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Argonne National Laboratory

A NEUTRON-DIFFRACTION STUDY OF URANYL NITRATE HEXAHYDRATE

by

J. C. Taylor and M. H. Mueller

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A NEUTRON-DIFFRACTION STUDY OF URANYL NITRATE HEXAHYDRATE

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J. C. Taylor* and M. H. Mueller

ABSTRACT

The crystal structure of uranyl nitrate hexahydrate, $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, has been determined by neutron diffraction. The crystals are orthorhombic with $a = 13.197 \pm 0.003 \text{ \AA}$, $b = 8.035 \pm 0.002 \text{ \AA}$, $c = 11.467 \pm 0.003 \text{ \AA}$, and belong to the space group $\text{Cmc}2_1$. Complete neutron-diffraction data to $2\theta = 105^\circ$ were collected (1136 independent reflections, 25 unobservably small) with a neutron wavelength of $1.065 \text{ \AA}$. The structure was solved from the three-dimensional neutron Patterson and Fourier syntheses and refined by full-matrix least squares. Separate refinements were carried out with the following three different weighting schemes: $w = 1$, $w = |F|$, and a scheme based on the counting statistics. The final weighted R-factors were 7.5, 4.5, and 3.9%, respectively, and the results were within experimental error of each other.

Six oxygen atoms are bound to the uranyl grouping in its equatorial plane, forming an irregular hexagon around it. Four of these oxygens are from the two nonequivalent, bidentate nitrate groups, and the other two are reflection-equivalent, water-oxygen atoms. In the nitrate groups, the N-O bonds involving oxygens covalently bound to the uranium are about 0.03 to 0.05 $\text{\AA}$ longer than the N-O bonds not involved in U-O bonding; also, the O-N-O angles differ significantly from 120° .

All the hydrogen atoms are involved in hydrogen bonding that can be divided into (a) O(water)...O(water) hydrogen bonds of length 2.68-2.76 $\text{\AA}$ and (b) weaker O(water)...O(nitrate) hydrogen bonds of length 2.92 and 3.00 $\text{\AA}$. The hydrogen bond involving one nitrate oxygen atom is very bent, the O-H...O angle being 144.0° . The water molecules form infinite hydrogen-bonded sheets that are parallel to the bc plane. The observed O-H distances in the water molecule, when corrected for the effects of thermal motion, lie between 0.92 and 1.14 $\text{\AA}$. The water angles are 106.9 , 106.8 , and 114.6° .

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INTRODUCTION

The crystal structure of uranyl nitrate hexahydrate, $\text{UO}_2(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$, was first studied by Pauling and Dickinson¹ in 1924, by X-ray diffraction. These authors found the unit cell to be orthorhombic, with dimensions $13.15 \times 8.02 \times 11.42 \text{ \AA}$ and four molecules per unit cell. They believed the space group to be Cmcm ; however, Sasvari² reported a positive piezoelectric effect that suggested the crystal has the alternative, noncentric, space group $\text{Cmc}2_1$.

On the basis of the infrared spectrum, Gatehouse and Comyns³ suggested that the structure was $[\text{UO}_2(\text{H}_2\text{O})_6] \cdot 2\text{NO}_3$, and Vdovenko *et al.*⁴ proposed such a model in $\text{Cmc}2_1$ from X-ray diffraction data. On the other hand, Allpress and Hambly,⁵ also from the infrared spectrum, considered there was covalent bonding of the nitrate groups. Fleming and Lynton,⁶ in a two-dimensional X-ray study, proposed the structure $[\text{UO}_2(\text{NO}_3)_2(\text{H}_2\text{O})_2] \cdot 4\text{H}_2\text{O}$ but did not definitely locate the noncoordinated water molecules.

One of the authors (J.C.T.) collected neutron-diffraction data for the three axial projections at Lucas Heights, Sydney, Australia, through the courtesy of Mr. T. M. Sabine. Attempts to refine the coordinates of Fleming and Lynton by using these neutron data failed, and difference syntheses gave no clues as to the errors in the model. As a result, this work was discontinued.

To resolve the considerable doubts as to the overall structure, the present neutron-diffraction study was undertaken with use of the three-circle instrument at Argonne.⁷ This neutron technique was selected for the analysis for several reasons: The uranium atom does not have the dominant scattering power in neutron diffraction that it has in the X-ray case, the hydrogen atoms can also be located, and resolution is greatly increased with three-dimensional data. No preliminary X-ray study was made; it was considered that the structure could be solved directly from the neutron data. The results of this investigation were presented orally at the American Crystallographic Association meeting held at Bozeman, Montana, July 26-31, 1964, and a paper has been accepted by *Acta Crystallographica* for publication. However, since it was not possible or planned to include in the above publication many of the important results and experimental details or the listing of the final agreement between the observed and calculated structure factors of the 1136 reflections, this ANL report has been prepared.

It was brought to our attention after our work had been completed and this ANL report written that a report of a two-dimensional, neutron-diffraction study of this compound by Makarov and Melik'yan⁸ had just appeared in *Chemical Abstracts* (September 14, 1964). On the basis of $(hk0)$ and $(h0l)$ Fourier projections, these authors accepted the coordinates for U, N, and O proposed by Fleming and Lynton, and from the negative areas on their maps they deduced a set of coordinates for five of the six hydrogen

atoms. Their coordinates were not in agreement with the ones we had obtained in our three-dimensional study. The two sets of coordinates are compared later in the section on Hydrogen Bonding and Water Molecules.

EXPERIMENTAL

Large single crystals, weighing approximately 0.5 g, were readily obtained from slightly acidified aqueous solutions. One of these crystals was mounted on the three-circle neutron diffractometer at the CP-5 reactor. A wavelength of 1.065 Å was used from a beryllium monochromator. Two-theta values of 25 reflections (6 00l, 6 h00 and 13 hk0) were obtained by a simultaneous ϕ , 2θ maximization process, and a least-squares analysis based on the program of Mueller and Heaton⁹ led to the following values:

$$a = 13.197 \pm 0.003 \text{ Å},$$

$$b = 8.035 \pm 0.002 \text{ Å},$$

$$c = 11.467 \pm 0.003 \text{ Å}.$$

The best fit for the cell constants was obtained without the use of either a systematic correction term or weight, since these were relatively low-angle lines.

Intensity-data collection was then started, each peak being step-scanned over $6-7^\circ 2\theta$ in 0.1° steps. Time at each step was controlled by a monitor count, with a total time of about 15 min for each reflection. After the intensity of some 200 reflections had been collected, the low ambient humidity caused the crystal (covered lightly with grease, and enclosed in thin plastic sheeting) to lose water of crystallization. A new crystal was then grown (weight 870 mg) and shaped to a sphere (weight 540 mg) with a piece of damp filter paper. This crystal was mounted on the vanadium pin as before and then enclosed in a thin-walled vanadium can. No loss of intensity from this crystal was observed, even 6 months later. After 852 reflections had been observed, a 2-month reactor shutdown occurred. The structure was solved in essentials during this period by using the 852 reflections only. The data collection was continued after the shutdown to include all reflections within a 2θ of 105° , where the intensities were becoming very weak. Those reflections that had been taken with the first crystal were repeated with the second crystal to obtain a complete set of data with the second crystal. Of the 1136 independent reciprocal lattice points in the 2θ range, only 25 had unobservably small intensities. The observed F^2 and F values were placed on a near absolute scale by a comparison with the intensities from an MgO crystal of diameter 0.1555 in. The measured linear-absorption coefficient was 1.7 cm^{-1} ($\mu_r = 0.61$), giving about an 8% variation of the absorption factor over the 2θ range. Absorption corrections were applied at a later stage of the structure refinement (see section on Least-squares Refinement).

STRUCTURE ANALYSIS

Three-dimensional Patterson Map

The analysis was started during the shutdown period with 852 reflections only. A three-dimensional Patterson map was calculated by means of the MIFRI computer program¹⁰ from the $F_0^2(hkl)$ values. The highest peaks, as shown in Fig. 1, were concentrated in the section $x = 0$, indicating that many of the atoms may lie in the mirror planes (at $x = 0$ and $x = 1/2$). A large peak A ($0, 1/4, 1/2$) (Fig. 1), was consistent with the placement of the uranium atom at $(0, 1/8, 1/4)$ by Fleming and Lynton and was thus a U-U vector. Peak B (Fig. 1), $1.77 \text{ \AA}$ from the origin was clearly the superposition of the two U-O vectors in the (linear) uranyl group, lying in the mirror plane. There were only two peaks in the Patterson close enough to the origin to represent N-O distances in the nitrate groups--one in the zero level at C (Fig. 1), $1.23 \text{ \AA}$ from the origin, and one in the general location $(0.082, 0.087, 0)$, $1.29 \text{ \AA}$ from the origin.

Fig. 1. Section $x = 0$ of Three-dimensional Neutron Patterson

Since two crystallographically distinct nitrate groups must be present, while only two such N-O vectors were found, the nitrate groups evidently were similarly oriented within the unit cell. The nitrate groups were located with respect to the uranyl group by means of the vector D (Fig. 1), which was $2.95 \text{ \AA}$ from the origin and at right angles to the uranyl vector; this was thought to be the superposition of the two U-N vectors.

From the Patterson, a model for the $\text{UO}_2(\text{NO}_3)_2$ group was derived; the two nitrate groups were bidentate and bound to the uranium atom on

opposite sides of the uranyl group (see Fig. 2). The Patterson also suggested that two reflection-equivalent water oxygens were coordinated to the uranium atom, completing an irregular hexagon of six oxygen atoms in the uranyl equatorial plane (see Fig. 2).

Fig. 2. Configuration of Uranium Atom and Nitrate Groups

maps were then combined to give an M3 map. The minimum functions were somewhat smeared-out in appearance, but they supported the model already derived. The coordinates deduced from the Patterson and minimum functions showed fair agreement with those given by Fleming and Lynton,⁶ except for O_2 (0.48 Å difference in position) and O_6 (0.28 Å difference), as shown in Table I.

TABLE I. Comparison of Model Derived from the Patterson and Minimum Functions with Those Given by Fleming and Lynton

Atom	x	y	z
U	0 (0)*	0.125 (0.125)*	0.250 (0.250)*
N-1	0 (0)	0.461 (0.473)	0.147 (0.157)
N-2	0 (0)	0.789 (0.811)	0.353 (0.339)
O-5 (uranyl)	0 (0)	0.037 (0.044)	0.108 (0.107)
O-6 (uranyl)	0 (0)	0.213 (0.179)	0.392 (0.397)
O-1 (nitrate)	1/2 (1/2)	0.105 (0.122)	0.111 (0.115)
O-2 (nitrate)	1/2 (1/2)	0.145 (0.203)	0.389 (0.380)
O-3 (nitrate)	0.082 (0.082)	0.374 (0.369)	0.167 (0.176)
O-4 (nitrate)	0.082 (0.091)	0.876 (0.863)	0.333 (0.323)
O-7 (water)	0.185 (0.183)	0.125 (0.118)	0.250 (0.250)

*Fleming and Lynton values shown in parentheses.

Three-dimensional Fourier Maps

Structure factors were calculated for the Patterson and minimum function model, the U, N, and O atoms being given isotropic thermal

parameters of 2.0, 3.0, and 3.5 Å², respectively. The discrepancy factor R for the model was 40.7% for the 852 reflections, where

$$R = \frac{\sqrt{\sum w(F_0 - sF_C)^2}}{\sqrt{\sum wF_0^2}},$$

s being the scale factor, and the weights, w, in this case being unity. A three-dimensional Fourier synthesis of the neutron-scattering density was made with the calculated phase angles obtained from the above model and the $F_0(hkl)$ values; however, 189 $F_0(hkl)$ terms with small $F_C(hkl)$ values were left out. In this map, the positions of the remaining water oxygen atoms, O₈ and O₉, were apparent. The positions of the atomic centers in this map were determined by the peak-location program of Mueller, Clark, and Simonsen.¹² When O₈ and O₉ were added to the structure factor calculations, R dropped to 35%. The O₈ and O₉ coordinates found were in considerable disagreement with those proposed by Fleming and Lynton, as shown in Table II. This fact, together with the discrepancies for O₂ and O₆, mentioned in the preceding section, may have been the cause of the inability to solve the structure with the previous two-dimensional neutron data collected at Sydney.

TABLE II. Comparison of Water-Oxygen Coordinates of Fleming and Lynton with Those from the Present Investigation

Atom	x	y	z	Comments
F and L O ₅	0.183	0.118	0.250	0.08 Å away from present O ₇
Present O ₇	0.182	0.121	0.244	-
F and L O ₈ (first possibility)	0.208	0.457	0.075	Incorrect
F and L O ₈ (second possibility)	0.208	0.457	0.425	0.52 Å away from present O ₈
Present O ₈	0.206	0.523	0.427	-
F and L O ₉ (first possibility)	0.205	0.252	0.425	Incorrect
F and L O ₉ (second possibility)	0.205	0.252	0.075	1.19 Å away from present O ₉
Present O ₉	0.295	0.253	0.070	-

In a further three-dimensional Fourier synthesis (88 reflections omitted), the positions of the six hydrogen atoms in the asymmetric unit were apparent. Peak positions were determined as before, and with the hydrogen atoms included ($B_H = 3.5$ Å²), R dropped to 24.2%.

Least-squares Refinement

The Fourier coordinates were now refined by the full-matrix, Busing-Levy, least-squares program¹³ on an IBM-704 machine. The reflections were initially given unit weight, and the z-coordinate of the uranium atom was not refined since the choice of "z" for the first atom in $Cmc2_1$ is arbitrary. The scattering factors used were: $b_U = 0.85$, $b_N = 0.94$, $b_O = 0.577$, and $b_H = -0.378$ ($\times 10^{-12}$ cm). The refinement was based on F. Initially, the block of data with $\ell = 2, 3$, and 4 (268 reflections) was used to save computing time. After one cycle, in which the B's were not refined, R was 13.3%. Five more cycles, in which the B's were refined, were calculated, and R dropped to 8.3%. The refinement was continued on the CDC-3600 machine, with the FORTRAN version of the same program.¹⁴ Anisotropic temperature factors were now introduced, and symmetry relations were obtained for the β_{ij} terms by the method of Levy.¹⁵ At first, some β_{33} values became negative. This was due to the limited amount of data; when the additional 584 reflections were included, the refinement proceeded normally. The previous R of 8.3% became 14% with these included, and this dropped to 6.7% after two more cycles.

After the shutdown, complete data with 2θ less than 105° (1136 F_0 values) were collected on the spherical crystal; the data obtained from the first crystal were then discarded, and the new data were added. With the 1136 F's now included, R changed from 6.7 to 8.1%; after two cycles, R was steady at 7.5% and the unit weight parameters had ceased to change.

The variation of the R factor over the 2θ range was then determined and is shown in Table III(a). The R's were all about 5-6%, except for the higher regions $80-90^\circ$ (10.3%), $90-100^\circ$ (14.7%), and $100-105^\circ$ (20.7%). This increase in R was due mainly to the counting statistics since these high-angle reflections were weak. Two further cycles were therefore calculated

TABLE III. Variation of Weighted R-factors over the 2θ Range

(a) After unit-weight refinement

(b) After refinement with statistical weighting scheme

2θ Range (deg)	Number of Reflections	(a) R-factor (unit weights)	(b) R-factor (statistical weights)
0-10	2	0.366	0.474
10-20	14	0.068	0.044
20-30	29	0.048	0.031
30-40	54	0.059	0.038
40-50	84	0.058	0.037
50-60	115	0.046	0.030
60-70	148	0.051	0.043
70-80	174	0.063	0.060
80-90	204	0.103	0.077
90-100	202	0.147	0.114
100-105	110	0.207	0.119

with use of only the data with 2θ less than 80° ($615 F_0$); also, the (200) reflection was omitted as it suffered from extinction. The R factor for this set of data dropped from 5.5 to 4.8% in the two cycles.

The least-squares, unit-weight ($w_1 = 1$) coordinates were now compared with the coordinates obtained from F_0 and F_c Fourier maps and applying a backshift. The coordinates agreed well (see Appendix A, rows 1 and 4 for each atom). A difference map, calculated to check on the model, was featureless. The peak heights in these Fourier maps are listed in Table IV and show good agreement.

TABLE IV. Peak Heights in Observed and Calculated Fourier Syntheses
(arbitrary scale)

Atom	Height in Observed Map	Height in Calculated Map
U	1479	1484
N ₁	1409	1429
N ₂	1334	1357
O ₁	641	635
O ₂	691	692
O ₃	699	697
O ₄	704	714
O ₅	665	669
O ₆	690	721
O ₇	620	611
O ₈	561	558
O ₉	530	528
H ₁	-343	-340
H ₂	-349	-355
H ₃	-263	-258
H ₄	-270	-285
H ₅	-176	-179
H ₆	-247	-247

For the reasons given above, the scheme $w_2 = |F|$ was now used, to reduce the effect of the higher angle reflections. Statistical weights were also applied by the method of Evans¹⁶ in a separate refinement, in which the statistical weighting function is

$$w_3 = \frac{1}{[\sigma(F)]^2} \propto \frac{T - nb}{(T + nb) \sin 2\theta}$$

where T is the total count, n is the number of steps, b is the background height, and $\sigma(F)$ is the standard deviation in $|F|$. The structure factors in the statistical-weight refinement (but not in the w_1 and w_2 refinements) were corrected for absorption. The final R factors for w_2 and w_3 were 4.5 and 3.9%, respectively.

The parameters obtained with the various schemes are shown in Appendix A, together with those from the backshift Fouriers and isotropic least squares. The final R factors are given in Table V; the final list of F_0 and F_c for the statistical scheme is given in Appendix B. The bond lengths and angles with their standard errors are given in Appendixes C and D as calculated with the Busing, Martin, and Levy Function and Error Program.¹⁷ The effect of the unit-cell errors on the overall standard errors was insignificant; these are included only in the case of the statistical scheme. A flow sheet of the analysis is shown in Fig. 3.

TABLE V. Final Weighted R -factors

Amount of Data	Weighting Scheme		
	Unit	$w = F $	Statistical Scheme
615 reflections ($2\theta = 80^\circ$ or less)	4.8%		
1136 reflections (complete data to $2\theta = 105^\circ$)	7.5%	4.5%	3.9%

Fig. 3. Flow Sheet of Analysis

DISCUSSION

Uranyl Coordination

The configuration about the uranium atom is shown in Fig. 2; all distances quoted in the figures and in this discussion are from the results of the statistical weighting scheme. The uranyl group is perpendicular to the paper and is surrounded equatorially by an irregular hexagon of six oxygen atoms, four from the two crystallographically nonequivalent nitrate groups and two from symmetry-related water-oxygen atoms, O_7 .

The uranyl distances are not quite equivalent. The distance $U-O_5$ is 1.770 ± 0.007 Å; $U-O_6$ is 1.749 ± 0.007 Å. These distances may be compared with the distance of 1.78 Å found in the linear, symmetrical, uranyl group in rubidium uranyl nitrate.¹⁸ The uranyl angle of $179.1 \pm 0.5^\circ$ is close to linear. This hexagonal arrangement of oxygens about the uranyl group is similar to the arrangements found in rubidium uranyl nitrate¹⁸ (a neutron diffraction study) and in sodium uranyl acetate¹⁹ (an X-ray diffraction study).

Nitrate Groups

The dimensions of the nitrate groups are shown in Fig. 2. In each nitrate group, the N-O bonds are not equivalent; the N-O bonds involving coordinated oxygen atoms are 0.06 and 0.03 Å longer than those involving the noncoordinated oxygens.

The bond angles in the nitrate groups are also distorted from the ideal value of 120° by the bonding with uranium. Similar differences in the bond lengths and angles have been observed in the nitrate group in rubidium uranyl nitrate.¹⁸ The N-O distances may be compared with the distance of 1.218 Å found by Sass *et al.*²⁰ in sodium nitrate, and the distance of 1.268 Å found by Hamilton in lead nitrate.²¹

Least-squares Planes

Since the main structural aspects of this compound consist of a near planar arrangement of the uranium atom, the two water oxygens O_7 , and the two nitrate groups as indicated above, it was of interest to apply a least-squares plane analysis to this configuration. Several least-squares planes were calculated: one for each of the nitrate groups; one for the oxygen hexagon around the uranium; one for each nitrate group with U, O_7 , and O_7' ; and a final plane involving all these atoms. The equations of the least-squares planes were calculated by the method of Schomaker *et al.*²² and the computer program written by Normant.²³ The results are shown in Table VI, and the deviations of the atoms from the planes are also given.

TABLE VI. Least-squares Planes

Plane	Atoms	Equation of Plane
1	N ₁ , O ₁ , O ₃ , O ₃ ¹ : (NO ₃) _I	2.4575Y + 10.9106Z = 2.8951*
2	N ₂ , O ₂ , O ₄ , O ₄ ¹ : (NO ₃) _{II}	3.3241Y + 10.4331Z = 3.0518
3	Oxygen hexagon	3.1605Y + 10.5360Z = 3.0550
4	(NO ₃) _I , U, O ₇ , O ₇ ¹	2.6602Y + 10.8134Z = 2.9800
5	(NO ₃) _{II} , U, O ₇ , O ₇ ¹	3.4844Y + 10.3262Z = 2.9760
6	(NO ₃) _I , (NO ₃) _{II} , U, O ₇ , O ₇ ¹	3.0941Y + 10.5760Z = 3.1006

*Y and Z are fractional coordinates.

