1 | 5 | -3 | 1213 | -1160 |
| 1 | 5 | 4 | 1100 | 1284 |
| 1 | 5 | -4 | 4907 | -4631 |
| 1 | 7 | 0 | 1339 | -1254 |
| 1 | 7 | 1 | 2263 | 2226 |
| 1 | 7 | -1 | 2205 | 2175 |
| 1 | 7 | 2 | 993 | -933 |
| 1 | 7 | -2 | 1654 | -1555 |
| 1 | 7 | 3 | 3028 | 2911 |
| 1 | 7 | -3 | 691 | 490 |
| 1 | 7 | 4 | 1009 | 1102 |
| 1 | 7 | -4 | 2185 | -2277 |
| 2 | 0 | 0 | 3343 | -2654 |
| 2 | 0 | 2 | 4196 | -5075 |
| 2 | 0 | -2 | 1785 | 1457 |
| 2 | 0 | 4 | 3512 | -3682 |
| 2 | 0 | -4 | 2908 | 3141 |
| 2 | 0 | 6 | 4901 | -5245 |
| 2 | 0 | -6 | 3282 | 3079 |
| 2 | 0 | 8 | 2169 | -2191 |
| 2 | 0 | -8 | 4101 | 4020 |
| 2 | 0 | 10 | 1002 | -1086 |
| 2 | 0 | -10 | 1694 | 1902 |
| 2 | 2 | 0 | 1542 | -1280 |
| 2 | 2 | 1 | 2723 | -2810 |
| 2 | 2 | -1 | 6100 | -6790 |
| 2 | 2 | 2 | 1774 | -1724 |
| 2 | 2 | -2 | 0 | 233 |
| 2 | 2 | 3 | 2408 | -2625 |
| 2 | 2 | -3 | 4564 | -.704 |
| 2 | 2 | 4 | 1148 | -1136 |
| 2 | 2 | -4 | 1084 | 1039 |
| 2 | 2 | 5 | 912 | -860 |
| 2 | 2 | -5 | 2885 | -3024 |
| 2 | 2 | 6 | 2119 | -1971 |
| 2 | 2 | -6 | 1080 | 1118 |
| 2 | 2 | 7 | 1694 | 1574 |
| 2 | 2 | -7 | 1007 | -891 |
| 2 | 2 | 8 | 806 | -757 |
| 2 | 2 | -8 | 1945 | 1809 |
| 2 | 2 | 9 | 1776 | 1826 |
| 2 | 2 | -9 | 506 | 499 |
| 2 | 2 | -10 | 817 | 785 |
| 2 | 4 | 0 | 1514 | 1386 |
| 2 | 4 | 1 | 2603 | -2629 |
| 2 | 4 | -1 | 4107 | -4236 |
| 2 | 4 | 2 | 2408 | 2499 |
| 2 | 4 | -2 | 0 | -327 |
| 2 | 4 | 3 | 1998 | -1820 |
| 2 | 4 | -3 | 2912 | -2590 |
| 2 | 4 | 4 | 2159 | 2024 |
| 2 | 4 | -4 | 1449 | -1420 |
| 2 | 6 | 0 | 1319 | 1434 |
| 2 | 6 | 1 | 772 | 918 |
| 2 | 6 | -1 | 1602 | 1420 |
| 2 | 6 | 2 | 3190 | 2948 |
| 2 | 6 | -2 | 1289 | -1076 |
| 2 | 6 | 3 | 993 | 927 |
| 2 | 6 | -3 | 959 | 1051 |
| 2 | 6 | 4 | 2976 | 2772 |
| 2 | 6 | -4 | 1670 | -1508 |
| 2 | 8 | 0 | 360 | 385 |
| 2 | 8 | 1 | 2346 | 2323 |
| 2 | 8 | -1 | 3437 | 3470 |
| 2 | 8 | 2 | 0 | -108 |
| 2 | 8 | -2 | 545 | -282 |
| 2 | 8 | 3 | 1311 | 1581 |
| 2 | 8 | -3 | 2028 | 2333 |
| 3 | 1 | 0 | 3567 | -3723 |
| 3 | 1 | 1 | 0 | -427 |
| 3 | 1 | -1 | 1770 | -1453 |
| 3 | 1 | 2 | 5441 | -5840 |
| 3 | 1 | -2 | 3761 | -4486 |
| 3 | 1 | 3 | 1126 | 1112 |
| 3 | 1 | -3 | 1834 | -1989 |
| 3 | 1 | 4 | 2589 | -2722 |
| 3 | 1 | -4 | 1842 | -1966 |
| 3 | 1 | 5 | 1904 | 1909 |
| 3 | 1 | -5 | 2858 | -3128 |
| 3 | 1 | 6 | 1569 | -1531 |
| 3 | 1 | -6 | 0 | 566 |
| 3 | 1 | 7 | 1790 | 1780 |
| 3 | 1 | -7 | 1753 | -1807 |
| 3 | 1 | 8 | 0 | -195 |
| 3 | 1 | -8 | 1466 | 1380 |
| 3 | 1 | 9 | 1789 | 1779 |
| 3 | 1 | -9 | 1545 | -1303 |
| 3 | 1 | -10 | 1700 | 1733 |
| 3 | 3 | 0 | 0 | 377 |
| 3 | 3 | 1 | 799 | -493 |
| 3 | 3 | -1 | 2605 | -2609 |
| 3 | 3 | 2 | 865 | 587 |
| 3 | 3 | -2 | 1296 | 1191 |
| 3 | 3 | 3 | 2355 | 2405 |
| 3 | 3 | -3 | 3608 | -3428 |
| 3 | 3 | 4 | 996 | 865 |
| 3 | 3 | -4 | 538 | 391 |
| 3 | 3 | 5 | 3168 | 3021 |
| 3 | 3 | -5 | 4749 | -4899 |
| 3 | 3 | 6 | 549 | 384 |
| 3 | 3 | -6 | 0 | -173 |
| 3 | 3 | 7 | 2914 | 2757 |
| 3 | 3 | -7 | 3197 | -2988 |
| 3 | 3 | 8 | 0 | -207 |
| 3 | 3 | -8 | 296 | -340 |
| 3 | 3 | 9 | 3320 | 3016 |
| 3 | 3 | -9 | 2113 | -2238 |
| 3 | 5 | 0 | 3412 | 3379 |
| 3 | 5 | 1 | 594 | -386 |
| 3 | 5 | -1 | 731 | -606 |
| 3 | 5 | 2 | 4663 | 4701 |
| 3 | 5 | -2 | 3805 | 3684 |
| 3 | 5 | 3 | 903 | 948 |
| 3 | 5 | -3 | 647 | -656 |
| 3 | 5 | 4 | 2818 | 2612 |
| 3 | 5 | -4 | 1666 | 1421 |
| 3 | 7 | 0 | 1847 | 1793 |
| 3 | 7 | 1 | 0 | 29 |
| 3 | 7 | -1 | 1477 | 1445 |
| 3 | 7 | 2 | 2552 | 2477 |
| 3 | 7 | -2 | 1877 | 1628 |
| 3 | 7 | 3 | 1113 | -1002 |
| 3 | 7 | -3 | 2038 | 1968 |
| 3 | 7 | 4 | 1299 | 1164 |
| 3 | 7 | -4 | 892 | 855 |
| 4 | 0 | 0 | 4717 | -4118 |
| 4 | 0 | 2 | 1988 | -1999 |
| 4 | 0 | -2 | 6877 | -7102 |
| 4 | 0 | 4 | 0 | -99 |
| 4 | 0 | -4 | 4576 | -4717 |
| 4 | 0 | 6 | 2252 | 2279 |
| 4 | 0 | -6 | 3773 | -4095 |
| 4 | 0 | 8 | 2705 | 2516 |
| 4 | 0 | -8 | 1220 | -1217 |
| 4 | 0 | -10 | 493 | 414 |
| 4 | 2 | 0 | 1540 | -1616 |
| 4 | 2 | 1 | 3654 | 3884 |
| 4 | 2 | -1 | 2190 | 2100 |
| 4 | 2 | 2 | 1123 | -992 |
| 4 | 2 | -2 | 2381 | -2183 |
| 4 | 2 | 3 | 3889 | 4091 |
| 4 | 2 | -3 | 48 | 132 |
| 4 | 2 | 4 | 391 | -405 |
