lectures $\delta^+$ et $\delta^-$ relevées au galvanomètre fournissent par le rapport de leurs différence et somme (voir plus haut), pour le facteur de structure, une valeur d'autant plus proche de sa valeur unitaire *absolue* $|U(hk)|$ que l'on peut considérer comme ponctuelles les perforations circulaires qui ont servi à confectionner le modèle (leurs diamètres sont de l'ordre de 2 mm et leur identification à des points est valable dans une très large mesure).

Le procédé qui consiste à rechercher au déphaseur les extrémums de déviation s'appuie mathématiquement sur la méthode de la phase auxiliaire.

Sans apporter à ce travail un soin excessif on peut compter sur une précision de 5%, qui est au fond du même ordre que celle obtenue pour les valeurs expérimentales des facteurs de structure par diffraction des rayons X.

On a facilement soutenu le rythme de trois cycles d'essai-erreur par jour pour une structure non centrosymétrique comportant une soixantaine d'atomes (deux molécules) par maille. Il convient de noter cette particularité qu'*il n'y a jamais lieu, au cours du stade 'essai-erreur', de relever les valeurs numériques des coordonnées atomiques.*

## Présentation

Pour ne nécessiter que peu de modifications de fond en vue de son adaptation au calcul photométrique, le photosommateur n'en a pas moins dû, dans sa nouvelle version (Fig. 5), subir certaines consolidations et certains aménagements lui conférant de nouvelles souplesses de réglage (cadre porte-châssis centrable par vis micrométriques; possibilité d'ajuster le parallélisme du plan de grille par rapport à la fente). L'alimentation, devenue assez complexe, puisqu'elle nécessite alimentation générale stabilisée, rototransformateur, alimentation 2000 volts alternative pour la boîte porte-modèle, alimentation 2000 volts continue stabilisée pour le phototube, a été groupée en un meuble métallique distinct du photosommateur où le galvanomètre a également trouvé sa place.

Nous sommes avec reconnaissance redevables d'un secours technique précieux aux laboratoires d'électronique et de mécanique de l'Institut National de Recherche Chimique Appliquée ainsi qu'aux Établissements Beaudouin, à Paris.

## Référence

ELLER, G. VON (1955). *Bull. Soc. franç. Minér. Crist.* **78**, 157.

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*Acta Cryst.* (1965). **18**, 1004

# X-ray Crystal Analysis of the Substrates of Aconitase*

# V. Magnesium Citrate Decahydrate $[Mg(H_2O)_6][MgC_6H_5O_7(H_2O)]_2 . 2H_2O$†

BY CARROLL K. JOHNSON‡

*The Institute for Cancer Research, Philadelphia* 11, *Pennsylvania, U.S.A.*

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Magnesium citrate decahydrate crystallizes in the space group $P2_1/n$ with $a = 20{\cdot}222$, $b = 6{\cdot}686$, $c = 9{\cdot}135$ Å and $\beta = 96{\cdot}86°$. The unit cell contains two $[Mg(H_2O)_6]^{2+}$ ions and four units of $[MgC_6H_5O_7(H_2O)]^- . H_2O$. The structure was solved by multiple superposition. Least-squares refinement resulted in an $R$ value of 0·031 based on $F$ for the 2725 counter data. Each citrate chelates to one magnesium atom in a tridentate manner through one end carboxyl group, the central carboxyl group and the hydroxyl group oxygen, and bridges two other magnesium atoms with its remaining carboxyl group. This leads to an extended chelated strip with double bridging between magnesium atoms. Columns of hexaaquomagnesium ions are hydrogen bonded to the chelated strip.

## Introduction

Divalent metal ions such as magnesium, manganous, ferrous, cobaltous and zinc ions are known to be essential cofactors in many enzyme-catalyzed reactions. Several enzyme reactions involving citric acid as a substrate are dependent on certain of these divalent metals for activation. Aconitase, the enzyme involved in the citrate to isocitrate conversion, shows specific requirements for ferrous iron (Morrison, 1954). Other enzymes such as the citrate cleavage enzyme (Srere, 1961) and citratase* (Siva Raman, 1961) show less selective

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‡ Aided by a Postdoctoral Fellowship from the American Cancer Society. Present Address: Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

* These two enzymes are distinct from the condensing enzyme and from each other. They both cleave the citrate ion to form an oxaloacetate ion and an acetate ion. The acetate produced by the citrate cleavage enzyme system is in the form of acetyl coenzyme A.

metal requirements and are activated to various degrees by several of the metals mentioned above.

A mechanism suggested by Dagley & Dawes (1955) for the action mechanism of citratase requires that the citrate ion be chelated to the metal at the time of the enzymatic reaction. The present study was undertaken to clarify further the structural chemistry of the hydrated and chelated citrate ion.

## Experimental

Single crystals of several different hydrated citrates of divalent metals were grown and their cell dimensions* and space groups determined from precession photographs. One of four different magnesium citrate hydrates grown was selected for a detailed structural analysis. A magnesium salt was chosen because the relatively low atomic number of magnesium might permit the structure to be determined more accurately.

Solutions containing magnesium ion and citric acid in proportions expected to produce magnesium hydrogen citrate were layered under propanol at 90°. Crystals of magnesium citrate containing five molecules of water per citrate ion grew from this solution. Precession photographs indicated uniquely the symmetry elements of space group $P2_1/n$. The lattice constants were determined with a small crystal from the same crystallization crop as the crystal used for intensity data collection. Careful spectrometer measurements of 18 high-angle strong reflections yielded the following cell dimensions:

$$a=20{\cdot}222\,,\quad b=6{\cdot}686\,,\quad c=9{\cdot}135\text{ Å}\,;\quad \beta=96{\cdot}86^\circ\,.$$

The error was estimated to be 0·02% for $a$, $b$ and $c$ and ±0·03° for the $\beta$ angle. The density observed by flotation was 1·71 g.cm$^{-3}$ while the calculated density with 2 Mg at special positions and 4 units of $MgC_6H_5O_7\,.\,5H_2O$ at general positions was 1·709 g.cm$^{-3}$.

All intensity data were collected from one crystal which had been ground to the shape of a prolate ellipsoid with axes (diametral) 0·27 mm × 0·21 mm. The major axis was approximately normal to the (301) plane.

A General Electric XRD-5 X-ray unit with single crystal orienter, scintillation counter, and nickel-filtered copper radiation was used for intensity measurement with $2\theta$ scan technique and a 1° take-off angle. The scan rate was 2° per minute and the scan limits were set individually on each reflection to include both the $\alpha_1$ and $\alpha_2$ peaks. The scan time per reflection ranged from 40 to 100 seconds. A background measurement for each reflection was made at a higher $2\theta$ setting along the white radiation streak. Equal time was spent on a peak and its background. When an intense lower order reflection or when appreciable air scatter occurred, background measurements were made at both higher and lower $2\theta$ settings.

The 2725 unique reflections available for measurement with copper radiation were examined and 2484 (91%) were found to be above the experimental least count. During the period of data collection, the reference reflection 301 was measured on 174 occasions. The mean and standard deviation of the reference reflection were 36,250 ± 576 counts. Assuming the standard deviation to be a function of counting statistics and instrumental instability, the intensity error due to the latter is 1·5%.

The axis of the prolate ellipsoidal crystal was mounted along the goniometer head axis ($\varphi$ axis) so that the (301) plane was in reflecting position at $\chi=90°$. A test on the axial symmetry of the absorption effects about the $\varphi$ axis was made by measuring the 301 reflection at 20° steps about $\varphi$. A fractional standard deviation of 1·1% in intensity arises from this source. The higher order reflections of (301) are much less affected by this departure from symmetry about the $\varphi$ axis because of their higher $2\theta$ values (at $2\theta=180°$ the effect would disappear).

All angular settings for the Goniostat were machine computed*, but to minimize setting errors each reflection was individually checked for centering in the three-degree counter-aperture before scanning.

## Correction of counter data

An absorption program* using numerical integration was written to compute transmission factors for a crystal shaped as an ellipsoid of revolution and mounted with its unique axis along the G. E. Goniostat ($\varphi$) axis. A two-dimensional (11 × 11) table of transmission fac-

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* To be submitted for publication.

* Computations involved in this structure analysis were done on the IBM 1620 computer installed in the laboratory. The machine has a 20,000 decimal digit core memory and punched paper-tape input-output. The three-dimensional Fourier summation program (ICR No. 1) and the structure factor program (which produces block-diagonal least-square sums) (ICR No. 4), and The Fourier Data Tape Maker (ICR No. 6) were written by Dr Dick van der Helm. A program for calculating the least-squares best plane through a group of atoms and a general-plane Fourier program (ICR No. 8, 9) were written by Miss Nancy Burow. All other 1620 programs used in this structure analysis were written by the author.

Documented 1620 programs currently available for distribution from this laboratory include the programs mentioned above, a Goniostat coordinates program (ICR No. 2), an absorption program (ICR No. 10), two data reduction programs (ICR No. 11 and No. 12) and distances and angles programs (ICR No. 13 and No. 14).

Additional least-squares refinement with full-matrix least-squares was carried out on a CDC 1604 computer at the Oak Ridge National Laboratory with a modification of the ORFLS program by Dr W. R. Busing. Mrs K. O. Martin and Dr H. A. Levy. A modified version of the function and error program ORFFE by the same authors was used to obtain standard errors for individual structural features from the inverted matrix. A program which draws thermal ellipsoid plots (*e. g.*, Figs. 2 and 3) with an off-line $X$—$Y$ plotter was written by the author. The program can also produce pairs of perspective drawings for stereoscopic viewing.

tors ($\sin^2\theta$ *vs.* $\sin^2\chi$) was computed, then individual transmission factors were obtained in the data reduction program by two-way linear interpolation. The minimum and maximum absorption corrections differed in magnitude by about 8%. Lorentz–polarization corrections were computed for both $K\alpha_1$ and $K\alpha_2$ and a weighted mean was taken.

A variance for each non-zero structure factor was computed from the formula

$$\sigma^2(F_o)=\frac{F_o^2}{4}\left[\frac{(P+B)}{(P-B)^2}+n^2\left(\frac{\sigma(q)}{q}\right)^2+\left(\frac{\sigma(k)}{k}\right)^2\right] \qquad (1)$$

which was derived by the propagation of error technique from

$$F_o^2=k(P-B)q^n\,. \qquad (2)$$

In these expressions $P$ is the total number of counts in the peak; $B$ is the number of background counts in the peak; $q$ is the attenuation filter factor; $n$ is the number of attenuation filters used; $k$ is the combined scale, Lorentz–polarization and transmission factor. The term $\sigma(q)/q$ is the fractional standard deviation of the attenuation filter factor. $\sigma(k)/k$ is the corresponding factor for the combined effects of scale uncertainty due to instrumental instability, absorption, and Lorentz–polarization uncertainties. $\sigma(P)$ and $\sigma(B)$ are taken as $P^{\frac{1}{2}}$ and $B^{\frac{1}{2}}$.

From the analysis of experimental error discussed previously and an estimate of the error in the absorption correction, $\sigma(k)/k$ was assigned the value 0·02. The quantity $\sigma(q)/q$ was determined to be 0·01 from repeated measurements of the filter factor. Using equation (1) and these two values, an overall estimate on the reliability of the 2484 observed data was calculated as $\Sigma\sigma(F_o)/\Sigma F_o=0{\cdot}016$. The mean of the $\sigma(F_o)/F_o$ overall observed reflections was 0·030.

The unobserved reflections were given a count of one half the experimental least count. The standard error assigned was such that within $3\sigma$ the structure factor magnitude could be zero or the minimum measurable. The weighting system for the least-squares refinement was based on the experimental uncertainties with $w=1/\sigma^2(F_o)$.

## Solution of the structure

An initial attempt at solving the structure intuitively from a sharpened three-dimensional Patterson map was unsuccessful. A numerical superposition algorithm based on the Buerger minimum function was then coded for machine computation. The program uses three-way linear interpolation between the points of the three-dimensional Patterson map and allows an unlimited number of weighted superpositions to be made. The grid spacing on the gently sharpened Patterson map was roughly 0·2 Å in each direction.