Deviations
Δ(Å)

Atom	Plane 1	Plane 2	Plane 3	Plane 4	Plane 5	Plane 6
N ₁	-0.0101			-0.0146		0.0321
O ₁	0.0037			0.0313		0.1478
O ₃	0.0032		0.0520	-0.0196		-0.0125
O ₃ ¹	0.0032		0.0520	-0.0196		-0.0125
N ₂		0.0019			0.0060	0.0524
O ₂		-0.0007			-0.0238	0.0882
O ₄		-0.0006	0.0522		0.0182	0.0288
O ₄ ¹		-0.0006	0.0522		0.0182	0.0288
U			-0.0128*	0.0670	0.0556	-0.0569
O ₇			-0.1042	-0.0223	-0.0371	-0.1481
O ₇ ¹			-0.1042	-0.0223	-0.0371	-0.1481

*Not included in least-squares plane calculation.

Dihedral Angles			
Planes	Angle, (deg)	Planes	Angle, (deg)
1 and 2	6.63	1 and 3	5.35
4 and 5	6.37	2 and 3	1.28

The nitrate groups are both very close to planar. The oxygen hexagon is slightly puckered around the uranium level as the nitrate oxygens O_3 , O_3^I , O_4 , and O_4^I have significant deviations of $+0.05 \text{ \AA}$, while the water oxygens O_7 and O_7^I have significant deviations of $-0.10 \text{ \AA}$. The deviation of the uranium atom from the mean hexagon plane is only $-0.01 \text{ \AA}$, but this is probably not significant; the uranium atom was not used in the calculation of this plane. The nitrate groups lie approximately in the plane of the hexagon, the dihedral angles between $(NO_3)_I$ and $(NO_3)_{II}$, and the plane of the hexagon being 5.35 and 1.28° , respectively.

The whole equatorial system is bent about the $O_7-O_7^I$ line since planes 4 and 5, the "halves" of the hexagon, are inclined at an angle of 6.37° to each other. The nitrate group planes are inclined at 6.63° to each other.

The sixth plane calculated comprises all the atoms in the equator of the uranyl group. The larger deviations of the atoms here are a result of the bending already mentioned.

R-factors and Weighting Schemes

It was earlier decided from Table III(a) that the R-factor increased greatly with increasing 2θ when the unit weighting scheme (w_1) was used. This suggested the statistical weighting scheme w_3 and also the $w_2 = |F|$ scheme. From Table III(b) it is evident that the use of w_3 has reduced the effect of the low counting statistics at the higher angles. The large R for $2\theta < 10^\circ$ in Table III(a) and (b) is due to a large extinction effect in the (200) reflection. The other low-angle F_0 and F_C values were examined, and it was seen that the effect of extinction on the reflections other than (200) was not appreciable. The statistical and $w = |F|$ schemes, which emphasize the low angle data, would be sensitive to systematic errors in the data such as extinction and absorption.

The results for the three schemes are compared in Appendix A (positional and thermal parameters), Table V. (R-factors), Appendix C (bond lengths), and Appendix D (bond angles), and it can be concluded in this case that the three schemes led to essentially the same results, although the statistical scheme is the only one that is rigorously correct.

Thermal Parameters

The rms radial thermal displacement for all the atoms in the asymmetric unit are shown in Table VII. These values were obtained with the use of the ORFFE Function and Error computer program.¹⁷ The displacements vary somewhat according to type of atom--the U having the lowest value, N_1 and N_2 next, followed by the oxygens, with the hydrogens having

TABLE VII. Rms Radial Thermal Displacements and the rms Components along the Principal Axes R_i of the Vibration Ellipsoids

Atom	Rms Radial Displacement ($\text{\AA}$)	Displacements along		
		$R_1(\text{\AA})$	$R_2(\text{\AA})$	$R_3(\text{\AA})$
U	0.270(3)*	0.144(5)*	0.159(4)*	0.164(4)*
N ₁	0.295(4)	0.146(6)	0.178(4)	0.185(5)
N ₂	0.310(4)	0.153(6)	0.181(5)	0.199(5)
O ₁	0.370(6)	0.162(10)	0.235(7)	0.235(9)
O ₂	0.349(7)	0.156(10)	0.206(8)	0.235(8)
O ₃	0.343(4)	0.163(6)	0.171(6)	0.249(5)
O ₄	0.351(4)	0.164(6)	0.177(6)	0.255(6)
O ₅	0.365(7)	0.137(10)	0.204(9)	0.269(9)
O ₆	0.354(7)	0.138(10)	0.210(9)	0.249(8)
O ₇	0.388(4)	0.155(7)	0.194(6)	0.299(6)
O ₈	0.387(5)	0.190(7)	0.211(7)	0.262(7)
O ₉	0.401(5)	0.186(7)	0.224(7)	0.276(8)
H ₁	0.402(8)	0.181(10)	0.216(11)	0.286(11)
H ₂	0.408(8)	0.174(12)	0.236(11)	0.284(10)
H ₃	0.470(8)	0.212(12)	0.246(11)	0.340(12)
H ₄	0.459(8)	0.211(10)	0.244(13)	0.327(12)
H ₅	0.567(12)	0.219(13)	0.319(14)	0.414(16)
H ₆	0.497(10)	0.241(14)	0.273(13)	0.339(13)

*Standard errors ($\times 10^3$) in parentheses.

the greatest displacement. The hydrogens with the smallest displacements are H_1 and H_2 , which are attached to the O_7 atoms of the oxygen hexagon as shown in Fig. 4. There also seems to be a correlation between these radial displacements and the peak heights in the Fourier maps; that is, for a given kind of atom, the higher the rms value the lower the peak height. This is understandable since a higher rms value indicates a more smeared-out distribution.

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Fig. 4. Hydrogen Bonding

The rms components of thermal displacement along the principal axes of the atomic vibration ellipsoids are also listed in Table VII. The orientation of these ellipsoids in the unit cell are shown in Table VIII.

Table IX lists the rms displacements along the bond directions, and it may be noted that the magnitudes are nearly the same as the displacements along the shortest principal axes, indicating that the maximum vibration directions are more or less perpendicular to the bonds. Table IX also lists the angles between the shortest principal axis R_1 (and in some cases R_2) and the bond directions. The angles are small for the U-O and N-O bonds; for the O-H bonds they are somewhat larger.

TABLE VIII. Angles in Degrees between the Principal Axes R_i and the a, b, and c Directions

Atom	i	a	b	c	Atom	i	a	b	c
U	1	90	109	161	O_7	1	22	101	71
	2	90	19	109		2	111	138	55
	3	0	90	90		3	83	130	139
N_1	1	90	45	135	O_8	1	27	104	112
	2	0	90	90		2	77	118	31
	3	90	135	135		3	113	148	111
N_2	1	90	39	129	O_9	1	14	91	76
	2	0	90	90		2	104	94	15
	3	90	129	141		3	90	176	94
O_1	1	90	147	57	H_1	1	22	99	70
	2	0	90	90		2	112	114	33
	3	90	123	147		3	89	155	115
O_2	1	90	150	60	H_2	1	32	69	114
	2	0	90	90		2	120	36	108
	3	90	120	150		3	102	118	149
O_3	1	48	126	63	H_3	1	32	102	119
	2	138	125	70		2	64	102	29
	3	87	125	145		3	107	163	95
O_4	1	43	56	112	H_4	1	16	103	82
	2	133	50	111		2	104	122	36
	3	92	121	149		3	96	145	125
O_5	1	90	107	163	H_5	1	30	95	119
	2	90	17	107		2	72	132	47
	3	0	90	90		3	113	138	123
O_6	1	90	109	161	H_6	1	48	49	110
	2	90	19	109		2	138	54	108
	3	0	90	90		3	90	118	152

TABLE IX. Rms Components of Thermal Displacement along Bond Directions and Angles between Bonds and Shortest Principal Axes

Atom	Bond	Rms Component along Bond (Å)	Angle (deg)	
			R ₁	R ₂
O ₅	O ₅ -U	0.138(10)*	6	
O ₆	O ₆ -U	0.138(10)	2	
O ₁	O ₁ -N ₁	0.169(9)	16	
O ₃	O ₃ -N ₁	0.171(6)	20	
O ₂	O ₂ -N ₂	0.157(10)	5	
O ₄	O ₄ -N ₂	0.166(6)	75	16
H ₁	H ₁ -O ₇	0.193(12)	76	15
H ₂	H ₂ -O ₇	0.190(12)	86	34
H ₃	H ₃ -O ₈	0.225(11)	39	76
H ₄	H ₄ -O ₈	0.262(13)	78	32
H ₅	H ₅ -O ₉	0.235(13)	43	66
H ₆	H ₆ -O ₉	0.245(14)	63	27

*Standard errors ($\times 10^3$) in parentheses.

Bond distances derived from diffraction measurements are not in general the true separations but must be corrected for the effects of thermal motion, as has been shown by Busing and Levy.²⁴ Detailed knowledge of the dynamics of the system must be available for accurate corrections to be applied. Busing and Levy, however, show that corrections can be calculated for the case in which a lighter atom is assumed to "ride" on a heavier atom to which it is strongly bound (e.g., for O-H bonds) and the case in which the motions are independent. When corrected for "riding" motion, the O-H distances in the present analysis lie between 0.92 and 1.02 Å, and the difference in the uranyl bonds also persists when the oxygens are presumed to ride on the uranium. "Riding" and independent motion corrections are less justifiable for the other bonds; however, these corrections were calculated and are listed in Appendix C.

Hydrogen Bonding and Water Molecules

The uranyl coordination group is tied into the structure by four strong and four weak hydrogen bonds, as shown in Fig. 4. The strong bonds

are $O_7-H_2...O_8$ and $O_7-H_1...O_9$, and the weak bonds $O_2...H_3-O_8$ and $O_1...H_5-O_9$ involve the noncoordinated nitrate oxygens. The water molecules $H_3-O_8-H_4$ and $H_5-O_9-H_6$ form with $H_1-O_7-H_2$ an infinite aquo-complex sheet as shown in Fig. 5. The chains $...O_8-H_4...O_9-H_6...O_8-H_4$ in the direction of b and $...H_1-O_7-H_2...O_8...H_6-O_9...H_1-O_7-H_2...$ in the direction of c intertwine and form a "spider-web" network. These sheets are held together by hydrogen bonds only, and they lie roughly normal to the a axis. Figure 5 also shows the "up" and "down" weaker hydrogen bonds with the nitrate oxygens.

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Fig. 5. Water-molecule Sheets

There are two types of water molecules in the crystal, according to the classification of Wells.²⁵ The water molecule $H_1-O_7-H_2$ forms two strong hydrogen bonds with the water oxygens O_8 and O_9 , and one covalent bond to the uranium atom; it belongs in the type c(2) of Wells. The water molecules $H_3-O_8-H_4$ and $H_5-O_9-H_6$, on the other hand, have a distorted tetrahedral environment of hydrogen-bonded oxygen neighbors (see Appendix D) and are thus of type (b) in Wells. The water molecules of type (b) have higher thermal parameters than the more tightly bound molecule $H_1-O_7-H_2$.

The bond-distances and angles in the water molecules are shown in Appendixes C and D. The thermal vibrations have a considerable effect on the distances, as mentioned above. The water-molecule angles are 106.9, 106.8, and 114.6°. The $O-H...O$ angles lie between 164 and 177°,

except for the bond $O_9-H_5 \dots O_1$, which is greatly bent (144.0°) to accommodate $O_1-O_9-O_8$ angles of 81 and 140° . Similar bent-hydrogen bonds have been found in many hydrates including $Li_2SO_4 \cdot H_2O$ (Ref. 26) (two hydrogen bonds bent by 30°) and $CuSO_4 \cdot 5H_2O$ (Ref. 27) (one bond bent by 26°). The $O-O-O$ angle of 84° in oxalic acid dihydrate²⁸ forces one hydrogen bond to be bent by 24° .

The inelastic-neutron-scattering experiments of Rush²⁹ on uranyl nitrate gave a broad peak, due to the torsional oscillation of the water molecules, centered at about 450 wave numbers. The width of this peak, combined with an indication of splitting, suggests several different environments of the water molecules. The comparatively low frequency indicates that the hydrogen bonding is relatively weak.

An initial comparison of the hydrogen coordinates of Makarov and Melik'yan⁸ (hereafter referred to as M and M) with those of the present investigation revealed no correlation at all. M and M did not list any coordinates other than hydrogen; we thus had to correlate their hydrogen positions with the suggested water-oxygen positions of Fleming and Lynton (F and L), since M and M adopted the F and L model for the positive scatterers. This association was carried out by calculating $O_{\text{water}}(F \text{ and } L)-H(M \text{ and } M)$ distances, for the various $O_{\text{water}}(F \text{ and } L)$ positions. From the calculated distances shown in Table X, which are reasonable for O-H distances, it was concluded that:

- (a) The M and M H_1 and H_2 were attached to the F and L O_5 .
- (b) The M and M H_3 and H_6 were attached to the F and L O_8 (first of the two alternative positions suggested by F and L, Table I).
- (c) The M and M H_4 and H_5 were attached to the F and L O_9 (again the first suggested position of F and L).

Although the position of the F and L O_5 atom is in good agreement with our O_7 position (see Table II), the positions of the M and M H_1 and H_2 are vastly different from our H_1 and H_2 as shown in Table XI. Since the F and L O_8 and O_9 (first possibilities, our Table II) were shown to be incorrect in our earlier discussion, it is not surprising that the M and M H_3 , H_5 , H_4 , and H_6 hydrogen positions are again quite different than the results from our investigation, as shown in Table XI. The incorrect hydrogen coordinates of M and M well illustrate the dangers inherent in basing a neutron-diffraction study on incorrect structural information. In our analysis, we have found that the use of three-dimensional data greatly helps in the solution of the structure and also renders the final result more precise.

TABLE X. Oxygen-Hydrogen Distances in Model of Makarov and Melik'yan⁸

M and M Hydrogen	F and L Oxygen	Distance (Å)
H ₁	O ₅ *	0.88
H ₂	O ₅ *	1.30
H ₃	O ₈ **	-
H ₆	O ₈ **	0.96
H ₄	O ₉ **	0.80
H ₅	O ₉ **	1.01

*O₇ in present investigation.

**First possibility as shown in Table II.

TABLE XI. Comparison of Hydrogen Coordinates Reported by Makarov and Melik'yan (M and M) with Those of the Present Investigation (T and M)

Hydrogen Atom	x	y	z	$\Delta(\text{Å})$
M and M H ₁	0.13	0.17	0.28	1.65
T and M H ₁	0.225	0.174	0.186	
M and M H ₂	0.10	0.03	0.24	1.83
T and M H ₂	0.225	0.074	0.303	
M and M H ₃	0.22	0.08	-	0.73
M and M H ₄	0.22	0.18	0.47	
T and M H ₆	0.229	0.161	0.532*	
M and M H ₅	0.20	0.35	0.48	0.59 Å
T and M H ₄	0.202	0.420	0.463	
M and M H ₆	0.14	0.42	0.09	1.97 Å
T and M H ₃	0.136	0.437	-0.082*	

*Shifted to $1/2 - x$, $1/2 - y$, $1/2 + z$.

(0k ℓ) Fourier Projection

Although two-dimensional projections were not used in the solution of the crystal structure, it was thought worthwhile to calculate such a projection after completing the determination. The result is shown in Fig. 6 as an (0k ℓ) neutron Fourier that has some overlap but well illustrates the overall structure. Since this is a view in the plane of the oxygen hexagon, one can see a number of structural features such as: the relative orientation of the oxygen hexagon and uranyl group within the unit cell; the slight twist of the nitrate-group planes; the relative positions of the hydrogens; and the twist of H₁ and H₂, attached to the O₇'s of the hexagon, out of the plane of the hexagon.

Fig. 6. (0k ℓ) Fourier Projection

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PREVIOUS PRESENTATION

The results presented in this report have been given orally at the 1964 Annual Meeting of the American Crystallographic Association at Bozeman, Montana,³⁰ and have appeared in condensed form in *Acta Crystallographica*.³¹

APPENDIX A

Final Atomic Coordinates and Thermal Parameters

Basis: 1. w^{-1} , 2θ less than 80° ; 2. Statistical scheme (absorption-corrected data); 3. $w = |F|$; 4. Backshift Fourier; 5. Isotropic least squares

Basis	Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
1	U	0	0.1289(5)*	0.2500	0.0029(2)*	0.0079(4)*	0.0027(2)*	0	0	0.0000(2)*
2**		0	0.1292(5)	0.2500	0.0030(1)	0.0076(4)	0.0032(2)	0	0	-0.0003(2)
3		0	0.1291(4)	0.2500	0.0029(1)	0.0074(3)	0.0029(1)	0	0	-0.0001(2)
4		0	0.1290	0.2500						
5		0	0.1286(13)	0.2500	B = 2.0(1)					
1	N ₁	0	0.4720(4)	0.1577(5)*	0.0036(2)	0.0081(5)	0.0043(3)	0	0	0.0015(3)
2		0	0.4722(4)	0.1581(5)	0.0036(2)	0.0085(5)	0.0042(3)	0	0	0.0014(3)
3		0	0.4724(3)	0.1580(3)	0.0035(1)	0.0085(4)	0.0041(2)	0	0	0.0014(2)
4		0	0.4723	0.1575						
5		0	0.4728(10)	0.1586(26)	B = 2.3(2)					
1	N ₂	$\frac{1}{2}$	0.2924(5)	0.3581(5)	0.0035(2)	0.0090(5)	0.0050(3)	0	0	0.0018(3)
2		$\frac{1}{2}$	0.2919(5)	0.3590(5)	0.0037(2)	0.0092(5)	0.0050(3)	0	0	0.0017(3)
3		$\frac{1}{2}$	0.2922(4)	0.3586(3)	0.0036(1)	0.0088(4)	0.0051(2)	0	0	0.0017(2)
4		$\frac{1}{2}$	0.2921	0.3578						
5		$\frac{1}{2}$	0.2934(14)	0.3610(26)	B = 2.5(2)					
1	O ₁	$\frac{1}{2}$	0.1168(8)	0.1258(7)	0.0057(4)	0.0110(9)	0.0076(5)	0	0	0.0039(7)
2		$\frac{1}{2}$	0.1158(8)	0.1270(7)	0.0062(4)	0.0106(9)	0.0070(5)	0	0	0.0028(7)
3		$\frac{1}{2}$	0.1161(7)	0.1264(6)	0.0059(3)	0.0103(7)	0.0075(4)	0	0	0.0035(5)
4		$\frac{1}{2}$	0.1172	0.1258						
5		$\frac{1}{2}$	0.1170(19)	0.1231(41)	B = 2.8(3)					
1	O ₂	$\frac{1}{2}$	0.1535(8)	0.4026(8)	0.0047(4)	0.0105(10)	0.0076(5)	0	0	0.0034(6)
2		$\frac{1}{2}$	0.1523(8)	0.4032(8)	0.0048(4)	0.0098(10)	0.0072(5)	0	0	0.0029(6)
3		$\frac{1}{2}$	0.1526(7)	0.4028(6)	0.0046(3)	0.0097(8)	0.0074(4)	0	0	0.0031(5)
4		$\frac{1}{2}$	0.1525	0.4026						
5		$\frac{1}{2}$	0.1547(22)	0.3998(45)	B = 3.4(3)					
1	O ₃	0.0812(3)*	0.3923(5)*	0.1769(6)	0.0036(2)*	0.0115(6)*	0.0078(4)*	0.0002(3)*	0.0002(3)*	0.0032(4)*
2**		0.0810(3)	0.3913(5)	0.1775(5)	0.0032(2)	0.0119(7)	0.0076(3)	0.0000(3)	0.0003(2)	0.0034(4)
3		0.0811(3)	0.3923(4)	0.1771(4)	0.0032(2)	0.0115(5)	0.0077(3)	0.0002(2)	0.0002(2)	0.0031(5)
4		0.0815	0.3929	0.1766						
5		0.0818(9)	0.3890(15)	0.1769(25)	B = 2.9(2)					
1	O ₄	0.4195(3)	0.3673(5)	0.3331(6)	0.0029(2)	0.0116(7)	0.0084(4)	0.0002(3)	-0.0002(3)	0.0031(4)
2		0.4192(3)	0.3678(6)	0.3346(5)	0.0033(2)	0.0119(6)	0.0084(4)	0.0002(3)	-0.0003(2)	0.0034(5)
3		0.4194(2)	0.3675(5)	0.3335(4)	0.0031(1)	0.0121(5)	0.0083(3)	0.0002(2)	-0.0003(2)	0.0034(4)
4		0.4192	0.3676	0.3328						
5		0.4197(10)	0.3666(13)	0.3310(25)	B = 2.6(2)					
1	O ₅	0	0.0430(8)	0.1084(6)	0.0080(5)	0.0128(11)	0.0034(4)	0	0	-0.0021(6)
2		0	0.0426(8)	0.1080(6)	0.0082(5)	0.0121(11)	0.0031(4)	0	0	-0.0014(6)
3		0	0.0427(7)	0.1080(5)	0.0084(4)	0.0122(9)	0.0031(3)	0	0	-0.0018(4)
4		0	0.0427	0.1077						
5		0	0.0401(31)	0.1074(40)	B = 4.7(5)					
1	O ₆	0	0.2127(9)	0.3902(6)	0.0060(4)	0.0125(10)	0.0034(4)	0	0	-0.0008(5)
2		0	0.2114(9)	0.3913(6)	0.0070(5)	0.0127(11)	0.0033(4)	0	0	-0.0017(6)
3		0	0.2123(8)	0.3904(5)	0.0063(3)	0.0129(8)	0.0033(3)	0	0	-0.0013(4)
4		0	0.2182	0.3879						
5		0	0.2141(31)	0.3834(48)	B = 4.1(4)					
1	O ₇	0.1821(3)	0.1221(8)	0.2437(7)	0.0029(2)	0.0176(8)	0.0094(4)	0.0000(4)	0.0010(4)	0.0055(5)
2		0.1815(2)	0.1213(8)	0.2437(8)	0.0030(2)	0.0178(7)	0.0099(4)	0.0003(4)	0.0012(3)	0.0055(5)
3		0.1819(2)	0.1213(6)	0.2434(6)	0.0029(1)	0.0177(6)	0.0094(3)	0.0005(3)	0.0009(3)	0.0056(4)
4		0.1822	0.1216	0.2432						
5		0.1836(9)	0.1238(19)	0.2480(31)	B = 3.6(2)					
1	O ₈	0.2941(4)	0.0225(9)	0.4258(7)	0.0044(3)	0.0199(12)	0.0075(4)	-0.0016(5)	-0.0008(3)	0.0009(6)
2		0.2943(4)	0.0234(8)	0.4270(6)	0.0047(3)	0.0187(11)	0.0070(4)	-0.0018(5)	-0.0008(3)	0.0014(6)
3		0.2942(3)	0.0232(7)	0.4260(5)	0.0048(2)	0.0178(9)	0.0074(3)	-0.0013(4)	-0.0006(2)	0.0011(5)
4		0.2947	0.0225	0.4255						
5		0.2961(11)	0.0233(20)	0.4249(33)	B = 4.3(3)					
1	O ₉	0.2951(5)*	0.2520(10)*	0.0696(7)*	0.0040(3)*	0.0236(13)*	0.0075(4)*	-0.0003(5)*	0.0008(3)*	0.0000(7)
2**		0.2947(4)	0.2530(9)	0.0700(7)	0.0040(3)	0.0232(13)	0.0074(4)	0.0000(6)	0.0005(4)	0.0004(6)
3		0.2950(4)	0.2526(8)	0.0695(5)	0.0040(2)	0.0226(10)	0.0076(3)	-0.0004(4)	0.0006(3)	0.0002(5)
4		0.2952	0.2515	0.0695						
5		0.2952(12)	0.2517(21)	0.0666(30)	B = 3.9(3)					