| 4 | 2 | -4 | 1539 | -1462 |
| 4 | 2 | 5 | 4510 | 4740 |
| 4 | 2 | -5 | 1769 | -1743 |
| 4 | 2 | 6 | 899 | 934 |
| 4 | 2 | -6 | 1506 | -1402 |
| 4 | 2 | 7 | 1750 | 1675 |
| 4 | 2 | -7 | 2823 | -2685 |
| 4 | 2 | 8 | 1010 | 961 |
| 4 | 2 | -8 | 871 | -714 |
| 4 | 2 | 9 | 766 | 801 |
| 4 | 2 | -9 | 2832 | -2954 |
| 4 | 2 | -10 | 211 | -6 |
| 4 | 4 | 0 | 2329 | 2251 |
| 4 | 4 | 1 | 3052 | 3044 |
| 4 | 4 | -1 | 1961 | 2036 |
| 4 | 4 | 2 | 1348 | 1504 |
| 4 | 4 | -2 | 3156 | 3296 |
| 4 | 4 | 3 | 2515 | 2522 |
| 4 | 4 | -3 | 0 | -166 |
| 4 | 4 | 4 | 0 | 82 |
| 4 | 4 | -4 | 2341 | 2111 |
| 4 | 6 | 0 | 2791 | 2741 |
| 4 | 6 | 1 | 1304 | -1194 |
| 4 | 6 | -1 | 660 | -490 |
| 4 | 6 | 2 | 989 | 1016 |
| 4 | 6 | -2 | 4430 | 4307 |
| 4 | 6 | 3 | 1096 | -1041 |
| 4 | 6 | -3 | 289 | -214 |
| 4 | 6 | 4 | 0 | -52 |
| 4 | 6 | -4 | 2773 | 2679 |
| 4 | 8 | 0 | 239 | 112 |
| 4 | 8 | 1 | 2661 | -2674 |
| 4 | 8 | -1 | 1399 | -1418 |
| 4 | 8 | 2 | 0 | -52 |
| 4 | 8 | -2 | 0 | 217 |
| 4 | 8 | 3 | 2265 | -2360 |
| 4 | 8 | -3 | 294 | 236 |
| 5 | 1 | 0 | 0 | -219 |
| 5 | 1 | 1 | 3639 | 3570 |
| 5 | 1 | -1 | 1784 | 1806 |
| 5 | 1 | 2 | 2369 | 2479 |
| 5 | 1 | -2 | 1351 | -1196 |
| 5 | 1 | 3 | 1868 | 1852 |
| 5 | 1 | -3 | 2256 | 2236 |
| 5 | 1 | 4 | 3586 | 3618 |
| 5 | 1 | -4 | 3132 | -3290 |
| 5 | 1 | 5 | 1017 | 1043 |
| 5 | 1 | -5 | 1440 | 1603 |
| 5 | 1 | 6 | 2948 | 2837 |
| 5 | 1 | -6 | 3495 | -3642 |
| 5 | 1 | 7 | 0 | -89 |
| 5 | 1 | -7 | 470 | 558 |
| 5 | 1 | 8 | 2443 | 2471 |
| 5 | 1 | -8 | 2660 | -2568 |
| 5 | 1 | 9 | 833 | -906 |
| 5 | 1 | -9 | 782 | -712 |
| 5 | 1 | -10 | 2028 | -2195 |
| 5 | 3 | 0 | 0 | -31 |
| 5 | 3 | 1 | 5586 | 6159 |
| 5 | 3 | -1 | 4735 | 4917 |
| 5 | 3 | 2 | 0 | -180 |
| 5 | 3 | -2 | 0 | 427 |
| 5 | 3 | 3 | 2237 | 2273 |
| 5 | 3 | -3 | 4469 | 4439 |
| 5 | 3 | 4 | 1375 | -1291 |
| 5 | 3 | -4 | 399 | 362 |
| 5 | 3 | 5 | 1056 | 1025 |
| 5 | 3 | -5 | 1789 | 1720 |
| 5 | 3 | 6 | 269 | -347 |
| 5 | 3 | -6 | 1091 | 945 |
| 5 | 3 | 7 | 187 | -206 |
| 5 | 3 | -7 | 0 | 120 |
| 5 | 3 | 8 | 421 | -319 |
| 5 | 3 | -8 | 417 | 414 |
| 5 | 3 | -9 | 1215 | -1083 |
| 5 | 5 | 0 | 0 | -238 |
| 5 | 5 | 1 | 719 | 855 |
| 5 | 5 | -1 | 590 | 743 |
| 5 | 5 | 2 | 1588 | -1569 |
| 5 | 5 | -2 | 1766 | 1119 |
| 5 | 5 | 3 | 440 | 441 |
| 5 | 5 | -3 | 1281 | 1018 |
| 5 | 5 | 4 | 3626 | -3410 |
| 5 | 5 | -4 | 3098 | 2657 |
| 5 | 7 | 0 | 0 | -180 |
| 5 | 7 | 1 | 2912 | -2860 |
| 5 | 7 | -1 | 2255 | -2281 |
| 5 | 7 | 2 | 1306 | -1248 |
| 5 | 7 | -2 | 668 | 577 |
| 5 | 7 | 3 | 1583 | -1606 |
| 5 | 7 | -3 | 2538 | -2424 |
| 5 | 7 | 4 | 1558 | -1518 |
| 5 | 7 | -4 | 1753 | 1732 |
| 6 | 0 | 0 | 6133 | 6665 |
| 6 | 0 | 2 | 5820 | 6315 |
| 6 | 0 | -2 | 2072 | 1884 |
| 6 | 0 | 4 | 3941 | 4080 |
| 6 | 0 | -4 | 0 | -169 |
| 6 | 0 | 6 | 1822 | 1874 |
| 6 | 0 | -6 | 734 | -812 |
| 6 | 0 | 8 | 648 | 606 |
| 6 | 0 | -8 | 2942 | -2799 |
| 6 | 0 | -10 | 2321 | -2543 |
| 6 | 2 | 0 | 1290 | 1278 |
| 6 | 2 | 1 | 1599 | 1640 |
| 6 | 2 | -1 | 2402 | 2758 |
| 6 | 2 | 2 | 1792 | 1561 |
| 6 | 2 | -2 | 1516 | 1491 |
| 6 | 2 | 3 | 538 | -559 |
| 6 | 2 | -3 | 4956 | 5051 |
| 6 | 2 | 4 | 1456 | 1476 |
| 6 | 2 | -4 | 831 | 650 |
| 6 | 2 | 5 | 2270 | -2220 |
| 6 | 2 | -5 | 3400 | 3408 |
| 6 | 2 | 6 | 1198 | 1193 |
| 6 | 2 | -6 | 0 | -145 |
| 6 | 2 | 7 | 2814 | -2721 |
| 6 | 2 | -7 | 3470 | 3514 |
| 6 | 2 | 8 | 430 | 334 |
| 6 | 2 | -8 | 1295 | -1336 |
| 6 | 2 | 9 | 1414 | -1795 |
| 6 | 2 | -9 | 1370 | 1371 |
| 6 | 2 | -10 | 947 | -980 |
| 6 | 4 | 0 | 3296 | -3370 |
| 6 | 4 | 1 | 1346 | 952 |
| 6 | 4 | -1 | 1910 | 2077 |
| 6 | 4 | 2 | 2277 | -2269 |
| 6 | 4 | -2 | 1348 | -1042 |
| 6 | 4 | 3 | 0 | -387 |
| 6 | 4 | -3 | 3908 | 3636 |
| 6 | 4 | 4 | 2807 | -2629 |
| 6 | 4 | -4 | 1351 | -749 |
| 6 | 6 | 0 | 3749 | -3783 |
| 6 | 6 | 1 | 0 | -356 |
| 6 | 6 | -1 | 1196 | -961 |
| 6 | 6 | 2 | 2963 | -2871 |
| 6 | 6 | -2 | 1743 | -1749 |
| 6 | 6 | 3 | 255 | 220 |
| 6 | 6 | -3 | 1627 | -1477 |
| 6 | 6 | 4 | 3037 | -3152 |
| 6 | 6 | -4 | 0 | -326 |
| 6 | 8 | 0 | 208 | -97 |
| 6 | 8 | 1 | 759 | -506 |
| 6 | 8 | -1 | 1718 | -1779 |
