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Crystal Structure of Thorium Nitrate Pentahydrate by Neutron Diffraction

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The crystal structure of thorium nitrate pentahydrate, $Th(NO_3)_4 . 5H_2O$, has been determined by neutron diffraction. It is orthorhombic, space group *Fdd*2, with $a = 11{\cdot}191 \pm 0{\cdot}007$ Å, $b = 22{\cdot}889 \pm 0{\cdot}015$ Å and $c = 10{\cdot}579 \pm 0{\cdot}007$ Å. A total of 1642 independent reflections with $2\theta < 122°$ ($\lambda = 1{\cdot}065$ Å) were used. The structure was solved from the three-dimensional Patterson function and refined by the full-matrix least-squares method to $R = 4{\cdot}3$ % with the use of a statistical weighting scheme.

Eleven oxygen atoms are bound to the thorium atom, eight being from four bidentate nitrate groups and the other three from water molecules. The Th–O (water) distances, 2·438 and 2·473 Å, are shorter than the Th–O (nitrate) distances, 2·528 to 2·618 Å. The nitrate groups are planar and the N–O distances are found to be significantly different within the group. The structure is tied together by a simple hydrogen-bond scheme in which the hydrogen bonds are either 'strong' water–water hydrogen bonds (2·70 Å) or 'weak' water–nitrate oxygen hydrogen bonds (2·90–2·95 Å).

Introduction

Templeton & Dauben (1950) made an X-ray diffraction study of thorium nitrate pentahydrate, and found the space group to be *Fdd*2, with $a = 11{\cdot}2$, $b = 22{\cdot}8$, $c = 10{\cdot}6$ Å and 8 molecules per unit cell. The thorium atom only was located, at (0, 0, *z*) on the twofold axis. They considered the crystal to be the hexahydrate, admitting the exact composition was in doubt. Ferraro, Katzin & Gibson (1953) made a careful study of the ternary system thorium nitrate–water–nitric acid at 25 °C, and found that the stable hydrates at this temperature are the pentahydrate and tetrahydrate. Staritzky (1956) showed the number of water molecules in the crystal is five by density measurements and that its structure is apparently isomorphous with the plutonium and cerium analogues, $Pu(NO_3)_4 . 5H_2O$ and $Ce(NO_3)_4 . 5H_2O$ as determined from X-ray powder patterns.

The present neutron diffraction study was begun in order to determine accurately the complete structure including the hydrogen positions. At the time this neutron investigation was presented orally (Taylor, Mueller & Hitterman, 1965) it was found that an independent X-ray study of this compound had been carried out. This investigation by Ueki, Zalkin & Templeton (1966) is reported in an adjacent paper.

Experimental

Thorium nitrate pentahydrate was prepared according to the phase diagram of Ferraro, Katzin & Gibson (1953). Powder photos were obtained with a 114·6 mm diameter camera using Cr *Kα* and Cu *Kα* radiations. Nineteen lines from the Cu *Kα* photograph and 21 lines from the Cr*Kα* photograph were used with the least-squares lattice constant program of Mueller, Heaton & Miller (1960) to obtain the following cell dimensions and standard deviations (no systematic correction term):

$$a = 11{\cdot}191 \pm 0{\cdot}007 \text{ Å},$$
$$b = 22{\cdot}889 \pm 0{\cdot}015$$
$$c = 10{\cdot}579 \pm 0{\cdot}007.$$

A large single crystal was selected and shaped to a sphere of weight 1·62 g. This crystal was sealed in a thin-walled vanadium can and used to collect three-dimensional neutron diffraction data on the Argonne three-circle neutron instrument (Mueller, Heaton & Sidhu, 1963). Time at each step was controlled by a monitor count, with a counting time of about 12 minutes per reflection. The width of the 2θ scan varied from about 5° in the range 30–60° 2θ to about 9° in the range 90–122° 2θ. Complete data were collected within a 2θ of 122° ($\lambda = 1{\cdot}065$ Å) with the intensities still appreciable at the higher 2θ limit. A total of 1642 independent intensities were measured (20 unobservably small). Standard reflections were measured each day and the intensities were corrected for slight instrumental drifts. Absorption corrections were applied ($\mu = 1{\cdot}4$ cm^{-1}, $\mu r = 0{\cdot}72$), and the data were placed on a near absolute scale by comparison with the intensities from a magnesium oxide crystal.

No reflections were found which would violate the selection rules for *Fdd*2, although a search for these was made. It was concluded that the above space group is correct, in agreement with indexing of the powder photographs.

Structure analysis

Three-dimensional neutron Patterson map

Since the previous X-ray investigation had indicated the position of the thorium atoms only, an attempt

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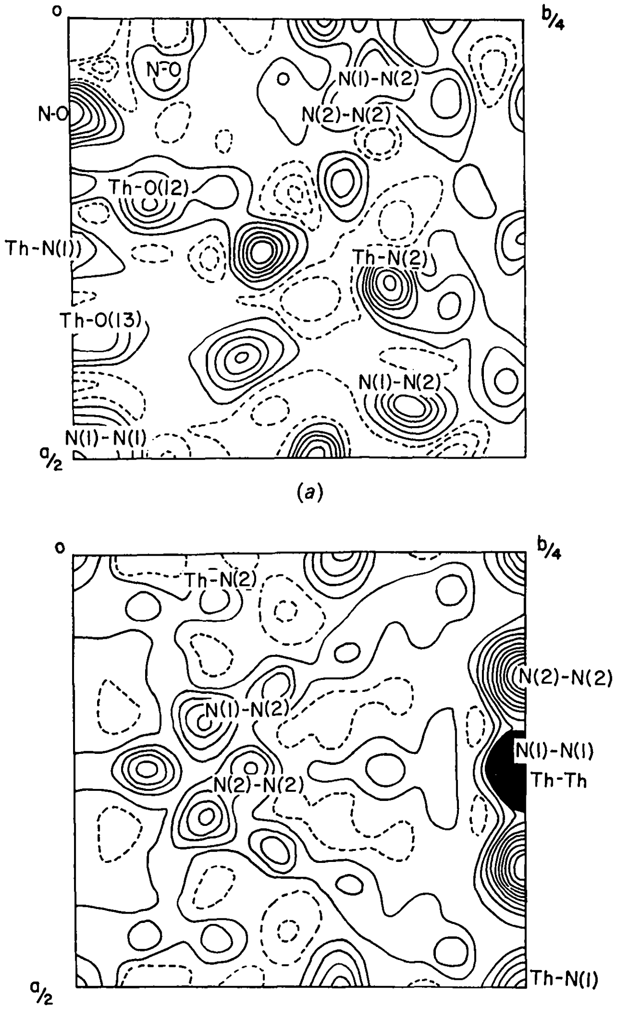
was made to unravel the structure from the three-dimensional neutron Patterson synthesis. With the thorium atoms in the special positions 8(*a*) at (0, 0, *z*; $\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}+z$) and 8[$Th(NO_3)_4 . 5H_2O$] per unit cell, it seemed most probable that all the remaining atoms would be in the general positions 16(*b*) except one water oxygen atom which would necessarily be in 8(*a*) because of the odd number of water molecules in the formula unit. This led to a total of 17 atoms in the asymmetric unit. The thorium atom was placed at the origin by giving it the arbitrary coordinate $z=0$.

A three-dimensional neutron Patterson map was calculated from 1278 reflections. The section $z=0$ of this is shown in Fig. 1(*a*). The N–O vectors in the nitrate groups appeared as two somewhat smeared-out peaks about 1·25 Å from the origin which are indicated in Fig. 1(*a*). The N–O peak lying along **a** lay around the level $z=0$, while the other N–O peak lay appreciably off this level at $z=3/60$, indicating a tilt of the nitrate groups with respect to the *ab* plane.



(*a*)

(*b*)

Fig. 1. (*a*) Section $z=0$, (*b*) section $z=\frac{1}{4}$ of the three-dimensional neutron Patterson synthesis.

One nitrate group consisting of the atoms N(1), O(11), O(12) and O(13), called $NO_3(1)$, was readily located through the Th–$NO_3(1)$ vectors. This nitrate group was coordinated to the thorium atom and was bidentate. Better estimates of the coordinates in $NO_3(1)$ were made by using the vectors from thorium to the $NO_3(1)$ related by the glide ($\frac{1}{4}+x$, $\frac{1}{4}-y$, $\frac{1}{4}+z$). The tilt of $NO_3(1)$ was mainly with respect to the *b* axis, and was made positive with respect to the positive direction of **b**.

In the second nitrate group comprising the atoms N(2), O(21), O(22) and O(23), called $NO_3(2)$, the atom N(2) was located at (0·305, 0·177, 0·077) by means of the strong Th–N and N–N vectors in the zero section [Fig. 1(*a*)] and the section $z=\frac{1}{4}$ [Fig. 1(*b*)]. Positions were derived from the Patterson map for the atoms O(21), O(22) and O(23), but these atoms were located with less confidence than the corresponding oxygens of $NO_3(1)$ because of the greater difficulty found in locating the vectors from the Th and N atoms to O(21), O(22) and O(23).

The vector at (0, 0, 0·233) was considered to be the one from the thorium atom to the water oxygen atom O(1), which is in the special position 8(*a*). A peak at (0, 0·103, 0·067), 2·46 Å from the origin, was considered to represent the vector between thorium and the second water oxygen atom O(2), which was placed at (0·250, 0·147, 0·317). A search was made of the remaining unidentified positive peaks in the Patterson map and two peaks at (0·050, 0·092, 0·392) and (0·208, 0·163, 0·142) were compatible with Th–O(3) vectors, where O(3) is the third and final water oxygen atom in the asymmetric unit. The O(3) atom was not bound to the thorium atom and the tetrahedral distribution of oxygen atoms around it indicated a reasonable hydrogen bonding scheme.

Some of the negative peaks in the Patterson map now suggested a set of hydrogen positions; however it was thought safer in view of the smaller size of these negative peaks to defer the hydrogen assignment until after the first Fourier calculation had been made.

Fourier and least-squares refinement

Structure factors were calculated including the Th, all N and all O atoms with $b_{Th}=1·01$, $b_N=0·940$, $b_O=0·577$ ($\times 10^{-12}$ cm) as given by Bacon (1962). This calculation, using the least-squares program of Busing, Martin & Levy (1962), resulted in an *R* of 49% where

$$R=\sqrt{\Sigma w(F_o-SF_c)^2}/\sqrt{\Sigma wF_o^2}$$

in which *S* is a scale factor and *w* is the statistical weight (Evans, 1961). A three-dimensional Fourier map was calculated with the observed structure factors and the calculated phase angles. There were bumps around the O(21), O(22) and O(23) oxygen peaks of the $NO_3(2)$ group indicating the need for appreciable corrections to these atomic coordinates. Initial hydrogen positions were also indicated in this Fourier map which were in agreement with the positions originally seen in the Patterson map. With the hydrogen atoms included as $b_H = -0{\cdot}378 \times 10^{-12}$ cm (Bacon, 1962) and without shifting the oxygen atoms of the $NO_3(2)$, R dropped to 40%. Two cycles of three-dimensional difference map refinement reduced R to 18%.

R dropped to 10·7% after two cycles of full-matrix isotropic least-squares refinement. At this stage, the positions of the hydrogen atoms were again checked by calculating a three-dimensional difference map. The hydrogen atoms appeared in this map at the positions assumed, indicating that the hydrogen assignment from the Patterson map and the first Fourier maps was correct. Up to this stage 1278 F_o values had been used in the least squares but now all 1642 F_o values were available and were included. After three more isotropic cycles with the complete data an R of 12·1% was obtained.