Basis	Atom	x	y	z	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
1	H ₁	0.2247(7)	0.1755(13)	0.1849(9)	0.0046(4)	0.0225(17)	0.0076(7)	-0.0002(8)	0.0006(5)	0.0026(10)
2		0.2252(6)	0.1738(13)	0.1859(9)	0.0039(4)	0.0230(18)	0.0077(7)	-0.0003(8)	0.0006(4)	0.0031(9)
3		0.2242(6)	0.1744(11)	0.1857(7)	0.0042(3)	0.0217(15)	0.0081(5)	-0.0003(6)	0.0007(3)	0.0031(7)
4		0.2246	0.1757	0.1849						
5		0.2267(17)	0.1726(28)	0.1914(38)	B = 3.8(4)					
1	H ₂	0.2252(7)	0.0754(11)	0.3034(10)	0.0045(4)	0.0161(13)	0.0104(8)	0.0005(7)	-0.0011(6)	0.0035(9)
2		0.2254(7)	0.0744(12)	0.3031(10)	0.0044(4)	0.0176(15)	0.0105(8)	0.0010(8)	-0.0017(5)	0.0029(9)
3		0.2251(6)	0.0749(10)	0.3040(8)	0.0047(3)	0.0168(11)	0.0105(6)	0.0008(6)	-0.0008(4)	0.0030(7)
4		0.2257	0.0758	0.3036						
5		0.2213(18)	0.0790(26)	0.2988(41)	B = 3.7(4)					
1	H ₃	0.3641(7)	0.0597(15)	0.4185(11)	0.0054(6)	0.0306(22)	0.0109(9)	-0.0020(9)	-0.0004(7)	0.0019(13)
2		0.3637(7)	0.0635(14)	0.4177(9)	0.0061(5)	0.0336(23)	0.0086(8)	-0.0033(10)	-0.0010(6)	0.0007(12)
3		0.3630(6)	0.0605(13)	0.4181(9)	0.0063(4)	0.0299(19)	0.0095(7)	-0.0025(7)	-0.0009(5)	0.0016(11)
4		0.3632	0.0595	0.4197						
5		0.3591(23)	0.0581(40)	0.4115(51)	B = 6.0(6)					
1	H ₄	0.2021(7)	0.4206(16)	0.4634(11)	0.0052(5)	0.0240(21)	0.0113(10)	-0.0005(9)	-0.0004(6)	0.0015(13)
2		0.2016(7)	0.4195(14)	0.4629(10)	0.0052(5)	0.0276(22)	0.0112(9)	-0.0014(9)	-0.0001(6)	0.0048(13)
3		0.2016(6)	0.4197(12)	0.4638(9)	0.0050(4)	0.0255(17)	0.0109(8)	-0.0009(7)	-0.0006(4)	0.0033(10)
4		0.2023	0.4206	0.4631						
5		0.1995(23)	0.4217(35)	0.4610(47)	B = 5.1(6)					
1	H ₅	0.3645(11)	0.2630(22)	0.0860(14)	0.0071(8)	0.0458(37)	0.0139(14)	-0.0037(13)	-0.0028(8)	0.0004(18)
2		0.3645(10)	0.2606(18)	0.0883(11)	0.0081(7)	0.0426(32)	0.0165(16)	-0.0045(14)	-0.0049(9)	0.0055(18)
3		0.3652(8)	0.2597(19)	0.0863(11)	0.0079(6)	0.0412(32)	0.0139(11)	-0.0039(12)	-0.0033(7)	0.0019(16)
4		0.3652	0.2627	0.0857						
5		0.3658(31)	0.2619(44)	0.0785(46)	B = 6.4(8)					
1	H ₆	0.2697(10)*	0.3412(16)*	0.0314(11)*	0.0083(8)*	0.0212(20)*	0.0120(11)*	0.0000(11)*	0.0007(8)*	0.0028(13)*
2**		0.2705(9)	0.3384(15)	0.0323(12)	0.0076(8)	0.0232(24)	0.0157(13)	0.0013(10)	-0.0005(8)	0.0044(13)
3~		0.2698(8)	0.3405(13)	0.0308(9)	0.0075(6)	0.0236(17)	0.0122(9)	0.0008(9)	0.0002(6)	0.0023(10)
4		0.2687	0.3428	0.0301						
5		0.2671(30)	0.3439(57)	0.0453(54)	B = 7.2(9)					

*Standard errors ($\times 10^4$) appear in parentheses.

**Statistical-scheme results also include effects of unit-cell errors.

APPENDIX B

Final Observed and Calculated Structure Factors
(Statistical Scheme)

H	K	L	Y(OBS)	Y(CALC)	A	B	OBS-CALC	SIG(O)
2	0	0	18.0060	25.2373	25.6258	0.0000	-7.2313	0.0000
4	0	0	14.4550	14.8997	15.1290	0.0000	-0.4447	0.3058
6	0	0	14.8940	15.1305	15.3634	0.0000	-0.2365	0.3847
8	0	0	1.9170	1.6904	-1.7165	0.0000	0.2266	1.5263
10	0	0	21.5700	22.1876	22.5292	0.0000	-0.6176	0.4798
12	0	0	15.5310	15.9241	16.1692	0.0000	-0.3931	0.5389
14	0	0	8.5160	8.2675	8.3948	0.0000	0.2485	0.6997
16	0	0	7.6090	7.4167	7.5308	0.0000	0.1923	0.7749
18	0	0	0.7950	0.0762	0.0773	0.0000	0.7188	4.8386
1	1	0	0.4710	0.6938	0.7045	0.0000	-0.2228	1.9275
3	1	0	2.0380	2.1785	-2.2120	0.0000	-0.1405	0.7537
5	1	0	3.9750	3.6624	-3.7187	0.0000	0.3126	0.6259
7	1	0	6.6090	6.2519	6.3482	0.0000	0.3571	0.5828
9	1	0	6.6550	6.6574	-6.7599	0.0000	-0.0024	0.6511
11	1	0	3.0240	3.5507	3.6054	0.0000	-0.5267	1.2726
13	1	0	3.6620	4.0521	-4.1145	0.0000	-0.3901	1.1651
15	1	0	1.3510	0.7142	0.7252	0.0000	0.6368	2.9911
17	1	0	1.1060	0.8171	0.8297	0.0000	0.2889	4.0300
19	1	0	1.6800	1.6135	-1.6383	0.0000	0.0665	2.5500
0	2	0	0.0000	0.5377	0.5460	0.0000	-0.5377	0.0000
2	2	0	0.3930	0.2294	-0.2330	0.0000	0.1636	3.8153
4	2	0	1.1240	0.7476	-0.7591	0.0000	0.3764	1.7852
6	2	0	1.6130	1.5712	-1.5954	0.0000	0.0418	1.7582
8	2	0	0.8010	0.8086	0.8210	0.0000	-0.0076	4.0929
10	2	0	1.4880	1.6453	-1.6706	0.0000	-0.1573	2.5545
12	2	0	0.5680	0.9770	0.9920	0.0000	-0.4090	7.4421
14	2	0	0.9900	0.5053	-0.5130	0.0000	0.4847	3.3644
1	3	0	6.3760	6.3505	-6.4483	0.0000	0.0255	0.4415
3	3	0	2.5590	2.2372	-2.2716	0.0000	0.3218	0.9057
5	3	0	6.5430	6.3845	-6.4827	0.0000	0.1585	0.5388
7	3	0	1.7520	1.9127	-1.9422	0.0000	-0.1607	1.9400
9	3	0	1.5860	1.2001	-1.2186	0.0000	0.3859	2.4019
11	3	0	8.5020	8.5309	-8.6622	0.0000	-0.0289	0.6327
13	3	0	1.1780	0.3862	-0.3922	0.0000	0.7918	3.7400
15	3	0	3.8650	4.5212	-4.5908	0.0000	-0.6562	1.0955
17	3	0	1.4610	1.2378	-1.2569	0.0000	0.2232	3.0000
19	3	0	1.3860	1.5469	-1.5707	0.0000	-0.1609	2.8839
0	4	0	3.1790	2.8940	-2.9385	0.0000	0.2850	0.8121
2	4	0	9.6220	9.8340	-9.9853	0.0000	-0.2120	0.4729
4	4	0	9.2080	9.1134	9.2536	0.0000	0.0946	0.5046
6	4	0	2.6250	2.5956	2.6355	0.0000	0.0294	1.2782
8	4	0	2.4600	2.3757	2.4123	0.0000	0.0843	1.8791
10	4	0	1.4210	0.8579	0.8711	0.0000	0.5631	3.1110
12	4	0	8.3970	8.7984	-8.9338	0.0000	-0.4014	0.7677
14	4	0	1.0400	1.1094	1.1264	0.0000	-0.0694	3.5919
16	4	0	2.0820	1.7832	-1.8106	0.0000	0.2988	1.8349
18	4	0	2.2060	2.1438	2.1768	0.0000	0.0622	1.8133

1	5	0	1.4270	1.4243	1.4462	0.0000	0.0027	2.0935
3	5	0	7.7350	7.8100	7.9303	0.0000	-0.0750	0.5820
5	5	0	3.7790	3.7117	-3.7689	0.0000	0.0673	0.9512
7	5	0	2.5660	2.4108	2.4479	0.0000	0.1552	1.4632
9	5	0	1.6300	1.5876	1.6120	0.0000	0.0424	2.5490
11	5	0	0.6260	0.4668	0.4740	0.0000	0.1592	6.2992
13	5	0	2.8520	2.6192	2.6595	0.0000	0.2328	1.7221
15	5	0	0.0000	0.5642	-0.5729	0.0000	-0.5642	26.5257
17	5	0	0.4390	0.2537	-0.2576	0.0000	0.1853	9.4420
0	6	0	1.7590	1.9782	2.0086	0.0000	-0.2192	1.8307
2	6	0	2.0130	2.4297	2.4671	0.0000	-0.4167	1.6682
4	6	0	1.1020	0.9032	0.9171	0.0000	0.1988	3.7864
6	6	0	3.8230	4.0301	4.0921	0.0000	-0.2071	1.0476
8	6	0	2.2800	2.5207	2.5595	0.0000	-0.2407	1.7681
10	6	0	1.7800	1.4996	1.5227	0.0000	0.2804	2.2278
12	6	0	0.7920	0.3243	0.3293	0.0000	0.4677	3.7580
14	6	0	1.9130	1.2189	1.2377	0.0000	0.6941	2.1154
16	6	0	1.7720	1.3910	1.4124	0.0000	0.3810	2.0907
1	7	0	2.8110	3.0361	-3.0828	0.0000	-0.2251	1.3111
3	7	0	3.5330	3.7850	-3.8432	0.0000	-0.2520	1.1119
5	7	0	6.0470	5.8732	-5.9637	0.0000	0.1738	0.7739
7	7	0	4.6070	4.6626	-4.7344	0.0000	-0.0556	0.9536
9	7	0	3.8430	3.7729	-3.8310	0.0000	0.0701	1.1214
11	7	0	0.4360	0.8617	-0.8750	0.0000	-0.4257	10.0129
13	7	0	1.0160	0.1266	-0.1286	0.0000	0.8894	3.5332
15	7	0	1.8630	2.1034	-2.1357	0.0000	-0.2404	2.1200
0	8	0	9.9310	10.0867	10.2420	0.0000	-0.1557	0.6298
2	8	0	0.9060	0.4138	-0.4202	0.0000	0.4922	4.0815
4	8	0	1.4150	1.5390	1.5627	0.0000	-0.1240	2.6537
6	8	0	0.4620	0.6748	-0.6852	0.0000	-0.2128	9.0185
8	8	0	2.2100	2.0344	-2.0657	0.0000	0.1756	1.7469
10	8	0	3.7370	3.7048	3.7619	0.0000	0.0322	1.2239
12	8	0	2.0600	2.4853	2.5236	0.0000	-0.4253	2.7084
14	8	0	2.4130	2.2537	2.2884	0.0000	0.1593	1.6005
1	9	0	1.7330	1.3681	1.3892	0.0000	0.3649	2.2864
3	9	0	1.0770	0.9577	0.9725	0.0000	0.1193	3.3934
5	9	0	4.0710	4.0328	4.0948	0.0000	0.0382	1.1916
7	9	0	1.5750	1.5543	1.5782	0.0000	0.0207	2.6791
9	9	0	1.8490	2.0832	2.1153	0.0000	-0.2342	1.7705
11	9	0	0.9810	0.7280	0.7393	0.0000	0.2530	3.6194
0	10	0	1.2140	0.7614	0.7731	0.0000	0.4526	2.9692
2	10	0	0.6320	0.4239	0.4304	0.0000	0.2081	6.5537
4	10	0	1.3450	0.3953	-0.4014	0.0000	0.9497	2.6391
6	10	0	0.5660	0.2767	-0.2810	0.0000	0.2893	5.8682
8	10	0	0.4000	0.1722	-0.1748	0.0000	0.2278	10.2266
10	10	0	0.6990	0.0606	0.0615	0.0000	0.6384	4.9461
1	11	0	2.7550	2.7153	-2.7571	0.0000	0.0397	4.2969
3	11	0	1.4630	0.9856	-1.0008	0.0000	0.4774	2.7900
5	11	0	0.8620	0.4625	-0.4696	0.0000	0.3995	2.9770
7	11	0	0.5040	0.2092	0.2124	0.0000	0.2948	7.3500
1	1	1	5.3930	5.1003	-0.9376	5.0933	0.2927	0.3043
3	1	1	2.5400	2.2816	1.5160	1.7519	0.2584	0.6365
5	1	1	3.5460	3.2054	2.4638	-2.1267	0.3406	0.7184
7	1	1	5.6280	5.4221	-5.4007	1.0696	0.2059	0.5986

9	1	1	5.0380	5.0685	4.9669	1.3478	-0.0305	0.7264
11	1	1	3.3680	3.7644	-3.1445	2.1731	-0.3964	1.0976
13	1	1	4.4170	4.2873	2.1753	3.7709	0.1297	0.9415
15	1	1	0.0000	0.4595	-0.1538	0.4405	-0.4595	3.3396
17	1	1	2.0660	1.7075	-1.2648	1.1858	0.3585	2.0849
19	1	1	1.9380	1.4792	1.2480	-0.8356	0.4588	2.0573
0	2	1	2.5050	2.2727	1.7386	1.5175	0.2323	0.6871
2	2	1	0.8880	1.1479	-0.8344	0.8138	-0.2599	1.7928
4	2	1	5.8190	5.4240	-5.3927	-1.1189	0.3950	0.4720
6	2	1	15.4540	15.6213	-15.8502	-0.6057	-0.1673	0.4134
8	2	1	4.3650	3.6638	-2.0540	3.1018	0.7012	0.8854
10	2	1	4.2030	4.1907	-3.0362	-2.9814	0.0123	1.0593
12	2	1	1.9150	1.7146	0.7421	1.5749	0.2004	2.1452
14	2	1	3.8440	3.9581	4.0131	-0.2176	-0.1141	1.0484
16	2	1	4.9700	4.7722	-4.8456	0.0212	0.1978	0.9793
18	2	1	2.9120	2.5060	-2.5444	-0.0283	0.4060	1.4004
1	3	1	6.8390	6.7003	-5.8226	3.5193	0.1387	0.4402
3	3	1	2.7500	2.5012	-1.5140	-2.0391	0.2488	0.9206
5	3	1	8.1400	7.9864	-4.0029	7.0526	0.1536	0.5259
7	3	1	10.3160	10.4260	-3.2371	-10.0794	-0.1100	0.4998
9	3	1	3.2380	3.1635	-0.2169	3.2049	0.0745	1.1185
11	3	1	6.8640	6.9632	-6.5500	2.6623	-0.0992	0.7140
13	3	1	0.9800	0.9716	-0.9159	0.3667	0.0084	3.8661
15	3	1	3.2810	3.0699	-2.6838	1.5855	0.2111	1.1980
17	3	1	2.6670	2.8906	-1.8135	-2.3077	-0.2236	1.5518
0	4	1	2.1840	2.1061	1.0403	-1.8684	0.0779	1.1364
2	4	1	3.2090	3.2089	1.1961	3.0308	0.0001	0.8837
4	4	1	1.8630	1.8382	-1.0948	-1.5117	0.0248	1.4137
6	4	1	1.8140	1.5613	-0.5859	1.4731	0.2527	1.7128
8	4	1	2.6630	2.7623	1.3887	2.4369	-0.0993	1.3301
10	4	1	2.2320	2.1862	-0.8729	-2.0410	0.0458	1.6176
12	4	1	1.1170	0.9770	0.9873	-0.0976	0.1400	3.4517
14	4	1	1.0920	1.0856	0.6312	-0.9038	0.0064	3.4463
16	4	1	0.6410	0.2798	0.1748	-0.2239	0.3612	5.4297
18	4	1	0.0000	0.3065	-0.2573	0.1752	-0.3065	0.0000
1	5	1	3.1720	2.9484	-2.9926	-0.0837	0.2236	0.9227
3	5	1	5.0640	4.8327	-4.6471	1.5761	0.2313	0.7064
5	5	1	4.6540	4.6087	3.5708	3.0246	0.0453	0.7963
7	5	1	3.6170	3.8287	-2.9573	2.5235	-0.2117	1.0512
9	5	1	1.8390	1.4169	-0.8335	1.1727	0.4221	1.9161
11	5	1	0.8140	0.1839	-0.1746	0.0661	0.6301	4.5851
13	5	1	2.6830	2.4480	-2.4511	-0.4128	0.2350	1.4998
15	5	1	0.0000	0.2043	-0.1574	0.1352	-0.2043	0.0000
17	5	1	1.1390	1.1331	0.4752	1.0478	0.0059	3.7100
0	6	1	4.8220	4.8597	4.5902	-1.8110	-0.0377	0.7778
2	6	1	2.3000	2.5598	2.0250	1.6294	-0.2598	1.4540
4	6	1	8.1720	7.9211	7.9253	-1.3710	0.2509	0.6032
6	6	1	10.9900	11.0017	11.1597	0.5025	-0.0117	0.5644
8	6	1	6.3240	6.2975	6.2111	1.5203	0.0265	0.7513
10	6	1	4.1270	4.2496	4.0683	-1.4381	-0.1226	1.0307
12	6	1	1.8070	1.9003	1.8294	0.6135	-0.0933	2.1079
14	6	1	0.7610	0.7894	0.6574	-0.4586	-0.0284	4.9250
16	6	1	3.8290	4.1677	4.2073	0.4556	-0.3387	1.0718
1	7	1	2.6950	2.6086	0.3552	2.6248	0.0864	1.4683