| 6 | 8 | 2 | 0 | -81 |
| 6 | 8 | -2 | 387 | -249 |
| 6 | 8 | -3 | 3037 | -3032 |
| 7 | 1 | 0 | 3733 | 3897 |
| 7 | 1 | 1 | 1871 | -1876 |
| 7 | 1 | -1 | 736 | -835 |
| 7 | 1 | 2 | 2781 | 2818 |
| 7 | 1 | -2 | 4960 | 4881 |
| 7 | 1 | 3 | 2574 | -2510 |
| 7 | 1 | -3 | 345 | 457 |
| 7 | 1 | 4 | 666 | 580 |
| 7 | 1 | -4 | 3953 | 4100 |
| 7 | 1 | 5 | 1561 | -1338 |
| 7 | 1 | -5 | 1399 | 1449 |
| 7 | 1 | 6 | 741 | -607 |
| 7 | 1 | -6 | 1504 | 1496 |
| 7 | 1 | 7 | 1959 | -1835 |
| 7 | 1 | -7 | 2109 | 2187 |
| 7 | 1 | 8 | 1643 | -1541 |
| 7 | 1 | -8 | 659 | 650 |
| 7 | 1 | 9 | 806 | -910 |
| 7 | 1 | -9 | 1580 | 1620 |
| 7 | 1 | -10 | 337 | -285 |
| 7 | 3 | 0 | 1617 | -1502 |
| 7 | 3 | 1 | 2749 | -2818 |
| 7 | 3 | -1 | 648 | -628 |
| 7 | 3 | 2 | 0 | -152 |
| 7 | 3 | -2 | 923 | -614 |
| 7 | 3 | 3 | 4580 | -4851 |
| 7 | 3 | -3 | 1307 | 1343 |
| 7 | 3 | 4 | 0 | -189 |
| 7 | 3 | -4 | 858 | -705 |
| 7 | 3 | 5 | 3101 | -2854 |
| 7 | 3 | -5 | 2769 | 2640 |
| 7 | 3 | 6 | 233 | 249 |
| 7 | 3 | -6 | 0 | -109 |
| 7 | 3 | 7 | 2885 | -2925 |
| 7 | 3 | -7 | 3454 | 3353 |
| 7 | 3 | 8 | 195 | 140 |
| 7 | 3 | -8 | 283 | -293 |
| 7 | 3 | -9 | 2360 | 2431 |
| 7 | 5 | 0 | 3710 | -3805 |
| 7 | 5 | 1 | 0 | -183 |
| 7 | 5 | -1 | 407 | -537 |
| 7 | 5 | 2 | 2050 | -2057 |
| 7 | 5 | -2 | 3542 | -3410 |
| 7 | 5 | 3 | 720 | -764 |
| 7 | 5 | -3 | 314 | -223 |
| 7 | 5 | 4 | 712 | -757 |
| 7 | 5 | -4 | 4431 | -4199 |
| 7 | 7 | 0 | 1880 | -1889 |
| 7 | 7 | 1 | 1654 | 1600 |
| 7 | 7 | -1 | 0 | 346 |
| 7 | 7 | 2 | 1596 | -1407 |
| 7 | 7 | -2 | 1744 | -1664 |
| 7 | 7 | 3 | 2242 | 2337 |
| 7 | 7 | -3 | 347 | -359 |
| 7 | 7 | 4 | 394 | -270 |
| 7 | 7 | -4 | 2019 | -2084 |
| 8 | 0 | 0 | 1120 | 719 |
| 8 | 0 | 2 | 1584 | -1704 |
| 8 | 0 | -2 | 3823 | 4023 |
| 8 | 0 | 4 | 2658 | -2607 |
| 8 | 0 | -4 | 4181 | 4069 |
| 8 | 0 | 6 | 3457 | -3349 |
| 8 | 0 | -6 | 4014 | 3835 |
| 8 | 0 | 8 | 2389 | -2528 |
| 8 | 0 | -8 | 3770 | 3702 |
| 8 | 0 | -10 | 1142 | 1364 |
| 8 | 2 | 0 | 0 | -95 |
| 8 | 2 | 1 | 3491 | -3453 |
| 8 | 2 | -1 | 5668 | -6000 |
| 8 | 2 | 2 | 619 | -490 |
| 8 | 2 | -2 | 1662 | 1548 |
| 8 | 2 | 3 | 3444 | -3595 |
| 8 | 2 | -3 | 2549 | -2463 |
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| 8 | 2 | -4 | 1357 | 1248 |
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| 8 | 2 | -5 | 820 | -787 |
| 8 | 2 | 6 | 1312 | -1228 |
| 8 | 2 | -6 | 1936 | 1741 |
| 8 | 2 | 7 | 382 | -295 |
| 8 | 2 | -7 | 591 | 504 |
| 8 | 2 | 8 | 972 | -961 |
| 8 | 2 | -8 | 1667 | 1561 |
| 8 | 2 | -9 | 1679 | 1731 |
| 8 | 4 | 0 | 483 | -505 |
| 8 | 4 | 1 | 2417 | -2526 |
| 8 | 4 | -1 | 3669 | -3606 |
| 8 | 4 | 2 | 1097 | 1098 |
| 8 | 4 | -2 | 1520 | -1545 |
| 8 | 4 | 3 | 2794 | -2812 |
| 8 | 4 | -3 | 1635 | -1496 |
| 8 | 4 | 4 | 1443 | 1324 |
| 8 | 4 | -4 | 2951 | -2891 |
| 8 | 6 | 0 | 692 | -574 |
| 8 | 6 | 1 | 831 | 918 |
| 8 | 6 | -1 | 1367 | 1268 |
| 8 | 6 | 2 | 961 | 906 |
| 8 | 6 | -2 | 2233 | -2144 |
| 8 | 6 | 3 | 1255 | 1125 |
| 8 | 6 | -3 | 1015 | 902 |
| 8 | 6 | 4 | 2005 | 1909 |
| 8 | 6 | -4 | 3015 | -2858 |
| 8 | 8 | 0 | 489 | 234 |
| 8 | 8 | 1 | 2167 | 2350 |
| 8 | 8 | -1 | 2578 | 2978 |
| 8 | 8 | 2 | 0 | -118 |
| 8 | 8 | -2 | 318 | -316 |
| 9 | 1 | 0 | 2551 | -2581 |
| 9 | 1 | 1 | 1510 | -1439 |
| 9 | 1 | -1 | 2523 | -2407 |
| 9 | 1 | 2 | 4056 | -4069 |
| 9 | 1 | -2 | 1946 | -1874 |
| 9 | 1 | 3 | 0 | -218 |
| 9 | 1 | -3 | 2373 | -2286 |
| 9 | 1 | 4 | 2970 | -2918 |
| 9 | 1 | -4 | 0 | 236 |
| 9 | 1 | 5 | 647 | 587 |
| 9 | 1 | -5 | 2949 | -2909 |
| 9 | 1 | 6 | 2525 | -2439 |
| 9 | 1 | -6 | 2474 | 2514 |
| 9 | 1 | 7 | 1162 | 1086 |
| 9 | 1 | -7 | 1144 | -1055 |
| 9 | 1 | 8 | 1081 | -1065 |
| 9 | 1 | -8 | 2412 | 2222 |
| 9 | 1 | -9 | 716 | -535 |
| 9 | 1 | -10 | 1719 | 2128 |
| 9 | 3 | 0 | 712 | 648 |
| 9 | 3 | 1 | 2395 | -2488 |
| 9 | 3 | -1 | 3996 | -4073 |
| 9 | 3 | 2 | 503 | 527 |
| 9 | 3 | -2 | 707 | 652 |
| 9 | 3 | 3 | 0 | 113 |
| 9 | 3 | -3 | 3939 | -3787 |
| 9 | 3 | 4 | 0 | 368 |
| 9 | 3 | -4 | 410 | -402 |
| 9 | 3 | 5 | 1221 | 1169 |
| 9 | 3 | -5 | 4615 | -4858 |
| 9 | 3 | 6 | 778 | 735 |
| 9 | 3 | -6 | 0 | -295 |