On attempting the first anisotropic cycle, the program stopped as the temperature factor of one of the hydrogen atoms, H(4), was not positive-definite. A difference map calculated with a set of structure factors for which H(4) had been omitted showed that H(4) was quite anisotropic in its thermal vibration. Three anisotropic cycles were calculated in which all parameters except the positional and thermal parameters (isotropic, converted to anisotropic) of H(4) were varied (R=9·6%). Then two more cycles were calculated in which the positional parameters of H(4) were allowed to vary (R=9·6%). When an attempt was made to vary the thermal parameters of H(4), the temperature factor again was not positive-definite. Half the calculated shifts in the thermal parameters were applied and when this was done, the refinement of the temperature factors of H(4) proceeded normally to R=8·1%. The atom H(4) was apparently so anisotropic in its vibration that the shifts in its temperature factors on going from isotropic to anisotropic refinement were too large, resulting in the failure of the positive-definite test.

At this stage 17 strong low-angle reflections were removed from the least-squares refinement, as they were apparently affected by extinction. As a result, the scale factor increased by 10%; however, there resulted a distinct improvement in R which became constant at 4·3% (statistical weight) and 6·5% (w=1) thus completing the least-squares refinement. At this stage a small scale adjustment was applied to the observed structure factors in order to make them absolute values comparable to the calculated structure factors.

At the end of the refinement, the r.m.s. standard deviation in an observed structure amplitude of unit weight, $[\Sigma w(F_o-F_c)^2/(m-n)]^{\frac{1}{2}}$ where m is the number of observations and n is the number of variables, was found to be 2·54 instead of unity. The fact that the number is greater than unity suggests that the standard deviations, as estimated from the counting statistics, are really an underestimate of the observational errors. Values greater than unity have been found by other workers; for example, 1·88 by Freeman & Snow (1965), 2·0 by Donohue & Marsh (1962), 3·18 by Freeman, Schoone & Sime (1965) and 4·07 by Peterson & Levy (1957). We have calculated a value of 1·20 for our neutron diffraction study of uranyl nitrate hexahydrate (Taylor & Mueller, 1965).

The final positional and thermal parameters are given in Table 1, interatomic distances and bond angles in Table 2. A complete listing of the final F_o and F_c values together with their phase angles is given in Table 3.

Discussion

Configuration of oxygen atoms around thorium

There are eleven oxygen atoms bound to the thorium atom – eight from four bidentate nitrate groups [two $NO_3(1)$ groups and two $NO_3(2)$ groups] and three from

Table 1. *Positional and thermal parameters*

The coordinates and their standard deviations in parentheses are multiplied by 10^4, and the anisotropic thermal parameters B_{ij} and their standard deviations are multiplied by 10^2. The temperature factor expression is: T.F.$=\exp(-\beta_{11}h^2-2\beta_{12}hk\ldots)$ where $4\beta_{12}=B_{12}a^*b^*$, *etc.*

Atom	x	y	z	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Th	0	0	0	96 (4)	78 (4)	122 (5)	−3 (4)	—	—
O(1)	0	0	2304 (4)	446 (20)	214 (13)	168 (13)	−119 (14)	—	—
O(2)	2428 (2)	1464 (1)	3161 (3)	177 (7)	115 (6)	322 (11)	−8 (6)	6 (9)	57 (7)
O(3)	0459 (3)	0883 (1)	3922 (3)	208 (10)	218 (8)	201 (9)	−13 (7)	19 (8)	26 (8)
N(1)	2644 (1)	0054 (1)	0509 (2)	103 (4)	151 (4)	221 (5)	1 (3)	−22 (4)	3 (4)
O(11)	2112 (2)	−0390 (1)	0058 (4)	124 (7)	153 (6)	367 (13)	10 (5)	−20 (8)	−50 (9)
O(12)	1973 (2)	0450 (1)	0907 (3)	170 (8)	195 (8)	261 (11)	10 (6)	−9 (8)	−65 (8)
O(13)	3715 (2)	0088 (1)	0527 (4)	102 (6)	272 (10)	403 (14)	−10(7)	−31 (9)	−80 (10)
N(2)	0477 (1)	0762 (1)	7727 (2)	184 (5)	132 (4)	161 (5)	−19(4)	25 (4)	18 (4)
O(21)	1309 (2)	0552 (1)	8397 (3)	180 (8)	222 (8)	239 (10)	−22 (6)	−1 (8)	77 (8)
O(22)	−0571 (2)	0623 (1)	8092 (3)	169 (8)	193 (6)	220 (9)	−6 (6)	12 (8)	85 (7)
O(23)	0656 (3)	1064 (1)	6814 (3)	282 (11)	258 (10)	214 (10)	3 (9)	55 (9)	79 (9)
H(1)	0178 (5)	0330 (2)	2821 (6)	506 (27)	291 (17)	330 (21)	−151 (18)	−60 (21)	35 (17)
H(2)	1710 (4)	1257 (2)	3412 (6)	281 (17)	214 (15)	408 (23)	−71 (12)	42 (18)	−20 (16)
H(3)	3091 (4)	1201 (2)	3074 (7)	237 (16)	279 (17)	608 (34)	36 (13)	40 (21)	54 (20)
H(4)	−0235 (5)	1113 (3)	4081 (7)	328 (23)	398 (25)	503 (30)	112 (18)	46 (22)	−110 (23)
H(5)	0629 (7)	0665 (3)	4702 (7)	537 (34)	518 (31)	324 (24)	−134 (27)	−128 (24)	139 (22)

water molecules, as shown in Fig. 2. The arrangement has a twofold axis of symmetry along the Th–O(1) line. The two O(2) water oxygen atoms, related by this axis, lie slightly above the thorium *z* level with the NO$_3$(1) pair also slightly above the thorium. The NO$_3$(2) pair hang well below the thorium level. The arrangement around the thorium is complex in that it cannot be described in terms of a coordination polyhedron; however, if the nitrate groups are thought of as single entities instead of bidentate groups then the arrangement somewhat resembles the NbF$_7^{2-}$ arrangement found in K$_2$NbF$_7$ as described by Brown, Walker & Levy (1964). Another view as seen along the Th–O(1) line (from underneath relative to Fig. 2) is shown in Fig. 3, which consists of the two halves of a stereoscopic drawing kindly computed at the Oak Ridge National

Table 2. *Interatomic distances and angles, uncorrected for thermal motion*

Standard deviations are given in parentheses, (× 10^3) for distances and (× 10) for angles.

Th–O (nitrate)	
Th–O(11)	2·528 (3) Å
Th–O(12)	2·618 (3)
Th–O(21)	2·573 (3)
Th–O(22)	2·554 (3)

Th–O (water)	
Th–O(1)	2·438 (5) Å
Th–O(2)	2·473 (3)

Nitrate groups	
N(1)–O(11)	1·270 (3) Å
N(1)–O(12)	1·250 (3)
N(1)–O(13)	1·202 (3)
N(2)–O(21)	1·264 (3)
N(2)–O(22)	1·275 (3)
N(2)–O(23)	1·206 (3)
O(11)–O(12)	2·127 (4)
O(12)–O(13)	2·156 (4)
O(11)–O(13)	2·158 (4)
O(21)–O(22)	2·135 (4)
O(21)–O(23)	2·171 (4)
O(22)–O(23)	2·175 (4)

Water molecules	
O(1)–H(1)	0·953 (6) Å
O(2)–H(2)	0·971 (5)
O(2)–H(3)	0·961 (6)
O(3)–H(4)	0·954 (6)
O(3)–H(5)	0·983 (7)

Other O–O distances	
O(2)—O(12)	3·368 (4) Å
O(2)—O(11)	3·215 (4)
O(2)—O(3)	3·517 (5)
O(3)—O(12)	3·745 (4)
O(3)—O(11)	3·159 (4)
O(3)—O(13)	3·163 (4)
O(3)—O(23)	3·095 (5)
O(13)–O(13)	2·904 (5)
O(13)–O(23)	3·050 (5)

Nitrate groups	
O(11)–N(1)–O(12)	115·2 (2)°
O(12)–N(1)–O(13)	123·2 (2)
O(11)–N(1)–O(13)	121·7 (2)
O(21)–N(2)–O(22)	114·5 (2)
O(21)–N(2)–O(23)	123·0 (2)
O(22)–N(2)–O(23)	122·5 (2)

Water molecules	
H(1)–O(1)–H(1)	110·0 (8)°
H(2)–O(2)–H(3)	111·0 (5)
H(4)–O(3)–H(5)	106·8 (7)

Hydrogen bonds	
O(1)–H(1) · · · O(3)	173·2 (5)°
O(2)–H(2) · · · O(3)	177·5 (6)
O(2)–H(3) · · · O(22)	173·6 (6)
O(3)–H(4) · · · O(23)	167·9 (6)
O(3)–H(5) · · · O(13)	147·9 (7)

Hydrogen bonds	
O(1)–O(3)	2·698 (4) Å
O(2)–O(3)	2·697 (4)
O(2)–O(22)	2·953 (4)
O(3)–O(13)	2·946 (4)
O(3)–O(23)	2·901 (4)
H(1)–O(3)	1·749 (6)
H(2)–O(3)	1·726 (5)
H(3)–O(22)	1·996 (5)
H(4)–O(23)	1·962 (6)
H(5)–O(13)	2·067 (8)

O–O distances between oxygen atoms bound to thorium	
O(1)–O(2)	2·941 (4) Å
O(1)–O(11)	3·469 (4)
O(1)–O(12)	2·850 (4)
O(2)–O(11)	2·795 (4)
O(12)–O(2)	2·665 (4)
O(22)–O(11)	2·755 (4)
O(22)–O(2)	2·931 (5)
O(21)–O(2)	3·058 (4)
O(21)–O(12)	2·768 (4)
O(21)–O(22)	2·833 (4)

Angles around water oxygen atom O(3)	
O(1)—O(3)–O(2)	109·6 (1)°
O(13)–O(3)–O(1)	82·0 (1)
O(13)–O(3)–O(2)	106·7 (1)
O(13)–O(3)–O(23)	60·0 (1)
O(23)–O(3)–O(2)	99·8 (1)
O(23)–O(3)–O(1)	137·8 (1)

O–Th–O angles	
O(11)–Th–O(21)	69·9 (1)°
O(11)–Th–O(22)	65·7 (1)
O(11)–Th–O(1)	88·6 (1)
O(11)–Th–O(2)	67·9 (1)
O(12)–Th–O(11)	48·8 (1)
O(12)–Th–O(21)	64·4 (1)
O(12)–Th–O(1)	68·5 (1)
O(12)–Th–O(2)	63·1 (1)
O(21)–Th–O(22)	67·1 (1)
O(21)–Th–O(22)	49·2 (1)
O(21)–Th–O(2)	74·6 (1)
O(22)–Th–O(2)	71·3 (1)
O(1)–Th–O(2)	73·6 (1)

Laboratory by Dr Carroll K. Johnson, which may be viewed best by means of an inexpensive stereoscope as described in the program (Johnson, 1965). In this figure the atoms are represented by ellipsoids of thermal displacement including 50% probability. This involves a scaling of the r.m.s. displacements by a factor of 1·54 relative to the scale of the bond lengths, with small adjustments for perspective.

The Th–O (nitrate) distances are 2·528–2·618 Å, which are longer than the Th–O (water) distances,

Table 3. *Observed and calculated structure factors*

Reflections indicated with an asterisk presumably suffer from extinction and were omitted from the final least-squares refinement.