3	7	1	3.8590	3.9705	-3.2612	2.3703	=0.1115	1.1381
5	7	1	6.9780	7.1009	-0.7574	7.1703	=0.1229	0.7424
7	7	1	3.7670	3.5257	-2.7634	2.2759	0.2413	1.2459
9	7	1	3.9400	3.9125	-1.2672	3.7652	0.0275	1.1228
11	7	1	1.7570	1.3029	0.6998	1.1227	0.4541	2.3844
13	7	1	0.0000	0.3559	0.1568	0.3256	=0.3559	0.0000
15	7	1	2.1850	1.7978	-0.5404	1.7436	0.3872	1.7742
0	8	1	2.4220	2.4544	-1.5210	=1.9742	=0.0324	1.7970
2	8	1	1.5000	1.2812	-0.2178	=1.2826	0.2188	2.8052
4	8	1	2.7590	2.6648	-0.5885	=2.6410	0.0942	1.5819
6	8	1	3.3810	3.2436	0.7597	=3.2048	0.1374	1.4074
8	8	1	1.9630	1.9282	0.0294	=1.9577	0.0348	2.2598
10	8	1	2.6180	1.8381	-0.5855	=1.7722	0.7799	1.7066
12	8	1	1.3500	0.7303	-0.3247	=0.6667	0.6197	2.9577
14	8	1	1.5450	1.5080	-0.7646	=1.3243	0.0390	2.4789
1	9	1	2.6160	3.0696	-2.2322	2.1754	=0.4536	1.6254
3	9	1	3.0370	3.1989	-2.9158	1.4312	=0.1619	1.3340
5	9	1	4.8030	4.8555	-4.9030	0.5174	=0.0525	1.1200
7	9	1	4.5580	4.1061	-4.1177	0.6540	0.4519	1.0542
9	9	1	2.9050	2.9805	-2.8955	0.8804	=0.0755	1.4212
11	9	1	1.2640	1.7346	-1.4716	0.9679	=0.4706	2.8268
0	10	1	1.0390	0.8084	-0.6653	-0.4807	0.2306	3.2855
2	10	1	1.2810	1.9195	1.7335	0.8910	=0.6385	3.2197
4	10	1	2.1260	1.7625	-1.7192	-0.4969	0.3635	1.9550
6	10	1	2.1010	2.1100	-2.1396	-0.1109	=0.0090	1.8620
8	10	1	0.0000	0.6887	-0.6966	-0.0616	-0.6887	0.0000
10	10	1	0.0000	0.2851	-0.1727	-0.2323	=0.2851	16.5253
1	11	1	2.0830	2.0355	-1.8241	0.9719	0.0475	2.0436
3	11	1	0.0000	0.5266	-0.5075	-0.1685	=0.5266	0.0000
5	11	1	0.6800	0.9264	-0.9295	0.1447	=0.2464	5.5095
7	11	1	0.8420	0.5953	-0.0790	-0.5993	0.2467	4.1462
0	0	2	10.6620	11.1402	-11.3053	-0.3811	=0.4782	0.2380
2	0	2	7.7550	7.3751	-7.4884	-0.0581	0.3799	0.3133
4	0	2	4.5470	4.2026	4.1544	-0.9752	0.3444	0.5380
6	0	2	4.9200	4.5035	-4.3191	1.5019	0.4165	0.6623
8	0	2	1.3430	1.4549	0.1040	-1.4737	=0.1119	2.2191
10	0	2	3.9670	2.9741	-2.9787	0.4970	0.9929	0.9098
12	0	2	8.8480	8.7197	-8.7764	-1.1697	0.1283	0.6772
14	0	2	1.5080	0.4021	-0.1240	-0.3890	1.1059	2.5947
16	0	2	4.7820	4.9170	-4.9910	0.1271	=0.1350	1.0004
18	0	2	1.4760	1.3947	1.2644	-0.6379	0.0813	3.4052
1	1	2	8.5670	8.3455	-0.4299	-8.4631	0.2215	0.2921
3	1	2	3.5450	3.4072	0.5079	-3.4222	0.1378	0.5471
5	1	2	6.0020	5.5408	-3.5235	4.3861	0.4612	0.4963
7	1	2	2.8890	2.4193	-0.9190	-2.2782	0.4697	1.0078
9	1	2	2.2710	2.0969	1.7537	-1.2076	0.1741	1.4547
11	1	2	5.5410	5.4458	-3.8597	-3.9598	0.0952	0.7961
13	1	2	5.9810	5.6910	1.7149	-5.5182	0.2900	0.7981
15	1	2	2.1620	2.2627	-0.7306	-2.1783	=0.1007	1.8396
17	1	2	1.1270	1.4451	-1.4424	-0.2694	-0.3181	3.3242
19	1	2	0.6590	1.2142	-0.1633	1.2221	=0.5552	5.6042
0	2	2	11.3520	11.9539	-1.3352	12.0642	-0.6019	0.3214
2	2	2	12.7560	12.7379	-0.8365	12.9070	0.0181	0.3387
4	2	2	6.0940	5.6332	-0.1726	5.7173	0.4608	0.5198

6	2	2	8.0630	7.6911	-1.7855	7.6026	0.3719	0.5169
8	2	2	12.6760	12.3306	1.0965	12.4724	0.3454	0.4790
10	2	2	2.5350	2.7155	-1.7110	2.1623	-0.1805	1.4338
12	2	2	7.4420	7.4684	-0.1116	7.5825	-0.0264	0.6917
14	2	2	4.3580	3.9171	-0.7732	3.9015	0.4409	1.0102
16	2	2	3.2620	3.2154	-0.4111	3.2389	0.0466	1.2840
18	2	2	2.4750	2.6922	0.2397	2.7231	-0.2172	1.5460
1	3	2	8.8360	8.5974	6.0397	6.3032	0.2386	0.4157
3	3	2	3.3340	3.2004	3.0129	-1.2176	0.1336	0.8546
5	3	2	4.7870	4.6861	4.0804	2.4477	0.1009	0.6752
7	3	2	8.0100	7.8306	4.7457	-6.3796	0.1794	0.5594
9	3	2	3.3120	2.9592	1.4087	2.6541	0.3528	1.0967
11	3	2	5.1410	5.0302	4.9537	1.2447	0.1108	0.8556
13	3	2	3.6560	3.8242	2.2596	3.1579	-0.1682	1.1519
15	3	2	1.8610	1.7327	1.6837	0.5105	0.1283	2.0966
17	3	2	3.1400	3.4463	2.9522	-1.8789	-0.3063	1.2757
0	4	2	11.8880	12.2462	12.4210	-0.5831	-0.3582	0.4352
2	4	2	2.9760	2.4966	-2.5053	0.3867	0.4794	0.8880
4	4	2	2.4670	2.2603	1.7091	1.5318	0.2067	1.1900
6	4	2	1.4550	1.6630	0.9535	-1.3936	-0.2080	2.1626
8	4	2	6.0370	5.7385	-5.8267	-0.0464	0.2985	0.7347
10	4	2	5.7680	5.7133	5.7494	0.7737	0.0547	0.8571
12	4	2	2.9450	2.2601	2.2350	0.5208	0.6849	1.4887
14	4	2	1.7730	1.7062	1.6794	0.4254	0.0668	2.2452
16	4	2	1.0940	1.1012	1.1178	0.0302	-0.0072	3.4507
18	4	2	1.2980	1.2658	-1.2470	0.3114	0.0322	2.6586
1	5	2	0.9310	1.1219	1.1382	-0.0467	-0.1909	3.3693
3	5	2	4.8550	4.9541	2.0911	-4.5752	-0.0991	0.7405
5	5	2	6.4780	6.4681	2.6667	-6.0020	0.0099	0.6827
7	5	2	7.9450	8.0914	4.1156	-7.1109	-0.1464	0.6453
9	5	2	3.6980	3.5893	-0.3029	-3.6319	0.1087	1.0846
11	5	2	2.7730	2.5904	2.6136	0.2953	0.1826	1.4676
13	5	2	1.4890	1.3078	-0.1272	-1.3219	0.1812	2.6805
15	5	2	0.9880	0.2095	0.1492	0.1516	0.7785	3.4769
17	5	2	4.1340	4.4145	2.5454	-3.6896	-0.2805	1.1244
0	6	2	8.3570	7.9773	0.1636	-8.0985	0.3797	0.6651
2	6	2	3.8090	3.6359	0.4377	3.6659	0.1731	1.0641
4	6	2	3.1910	3.3416	-2.3842	-2.4141	-0.1506	1.1953
6	6	2	1.8200	1.5676	0.4912	1.5140	0.2524	2.1043
8	6	2	2.7880	2.4712	-1.5117	2.0027	0.3168	1.3852
10	6	2	2.4860	2.5166	0.1666	-2.5499	-0.0306	1.5908
12	6	2	0.5570	0.5390	-0.1661	0.5215	0.0180	7.1085
14	6	2	1.6550	1.8186	-0.2258	-1.8327	-0.1636	2.2768
16	6	2	0.9320	0.7914	0.0339	0.8029	0.1406	3.5894
1	7	2	4.2720	4.2067	-3.9757	1.5617	0.0653	0.9636
3	7	2	2.5910	2.5012	1.1394	2.2698	0.0898	1.4317
5	7	2	5.3500	5.2499	-3.3342	4.1593	0.1001	0.9192
7	7	2	4.9010	5.0945	1.3997	4.9800	-0.1935	1.0094
9	7	2	2.6770	2.3714	-1.7619	1.6413	0.3056	1.5383
11	7	2	1.9010	2.1017	-1.8134	-1.1250	-0.2007	2.2290
13	7	2	1.2070	1.2722	-1.2199	-0.4249	-0.0652	3.0510
15	7	2	2.5320	1.9712	-1.0393	1.7106	0.5608	1.6820
0	8	2	5.1340	5.1544	-5.1078	1.1412	-0.0204	0.8826
2	8	2	2.9120	2.9714	-2.6345	1.4705	-0.0594	1.3832

4	8	2	3.3180	3.0436	-1.8043	2.5090	0.2744	1.3106
6	8	2	2.4130	2.1681	-1.1134	1.8992	0.2449	1.5872
8	8	2	1.8770	1.6660	-0.8684	1.4517	0.2110	2.4726
10	8	2	2.6350	2.2875	-1.9390	1.2788	0.3475	1.7414
12	8	2	3.3330	3.3229	-3.2715	0.8258	0.0101	1.2839
14	8	2	1.5260	1.2758	-1.1279	0.6372	0.2502	2.5620
1	9	2	5.0730	5.4007	-0.6962	-5.4395	-0.3277	0.9404
3	9	2	4.2960	4.4343	0.2905	-4.4932	-0.1383	1.0256
5	9	2	2.6540	2.8588	-2.5043	-1.4679	-0.2048	1.4772
7	9	2	2.0710	2.0642	-1.2156	-1.7075	0.0068	1.8419
9	9	2	2.1230	2.1938	-0.4476	-2.1822	-0.0708	1.7677
11	9	2	2.8870	3.0418	-0.6663	-3.0159	-0.1548	1.3327
0	10	2	1.0660	0.6514	-0.6485	-0.1304	0.4146	4.0300
2	10	2	0.6960	0.7239	0.0525	-0.7332	-0.0279	5.2049
4	10	2	1.3800	1.7605	0.0722	-1.7861	-0.3805	2.6492
6	10	2	2.3120	2.4522	0.1797	-2.4835	-0.1402	1.6288
8	10	2	1.2970	1.4980	0.4885	-1.4405	-0.2010	2.8812
10	10	2	0.8460	0.8147	-0.2896	-0.7749	0.0313	9.6128
1	11	2	2.0300	2.0808	1.9370	0.8439	-0.0508	1.8181
3	11	2	0.4480	0.7160	0.7063	0.1723	-0.2680	9.0600
5	11	2	1.0540	0.7442	0.6918	-0.3040	0.3098	3.1913
7	11	2	0.7590	0.2033	-0.0061	-0.2063	0.5557	4.7504
1	1	3	8.6830	8.2621	4.5296	-7.0613	0.4209	0.3417
3	1	3	3.6950	3.3072	1.0727	-3.1822	0.3878	0.5948
5	1	3	11.0450	10.8008	10.3525	3.6197	0.2442	0.4165
7	1	3	2.3580	1.9273	-1.9438	0.2263	0.4307	1.3668
9	1	3	2.5990	2.3085	2.1590	0.9128	0.2905	1.3668
11	1	3	10.1490	9.9457	8.0046	-6.1572	0.2033	0.5898
13	1	3	3.7250	4.0142	-0.8445	-3.9876	-0.2892	0.9045
15	1	3	4.2150	4.5009	3.8274	-2.4974	-0.2859	1.0862
17	1	3	1.3330	1.1988	0.7447	0.9629	0.1342	3.1351
19	1	3	1.9640	1.8129	1.7193	0.6577	0.1511	1.9132
0	2	3	2.5920	2.4843	-1.5777	-1.9683	0.1077	0.8144
2	2	3	1.9730	1.7356	0.9855	-1.4610	0.2374	1.0451
4	2	3	5.4790	5.4109	-5.4929	-0.1171	0.0681	0.5281
6	2	3	5.9250	5.8245	5.2287	-2.7637	0.1005	0.6036
8	2	3	2.6100	2.0212	-1.8217	0.9452	0.5888	1.2685
10	2	3	2.2560	1.8908	-0.1457	-1.9144	0.3652	1.5172
12	2	3	1.6840	1.9670	1.9938	-0.1180	-0.2830	2.2518
14	2	3	2.4520	2.1966	-2.2103	-0.2986	0.2554	1.6319
16	2	3	2.7420	3.1521	3.1502	-0.5659	-0.4101	1.5402
18	2	3	0.3530	0.3010	0.3045	0.0265	0.0520	11.9700
1	3	3	6.3620	5.9536	3.8684	-4.6455	0.4084	0.5054
3	3	3	1.4350	1.2077	0.7828	-0.9439	0.2273	1.5530
5	3	3	5.6590	5.5711	2.0270	5.2812	0.0879	0.6255
7	3	3	4.8200	4.3986	1.7810	4.0958	0.4214	0.7731
9	3	3	0.3980	0.9021	-0.6951	0.5966	-0.5041	9.4398
11	3	3	4.8470	5.0944	4.7632	-2.0176	-0.2474	0.8986
13	3	3	4.1160	4.2717	0.2453	-4.3305	-0.1557	1.0898
15	3	3	1.0900	1.2014	0.5447	1.0915	-0.1114	3.6541
17	3	3	2.0130	1.6456	1.6148	0.4294	0.3674	1.9606
0	4	3	2.0330	2.2320	-1.1780	-1.9361	-0.1990	1.4376
2	4	3	9.4670	9.4023	0.9790	9.4967	0.0647	0.4786
4	4	3	3.9390	3.8687	-3.0275	-2.5031	0.0703	0.9052

6	4	3	2.4920	2.5822	0.4541	2.5823	-0.0902	1.3383
8	4	3	2.7260	2.4427	2.0121	1.4502	-0.2833	1.3268
10	4	3	3.5080	3.3169	-2.9404	1.6423	0.1911	1.1827
12	4	3	4.3200	4.4203	0.7057	4.4325	-0.1003	1.0432
14	4	3	1.8090	1.4860	-0.7172	1.3275	0.3230	2.2185
16	4	3	1.7680	2.0063	0.3730	2.0028	-0.2383	2.1692
18	4	3	0.6030	0.3763	-0.2055	-0.3222	0.2267	2.8279
1	5	3	6.8840	6.8609	-6.9284	-0.7277	0.0231	0.6111
3	5	3	6.4630	6.4702	-6.2465	-2.0353	-0.0072	0.6546
5	5	3	7.8820	7.8290	-2.2386	-7.6278	0.0530	0.6209
7	5	3	10.5220	10.3419	-9.8186	-3.7241	0.1801	0.5888
9	5	3	5.0740	4.9536	-1.8125	-4.6919	0.1204	0.8673
11	5	3	4.2110	4.2612	-4.0217	1.5962	-0.0502	1.0196
13	5	3	3.0560	2.9754	-2.8259	-1.0686	0.0806	1.3343
15	5	3	1.6760	1.1076	-1.1090	-0.1871	0.5684	2.2506
17	5	3	3.9600	4.1629	-3.4928	-2.3808	-0.2029	1.0977
0	6	3	5.0390	5.1777	-5.2424	0.3959	-0.1387	0.8574
2	6	3	1.9630	1.9562	1.3525	1.4548	0.0068	1.8152
4	6	3	2.6070	2.5483	-2.5800	0.1970	0.0587	1.4610
6	6	3	3.4290	3.0636	-3.0985	0.2753	0.3654	1.1326
8	6	3	1.8000	1.4045	1.3389	0.4909	0.3955	2.1837
10	6	3	2.7880	2.2995	-2.3348	-0.0259	0.4885	1.4299
12	6	3	1.1500	1.3110	-0.7518	1.0986	-0.1610	3.4543
14	6	3	0.7600	0.0458	0.0363	-0.0290	0.7142	4.7213
16	6	3	1.4210	0.8399	-0.7960	0.3061	0.5811	2.5248
1	7	3	4.1600	4.1793	-4.2118	-0.5194	-0.0193	0.9934
3	7	3	5.1650	5.1662	-1.0098	-5.1476	-0.0012	0.9080
5	7	3	5.7180	5.6193	-3.4056	-4.5780	0.0987	0.8321
7	7	3	7.2360	7.3182	-0.7246	-7.3955	-0.0822	0.7543
9	7	3	2.3690	2.5896	-1.4012	-2.2251	-0.2206	1.6757
11	7	3	2.7360	2.9820	-2.7632	-1.2401	-0.2468	1.4631
13	7	3	0.9760	1.1390	-1.0242	0.5371	-0.1630	3.7527
15	7	3	1.7870	1.6514	-0.7795	-1.4846	0.1356	2.1090
0	8	3	3.3160	3.3363	-1.7836	2.8801	-0.0203	1.2907
2	8	3	0.7500	0.9777	0.8068	0.5784	-0.2277	4.8262
4	8	3	5.2740	5.0642	-1.3392	4.9647	0.2098	0.9147
6	8	3	4.2550	4.4115	-0.7552	4.4152	-0.1565	1.0256
8	8	3	3.4890	3.7218	0.1035	3.7777	-0.2328	1.1975
10	8	3	1.6300	1.9361	-0.8750	1.7605	-0.3061	2.3415
12	8	3	0.9390	0.8399	0.3728	0.7671	0.0991	3.7036
14	8	3	1.1080	1.0938	-0.4745	1.0041	0.0142	8.7677
1	9	3	2.6070	2.7478	1.5067	-2.3483	-0.1408	1.4928
3	9	3	1.4110	1.5141	-0.4079	-1.4823	-0.1031	2.7614
5	9	3	3.1350	3.2518	3.2959	0.1982	-0.1168	1.2871
7	9	3	0.7940	0.1932	0.1392	-0.1383	0.6008	5.0120
9	9	3	1.5270	1.5554	1.4808	-0.5492	-0.0284	2.3788
11	9	3	1.3610	1.7376	0.7378	-1.6027	-0.3766	2.5745
0	10	3	1.9550	1.8819	1.9093	-0.0764	0.0731	1.9073
2	10	3	0.5970	0.8188	0.7778	0.2938	-0.2218	6.1896
4	10	3	0.9710	1.2506	1.1046	0.6263	-0.2796	3.6658
6	10	3	1.2140	1.4086	1.1048	0.9084	-0.1946	2.9652
8	10	3	0.8990	0.9330	0.7066	0.6311	-0.0340	3.7555
10	10	3	1.0280	1.0619	1.0044	0.3923	-0.0339	7.9628
1	11	3	2.4510	2.8665	1.0101	-2.7297	-0.4155	1.5246