The two magnesium positions (one in a twofold special position and one in a general position) were found by inspection of the Patterson map. Two oxygen atoms [O(8) and O(9)], one from each coordination sphere, were also located in this manner. Using these four atoms and their symmetry equivalents, a fourteen-shift three-dimensional weighted-minimum-function map was computed in seven sections with a grid spacing of roughly 0·4 Å. In this map the thirteen highest peaks were the two magnesium positions and eleven of the twelve oxygens. The carbons and the remaining oxygen were all represented, but their peak heights were not above the spurious peak noise level. The known chemistry of the molecule allowed the correct carbon peaks to be chosen. The structure derived in this manner lacked one water oxygen but gave an initial reliability index, $R$, of 0·36. A three-dimensional $F_o$ Fourier synthesis located the remaining water oxygen atoms and indicated initial parameter shifts. At this point a structure factor calculation gave an $R$ value of 0·21.

## Refinement of the structure

Least-squares three-dimensional refinement based on the block diagonal approximation was performed with the full set of 2725 data. The final refinement steps utilized full-matrix methods. The progress of the refinement is shown in Table 1. Using isotropic temperature

Table 1. *Refinement of* $[Mg(H_2O)_6][MgC_6H_5O_7\,.\,H_2O]_2\,.\,2H_2O$

| Refinement Step | Result $R$ | $R'$* |
|---|---|---|
| 3-D Minimum function | 0·36 | 0·37 |
| 3-D $F_o$ Fourier synthesis | 0·21 | 0·23 |
| (Found remaining water) | | |
| Least-squares 1 | 0·13 | 0·13 |
| (Mg, O and C isotropic) | | |
| Least-squares 2 | 0·096 | 0·103 |
| Least-squares 3 | 0·091 | 0·096 |
| 3-D Difference Fourier synthesis | 0·073 | 0·077 |
| (Found all 15 H atoms) | | |
| Least-squares 4 | 0·072 | 0·076 |
| Least-squares 5 | 0·048 | 0·047 |
| (Mg and O anisotropic) | | |
| Least-squares 6 | 0·046 | 0·046 |
| Least-squares 7 | 0·041 | 0·039 |
| (Mg, O and C anisotropic) | | |
| (H refined isotropically) | | |
| · | | |
| · | | |
| · | | |
| 3-D Difference Fourier synthesis | | |
| · | | |
| · | | |
| Block-diagonal least-squares best fit | | |
| for all 2725 data | | |
| (without extinction correction) | 0·036 | 0·036 |
| for all 2725 data | | |
| (with extinction correction) | 0·034 | 0·035 |
| without unobserved (2484 data) | | |
| (with extinction correction) | 0·030 | 0·034 |
| Full-matrix least-squares best fit | | |
| for all 2725 data | | |
| (with extinction correction) | 0·031 | 0·036 |
| for the 2484 observed data | | |
| (with extinction correction) | 0·028 | 0·036 |

* See footnote of p .1009.

Table 2. *Experimental and calculated structure factors from block-diagonal least-squares refinement*

An asterisk designates that a reflection was too weak for measurement and was assigned an $F_o$ corresponding to half the experimental least count. The values of $F_o$ and $F_c$ are given in electrons.