| 9 | 3 | 7 | 1740 | 1680 |
| 9 | 3 | -7 | 1743 | -1810 |
| 9 | 3 | 8 | 0 | 125 |
| 9 | 3 | -8 | 668 | -616 |
| 9 | 3 | -9 | 797 | -873 |
| 9 | 5 | 0 | 2301 | 2309 |
| 9 | 5 | 1 | 1090 | -928 |
| 9 | 5 | -1 | 387 | -658 |
| 9 | 5 | 2 | 3835 | 3871 |
| 9 | 5 | -2 | 1517 | 1427 |
| 9 | 5 | 3 | 0 | 135 |
| 9 | 5 | -3 | 434 | -568 |
| 9 | 5 | 4 | 2570 | 2691 |
| 9 | 5 | -4 | 648 | -442 |
| 9 | 7 | 0 | 1276 | 1121 |
| 9 | 7 | 1 | 1329 | 1268 |
| 9 | 7 | -1 | 2356 | 2466 |
| 9 | 7 | 2 | 2054 | 2118 |
| 9 | 7 | -2 | 725 | 576 |
| 9 | 7 | 3 | 0 | 79 |
| 9 | 7 | -3 | 1924 | 2018 |
| 9 | 7 | -4 | 348 | 146 |
| 10 | 0 | 0 | 4196 | -4269 |
| 10 | 0 | 2 | 3297 | -3553 |
| 10 | 0 | -2 | 5932 | -6308 |
| 10 | 0 | 4 | 1961 | -1830 |
| 10 | 0 | -4 | 3018 | -2913 |
| 10 | 0 | 6 | 0 | 200 |
| 10 | 0 | -6 | 1723 | -1698 |
| 10 | 0 | 8 | 1202 | 1101 |
| 10 | 0 | -8 | 537 | 339 |
| 10 | 0 | -10 | 1732 | 1809 |
| 10 | 2 | 0 | 1583 | -1502 |
| 10 | 2 | 1 | 1649 | 1520 |
| 10 | 2 | -1 | 709 | 391 |
| 10 | 2 | 2 | 1587 | -1372 |
| 10 | 2 | -2 | 2192 | -2021 |
| 10 | 2 | 3 | 2134 | 2091 |
| 10 | 2 | -3 | 2447 | -2236 |
| 10 | 2 | 4 | 1094 | -971 |
| 10 | 2 | -4 | 915 | -805 |
| 10 | 2 | 5 | 3879 | 3812 |
| 10 | 2 | -5 | 3326 | -3342 |
| 10 | 2 | 6 | 0 | 34 |
| 10 | 2 | -6 | 952 | -869 |
| 10 | 2 | 7 | 2001 | 2156 |
| 10 | 2 | -7 | 2877 | -2922 |
| 10 | 2 | -8 | 257 | -260 |
| 10 | 2 | -9 | 2830 | -3127 |
| 10 | 4 | 0 | 2074 | 2142 |
| 10 | 4 | 1 | 1455 | 1419 |
| 10 | 4 | -1 | 0 | 322 |
| 10 | 4 | 2 | 2432 | 2399 |
| 10 | 4 | -2 | 2991 | 1916 |
| 10 | 4 | 3 | 1628 | 1665 |
| 10 | 4 | -3 | 2068 | -2087 |
| 10 | 4 | 4 | 1189 | 1113 |
| 10 | 4 | -4 | 2103 | 1847 |
| 10 | 6 | 0 | 2893 | 3046 |
| 10 | 6 | 1 | 423 | -500 |
| 10 | 6 | -1 | 0 | 81 |
| 10 | 6 | 2 | 2654 | 2533 |
| 10 | 6 | -2 | 3827 | 3814 |
| 10 | 6 | 3 | 816 | -731 |
| 10 | 6 | -3 | 333 | 334 |
| 10 | 6 | 4 | 1006 | 1107 |
| 10 | 6 | -4 | 1338 | 1818 |
| 11 | 1 | 0 | 1988 | -1851 |
| 11 | 1 | 1 | 2852 | 2583 |
| 11 | 1 | -1 | 1149 | 1121 |
| 11 | 1 | 2 | 0 | 128 |
| 11 | 1 | -2 | 3076 | -3002 |
| 11 | 1 | 3 | 1908 | 1828 |
| 11 | 1 | -3 | 1520 | 1457 |
| 11 | 1 | 4 | 1661 | 1632 |
| 11 | 1 | -4 | 3420 | -3216 |
| 11 | 1 | 5 | 1667 | 1582 |
| 11 | 1 | -5 | 908 | 718 |
| 11 | 1 | 6 | 1940 | 1805 |
| 11 | 1 | -6 | 4231 | -4051 |
| 11 | 1 | 7 | 805 | 722 |
| 11 | 1 | -7 | 1170 | -1063 |
| 11 | 1 | -8 | 1748 | -1657 |
| 11 | 1 | -9 | 1478 | -1476 |
| 11 | 3 | 0 | 0 | 180 |
| 11 | 3 | 1 | 5103 | 5308 |
| 11 | 3 | -1 | 2821 | 2751 |
| 11 | 3 | 2 | 0 | 216 |
| 11 | 3 | -2 | 498 | 616 |
| 11 | 3 | 3 | 3068 | 3072 |
| 11 | 3 | -3 | 2092 | 1890 |
| 11 | 3 | 4 | 246 | -345 |
| 11 | 3 | -4 | 899 | 747 |
| 11 | 3 | 5 | 2201 | 2124 |
| 11 | 3 | -5 | 554 | 289 |
| 11 | 3 | 6 | 659 | -623 |
| 11 | 3 | -6 | 827 | 643 |
| 11 | 3 | 7 | 988 | 1076 |
| 11 | 3 | -7 | 2109 | -2072 |
| 11 | 3 | -8 | 284 | 411 |
| 11 | 3 | -9 | 2240 | -2106 |
| 11 | 5 | 0 | 1164 | 1453 |
| 11 | 5 | 1 | 1205 | 1011 |
| 11 | 5 | -1 | 371 | 509 |
| 11 | 5 | 2 | 0 | -121 |
| 11 | 5 | -2 | 2751 | 2779 |
| 11 | 5 | 3 | 324 | 516 |
| 11 | 5 | -3 | 480 | 376 |
| 11 | 5 | 4 | 1285 | -1240 |
| 11 | 5 | -4 | 3119 | 3096 |
| 11 | 7 | 0 | 992 | 1054 |
| 11 | 7 | 1 | 2423 | -2598 |
| 11 | 7 | -1 | 1603 | -1622 |
| 11 | 7 | 2 | 557 | -542 |
| 11 | 7 | -2 | 1617 | 1484 |
| 11 | 7 | -3 | 1160 | -1209 |
| 11 | 7 | -4 | 1537 | 1685 |
| 12 | 0 | 0 | 2496 | 2465 |
| 12 | 0 | 2 | 3267 | 3250 |
| 12 | 0 | -2 | 612 | -196 |
| 12 | 0 | 4 | 4804 | 4659 |
| 12 | 0 | -4 | 1936 | -1805 |
| 12 | 0 | 6 | 2015 | 2000 |
| 12 | 0 | -6 | 3068 | -2850 |
| 12 | 0 | -8 | 3034 | -2952 |
| 12 | 2 | 0 | 1107 | 1084 |
| 12 | 2 | 1 | 2663 | 2688 |
| 12 | 2 | -1 | 3295 | 3218 |
| 12 | 2 | 2 | 805 | 633 |
| 12 | 2 | -2 | 548 | 584 |
| 12 | 2 | 3 | 1690 | 1628 |
| 12 | 2 | -3 | 4650 | 4786 |
| 12 | 2 | 4 | 1809 | 1618 |
| 12 | 2 | -4 | 701 | -564 |
| 12 | 2 | 5 | 663 | -638 |
| 12 | 2 | -5 | 2529 | 2415 |
| 12 | 2 | 6 | 851 | 834 |
| 12 | 2 | -6 | 1320 | -1157 |
| 12 | 2 | 7 | 1264 | -1323 |
| 12 | 2 | -7 | 2160 | 1919 |