H	K	L	FOBS	FCAL
*0	0	4	32.94	43.33
0	0	8	15.17	14.94
0	0	12	9.58	8.57
0	0	16	7.30	6.81
*0	2	2	21.09	24.04
0	2	6	21.77	22.75
0	2	10	1.23	0.26
0	2	14	6.18	5.85
*0	4	0	25.69	34.29
*0	4	4	25.33	28.49
0	4	8	9.54	8.14
0	4	12	11.26	10.94
0	4	16	8.62	8.62
*0	6	2	34.86	49.54
0	6	6	18.87	19.17
0	6	10	20.26	19.57
0	6	14	5.01	4.97
0	8	0	7.07	5.74
*0	8	4	24.57	26.90
0	8	8	6.82	6.59
0	8	12	16.38	15.06
0	8	16	14.81	15.48
*0	10	2	26.17	29.59
0	10	6	28.22	29.39
0	10	10	19.26	18.26
0	10	14	10.37	8.45
*0	12	0	35.13	43.07
0	12	4	22.77	22.66
0	12	8	23.73	23.97
0	12	12	12.03	11.06
0	12	16	1.76	1.80
0	14	2	23.50	24.51
0	14	6	11.32	11.48
0	14	10	6.86	7.50
0	14	14	10.88	10.75
0	16	0	13.99	13.63
0	16	4	27.53	28.72
0	16	8	9.09	8.21
0	16	12	4.93	3.43
0	18	2	22.81	22.69
0	18	6	20.61	20.60
0	18	10	7.04	7.28
0	18	14	4.20	4.15
*0	20	0	37.21	41.65
0	20	4	19.12	19.37
0	20	8	17.96	17.28
0	20	12	14.87	14.58
0	22	2	25.86	27.34
0	22	6	12.34	12.27
0	22	10	7.22	6.62
0	22	14	3.36	3.97
0	24	0	13.23	13.24
0	24	4	17.25	17.08
0	24	8	19.52	20.20
0	24	12	0.00	1.29
0	26	2	16.00	15.87
0	26	6	4.71	3.41
0	26	10	5.21	5.03
0	28	0	24.18	24.54
0	28	4	20.52	20.50
0	28	8	4.25	2.12
0	30	2	12.24	13.08
0	30	6	8.64	8.28
0	32	0	4.54	3.21
0	32	4	6.65	5.47
0	32	8	4.19	5.10
0	34	2	10.36	11.12
0	34	6	10.84	12.06
0	36	0	6.42	7.35
0	36	4	1.67	2.89
*1	1	1	19.87	24.45
1	1	3	11.19	10.37
1	1	5	21.27	22.51
1	1	7	16.09	16.01
1	1	9	11.26	10.32
1	1	11	6.01	5.11
1	1	13	15.10	14.87
1	1	15	3.09	2.34
1	1	17	3.73	3.71
1	3	1	12.42	12.41
1	3	3	7.13	6.41
1	3	5	15.15	15.11
1	3	7	6.83	5.84
1	3	9	17.89	17.88
1	3	11	9.25	9.21
1	3	13	10.51	9.90
1	3	15	5.03	4.40
1	3	17	1.63	2.53
1	5	1	9.06	7.84
1	5	3	23.12	24.52
1	5	5	9.81	9.06
1	5	7	16.37	15.64
1	5	9	6.78	5.37
1	5	11	11.35	10.85
1	5	13	3.92	2.72
1	5	15	4.40	3.88
1	5	17	2.78	4.35
1	7	1	20.88	22.43
1	7	3	19.82	20.21
1	7	5	14.47	14.16
1	7	7	19.10	18.88
1	7	9	14.14	13.89
1	7	11	8.41	7.71
1	7	13	2.64	2.05
1	7	15	7.16	7.01
1	7	17	0.00	2.52
1	9	1	6.73	5.74
1	9	3	20.17	20.28
1	9	5	12.88	11.92
1	9	7	8.28	7.94
1	9	9	11.13	11.82
1	9	11	2.79	2.04
1	9	13	7.81	6.53
1	9	15	5.17	4.94
1	11	1	9.16	8.39
1	11	3	18.56	18.25
1	11	5	6.16	6.52
1	11	7	3.25	2.48
1	11	9	6.55	6.40
1	11	11	6.51	6.21
1	11	13	14.43	13.40
1	11	15	5.52	4.64
1	13	1	1.41	0.98
1	13	3	13.97	13.49
1	13	5	25.28	26.50
1	13	7	9.61	8.70
1	13	9	16.70	16.33
1	13	11	2.37	2.94
1	13	13	9.37	9.03
1	13	15	1.11	0.48
1	15	1	7.34	6.07
1	15	3	22.41	21.89
1	15	5	17.65	17.74
1	15	7	18.60	19.28
1	15	9	5.15	4.18
1	15	11	7.09	6.86
1	15	13	3.81	3.91
1	15	15	6.98	6.86
1	17	1	18.57	18.07
1	17	3	8.26	8.01
1	17	5	4.89	4.43
1	17	7	4.76	5.12
1	17	9	9.37	9.01
1	17	11	10.48	10.82
1	17	13	4.95	3.55
1	17	15	6.09	6.89
1	19	1	22.11	21.93
1	19	3	16.77	17.21
1	19	5	24.07	24.67
1	19	7	16.37	16.84
1	19	9	3.80	2.79
1	19	11	6.83	7.01
1	19	13	6.82	5.32
1	21	1	4.95	4.92
1	21	3	11.15	10.23
1	21	5	12.97	13.01
1	21	7	5.22	4.97
1	21	9	4.36	3.74
1	21	11	7.57	7.20
1	21	13	1.93	0.99
1	23	1	20.22	19.95
1	23	3	13.05	12.04
1	23	5	5.94	5.25
1	23	7	10.31	9.73
1	23	9	10.95	10.42
1	23	11	7.78	6.95
1	23	13	11.00	10.58
1	25	1	11.89	11.40
1	25	3	3.94	3.45
1	25	5	20.85	21.53
1	25	7	3.14	4.12
1	25	9	12.95	13.21
1	25	11	4.06	3.17
1	27	1	8.29	8.14
1	27	3	16.65	16.95
1	27	5	4.36	5.13
1	27	7	12.10	12.23
1	27	9	13.76	13.90
1	27	11	4.98	4.91
1	29	1	13.98	14.13
1	29	3	5.76	5.85
1	29	5	8.35	7.97
1	29	7	9.43	8.84
1	29	9	9.17	8.44
1	29	11	6.83	7.42
1	31	1	4.15	4.98
1	31	3	10.08	10.45
1	31	5	5.97	4.38
1	31	7	8.23	8.65
1	31	9	1.95	1.25
1	33	1	4.49	2.97
1	33	3	6.59	6.33
1	33	5	11.62	12.43
1	33	7	9.17	10.25
1	35	1	4.73	4.03
1	35	3	6.41	6.36
1	35	5	2.54	2.64
1	37	1	6.93	8.52
*2	0	2	30.75	39.78
2	0	6	8.37	8.56
2	0	10	12.82	12.73
2	0	14	3.93	2.93
2	2	0	6.26	5.66
2	2	2	13.69	13.66
2	2	4	14.55	14.35
2	2	6	7.18	6.77
2	2	8	12.72	12.67
2	2	10	9.73	9.71
2	2	12	7.97	7.53
2	2	14	4.90	5.21
2	2	16	5.40	5.46
2	4	0	13.13	12.57
2	4	2	13.49	12.35
2	4	4	14.30	13.71
2	4	6	12.49	12.64
2	4	8	4.67	3.89
2	4	10	17.92	18.15
2	4	12	12.04	12.32
2	4	14	11.18	11.18
2	4	16	6.75	7.70
*2	6	0	27.38	32.27
2	6	2	6.35	5.59
2	12	4	16.63	15.78
2	12	6	13.01	12.52
2	12	8	6.18	6.10
2	12	10	22.70	22.61
2	12	12	5.40	5.18
2	12	14	8.85	8.84
2	12	16	4.02	5.21
2	14	0	16.64	16.19
2	14	2	10.35	9.69
2	14	4	17.26	17.75
2	14	6	5.99	6.11
2	14	8	26.67	27.63
2	14	10	7.22	7.31
2	14	12	14.33	13.80
2	14	14	3.01	3.52
2	14	16	5.94	6.59
2	16	0	12.59	11.62
2	16	2	20.32	20.08
2	16	4	10.57	10.22
2	16	6	25.45	25.90
2	16	8	16.70	16.51
2	16	10	18.37	17.55
2	16	12	5.05	5.06
2	16	14	10.61	10.15
2	18	0	3.62	1.95
*2	6	4	26.84	28.65
2	6	6	4.77	4.02
2	6	8	28.56	30.61
2	6	10	9.42	8.46
2	6	12	12.62	11.95
2	6	14	4.20	4.49
2	6	16	2.18	3.30
2	8	0	17.37	17.64
2	8	2	11.93	10.97
2	8	4	9.88	9.31
2	8	6	17.27	17.32
2	8	8	17.24	16.95
2	8	10	11.81	11.32
2	8	12	4.11	4.23
2	8	14	11.05	10.79
2	8	16	0.00	1.07
2	10	0	26.77	27.70
2	10	2	6.29	5.47
2	10	4	9.98	9.38
2	10	6	9.10	8.54
2	10	8	17.23	17.63
2	10	10	9.63	9.12
2	10	12	15.66	15.16
2	10	14	8.14	7.93
2	10	16	5.33	5.00
2	12	0	3.50	2.34
2	12	2	10.98	9.08
2	18	2	7.71	6.90
2	18	4	11.86	13.11
2	18	6	5.83	6.01
2	18	8	10.07	9.77
2	18	10	1.36	2.61
2	18	12	8.49	8.36
2	18	14	6.60	6.83
2	20	0	6.52	6.03
2	20	2	10.99	8.36
2	20	4	7.94	7.76
2	20	6	11.01	10.06
2	20	8	5.35	5.55
2	20	10	9.83	9.87
2	20	12	9.13	9.38
2	20	14	7.37	7.99
2	22	0	11.48	10.02
2	22	2	4.24	3.94
2	22	4	21.16	21.02
2	22	6	14.36	14.81
2	22	8	15.91	16.54
2	22	10	3.23	4.24
2	22	12	6.74	6.81
2	24	0	4.21	4.37
2	24	2	21.09	21.30
2	24	4	9.62	9.61
2	24	6	7.37	6.95
2	24	8	9.45	9.35
2	24	10	5.22	4.56
2	24	12	6.61	7.15
2	26	0	1.99	2.88
2	26	2	7.61	6.82
2	26	4	12.56	13.15
2	26	6	7.51	7.41
2	26	8	12.71	10.75
2	26	10	5.42	6.26
2	26	12	5.88	7.61
2	28	0	5.51	5.01
2	28	2	10.67	9.04
2	28	4	2.94	3.57
2	28	6	0.63	1.58
2	28	8	1.68	1.14
2	28	10	3.44	4.06
2	30	0	5.40	4.68
2	30	2	11.19	11.27
2	30	4	0.00	0.33
2	30	6	10.25	10.06
2	30	8	6.70	7.61
2	32	0	8.37	8.28
2	32	2	7.98	7.47
2	32	4	6.65	6.04
2	32	6	6.46	7.38
2	32	8	2.99	3.02
2	34	0	0.00	1.10
2	34	2	2.57	1.86
2	34	4	5.06	5.41
2	34	6	3.25	3.42
2	36	0	9.26	9.55
2	36	2	5.48	5.72
2	36	4	6.49	7.40
3	1	1	15.27	14.85
3	1	3	15.07	14.56
3	1	5	17.10	16.94
3	1	7	18.30	20.11
3	1	9	11.50	11.50
3	1	11	8.22	6.76
3	1	13	5.88	5.09
3	1	15	4.17	3.46
3	1	17	4.18	5.09
3	3	1	6.35	5.59
3	3	3	13.58	12.62
3	3	5	8.24	7.58
3	3	7	9.34	8.68
3	3	9	3.42	2.56
3	3	11	18.69	18.70
3	3	13	12.54	11.97
3	3	15	7.55	7.85
3	3	17	5.67	7.36
3	5	1	17.09	17.09
3	5	3	12.57	12.09
3	5	5	21.71	22.30
3	5	7	12.91	13.01
3	5	9	8.43	7.72
3	5	11	8.11	8.19
3	5	13	6.82	5.76
3	5	15	4.54	4.22
3	7	1	14.50	13.65
3	7	3	18.88	18.77
3	7	5	9.33	8.42
3	7	7	8.82	8.94
3	7	9	3.45	3.30
3	7	11	6.05	4.86
3	7	13	3.04	1.88
3	7	15	4.34	3.56
3	9	1	23.27	23.96
3	9	3	9.17	7.58
3	9	5	17.53	17.05
3	9	7	9.03	8.43
3	9	9	6.25	6.08
3	9	11	9.42	9.08
3	9	13	11.81	12.03
3	9	15	6.70	7.18
3	11	1	24.26	24.84
3	11	3	20.89	20.47
3	11	5	20.79	20.32
3	11	7	7.20	6.73
3	11	9	11.09	10.52
3	11	11	10.40	9.82
3	11	13	12.19	11.29
3	11	15	5.90	6.31
3	13	1	17.17	16.09
3	13	3	16.48	16.17
3	13	5	15.47	14.93
3	13	7	4.05	3.54
3	13	9	2.51	1.58
3	13	11	2.46	2.40
3	13	13	4.35	6.19
3	13	15	6.03	5.24
3	15	1	10.65	9.57
3	15	3	6.76	5.91
3	15	5	9.49	8.70
3	15	7	8.84	8.20
3	15	9	8.34	7.81
3	15	11	4.80	5.10
3	15	13	6.45	6.79
3	15	15	3.49	1.97
3	17	1	14.42	13.80
3	17	3	15.10	14.51
3	17	5	14.53	14.46
3	17	7	12.31	11.67
3	17	9	18.00	18.49
3	17	11	4.88	5.22
3	17	13	6.91	6.24
3	17	15	5.19	5.98
3	19	1	15.14	14.47
3	19	3	16.28	15.36
3	19	5	21.52	21.48
3	19	7	2.56	1.12
3	19	9	6.74	6.32
3	19	11	6.97	7.57
3	19	13	7.90	6.75