| H | OBS | CALC |
|---|---|---|
| (H,0,0) | | |
| 2 | 57.6 | -53.2 |
| 4 | 9.0 | 5.3 |
| 6 | 28.6 | 27.8 |
| 8 | 7.4 | -8.7 |
| 10 | 21.3 | -19.6 |
| 12 | 18.2 | -16.7 |
| 14 | 9.0 | 9.6 |
| 16 | 8.7 | -8.1 |
| 18 | 4.4 | 4.3 |
| 20 | 27.3 | -27.2 |
| 22 | 18.0 | 17.9 |
| 24 | 15.5 | 15.2 |
| (H,1,0) | | |
| 1 | 28.4 | 28.9 |
| 2 | 30.9 | -32.4 |
| 3 | 17.2 | -19.2 |
| 4 | 7.2 | 7.2 |
| 5 | 28.7 | 29.7 |
| 6 | 35.8 | 36.7 |
| 7 | 3.6 | -2.4 |
| 8 | 41.2 | 41.1 |
| 9 | 33.3 | -34.3 |
| 10 | 28.7 | 28.1 |
| 11 | 77.8 | 79.2 |
| 12 | 37.5 | 37.0 |
| 13 | 20.2 | -20.3 |
| 14 | 43.6 | -43.7 |
| 15 | 19.0 | -18.5 |
| 16 | 5.2 | 5.1 |
| 17 | 41.5 | 41.1 |
| 18 | 30.0 | -29.8 |
| 19 | 3.9 | 2.8 |
| 20 | 3.4 | 4.6 |
| 21 | 28.3 | 28.0 |
| 22 | 11.7 | -11.2 |
| 23 | 1.3* | -1.5 |
| 24 | 7.1 | 6.9 |
| 25 | 19.6 | 19.4 |
| (H,2,0) | | |
| 0 | 55.3 | 55.7 |
| 1 | 40.4 | -41.4 |
| 2 | 10.3 | 9.5 |
| 3 | 23.4 | 23.6 |
| 4 | 38.7 | -37.5 |
| 5 | 8.7 | 8.0 |
| 6 | 70.8 | 69.2 |
| 7 | 64.5 | 64.2 |
| 8 | 29.7 | 28.7 |
| 9 | 13.9 | -13.0 |
| 10 | 42.5 | 43.7 |
| 11 | 1.8 | -0.7 |
| 12 | 14.8 | -14.9 |
| 13 | 8.1 | 8.6 |
| 14 | 21.1 | 21.8 |
| 15 | 7.5 | -7.3 |
| 16 | 7.7 | 7.2 |
| 17 | 21.9 | -22.7 |
| 18 | 8.3 | 7.7 |
| 19 | 7.1 | 7.0 |
| 20 | 15.6 | -15.2 |
| 21 | 8.9 | 8.9 |
| 22 | 8.5 | 8.2 |
| 23 | 13.7 | -13.3 |
| 24 | 2.8 | 3.1 |
| 25 | 7.4 | -7.5 |
| (H,3,0) | | |
| 1 | 43.7 | -44.1 |
| 2 | 42.2 | 42.4 |
| 3 | 4.5 | 5.3 |
| 4 | 17.2 | -17.8 |
| 5 | 15.1 | 14.5 |
| 6 | 26.9 | -27.5 |
| 7 | 42.7 | 44.4 |
| 8 | 18.2 | 19.3 |
| 9 | 38.5 | -39.1 |
| 10 | 9.6 | 8.3 |
| 11 | 67.3 | 66.8 |
| 12 | 15.3 | -15.3 |
| 13 | 4.1 | -4.4 |
| 14 | 3.4 | 0.8 |
| 15 | 13.6 | 12.9 |
| 16 | 12.5 | -13.3 |
| 17 | 16.6 | 15.9 |
| 18 | 14.9 | 14.7 |
| 19 | 33.4 | 33.9 |
| 20 | 1.4* | -0.9 |
| 21 | 3.5 | 3.6 |
| 22 | 5.5 | 5.2 |
| 23 | 19.1 | -18.9 |
| 24 | 2.9 | -3.0 |
| (H,4,0) | | |
| 0 | 86.4 | 93.6 |
| 1 | 22.3 | 21.4 |
| 2 | 17.0 | -16.6 |
| 3 | 7.6 | -7.8 |
| 4 | 40.1 | 41.2 |
| 5 | 43.7 | 45.6 |
| 6 | 17.1 | 16.1 |
| 7 | 16.2 | -16.6 |
| 8 | 9.7 | 9.8 |
| 9 | 23.7 | -23.3 |
| 10 | 14.5 | 14.4 |
| 11 | 5.0 | 4.8 |
| 12 | 22.4 | -22.2 |
| 13 | 13.1 | 12.8 |
| 14 | 32.7 | 34.9 |
| 15 | 7.0 | -7.9 |
| 16 | 11.0 | -10.9 |
| 17 | 11.3 | 11.4 |
| 18 | 18.8 | 18.7 |
| 19 | 1.4* | 0.3 |
| 20 | 3.2 | -3.3 |
| 21 | 4.5 | -4.7 |
| 22 | 10.8 | -10.6 |
| (H,5,0) | | |
| 1 | 13.3 | -12.4 |
| 2 | 40.6 | 41.1 |
| 3 | 17.3 | 17.2 |
| 4 | 21.0 | -21.0 |
| 5 | 16.5 | -17.4 |
| 6 | 12.3 | -12.7 |
| 7 | 12.3 | 12.6 |
| 8 | 1.6 | -1.7 |
| 9 | 3.5 | 2.6 |
| 10 | 24.9 | 25.3 |
| 11 | 23.7 | 23.3 |
| 12 | 9.4 | 9.9 |
| 13 | 11.4 | 11.6 |
| 14 | 16.4 | -16.6 |
| 15 | 12.4 | 12.7 |
| 16 | 6.1 | 5.6 |
| 17 | 18.9 | 19.3 |
| 18 | 4.3 | -4.1 |
| 19 | 3.0 | -2.7 |
| 20 | 14.0 | -13.7 |
| (H,6,0) | | |
| 0 | 32.3 | 33.7 |
| 1 | 3.2 | 2.7 |
| 2 | 14.9 | -14.8 |
| 3 | 7.7 | 7.9 |
| 4 | 8.4 | 7.4 |
| 5 | 5.6 | -6.2 |
| 6 | 14.7 | 14.6 |
| 7 | 5.2 | 5.4 |
| 8 | 21.3 | 21.2 |
| 9 | 18.6 | -18.5 |
| 10 | 15.3 | 14.6 |
| 11 | 3.6 | -3.7 |
| 12 | 7.6 | 8.3 |
| 13 | 12.7 | 12.8 |
| 14 | 8.7 | 8.6 |
| 15 | 2.0 | -2.6 |
| 16 | 6.6 | -6.0 |
| 17 | 1.0* | 0.8 |
| 18 | 4.8 | 4.9 |
| (H,7,0) | | |
| 1 | 16.7 | 17.2 |
| 2 | 3.3 | 2.9 |
| 3 | 11.9 | -12.5 |
| 4 | 9.3 | -8.6 |
| 5 | 4.6 | -4.8 |
| 6 | 13.7 | -13.0 |
| 7 | 17.1 | 16.9 |
| 8 | 8.7 | -8.7 |
| 9 | 17.6 | -17.7 |
| 10 | 1.2* | -0.8 |
| 11 | 26.0 | 25.8 |
| 12 | 3.0 | 2.6 |
| 13 | 6.2 | 5.7 |
| 14 | 12.5 | -12.5 |
| (H,8,0) | | |
| 0 | 32.5 | 33.4 |
| 1 | 4.3 | -3.7 |
| 2 | 2.7 | -2.7 |
| 3 | 11.8 | -12.0 |
| 4 | 23.7 | 23.6 |
| 5 | 3.6 | 3.0 |
| 6 | 10.8 | 10.2 |
| 7 | 2.6 | 2.6 |
| 8 | 11.1 | -10.4 |
| 9 | 12.6 | -12.9 |
| (H,0,1) | | |
| -25 | 11.2 | 11.4 |
| -23 | 1.3* | 0.1 |
| -21 | 31.8 | 31.4 |
| -19 | 1.6* | 0.8 |
| -17 | 3.6 | -1.6 |
| -15 | 5.0 | 4.8 |
| -13 | 1.4* | 1.5 |
| -11 | 17.4 | 16.5 |
| -9 | 59.9 | 60.7 |
| -7 | 23.1 | 23.7 |
| -5 | 32.8 | 34.7 |
| -3 | 157.4 | 152.2 |
| -1 | 30.7 | -31.7 |
| 1 | 12.3 | -14.2 |
| 3 | 70.3 | 69.8 |
| 5 | 74.6 | -74.8 |
| 7 | 48.1 | 49.7 |
| 9 | 83.2 | -84.1 |
| 11 | 60.9 | 62.4 |
| 13 | 24.3 | -24.9 |
| 15 | 1.5* | 1.4 |
| 17 | 25.9 | -26.5 |
| 19 | 4.0 | 3.5 |
| 21 | 56.1 | 57.3 |
| 23 | 1.3* | -1.0 |
| 25 | 18.0 | 18.1 |
| (H,1,1) | | |
| -25 | 10.8 | 10.7 |
| -24 | 12.4 | 12.7 |
| -23 | 1.3* | -0.4 |
| -22 | 5.0 | 4.5 |
| -21 | 6.0 | 5.5 |
| -20 | 9.7 | 9.1 |
| -19 | 1.6* | -0.1 |
| -18 | 8.7 | -8.8 |
| -17 | 10.3 | -10.4 |
| -16 | 38.1 | -37.8 |
| -15 | 9.4 | 10.3 |
| -14 | 56.6 | 56.5 |
| -13 | 17.5 | 17.9 |
| -12 | 26.9 | -26.7 |
| -11 | 17.6 | 17.8 |
| -10 | 23.8 | 24.4 |
| -9 | 58.3 | -58.3 |
| -8 | 1.4 | 2.5 |
| -7 | 1.2 | -1.0 |
| -6 | 3.8 | -4.1 |
| -5 | 48.4 | -46.7 |
| -4 | 62.3 | 62.0 |
| -3 | 18.7 | -19.0 |
| -2 | 38.0 | -37.7 |
| -1 | 38.3 | -39.3 |
| 0 | 70.2 | 65.1 |
| 1 | 29.3 | 30.1 |
| 2 | 53.4 | 55.3 |
| 3 | 37.4 | 40.2 |
| 4 | 90.2 | 90.5 |
| 5 | 27.7 | -28.2 |
| 6 | 57.3 | -59.8 |
| 7 | 100.4 | 102.4 |
| 8 | 1.5 | 2.4 |
| 9 | 13.1 | 12.4 |
| 10 | 48.4 | 47.9 |
| 11 | 20.1 | -18.9 |
| 12 | 19.3 | 20.2 |
| 13 | 11.5 | -10.5 |
| 14 | 14.5 | 14.9 |
| 15 | 11.9 | -12.0 |
| 16 | 10.9 | 10.4 |
| 17 | 8.2 | -8.3 |
| 18 | 28.3 | 28.0 |
| 19 | 12.9 | 12.7 |
| 20 | 10.6 | -9.9 |
| 21 | 7.3 | -7.6 |
| 22 | 9.5 | 8.9 |
| 23 | 4.9 | 5.3 |
| 24 | 6.2 | 6.2 |
| 25 | 6.8 | -7.1 |
| (H,2,1) | | |
| -25 | 15.4 | 15.5 |
| -24 | 1.6 | -1.4 |
| -23 | 29.7 | -29.0 |
| -22 | 1.4* | 0.2 |
| -21 | 20.3 | 20.1 |
| -20 | 7.4 | 7.0 |
| -19 | 4.5 | -4.5 |
| -18 | 11.7 | -12.6 |
| -17 | 10.3 | 10.0 |
| -16 | 5.5 | -6.0 |
| -15 | 42.8 | 43.4 |
| -14 | 35.3 | 35.5 |