**Table II.** (Continued)

| H | K | L | 10F0 | 10FC | H | K | L | 10F0 | 10FC | H | K | L | 10F0 | 10FC | H | K | L | 10F0 | 10FC | H | K | L | 10F0 | 10FC | H | K | L | 10F0 | 10FC |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 12 | 2 | -8 | 1178 | -1185 | 13 | 3 | -4 | 0 | -151 | 14 | 4 | -1 | 1827 | -1725 | 15 | 5 | -1 | 582 | -719 | 17 | 1 | -5 | 807 | -782 | 19 | 1 | 1 | 707 | 675 |
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| 12 | 4 | 0 | 1289 | -1221 | 13 | 3 | -5 | 3451 | 3106 | 14 | 4 | -2 | 2286 | -2176 | 15 | 5 | 3 | 474 | -359 | 17 | 1 | -7 | 1580 | -1646 | 19 | 1 | 2 | 2196 | 2176 |
| 12 | 4 | 1 | 1778 | 1697 | 13 | 3 | 6 | 138 | 49 | 14 | 4 | 3 | 2460 | -2647 | 15 | 5 | -3 | 590 | -548 | 17 | 1 | -8 | 735 | -698 | 19 | 1 | -2 | 1164 | 1149 |
| 12 | 4 | -1 | 2430 | 2545 | 13 | 3 | -6 | 222 | -79 | 14 | 4 | -3 | 893 | -866 | 15 | 5 | -4 | 1720 | -1793 | 17 | 3 | 0 | 442 | 321 | 19 | 1 | 3 | 278 | -260 |
| 12 | 4 | 2 | 1895 | -1881 | 13 | 3 | -7 | 3783 | 3773 | 14 | 4 | 4 | 505 | 569 | 16 | 0 | 0 | 3079 | -3119 | 17 | 3 | 1 | 2991 | 2817 | 19 | 1 | -3 | 1804 | 1763 |
| 12 | 4 | -2 | 0 | -221 | 13 | 3 | -8 | 0 | 63 | 14 | 4 | -4 | 2614 | -2663 | 16 | 0 | 2 | 4002 | -3960 | 17 | 3 | -1 | 1154 | 1084 | 19 | 1 | -4 | 186 | 169 |
| 12 | 4 | 3 | 1304 | 1287 | 13 | 5 | 0 | 3510 | -3764 | 14 | 6 | 0 | 1583 | -1727 | 16 | 0 | -2 | 3564 | -3373 | 17 | 3 | 2 | 371 | 318 | 19 | 1 | -5 | 1615 | 1642 |
| 12 | 4 | -3 | 3775 | 3591 | 13 | 5 | 1 | 592 | -527 | 14 | 6 | 1 | 624 | 731 | 16 | 0 | 4 | 1956 | -1991 | 17 | 3 | -2 | 773 | 744 | 19 | 1 | -6 | 705 | -718 |
| 12 | 4 | 4 | 2282 | -2266 | 13 | 5 | -1 | 322 | 402 | 14 | 6 | -1 | 1015 | 961 | 16 | 0 | -4 | 1202 | -1113 | 17 | 3 | 3 | 2360 | 2459 | 19 | 3 | 0 | 598 | -536 |
| 12 | 4 | -4 | 677 | 642 | 13 | 5 | 2 | 2336 | -2416 | 14 | 6 | -2 | 2360 | -2371 | 16 | 0 | -6 | 785 | 773 | 17 | 3 | -3 | 362 | -235 | 19 | 3 | 1 | 1002 | 1137 |
| 12 | 6 | 0 | 1692 | -1723 | 13 | 5 | -2 | 2746 | -2730 | 14 | 6 | -3 | 310 | -197 | 16 | 0 | -8 | 1991 | 1807 | 17 | 3 | 4 | 0 | 54 | 19 | 3 | -1 | 2209 | 2292 |
| 12 | 6 | 1 | 779 | -1132 | 13 | 5 | 3 | 0 | -144 | 14 | 6 | -4 | 2601 | -3242 | 16 | 2 | 0 | 1039 | -994 | 17 | 3 | -4 | 531 | 493 | 19 | 3 | 2 | 428 | -357 |
| 12 | 6 | -1 | 1090 | -974 | 13 | 5 | -3 | 343 | 267 | 15 | 1 | 0 | 1148 | -1169 | 16 | 2 | 1 | 576 | -309 | 17 | 3 | -5 | 1541 | -1587 | 19 | 3 | -2 | 0 | -93 |
| 12 | 6 | 2 | 2154 | -2136 | 13 | 5 | 4 | 1447 | -1832 | 15 | 1 | 1 | 1647 | -1597 | 16 | 2 | -1 | 1680 | -1602 | 17 | 3 | -6 | 400 | 473 | 19 | 3 | -3 | 2835 | 2996 |
| 12 | 6 | -2 | 382 | -415 | 13 | 5 | -4 | 2044 | -2044 | 15 | 1 | -1 | 2696 | -2479 | 16 | 2 | 2 | 1745 | -1553 | 17 | 3 | -7 | 2544 | -2619 | 19 | 3 | -4 | 0 | -48 |
| 12 | 6 | 3 | 386 | -119 | 13 | 7 | 0 | 1780 | -1964 | 15 | 1 | 2 | 2491 | -2171 | 16 | 2 | -2 | 1216 | -1029 | 17 | 5 | 0 | 1770 | 2050 | 19 | 3 | -5 | 2316 | 2671 |
| 12 | 6 | -3 | 1220 | -1171 | 13 | 7 | -1 | 697 | -543 | 15 | 1 | -2 | 537 | 683 | 16 | 2 | 3 | 840 | 786 | 17 | 5 | -1 | 369 | 290 | 20 | 0 | 0 | 2724 | 2971 |
| 12 | 6 | -4 | 1453 | 1516 | 13 | 7 | -2 | 1400 | -1290 | 15 | 1 | 3 | 1395 | -1003 | 16 | 2 | -3 | 3076 | -2927 | 17 | 5 | -2 | 3019 | 3253 | 20 | 0 | 2 | 1800 | 2081 |
| 13 | 1 | 0 | 4582 | 4663 | 14 | 0 | 0 | 2931 | 3070 | 15 | 1 | -3 | 1843 | -1685 | 16 | 2 | 4 | 901 | -825 | 17 | 5 | -3 | 109 | -70 | 20 | 0 | -2 | 2859 | 2890 |
| 13 | 1 | 1 | 408 | -555 | 14 | 0 | 2 | 1068 | 881 | 15 | 1 | 4 | 1964 | -1816 | 16 | 2 | -4 | 524 | -542 | 17 | 5 | -4 | 2147 | 2374 | 20 | 0 | -4 | 3185 | 3188 |