3	21	1	5.50	5.04
3	21	3	4.53	4.64
3	21	5	6.78	6.13
3	21	7	6.96	7.06
3	21	9	0.59	0.92
3	21	11	2.46	2.78
3	21	13	4.52	3.75
3	23	1	12.01	11.33
3	23	3	14.68	14.39
3	23	5	13.46	12.95
3	23	7	14.14	13.86
3	23	9	6.49	5.91
3	23	11	8.96	8.39
3	23	13	4.11	4.41
3	25	1	10.91	10.40
3	25	3	7.37	6.89
3	25	5	9.41	8.78
3	25	7	3.16	2.95
3	25	9	6.39	6.17
3	25	11	5.47	4.96
3	27	1	8.00	7.71
3	27	3	3.66	3.47
3	27	5	3.62	3.43
3	27	7	3.79	2.86
3	27	9	5.84	5.84
3	27	11	4.35	4.40
3	29	1	18.98	19.18
3	29	3	6.35	6.01
3	29	5	13.95	14.01
3	29	7	2.22	2.11
3	29	9	4.13	4.90
3	31	1	4.94	5.79
3	31	3	2.84	3.73
3	31	5	3.62	3.04
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3	31	9	9.74	10.05
3	33	1	5.24	3.77
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3	33	5	8.25	9.00
3	33	7	7.67	8.50
3	35	1	10.01	10.33
3	35	3	8.45	8.91
3	35	5	3.81	3.27
3	37	1	2.25	2.05
*4	0	0	23.38	25.48
4	0	4	20.45	21.45
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4	0	12	9.49	8.57
4	0	16	6.41	7.39
4	2	0	14.76	14.77
4	2	2	21.02	21.55
4	2	4	15.73	15.64
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4	2	8	19.88	20.52
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4	2	12	11.62	11.37
4	2	14	4.24	3.82
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4	4	6	12.19	11.60
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4	6	4	18.42	17.74
4	6	6	17.09	16.90
4	6	8	14.75	15.02
4	6	10	12.36	11.46
4	6	12	2.90	2.45
4	6	14	3.93	3.77
4	6	16	2.55	1.94
4	8	0	18.05	17.79
4	8	2	19.00	17.86
4	8	4	13.85	13.46
4	8	6	15.15	15.11
4	8	8	10.10	9.51
4	8	10	14.69	15.28
4	8	12	7.66	7.45
4	8	14	5.25	4.69
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4	10	0	3.07	2.35
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4	10	8	16.88	17.12
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4	10	12	9.00	8.10
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4	12	12	4.62	3.65
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4	12	16	2.07	1.83
4	14	0	21.93	22.27
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4	14	10	3.79	3.24
4	14	12	5.22	5.13
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4	16	0	7.36	7.04
4	16	2	8.97	8.21
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4	16	10	9.89	9.38
4	16	12	3.28	2.64
4	16	14	4.32	4.23
4	18	0	1.40	0.24
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4	18	4	13.25	12.36
4	18	6	6.83	6.17
4	18	8	3.33	2.99
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4	18	12	10.35	9.58
4	18	14	4.98	5.18
4	20	0	16.27	14.97
4	20	2	17.25	16.96
4	20	4	11.74	11.64
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4	20	8	3.26	2.32
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4	20	12	8.11	8.30
4	20	14	4.33	3.68
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4	22	2	13.76	13.19
4	22	4	13.36	12.94
4	22	6	9.11	9.03
4	22	8	7.32	7.23
4	22	10	6.52	5.47
4	22	12	2.09	1.76
4	24	0	16.79	17.26
4	24	2	8.68	8.28
4	24	4	9.90	9.75
4	24	6	7.45	7.21
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4	24	10	6.21	7.07
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4	26	6	10.28	10.24
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4	26	10	4.18	3.24
4	28	0	18.68	19.16
4	28	2	8.13	7.99
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4	34	2	5.18	5.48
4	34	4	2.35	1.47
4	34	6	5.73	6.24
4	36	0	2.43	3.15
4	36	2	13.66	14.85
5	1	1	25.77	26.82
5	1	3	16.85	16.36
5	1	5	4.15	4.25
5	1	7	2.96	1.12
5	1	9	13.87	13.87
5	1	11	10.97	11.28
5	1	13	11.66	10.77
5	1	15	4.64	4.16
5	3	1	13.27	12.49
5	3	3	22.69	22.89
5	3	5	23.13	24.25
5	3	7	2.86	4.40
5	3	9	21.79	21.89
5	3	11	15.27	15.57
5	3	13	12.58	12.39
5	3	15	5.07	5.22
5	5	1	3.04	2.03
5	5	3	2.74	0.97
5	5	5	4.40	3.41
5	5	7	14.75	14.41
5	5	9	7.21	6.44
5	5	11	9.44	9.02
5	5	13	7.11	5.98
5	5	15	4.82	5.33
5	7	1	3.96	3.09
5	7	3	8.47	7.80
5	7	5	11.33	10.46
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5	9	1	13.16	12.89
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5	9	9	3.75	3.21
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5	9	13	4.86	5.12
5	9	15	1.19	0.60
5	11	1	4.44	4.20
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5	11	5	5.01	4.84
5	11	7	5.88	8.89
5	11	9	10.87	9.64
5	11	11	5.21	4.39
5	11	13	11.43	10.19
5	11	15	6.24	7.75
5	13	1	20.17	20.05
5	13	3	15.87	15.78
5	13	5	18.39	18.52
5	13	7	15.90	15.73
5	13	9	11.49	11.23
5	13	11	4.46	4.21
5	13	13	4.32	4.02
5	15	1	7.02	6.43
5	15	3	13.35	13.00
5	15	5	11.32	10.85
5	15	7	7.58	7.52
5	15	9	8.35	8.16
5	15	11	6.02	5.17
5	15	13	4.83	4.11
5	15	15	4.75	5.17
5	17	1	1.11	1.44
5	17	3	7.84	7.95
5	17	5	11.09	10.73
5	17	7	7.65	7.77
5	17	9	5.53	5.04
5	17	11	6.21	6.42
5	17	13	7.55	6.58
5	19	1	17.16	16.29
5	19	3	8.98	8.61
5	19	5	5.12	3.86
5	19	7	5.88	4.99
5	19	9	7.02	6.45
5	19	11	2.89	3.51
5	19	13	6.06	6.27
5	21	1	15.66	14.77
5	21	3	19.19	18.33
5	21	5	14.50	13.59
5	21	7	1.86	1.67
5	21	9	6.75	6.72
5	21	11	7.45	7.57
5	21	13	6.73	6.03
5	23	1	2.93	4.12
5	23	3	7.91	8.02
5	23	5	6.49	6.02
5	23	7	13.10	13.58
5	23	9	10.24	10.51
5	23	11	6.56	6.05
5	25	1	17.11	16.98
5	25	3	4.70	3.58
5	25	5	9.98	9.38
5	25	7	8.30	8.10
5	25	9	13.77	13.11
5	25	11	6.19	7.45
5	27	1	9.21	9.43
5	27	3	10.64	9.50
5	27	5	9.04	8.21
5	27	7	6.93	6.15
5	27	9	6.38	6.78
5	27	11	2.98	3.31
5	29	1	3.84	3.82
5	29	3	5.05	5.50
5	29	5	8.17	8.34
5	29	7	4.63	5.21
5	29	9	4.93	5.36
5	31	1	12.24	11.99
5	31	3	6.65	6.91
5	31	5	3.37	4.09
5	31	7	6.62	7.03
5	33	1	3.94	4.36
5	33	3	5.92	5.91
5	33	5	7.02	7.17
5	35	1	10.27	10.09
5	35	3	8.67	8.95
6	0	2	21.90	21.63
6	0	6	4.85	4.68
6	0	10	4.73	3.51
6	0	14	10.03	10.44
6	2	0	3.77	2.84
6	2	2	11.31	11.30
6	2	4	12.83	12.13
6	2	6	19.56	19.69
6	2	8	21.01	21.97
6	2	10	15.36	15.76
6	2	12	12.21	11.93
6	2	14	3.52	4.18
6	2	16	2.65	2.87
6	4	0	3.04	2.40
6	4	2	20.13	19.96
6	4	4	9.35	8.54
6	4	6	17.37	17.45
6	4	8	15.14	15.15
6	4	10	16.47	15.95
6	4	12	8.36	7.92
6	4	14	5.93	4.90
6	4	16	5.73	6.91
6	6	0	4.05	2.81
6	6	2	20.94	20.08
6	6	4	17.66	16.91
6	6	6	21.89	22.42
6	6	8	13.42	13.45
6	6	10	8.89	8.23
6	6	12	10.25	10.11
6	6	14	1.54	2.24
6	6	16	1.76	2.58
6	8	0	24.13	24.80
6	8	2	5.11	4.15
6	8	4	9.98	9.44
6	8	6	9.62	9.18
6	8	8	19.54	19.67
6	8	10	13.29	12.76
6	8	12	3.69	3.10
6	8	14	10.75	10.88
6	8	16	3.11	3.99
6	10	0	2.16	0.41
6	10	2	6.86	6.20
6	10	4	13.31	12.38
6	10	6	11.85	11.43
6	10	8	12.83	12.56
6	10	10	10.90	10.77
6	10	12	8.22	7.78
6	10	14	6.73	7.10
6	12	0	12.99	11.87
6	12	2	14.00	13.20
6	12	4	12.77	12.44
6	12	6	14.95	14.02
6	12	8	9.56	9.39
6	12	10	11.81	11.31
6	12	12	6.13	5.40
6	12	14	7.81	7.52
6	14	0	1.33	1.07
6	14	2	18.25	17.55
6	14	4	25.89	26.09
6	14	6	8.22	7.76
6	14	8	14.64	14.83
6	14	10	0.00	0.79
6	14	12	10.15	9.54
6	14	14	5.92	3.86
6	16	0	12.20	11.60
6	16	2	2.77	1.69
6	16	4	16.90	16.49
6	16	6	9.43	8.86
6	16	8	14.87	13.96
6	16	10	9.29	8.55
6	16	12	4.93	5.10
6	16	14	5.43	5.53
6	18	0	6.00	4.97
6	18	2	1.62	1.80
6	18	4	7.55	7.36
6	18	6	3.80	3.07
6	18	8	14.71	14.42
6	18	10	3.78	3.86
6	18	12	7.53	7.74
6	18	14	6.65	7.74
6	20	0	6.91	6.69
6	20	2	7.24	6.12
6	20	4	13.59	13.61
6	20	6	4.20	4.47
6	20	8	4.98	4.66
6	20	10	7.68	6.73
6	20	12	5.94	5.09
6	22	0	9.89	8.84
6	22	2	18.46	18.80
6	22	4	5.92	6.27
6	22	6	9.02	8.86
6	22	8	7.94	8.37
6	22	10	3.99	3.66
6	22	12	8.45	8.83
6	24	0	5.63	5.65
6	24	2	5.15	4.83
6	24	4	7.94	7.49
6	24	6	11.26	10.68
6	24	8	3.67	3.79
6	24	10	12.84	12.71
6	24	12	7.14	6.81
6	26	0	3.33	2.62
6	26	2	4.27	3.91
6	26	4	7.90	7.32
6	26	6	5.89	5.39
6	26	8	9.96	9.64
6	26	10	5.84	6.57
6	28	0	13.75	13.89
6	28	2	7.07	6.25
6	28	4	10.58	10.33
6	28	6	3.05	3.06
6	28	8	3.22	2.34
6	28	10	3.87	4.80
6	30	0	5.22	3.81
6	30	2	13.99	14.45