| -13 | 20.9 | 20.4 |
| -12 | 27.6 | -28.2 |
| -11 | 22.1 | 21.5 |
| -10 | 12.3 | -12.1 |
| -9 | 22.6 | 22.1 |
| -8 | 33.8 | -32.6 |
| -7 | 79.3 | 84.3 |
| -6 | 38.1 | -38.6 |
| -5 | 1.5 | -0.2 |
| -4 | 41.5 | 41.7 |
| -3 | 49.2 | 49.8 |
| -2 | 82.6 | 85.4 |
| -1 | 22.4 | 21.9 |
| 0 | 34.9 | -34.9 |
| 1 | 42.8 | -44.0 |
| 2 | 40.5 | 42.4 |
| 3 | 47.2 | -50.0 |
| 4 | 4.6 | -4.2 |
| 5 | 41.5 | 41.0 |
| 6 | 9.2 | -9.1 |
| 7 | 22.0 | -19.0 |
| 8 | 12.1 | 11.1 |
| 9 | 42.7 | -42.9 |
| 10 | 17.7 | 17.0 |
| 11 | 23.8 | 25.0 |
| 12 | 9.5 | -9.9 |
| 13 | 14.6 | 15.6 |
| 14 | 17.9 | -18.6 |
| 15 | 8.8 | 8.6 |
| 16 | 14.2 | -14.0 |
| 17 | 20.9 | 20.6 |
| 18 | 1.6* | -1.4 |
| 19 | 1.6* | 2.6 |
| 20 | 1.5* | 0.3 |
| 21 | 27.4 | 27.5 |
| 22 | 1.3* | -2.6 |
| 23 | 1.1* | -1.1 |
| 24 | 11.1 | 10.8 |
| (H,3,1) | | |
| -24 | 13.3 | 13.3 |
| -23 | 2.2 | 2.1 |
| -22 | 5.2 | 5.3 |
| -21 | 8.3 | 8.3 |
| -20 | 1.5* | -0.1 |
| -19 | 11.3 | 11.9 |
| -18 | 7.3 | 7.0 |
| -17 | 23.7 | -23.9 |
| -16 | 4.8 | 5.1 |
| -15 | 2.4 | -2.8 |
| -14 | 34.6 | 34.9 |
| -13 | 6.1 | -5.3 |
| -12 | 33.9 | -35.0 |
| -11 | 44.1 | -44.5 |
| -10 | 4.2 | 4.6 |
| -9 | 29.8 | 29.4 |
| -8 | 1.5 | 0.2 |
| -7 | 22.1 | -21.0 |
| -6 | 4.2 | 4.1 |
| -5 | 32.1 | 31.7 |
| -4 | 27.6 | 28.0 |
| -3 | 35.8 | 36.1 |
| -2 | 46.5 | -45.8 |
| -1 | 26.0 | 25.7 |
| 0 | 32.1 | 33.7 |
| 1 | 6.6 | 6.2 |
| 2 | 21.5 | 21.0 |
| 3 | 9.7 | 10.0 |
| 4 | 49.1 | 49.8 |
| 5 | 23.5 | -23.4 |
| 6 | 37.9 | 38.3 |
| 7 | 4.3 | 4.0 |
| 8 | 26.4 | 25.4 |
| 9 | 4.0 | -5.1 |
| 10 | 54.3 | 53.8 |
| 11 | 30.1 | -30.0 |
| 12 | 17.8 | -17.3 |
| 13 | 12.8 | -12.8 |
| 14 | 24.1 | 23.9 |
| 15 | 8.4 | 8.2 |
| 16 | 17.8 | 18.2 |
| 17 | 1.6* | -0.5 |
| 18 | 15.7 | 16.1 |
| 19 | 6.0 | -5.9 |
| 20 | 23.7 | -24.1 |
| 21 | 4.0 | 4.6 |
| 22 | 21.6 | 22.0 |
| 23 | 9.2 | 9.1 |
| (H,4,1) | | |
| -22 | 4.4 | -4.1 |
| -21 | 16.1 | 16.3 |
| -20 | 1.3* | -0.3 |
| -19 | 10.8 | 10.5 |
| -18 | 11.0 | 11.3 |
| -17 | 16.5 | 16.4 |
| -16 | 8.9 | -9.1 |
| -15 | 22.0 | 22.4 |
| -14 | 12.1 | -12.6 |
| -13 | 7.6 | -5.4 |
| -12 | 11.3 | 12.0 |
| -11 | 14.7 | 14.7 |
| -10 | 6.8 | -7.1 |
| -9 | 9.8 | -9.8 |
| -8 | 3.8 | -4.3 |
| -7 | 45.7 | 46.8 |
| -6 | 18.6 | -17.8 |
| -5 | 25.7 | -25.9 |
| -4 | 23.9 | 24.0 |
| -3 | 43.8 | 45.5 |
| -2 | 9.0 | 8.5 |
| -1 | 20.1 | -20.4 |
| 0 | 2.5 | 1.2 |
| 1 | 6.1 | 5.3 |
| 2 | 3.1 | 0.9 |
| 3 | 17.1 | 16.2 |
| 4 | 13.0 | 12.5 |
| 5 | 27.6 | 28.0 |
| 6 | 2.5 | -0.7 |
| 7 | 55.0 | 56.4 |
| 8 | 7.6 | -7.6 |
| 9 | 39.1 | -38.6 |
| 10 | 29.2 | -29.8 |
| 11 | 47.9 | 48.0 |
| 12 | 25.6 | 25.5 |
| 13 | 39.5 | -40.0 |
| 14 | 8.1 | 7.7 |
| 15 | 10.5 | 10.0 |
| 16 | 14.4 | -14.3 |
| 17 | 1.5* | -0.7 |
| 18 | 1.4* | -0.3 |
| 19 | 16.3 | -16.4 |
| 20 | 1.2* | -0.4 |
| 21 | 24.9 | 24.4 |
| 22 | 3.3 | -3.3 |
| (H,5,1) | | |
| -21 | 3.8 | 4.8 |
| -20 | 13.2 | 13.6 |
| -19 | 1.1* | 2.1 |
| -18 | 10.2 | 9.6 |
| -17 | 5.8 | 5.6 |
| -16 | 11.1 | -10.9 |
| -15 | 12.6 | -12.8 |
| -14 | 33.1 | 33.1 |
| -13 | 1.6* | -0.4 |
| -12 | 18.4 | -18.6 |
| -11 | 23.2 | 24.1 |
| -10 | 1.6* | 0.7 |
| -9 | 2.7 | 3.0 |
| -8 | 6.1 | -6.5 |
| -7 | 21.2 | 20.8 |
| -6 | 9.4 | 9.1 |
| -5 | 36.5 | -37.2 |
| -4 | 11.4 | -11.3 |
| -3 | 13.0 | -13.0 |
| -2 | 5.6 | -6.3 |
| -1 | 26.4 | -26.1 |
| 0 | 43.5 | 43.7 |
| 1 | 2.6 | -2.5 |
| 2 | 19.0 | -18.7 |
| 3 | 1.5* | 0.0 |
| 4 | 50.6 | 51.5 |
| 5 | 26.7 | 27.3 |
| 6 | 23.8 | 23.7 |
| 7 | 18.2 | 18.4 |
| 8 | 8.2 | 8.7 |
| 9 | 7.7 | -7.7 |
| 10 | 34.3 | 34.7 |
| 11 | 20.7 | -21.0 |
| 12 | 12.3 | 12.2 |
| 13 | 16.5 | 16.4 |
| 14 | 1.5* | 1.3 |
| 15 | 5.4 | 5.5 |
| 16 | 1.9 | 2.6 |
| 17 | 9.3 | 8.9 |
| 18 | 9.7 | 9.6 |
| 19 | 11.5 | -11.5 |
| 20 | 14.5 | -14.5 |
| (H,6,1) | | |
| -18 | 2.5 | 1.9 |
| -17 | 9.0 | 8.9 |
| -16 | 1.1* | 2.0 |
| -15 | 6.4 | 6.5 |
| -14 | 1.8 | 1.3 |
| -13 | 22.8 | 22.7 |
| -12 | 12.8 | 12.8 |
| -11 | 29.9 | 29.7 |
| -10 | 3.1 | 3.3 |
| -9 | 10.3 | 10.1 |
| -8 | 1.6* | 1.9 |
| -7 | 3.0 | 2.3 |
| -6 | 10.6 | -10.3 |
| -5 | 5.9 | -5.3 |
| -4 | 8.1 | 8.2 |
| -3 | 15.7 | 15.5 |
| -2 | 3.5 | 3.3 |
| -1 | 6.3 | 5.6 |
| 0 | 14.8 | -15.2 |
| 1 | 1.6* | 0.0 |
| 2 | 11.8 | -11.6 |
| 3 | 20.7 | 21.1 |
| 4 | 7.1 | 6.9 |
| 5 | 8.1 | -8.1 |
| 6 | 6.3 | 6.0 |
| 7 | 13.5 | -13.5 |
| 8 | 22.4 | -22.3 |
| 9 | 9.6 | -9.8 |
| 10 | 16.3 | 16.3 |
| 11 | 22.6 | 22.0 |
| 12 | 11.1 | 11.0 |
| 13 | 6.7 | 6.4 |
| 14 | 1.9 | 2.6 |
| 15 | 8.9 | 8.7 |
| 16 | 1.1* | 0.7 |
| 17 | 14.5 | 14.4 |
| 18 | 0.7* | -0.5 |
| (H,7,1) | | |
| -15 | 6.4 | -6.4 |
| -14 | 11.0 | 11.3 |
| -13 | 8.8 | 8.6 |
| -12 | 9.2 | -9.0 |
| -11 | 1.2* | -1.4 |
| -10 | 9.4 | 8.9 |
| -9 | 1.9 | -1.5 |
| -8 | 9.7 | 10.0 |
| -7 | 2.9 | 2.7 |
| -6 | 11.2 | -11.0 |
| -5 | 17.1 | 17.0 |
| -4 | 26.0 | 26.1 |
| -3 | 6.7 | -6.2 |
| -2 | 7.1 | -7.4 |
| -1 | 7.6 | 8.3 |
| 0 | 18.9 | 18.3 |
| 1 | 6.2 | -5.6 |
| 2 | 5.7 | -5.7 |
| 3 | 17.5 | -17.6 |
| 4 | 19.8 | 19.8 |
| 5 | 10.8 | -10.9 |
| 6 | 9.3 | -9.0 |
| 7 | 8.5 | 8.5 |
| 8 | 21.0 | 20.5 |
| 9 | 6.5 | -6.4 |
| 10 | 14.0 | 13.7 |
| 11 | 1.1* | -0.7 |
| 12 | 4.8 | 5.0 |
| 13 | 3.4 | 3.7 |
| 14 | 12.3 | 12.6 |
| (H,8,1) | | |
| -9 | 5.6 | 5.8 |
| -8 | 9.1 | -9.0 |
| -7 | 22.0 | 22.2 |
| -6 | 7.8 | 7.6 |
| -5 | 12.7 | -12.6 |
| -4 | 5.8 | 5.9 |
| -3 | 22.8 | 22.9 |
| -2 | 3.1 | 2.9 |
| -1 | 1.1* | 1.0 |
| 0 | 6.7 | -6.7 |
| 1 | 4.9 | 4.8 |
| 2 | 2.3 | 2.6 |
| 3 | 10.7 | 10.8 |
| 4 | 6.4 | -6.7 |
| 5 | 7.0 | -6.7 |
| 6 | 5.7 | -4.6 |
| 7 | 9.3 | 9.3 |
| 8 | 6.3 | 6.6 |
| (H,0,2) | | |
| -24 | 3.8 | 3.7 |
| -22 | 22.9 | 23.0 |
| -20 | 14.0 | 14.4 |
| -18 | 9.8 | -10.1 |
| -16 | 9.6 | 9.7 |
| -14 | 60.7 | 64.4 |
| -12 | 23.7 | -25.2 |
| -10 | 57.8 | 60.4 |
| -8 | 34.9 | 35.2 |
| -6 | 113.7 | -115.9 |