3	11	3	1.4470	1.5628	-0.2723	-1.5633	-0.1158	2.4199
5	11	3	0.9750	0.8992	0.7543	-0.5145	0.0758	3.4181
0	0	4	11.9640	12.1441	-12.0135	-2.7804	-0.1801	0.3360
2	0	4	10.2160	9.9022	-9.6123	-2.9493	0.3138	0.3931
4	0	4	13.2680	13.4003	-13.2996	-2.8739	-0.1323	0.4027
6	0	4	2.2180	0.8301	-0.6083	-0.5834	1.3879	1.4464
8	0	4	7.0860	6.5514	-5.9202	-3.0338	0.5346	0.7466
10	0	4	7.7980	7.6155	-7.6845	-0.8619	0.1825	0.6891
12	0	4	5.7400	5.4005	-4.2931	-3.4116	0.3395	0.9357
14	0	4	6.2520	6.1321	-6.2247	-0.1482	0.1199	0.8797
16	0	4	1.3750	0.8645	-0.1803	-0.8591	0.5105	3.3139
1	1	4	8.8410	8.4457	4.1237	7.5192	0.3953	0.3895
3	1	4	5.8710	5.7836	0.4525	5.8552	0.0874	0.5464
5	1	4	8.5420	8.2235	8.2932	0.9731	0.3185	0.4662
7	1	4	3.6310	3.5637	2.0849	-2.9575	0.0673	0.9056
9	1	4	3.0650	3.0578	1.3786	2.7820	0.0072	1.1127
11	1	4	8.7370	8.4119	5.6546	6.4016	0.3251	0.6442
13	1	4	3.6830	3.9146	-0.1809	3.9707	-0.2316	1.1419
15	1	4	3.5680	3.9352	2.7175	2.9294	-0.3672	1.2017
17	1	4	2.4090	2.4180	2.1518	-1.1823	-0.0090	1.7099
19	1	4	1.2420	1.1496	1.1535	0.1790	0.0924	3.0927
0	2	4	8.3840	8.4902	-0.3763	-8.6127	-0.1062	0.4401
2	2	4	4.9880	5.1659	1.2660	5.0904	-0.1779	0.5688
4	2	4	7.8160	7.7675	0.7595	-7.8505	0.0485	0.4899
6	2	4	0.7920	0.5531	-0.1979	0.5256	0.2389	3.6893
8	2	4	4.2940	3.8027	1.2258	3.6615	0.4913	0.9399
10	2	4	6.9460	6.5877	0.1998	-6.6862	0.3583	0.7111
12	2	4	1.1980	1.1402	0.7845	0.8515	0.0578	3.1776
14	2	4	3.2240	3.7121	-0.0835	-3.7683	-0.4881	1.2873
16	2	4	0.7580	0.8905	0.3806	0.8202	-0.1325	3.7636
18	2	4	0.9570	1.0232	0.3493	-0.9785	-0.0662	3.7222
1	3	4	2.9900	2.5308	-1.1398	-2.3032	0.4592	0.8559
3	3	4	1.2770	0.7408	0.6795	-0.3226	0.5362	2.1142
5	3	4	6.2710	5.9995	-1.2532	5.9616	0.2715	0.6394
7	3	4	3.8480	3.7112	-2.4584	2.8559	0.1368	0.9853
9	3	4	1.5850	1.6179	1.4385	0.7933	-0.0329	2.4983
11	3	4	2.2080	1.3735	-1.2809	-0.5516	0.8345	1.6691
13	3	4	3.2780	2.9409	0.8599	-2.8596	0.3371	1.3551
15	3	4	1.1360	0.9474	0.2456	0.9301	0.1886	2.9436
17	3	4	1.2910	1.2890	-1.2188	0.4773	0.0020	3.1211
0	4	4	4.8750	4.8670	-4.9403	-0.1276	0.0080	0.6609
2	4	4	2.0920	1.0790	-0.8597	-0.6792	1.0130	1.4760
4	4	4	6.1810	5.7274	-5.7426	0.9183	0.4536	0.6622
6	4	4	9.1000	8.9153	-9.0051	-0.9251	0.1847	0.5796
8	4	4	1.4060	1.6475	-1.5684	-0.5818	-0.2415	3.1870
10	4	4	4.8150	4.4561	-4.5233	-0.1126	0.3589	0.9381
12	4	4	1.7820	1.6838	-1.6264	0.5274	0.0982	2.2080
14	4	4	0.9890	0.6027	0.0371	-0.6109	0.3863	3.5701
16	4	4	2.7990	3.4287	-3.4577	-0.4062	-0.6297	1.4969
1	5	4	6.4800	6.1307	-6.2220	0.1976	0.3493	0.6374
3	5	4	4.4640	4.7729	-4.3397	-2.1574	-0.3089	0.8673
5	5	4	12.0020	11.8915	-7.5764	9.4017	0.1105	0.5472
7	5	4	4.7610	4.5371	-4.3069	1.6352	0.2239	0.9201
9	5	4	5.4770	5.2705	-3.4941	4.0536	0.2065	0.8616

11	5	4	4.8010	4.5618	-4.3963	-1.4589	0.2392	0.9733
13	5	4	2.3240	1.9094	-1.6787	-0.9701	0.4146	1.9054
15	5	4	2.1360	1.9072	-1.7708	0.7838	0.2288	1.9571
17	5	4	3.1590	3.0504	-2.5685	1.7310	0.1086	1.3103
0	6	4	1.8550	2.1072	-1.3569	-1.6544	-0.2522	1.8452
2	6	4	0.9070	0.3827	-0.3865	0.0405	0.5243	3.7366
4	6	4	3.2680	3.4326	-0.2610	-3.4756	-0.1646	1.2250
6	6	4	5.5270	5.4165	-0.7871	-5.4432	0.1105	0.8712
8	6	4	2.0470	1.4667	-1.0045	-1.0995	0.5803	1.8644
10	6	4	2.8700	2.8255	-0.1300	-2.8661	0.0445	1.5276
12	6	4	2.1200	1.8498	-0.5486	1.7964	0.2702	1.9858
14	6	4	0.9020	1.0801	-0.2883	-1.0581	-0.1781	4.2605
16	6	4	1.3850	1.4487	-0.3354	-1.4322	-0.0637	2.7652
1	7	4	7.6450	7.7141	7.0417	3.4305	-0.0691	0.6955
3	7	4	5.7010	5.6339	5.6477	-0.9108	0.0671	0.8429
5	7	4	7.1680	7.3351	7.3831	0.9814	-0.1671	0.7764
7	7	4	6.0940	5.9610	5.7941	-1.7505	0.1330	0.8255
9	7	4	4.5210	4.5560	4.5061	1.0469	-0.0350	1.0497
11	7	4	4.4280	4.4150	4.3543	1.0660	0.0130	1.0726
13	7	4	2.7540	3.0533	2.8170	1.2948	-0.2993	1.5520
15	7	4	2.7370	2.6074	2.5150	0.8271	0.1296	1.4840
0	8	4	2.4020	2.2610	2.2202	-0.5842	0.1410	1.8445
2	8	4	0.8310	0.9945	0.2020	-0.9894	-0.1635	4.1535
4	8	4	3.0310	3.1642	3.2129	-0.0007	-0.1332	1.3822
6	8	4	4.1490	4.3112	4.1580	-1.3690	-0.1622	1.0394
8	8	4	2.1320	2.1185	1.9748	-0.8527	0.0135	1.8258
10	8	4	1.7090	1.4092	1.4173	-0.1970	0.2998	2.2911
12	8	4	0.9380	1.0729	0.9535	-0.5269	-0.1349	3.9798
1	9	4	1.2910	1.4142	0.4701	1.3569	-0.1232	3.1648
3	9	4	0.9970	0.9000	-0.8751	-0.2634	0.0970	4.0974
5	9	4	1.6900	1.8649	1.0183	-1.5965	-0.1749	2.3615
7	9	4	1.3430	1.7124	-0.0536	-1.7379	-0.3694	3.0391
9	9	4	0.4080	0.1519	-0.1390	-0.0667	0.2561	9.1097
11	9	4	1.2750	0.8225	0.2200	0.8056	0.4525	3.1031
0	10	4	2.1960	1.8432	-0.7977	-1.6931	0.3528	1.7915
2	10	4	1.2840	1.1420	-1.1589	0.0410	0.1420	2.8308
4	10	4	1.6180	1.6006	-0.7769	1.4276	0.0174	2.4624
6	10	4	1.7150	1.8206	-0.7400	1.6941	-0.1056	2.3237
8	10	4	1.7890	1.9694	-0.8198	1.8240	-0.1804	2.1738
1	11	4	1.6240	1.6186	-0.9238	-1.3592	0.0054	2.3657
3	11	4	0.8830	1.0905	-0.8571	-0.7010	-0.2075	4.2385
5	11	4	1.6370	1.4965	-1.3699	-0.6574	0.1405	2.4140
1	1	5	7.3490	6.9139	-6.4693	2.7264	0.4351	0.4773
3	1	5	3.6290	3.9230	-3.8406	-1.0571	-0.2940	0.9035
5	1	5	3.3200	2.5102	-2.5410	-0.1998	0.8098	1.0103
7	1	5	7.7630	7.2527	-5.7341	-4.6210	0.5103	0.6231
9	1	5	2.5720	2.4848	-2.4824	-0.4511	0.0872	1.5405
11	1	5	4.5550	4.3921	-3.8389	2.2699	0.1629	1.0951
13	1	5	3.9100	3.7208	-3.7541	0.4252	0.1892	1.1877
15	1	5	1.1400	0.7473	-0.4787	0.5887	0.3927	3.7428
17	1	5	3.8900	4.1906	-3.9398	-1.6075	-0.3006	1.1332
0	2	5	16.0800	16.6903	-16.9035	-1.2177	-0.6103	0.3964
2	2	5	2.0580	1.8915	-0.5083	-1.8521	0.1665	1.2929
4	2	5	5.5210	5.0942	-4.6899	2.1819	0.4268	0.6548

6	2	5	0.8190	0.1362	0.0055	0.1382	0.6828	4.1964
8	2	5	2.9120	2.8566	2.8259	-0.6540	0.0554	1.3597
10	2	5	7.2410	7.3278	-7.4402	0.0739	-0.0868	0.7290
12	2	5	5.9360	5.7127	-5.7999	-0.0933	0.2233	0.8354
14	2	5	3.4520	3.7002	-3.6349	-0.9505	-0.2482	1.3804
16	2	5	2.0460	2.1197	-2.1455	0.1721	-0.0737	2.0969
18	2	5	0.0000	0.9390	-0.0871	0.9495	-0.9390	0.0000
1	3	5	3.3010	3.2806	-0.7350	3.2490	0.0204	1.0189
3	3	5	4.8150	4.7066	3.0988	-3.6382	0.1084	0.7661
5	3	5	4.8200	4.4364	-1.6441	-4.1940	0.3836	0.7999
7	3	5	2.0910	1.5735	0.7491	-1.4112	0.5175	1.5942
9	3	5	1.4250	1.6220	1.5046	-0.6699	-0.1970	2.8546
11	3	5	1.5190	0.8830	-0.6583	-0.6086	0.6360	2.7760
13	3	5	2.9570	3.0261	0.8028	2.9659	-0.0691	1.5269
15	3	5	1.2270	0.7564	0.3207	-0.6979	0.4706	3.4050
17	3	5	0.3630	0.2756	-0.0698	0.2710	0.0874	11.0470
0	4	5	3.4500	3.3418	0.3053	-3.3794	0.1082	1.0187
2	4	5	7.9240	7.6972	1.8568	-7.5919	0.2268	0.6057
4	4	5	0.6030	0.7168	0.7252	0.0611	-0.1138	5.8776
6	4	5	2.3580	2.4303	0.2912	-2.4505	-0.0723	1.3713
8	4	5	3.9040	3.8719	3.3132	-2.1164	0.0321	1.1645
10	4	5	2.1280	2.3407	-1.3814	-1.9341	-0.2127	1.9938
12	4	5	3.2100	3.0465	1.5879	-2.6548	0.1635	1.4040
14	4	5	1.4130	1.1720	0.0648	-1.1883	0.2410	1.9512
16	4	5	1.5750	1.4022	0.4210	-1.3602	0.1728	1.6628
1	5	5	7.0860	6.7191	6.8213	-0.1300	0.3669	0.6822
3	5	5	1.2560	1.1626	0.4562	-1.0888	0.0934	3.5285
5	5	5	9.4160	9.3555	8.7979	3.5830	0.0605	0.6764
7	5	5	1.2820	1.5013	-1.4862	0.3389	-0.2193	3.4442
9	5	5	5.0260	5.0328	4.6300	2.1629	-0.0068	0.9591
11	5	5	4.5480	3.9018	3.8406	-0.9730	0.6462	1.1008
13	5	5	1.9990	2.2555	2.2831	-0.1803	-0.2565	2.0601
15	5	5	2.3510	2.2727	2.2844	0.3271	0.0783	1.6450
0	6	5	2.9770	2.9568	2.9275	-0.6661	0.0202	1.1901
2	6	5	1.9980	2.0099	-1.3579	-1.5236	-0.0119	1.9558
4	6	5	4.4370	4.4796	-4.5485	-0.0149	-0.0426	0.9998
6	6	5	4.4140	4.5694	-4.2354	-1.8941	-0.1554	1.0286
8	6	5	5.0180	4.6935	-4.5527	-1.4091	0.3245	0.9613
10	6	5	1.2870	0.7866	-0.7677	0.2206	0.5004	3.2912
12	6	5	2.0610	2.1270	1.9498	-0.9289	-0.0660	2.2445
14	6	5	1.2960	1.0080	-1.0235	-0.0026	0.2880	2.1364
16	6	5	0.7030	0.9590	-0.3446	-0.9107	-0.2560	2.5268
1	7	5	5.6670	5.7207	4.1729	-4.0409	-0.0537	0.8493
3	7	5	3.1130	3.0577	3.0675	-0.4800	0.0553	1.2784
5	7	5	5.3520	5.0487	4.3961	-2.6371	0.3033	0.8879
7	7	5	4.2900	4.0914	3.8286	1.6126	0.1986	0.9780
9	7	5	2.6750	2.5054	2.0464	-1.5113	0.1696	1.4991
11	7	5	3.6940	3.6775	3.2180	-1.8941	0.0165	1.1465
13	7	5	2.0660	2.0752	1.4108	-1.5652	-0.0092	1.8156
0	8	5	2.0420	2.2481	-1.8382	1.3535	-0.2061	2.0133
2	8	5	0.8510	1.0112	-0.0039	1.0268	-0.1602	4.3192
4	8	5	1.9850	2.1003	-1.8118	-1.1249	-0.1153	2.0975
6	8	5	1.9820	1.9258	-0.8034	-1.7828	0.0562	2.1387
8	8	5	1.3610	1.5022	-1.1366	-1.0172	-0.1412	2.9109

10	8	5	1.1350	1.2173	-0.9233	0.8217	=0.0823	3.0392
12	8	5	1.0410	0.8140	-0.1688	0.8091	0.2270	3.3334
1	9	5	0.6110	0.6890	0.2099	-0.6674	-0.0780	6.3134
3	9	5	0.7500	0.8980	0.9114	0.0290	-0.1480	5.4245
5	9	5	2.0820	2.4161	2.0175	-1.3959	-0.3341	2.1061
7	9	5	0.3440	0.9979	0.9716	-0.2877	-0.6539	10.5380
9	9	5	1.5240	1.6152	1.5317	-0.5862	=0.0912	2.4615
11	9	5	0.4620	0.4364	-0.4209	0.1385	0.0256	8.5233
0	10	5	4.5180	4.8341	-4.8996	-0.2964	-0.3161	1.1619
2	10	5	2.7420	2.8999	-2.8357	-0.7930	-0.1579	1.4171
4	10	5	1.5400	1.6279	-1.4816	-0.7331	-0.0879	2.5550
6	10	5	1.5810	1.3776	-1.3525	-0.3569	0.2034	2.4580
8	10	5	0.8780	1.1167	-0.6126	-0.9542	-0.2387	4.5900
1	11	5	1.3610	1.6679	-0.7300	1.5282	-0.3069	3.0200
3	11	5	1.7430	1.5873	-0.6461	1.4765	0.1557	2.3245
5	11	5	1.2830	1.1757	-1.1581	0.2900	0.1073	3.0842
0	0	6	6.3750	6.3122	-4.6155	4.4472	0.0628	0.5550
2	0	6	11.8910	11.4004	11.5759	0.0397	0.4906	0.4654
4	0	6	12.7960	12.3092	-12.4732	-0.7987	0.4868	0.4814
6	0	6	7.9050	8.0652	-7.9610	1.9203	-0.1602	0.6241
8	0	6	3.2810	3.7496	3.0867	-2.2289	-0.4686	1.1117
10	0	6	6.2960	6.1967	-5.8337	2.3575	0.0993	0.7741
12	0	6	5.3140	5.8122	5.7271	1.4249	-0.4982	0.9743
14	0	6	2.2750	2.1057	1.7185	1.2721	0.1693	1.9135
16	0	6	0.9670	0.6432	-0.6053	0.2454	0.3238	4.1345
18	0	6	2.6490	2.7709	-2.7866	-0.3889	-0.1219	1.5830
1	1	6	6.9550	6.8578	-6.9299	0.6820	0.0972	0.5738
3	1	6	3.7060	3.3228	-3.2714	0.8257	0.3832	0.8827
5	1	6	4.6250	4.3357	-3.8209	2.1868	0.2893	0.7716
7	1	6	6.4740	6.5301	-6.3762	1.8190	-0.0561	0.7128
9	1	6	3.3090	3.0945	-2.8617	1.2975	0.2145	1.3128
11	1	6	3.1170	2.9426	-2.9764	0.2617	0.1744	1.4825
13	1	6	3.4990	3.4671	-3.4272	0.8049	0.0319	1.3675
15	1	6	1.0080	1.0791	-1.0955	-0.0243	-0.0711	4.1331
17	1	6	3.3160	3.5179	-3.3067	1.3512	-0.2019	1.3499
0	2	6	4.7390	4.9682	2.3131	-4.4832	-0.2292	0.6839
2	2	6	7.2200	6.7613	1.5851	-6.6799	0.4587	0.5725
4	2	6	5.5010	5.3582	2.2346	-4.9607	0.1428	0.7304
6	2	6	7.1360	6.9595	0.8707	-7.0128	0.1765	0.6984
8	2	6	4.2560	4.1707	1.9490	-3.7598	0.0853	0.9921
10	2	6	4.7820	4.3132	0.9774	-4.2692	0.4688	0.9547
12	2	6	2.3790	2.0127	1.3778	-1.5094	0.3663	1.7897
14	2	6	2.8620	3.0081	1.2140	-2.8028	-0.1461	1.5144
16	2	6	1.9130	1.7017	0.6104	-1.6165	0.2113	2.1988
18	2	6	0.9110	1.2010	0.6568	-1.0276	-0.2900	3.9210
1	3	6	3.1900	3.0997	-1.9845	-2.4430	0.0903	1.1389
3	3	6	7.9230	7.9025	-6.6574	-4.4796	0.0205	0.5723
5	3	6	4.2360	4.1567	4.1810	-0.5775	0.0793	0.9713
7	3	6	8.1110	7.7266	-5.5466	-5.5487	0.3844	0.6575
9	3	6	0.6290	0.6644	-0.3724	0.5625	-0.0354	5.8598
11	3	6	3.1970	3.1895	-1.2713	-2.9786	0.0075	1.3358
13	3	6	2.5770	2.3091	-2.3439	-0.0571	0.2679	1.7199
15	3	6	1.2810	1.3073	-0.8814	-0.9925	-0.0263	3.1529
17	3	6	0.0000	0.5972	-0.1655	-0.5834	-0.5972	0.0000

0	4	6	1.1780	0.2533	0.1789	0.1848	0.9247	3.0803
2	4	6	3.5590	3.8422	3.8612	0.5579	-0.2832	1.1400
4	4	6	6.4290	6.0366	5.6721	2.3234	0.3924	0.6898
6	4	6	10.6860	10.5624	10.6221	1.4818	0.1236	0.5779
8	4	6	8.7010	8.4940	8.4215	1.8614	0.2070	0.6675
10	4	6	0.4050	0.7872	0.7869	0.1401	-0.3822	10.9519
12	4	6	2.6620	2.6529	2.6474	-0.4977	0.0091	1.7229
14	4	6	0.7430	1.2182	-0.9903	0.7412	-0.4752	5.6151
1	5	6	3.8560	3.6723	2.6000	2.6728	0.1837	0.9904
3	5	6	3.2030	3.2951	-2.4756	2.2508	-0.0921	1.1919
5	5	6	2.3920	2.3322	2.0563	1.1745	0.0598	1.6735
7	5	6	2.0590	1.6947	-0.7904	1.5286	0.3643	1.8604
9	5	6	1.2450	1.4728	-0.2457	1.4752	-0.2278	3.3805
11	5	6	2.8220	3.0163	2.1362	2.1948	-0.1943	1.5203
13	5	6	1.0380	0.6541	0.0353	0.6632	0.3839	3.6138
15	5	6	2.0410	2.5250	1.1690	2.3819	-0.4840	1.9376
0	6	6	5.8630	5.8222	-1.5674	-5.7003	0.0408	0.7701
2	6	6	4.1520	3.9491	0.0012	4.0099	0.2029	1.0222
4	6	6	1.6640	1.2286	0.5325	-1.1282	0.4354	2.3588
6	6	6	2.1510	2.2093	0.2879	2.2248	-0.0583	1.9002
8	6	6	1.9580	1.9729	-0.6409	1.8980	-0.0149	2.1152
10	6	6	1.4120	1.0830	0.5567	-0.9484	0.3290	2.8191
12	6	6	0.4500	0.3713	-0.3495	0.1413	0.0787	9.5007
14	6	6	0.3420	0.8131	-0.3563	-0.7448	-0.4711	10.6619
1	7	6	2.3320	2.4583	-0.8337	-2.3528	-0.1263	1.7490
3	7	6	2.9800	2.8378	-2.0510	-2.0240	0.1422	1.4000
5	7	6	4.6220	4.2534	-3.2472	-2.8475	0.3686	0.9564
7	7	6	3.6250	3.7050	-3.3416	-1.7281	-0.0800	1.2830
9	7	6	2.4260	2.5274	-1.2168	-2.2595	-0.1014	1.7157
11	7	6	2.0060	1.8007	-1.7002	-0.6727	0.2053	1.9968
13	7	6	1.5830	1.7161	-0.6720	-1.6077	-0.1331	2.3878
0	8	6	1.0240	0.6441	0.2108	-0.6192	0.3799	3.6592
2	8	6	1.5240	1.8371	1.5706	-1.0063	-0.3131	2.6374
4	8	6	2.2580	2.0881	-1.7070	-1.2576	0.1699	1.7972
6	8	6	4.8460	4.8546	-4.7880	-1.1720	-0.0086	0.9283
8	8	6	1.4290	1.3041	-0.8469	-1.0179	0.1249	2.7513
10	8	6	1.4410	1.1603	-1.0244	-0.5819	0.2807	2.8677
12	8	6	1.2420	0.9432	0.9277	-0.2377	0.2988	3.1388
1	9	6	2.6450	2.8646	-1.4274	2.5343	-0.2196	1.5010
3	9	6	1.8480	1.7536	-0.3876	1.7379	0.0944	2.3467
5	9	6	2.3470	2.3617	-0.2317	2.3868	-0.0147	1.6493
7	9	6	1.5540	1.7307	0.0147	1.7573	-0.1767	2.6266
9	9	6	1.1810	1.0940	0.0873	1.1074	0.0870	3.3096
0	10	6	2.9520	3.0453	1.6326	2.6261	-0.0933	1.4973
2	10	6	1.6080	1.8789	1.2382	1.4514	-0.2709	2.5690
4	10	6	1.3320	1.4038	1.2290	0.7221	-0.0718	3.0552
6	10	6	0.3810	0.8358	0.7544	0.3889	-0.4548	8.3198
8	10	6	0.8160	0.6807	0.6403	0.2602	0.1353	4.6220
1	11	6	0.2490	0.7524	0.6755	-0.3569	-0.5034	13.7160
3	11	6	1.2800	1.1182	1.1314	-0.0959	0.1618	3.0893
1	1	7	5.5490	5.1182	4.1613	3.1132	0.4308	0.7502
3	1	7	1.8130	2.0671	-2.0900	0.1934	-0.2541	1.9244
5	1	7	6.0460	5.8955	5.0766	3.1722	0.1505	0.7364
7	1	7	2.4200	1.9341	0.5095	-1.8966	0.4859	1.7388