Table 3 (*cont.*)

H	K	L	FOBS	FCAL
6	30	4	5.69	5.56
6	30	6	9.87	10.58
6	30	8	5.56	7.43
6	32	0	1.26	2.58
6	32	2	0.00	0.95
6	32	4	3.12	3.01
6	32	6	4.23	4.17
6	34	0	0.00	0.88
6	34	2	2.25	0.35
6	34	4	9.73	10.43
7	1	1	9.31	8.73
7	1	3	7.63	6.82
7	1	5	14.97	14.91
7	1	7	8.83	8.28
7	1	9	4.59	3.56
7	1	11	4.89	5.25
7	1	13	0.00	1.27
7	1	15	3.25	3.28
7	3	1	9.74	9.40
7	3	3	12.18	11.56
7	3	5	7.50	6.89
7	3	7	10.89	10.20
7	3	9	5.31	5.08
7	3	11	8.96	8.64
7	3	13	12.19	11.93
7	3	15	4.68	5.24
7	5	1	12.21	11.39
7	5	3	14.40	14.30
7	5	5	22.17	22.25
7	5	7	6.36	6.39
7	5	9	19.38	19.86
7	5	11	6.59	6.86
7	5	13	4.92	4.14
7	5	15	2.28	2.21
7	7	1	16.72	16.42
7	7	3	11.43	10.77
7	7	5	13.91	13.30
7	7	7	10.26	9.69
7	7	9	6.44	5.52
7	7	11	3.79	3.73
7	7	13	4.49	3.98
7	7	15	0.00	1.88
7	9	1	24.27	24.04
7	9	3	15.36	14.29
7	9	5	9.35	8.99
7	9	7	11.32	11.04
7	9	9	4.06	4.57
7	9	11	14.48	14.52
7	9	13	2.76	2.94
7	9	15	5.57	6.95
7	11	1	21.03	20.65
7	11	3	19.10	18.84
7	11	5	7.80	7.26
7	11	7	16.24	15.72
7	11	9	9.58	8.82
7	11	11	6.52	5.54
7	11	13	4.99	4.99
7	11	15	3.78	4.20
7	13	1	11.28	10.91
7	13	3	16.09	15.44
7	13	5	13.60	13.73
7	13	7	6.39	6.07
7	13	9	6.86	7.00
7	13	11	8.24	7.32
7	13	13	0.98	1.40
7	15	1	11.71	10.98
7	15	3	14.45	13.79
7	15	5	7.87	7.50
7	15	7	14.45	14.27
7	15	9	6.93	6.23
7	15	11	4.64	4.25
7	15	13	10.31	8.56
7	17	1	19.58	19.94
7	17	3	6.34	6.29
7	17	5	20.45	20.66
7	17	7	9.33	9.44
7	17	9	5.44	5.01
7	17	11	7.21	6.96
7	17	13	6.22	6.33
7	19	1	7.52	8.01
7	19	3	8.66	8.48
7	19	5	6.48	5.19
7	19	7	8.94	8.34
7	19	9	7.46	7.57
7	19	11	1.33	1.27
7	19	13	7.06	6.75
7	21	1	12.87	12.56
7	21	3	10.12	9.83
7	21	5	13.01	13.11
7	21	7	4.60	5.90
7	21	9	5.25	5.46
7	21	11	6.56	5.63
7	23	1	9.15	9.20
7	23	3	11.16	10.88
7	23	5	7.84	8.01
7	23	7	8.13	7.75
7	23	9	6.38	6.49
7	23	11	5.89	4.97
7	25	1	8.40	7.97
7	25	3	4.36	3.45
7	25	5	6.39	6.32
7	25	7	8.05	7.70
7	25	9	5.06	5.24
7	25	11	7.20	7.82
7	27	1	8.18	8.00
7	27	3	7.22	6.87
7	27	5	1.77	0.34
7	27	7	4.90	3.86
7	27	9	2.66	2.43
7	29	1	13.09	12.96
7	29	3	12.62	12.22
7	29	5	8.47	8.60
7	29	7	7.64	7.63
7	31	1	5.76	5.59
7	31	3	4.77	6.14
7	31	5	6.71	6.12
7	31	7	2.29	2.64
7	33	1	9.42	9.25
7	33	3	4.67	4.77
7	33	5	6.70	5.89
8	0	0	11.96	11.86
8	0	4	21.90	21.46
8	0	8	15.88	15.76
8	0	12	13.27	12.93
8	2	0	8.59	8.41
8	2	2	24.80	25.80
8	2	4	7.39	6.98
8	2	6	22.49	22.58
8	2	8	15.05	15.50
8	2	10	16.98	16.57
8	2	12	2.22	2.06
8	2	14	7.76	8.77
8	4	0	22.18	22.12
8	4	2	11.10	10.41
8	4	4	13.47	12.43
8	4	6	2.98	2.17
8	4	8	12.44	11.50
8	4	10	2.84	2.77
8	4	12	4.23	2.74
8	4	14	5.10	4.62
8	6	0	8.28	7.45
8	6	2	5.46	5.21
8	6	4	10.31	9.90
8	6	6	9.51	9.06
8	6	8	4.01	2.30
8	6	10	6.66	6.58
8	6	12	4.01	3.27
8	6	14	4.24	3.60
*8	8	0	37.62	41.73
8	8	2	15.81	15.53
*8	8	4	34.44	38.70
8	8	6	15.13	15.03
8	8	8	13.19	12.56
8	8	10	6.62	6.74
8	8	12	9.10	8.69
8	8	14	2.01	1.73
8	10	0	9.68	9.11
8	10	2	29.96	30.48
8	10	4	5.33	4.54
8	10	6	12.99	12.78
8	10	8	4.80	4.24
8	10	10	3.35	2.28
8	10	12	6.08	5.96
8	10	14	7.95	9.24
8	12	0	16.44	15.75
8	12	2	9.93	9.29
8	12	4	14.48	13.44
8	12	6	4.53	4.10
8	12	8	4.54	4.17
8	12	10	4.30	5.34
8	12	12	5.45	5.40
8	12	14	3.12	3.10
8	14	0	10.04	9.37
8	14	2	25.78	26.07
8	14	4	7.19	6.12
8	14	6	17.28	16.65
8	14	8	4.64	4.00
8	14	10	1.60	1.93
8	14	12	3.98	2.69
8	14	14	1.84	0.74
8	16	0	26.25	26.82
8	16	2	8.48	8.07
8	16	4	6.77	6.41
8	16	6	10.85	11.36
8	16	8	5.34	5.79
8	16	10	9.67	9.72
8	16	12	3.63	3.74
8	18	0	1.57	0.06
8	18	2	12.12	11.59
8	18	4	6.98	5.77
8	18	6	9.22	9.03
8	18	8	6.20	4.99
8	18	10	7.10	6.91
8	18	12	4.60	4.64
8	20	0	20.18	20.08
8	20	2	3.89	3.64
8	20	4	20.49	19.51
8	20	6	4.18	4.29
8	20	8	5.13	4.56
8	20	10	6.38	6.47
8	20	12	3.72	3.30
8	22	0	6.09	5.55
8	22	2	2.15	1.85
8	22	4	7.38	7.68
8	22	6	7.67	6.85
8	22	8	6.71	6.20
8	22	10	2.41	2.34
8	24	0	5.30	4.87
8	24	2	4.33	3.95
8	24	4	8.56	8.17
8	24	6	7.39	6.21
8	24	8	4.51	4.10
8	24	10	3.82	3.97
8	26	0	6.37	5.84
8	26	2	9.74	9.06
8	26	4	4.88	4.45
8	26	6	7.70	7.72
8	26	8	6.17	6.28
8	26	10	5.16	5.34
8	28	0	2.08	2.34
8	28	2	2.52	1.51
8	28	4	5.00	3.96
8	28	6	0.46	1.11
8	28	8	0.97	1.97
8	30	0	8.52	8.76
8	30	2	14.89	14.16
8	30	4	10.67	10.88
8	30	6	9.19	9.15
8	32	0	13.82	12.84
8	32	2	5.14	5.07
8	32	4	6.44	6.24
9	1	1	14.05	14.03
9	1	3	15.64	14.78
9	1	5	7.67	7.37
9	1	7	11.61	11.07
9	1	9	7.47	7.30
9	1	11	10.90	10.84
9	1	13	6.72	6.09
9	1	15	4.30	5.95
9	3	1	6.27	5.61
9	3	3	9.82	9.35
9	3	5	11.99	11.51
9	3	7	19.65	20.13
9	3	9	13.24	12.91
9	3	11	14.30	14.28
9	3	13	10.80	10.26
9	3	15	4.00	4.09
9	5	1	24.61	24.41
9	5	3	6.82	6.19
9	5	5	26.96	28.21
9	5	7	11.41	11.13
9	5	9	19.03	19.19
9	5	11	2.62	1.01
9	5	13	6.85	7.00
9	7	1	6.72	5.96
9	7	3	4.51	3.26
9	7	5	14.10	14.02
9	7	7	11.15	10.27
9	7	9	9.06	8.55
9	7	11	3.33	2.49
9	7	13	11.62	11.57
9	9	1	7.64	7.31
9	9	3	4.33	4.23
9	9	5	16.08	16.24
9	9	7	6.95	7.03
9	9	9	12.40	11.94
9	9	11	11.10	11.03
9	9	13	4.74	4.68
9	11	1	11.18	10.41
9	11	3	20.37	19.39
9	11	5	3.68	2.58
9	11	7	10.34	9.83
9	11	9	6.52	6.08
9	11	11	7.33	7.66
9	11	13	2.72	3.30
9	13	1	5.26	4.91
9	13	3	14.58	14.66
9	13	5	7.67	7.46
9	13	7	15.82	15.76
9	13	9	4.81	4.99
9	13	11	9.31	8.61
9	13	13	4.74	3.65
9	15	1	17.90	17.52
9	15	3	21.60	22.30
9	15	5	8.29	7.98
9	15	7	12.92	12.82
9	15	9	7.76	7.44
9	15	11	8.40	7.89
9	15	13	5.56	4.79
9	17	1	5.34	5.40
9	17	3	9.83	9.64
9	17	5	7.87	7.34
9	17	7	11.73	11.69
9	17	9	4.99	4.31
9	17	11	5.00	4.69
9	19	1	4.56	3.53
9	19	3	4.61	3.86
9	19	5	11.43	11.03
9	19	7	5.40	5.40
9	19	9	11.77	11.57
9	19	11	3.40	3.66
9	21	1	14.92	13.95
9	21	3	3.94	3.95
9	21	5	14.90	14.85
9	21	7	2.29	2.17
9	21	9	8.68	8.74
9	21	11	3.13	3.32
9	23	1	4.24	3.35
9	23	3	3.61	4.06
9	23	5	4.13	4.25
9	23	7	8.89	8.39
9	23	9	10.68	10.69
9	25	1	4.12	4.17
9	25	3	4.94	4.74
9	25	5	12.31	12.36
9	25	7	7.89	8.10
9	25	9	14.77	15.65
9	27	1	8.32	8.16
9	27	3	13.84	13.46
9	27	5	5.05	4.36
9	27	7	11.03	10.56
9	29	1	4.14	4.37
9	29	3	5.51	4.93
9	29	5	6.22	7.13
9	29	7	3.63	3.90
9	31	1	4.30	4.64
9	31	3	6.95	6.88
10	0	2	31.81	34.48
10	0	6	6.92	7.17
10	0	10	9.64	10.13
10	0	14	9.38	11.66
10	2	0	4.43	4.23
10	2	2	17.84	17.59
10	2	4	12.73	12.49
10	2	6	3.63	2.79
10	2	8	18.96	19.90
10	2	10	5.68	5.28
10	2	12	10.88	11.57
10	2	14	0.00	1.16
10	4	0	2.83	0.90
10	4	2	12.55	11.11
10	4	4	7.21	6.92
10	4	6	12.66	12.39
10	4	8	5.52	4.87
10	4	10	15.68	16.30
10	4	12	3.29	1.18
10	4	14	5.14	5.01
10	6	0	17.64	16.97
10	6	2	11.12	11.24
10	6	4	10.49	10.58
10	6	6	6.33	6.25
10	6	8	17.59	18.29
10	6	10	1.46	1.45
10	6	12	8.09	8.19
10	6	14	1.79	2.28
10	8	0	9.90	9.10
10	8	2	20.96	21.00
10	8	4	8.02	7.66
10	8	6	10.92	10.96
10	8	8	7.90	8.42
10	8	10	5.19	6.62
10	8	12	2.28	2.41
10	8	14	4.61	4.97
10	10	0	6.14	5.56
10	10	2	4.70	4.32
10	10	4	9.24	8.40
10	10	6	1.64	2.33
10	10	8	6.11	6.05
10	10	10	2.30	2.43
10	10	12	5.03	4.19
10	12	0	22.38	22.10
10	12	2	7.51	6.24
10	12	4	12.09	12.65
10	12	6	15.56	16.14
10	12	8	9.69	9.39
10	12	10	9.48	9.67
10	12	12	0.00	0.70
10	14	0	19.46	18.39
10	14	2	3.30	3.10
10	14	4	22.24	22.21
10	14	6	7.78	7.11
10	14	8	10.13	9.78
10	14	10	8.53	8.21
10	14	12	4.46	4.99
10	16	0	2.59	2.99
10	16	2	5.55	4.66
10	16	4	7.70	7.43
10	16	6	2.92	4.45
10	16	8	4.83	4.16
10	16	10	6.63	6.02
10	16	12	5.47	5.00
10	18	0	7.74	6.76
10	18	2	5.43	5.27
10	18	4	7.19	6.92
10	18	6	9.19	8.26
10	18	8	12.61	13.43
10	18	10	5.91	5.12
10	20	0	1.62	2.42
10	20	2	4.61	1.60
10	20	4	2.17	3.70
10	20	6	8.34	8.24
10	20	8	7.30	7.94
10	20	10	9.33	9.31
10	22	0	13.34	12.63
10	22	2	12.39	12.06
10	22	4	11.64	10.34
10	22	6	12.44	12.42
10	22	8	6.20	7.23
10	22	10	7.13	7.77
10	24	0	3.66	3.58
10	24	2	4.35	3.64
10	24	4	5.32	4.87