| -4 | 65.0 | -67.2 |
| -2 | 16.9 | -15.1 |
| 0 | 71.8 | 70.3 |
| 2 | 6.0 | -4.9 |
| 4 | 35.5 | 36.0 |
| 6 | 45.1 | -43.9 |
| 8 | 84.2 | 80.9 |
| 10 | 21.3 | -21.7 |
| 12 | 33.2 | 33.3 |
| 14 | 49.0 | 47.9 |
| 16 | 13.6 | 14.1 |
| 18 | 35.8 | 35.2 |
| 20 | 22.5 | -23.4 |
| 22 | 22.1 | 22.5 |
| 24 | 1.0* | -2.8 |
| (H,1,2) | | |
| -25 | 8.1 | 8.2 |
| -24 | 2.7 | -3.1 |
| -23 | 21.3 | -20.9 |
| -22 | 1.4* | -0.9 |
| -21 | 12.1 | 12.1 |
| -20 | 17.3 | -17.0 |
| -19 | 2.2 | -2.1 |
| -18 | 12.4 | 12.5 |
| -17 | 20.4 | 19.9 |
| -16 | 2.8 | 2.6 |
| -15 | 3.9 | -4.4 |
| -14 | 20.5 | 19.8 |
| -13 | 7.0 | 7.4 |
| -12 | 10.9 | -10.8 |
| -11 | 48.0 | 48.7 |
| -10 | 33.9 | 34.6 |
| -9 | 54.7 | 54.1 |
| -8 | 53.1 | -52.1 |
| -7 | 14.5 | -12.8 |
| -6 | 17.9 | 17.1 |
| -5 | 23.7 | 24.2 |
| -4 | 8.9 | 8.1 |
| -3 | 132.4 | 136.0 |
| -2 | 51.0 | 53.2 |
| -1 | 23.0 | -22.5 |
| 0 | 3.6 | 2.4 |
| 1 | 40.9 | 39.3 |
| 2 | 68.4 | -68.3 |
| 3 | 15.1 | 13.4 |
| 4 | 7.7 | -8.5 |
| 5 | 67.0 | -68.5 |
| 6 | 51.1 | -52.2 |
| 7 | 79.7 | 81.0 |
| 8 | 7.4 | 7.0 |
| 9 | 19.2 | -18.7 |
| 10 | 32.7 | 33.5 |
| 11 | 23.1 | 25.1 |
| 12 | 1.4* | -0.4 |
| 13 | 7.2 | 5.7 |
| 14 | 8.4 | 8.5 |
| 15 | 15.9 | 16.6 |
| 16 | 7.1 | 6.6 |
| 17 | 8.9 | -9.1 |
| 18 | 11.5 | -11.9 |
| 19 | 8.3 | -8.9 |
| 20 | 3.8 | 3.2 |
| 21 | 15.7 | 15.4 |
| 22 | 3.1 | 3.3 |
| 23 | 2.2 | 2.5 |
| 24 | 7.4 | -7.2 |
| (H,2,2) | | |
| -25 | 6.4 | 6.4 |
| -24 | 17.8 | 17.2 |
| -23 | 9.7 | 9.5 |
| -22 | 9.1 | 9.2 |
| -21 | 24.6 | -24.1 |
| -20 | 7.4 | 7.5 |
| -19 | 3.3 | 3.4 |
| -18 | 15.6 | 15.4 |
| -17 | 7.7 | 7.1 |
| -16 | 18.4 | -19.2 |
| -15 | 21.4 | -21.1 |
| -14 | 40.6 | 41.2 |
| -13 | 4.5 | -4.0 |
| -12 | 35.6 | -36.0 |
| -11 | 5.7 | 6.5 |
| -10 | 66.1 | 68.6 |
| -9 | 11.3 | -11.9 |
| -8 | 7.2 | 6.7 |
| -7 | 28.8 | 29.8 |
| -6 | 23.5 | 24.8 |
| -5 | 3.4 | -2.8 |
| -4 | 62.2 | 63.3 |
| -3 | 29.7 | 28.4 |
| -2 | 67.4 | -67.9 |
| -1 | 82.5 | 82.0 |
| 0 | 17.8 | -15.0 |
| 1 | 43.5 | -45.0 |
| 2 | 3.0 | -2.3 |
| 3 | 32.8 | -33.1 |
| 4 | 49.1 | -45.7 |
| 5 | 5.6 | 5.7 |
| 6 | 16.2 | 15.7 |
| 7 | 1.9 | -0.5 |
| 8 | 54.8 | 49.8 |
| 9 | 22.2 | -21.1 |
| 10 | 1.4* | 1.0 |
| 11 | 14.8 | 15.1 |
| 12 | 2.4 | 2.1 |
| 13 | 22.7 | -22.3 |
| 14 | 42.3 | 43.7 |
| 15 | 9.4 | -9.1 |
| 16 | 8.8 | 8.8 |
| 17 | 1.6* | 1.2 |
| 18 | 30.2 | 29.9 |
| 19 | 12.7 | 12.0 |
| 20 | 9.4 | 9.8 |
| 21 | 12.0 | 11.6 |
| 22 | 7.6 | 7.2 |
| 23 | 1.0* | 2.1 |
| 24 | 5.7 | 5.1 |
| (H,3,2) | | |
| -24 | 10.1 | 10.1 |
| -23 | 16.0 | -15.6 |
| -22 | 4.8 | -5.0 |
| -21 | 9.5 | 9.2 |
| -20 | 9.3 | -9.3 |
| -19 | 6.3 | 7.1 |
| -18 | 5.6 | -5.7 |
| -17 | 13.1 | 13.2 |
| -16 | 19.5 | -19.6 |
| -15 | 3.5 | 2.6 |
| -14 | 14.3 | -15.0 |
| -13 | 9.1 | -8.7 |
| -12 | 27.6 | 27.4 |
| -11 | 23.3 | 23.9 |
| -10 | 40.8 | -40.5 |
| -9 | 10.6 | -11.4 |
| -8 | 18.2 | 17.1 |
| -7 | 36.2 | 38.2 |
| -6 | 20.9 | 21.7 |
| -5 | 2.6 | -0.8 |
| -4 | 19.3 | -18.6 |
| -3 | 125.7 | 130.7 |
| -2 | 45.4 | 45.4 |
| -1 | 30.2 | -29.4 |
| 0 | 29.0 | 30.1 |
| 1 | 16.8 | 17.6 |
| 2 | 38.9 | 38.0 |
| 3 | 37.7 | 36.9 |
| 4 | 25.4 | -25.5 |
| 5 | 17.2 | 16.7 |
| 6 | 8.0 | 6.8 |
| 7 | 41.0 | 42.9 |
| 8 | 33.7 | -34.1 |
| 9 | 10.9 | -17.9 |
| 10 | 5.6 | -5.4 |
| 11 | 15.0 | 15.7 |
| 12 | 16.6 | -17.9 |
| 13 | 19.2 | -17.7 |
| 14 | 14.2 | -13.9 |
| 15 | 1.6* | 0.4 |
| 16 | 3.7 | 3.7 |
| 17 | 5.2 | 4.4 |
| 18 | 7.0 | 7.1 |
| 19 | 3.7 | 3.6 |
| 20 | 6.4 | 6.2 |
| 21 | 1.2* | 1.1 |
| 22 | 7.9 | 7.7 |
| 23 | 1.5 | -1.5 |
| (H,4,2) | | |
| -22 | 6.2 | 6.4 |
| -21 | 2.5 | 2.0 |
| -20 | 16.2 | 15.7 |
| -19 | 2.2 | -2.2 |
| -18 | 15.0 | 14.8 |
| -17 | 11.7 | 11.4 |
| -16 | 12.2 | 12.0 |
| -15 | 5.7 | -5.1 |
| -14 | 19.9 | 19.7 |
| -13 | 24.8 | -25.6 |
| -12 | 8.0 | -8.1 |
| -11 | 4.0 | -3.6 |
| -10 | 8.7 | -8.9 |
| -9 | 23.2 | 23.5 |
| -8 | 21.3 | -22.0 |
| -7 | 19.1 | 18.7 |
| -6 | 20.5 | -20.8 |
| -5 | 14.7 | -15.1 |
| -4 | 19.5 | 19.6 |
| -3 | 10.8 | 10.8 |
| -2 | 16.2 | -16.4 |
| -1 | 10.0 | -9.9 |
| 0 | 23.3 | 24.6 |
| 1 | 5.8 | -5.1 |
| 2 | 20.2 | 19.5 |
| 3 | 12.7 | 13.0 |
| 4 | 51.3 | 52.9 |
| 5 | 2.7 | -2.1 |
| 6 | 3.0 | -0.7 |
| 7 | 13.6 | -13.6 |
| 8 | 43.5 | 43.0 |
| 9 | 21.1 | 22.0 |
| 10 | 1.6* | -1.2 |
| 11 | 24.0 | -25.1 |
| 12 | 7.1 | -7.1 |
| 13 | 10.2 | -11.2 |
| 14 | 22.7 | 22.4 |
| 15 | 3.7 | 3.5 |
| 16 | 10.7 | -11.2 |
| 17 | 7.8 | 8.2 |
| 18 | 35.6 | 35.8 |
| 19 | 2.7 | 2.4 |
| 20 | 18.2 | -17.5 |
| 21 | 0.9* | -1.1 |
| (H,5,2) | | |
| -21 | 7.8 | 7.8 |
| -20 | 8.6 | 8.8 |
| -19 | 7.3 | -6.8 |
| -18 | 4.9 | 4.9 |
| -17 | 21.3 | 21.7 |
| -16 | 1.4* | 0.5 |
| -15 | 11.6 | -10.1 |
| -14 | 18.3 | 18.6 |
| -13 | 3.3 | 2.6 |
| -12 | 2.2 | -1.6 |
| -11 | 16.2 | 16.1 |
| -10 | 6.2 | -7.4 |
| -9 | 4.8 | 4.8 |
| -8 | 7.4 | 7.5 |
| -7 | 5.2 | 4.3 |
| -6 | 8.0 | -6.4 |
| -5 | 2.3 | 2.8 |
| -4 | 3.3 | -3.2 |
| -3 | 42.3 | 42.3 |
| -2 | 33.5 | -33.0 |
| -1 | 5.4 | -4.6 |
| 0 | 12.2 | 12.4 |
| 1 | 48.9 | 49.4 |
| 2 | 4.6 | 2.9 |
| 3 | 21.1 | 20.9 |
| 4 | 5.7 | 5.1 |
| 5 | 3.4 | 2.8 |
| 6 | 36.2 | -37.7 |
| 7 | 41.3 | 41.9 |
| 8 | 29.8 | 29.7 |
| 9 | 15.8 | -15.5 |
| 10 | 3.2 | 2.8 |
| 11 | 2.2 | -1.9 |
| 12 | 9.7 | 10.0 |
| 13 | 2.3 | -2.2 |
| 14 | 18.3 | 17.9 |
| 15 | 5.2 | 4.9 |
| 16 | 1.3* | 0.7 |
| 17 | 12.6 | -12.5 |
| 18 | 1.1* | 0.8 |
| 19 | 2.0 | -2.0 |
| (H,6,2) | | |
| -18 | 11.2 | 11.4 |
| -17 | 8.9 | 9.0 |
| -16 | 12.0 | -11.7 |
| -15 | 1.2* | 0.4 |
| -14 | 23.9 | 23.8 |
| -13 | 1.4* | 2.1 |
| -12 | 22.7 | -22.3 |
| -11 | 12.7 | -13.3 |
| -10 | 26.7 | 26.9 |
| -9 | 20.9 | 20.9 |
| -8 | 1.6* | 0.5 |
| -7 | 4.2 | 4.6 |
| -6 | 4.2 | 3.4 |
| -5 | 15.3 | -16.0 |
| -4 | 16.5 | 16.8 |
| -3 | 9.8 | -10.1 |
| -2 | 9.6 | -8.6 |
| -1 | 5.4 | -5.6 |