| 13 | 1 | -1 | 1216 | 972 | 14 | 0 | -2 | 3211 | 3220 | 15 | 1 | -4 | 2285 | 2220 | 16 | 2 | 5 | 1849 | 1791 | 18 | 0 | 0 | 397 | -310 | 20 | 0 | -6 | 1350 | 1305 |
| 13 | 1 | 2 | 2361 | 2323 | 14 | 0 | 4 | 1050 | -1094 | 15 | 1 | 5 | 386 | -378 | 16 | 2 | -5 | 3623 | -3657 | 18 | 0 | 2 | 1446 | 1375 | 20 | 2 | 0 | 946 | 912 |
| 13 | 1 | -2 | 2522 | 2447 | 14 | 0 | -4 | 4949 | 4899 | 15 | 1 | -5 | 1725 | -1549 | 16 | 2 | -6 | 0 | -60 | 18 | 0 | -2 | 1494 | -1427 | 20 | 2 | 1 | 1160 | -1305 |
| 13 | 1 | 3 | 1527 | -1384 | 14 | 0 | 6 | 1772 | -1635 | 15 | 1 | 6 | 2585 | -2566 | 16 | 2 | -7 | 2141 | -2302 | 18 | 0 | 4 | 2228 | 2557 | 20 | 2 | -1 | 551 | -523 |
| 13 | 1 | -3 | 1400 | 1403 | 14 | 0 | -6 | 2642 | 2612 | 15 | 1 | -6 | 2456 | 2400 | 16 | 2 | -8 | 705 | 614 | 18 | 0 | -4 | 2766 | -2735 | 20 | 2 | 2 | 827 | 888 |
| 13 | 1 | 4 | 2034 | 2025 | 14 | 0 | -8 | 2197 | 2240 | 15 | 1 | -7 | 615 | -376 | 16 | 4 | 0 | 1595 | 1619 | 18 | 0 | -6 | 3348 | -3365 | 20 | 2 | -2 | 1203 | 1195 |
| 13 | 1 | -4 | 2207 | 2107 | 14 | 2 | 0 | 1217 | 1072 | 15 | 1 | -8 | 2818 | 2869 | 16 | 4 | -1 | 1235 | -1273 | 18 | 2 | 0 | 0 | 85 | 20 | 2 | -3 | 984 | 1037 |
| 13 | 1 | 5 | 1143 | -1077 | 14 | 2 | 1 | 2939 | -2741 | 15 | 3 | 0 | 0 | 342 | 16 | 4 | -2 | 2112 | 1916 | 18 | 2 | 1 | 2955 | 2972 | 20 | 2 | -4 | 1252 | 1291 |
| 13 | 1 | -5 | 1899 | 1855 | 14 | 2 | -1 | 2925 | -2820 | 15 | 3 | 1 | 2736 | -2799 | 16 | 4 | 3 | 815 | 898 | 18 | 2 | -1 | 2622 | 2610 | 20 | 2 | -5 | 2012 | 1969 |
| 13 | 1 | 6 | 781 | 709 | 14 | 2 | 2 | 805 | 452 | 15 | 3 | -1 | 4355 | -4246 | 16 | 4 | -3 | 2166 | -2168 | 18 | 2 | 2 | 520 | 527 | 21 | 1 | 0 | 176 | 314 |
| 13 | 1 | -6 | 442 | 429 | 14 | 2 | -2 | 1096 | 1022 | 15 | 3 | 2 | 540 | 424 | 16 | 4 | -4 | 872 | 801 | 18 | 2 | -2 | 388 | -341 | 21 | 1 | 1 | 1401 | -1338 |
| 13 | 1 | 7 | 1342 | -1412 | 14 | 2 | 3 | 3446 | -3489 | 15 | 3 | -2 | 0 | -120 | 16 | 6 | -1 | 607 | 533 | 18 | 2 | 3 | 1697 | 1862 | 21 | 1 | -1 | 1710 | -1688 |
| 13 | 1 | -7 | 2471 | 2430 | 14 | 2 | -3 | 696 | -607 | 15 | 3 | 3 | 1625 | -1563 | 16 | 6 | -2 | 2113 | 2104 | 18 | 2 | -3 | 3009 | 3008 | 21 | 1 | -2 | 1880 | 2039 |
| 13 | 1 | -8 | 983 | -887 | 14 | 2 | 4 | 484 | -400 | 15 | 3 | -3 | 3165 | -2954 | 16 | 6 | -3 | 407 | 894 | 18 | 2 | -4 | 1204 | -1158 | 21 | 1 | -3 | 706 | -746 |
| 13 | 1 | -9 | 1169 | 1219 | 14 | 2 | -4 | 2236 | 2061 | 15 | 3 | 4 | 274 | 295 | 17 | 1 | 0 | 2138 | -2154 | 18 | 2 | -5 | 1064 | 1072 | 21 | 1 | -4 | 1806 | 2242 |
| 13 | 3 | 0 | 766 | -679 | 14 | 2 | 5 | 1950 | -1996 | 15 | 3 | -4 | 412 | -531 | 17 | 1 | 1 | 1522 | 1342 | 18 | 2 | -6 | 1196 | -1251 | 21 | 1 | -5 | 517 | -420 |
| 13 | 3 | 1 | 834 | -823 | 14 | 2 | -5 | 1462 | 1311 | 15 | 3 | 5 | 473 | -507 | 17 | 1 | -1 | 690 | 640 | 18 | 2 | -7 | 148 | 142 | 21 | 3 | -2 | 0 | -285 |
| 13 | 3 | -1 | 2094 | 2006 | 14 | 2 | 6 | 598 | -688 | 15 | 3 | -5 | 2662 | -2658 | 17 | 1 | 2 | 1280 | -1220 | 18 | 4 | 0 | 0 | 56 | 22 | 0 | -2 | 1088 | -995 |
| 13 | 3 | 2 | 906 | -757 | 14 | 2 | -6 | 1160 | 1073 | 15 | 3 | -6 | 529 | -546 | 17 | 1 | -2 | 3514 | -3397 | 18 | 4 | -1 | 1993 | 2069 | | | | | |
| 13 | 3 | -2 | 547 | -589 | 14 | 2 | -7 | 1742 | 1706 | 15 | 3 | -7 | 587 | 622 | 17 | 1 | 3 | 1331 | 1256 | 18 | 4 | -2 | 1085 | 698 | | | | | |
| 13 | 3 | 3 | 2360 | 2280 | 14 | 2 | -8 | 981 | 880 | 15 | 3 | -8 | 427 | -421 | 17 | 1 | -3 | 0 | 287 | 18 | 4 | -3 | 2031 | 2107 | | | | | |
| 13 | 3 | -3 | 2534 | 2491 | 14 | 4 | 0 | 1466 | -1619 | 15 | 5 | 0 | 949 | 928 | 17 | 1 | 4 | 228 | -279 | 18 | 4 | -4 | 1290 | 1402 | | | | | |
| 13 | 3 | 4 | 255 | -328 | 14 | 4 | 1 | 1821 | -1785 | 15 | 5 | 1 | 605 | -668 | 17 | 1 | -4 | 2682 | -2658 | 19 | 1 | 0 | 2608 | 2567 | | | | | |