10	24	6	14.84	14.90
10	24	8	5.10	5.19
10	26	0	3.00	1.49
10	26	2	7.57	8.75
10	26	4	6.19	5.63
10	26	6	5.82	5.30
10	26	8	9.28	9.45
10	28	0	8.85	8.96
10	28	2	12.32	11.91
10	28	4	6.46	7.22
10	28	6	7.50	7.50
10	30	0	8.19	8.94
10	30	2	6.17	6.59
10	30	4	5.49	5.72
11	1	1	21.62	21.62
11	1	3	18.35	17.54
11	1	5	17.90	18.82
11	1	7	11.20	10.76
11	1	9	3.78	3.85
11	1	11	7.52	8.42
11	1	13	6.30	6.03
11	3	1	16.05	15.24
11	3	3	9.39	8.27
11	3	5	6.23	6.11
11	3	7	3.48	2.90
11	3	9	4.70	4.81
11	3	11	3.16	3.19
11	3	13	0.00	1.55
11	5	1	13.79	13.19
11	5	3	23.74	23.61
11	5	5	9.42	9.15
11	5	7	11.40	11.11
11	5	9	1.88	1.65
11	5	11	5.70	5.71
11	5	13	3.56	3.97
11	7	1	13.93	13.15
11	7	3	10.80	9.97
11	7	5	23.02	23.92
11	7	7	2.89	2.59
11	7	9	1.41	2.10
11	7	11	4.95	4.64
11	7	13	6.14	6.59
11	9	1	21.02	21.17
11	9	3	13.72	13.27
11	9	5	13.90	13.89
11	9	7	10.97	10.78
11	9	9	3.45	3.54
11	9	11	3.79	3.24
11	9	13	5.80	5.64
11	11	1	22.39	22.27
11	11	3	8.50	7.46
11	11	5	13.13	12.61
11	11	7	4.63	4.12
11	11	9	7.29	6.96
11	11	11	5.94	5.60
11	13	1	9.99	9.81
11	13	3	9.72	8.89
11	13	5	14.58	15.08
11	13	7	10.05	10.18
11	13	9	5.30	5.68
11	13	11	3.82	5.07
11	15	1	10.65	10.68
11	15	3	18.48	18.11
11	15	5	7.43	7.26
11	15	7	8.68	8.00
11	15	9	3.46	2.55
11	15	11	1.93	1.31
11	17	1	13.22	13.18
11	17	3	11.84	11.51
11	17	5	4.92	5.06
11	17	7	2.73	1.80
11	17	9	4.03	3.77
11	17	11	2.43	2.27
11	19	1	9.34	9.15
11	19	3	17.06	17.02
11	19	5	9.21	8.94
11	19	7	11.80	11.69
11	19	9	5.28	6.07
11	21	1	14.20	13.69
11	21	3	12.27	12.08
11	21	5	9.57	9.83
11	21	7	7.00	5.98
11	21	9	3.98	4.48
11	23	1	7.62	7.59
11	23	3	1.49	1.63
11	23	5	2.65	1.65
11	23	7	3.36	3.92
11	25	1	5.67	6.47
11	25	3	7.05	6.29
11	25	5	3.32	4.16
11	25	7	4.13	4.05
11	27	1	7.97	7.77
11	27	3	3.50	2.96
11	27	5	10.59	11.46
11	29	1	3.36	3.00
11	29	3	6.66	6.60
12	0	0	20.01	20.10
12	0	4	11.78	11.74
12	0	8	4.66	5.33
12	0	12	7.13	7.21
12	2	0	1.99	0.51
12	2	2	7.95	6.85
12	2	4	3.29	4.21
12	2	6	4.38	3.66
12	2	8	4.05	3.22
12	2	10	2.03	1.81
12	2	12	5.09	5.16
12	4	0	3.55	2.13
12	4	2	7.12	7.01
12	4	4	5.97	5.70
12	4	6	3.64	3.31
12	4	8	9.29	9.67
12	4	10	6.03	5.71
12	4	12	1.97	2.36
12	6	0	9.26	8.64
12	6	2	14.10	13.10
12	6	4	3.70	3.28
12	6	6	4.76	3.75
12	6	8	3.31	6.20
12	6	10	5.14	5.39
12	6	12	1.42	1.51
12	8	0	25.90	26.16
12	8	2	10.54	10.34
12	8	4	13.30	13.69
12	8	6	5.21	5.14
12	8	8	5.05	4.87
12	8	10	5.32	6.30
12	8	12	5.06	5.33
12	10	0	7.10	6.81
12	10	2	11.19	10.08
12	10	4	5.06	4.73
12	10	6	8.77	8.62
12	10	8	5.94	5.40
12	10	10	3.97	3.92
12	10	12	0.00	1.83
12	12	0	11.31	10.64
12	12	2	4.00	5.20
12	12	4	6.80	6.85
12	12	6	4.20	5.25
12	12	8	10.67	10.94
12	12	10	5.43	5.58
12	14	0	4.88	5.46
12	14	2	16.99	16.32
12	14	4	2.27	0.73
12	14	6	11.86	11.73
12	14	8	2.71	1.40
12	14	10	10.24	10.55
12	16	0	4.46	4.30
12	16	2	7.15	7.08
12	16	4	11.98	11.60
12	16	6	11.28	11.37
12	16	8	11.99	12.01
12	16	10	7.46	7.55
12	18	0	7.81	7.53
12	18	2	6.22	5.44
12	18	4	6.06	5.82
12	18	6	3.79	3.61
12	18	8	9.47	10.22
12	18	10	7.31	7.75
12	20	0	12.99	12.81
12	20	2	5.13	4.88
12	20	4	11.36	11.32
12	20	6	3.32	1.95
12	20	8	6.09	6.61
12	22	0	4.64	4.33
12	22	2	2.37	0.87
12	22	4	8.21	8.02
12	22	6	4.87	4.28
12	22	8	5.94	7.04
12	24	0	6.85	6.74
12	24	2	5.76	5.77
12	24	4	5.69	5.11
12	24	6	4.66	4.82
12	26	0	7.23	7.83
12	26	2	4.96	5.42
12	26	4	5.96	6.57
12	28	0	9.45	9.79
12	28	2	10.50	11.62
13	1	1	0.00	1.07
13	1	3	12.96	12.73
13	1	5	4.06	3.58
13	1	7	7.77	7.31
13	1	9	7.54	7.19
13	1	11	5.35	5.89
13	3	1	5.46	5.25
13	3	3	8.70	8.30
13	3	5	6.62	6.15
13	3	7	9.62	10.12
13	3	9	2.48	2.61
13	3	11	6.11	5.79
13	5	1	4.72	4.06
13	5	3	2.06	1.89
13	5	5	14.13	14.60
13	5	7	5.03	4.68
13	5	9	14.46	15.05
13	5	11	9.94	10.12
13	7	1	3.63	3.49
13	7	3	6.00	5.73
13	7	5	9.77	10.04
13	7	7	4.60	4.46
13	7	9	5.31	5.17
13	7	11	4.11	4.11
13	9	1	5.95	5.40
13	9	3	7.53	6.81
13	9	5	5.82	5.83
13	9	7	4.65	5.43
13	9	9	6.76	7.45
13	9	11	4.42	5.54
13	11	1	8.74	7.68
13	11	3	3.42	2.87
13	11	5	6.60	6.24
13	11	7	8.89	9.68
13	11	9	10.92	11.44
13	11	11	8.80	10.12
13	13	1	5.96	5.99
13	13	3	11.17	11.42
13	13	5	2.66	3.86
13	13	7	5.83	6.12
13	13	9	2.88	3.32
13	15	1	4.58	2.57
13	15	3	5.38	5.89
13	15	5	11.60	11.80
13	15	7	8.62	8.27
13	15	9	6.64	7.33
13	17	1	1.38	1.45
13	17	3	4.76	4.68
13	17	5	11.86	11.94
13	17	7	9.31	9.46
13	17	9	7.61	7.93
13	19	1	6.89	6.73
13	19	3	9.12	8.64
13	19	5	6.72	7.19
13	19	7	4.30	4.49
13	21	1	3.38	2.67
13	21	3	6.61	7.30
13	21	5	5.08	5.83
13	21	7	4.24	4.96
13	23	1	7.26	7.24
13	23	3	6.06	6.35
13	23	5	10.46	10.99
13	25	1	3.80	3.65
13	5	3	5.95	6.51
14	0	2	9.68	9.64
14	0	6	15.18	15.66
14	0	10	8.05	8.01
14	2	0	11.41	11.43
14	2	2	5.27	5.16
14	2	4	7.43	7.82
14	2	6	5.20	4.81
14	2	8	6.15	6.07
14	2	10	6.99	7.67
14	4	0	13.46	12.96
14	4	2	7.78	7.01
14	4	4	6.69	6.27
14	4	6	6.85	5.81
14	4	8	2.64	2.80
14	4	0	7.21	7.09
14	6	0	4.37	4.85
14	6	2	3.05	1.87
14	6	4	9.54	9.27
14	6	6	6.55	7.09
14	6	8	12.31	13.31
14	6	10	3.21	2.41
14	8	0	5.02	4.90
14	8	2	2.03	0.20
14	8	4	4.38	3.83
14	8	6	1.30	0.95
14	8	8	9.38	8.83
14	8	10	4.60	5.14
14	10	0	1.92	2.55
14	10	2	3.64	3.63
14	10	4	5.54	4.98
14	10	6	4.87	5.47
14	10	8	0.00	1.88
14	10	10	4.49	4.77
14	12	0	3.05	2.41
14	12	2	4.44	5.09
14	12	4	0.00	1.50
14	12	6	3.45	2.85
14	12	8	6.52	6.31
14	14	0	8.84	8.72
14	14	2	2.45	2.05
14	14	4	2.85	3.15
14	14	6	4.03	3.94
14	14	8	3.91	5.80
14	16	0	1.76	0.67
14	16	2	8.55	7.83
14	16	4	6.68	7.25
14	16	6	4.87	5.15
14	16	8	9.40	10.82
14	18	0	12.90	13.28
14	18	2	4.71	5.10
14	18	4	2.54	3.06
14	18	6	3.10	1.23
14	20	0	2.13	2.68
14	20	2	4.14	3.73
14	20	4	2.35	3.51
14	20	6	2.80	1.68
14	22	0	4.10	3.18
14	22	2	9.86	10.23
14	22	4	7.65	8.19
14	24	0	2.83	2.74
15	1	1	13.07	12.43
15	1	3	6.81	6.70
15	1	5	7.52	7.64
15	1	7	4.61	4.21
15	1	9	2.53	0.85
15	3	1	12.21	12.78
15	3	3	9.22	9.06
15	3	5	10.91	11.27
15	3	7	4.56	4.45
15	3	9	4.52	4.84
15	5	1	7.08	7.13
15	5	3	4.02	5.41
15	5	5	4.57	5.86
15	5	7	4.53	4.51
15	5	9	2.04	2.49
15	7	1	6.99	7.25
15	7	3	7.65	7.55
15	7	5	3.35	2.87
15	7	7	3.37	3.12
15	7	9	3.01	3.92
15	9	1	3.94	3.79
15	9	3	16.45	16.59
15	9	5	5.29	5.67
15	9	7	9.90	10.18
15	9	9	3.92	4.70
15	11	1	6.57	6.53
15	11	3	5.64	5.55
15	11	5	4.23	5.00
15	11	7	3.03	3.17
15	13	1	5.78	5.34
15	13	3	2.32	2.46
15	13	5	7.39	7.57
15	13	7	4.13	3.99
15	15	1	6.10	5.45
15	15	3	6.19	6.49
15	15	5	10.05	10.51
15	15	7	4.64	6.04
15	17	1	2.32	2.88
15	17	3	0.00	1.50
15	17	5	3.95	2.87
15	19	1	11.99	12.10
15	19	3	9.02	9.63
15	21	1	11.82	12.49
16	0	0	19.84	20.63
16	0	4	12.16	11.36
16	0	8	6.68	7.69
16	2	0	3.25	3.58
16	2	2	5.09	4.60
16	2	4	5.64	5.16
16	2	6	3.13	2.61
16	2	8	8.01	9.19
16	4	0	7.90	7.76
16	4	2	2.17	2.83
16	4	4	7.83	8.24
16	4	6	2.95	3.88
16	4	8	0.00	2.23
16	6	0	1.16	0.97
16	6	2	11.36	10.61
16	6	4	8.25	8.23
16	6	6	4.68	4.21
16	6	8	5.23	6.11
16	8	0	5.80	6.21
16	8	2	2.68	1.80
16	8	4	8.71	8.72
16	8	6	8.40	8.38
16	10	0	7.52	8.06
16	10	2	16.31	16.35
16	10	4	2.68	2.46
16	10	6	6.69	7.32
16	12	0	10.79	10.35
16	12	2	2.22	2.35
16	12	4	10.32	10.37
16	12	6	2.91	2.17
16	14	0	8.86	9.31
16	14	2	7.27	6.91
16	14	4	5.69	5.88
16	16	0	11.54	11.94
16	16	2	10.27	10.99
16	16	4	7.72	8.47
16	18	0	4.67	4.71
16	18	2	5.56	5.98
17	1	1	8.82	9.67
17	1	3	5.00	5.38
17	1	5	7.84	7.72
17	3	1	5.54	5.55
17	3	3	8.80	9.62
17	3	5	9.18	10.02
17	5	1	7.29	7.70
17	5	3	9.50	9.64
17	5	5	8.02	9.43
17	7	1	8.40	9.17
17	7	3	9.79	10.54
17	7	5	4.33	4.68
17	9	1	1.52	2.10
17	9	3	3.62	4.13
17	9	5	5.43	6.70
17	11	1	2.60	2.82
17	11	3	7.26	8.20
17	13	1	1.61	2.18
18	0	2	4.60	4.72
18	2	0	5.53	5.88
18	2	2	0.00	0.63
18	4	0	3.06	3.82
18	4	2	4.32	4.38
18	6	0	2.83	3.51
18	6	2	4.23	4.42