| 0 | 17.9 | 17.6 |
| 1 | 6.0 | -5.2 |
| 2 | 9.4 | -9.5 |
| 3 | 5.2 | 5.3 |
| 4 | 2.7 | 2.4 |
| 5 | 12.3 | -12.5 |
| 6 | 10.9 | -11.1 |
| 7 | 24.6 | 24.7 |
| 8 | 23.8 | 23.4 |
| 9 | 6.5 | 6.6 |
| 10 | 9.9 | 10.5 |
| 11 | 9.6 | -9.2 |
| 12 | 11.1 | 10.6 |
| 13 | 13.2 | 13.2 |
| 14 | 13.3 | 13.0 |
| 15 | 10.5 | -10.7 |
| 16 | 2.4 | 2.1 |
| 17 | 1.5 | 2.1 |
| (H,7,2) | | |
| -14 | 1.4 | 1.5 |
| -13 | 1.0* | -1.4 |
| -12 | 1.1* | 0.9 |
| -11 | 11.0 | 11.2 |
| -10 | 2.8 | 2.4 |
| -9 | 17.6 | 17.8 |
| -8 | 1.3* | 0.5 |
| -7 | 20.2 | 19.6 |
| -6 | 15.9 | -16.0 |
| -5 | 12.5 | -12.9 |
| -4 | 2.1 | -1.3 |
| -3 | 20.3 | 20.3 |
| -2 | 8.7 | 9.1 |
| -1 | 10.6 | 11.4 |
| 0 | 17.9 | -18.3 |
| 1 | 8.9 | 8.9 |
| 2 | 27.5 | 27.1 |
| 3 | 18.9 | 18.3 |
| 4 | 5.5 | -5.9 |
| 5 | 12.2 | -11.9 |
| 6 | 2.5 | -0.9 |
| 7 | 19.3 | 19.3 |
| 8 | 9.7 | 9.6 |
| 9 | 16.7 | -16.4 |
| 10 | 1.1* | 1.6 |
| 11 | 12.9 | 13.1 |
| 12 | 5.9 | -5.8 |
| 13 | 2.5 | -2.5 |
| (H,8,2) | | |
| -8 | 12.4 | -12.9 |
| -7 | 0.8* | -0.9 |
| -6 | 0.9* | 0.0 |
| -5 | 13.9 | -13.5 |
| -4 | 12.1 | 12.4 |
| -3 | 10.2 | 10.1 |
| -2 | 10.3 | -10.2 |
| -1 | 5.5 | 5.5 |
| 0 | 6.6 | 6.7 |
| 1 | 5.6 | -5.4 |
| 2 | 4.0 | 3.8 |
| 3 | 1.0* | 0.5 |
| 4 | 5.8 | 5.6 |
| 5 | 4.9 | -4.9 |
| 6 | 10.7 | -10.6 |
| 7 | 3.9 | 4.2 |
| (H,0,3) | | |
| -25 | 9.2 | 9.8 |
| -23 | 21.2 | 20.8 |
| -21 | 16.0 | -16.0 |
| -19 | 21.9 | 22.0 |
| -17 | 34.9 | 35.6 |
| -15 | 18.1 | -19.3 |
| -13 | 37.3 | 32.0 |
| -11 | 10.3 | 11.9 |
| -9 | 19.2 | -19.5 |
| -7 | 22.4 | 23.9 |
| -5 | 56.1 | -58.4 |
| -3 | 70.4 | -72.6 |
| -1 | 93.2 | 96.4 |
| 1 | 4.1 | 2.3 |
| 3 | 22.9 | 22.5 |
| 5 | 23.6 | 23.6 |
| 7 | 100.3 | 96.7 |
| 9 | 5.8 | -6.3 |
| 11 | 104.2 | 104.6 |
| 13 | 20.0 | 20.5 |
| 15 | 12.8 | 12.5 |
| 17 | 41.8 | -42.3 |
| 19 | 7.3 | 8.3 |
| 21 | 8.3 | -3.8 |
| 23 | 8.9 | -9.3 |
| (H,1,3) | | |
| -25 | 5.9 | -5.7 |
| -24 | 18.0 | 17.6 |
| -23 | 6.4 | 6.2 |
| -22 | 5.4 | 4.9 |
| -21 | 10.1 | -10.5 |
| -20 | 10.1 | 9.9 |
| -19 | 4.7 | -5.0 |
| -18 | 35.9 | 37.2 |
| -17 | 29.3 | -29.8 |
| -16 | 30.4 | -30.2 |
| -15 | 29.8 | 30.5 |
| -14 | 52.3 | 53.1 |
| -13 | 21.3 | 22.0 |
| -12 | 34.7 | 34.6 |
| -11 | 15.5 | 15.8 |
| -10 | 20.9 | 22.1 |
| -9 | 2.5 | 1.0 |
| -8 | 2.4 | -2.4 |
| -7 | 68.8 | 69.8 |
| -6 | 76.3 | 77.3 |
| -5 | 40.1 | -39.6 |
| -4 | 41.7 | -42.7 |
| -3 | 16.5 | 15.9 |
| -2 | 59.9 | -61.2 |
| -1 | 55.6 | -54.9 |
| 0 | 4.0 | -2.5 |
| 1 | 1.6 | -1.0 |
| 2 | 33.7 | 33.6 |
| 3 | 84.0 | -86.4 |
| 4 | 36.8 | 39.9 |
| 5 | 10.6 | -11.0 |
| 6 | 69.5 | -69.9 |
| 7 | 22.2 | 21.3 |
| 8 | 29.7 | 31.3 |
| 9 | 1.3* | 1.0 |
| 10 | 29.4 | 29.5 |
| 11 | 27.9 | 28.0 |
| 12 | 15.6 | 15.4 |
| 13 | 18.0 | -17.9 |
| 14 | 3.7 | -4.1 |
| 15 | 12.2 | 11.7 |
| 16 | 1.8* | 1.9 |
| 17 | 1.6* | 1.8 |
| 18 | 41.7 | 41.9 |
| 19 | 19.0 | 18.8 |
| 20 | 9.6 | -9.3 |
| 21 | 5.8 | -6.1 |
| 22 | 5.7 | 5.4 |
| 23 | 10.8 | 10.7 |
| (H,2,3) | | |
| -24 | 6.7 | 6.3 |
| -23 | 4.0 | -4.2 |
| -22 | 2.8 | -2.8 |
| -21 | 3.8 | -4.1 |
| -20 | 13.8 | -13.5 |
| -19 | 32.4 | -32.0 |
| -18 | 14.6 | -14.6 |
| -17 | 45.1 | 44.9 |
| -16 | 5.0 | 5.3 |
| -15 | 10.3 | -9.7 |
| -14 | 6.5 | 6.5 |
| -13 | 4.8 | 4.0 |
| -12 | 26.8 | 26.5 |
| -11 | 6.2 | -5.7 |
| -10 | 19.0 | 18.8 |
| -9 | 2.4 | 2.3 |
| -8 | 25.3 | -24.5 |
| -7 | 70.8 | 72.6 |
| -6 | 14.0 | 13.2 |
| -5 | 79.3 | -80.1 |
| -4 | 19.1 | 18.3 |
| -3 | 116.9 | 123.8 |
| -2 | 12.4 | 11.5 |
| -1 | 21.5 | 20.4 |
| 0 | 47.7 | -46.0 |
| 1 | 60.7 | 62.1 |
| 2 | 19.3 | 18.8 |
| 3 | 3.5 | -2.9 |
| 4 | 49.3 | -48.5 |
| 5 | 18.1 | 19.4 |
| 6 | 18.8 | -17.9 |
| 7 | 36.3 | 37.1 |
| 8 | 6.3 | -6.3 |
| 9 | 22.5 | -23.5 |
| 10 | 17.1 | 17.1 |
| 11 | 16.4 | 17.3 |
| 12 | 2.9 | -1.3 |
| 13 | 19.4 | 19.8 |
| 14 | 21.2 | 20.4 |
| 15 | 8.1 | 8.8 |
| 16 | 8.4 | -9.6 |
| 17 | 10.1 | 9.9 |
| 18 | 15.3 | 15.7 |
| 19 | 5.5 | 5.1 |
| 20 | 4.2 | 4.5 |
| 21 | 9.2 | 9.0 |
| 22 | 5.3 | -5.1 |
| 23 | 3.7 | -3.1 |
| (H,3,3) | | |
| -24 | 17.7 | 19.1 |
| -23 | 2.0 | 1.5 |
| -22 | 10.3 | -10.4 |
| -21 | 9.1 | 8.6 |
| -20 | 10.7 | 11.3 |
| -19 | 13.2 | -13.2 |
| -18 | 14.7 | 15.2 |
| -17 | 10.6 | 10.3 |
| -16 | 5.3 | 5.1 |
| -15 | 6.2 | 6.4 |
| -14 | 19.5 | 19.4 |
| -13 | 7.1 | -7.0 |
| -12 | 8.2 | 7.9 |
| -11 | 18.2 | -18.6 |
| -10 | 3.5 | 1.6 |
| -9 | 15.8 | -15.5 |
| -8 | 13.2 | 13.4 |
| -7 | 12.3 | 12.0 |
| -6 | 47.7 | 48.8 |
| -5 | 41.9 | 41.2 |
| -4 | 39.6 | 40.2 |
| -3 | 12.7 | -13.1 |
| -2 | 49.2 | -49.2 |
| -1 | 31.3 | 30.7 |
| 0 | 48.1 | 48.8 |
| 1 | 1.4 | -0.9 |
| 2 | 14.1 | -13.9 |
| 3 | 5.4 | -4.8 |
| 4 | 1.3* | 2.8 |
| 5 | 35.8 | -36.1 |
| 6 | 14.3 | -14.8 |
| 7 | 9.1 | 8.1 |
| 8 | 31.0 | 30.1 |
| 9 | 21.0 | 20.8 |
| 10 | 24.5 | -25.1 |
| 11 | 30.0 | -29.1 |
| 12 | 2.4 | -1.7 |
| 13 | 16.8 | 18.1 |
| 14 | 15.3 | 15.1 |
| 15 | 5.7 | -6.3 |
| 16 | 19.1 | -18.1 |
| 17 | 4.0 | -3.7 |
| 18 | 52.7 | 52.9 |
| 19 | 2.3 | -1.6 |
| 20 | 4.5 | -4.0 |
| 21 | 4.1 | 4.3 |
| 22 | 10.2 | 10.6 |
| (H,4,3) | | |
| -22 | 0.8* | 1.0 |
| -21 | 4.2 | 4.2 |
| -20 | 1.2* | -1.7 |
| -19 | 2.5 | -1.9 |
| -18 | 9.2 | 9.0 |
| -17 | 19.2 | 18.9 |
| -16 | 12.8 | -12.8 |
| -15 | 1.6* | 1.6 |
| -14 | 2.7 | -2.7 |
| -13 | 16.7 | -16.5 |
| -12 | 13.4 | 13.8 |
| -11 | 8.2 | -8.9 |
| -10 | 3.7 | 3.0 |
| -9 | 4.9 | 5.2 |
| -8 | 3.5 | 3.0 |
| -7 | 18.8 | 18.8 |
| -6 | 14.9 | -16.0 |
| -5 | 1.4* | 1.0 |
| -4 | 10.1 | 10.9 |
| -3 | 30.3 | 31.9 |
| -2 | 6.9 | -6.7 |
| -1 | 8.2 | 7.9 |
| 0 | 4.9 | -5.1 |
| 1 | 37.4 | 38.0 |
| 2 | 19.1 | -19.2 |
| 3 | 4.8 | -4.4 |
| 4 | 54.8 | 55.9 |
| 5 | 22.2 | 21.5 |
| 6 | 11.6 | -11.9 |
| 7 | 67.6 | 68.2 |
| 8 | 32.5 | -32.9 |
| 9 | 7.4 | -7.7 |
| 10 | 10.9 | -10.9 |
| 11 | 14.3 | 14.7 |
| 12 | 24.4 | 25.6 |