the phosphate groups is very close in the whole unit cell except along twofold axes between phosphate groups where there are channels parallel to the c-axis, Figure 1. These channels are so large that any of alkaline metal cation fit inside their and leave the unit cell practically unchanged.[3] Figure 2 represents a perspective view of the cavity. The centre of the cavity is surrounded by eight oxygen atoms of six phosphate groups, two of which are bidentate and the others monodentate. A twofold axes passes through the cavity (in the case of C2/c space group) and relates the oxygen atoms of the bidentate phosphate groups.

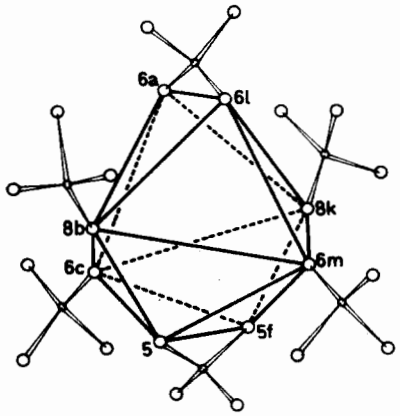


Figure 2. A view down the polyhedron of oxygen atoms around the alkali metal atom (which is omitted in the figure).

In the structure of $KTh_2(PO_4)_3$ potassium atom is located on the twofold axis close to the centre of the cavity.

When a smaller, sodium atom is in the cavity, it is out of two fold axes and farther from the centre. The closest sodium-oxygen distance is 2.49 Å. In the case of $NaTh_2(PO_4)_3$ the results of the least squares refinement suggest that each of two sodium atoms occupies half of positions which are out, but close to twofold axes. Figure 3 shows both positions of two half sodium atoms in the cavity and the empty site where, in $KTh_2(PO_4)_3$, potassium atom is located. Figure 4 is the projection of the structure of $NaTh_2(PO_4)_3$ on a plane normal to *b* axis. The atomic positions are the

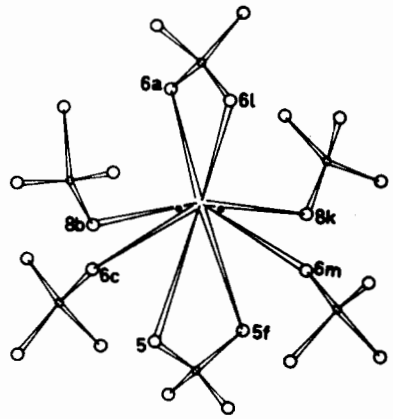


Figure 3. The positions of two sodium atoms (black circles) in the structure of $NaTh_2(PO_4)_3$ in comparison with the empty site where, in $KTh_2(PO_4)_3$, potassium atom is located. The empty site of potassium atom and coordinated oxygen atoms from phosphates groups are connected by full lines.