2·438 and 2·473 Å, in agreement with spectroscopic evidence (Ferraro, 1965). The Th–O distances are longer than the corresponding distance of 2·418 Å in the ThO_2 fluorite structure.

Several other thorium salts have been the subject of two-dimensional X-ray diffraction studies. A square antiprism arrangement (two almost parallel squares rotated 45° to each other) was found in $Th(OH)_2SO_4$ (Lundgren, 1951), $Th(OH)_2CrO_4 . H_2O$ (Lundgren & Sillen, 1949) and Th(IV) acetylacetonate (Grdenić & Matković, 1958). In the double salt $Mg(H_2O)_6 . Th(NO_3)_6 . 2H_2O$ (Šćavničar & Prodić, 1965) the thorium atom is surrounded by twelve oxygen atoms from six bidentate nitrate groups and the oxygen atoms form an irregular icosahedron. If the nitrate groups in the above double salt are considered as single groups bonded to thorium as above, then they are really arranged in octahedral fashion about the thorium atom. Thorium nitrate pentahydrate thus has the most irregular coordination about the thorium atom of any thorium salt so far studied.

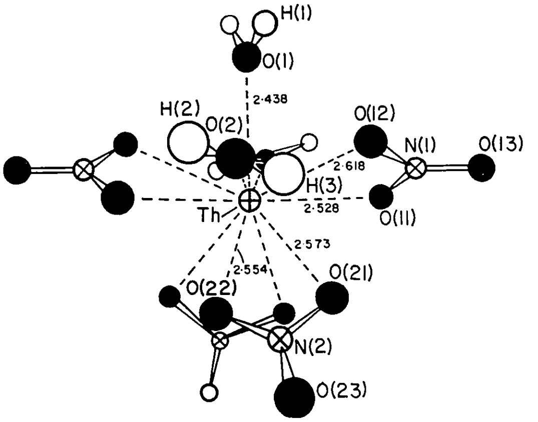

Fig. 2. Oxygen arrangement around the thorium atom as viewed in the **b** direction.

Nitrate groups

The bonds and angles in the nitrate groups are denoted as shown in Fig. 4.

In Table 4 we have summarized the distances and angles found in the nitrate groups in thorium nitrate pentahydrate, uranyl nitrate hexahydrate (Taylor & Mueller, 1965), rubidium uranyl nitrate (Barclay, Sabine & Taylor, 1965) and cerium magnesium nitrate hydrate (Zalkin, Forrester & Templeton, 1963). The latter study is by X-ray diffraction, while the others are neutron diffraction studies. It is seen that r_1 and r_2 are always greater than r_3 by about 0·05 Å, while θ_1 and θ_2 are greater than θ_3 by about 6°.

Ferraro (1960) found, by infrared spectroscopy, a lowering of the nitrate symmetry from D_{3h} to C_{2v} in going from a monovalent to a tetravalent metallic nitrate and that thorium nitrate pentahydrate showed

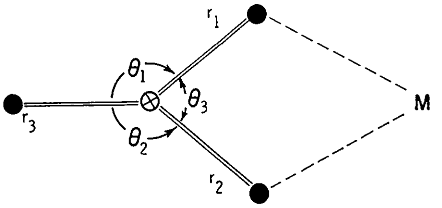

Fig. 4. Bond lengths and angles in nitrate groups.

Table 4. *Bond lengths and angles of the coordinated nitrate groups*

Compound	r_1 (Å)	r_2 (Å)	r_3 (Å)	θ_1 (°)	θ_2 (°)	θ_3 (°)
Thorium nitrate pentahydrate: $NO_3(1)$	1·250	1·270	1·202	123·2	121·7	115·2
$NO_3(2)$	1·264	1·275	1·206	123·0	122·5	114·5
Uranyl nitrate hexahydrate: $NO_3(1)$	1·271	1·271	1·208	122·7	122·7	114·6
$NO_3(2)$	1·260	1·260	1·231	122·2	122·2	115·6
Rubidium uranyl nitrate: $NO_3(1)$	1·26	1·26	1·21	121·2	121·2	117·5
Cerium magnesium nitrate hydrate: $NO_3(1)$	1·259	1·268	1·220	122·8	121·2	116·1
$NO_3(2)$	1·262	1·257	1·225	120·8	121·8	117·4
Average	1·263		1·215	122·1		115·8

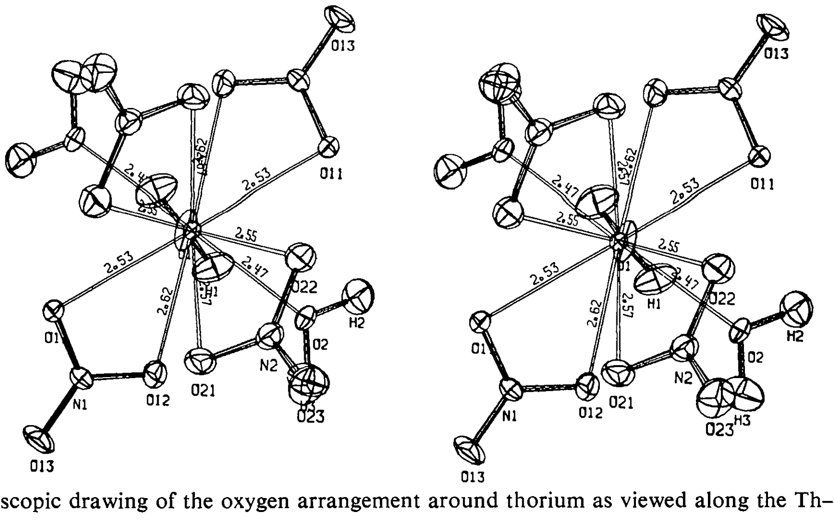

Fig. 3. Stereoscopic drawing of the oxygen arrangement around thorium as viewed along the Th–O(1) bond.

typical C_{2v} symmetry. Cho & Wadsworth (1962) also noted C_{2v} symmetry in this compound and a shift from C_{2v} to D_{3h} upon dehydration. Cho & Wadsworth felt that the distortion of the nitrate group was due to hydrogen bonding with the nitrate oxygen atoms; however since a similar distortion occurs in rubidium uranyl nitrate (Barclay, Sabine & Taylor, 1965), where there is no hydrogen bonding, it seems probable that the effect is largely due to the interaction with the metal atom. This is one of the mechanisms proposed by Ferraro & Walker (1965).

Table 5 shows the least-squares planes of the nitrate groups, which are very close to planar with small coefficients in X. These planes were calculated by the method of Schomaker, Waser, Marsh & Bergman (1959) with the computer program of Norment (1963). The quantity on the right hand side of each equation is the origin-to-plane distance in Å.

Water molecules and hydrogen bonds

The distances of 0·953–0·983 Å and angles of 106·8–111·0° found in the water molecules (uncorrected for thermal motion) as given in Table 2 appear to be normal.