9	1	7	3.1470	2.9378	1.8012	2.3779	0.2092	1.2094
11	1	7	2.3530	1.8185	0.7786	1.6743	0.5345	1.7733
13	1	7	1.8790	1.7699	0.9460	1.5280	0.1091	2.3120
15	1	7	1.8780	2.2706	0.7854	2.1676	-0.3926	2.1672
17	1	7	1.1800	1.3103	1.0922	-0.7597	-0.1303	3.3697
0	2	7	14.3260	14.9259	14.9059	2.7401	-0.5999	0.4699
2	2	7	8.9580	8.6038	8.2147	2.9732	0.3542	0.5859
4	2	7	5.7840	5.6345	4.9387	2.8883	0.1495	0.7324
6	2	7	2.9570	2.4108	2.4425	-0.1638	0.5462	1.4894
8	2	7	1.4420	1.1930	1.1650	0.3321	0.2490	3.0523
10	2	7	7.1950	6.9739	6.2712	3.2888	0.2211	0.8092
12	2	7	7.9710	7.9144	7.9597	1.1060	0.0566	0.7639
14	2	7	4.1650	4.1510	3.8524	1.7100	0.0140	1.1904
16	2	7	2.0390	1.8777	1.9062	0.0388	0.1613	1.9881
1	3	7	0.6820	0.8337	-0.1857	-0.8259	-0.1517	5.1034
3	3	7	3.6560	3.4160	-3.1915	1.3583	0.2400	1.0531
5	3	7	8.3540	8.4534	3.6366	-7.7751	-0.0994	0.6462
7	3	7	3.4670	3.2935	-0.8848	3.2251	0.1735	1.2124
9	3	7	2.7660	2.9324	0.2394	-2.9679	-0.1664	1.5849
11	3	7	0.9760	0.5879	0.1609	-0.5748	0.3881	2.6508
13	3	7	2.1520	1.6518	-1.6618	0.2274	0.5002	2.0296
15	3	7	0.0000	0.3148	0.2161	-0.2355	-0.3148	0.0000
17	3	7	1.3740	1.1642	1.1362	-0.3263	0.2098	3.2331
0	4	7	5.6090	5.8297	-0.3580	-5.9086	-0.2207	0.7705
2	4	7	2.9830	2.8254	1.5807	-2.3941	0.1576	1.2336
4	4	7	4.2280	4.0238	1.0662	-3.9442	0.2042	1.0835
6	4	7	3.9480	3.9182	-0.4159	-3.9568	0.0298	1.0719
8	4	7	4.4830	4.4059	0.3679	-4.4586	0.0771	1.0192
10	4	7	1.8390	1.6442	0.1869	-1.6590	0.1948	2.3616
12	4	7	2.8770	2.7223	1.1569	-2.5105	0.1547	1.5169
14	4	7	1.5000	1.4316	0.0456	-1.4529	0.0684	2.6379
16	4	7	1.6510	1.8010	0.1633	-1.8214	-0.1500	2.6304
1	5	7	2.2180	2.1588	-0.3466	2.1645	0.0592	1.8359
3	5	7	2.9830	2.8217	0.4250	2.8335	0.1613	1.3533
5	5	7	3.6840	3.7891	0.7227	3.7790	-0.1051	1.2009
7	5	7	4.3680	4.3587	0.9220	4.3287	0.0093	1.0695
9	5	7	2.5910	2.1349	1.1454	1.8405	0.4561	1.5520
11	5	7	2.6550	2.7559	-2.2876	1.6118	-0.1009	1.4548
13	5	7	0.9920	0.8324	-0.7729	0.3420	0.1596	3.7470
15	5	7	2.0000	1.8071	-0.1737	1.8267	0.1929	1.9192
0	6	7	4.9340	4.6576	-4.7291	0.0482	0.2764	0.9660
2	6	7	2.0590	2.2974	-0.9575	-2.1272	-0.2384	1.8400
4	6	7	2.4610	1.8969	1.7190	0.8688	0.5641	1.6480
6	6	7	1.4880	1.5321	1.4737	0.4984	-0.0441	2.6102
8	6	7	2.7950	2.5398	2.4551	-0.7896	0.2552	1.5805
10	6	7	2.0050	1.7810	-1.8006	0.1678	0.2240	2.0634
12	6	7	2.9620	3.1889	-3.1392	-0.7937	-0.2269	1.4065
14	6	7	0.9570	0.7300	-0.7177	-0.1854	0.2270	3.8603
1	7	7	1.3960	1.6522	-0.1204	1.6733	-0.2562	2.9825
3	7	7	2.6810	2.6986	-0.0011	2.7402	-0.0176	1.5758
5	7	7	3.4060	3.4340	-3.0611	1.6697	-0.0280	1.2162
7	7	7	4.4640	4.6456	-2.0729	4.2372	-0.1816	1.1137
9	7	7	1.2040	1.0784	-0.6520	0.8797	0.1256	3.2947
11	7	7	1.5500	1.6951	-1.0117	1.3925	-0.1451	2.6476

13	7	7	0.3990	0.9423	0.2036	0.9349	-0.5433	10.0661
0	8	7	1.1800	1.7285	1.0546	-1.4029	-0.5485	3.3603
2	8	7	3.7810	4.0158	1.5714	-3.7627	-0.2348	1.1219
4	8	7	1.8590	2.3298	1.6333	-1.7114	-0.4708	2.3181
6	8	7	2.0820	2.4479	2.1072	-1.3183	-0.3659	1.9947
8	8	7	2.3560	2.6228	1.2781	-2.3365	-0.2668	1.7385
10	8	7	1.3820	1.9016	1.2714	-1.4532	-0.5196	2.6583
12	8	7	1.5850	1.9479	0.6362	-1.8728	-0.3629	2.6890
1	9	7	1.6900	1.5644	1.4250	0.7019	0.1256	2.3081
3	9	7	0.6250	0.2368	0.1786	-0.1611	0.3882	6.3604
5	9	7	1.1590	1.2372	-0.9100	-0.8660	-0.0782	3.3103
7	9	7	0.5000	0.8885	-0.3642	-0.8254	-0.3885	9.2965
9	9	7	0.6590	0.7434	-0.6571	-0.3715	-0.0844	6.6662
0	10	7	4.4040	4.8876	4.9123	0.7066	-0.4836	1.0795
2	10	7	3.3970	3.6368	3.6414	-0.6138	-0.2398	1.3576
4	10	7	1.7110	2.1802	2.2137	0.0208	-0.4692	2.3142
6	10	7	2.3050	2.3918	2.3763	-0.5013	-0.0868	1.5999
0	0	8	6.9650	6.8592	6.9646	0.0533	0.1058	0.6340
2	0	8	6.2820	6.3804	5.9037	2.6682	-0.0984	0.7056
4	0	8	8.8620	8.7030	8.4720	2.5136	0.1590	0.6363
6	0	8	11.1410	10.9932	10.4728	3.8626	0.1478	0.5670
8	0	8	9.4970	9.7886	9.8993	0.8910	-0.2916	0.6601
10	0	8	3.4310	3.3503	2.0406	2.7219	0.0807	1.3134
12	0	8	4.2590	4.0316	4.0814	-0.3175	0.2274	1.1652
14	0	8	1.6940	1.4580	0.2792	1.4539	0.2360	2.5217
16	0	8	4.0200	3.9641	3.8382	1.2125	0.0559	1.2775
1	1	8	9.4630	9.0532	4.9286	-7.7597	0.4098	0.5789
3	1	8	2.8710	2.9068	-0.3650	-2.9289	-0.0358	1.3552
5	1	8	9.0860	9.0630	6.3143	-6.6946	0.0230	0.6195
7	1	8	3.4840	3.0291	-2.6696	1.5277	0.4549	1.2031
9	1	8	5.5860	5.4334	3.7631	-4.0345	0.1526	0.9320
11	1	8	5.4000	5.5083	2.5686	-4.9684	-0.1083	0.9084
13	1	8	3.6010	3.8745	1.8766	-3.4578	-0.2735	1.3929
15	1	8	2.6120	2.2870	1.0486	-2.0720	0.3250	1.7255
17	1	8	1.2490	1.2059	0.9093	-0.8200	0.0431	3.4761
0	2	8	3.0890	2.8519	-1.7298	2.3224	0.2371	1.3023
2	2	8	2.3310	2.0954	-2.1021	-0.3287	0.2356	1.2576
4	2	8	4.3970	4.3158	-1.8693	3.9635	0.0812	1.0230
6	2	8	1.5630	1.5459	-0.7554	1.3760	0.0171	2.6190
8	2	8	1.8690	1.9624	-1.7025	-1.0355	-0.0934	2.2643
10	2	8	4.4760	4.3153	-1.4257	4.1433	0.1607	1.0754
12	2	8	1.2170	1.5504	-1.4808	0.5344	-0.3334	3.9077
14	2	8	1.9590	1.8773	-0.6885	1.7775	0.0817	2.4003
16	2	8	1.1950	1.2840	-0.8171	1.0160	-0.0890	3.3257
1	3	8	2.5250	2.1599	-2.0161	0.8635	0.3651	1.6832
3	3	8	0.7070	1.6129	-1.5095	-0.6352	-0.9059	5.0603
5	3	8	4.5360	4.3303	-1.9336	-3.9490	0.2057	0.9292
7	3	8	3.2950	3.4220	-2.6574	-2.2386	-0.1270	1.3061
9	3	8	1.5030	1.4624	-1.1985	-0.8766	0.0406	2.8710
11	3	8	1.9610	1.6841	-1.6963	0.2156	0.2769	2.5844
13	3	8	2.1640	2.3355	-1.7894	1.5563	-0.1715	2.2329
15	3	8	0.9710	0.6619	0.0825	-0.6670	0.3091	4.6557
0	4	8	6.2590	6.4458	-6.0897	2.3986	-0.1868	0.7952
2	4	8	3.9910	4.5015	4.5001	-0.8006	-0.5105	1.1388

4	4	8	5.5400	5.6327	-5.6848	-0.6288	-0.0927	0.8152
6	4	8	6.0440	5.8352	-5.9146	-0.3521	0.2088	0.7913
8	4	8	1.3210	0.3482	-0.2275	-0.2706	0.9728	3.2458
10	4	8	3.8180	3.6814	-3.7331	-0.1927	0.1366	1.3300
12	4	8	1.7730	1.6753	1.4089	0.9532	0.0977	2.2047
14	4	8	0.9850	0.6894	-0.6900	0.1179	0.2956	4.8200
16	4	8	1.6880	1.5826	-1.6063	-0.0440	0.1054	2.6013
1	5	8	1.5080	1.2509	1.2428	-0.2624	0.2571	2.8300
3	5	8	3.7790	3.6814	2.7290	-2.5546	0.0976	1.2278
5	5	8	4.8930	5.2668	4.1144	-3.4163	-0.3738	1.0251
7	5	8	4.6970	4.5129	2.9505	-3.5061	0.1841	1.0714
9	5	8	3.6860	3.7266	2.6922	-2.6590	-0.0406	1.3615
11	5	8	0.9210	0.4969	-0.4782	0.1609	0.4241	5.3516
13	5	8	0.0000	0.2115	0.1287	-0.1720	-0.2115	0.0000
15	5	8	1.4940	1.8215	1.1320	-1.4626	-0.3275	2.9327
0	6	8	2.6460	3.1718	0.1305	3.2180	-0.5258	1.7068
2	6	8	2.1080	1.7201	-0.2213	1.7325	0.3879	1.9219
4	6	8	2.2000	2.2099	0.0044	2.2439	-0.0099	2.0526
6	6	8	3.4740	3.3168	-0.8865	3.2491	0.1572	1.3463
8	6	8	1.4370	1.2891	-0.5094	1.2057	0.1479	3.3446
10	6	8	2.0720	1.8608	0.1242	1.8854	0.2112	2.3477
12	6	8	0.8650	1.2774	0.2913	1.2640	-0.4124	5.5043
14	6	8	0.5620	0.5753	0.1867	0.5535	-0.0133	7.3311
1	7	8	2.3840	2.6610	-0.8898	-2.5512	-0.2770	1.8788
3	7	8	1.6830	1.9591	-1.8299	-0.7804	-0.2761	2.7728
5	7	8	1.6480	1.4871	1.2333	0.8711	0.1609	2.7962
7	7	8	0.0000	0.7200	0.5840	0.4398	-0.7200	0.0000
9	7	8	0.8680	0.7950	-0.6142	-0.5238	0.0730	5.3574
11	7	8	0.5250	0.9915	0.2813	-0.9666	-0.4665	7.8642
13	7	8	1.8850	1.8215	-1.1912	-1.4148	0.0635	2.3363
0	8	8	1.0450	0.8878	-0.1893	0.8813	0.1572	3.6662
2	8	8	2.0430	1.4396	1.2551	0.7493	0.6034	1.9656
4	8	8	1.4110	1.5333	0.9403	1.2408	-0.1223	3.0886
6	8	8	3.1690	2.9147	2.8206	0.8964	0.2543	1.5499
8	8	8	1.9310	1.8352	1.1759	1.4456	0.0958	2.1617
10	8	8	1.0950	0.5009	0.3928	0.3230	0.5941	3.6235
1	9	8	2.2980	2.2942	2.2101	-0.7362	0.0038	1.7578
3	9	8	1.1970	1.0836	0.6672	0.8749	0.1134	3.3602
5	9	8	1.0270	1.1760	0.0154	1.1940	-0.1490	4.0441
7	9	8	1.0000	1.1018	0.2432	1.0920	-0.1018	4.4180
9	9	8	0.6360	0.9545	0.1303	0.9604	-0.3185	6.5943
0	10	8	1.0350	0.4016	0.3226	-0.2495	0.6334	4.5711
2	10	8	1.4490	0.7775	-0.1427	-0.7765	0.6715	3.1377
4	10	8	1.0460	0.8567	0.6567	-0.5704	0.1893	3.9467
1	1	9	4.1600	3.7124	0.6633	-3.7107	0.4476	0.9880
3	1	9	4.3460	4.4038	2.8767	-3.4234	-0.0578	0.9784
5	1	9	5.4510	5.4201	-4.8935	2.5185	0.0309	0.9061
7	1	9	3.6350	3.7124	3.7578	-0.2963	-0.0774	1.0351
9	1	9	1.5170	1.3103	-1.2429	-0.4746	0.2067	2.4521
11	1	9	2.8030	2.7434	0.3782	-2.7599	0.0596	1.5516
13	1	9	2.3600	1.9666	0.3816	-1.9601	0.3934	1.7202
15	1	9	0.9920	0.9013	0.4080	-0.8192	0.0907	4.9529
0	2	9	7.5750	7.7581	-7.3916	2.7237	-0.1831	0.6498
2	2	9	3.4140	3.1791	3.0047	-1.1800	0.2349	1.2484

4	2	9	2.5650	1.7477	-1.1944	1.3125	0.8173	1.6505
6	2	9	1.1980	1.1470	0.0404	1.1639	0.0510	3.2548
8	2	9	0.5280	0.5634	0.5664	-0.0806	-0.0354	8.1243
10	2	9	1.3680	1.3370	-1.1220	0.7644	0.0310	3.5129
12	2	9	1.3870	1.0153	-1.0308	0.0146	0.3717	3.6595
14	2	9	0.9970	0.5491	-0.5514	0.0821	0.4479	4.6524
16	2	9	1.0450	0.5856	-0.5849	0.1071	0.4594	4.2988
1	3	9	2.4700	2.0996	-1.4470	-1.5657	0.3704	1.6268
3	3	9	3.5690	3.7910	-3.1964	2.1450	-0.2220	1.1460
5	3	9	4.4340	4.5316	-4.4159	1.2931	-0.0976	0.9421
7	3	9	6.1770	6.2135	-3.9218	4.9422	-0.0365	0.8578
9	3	9	2.4440	2.3532	-2.2931	-0.6717	0.0908	1.8504
11	3	9	1.9590	1.5985	-1.5942	-0.3047	0.3605	2.2613
13	3	9	2.0410	1.6947	-1.3533	-1.0628	0.3463	2.1222
15	3	9	1.1660	1.6645	-0.6301	-1.5683	-0.4985	3.5700
0	4	9	6.6520	6.5944	-1.9401	6.4087	0.0576	0.8261
2	4	9	4.3920	4.3691	-2.3113	3.7866	0.0229	0.9308
4	4	9	3.8820	4.0738	0.3009	4.1256	-0.1918	1.2754
6	4	9	3.7390	3.4467	-1.5954	3.1149	0.2923	1.3477
8	4	9	2.3080	2.2932	-1.2859	1.9412	0.0148	2.0905
10	4	9	3.5170	3.2687	-0.8136	3.2177	0.2483	1.3404
12	4	9	2.6360	2.5196	-0.8391	2.4168	0.1164	1.6740
14	4	9	1.7580	1.5473	-0.8802	1.3014	0.2107	2.4303
1	5	9	2.5300	2.6103	2.5999	0.5151	-0.0803	1.8547
3	5	9	2.1540	1.9704	0.8466	-1.8127	0.1836	2.1789
5	5	9	2.9410	2.9535	0.5976	-2.9388	-0.0125	1.6078
7	5	9	3.7380	4.1500	2.5690	-3.3402	-0.4120	1.3513
9	5	9	1.5960	1.7456	0.2121	-1.7598	-0.1496	2.9757
11	5	9	1.8770	1.4645	1.4803	0.1414	0.4125	2.5310
13	5	9	1.2140	1.1474	1.1651	-0.0084	0.0666	3.7305
0	6	9	7.2630	7.1916	6.9724	2.1703	0.0714	0.7491
2	6	9	4.4760	4.9043	4.9156	0.7969	-0.4283	1.1447
4	6	9	5.3660	5.4598	5.2616	1.7464	-0.0938	1.0044
6	6	9	5.3620	5.6382	5.7096	0.4195	-0.2762	0.9072
8	6	9	2.8300	3.0658	2.8922	1.1515	-0.2358	1.5122
10	6	9	4.5150	4.6291	4.5437	1.2036	-0.1141	1.1473
12	6	9	3.4310	3.6582	3.7048	0.2683	-0.2272	1.3945
1	7	9	2.1840	1.8466	-1.1347	1.4927	0.3374	2.4520
3	7	9	1.4810	1.4276	-0.2880	1.4206	0.0534	3.3735
5	7	9	2.8020	2.3654	1.1539	-2.1065	0.4366	1.7644
7	7	9	2.0490	1.8784	1.5976	-1.0418	0.1706	2.3666
9	7	9	1.1900	0.6932	-0.7039	-0.0055	0.4968	3.6800
11	7	9	0.5310	0.2999	0.2093	0.2212	0.2311	8.0174
0	8	9	1.4150	1.5021	0.9256	1.2123	-0.0871	3.5813
2	8	9	1.6280	1.7599	-0.4821	1.7208	-0.1319	3.2223
4	8	9	3.1280	2.9755	0.0391	3.0210	0.1525	1.7644
6	8	9	2.2580	2.2563	-0.4099	2.2541	0.0017	2.3907
8	8	9	2.7790	2.6033	-0.6463	2.5632	0.1757	1.7535
10	8	9	0.6310	1.2734	0.5039	1.1907	-0.6424	6.7803
1	9	9	3.7160	3.9502	-3.8782	-1.0239	-0.2342	1.3736
3	9	9	1.6580	1.9203	-1.9405	0.1901	-0.2623	2.8528
5	9	9	2.9610	3.1457	-3.1132	0.7147	-0.1847	1.7573
7	9	9	1.5620	1.7568	-1.5772	0.8335	-0.1948	2.7810
0	10	9	1.0710	0.7524	-0.2568	0.7195	0.3186	4.1749