**Table III.** Interatomic distances and angles in $NaTh_2(PO_4)_3$ Standard errors are in parentheses

| A | B | C | Distances (Å) A-B | A-C | Angles (degrees) A-B-C |
|---|---|---|---|---|---|
| | | | Within Th-polyhedron | | |
| O(6c) | Th(1) | O(5e) | 2.44(2) | 2.42(3)* | 57.5(7) |
| O(7) | Th(1) | O(9) | 2.51(2) | 2.38(2)* | 56.3(4) |
| O(5e) | Th(1) | O(7e) | 2.58(2) | 2.60(3) | 61.5(6) |
| O(5) | Th(1) | O(7) | 2.45(2) | | 63.1(6) |
| O(9g) | Th(1) | O(9) | 2.42(1) | 2.76(2) | 67.4(4) |
| O(9) | Th(1) | O(7e) | 2.54(1) | 2.84(2) | 68.5(4) |
| O(7e) | Th(1) | O(9g) | 2.50(2) | 2.81(2) | 69.6(5) |
| O(8b) | Th(1) | O(9g) | 2.35(2) | 2.76(1) | 70.6(4) |
| O(10h) | Th(1) | O(5) | 2.27(1) | 2.74(2) | 70.8(6) |
| O(5) | Th(1) | O(6c) | | 3.05(3) | 77.0(7) |
| O(8b) | Th(1) | O(6c) | | 2.82(3) | 71.9(7) |
| O(7) | Th(1) | O(10h) | | 2.91(2) | 74.9(4) |
| O(10h) | Th(1) | O(7e) | | 2.95(2) | 76.2(5) |
| O(8b) | Th(1) | O(5) | | 2.89(3) | 74.0(6) |
| O(7) | Th(1) | O(8b) | | 3.01(2) | 76.5(5) |
| O(10h) | Th(1) | O(5e) | | 3.12(2) | 79.8(5) |
| O(8b) | Th(1) | O(9) | | 3.34(2) | 85.9(6) |
| O(5e) | Th(1) | O(9g) | | 3.40(3) | 85.6(5) |
| O(6c) | Th(1) | O(9g) | | 3.25(3) | 83.6(7) |
| O(10h) | Th(1) | O(9) | | 3.65(2) | 98.5(6) |
| O(5) | Th(1) | O(5e) | | 4.09(1) | 108.6(7) |
| O(7) | Th(1) | O(7e) | | 4.13(1) | 111.1(6) |
| O(10h) | Th(1) | O(6c) | | 3.94(3) | 113.0(8) |
| O(6c) | Th(1) | O(7e) | | 4.15(3) | 114.4(7) |
| O(7) | Th(1) | O(9g) | | 4.17(2) | 115.6(5) |
| O(5) | Th(1) | O(9) | | 4.31(2) | 119.0(5) |
| O(8b) | Th(1) | O(5e) | | 4.39(2) | 126.0(5) |
| O(5e) | Th(1) | O(9) | | 4.62(2) | 128.9(5) |
| O(7) | Th(1) | O(6c) | | 4.56(3) | 134.4(7) |
| O(8b) | Th(1) | O(7e) | | 4.53(2) | 138.5(6) |
| O(10h) | Th(1) | O(8b) | | 4.37(2) | 141.9(3) |
| O(5) | Th(1) | O(9g) | | 4.63(2) | 143.5(6) |
| O(10h) | Th(1) | O(9g) | | 4.49(2) | 145.7(5) |
| O(5) | Th(1) | O(7e) | | 4.74(3) | 146.8(6) |
| O(6c) | Th(1) | O(9) | | 4.80(3) | 148.3(7) |
| O(7) | Th(1) | O(5e) | | 4.96(3) | 154.7(6) |
| | | | Within the phosphate groups | | |
| O(6) | P(4) | O(5f) | 1.53(3) | 2.42(3) | 102(1) |
| O(6f) | P(4) | O(5) | | | |
| O(5) | P(4) | O(6) | | | |
| O(5f) | P(4) | O(6f) | 1.59(2) | 2.61(3) | 114(1) |
| O(5) | P(4) | O(5f) | | 2.60(4) | 110(1) |
| O(6) | P(4) | O(6f) | | 2.59(5) | 116(2) |
| O(7) | P(3) | O(9) | 1.53(2) | 2.38(2) | 100(1) |
| O(9) | P(3) | O(10) | 1.57(1) | 2.46(1) | 104(1) |
| O(8) | P(3) | O(7) | 1.52(2) | 2.55(2) | 114(1) |
| O(10) | P(3) | O(7) | 1.55(1) | 2.54(2) | 112(1) |
| O(8) | P(3) | O(9) | | 2.53(2) | 110(1) |
| O(8) | P(3) | O(10) | | 2.58(2) | 115(1) |

* Also within the phosphate group.

mean values from the least squares refinement carried out in the space group C2/c. The $[Th_2(PO_4)_3]$ groupings in $NaTh_2(PO_4)_3$ are not significantly different from those in $KTh_2(PO_4)_3$. The interatomic distances and angles in $NaTh_2(PO_4)_3$ are represented in Table III. Thorium-oxygen distances are from 2.27 to 2.58 Å. Phosphorus-oxygen distances within the phosphate groups vary from 1.52 to 1.59 Å. From the results obtained in the idealized structure it is obvious that the bond lengths and angles in $PO_4$ tetrahedra deviate to some small extent from the results obtained and discussed before.[4]

**Table III.** (Continued)

| Sodium-oxygen distances ⩽4.02 Å Standard errors are 0.06 Å | | |
|---|---|---|
| Na(2) | O(6m) | 2.49 |
| Na(2f) | O(6c) | |
| Na(2) | O(8k) | 2.71 |
| Na(2f) | O(8b) | |
| Na(2) | O(6l) | 2.69 |
| Na(2f) | O(6a) | |
| Na(2) | O(5) | 2.80 |
| Na(2f) | O(5f) | |
| Na(2) | O(8b) | 2.80 |
| Na(2f) | O(8k) | |
| Na(2) | O(10j) | 2.91 |
| Na(2f) | O(10d) | |
| Na(2) | O(5f) | 2.96 |
| Na(2f) | O(5) | |
| Na(2) | O(8j) | 3.30 |
| Na(2f) | O(8d) | |
| Na(2) | O(6a) | 3.38 |
| Na(2f) | O(6l) | |
| Na(2) | O(9b) | 3.60 |
| Na(2f) | O(9k) | |
| Na(2) | O(6c) | 3.75 |
| Na(2f) | O(6m) | |
| Na(2) | O(10k) | 4.02 |
| Na(2f) | O(10b) | |

Numbering of the Atoms

Small letters indicate symmetry transformations or cell translations:

a: x, y+1, z
b: ½−x, ½+y, ½−z
c: −x, −y, −z
d: ½+x−1, ½−y, ½+z−1
e: x, −y, ½+z−1
f: −x, y, ½−z
g: ½−x, ½−y, −z
h: ½−x, ½+y−1, ½−z
i: ½+x−1, ½+y−1, z
j: ½−x, ½−y, 1−z
k: ½+x−1, ½+y, z
l: −x, y+1, ½−z
m: x, −y, ½+z.

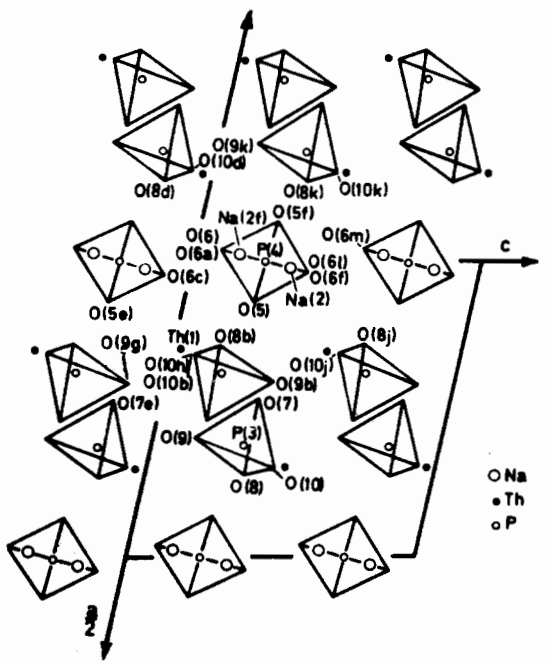


Figure 4. Projection of the structure of $NaTh_2(PO_4)_3$ on a plane normal to b-axis. Oxygen atoms from the phosphates groups are connected by full lines. Only those atoms are numbered which are mentioned in the text or tables.

The present paper describes without any ambiguity the structural model of a hitherto unknown ferroelectric compound . Bond lengths and angles do not represent the absolute truth because they were obtained on the assumption that the shifts of atoms in domains do not have significant value. The standard deviations of bond lengths and angles, which were obtained from the least squares refinement, are probably under estimated. More precise structural studies of a monodomain ferroelectric sample stabilized by an electric field are planned in order to give more accurate values for bond lengths and angles and to completely explain why the crystals of $NaTh_2(PO_4)_3$ exhibit ferroelectric properties.