Table 5. *Least-squares planes of nitrate groups; equations and deviations of atoms from the planes*

Equations*

$\mathrm{NO_3}(1)$: $0{\cdot}0793X-9{\cdot}6769Y+9{\cdot}5868Z=0{\cdot}4514$

$\mathrm{NO_3}(2)$: $-0{\cdot}2831X-18{\cdot}6270Y+6{\cdot}1421Z=-3{\cdot}1847$

Deviations

Plane	Atom	Deviation
$\mathrm{NO_3}(1)$	N(1)	0·0053 Å
	O(11)	−0·0017
	O(12)	−0·0017
	O(13)	−0·0019
$\mathrm{NO_3}(2)$	N(2)	0·0024
	O(21)	−0·0008
	O(22)	−0·0008
	O(23)	−0·0009

* X, Y and Z are fractional coordinates.

The hydrogen bond scheme is given in Fig. 5. This scheme is quite simple, and the hydrogen bonds fall into two classes: (*a*) two 'strong' water–water hydrogen bonds, O(1)–H(1) · · · O(3) (2·698 Å) and O(2)–H(2) · · · O(3) (2·697 Å) and (*b*) the three 'weak' water–nitrate oxygen hydrogen bonds O(2)–H(3) · · · O(22) (2·953 Å), O(3)–H(4) · · · O(23) (2·901 Å) and O(3)–H(5) · · · O(13) (2·946 Å). The water oxygen atom O(3), which is not bonded to the thorium atom, has approximately a tetrahedral disposition of hydrogen bonds about it, as shown by the O–O–O angles in Table 2. One of the hydrogen bonds is directed to the nitrate oxygen atom O(22) which is also bound to thorium. This does not appear to be unusual, since a hydrogen bond occurs in $\mathrm{CuSO_4 . 5H_2O}$ which involves a sulphate oxygen atom already bound to the copper atom (Bacon & Curry, 1962). Table 2 lists the hydrogen bond angles, which are nearly linear except for O(3)–H(5) · · · O(13) (147·9°). The hydrogen bond scheme is in accord with the infrared observations of Cho & Wadsworth (1962), who found a broad band at 3100 $\mathrm{cm^{-1}}$ corresponding to strongly hydrogen bonded water with more weakly hydrogen bonded water in evidence at 3440 $\mathrm{cm^{-1}}$.

Thermal parameters

The r.m.s. radial thermal displacements are given in Table 6. The displacements are 0·18 Å for thorium, 0·23 Å for the nitrogen atoms, 0·25–0·30 Å for the oxygen atoms (with not much difference between nitrate and water oxygen) and finally 0·30–0·40 Å for the hydrogen atoms. For comparison in uranyl nitrate hexahydrate (Taylor & Mueller, 1965) the values are 0·27 Å for uranium, 0·30 Å for the nitrogen atoms, 0·34–0·40 Å for the oxygen atoms, and 0·40–0·56 Å for the hydrogen atoms; thus in the present case the thermal displacements are much lower.

Table 6. *R.M.S. radial thermal displacements and the components along the principal axes, R_1, R_2 and R_3 of the vibrational ellipsoids*

Standard deviations (× 10³) are given in parentheses

Atom	R.M.S. radial displacement (Å)	Component along R_1 (Å)	R_2 (Å)	R_3 (Å)
Th	0·194 (2)	0·099 (3)	0·111 (2)	0·125 (3)
O(1)	0·324 (4)	0·144 (6)	0·146 (5)	0·251 (6)
O(2)	0·279 (3)	0·112 (4)	0·150 (3)	0·207 (4)
O(3)	0·282 (3)	0·146 (4)	0·168 (4)	0·174 (4)
N(1)	0·245 (2)	0·112 (2)	0·138 (2)	0·169 (2)
O(11)	0·285 (3)	0·123 (3)	0·135 (4)	0·219 (4)
O(12)	0·282 (3)	0·140 (4)	0·147 (3)	0·196 (4)
O(13)	0·314 (3)	0·111 (4)	0·173 (4)	0·237 (4)
N(2)	0·246 (2)	0·119 (2)	0·145 (2)	0·159 (2)
O(21)	0·285 (3)	0·136 (4)	0·153 (3)	0·198 (4)
O(22)	0·271 (2)	0·122 (4)	0·148 (3)	0·192 (3)
O(23)	0·309 (3)	0·133 (4)	0·185 (4)	0·208 (4)
H(1)	0·378 (5)	0·165 (6)	0·199 (7)	0·276 (7)
H(2)	0·338 (5)	0·146 (6)	0·196 (6)	0·233 (7)
H(3)	0·377 (6)	0·165 (6)	0·190 (6)	0·281 (8)
H(4)	0·395 (6)	0·163 (7)	0·238 (8)	0·270 (8)
H(5)	0·418 (6)	0·174 (8)	0·223 (8)	0·308 (9)

The r.m.s. components of thermal displacement along the principal axes of the vibration ellipsoids are given in Table 6. For the atoms which are bound to the thorium, the longest principal axis R_3 always lines up in a direction nearly perpendicular to the Th–O bond (and also the N–O bond with nitrate oxygen atoms) as shown in Table 7. Table 8 gives the orientation of the vibration ellipsoids in the unit cell.

Table 7. *Angles between the R_3 (longest principal) axes of the coordinated oxygen atoms and their respective* O–Th *and* O–N *bond vectors*

Atom	(*a*) N–O vector	(*b*) Th–O vector
O(1)	—	90·0°
O(2)	—	88·5
O(11)	77·0°	82·1
O(12)	81·4	78·7
O(21)	75·8	85·2
O(22)	83·1	76·5

X-ray study of Ueki, Zalkin & Templeton

Since it is unusual to have independent neutron and X-ray investigations of the same compound reported together, the authors of the two papers have, at the suggestion of the editor and reviewer, standardized on certain aspects such as atom designation, particular atoms in the asymmetric unit, temperature factor expression, listing order of the reflection, *etc.*, for convenience of comparison for the reader. Ueki, Zalkin & Templeton first corrected the Th atom scattering curve for the real anomalous dispersion correction $\Delta f'$ only and then later the imaginary term $\Delta f''$ was included as well. It can be noted in Table 9 that the inclusion of the imaginary dispersion correction reduces the average deviation between the neutron and X-ray coordinates from 0·065 Å to 0·026 Å for the nitrogen and oxygen atoms. This is certainly a very good agree-

Table 8. *Angles in degrees between principal axes R_1, R_2, R_3 of vibration ellipsoids and unit cell edges*

Errors in degrees are shown in parentheses

Angle between

Atom	R_1, **a**	R_1, **b**	R_1, **c**	R_2, **a**	R_2, **b**	R_2, **c**	R_3, **a**	R_3, **b**	R_3, **c**
Th	82 (11)	172 (11)	90 (0)	172 (11)	98 (11)	90 (0)	90 (0)	90 (0)	180 (0)
N(1)	11 (2)	88 (3)	100 (2)	92 (3)	3 (3)	92 (3)	100 (2)	92 (3)	169 (2)
N(2)	112 (2)	38 (4)	119 (3)	110 (6)	127 (4)	136 (5)	30 (4)	84 (4)	119 (5)
O(1)	67 (2)	157 (2)	90 (0)	90 (0)	90 (0)	0 (0)	23 (2)	67 (2)	90 (0)
O(2)	82 (4)	163 (3)	75 (2)	172 (4)	98 (4)	89 (3)	89 (3)	105 (2)	165 (2)
O(3)	60 (8)	121 (6)	46 (6)	150 (8)	109 (22)	67 (17)	88 (22)	143 (14)	127 (13)
O(11)	164 (13)	106 (13)	89 (4)	106 (14)	21 (11)	76 (2)	95 (2)	77 (2)	166 (2)
O(12)	102 (23)	147 (6)	120 (6)	167 (21)	83 (20)	79 (12)	84 (3)	121 (3)	32 (3)
O(13)	10 (3)	97 (3)	98 (2)	81 (3)	26 (3)	66 (3)	86 (2)	115 (3)	25 (3)
O(21)	115 (9)	45 (4)	125 (5)	154 (9)	104 (7)	69 (6)	83 (3)	48 (3)	43 (3)
O(22)	103 (7)	43 (3)	129 (2)	166 (7)	102 (6)	83 (5)	93 (4)	50 (2)	40 (2)
O(23)	107 (3)	58 (3)	143 (2)	140 (7)	129 (6)	97 (5)	124 (7)	55 (6)	54 (2)
H(1)	63 (3)	153 (3)	88 (9)	103 (6)	95 (9)	14 (4)	149 (3)	117 (3)	104 (4)
H(2)	57 (5)	147 (5)	89 (4)	40 (6)	60 (5)	66 (8)	69 (7)	78 (5)	156 (8)
H(3)	150 (10)	120 (11)	91 (4)	119 (11)	31 (10)	102 (3)	83 (3)	100 (3)	168 (3)
H(4)	45 (4)	52 (4)	70 (3)	46 (4)	122 (7)	119 (9)	96 (7)	54 (7)	144 (8)
H(5)	76 (6)	70 (5)	155 (3)	136 (5)	46 (5)	86 (7)	131 (4)	129 (4)	114 (3)

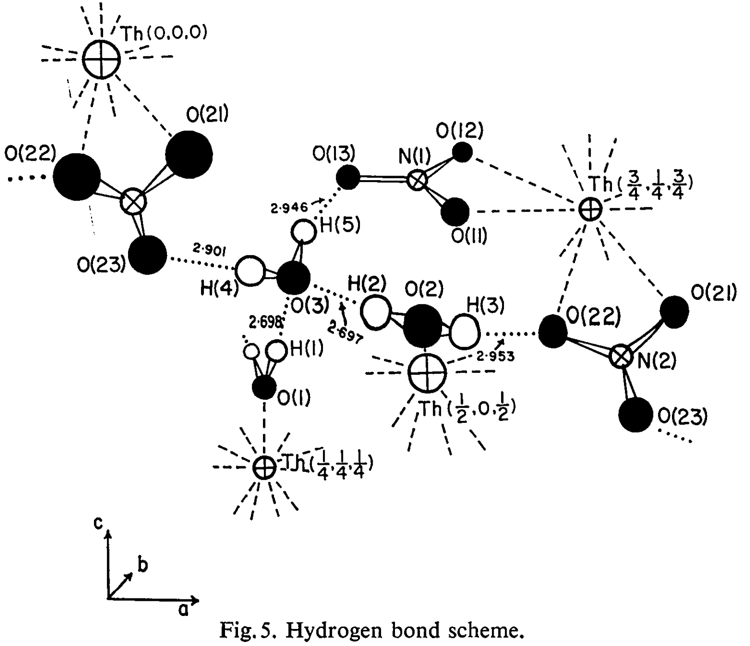

Fig. 5. Hydrogen bond scheme.

ment. The differences in the hydrogen atoms are much greater with an average deviation of 0·37 Å and are indicative of the limitations of the X-ray method in locating hydrogen atoms in the presence of heavy atoms. The two completely independent analyses make an interesting comparison; the X-ray analysis of Ueki, Zalkin & Templeton (1966) is published in an adjoining paper.

Table 9. *Deviations between the neutron and X-ray coordinates*

(1) Without X-ray dispersion correction, $\Delta f''$
(2) With dispersion correction, $\Delta f''$

Atom	Deviation (Å)	
	(1)	(2)
O(1)	0·085	0·029
O(2)	0·070	0·036
O(3)	0·041	0·024
N(1)	0·054	0·020
O(11)	0·088	0·045
O(12)	0·050	0·011
O(13)	0·044	0·026
N(2)	0·048	0·016
O(21)	0·075	0·020
O(22)	0·075	0·026
O(23)	0·082	0·037
Mean deviation	0·065	0·026

Atom	Deviation (Å)
H(1)	0·52
H(2)	0·32
H(3)	0·23
H(4)	0·31
H(5)	0·48
Mean deviation	0·37

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