2	10	9	1.5540	1.3593	-1.3036	0.4536	0.1947	2.9111
0	0	10	7.5530	7.8995	-8.0063	-0.4866	-0.3465	0.6499
2	0	10	2.8410	2.5072	-0.0592	-2.5451	0.3338	1.5237
4	0	10	3.3810	2.9959	-3.0416	0.0505	0.3851	1.2785
6	0	10	2.7760	2.4672	-2.4181	-0.6550	0.3088	1.5379
8	0	10	2.9000	2.8919	-2.3154	-1.8060	0.0081	1.4395
10	0	10	3.3160	2.9895	-3.0037	-0.4385	0.3265	1.4651
12	0	10	3.0470	2.7604	-2.5731	-1.1115	0.2866	1.4905
14	0	10	2.3870	3.2376	-2.9239	-1.5026	-0.8506	1.7295
1	1	10	3.0980	2.8776	-0.3036	2.9061	0.2204	1.2909
3	1	10	3.0800	2.7784	2.4801	1.3445	0.3016	1.4419
5	1	10	3.9790	3.9946	-0.2488	-4.0485	-0.0156	1.1779
7	1	10	2.7940	3.0869	2.9204	1.1384	-0.2929	1.4126
9	1	10	1.5230	1.3865	0.4812	-1.3231	0.1365	2.6297
11	1	10	2.2900	1.7176	-1.0234	1.4123	0.5724	2.1805
13	1	10	2.3020	2.6120	-0.3683	2.6266	-0.3100	2.1106
15	1	10	0.5630	0.6004	0.3342	-0.5099	-0.0374	7.9900
0	2	10	3.8630	3.9966	0.4714	4.0306	-0.1336	1.1671
2	2	10	2.9130	2.8176	-0.8508	-2.7315	0.0954	1.5690
4	2	10	3.7400	3.7874	-0.3528	3.8295	-0.0474	1.2361
6	2	10	2.3740	2.0646	-0.1084	2.0936	0.3094	1.9018
8	2	10	2.0800	2.2043	-0.9708	-2.0167	-0.1243	1.9640
10	2	10	2.9230	3.1063	-0.0850	3.1529	-0.1833	1.3855
12	2	10	1.8460	1.4824	-0.2394	-1.4861	0.3636	2.6427
14	2	10	0.0000	0.4797	-0.0258	0.4864	-0.4797	0.0000
1	3	10	6.2320	6.5321	6.4871	1.3815	-0.3001	0.8534
3	3	10	5.9080	5.9964	3.6596	4.8661	-0.0884	0.8500
5	3	10	6.4000	6.2935	5.6183	3.0451	0.1065	0.8445
7	3	10	7.1990	7.3599	3.7558	6.4608	-0.1609	0.8215
9	3	10	4.2040	4.4755	4.0670	2.0277	-0.2715	1.1692
11	3	10	4.1420	3.9977	3.9494	0.9370	0.1443	1.1764
13	3	10	2.8250	2.9705	2.9663	0.5465	-0.1455	1.6331
15	3	10	2.3270	2.2195	2.1270	0.7448	0.1075	2.0295
0	4	10	2.5060	2.6244	1.4509	-2.2352	-0.1184	1.5360
2	4	10	1.9140	1.9411	0.7671	-1.8156	-0.0271	2.3065
4	4	10	1.9810	2.4740	-0.4829	-2.4653	-0.4930	2.0719
6	4	10	2.5870	2.5933	0.2358	-2.6226	-0.0063	1.5480
8	4	10	1.5010	1.7634	-1.1296	-1.3893	-0.2624	2.4115
10	4	10	1.9970	1.3891	0.3223	-1.3731	0.6079	2.1236
12	4	10	1.7160	2.0634	1.6187	-1.3302	-0.3474	2.2882
14	4	10	0.8780	1.0069	-0.8667	-0.5424	-0.1289	5.2472
1	5	10	4.0070	3.9891	3.3351	-2.2986	0.0179	1.1766
3	5	10	1.3110	1.8378	1.1920	1.4358	-0.5268	2.9060
5	5	10	2.0420	1.7937	1.7326	0.5613	0.2483	2.0174
7	5	10	1.5710	1.7670	0.1017	1.7913	-0.1960	2.7438
9	5	10	1.3200	1.3841	1.0699	0.9114	-0.0641	3.8862
11	5	10	2.8490	2.9764	2.4622	-1.7526	-0.1274	1.6940
13	5	10	1.5360	1.1592	1.0114	-0.6020	0.3768	3.0093
0	6	10	2.2980	2.1303	-0.4212	2.1217	0.1677	1.7792
2	6	10	1.6820	1.3304	-0.9621	-0.9482	0.3516	2.4608
4	6	10	1.0170	0.3709	-0.0406	-0.3744	0.6461	4.8613
6	6	10	2.0630	1.9986	-0.2953	-2.0078	0.0644	2.0013
8	6	10	1.4590	1.3816	0.0656	-1.4014	0.0774	3.1910
10	6	10	1.3860	0.8991	-0.5963	0.6913	0.4869	3.2294

12	6	10	1.0850	0.9987	-0.7537	-0.6784	0.0863	4.2758
1	7	10	2.4320	2.6900	-1.3565	2.3708	-0.2580	1.8315
3	7	10	2.0880	2.0797	-0.8650	1.9265	0.0083	2.2032
5	7	10	1.3060	1.2427	-1.2291	0.2857	0.0633	3.6831
7	7	10	1.7290	1.5960	-1.6147	0.1368	0.1330	2.8433
9	7	10	0.9330	1.1466	-0.0120	1.1642	-0.2136	4.7198
11	7	10	1.6040	1.9652	-1.4886	1.3289	-0.3612	2.5397
0	8	10	3.0640	3.0167	-3.0549	0.2251	0.0473	1.6146
2	8	10	2.5090	2.5457	-2.5101	0.6173	-0.0367	1.9347
4	8	10	0.9420	0.8466	-0.8586	-0.0420	0.0954	4.9656
6	8	10	1.5740	1.7742	-1.6231	0.7816	-0.2002	2.7401
8	8	10	0.2620	0.3613	-0.1234	0.3455	-0.0993	15.8909
1	9	10	2.0830	2.1366	-2.1603	0.1996	-0.0536	2.0727
3	9	10	1.1860	1.2668	-0.9896	-0.8217	-0.0808	3.8349
5	9	10	1.5940	1.5766	-1.0261	-1.2288	0.0174	2.8858
1	1	11	0.0000	0.1827	-0.1699	0.0745	-0.1827	3.4367
3	1	11	0.6970	0.5787	0.5667	0.1553	0.1183	6.5980
5	1	11	3.1470	3.3519	-0.1785	-3.3989	-0.2049	1.5772
7	1	11	2.3620	2.5245	2.2596	-1.2104	-0.1625	1.9671
9	1	11	0.9930	1.4723	-0.3593	-1.4512	-0.4793	4.8442
11	1	11	0.7580	0.6101	0.5742	0.2327	0.1479	6.5196
13	1	11	0.7260	0.4352	0.4266	0.1153	0.2908	4.3358
0	2	11	3.5110	3.8364	-1.5736	-3.5634	-0.3254	1.3713
2	2	11	3.4350	3.8438	-3.2562	-2.1519	-0.4088	1.4255
4	2	11	2.1350	2.5889	0.8549	-2.4859	-0.4539	2.1487
6	2	11	2.3460	1.6770	1.4686	-0.8619	0.6690	2.1431
8	2	11	1.2690	1.1162	-0.2680	-1.1013	0.1528	4.3044
10	2	11	1.9330	1.5873	0.0034	-1.6117	0.3457	2.8645
12	2	11	2.5220	2.7217	-0.9808	-2.5837	-0.1997	2.1712
14	2	11	1.0560	1.3837	-1.2532	-0.6354	-0.3277	4.5506
1	3	11	5.0270	5.0496	4.1621	2.9943	-0.0226	1.0023
3	3	11	3.5840	4.0207	1.7436	3.6915	-0.4367	1.3352
5	3	11	5.8470	5.9743	6.0054	0.8578	-0.1273	0.9551
7	3	11	2.5750	2.8173	2.8452	-0.2964	-0.2423	1.8479
9	3	11	3.4100	3.4948	2.9973	1.8997	-0.0848	1.3729
11	3	11	3.2040	3.0002	2.3090	1.9871	0.2038	1.5069
13	3	11	2.5410	2.4714	1.3996	2.0829	0.0696	1.7681
0	4	11	3.0170	3.4397	-0.4062	3.4689	-0.4227	1.4776
2	4	11	2.5460	2.6787	-2.1458	1.6715	-0.1327	1.8735
4	4	11	4.1440	4.1513	-0.4174	4.1945	-0.0073	1.1510
6	4	11	3.0880	3.7076	-2.0473	3.1593	-0.6196	1.5658
8	4	11	3.8410	3.8792	-1.1678	3.7618	-0.0382	1.2230
10	4	11	1.5630	1.7298	-0.2968	1.7312	-0.1668	3.2401
12	4	11	0.0000	0.9792	-0.9723	0.2077	-0.9792	39.4361
1	5	11	3.4030	3.2494	-2.5727	-2.0659	0.1536	1.5610
3	5	11	1.6890	1.5293	-0.9439	-1.2331	0.1597	2.9808
5	5	11	3.9300	4.0275	-4.0891	0.0609	-0.0975	1.2581
7	5	11	1.7260	1.2391	-0.9405	-0.8357	0.4869	3.0191
9	5	11	1.3000	1.3606	-1.3560	-0.2643	-0.0606	4.1059
11	5	11	2.3770	2.5023	-1.8205	-1.7723	-0.1253	2.0019
0	6	11	3.0670	3.2440	-3.2519	0.5244	-0.1770	1.7653
2	6	11	4.3700	4.0709	-4.1336	0.0198	0.2991	1.3478
4	6	11	4.1890	4.4825	-4.4179	-1.0947	-0.2935	1.2943
6	6	11	6.2690	6.5424	-6.6237	-0.5074	-0.2734	0.9701

8	6	11	3.8570	3.9369	-3.9680	-0.4846	-0.0799	1.5347
10	6	11	2.3730	2.6016	-2.6183	-0.3500	-0.2286	2.0306
1	7	11	1.4950	1.4471	-0.5438	-1.3651	0.0479	3.4362
3	7	11	1.4490	1.2963	-0.2550	-1.2913	0.1527	3.4910
5	7	11	1.4100	1.1706	-1.0859	0.4834	0.2394	3.4566
7	7	11	0.7390	0.5708	-0.5524	0.1756	0.1682	6.5593
9	7	11	1.6370	1.1670	-0.1027	-1.1805	0.4700	2.8621
0	8	11	1.9450	1.8710	-0.0499	1.8991	0.0740	2.5815
2	8	11	1.4860	2.0421	-0.8142	1.9070	-0.5561	3.3630
4	8	11	0.9110	0.3828	-0.1596	-0.3544	0.5282	4.6678
6	8	11	0.0000	0.1994	0.1942	0.0575	-0.1994	3.8575
1	9	11	2.4870	2.7094	2.1006	1.7766	-0.2224	1.9369
0	0	12	7.1300	7.2096	7.3100	-0.3944	-0.0796	0.7542
2	0	12	2.1920	1.3165	-0.0682	1.3351	0.8755	2.2051
4	0	12	3.2270	3.3253	3.1783	-1.1400	-0.0983	1.4824
6	0	12	1.5980	1.7756	0.1239	-1.7987	-0.1776	3.0417
8	0	12	2.0120	2.1662	-2.1101	-0.6208	-0.1542	2.2261
10	0	12	4.3320	4.4115	4.4361	0.6209	-0.0795	1.0712
12	0	12	2.5350	2.5494	2.5846	0.1448	-0.0144	1.9884
1	1	12	1.7860	1.8485	0.0388	1.8766	-0.0625	2.7258
3	1	12	3.8290	4.2306	-0.5312	4.2627	-0.4016	1.3018
5	1	12	2.0240	2.3478	-1.4855	1.8645	-0.3238	2.3339
7	1	12	3.7490	4.0437	0.8698	4.0127	-0.2947	1.4410
9	1	12	2.1170	1.7992	-0.6689	1.7000	0.3178	2.3927
11	1	12	1.2030	1.1884	-0.3713	1.1482	0.0146	3.6610
13	1	12	1.2720	1.2168	0.3816	1.1751	0.0552	3.4534
0	2	12	3.6810	4.1188	1.8890	3.7313	-0.4378	1.3276
2	2	12	2.6950	2.6449	1.0288	-2.4808	0.0501	1.6955
4	2	12	2.2800	2.5448	2.2081	1.3422	-0.2648	1.9864
6	2	12	1.9440	1.7998	1.3772	-1.2012	0.1442	2.4508
8	2	12	1.7510	1.6779	1.0045	-1.3761	0.0731	2.7668
10	2	12	2.1060	1.8069	1.5609	0.9643	0.2991	2.3690
12	2	12	1.7600	1.9174	0.6369	-1.8398	-0.1574	2.7053
1	3	12	3.3350	3.3375	-3.2162	1.0679	-0.0025	1.5734
3	3	12	1.3900	1.4975	-1.2593	0.8522	-0.1075	3.0822
5	3	12	3.4600	3.4489	-3.5006	0.0995	0.0111	1.4509
7	3	12	1.2630	1.0465	-0.9958	0.3709	0.2165	3.7179
9	3	12	2.1480	1.5287	-1.5161	0.3328	0.6193	2.3471
11	3	12	2.7050	2.6202	-2.6578	-0.1198	0.0848	1.6905
13	3	12	1.4420	1.3253	-0.9015	0.9992	0.1167	3.1974
0	4	12	3.1800	2.8243	-2.8671	0.0611	0.3557	1.6316
2	4	12	2.5140	2.4392	-2.4724	0.1459	0.0748	1.9635
4	4	12	1.1840	1.1221	0.6230	-0.9540	0.0619	3.5935
6	4	12	1.0630	1.8485	0.7230	1.7321	-0.7855	4.6592
8	4	12	0.0000	0.7301	0.1491	0.7262	-0.7301	0.0000
10	4	12	1.2560	0.6359	-0.6447	-0.0369	0.6201	3.9765
12	4	12	2.5200	2.6320	-2.6711	0.0886	-0.1120	1.6513
1	5	12	4.0720	4.3343	-4.2058	1.2965	-0.2623	1.2823
3	5	12	3.0700	3.2398	-3.0638	1.1980	-0.1698	1.5791
5	5	12	4.1030	4.2476	-4.3119	-0.0949	-0.1446	1.1921
7	5	12	3.1970	3.4259	-3.1890	1.3897	-0.2289	1.5125
9	5	12	2.4450	2.7007	-2.7089	-0.4267	-0.2557	1.8369
11	5	12	3.1290	3.2428	-2.5807	2.0451	-0.1138	1.6722
0	6	12	2.1430	2.4023	1.6787	-1.7698	-0.2593	2.1805

2	6	12	1.9890	2.4443	1.6457	-1.8578	-0.4553	2.7310
4	6	12	1.6360	1.1442	0.7197	-0.9120	0.4918	3.3840
6	6	12	1.6470	1.7599	1.4251	1.0781	-0.1129	2.5367
8	6	12	1.2240	1.6105	1.1158	-1.1955	-0.3865	4.1424
1	7	12	1.5230	1.5172	1.5210	0.2450	0.0058	3.0788
3	7	12	0.9160	1.0442	1.0595	0.0420	-0.1282	5.2173
5	7	12	0.6810	0.8181	0.8111	-0.1793	-0.1371	6.8701
7	7	12	0.8740	0.8741	0.8875	0.0143	-0.0001	5.2849
0	8	12	3.2810	3.5590	3.5402	-0.7258	-0.2780	1.6207
2	8	12	1.6900	1.6901	1.6867	-0.3161	-0.0001	2.8285
4	8	12	1.1950	1.0180	0.5718	-0.8611	0.1770	4.0130
1	1	13	4.4880	4.5835	-4.1360	2.1339	-0.0955	1.3000
3	1	13	3.2600	3.4995	-2.2339	2.7633	-0.2395	1.6359
5	1	13	4.0520	4.1086	-4.0503	1.0000	-0.0566	1.4997
7	1	13	3.2310	3.1928	-2.4588	2.1129	0.0382	1.7604
9	1	13	2.5850	2.7246	-2.4954	1.1944	-0.1396	2.0243
11	1	13	2.6970	2.6384	-2.3692	1.2507	0.0586	1.8584
0	2	13	2.3480	1.9590	-1.6856	1.0560	0.3890	2.1295
2	2	13	2.1020	2.2423	-2.2426	-0.3933	-0.1403	2.3766
4	2	13	4.5160	4.2112	-3.9377	-1.6671	0.3048	1.1702
6	2	13	5.3990	5.3458	-5.3527	-0.9015	0.0532	1.0899
8	2	13	3.2320	3.2502	-3.1506	-0.9826	-0.0182	1.7352
10	2	13	1.9920	1.9334	-1.9468	-0.2528	0.0586	2.6261
12	2	13	1.1120	1.4023	-1.2733	0.6372	-0.2903	4.0600
1	3	13	1.6660	1.7907	-1.5218	-0.9951	-0.1247	3.2458
3	3	13	1.7810	1.5707	-0.7497	-1.4077	0.2103	2.7568
5	3	13	0.6210	0.3345	-0.3131	0.1317	0.2865	8.8698
7	3	13	1.7160	1.4518	-0.4818	-1.3932	0.2642	3.0805
9	3	13	1.2290	1.0548	-0.3894	-0.9978	0.1742	4.0210
11	3	13	1.2870	1.2006	-1.0831	0.5595	0.0864	3.3965
0	4	13	2.6190	3.3626	-2.0889	-2.7008	-0.7436	1.8103
2	4	13	2.3990	2.8476	1.8042	-2.2594	-0.4486	2.1381
4	4	13	3.7610	4.4260	1.4178	-4.2647	-0.6650	1.4266
6	4	13	2.5150	2.9633	1.9522	-2.3162	-0.4683	2.0227
8	4	13	2.9610	3.1032	1.4164	-2.8147	-0.1422	1.8976
10	4	13	2.0300	2.2441	1.3022	-1.8699	-0.2141	2.3049
1	5	13	0.4800	0.5303	-0.3068	0.4426	-0.0503	9.7082
3	5	13	1.1320	1.5904	0.2182	1.6001	-0.4584	3.7522
5	5	13	1.1190	1.2544	0.1490	1.2649	-0.1354	4.4148
7	5	13	1.7820	1.9511	1.0582	1.6748	-0.1691	2.8253
9	5	13	0.7370	1.0528	-0.7121	0.7972	-0.3158	6.0444
0	6	13	1.7620	2.1673	-1.3967	-1.7006	-0.4053	3.0976
2	6	13	1.0100	1.4097	-1.3758	-0.3949	-0.3997	4.3232
4	6	13	0.0000	0.3560	0.0059	-0.3614	-0.3560	5.0675
6	6	13	1.7620	1.5754	1.5660	-0.3263	0.1866	2.9076
8	6	13	0.5610	0.3735	0.0749	0.3717	0.1875	7.3757
1	7	13	1.0100	0.7254	0.7135	0.1830	0.2846	4.5863
3	7	13	1.4160	0.3040	-0.3087	-0.0042	1.1120	3.1962
5	7	13	0.5370	1.1317	-0.2027	1.1311	-0.5947	8.4847
0	0	14	2.0300	1.8582	-1.8217	0.4913	0.1718	2.5235
2	0	14	5.5940	5.6446	-5.6987	0.6115	-0.0506	1.1670
4	0	14	0.8250	0.7152	-0.0966	0.7198	0.1098	6.8975
6	0	14	2.5010	2.2163	-1.3938	1.7668	0.2847	2.3567
8	0	14	2.2140	2.3464	-1.9934	1.3049	-0.1324	2.4045