Table 2 (*cont.*)

| H | OBS | CALC |
|---|---|---|
| (H,4,3) | | |
| 13 | 8.9 | 9.5 |
| 14 | 3.9 | -3.9 |
| 15 | 1.5* | 0.4 |
| 16 | 1.5* | -0.1 |
| 17 | 12.9 | -12.9 |
| 18 | 2.7 | 3.1 |
| 19 | 12.4 | 12.1 |
| 20 | 7.5 | 7.1 |
| 21 | 2.6 | -2.1 |
| (H,5,3) | | |
| -20 | 2.1 | 1.9 |
| -19 | 3.6 | -3.3 |
| -18 | 10.7 | 10.3 |
| -17 | 4.7 | 4.9 |
| -16 | 3.9 | -4.3 |
| -15 | 3.8 | -4.1 |
| -14 | 28.2 | 28.3 |
| -13 | 3.1 | 3.2 |
| -12 | 12.4 | -12.4 |
| -11 | 6.4 | -6.2 |
| -10 | 32.1 | 31.8 |
| -9 | 6.3 | 6.6 |
| -8 | 7.1 | -6.7 |
| -7 | 25.4 | 25.2 |
| -6 | 19.9 | 19.6 |
| -5 | 1.6* | -2.2 |
| -4 | 19.0 | 18.1 |
| -3 | 21.0 | -20.9 |
| -2 | 8.0 | 8.4 |
| -1 | 12.2 | -13.2 |
| 0 | 8.0 | 7.8 |
| 1 | 8.0 | -7.9 |
| 2 | 8.4 | 8.4 |
| 3 | 1.6* | 0.7 |
| 4 | 12.4 | 12.4 |
| 5 | 13.9 | 14.2 |
| 6 | 28.0 | -27.8 |
| 7 | 7.0 | 6.7 |
| 8 | 14.6 | 14.5 |
| 9 | 1.6* | -1.1 |
| 10 | 9.3 | -9.2 |
| 11 | 1.6* | -1.0 |
| 12 | 12.7 | 12.6 |
| 13 | 5.6 | -5.6 |
| 14 | 1.4* | 0.8 |
| 15 | 10.7 | 10.2 |
| 16 | 4.1 | -4.3 |
| 17 | 9.6 | -9.6 |
| 18 | 23.4 | 22.9 |
| 19 | 0.7* | -0.3 |
| (H,6,3) | | |
| -18 | 3.7 | 3.9 |
| -17 | 4.9 | 4.9 |
| -16 | 4.0 | 2.8 |
| -15 | 21.2 | -21.1 |
| -14 | 13.8 | -14.4 |
| -13 | 13.7 | 14.4 |
| -12 | 13.9 | 14.1 |
| -11 | 14.9 | 15.0 |
| -10 | 4.1 | 3.9 |
| -9 | 7.9 | -7.8 |
| -8 | 18.5 | -19.1 |
| -7 | 24.4 | 25.3 |
| -6 | 2.1 | 1.4 |
| -5 | 6.4 | -6.4 |
| -4 | 2.0 | -1.1 |
| -3 | 25.0 | 24.3 |
| -2 | 3.0 | 3.0 |
| -1 | 3.6 | 3.4 |
| 0 | 16.3 | -16.6 |
| 1 | 35.2 | 35.5 |
| 2 | 10.7 | 10.7 |
| 3 | 19.9 | 19.8 |
| 4 | 25.8 | 26.0 |
| 5 | 6.8 | -6.8 |
| 6 | 6.0 | -6.0 |
| 7 | 18.8 | 18.4 |
| 8 | 16.1 | -16.1 |
| 9 | 23.4 | -23.7 |
| 10 | 7.5 | 7.3 |
| 11 | 17.4 | 17.1 |
| 12 | 1.3* | 0.0 |
| 13 | 1.2* | -0.5 |
| 14 | 11.0 | 10.6 |
| 15 | 7.1 | 7.5 |
| 16 | 9.4 | -8.6 |
| (H,7,3) | | |
| -14 | 11.6 | 12.2 |
| -13 | 1.6 | -2.2 |
| -12 | 14.0 | 14.1 |
| -11 | 16.6 | -16.3 |
| -10 | 10.1 | 9.8 |
| -9 | 23.7 | -23.7 |
| -8 | 8.8 | -8.7 |
| -7 | 13.4 | 13.8 |
| -6 | 17.0 | 17.0 |
| -5 | 1.4* | -0.2 |
| -4 | 1.4 | 1.5 |
| -3 | 6.4 | -6.3 |
| -2 | 1.4* | -0.7 |
| -1 | 23.8 | 24.1 |
| 0 | 25.0 | 25.0 |
| 1 | 3.8 | 3.1 |
| 2 | 16.6 | -16.5 |
| 3 | 5.6 | 5.6 |
| 4 | 10.3 | 9.8 |
| 5 | 1.3* | 1.7 |
| 6 | 11.7 | -11.7 |
| 7 | 3.9 | -3.7 |
| 8 | 1.2* | -0.6 |
| 9 | 11.3 | 11.2 |
| 10 | 4.8 | 4.3 |
| 11 | 5.5 | -5.4 |
| 12 | 11.1 | 10.7 |
| (H,8,3) | | |
| -7 | 14.9 | 15.3 |
| -6 | 1.1 | -1.1 |
| -5 | 7.5 | -7.3 |
| -4 | 0.9* | 1.4 |
| -3 | 3.9 | 3.5 |
| -2 | 2.5 | 2.6 |
| -1 | 2.8 | -2.8 |
| 0 | 1.5 | 1.7 |
| 1 | 0.9* | 1.1 |
| 2 | 0.9* | -0.3 |
| 3 | 6.9 | 6.6 |
| 4 | 8.2 | 7.9 |
| 5 | 18.5 | 18.7 |
| (H,0,4) | | |
| -24 | 10.2 | 10.5 |
| -22 | 12.1 | 12.4 |
| -20 | 9.0 | 8.7 |
| -18 | 9.6 | 9.2 |
| -16 | 6.6 | 8.3 |
| -14 | 22.5 | 24.3 |
| -12 | 13.2 | 12.5 |
| -10 | 63.0 | 65.5 |
| -8 | 3.6 | -4.5 |
| -6 | 34.4 | -34.4 |
| -4 | 2.0 | 0.7 |
| -2 | 36.7 | 35.7 |
| 0 | 30.1 | -29.6 |
| 2 | 51.8 | 52.8 |
| 4 | 73.2 | 74.2 |
| 6 | 14.8 | 15.9 |
| 8 | 1.3* | 0.4 |
| 10 | 6.8 | 7.2 |
| 12 | 7.1 | 7.5 |
| 14 | 17.0 | 17.0 |
| 16 | 27.7 | -27.7 |
| 18 | 10.0 | 9.6 |
| 20 | 7.5 | -7.8 |
| 22 | 13.8 | 13.5 |
| (H,1,4) | | |
| -25 | 6.5 | 6.9 |
| -24 | 8.7 | -8.8 |
| -23 | 6.2 | 6.4 |
| -22 | 4.4 | -3.9 |
| -21 | 24.6 | 24.2 |
| -20 | 8.4 | -8.4 |
| -19 | 7.3 | -7.2 |
| -18 | 1.6* | 0.3 |
| -17 | 15.3 | 15.2 |
| -16 | 15.6 | 15.9 |
| -15 | 1.6* | 1.5 |
| -14 | 10.4 | -11.2 |
| -13 | 25.8 | 25.9 |
| -12 | 42.1 | 42.8 |
| -11 | 2.8 | -3.8 |
| -10 | 7.6 | 7.5 |
| -9 | 24.0 | -24.4 |
| -8 | 12.3 | -12.8 |
| -7 | 24.1 | 25.2 |
| -6 | 9.6 | -9.0 |
| -5 | 78.4 | -78.6 |
| -4 | 17.5 | 18.2 |
| -3 | 18.6 | 19.4 |
| -2 | 3.1 | -3.9 |
| -1 | 18.4 | 17.7 |
| 0 | 1.2 | 1.1 |
| 1 | 40.4 | 43.4 |
| 2 | 33.8 | -33.9 |
| 3 | 17.0 | 16.9 |
| 4 | 40.7 | -41.7 |
| 5 | 17.7 | 17.0 |
| 6 | 11.2 | -10.8 |
| 7 | 43.4 | 43.3 |
| 8 | 12.7 | 13.4 |
| 9 | 6.8 | 6.3 |
| 10 | 9.7 | -9.6 |
| 11 | 33.0 | 32.9 |
| 12 | 26.5 | 27.4 |
| 13 | 10.5 | 10.9 |
| 14 | 20.2 | 20.4 |
| 15 | 41.6 | 42.5 |
| 16 | 6.0 | -6.3 |
| 17 | 13.9 | -14.0 |
| 18 | 7.6 | 7.4 |
| 19 | 2.7 | -2.0 |
| 20 | 1.3* | -0.4 |
| 21 | 1.2* | -1.9 |
| 22 | 1.0* | 0.6 |
| 23 | 15.9 | 16.0 |
| (H,2,4) | | |
| -24 | 6.6 | 6.7 |
| -23 | 10.7 | -10.3 |
| -22 | 1.2* | 0.9 |
| -21 | 4.6 | 4.2 |
| -20 | 20.5 | 19.9 |
| -19 | 2.1 | -2.3 |
| -18 | 10.2 | 10.4 |
| -17 | 2.6 | 2.8 |
| -16 | 23.5 | -24.1 |
| -15 | 16.9 | 16.5 |
| -14 | 23.5 | 23.4 |
| -13 | 2.8 | -2.5 |
| -12 | 11.2 | -11.3 |
| -11 | 22.5 | 22.6 |
| -10 | 18.5 | 18.5 |
| -9 | 8.4 | -8.7 |
| -8 | 1.3* | 1.4 |
| -7 | 27.1 | -27.7 |
| -6 | 84.9 | 88.0 |
| -5 | 9.0 | -9.2 |
| -4 | 25.3 | 25.7 |
| -3 | 24.7 | 23.8 |
| -2 | 62.7 | 63.0 |
| -1 | 15.9 | -16.8 |
| 0 | 10.2 | 10.6 |
| 1 | 16.3 | -14.3 |
| 2 | 60.1 | -61.0 |
| 3 | 30.3 | -30.4 |
| 4 | 107.5 | 111.2 |
| 5 | 11.2 | 10.2 |
| 6 | 44.3 | -44.0 |
| 7 | 17.5 | -13.0 |
| 8 | 15.8 | 16.7 |
| 9 | 31.8 | 32.1 |
| 10 | 14.7 | -14.6 |
| 11 | 23.7 | 23.7 |
| 12 | 7.7 | 8.1 |
| 13 | 1.6* | -0.6 |
| 14 | 8.7 | -9.9 |
| 15 | 7.7 | -7.3 |
| 16 | 22.1 | -22.6 |
| 17 | 3.3 | 3.2 |
| 18 | 22.3 | 22.4 |
| 19 | 1.4* | -2.7 |
| 20 | 2.3 | 2.3 |
| 21 | 1.1* | -1.1 |
| 22 | 10.4 | 10.4 |
| (H,3,4) | | |
| -23 | 0.8* | 0.5 |
| -22 | 6.2 | 6.0 |
| -21 | 13.1 | 13.0 |
| -20 | 8.7 | 8.7 |
| -19 | 9.9 | -9.1 |
| -18 | 9.7 | -9.5 |
| -17 | 21.0 | 21.0 |
| -16 | 1.6* | 2.2 |
| -15 | 10.0 | -10.1 |
| -14 | 2.7 | 2.7 |
| -13 | 35.5 | 36.1 |
| -12 | 7.7 | -7.4 |
| -11 | 19.0 | -18.9 |
| -10 | 29.9 | 30.2 |
| -9 | 10.4 | -11.5 |
| -8 | 8.1 | -8.3 |
| -7 | 38.3 | 39.7 |
| -6 | 23.2 | -24.0 |
| -5 | 17.6 | -17.6 |
| -4 | 27.0 | -27.1 |
| -3 | 46.2 | 46.4 |
| -2 | 7.9 | -7.4 |
| -1 | 14.0 | -13.7 |
| 0 | 2.7 | 3.3 |
| 1 | 10.2 | -8.3 |
| 2 | 9.1 | -8.8 |
| 3 | 21.3 | 20.0 |
| 4 | 16.4 | 15.6 |
| 5 | 11.4 | 10.3 |
| 6 | 45.7 | 46.6 |
| 7 | 1.5* | 1.3 |
| 8 | 12.3 | -11.1 |
| 9 | 27.7 | 29.0 |
| 10 | 10.5 | 10.5 |
| 11 | 14.2 | 14.7 |
| 12 | 16.8 | -17.0 |
| 13 | 13.2 | -13.8 |
| 14 | 2.9 | 3.3 |
| 15 | 47.2 | 46.6 |
| 16 | 1.5* | 0.4 |
| 17 | 7.6 | 7.7 |
| 18 | 7.7 | -8.2 |
| 19 | 1.2* | 0.5 |
| 20 | 4.0 | 4.3 |
| 21 | 17.2 | 17.3 |
| (H,4,4) | | |
| -22 | 11.8 | -12.7 |
| -21 | 1.6 | 1.7 |
| -20 | 3.2 | 3.4 |
| -19 | 5.3 | 5.1 |
| -18 | 7.6 | 7.5 |
| -17 | 12.4 | 12.3 |
| -16 | 2.9 | -3.5 |
| -15 | 6.0 | -6.6 |
| -14 | 29.4 | 29.3 |
| -13 | 3.6 | -3.4 |
| -12 | 28.1 | 28.9 |
| -11 | 6.7 | 6.7 |
| -10 | 3.0 | 2.6 |
| -9 | 13.6 | -14.6 |
| -8 | 25.0 | 25.1 |
| -7 | 3.1 | 2.9 |
| -6 | 18.5 | 18.6 |
| -5 | 19.9 | 19.3 |
| -4 | 18.6 | 18.1 |
| -3 | 21.7 | -22.1 |
| -2 | 20.1 | 19.0 |
| -1 | 1.5* | -0.7 |
| 0 | 8.9 | -8.6 |
| 1 | 1.5* | 1.9 |
| 2 | 19.3 | -19.3 |
| 3 | 3.0 | 2.4 |
| 4 | 57.1 | 58.8 |
| 5 | 14.5 | -14.6 |
| 6 | 29.4 | -28.8 |
| 7 | 17.8 | 18.6 |
| 8 | 2.4 | 1.8 |
| 9 | 8.7 | 8.9 |
| 10 | 15.1 | 14.7 |
| 11 | 1.6* | 0.3 |
| 12 | 9.8 | -9.7 |
| 13 | 9.3 | -9.4 |
| 14 | 10.8 | 10.3 |
| 15 | 7.8 | 7.3 |
| 16 | 9.2 | 9.5 |
| 17 | 1.3* | 1.0 |
| 18 | 13.6 | 13.7 |
| 19 | 5.5 | -5.3 |
| 20 | 0.6* | 0.0 |
| (H,5,4) | | |
| -20 | 3.6 | -3.7 |
| -19 | 0.9* | -1.2 |
| -18 | 4.6 | 4.8 |
| -17 | 8.4 | 8.4 |
| -16 | 3.0 | -2.7 |
| -15 | 7.4 | -7.7 |
| -14 | 7.3 | -7.0 |
| -13 | 23.1 | 23.0 |
| -12 | 3.4 | 3.5 |
| -11 | 1.6* | -1.5 |
| -10 | 3.4 | 3.2 |
| -9 | 4.2 | -4.1 |
| -8 | 14.5 | 15.7 |
| -7 | 48.3 | 49.5 |
| -6 | 6.9 | 6.2 |
| -5 | 35.5 | -34.8 |
| -4 | 12.6 | -13.7 |
| -3 | 17.4 | 17.0 |
| -2 | 6.1 | 6.1 |
| -1 | 8.7 | 8.4 |
| 0 | 12.9 | 13.9 |
| 1 | 9.3 | -9.2 |
| 2 | 22.2 | -22.1 |
| 3 | 5.8 | -5.3 |
| 4 | 6.5 | 6.3 |
| 5 | 24.0 | 23.7 |
| 6 | 8.7 | -8.4 |
| 7 | 3.2 | 2.3 |
| 8 | 3.2 | -2.9 |
| 9 | 7.3 | 7.0 |
| 10 | 23.1 | -23.1 |
| 11 | 23.7 | 22.9 |
| 12 | 1.5* | 0.8 |
| 13 | 1.4* | -1.8 |
| 14 | 12.4 | 12.3 |
| 15 | 29.7 | 30.0 |
| 16 | 21.3 | 21.0 |
| 17 | 0.9* | 0.5 |
| (H,6,4) | | |
| -17 | 0.7* | -1.5 |
| -16 | 9.7 | -9.7 |
| -15 | 6.4 | -6.6 |
| -14 | 15.1 | 15.6 |
| -13 | 1.2* | -0.8 |
| -12 | 11.8 | -12.0 |
| -11 | 9.4 | -9.5 |
| -10 | 32.6 | 32.8 |
| -9 | 1.5* | -0.3 |
| -8 | 2.0 | -1.2 |
| -7 | 3.5 | 4.2 |
| -6 | 29.9 | 30.1 |
| -5 | 7.6 | 7.6 |
| -4 | 2.3 | -1.9 |
| -3 | 1.6* | 0.2 |
| -2 | 32.9 | 32.8 |
| -1 | 18.3 | 18.4 |