10	0	14	1.6650	0.2166	-0.1953	0.1012	1.4484	3.2752
1	1	14	2.9000	2.7118	-2.2935	-1.5237	0.1882	1.9829
3	1	14	1.6790	1.7890	-1.5144	-1.0032	-0.1100	3.3146
5	1	14	3.8660	3.9886	-4.0500	0.0058	-0.1226	1.6581
7	1	14	1.4520	1.3891	-1.3202	-0.4964	0.0629	3.2759
9	1	14	1.8850	2.1635	-1.8570	-1.1736	-0.2785	2.3422
11	1	14	1.4230	1.5184	-1.5267	-0.2149	-0.0954	3.8043
0	2	14	1.5100	1.5052	-1.0497	1.1109	0.0048	3.4901
2	2	14	1.7780	1.4021	-0.6668	1.2579	0.3759	3.5015
4	2	14	1.0100	0.9670	-0.8074	0.5587	0.0430	5.9193
6	2	14	1.7210	1.5210	-0.4858	1.4660	0.2000	3.1188
8	2	14	0.7760	1.4511	-0.8487	1.2045	-0.6751	7.1900
10	2	14	1.1460	0.7090	-0.2087	0.6890	0.4370	4.2471
1	3	14	1.6020	1.8586	-0.1595	-1.8804	-0.2566	3.6494
3	3	14	2.2990	2.1883	0.5676	-2.1482	0.1107	2.3055
5	3	14	2.6680	3.0162	-0.8330	-2.9472	-0.3482	2.2411
7	3	14	2.5270	2.7973	1.2227	-2.5637	-0.2703	2.2354
9	3	14	2.2110	2.2894	-1.0108	-2.0934	-0.0784	2.3374
0	4	14	4.2220	4.4686	4.1246	1.9391	-0.2666	1.5473
2	4	14	2.4510	2.4281	0.9683	2.2674	0.0229	2.9077
4	4	14	1.9230	2.0384	1.2879	1.6202	-0.1154	2.9082
6	4	14	1.1250	1.4417	1.2998	0.6734	-0.3167	4.6782
8	4	14	1.7710	1.4713	-0.3458	1.4534	0.2997	3.1006
1	5	14	0.5000	0.7112	0.0025	-0.7221	-0.2112	11.0363
3	5	14	1.4070	1.1627	0.8136	-0.8555	0.2443	8.2366
5	5	14	2.2740	1.9333	1.5449	-1.2111	0.3407	2.6454
7	5	14	1.8480	2.1605	1.6082	-1.4921	-0.3125	2.6238
0	6	14	0.7140	0.5341	-0.1209	0.5287	0.1799	3.6177
2	6	14	1.5310	0.5447	-0.2356	0.5004	0.9863	2.8654
4	6	14	0.0000	0.6944	-0.1468	0.6896	-0.6944	0.0000
1	1	15	2.8470	3.0059	3.0135	-0.4842	-0.1589	2.1117
3	1	15	2.8310	2.7926	2.5208	1.2985	0.0384	2.0881
5	1	15	2.4300	2.2757	2.2910	0.3019	0.1543	2.3946
7	1	15	2.2330	2.4443	1.8604	1.6428	-0.2113	2.5822
9	1	15	0.8320	1.3915	1.3583	0.3890	-0.5595	6.0936
0	2	15	2.4500	2.9139	2.7915	0.9809	-0.4639	2.3622
2	2	15	3.3160	3.2102	2.8691	1.5470	0.1058	1.8128
4	2	15	2.7900	2.9707	2.5652	1.5871	-0.1807	2.0838
6	2	15	3.5740	3.9594	3.7975	1.3201	-0.3854	1.7836
8	2	15	2.1820	2.7469	2.3982	1.4240	-0.5649	2.5449
1	3	15	2.6640	2.7161	-0.1251	-2.7551	-0.0521	2.3471
3	3	15	2.1960	2.6228	-0.4931	-2.6171	-0.4268	2.8310
5	3	15	0.6700	1.4602	-1.2253	-0.8349	-0.7902	9.6358
7	3	15	2.1480	2.4630	-1.2997	-2.1367	-0.3150	2.7428
0	4	15	0.9190	1.7142	0.5446	-1.6532	-0.7952	23.0296
2	4	15	1.8920	1.7274	0.1535	-1.7473	0.1646	3.4434
4	4	15	1.6960	1.4627	0.4682	-1.4095	0.2333	3.4719
6	4	15	1.4240	1.7492	0.1825	-1.7668	-0.3252	3.7834
1	5	15	1.3780	0.8603	-0.8268	0.2819	0.5177	3.7505
3	5	15	0.5440	0.6374	-0.6065	-0.2258	-0.0934	8.8906
0	0	16	1.3670	1.5970	1.0498	-1.2359	-0.2300	3.2741
2	0	16	0.5880	1.2228	-0.6368	-1.0660	-0.6348	9.4815
4	0	16	1.6300	1.0556	-0.0308	-1.0714	0.5744	2.9585
6	0	16	0.0000	1.1400	0.4595	-1.0624	-1.1400	0.0000

1	1	16	1.5530	1.3774	1.3635	-0.3113	0.1756	3.6416
3	1	16	2.0300	2.5088	2.3345	-1.0195	-0.4788	2.9751
5	1	16	2.1400	2.0068	1.9820	-0.4731	0.1332	2.7739
0	2	16	1.7760	2.1430	-0.7874	-2.0286	-0.3670	3.3478
2	2	16	1.6100	1.0603	-1.0190	-0.3476	0.5497	3.6884
4	2	16	1.5670	1.5513	-0.9186	-1.2796	0.0157	3.7626
1	3	16	0.8090	0.6090	-0.1743	-0.5933	0.2000	7.1205
3	3	16	0.5370	0.4027	0.2091	-0.3514	0.1343	12.3644
0	4	16	1.5540	1.9044	-1.7513	-0.8201	-0.3504	4.1283

AGREEMENT FACTORS BASED ON PARAMETERS BEFORE CYCLE 1

SUM(W*(O-C)**2) IS 7.3457+001

SQRTF(SUM(W*(O-C)**2)/(NO-NV)) IS 0.2716

	NUMERATOR	DENOMINATOR	R
R FACTOR INCLUDING ZEROS	2.8195790+002	3.4241510+003	0.082
R FACTOR OMITTING ZEROS	2.7048548+002	3.4241510+003	0.079
WEIGHTED R FACTOR INCLUDING ZEROS	8.5706883+000	2.1757945+002	0.039
WEIGHTED R FACTOR OMITTING ZEROS	8.5688956+000	2.1757945+002	0.039

APPENDIX C

Bond Lengths

Bond	Apparent Distance, Å*	Distance Averaged over Thermal Motion, in Å*		Weighting Scheme**
		Second Atom Rides on First	Atoms Move Independently	
<u>URANYL BONDS</u>				
U-O ₅	1.770(7)	1.788(7)	1.817(7)	1
	1.769(6)	1.788(6)	1.816(6)	2
	1.764(7)	1.783(7)	1.811(7)	3
U-O ₆	1.749(7)	1.765(7)	1.794(7)	1
	1.743(6)	1.757(6)	1.785(6)	2
	1.742(7)	1.754(7)	1.783(7)	3
<u>OTHER U-O BONDS</u>				
U-O ₃	2.504(5)	2.513(5)	2.532(5)	1
	2.513(5)	2.522(5)	2.540(5)	2
	2.516(5)	2.525(5)	2.543(5)	3
U-O ₄	2.547(6)	2.556(6)	2.574(6)	1
	2.542(5)	2.551(5)	2.569(5)	2
	2.541(5)	2.550(5)	2.567(5)	3
U-O ₇	2.397(3)	2.413(3)	2.433(3)	1
	2.403(3)	2.419(3)	2.437(3)	2
	2.405(4)	2.421(4)	2.439(4)	3
<u>U-N DISTANCES</u>				
U-N ₁	2.951(6)	2.954(6)	2.970(6)	1
	2.954(4)	2.957(4)	2.972(4)	2
	2.953(5)	2.957(5)	2.972(5)	3
U-N ₂	2.984(6)	2.988(6)	3.004(6)	1
	2.979(4)	2.983(4)	2.998(4)	2
	2.975(6)	2.979(6)	2.994(6)	3
<u>DISTANCES IN NITRATE GROUPS</u>				
N ₁ -O ₁	1.207(8)	1.226(8)	1.278(8)	1
	1.210(6)	1.230(7)	1.281(6)	2
	1.219(8)	1.238(8)	1.291(8)	3
N ₁ -O ₃	1.271(4)	1.284(5)	1.329(4)	1
	1.268(4)	1.280(4)	1.325(4)	2
	1.268(5)	1.280(5)	1.326(5)	3
O ₁ -O ₃	2.176(7)	2.172(7)	2.219(7)	1
	2.172(6)	2.168(6)	2.216(6)	2
	2.178(7)	2.175(7)	2.223(7)	3
O ₃ -O ₃	2.139(8)	2.139(8)	2.181(8)	1
	2.140(7)	2.140(7)	2.181(7)	2
	2.142(9)	2.142(9)	2.184(9)	3
N ₂ -O ₂	1.231(7)	1.242(7)	1.300(7)	1
	1.231(6)	1.242(6)	1.299(6)	2
	1.227(7)	1.240(8)	1.296(8)	3
N ₂ -O ₄	1.260(4)	1.272(5)	1.324(4)	1
	1.257(4)	1.269(4)	1.320(4)	2
	1.255(5)	1.266(5)	1.318(5)	3

Bond	Apparent Distance, Å*	Distance Averaged over Thermal Motion, in Å*		Weighting Scheme**
		Second Atom Rides on First	Atoms Move Independently	
O ₄ -O ₂	2.181(7)	2.181(7)	2.224(7)	1
	2.178(6)	2.178(6)	2.221(6)	2
	2.171(7)	2.173(7)	2.215(7)	3
O ₄ -O ₄	2.133(8)	2.133(8)	2.177(8)	1
	2.127(6)	2.127(6)	2.171(6)	2
	2.126(8)	2.126(8)	2.170(8)	3
<u>WATER MOLECULES</u>				
O ₇ -H ₁	0.974(12)	0.975(12)	1.100(12)	1
	0.964(9)	0.968(9)	1.089(9)	2
	0.977(13)	0.980(13)	1.101(14)	3
O ₇ -H ₂	0.970(13)	0.982(13)	1.093(13)	1
	0.973(10)	0.982(10)	1.091(9)	2
	0.966(14)	0.975(14)	1.003(15)	3
O ₈ -H ₃	0.977(11)	1.008(12)	1.121(12)	1
	0.961(9)	0.989(10)	1.104(10)	2
	0.974(12)	1.003(13)	1.123(13)	3
O ₈ -H ₄	0.932(15)	0.957(16)	1.060(16)	1
	0.939(14)	0.958(14)	1.062(14)	2
	0.927(18)	0.944(20)	1.047(19)	3
O ₉ -H ₅	0.947(15)	1.022(17)	1.152(16)	1
	0.947(13)	1.009(14)	1.137(13)	2
	0.940(17)	1.008(18)	1.140(18)	3
O ₉ -H ₆	0.872(17)	0.924(18)	1.035(18)	1
	0.898(15)	0.933(16)	1.039(16)	2
	0.904(21)	0.939(22)	1.044(22)	3
<u>HYDROGEN BONDS</u>				
O ₇ -O ₉	2.705(9)	2.705(9)	2.750(9)	1
	2.704(7)	2.704(7)	2.746(7)	2
	2.701(9)	2.701(9)	2.744(9)	3
O ₉ -H ₁	1.737(11)	1.739(11)	1.805(11)	1
	1.744(9)	1.746(9)	1.813(9)	2
	1.728(12)	1.730(12)	1.800(12)	3
O ₇ -O ₈	2.692(9)	2.693(9)	2.731(9)	1
	2.683(7)	2.684(7)	2.722(7)	2
	2.679(10)	2.681(10)	2.719(10)	3
O ₈ -H ₂	1.736(11)	1.740(11)	1.803(11)	1
	1.720(9)	1.723(9)	1.785(9)	2
	1.724(13)	1.726(12)	1.790(12)	3
O ₈ -O ₂	2.918(6)	2.913(6)	2.952(6)	1
	2.921(5)	2.916(5)	2.954(5)	2
	2.926(6)	2.921(6)	2.961(6)	3
O ₂ -H ₃	1.942(9)	1.965(9)	2.007(9)	1
	1.961(8)	1.981(8)	2.024(8)	2
	1.954(10)	1.976(10)	2.021(10)	3
O ₈ -O ₉	2.760(10)	2.759(10)	2.795(10)	1
	2.760(9)	2.759(9)	2.795(9)	2
	2.754(11)	2.753(11)	2.789(11)	3
O ₉ -H ₄	1.852(12)	1.867(12)	1.918(11)	1
	1.840(11)	1.852(11)	1.904(11)	2
	1.845(15)	1.854(14)	1.907(14)	3

Bond	Apparent Distance, Å*	Distance Averaged over Thermal Motion, in Å*		Weighting Scheme**
		Second Atom Rides on First	Atoms Move Independently	
O ₉ -O ₁	2.997(7)	2.992(7)	3.031(7)	1
	2.990(6)	2.986(6)	3.025(6)	2
	2.985(8)	2.980(8)	3.020(8)	3
O ₁ -H ₅	2.179(14)	2.210(14)	2.251(13)	1
	2.170(14)	2.194(13)	2.237(13)	2
	2.187(17)	2.213(16)	2.256(16)	3
O ₈ -O ₉	2.701(9)	2.704(9)	2.735(9)	1
	2.709(8)	2.711(8)	2.744(9)	2
	2.717(11)	2.719(11)	2.752(11)	3
O ₈ -H ₆	1.849(13)	1.876(12)	1.922(12)	1
	1.832(12)	1.851(11)	1.899(11)	2
	1.837(16)	1.855(15)	1.904(14)	3
<u>CONTACTS</u>				
O ₅ -O ₆	3.214(9)	3.210(9)	3.245(9)	1
	3.227(7)	3.222(7)	3.258(7)	2
	3.236(9)	3.232(9)	3.267(9)	3
O ₇ -O ₃	2.653(7)	2.649(7)	2.691(7)	1
	2.663(6)	2.659(6)	2.699(6)	2
	2.660(7)	2.657(7)	2.697(7)	3
O ₇ -O ₄	2.645(7)	2.641(7)	2.686(7)	1
	2.649(5)	2.645(6)	2.688(5)	2
	2.653(7)	2.649(7)	2.692(7)	3
O ₇ -O ₈	3.867(9)	3.870(9)	3.887(9)	1
	3.861(8)	3.864(8)	3.880(8)	2
	3.848(9)	3.851(9)	3.867(9)	3
O ₇ -O ₉	3.580(10)	3.584(10)	3.602(10)	1
	3.583(8)	3.587(8)	3.605(8)	2
	3.594(10)	3.598(10)	3.616(10)	3

*Standard errors ($\times 10^3$) appear in parentheses.

**Statistical-scheme results also include effect of unit-cell errors.

APPENDIX D

Bond Angles

Weighting Scheme: 1. Statistical scheme; 2. $w = |F|$;
 3. $w = 1$, 2θ less than 80°

Angle	Deg.*	Weighting Scheme**
<u>URANYL ANGLE</u>		
O ₅ -U-O ₆	179.1(5)	1
	179.4(4)	2
	179.7(4)	3
<u>OTHER ANGLES ABOUT URANIUM</u>		
O ₆ -U-O ₇	92.2(2)	1
	92.2(2)	2
	92.1(2)	3
O ₆ -U-O ₃	89.4(3)	1
	89.1(2)	2
	89.0(3)	3
O ₆ -U-O ₄	87.7(3)	1
	88.3(2)	2
	88.5(3)	3
O ₆ -U-N ₁	88.7(3)	1
	88.4(2)	2
	88.3(3)	3
O ₆ -U-N ₂	87.4(3)	1
	87.9(2)	2
	88.1(3)	3
O ₆ -U-O ₁	87.6(3)	1
	87.3(2)	2
	87.2(3)	3
O ₆ -U-O ₂	87.6(3)	1
	88.0(2)	2
	88.1(3)	3
O ₅ -U-O ₃	91.5(3)	1
	91.4(2)	2
	91.3(3)	3
O ₅ -U-O ₄	91.5(3)	1
	91.2(2)	2
	91.2(3)	3

Angle	Deg.*	Weighting Scheme**
O ₅ -U-N ₁	92.2(3)	1
	92.2(2)	2
	92.1(3)	3
O ₅ -U-N ₂	91.6(3)	1
	91.6(2)	2
	91.6(3)	3
O ₅ -U-O ₁	93.3(3)	1
	93.2(2)	2
	93.1(3)	3
O ₅ -U-O ₂	91.5(3)	1
	91.5(2)	2
	91.5(3)	3
<u>WATER-MOLECULE ANGLES.</u>		
H ₁ -O ₇ -H ₂	106.9(5)	1
	108.6(5)	2
	108.7(7)	3
H ₃ -O ₈ -H ₄	106.8(9)	1
	105.2(8)	2
	105.1(10)	3
H ₅ -O ₉ -H ₆	114.6(12)	1
	114.5(12)	2
	112.5(14)	3
<u>HYDROGEN BOND ANGLES</u>		
O ₇ -H ₁ ...O ₉	172.8(9)	1
	173.1(9)	2
	173.3(10)	3
O ₇ -H ₂ ...O ₈	168.2(10)	1
	169.6(9)	2
	169.3(10)	3
O ₈ -H ₃ ...O ₂	177.4(10)	1
	176.0(10)	2
	175.2(11)	3
O ₈ -H ₄ ...O ₉	164.0(10)	1
	165.5(9)	2
	165.8(11)	3

Angle	Deg.*	Weighting Scheme**
O ₉ -H ₅ ...O ₁	144.0(13)	1
	144.3(14)	2
	142.0(15)	3
O ₉ -H ₆ ...O ₈	164.9(12)	1
	164.8(10)	2
	164.1(12)	3
<u>NITRATE GROUP ANGLES</u>		
O ₁ -N ₁ -O ₃	122.7(2)	1
	122.4(2)	2
	122.3(2)	3
O ₃ -N ₁ -O ₃	114.6(5)	1
	115.1(4)	2
	115.4(5)	3
O ₄ -N ₂ -O ₂	122.2(2)	1
	122.2(2)	2
	122.1(2)	3
O ₄ -N ₂ -O ₄	115.6(5)	1
	115.6(4)	2
	115.8(5)	3
<u>O-O-O ANGLES AROUND WATER OXYGENS</u>		
O ₉ -O ₇ -O ₈	112.5(2)	1
	112.6(2)	2
	112.7(2)	3
O ₇ -O ₈ -O ₂	109.7(3)	1
	109.8(2)	2
	109.5(3)	3
O ₇ -O ₈ -O ₉	92.2(3)	1
	92.2(2)	2
	92.0(3)	3
O ₇ -O ₈ -O ₉	134.4(3)	1
	134.7(3)	2
	135.1(3)	3
O ₉ -O ₈ -O ₂	103.0(3)	1
	102.9(2)	2
	102.6(3)	3

Angle	Deg.*	Weighting Scheme**
O ₉ -O ₈ -O ₂	109.8(3)	1
	109.7(2)	2
	109.8(3)	3
O ₉ -O ₈ -O ₉	100.2(2)	1
	100.0(2)	2
	100.0(3)	3
O ₁ -O ₉ -O ₈	140.4(2)	1
	140.3(2)	2
	140.0(3)	3
O ₁ -O ₉ -O ₈	80.5(2)	1
	80.7(2)	2
	80.9(3)	3
O ₇ -O ₉ -O ₁	101.2(3)	1
	101.3(2)	2
	101.6(3)	3
O ₈ -O ₉ -O ₇	96.9(3)	1
	97.1(3)	2
	97.5(3)	3
O ₈ -O ₉ -O ₇	117.8(2)	1
	117.8(2)	2
	117.8(3)	3
O ₈ -O ₉ -O ₈	100.0(2)	1
	99.8(2)	2
	99.7(3)	

*Standard errors ($\times 10$) are shown in parentheses.

**Statistical-scheme results also include effects of unit-scale errors.

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REFERENCES

1. Pauling, L., and Dickinson, R. G., J. Amer. Chem. Soc. 46, 1615 (1924).
2. Sasvari, K., Acta Geologica Acad. Sc. Hung. 4, No. 3, 467 (1957).
3. Gatehouse, B. M., and Comyns, A. E., J. Chem. Soc. 802, 3965 (1958).
4. Vdovenko, V. M., et al., Radiokhimiya 2, 24 (1960).
5. Allpress, J. G., and Hambly, A. N., Austral. J. Chem. 12, 569 (1959).
6. Fleming, J. E., and Lynton, H., Chem. and Ind. 79, 1416 (1960).
7. Mueller, M. H., Heaton, L., and Sidhu, S. S., Rev. Sci. Instr. 34, 74 (1963).
8. Makarov, E. S., and Melikyan, A. A., Proceedings of the Working Conference on Slow Neutron Physics, held Dec. 7-12, 1961. AEC-tr-5734 issued May 1963.
9. Mueller, M. H., and Heaton, L., Determination of Lattice Parameters with the Aid of a Computer, ANL-6176 (Jan 1961).
10. Sly, W. G., and Shoemaker, D. P., MIFRI: Two and Three-Dimensional Crystallographic Fourier Summation Program for the IBM-704 Computer, Dept. of Chemistry, Massachusetts Institute of Technology, Cambridge, Mass.
11. Penfold, B. R., Patterson Superposition Program, Harvard University, (Mar 1960).
12. Mueller, M. H., Clark, F. L., and Simonsen, S. H., Program for the Location of Fourier Peak Centers, ANL-6699 (July 1963).
13. Busing, W. R. and Levy, H. A., A Crystallographic Least-squares Refinement Program for the IBM-704, ORNL-59-4-37 (1959).
14. Busing, W. R., Martin, K. O., and Levy, H. A., A Fortran Crystallographic Least-squares Program, ORNL-TM-305 (1962).
15. Levy, H. A., Acta Cryst. 9, 679 (1956).
16. Evans, H. T., Acta Cryst. 14, 689 (1961).
17. Busing, W. R., Martin, K. O., and Levy, H. A., A Fortran Crystallographic Function and Error Program, ORNL-TM-306 (1964).
18. Barclay, G. A., Sabine, T. M., and Taylor, J. C., to be published.
19. Zachariasen, W. and Plettinger, H., Acta Cryst. 12, 526 (1959).
20. Sass, R. L., Vidale, R., and Donohue, J., Acta Cryst. 10, 567 (1957).
21. Hamilton, W. C., Acta Cryst. 10, 103 (1957).
22. Schomaker, V., Waser, J., Marsh, R. E., and Bergman, G., Acta Cryst. 12, 600 (1959).

23. Norment, N. G., NRL-5885 (Apr 1963).
24. Busing, W. R., and Levy, H. A., Acta Cryst. 17, 142 (1964).
25. Wells, A. F., Structural Inorganic Chemistry, 3rd ed., Oxford (1962), p. 577.
26. Smith, H. G., Peterson, S. W., and Levy, H. A., Abstract Amer. Cryst. Assoc. (1961).
27. Bacon, G. E., and Curry, N. A., Proc. Roy. Soc. (London), A 266, 95 (1962).
28. Garrett, B. S., ORNL-1745 (Aug 1954).
29. Rush, J. J., private communication. Material presented at Mid-America Symposium on Spectroscopy, Chicago, Illinois (June 1965).
30. Taylor, J. C., and Mueller, M. H., American Crystallographic Association Program and Abstracts, Paper H-12, p. 70 (July 1964).
31. Taylor, J. C., and Mueller, M. H., Acta Cryst., 19, 536 (1965).