| 0 | 15.3 | 15.4 |
| 1 | 7.7 | -7.6 |
| 2 | 10.2 | -9.8 |
| 3 | 1.6* | -0.2 |
| 4 | 23.6 | 23.1 |
| 5 | 5.6 | 5.1 |
| 6 | 28.7 | -28.1 |
| 7 | 16.7 | -16.7 |
| 8 | 8.5 | 8.2 |
| 9 | 10.5 | 10.6 |
| 10 | 2.9 | -2.6 |
| 11 | 1.2* | 0.3 |
| 12 | 1.2* | 0.5 |
| 13 | 15.9 | -15.6 |
| 14 | 9.9 | 9.4 |
| 15 | 4.8 | 5.0 |
| (H,7,4) | | |
| -13 | 4.4 | -4.3 |
| -12 | 5.3 | 5.1 |
| -11 | 1.3 | -1.3 |
| -10 | 6.1 | 6.0 |
| -9 | 11.3 | 12.3 |
| -8 | 7.1 | -7.1 |
| -7 | 4.5 | 4.2 |
| -6 | 2.8 | -2.5 |
| -5 | 13.9 | -14.4 |
| -4 | 2.9 | -2.5 |
| -3 | 15.3 | 15.2 |
| -2 | 8.8 | 9.0 |
| -1 | 4.3 | -4.3 |
| 0 | 9.2 | 9.2 |
| 1 | 10.0 | 9.7 |
| 2 | 6.0 | -5.8 |
| 3 | 7.4 | 7.3 |
| 4 | 6.8 | 6.8 |
| 5 | 1.2* | 1.7 |
| 6 | 18.2 | 18.0 |
| 7 | 20.2 | 19.7 |
| 8 | 11.6 | -11.3 |
| 9 | 4.2 | -4.3 |
| 10 | 1.6 | -1.7 |
| 11 | 17.1 | 17.5 |
| (H,8,4) | | |
| -4 | 0.6* | -1.8 |
| -3 | 6.9 | 7.3 |
| -2 | 0.7* | 0.1 |
| -1 | 4.2 | 4.5 |
| 0 | 18.9 | 19.4 |
| 1 | 2.0 | 1.9 |
| 2 | 5.5 | 5.2 |
| (H,0,5) | | |
| -23 | 10.4 | 10.3 |
| -21 | 27.3 | 27.0 |
| -19 | 10.6 | -10.3 |
| -17 | 22.8 | 22.7 |
| -15 | 3.5 | 1.7 |
| -13 | 1.6* | 2.6 |
| -11 | 27.0 | 27.3 |
| -9 | 20.0 | 20.7 |
| -7 | 34.2 | 36.6 |
| -5 | 48.1 | -49.7 |
| -3 | 16.6 | 16.9 |
| -1 | 25.3 | 25.5 |
| 1 | 2.0 | 3.8 |
| 3 | 15.1 | 15.7 |
| 5 | 23.2 | -22.6 |
| 7 | 11.5 | -10.9 |
| 9 | 13.0 | 13.6 |
| 11 | 32.2 | 31.6 |
| 13 | 12.6 | -12.4 |
| 15 | 38.4 | 38.1 |
| 17 | 1.5* | -1.2 |
| 19 | 9.1 | 8.6 |
| 21 | 1.0* | -0.7 |
| (H,1,5) | | |
| -24 | 0.8* | -1.5 |
| -23 | 10.7 | 10.4 |
| -22 | 4.4 | 4.5 |
| -21 | 4.6 | -5.1 |
| -20 | 16.0 | 16.3 |
| -19 | 6.7 | -6.6 |
| -18 | 1.6* | 0.9 |
| -17 | 21.6 | -22.4 |
| -16 | 3.6 | -4.2 |
| -15 | 26.0 | 25.8 |
| -14 | 5.6 | -6.0 |
| -13 | 13.7 | -13.3 |
| -12 | 14.1 | -13.8 |
| -11 | 4.4 | 4.6 |
| -10 | 39.6 | 40.2 |
| -9 | 1.4* | 0.6 |
| -8 | 35.1 | -36.3 |
| -7 | 14.7 | 14.1 |
| -6 | 58.9 | 58.7 |
| -5 | 14.6 | -15.2 |
| -4 | 22.0 | 21.8 |
| -3 | 14.5 | 14.2 |
| -2 | 29.4 | 29.3 |
| -1 | 12.0 | 12.4 |
| 0 | 37.7 | 38.1 |
| 1 | 11.2 | -10.6 |
| 2 | 33.1 | 32.6 |
| 3 | 2.3 | -2.2 |
| 4 | 46.0 | 45.1 |
| 5 | 6.5 | -6.3 |
| 6 | 23.5 | -24.0 |
| 7 | 16.5 | -16.6 |
| 8 | 45.3 | 46.9 |
| 9 | 36.6 | 37.5 |
| 10 | 11.1 | 10.9 |
| 11 | 8.2 | -8.1 |
| 12 | 13.9 | -14.3 |
| 13 | 17.6 | -17.5 |
| 14 | 7.9 | 8.2 |
| 15 | 8.7 | 9.3 |
| 16 | 10.3 | -9.9 |
| 17 | 9.4 | -8.8 |
| 18 | 2.1 | 0.8 |
| 19 | 2.1 | 1.4 |
| 20 | 4.2 | 4.2 |
| 21 | 8.4 | 8.0 |
| (H,2,5) | | |
| -23 | 8.1 | 7.6 |
| -22 | 7.5 | -7.9 |
| -21 | 7.5 | 7.6 |
| -20 | 5.5 | 5.7 |
| -19 | 21.1 | -20.4 |
| -18 | 1.5* | 0.1 |
| -17 | 42.3 | 41.9 |
| -16 | 5.5 | -4.5 |
| -15 | 3.8 | -3.4 |
| -14 | 7.9 | 8.3 |
| -13 | 1.6* | 1.7 |
| -12 | 10.6 | 10.4 |
| -11 | 15.6 | 16.2 |
| -10 | 24.0 | -24.9 |
| -9 | 17.0 | 16.3 |
| -8 | 7.4 | 7.5 |
| -7 | 2.1 | -4.3 |
| -6 | 14.6 | -14.7 |
| -5 | 18.3 | -19.0 |
| -4 | 18.3 | -18.2 |
| -3 | 39.5 | 40.8 |
| -2 | 4.1 | 4.1 |
| -1 | 15.5 | -16.5 |
| 0 | 11.5 | 11.1 |
| 1 | 66.7 | 68.4 |
| 2 | 3.8 | 3.3 |
| 3 | 24.2 | -23.9 |
| 4 | 1.9 | 2.2 |
| 5 | 17.5 | 17.2 |
| 6 | 5.8 | 5.7 |
| 7 | 1.5* | 1.7 |
| 8 | 10.6 | 11.3 |
| 9 | 3.1 | 2.1 |
| 10 | 15.9 | 16.4 |
| 11 | 8.4 | -9.3 |
| 12 | 15.9 | -15.5 |
| 13 | 20.5 | -19.5 |
| 14 | 1.6* | -1.4 |
| 15 | 45.7 | 46.5 |
| 16 | 4.7 | -4.4 |
| 17 | 8.5 | -8.9 |
| 18 | 5.5 | -5.3 |
| 19 | 23.2 | 23.0 |
| 20 | 2.5 | 2.1 |
| 21 | 10.1 | 10.5 |
| (H,3,5) | | |
| -22 | 7.9 | -7.9 |
| -21 | 2.2 | 2.5 |
| -20 | 8.8 | 8.8 |
| -19 | 2.0 | 1.6 |
| -18 | 2.8 | 3.1 |
| -17 | 18.2 | 17.7 |
| -16 | 17.0 | 16.7 |
| -15 | 9.1 | 9.4 |
| -14 | 3.6 | 2.9 |
| -13 | 23.5 | 22.8 |
| -12 | 7.7 | -7.8 |
| -11 | 34.8 | -35.5 |
| -10 | 22.1 | 22.3 |
| -9 | 20.4 | -21.3 |
| -8 | 3.4 | -2.8 |
| -7 | 5.2 | -5.5 |
| -6 | 22.9 | 22.6 |
| -5 | 29.1 | -28.8 |
| -4 | 19.2 | 19.0 |
| -3 | 6.4 | -6.7 |
| -2 | 23.6 | 23.8 |
| -1 | 12.1 | 11.6 |
| 0 | 23.0 | 22.0 |
| 1 | 23.4 | 23.0 |
| 2 | 30.1 | -30.0 |
| 3 | 3.9 | -3.0 |
| 4 | 51.9 | 52.6 |
| 5 | 2.8 | 2.4 |
| 6 | 2.1 | -1.2 |
| 7 | 4.9 | 4.3 |
| 8 | 46.9 | 46.6 |
| 9 | 17.1 | 16.4 |
| 10 | 3.2 | -4.1 |
| 11 | 12.6 | 12.7 |
| 12 | 8.2 | 8.4 |
| 13 | 4.6 | 4.7 |
| 14 | 2.8 | 2.3 |
| 15 | 7.2 | -7.5 |
| 16 | 3.7 | -3.7 |
| 17 | 6.7 | -6.1 |
| 18 | 11.3 | 11.6 |
| 19 | 15.0 | -14.9 |
| 20 | 4.4 | -3.7 |
| (H,4,5) | | |
| -21 | 13.3 | 13.8 |
| -20 | 3.2 | 3.3 |
| -19 | 9.4 | -9.3 |
| -18 | 6.9 | 6.3 |
| -17 | 38.0 | 38.6 |
| -16 | 1.4* | 0.5 |
| -15 | 6.2 | 6.5 |
| -14 | 7.6 | -7.8 |
| -13 | 14.0 | 13.5 |
| -12 | 13.6 | -13.2 |
| -11 | 10.5 | 9.6 |
| -10 | 21.7 | 22.5 |
| -9 | 22.0 | 22.2 |
| -8 | 1.6* | -2.6 |
| -7 | 16.8 | 15.8 |
| -6 | 6.8 | -6.7 |
| -5 | 5.3 | -5.1 |
| -4 | 6.4 | 6.2 |
| -3 | 4.9 | 5.1 |
| -2 | 15.0 | -15.6 |
| -1 | 14.8 | -14.2 |
| 0 | 12.2 | -12.8 |
| 1 | 21.8 | -21.9 |
| 2 | 6.8 | 7.4 |
| 3 | 22.5 | -22.3 |
| 4 | 32.6 | 32.3 |
| 5 | 7.8 | -8.1 |
| 6 | 4.3 | -4.9 |
| 7 | 29.7 | 29.2 |
| 8 | 2.0 | -2.8 |
| 9 | 15.7 | 15.2 |
| 10 | 4.0 | 4.8 |
| 11 | 19.2 | 20.1 |
| 12 | 6.9 | -6.8 |
| 13 | 9.6 | 9.8 |
| 14 | 8.0 | -8.1 |
| 15 | 24.2 | 23.3 |
| 16 | 6.9 | 6.8 |
| 17 | 5.6 | 5.5 |
| 18 | 2.2 | -2.5 |
| (H,5,5) | | |
| -19 | 4.0 | -4.1 |
| -18 | 4.9 | 5.3 |
| -17 | 7.5 | -7.8 |
| -16 | 1.2* | 1.5 |
| -15 | 10.8 | 10.9 |
| -14 | 9.2 | 8.7 |
| -13 | 18.4 | -18.8 |
| -12 | 2.0 | -1.9 |
| -11 | 6.6 | 6.9 |
| -10 | 41.6 | 42.3 |
| -9 | 10.0 | 10.0 |
| -8 | 23.1 | -23.4 |
| -7 | 4.2 | 3.8 |
| -6 | 24.4 | 23.7 |
| -5 | 27.3 | 28.5 |
| -4 | 9.8 | 8.9 |
| -3 | 20.3 | -20.1 |
| -2 | 1.6* | -0.9 |
| -1 | 1.6* | 0.9 |
| 0 | 10.1 | 10.1 |
| 1 | 1.3 | -1.4 |
| 2 | 7.5 | 7.7 |
| 3 | 1.6* | -0.2 |
| 4 | 20.0 | 19.6 |
| 5 | 10.7 | -10.3 |
| 6 | 8.9 | -8.7 |
| 7 | 2.8 | -2.8 |
| 8 | 30.0 | 29.4 |
| 9 | 15.1 | -14.5 |
| 10 | 1.5* | 0.4 |
| 11 | 13.6 | 13.6 |
| 12 | 11.7 | 11.6 |
| 13 | 3.7 | -3.7 |
| 14 | 14.2 | 14.0 |
| 15 | 2.5 | -2.0 |
| 16 | 0.8* | -0.2 |
| (H,6,5) | | |
| -16 | 0.7* | -0.9 |
| -15 | 3.2 | 3.2 |
| -14 | 11.1 | -11.3 |
| -13 | 11.4 | 11.1 |
| -12 | 4.5 | -4.3 |
| -11 | 7.9 | 7.5 |
| -10 | 17.4 | 17.6 |
| -9 | 1.4* | 0.0 |
| -8 | 2.5 | -2.9 |
| -7 | 13.1 | 13.7 |
| -6 | 16.5 | 15.8 |
| -5 | 10.6 | -10.6 |
| -4 | 6.7 | 6.8 |
| -3 | 14.9 | 15.1 |
| -2 | 13.7 | -13.9 |
| -1 | 19.0 | -19.1 |
| 0 | 6.0 | 5.9 |
| 1 | 32.0 | 31.4 |
| 2 | 6.3 | 6.5 |
| 3 | 3.3 | -3.4 |
| 4 | 16.8 | -16.5 |
| 5 | 5.8 | 5.4 |
| 6 | 14.0 | 14.0 |
| 7 | 2.5 | -2.2 |
| 8 | 19.1 | -18.6 |
| 9 | 1.2* | 0.9 |
| 10 | 8.0 | -7.7 |
| 11 | 13.0 | 12.6 |
| 12 | 10.2 | 10.0 |
| 13 | 15.1 | -14.6 |
| (H,7,5) | | |
| -11 | 3.7 | -3.7 |
| -10 | 12.4 | 12.1 |
| -9 | 4.1 | -4.0 |
| -8 | 6.2 | -6.4 |
| -7 | 2.3 | -2.4 |
| -6 | 7.5 | 7.4 |
| -5 | 1.8 | 2.2 |
| -4 | 2.7 | -2.4 |
| -3 | 1.5 | 1.7 |
| -2 | 16.3 | 16.5 |
| -1 | 5.3 | -5.2 |
| 0 | 10.1 | 10.3 |
| 1 | 21.3 | 21.5 |
| 2 | 14.3 | 14.0 |
| 3 | 12.0 | -11.3 |
| 4 | 24.6 | 24.4 |
| 5 | 10.9 | -10.6 |
| 6 | 9.4 | -9.3 |
| 7 | 4.5 | -4.3 |
| 8 | 3.5 | 3.7 |
| (H,0,6) | | |
| -22 | 34.7 | -33.9 |
| -20 | 13.7 | 13.3 |
| -18 | 1.5* | -2.1 |
| -16 | 2.5 | 3.7 |
| -14 | 9.3 | -9.1 |
| -12 | 17.4 | 16.9 |
| -10 | 50.8 | 53.2 |
| -8 | 27.2 | -27.7 |
| -6 | 43.3 | 44.2 |
| -4 | 2.4 | -1.2 |
| -2 | 13.0 | 14.4 |
| 0 | 21.5 | 20.9 |
| 2 | 17.4 | -17.5 |
| 4 | 20.1 | 22.3 |
| 6 | 9.8 | 8.8 |
| 8 | 18.5 | -19.9 |
| 10 | 12.1 | 12.3 |
| 12 | 33.4 | 34.0 |
| 14 | 34.4 | 33.3 |
| 16 | 17.3 | -17.3 |
| 18 | 23.2 | 22.9 |
| 20 | 16.5 | 15.4 |
| (H,1,6) | | |
| -23 | 8.2 | 8.1 |
| -22 | 3.1 | -3.0 |
| -21 | 11.6 | 11.2 |
| -20 | 2.8 | 2.4 |
| -19 | 13.7 | -14.0 |
| -18 | 6.0 | -5.7 |
| -17 | 4.7 | 4.6 |
| -16 | 4.5 | -4.1 |
| -15 | 3.5 | 3.3 |
| -14 | 6.5 | -7.2 |
| -13 | 27.9 | 26.7 |
| -12 | 11.4 | 11.2 |
| -11 | 8.9 | 8.3 |
| -10 | 27.6 | -27.4 |
| -9 | 17.6 | 18.3 |
| -8 | 10.9 | 11.1 |
| -7 | 57.6 | 57.4 |
| -6 | 27.9 | -28.2 |
| -5 | 3.3 | 3.6 |
| -4 | 44.4 | 45.3 |
| -3 | 6.4 | 7.2 |
| -2 | 1.4* | 2.1 |
| -1 | 5.7 | -6.4 |
| 0 | 52.0 | 52.5 |
| 1 | 66.1 | 67.3 |
| 2 | 23.4 | -22.4 |
| 3 | 31.5 | -30.1 |
| 4 | 3.6 | -3.1 |
| 5 | 10.3 | 9.7 |
| 6 | 10.4 | 10.2 |
| 7 | 16.9 | -16.8 |
| 8 | 30.4 | -31.6 |
| 9 | 14.8 | -14.9 |
| 10 | 6.6 | -6.6 |
| 11 | 11.5 | 11.1 |
| 12 | 10.8 | 11.9 |
| 13 | 14.2 | -14.6 |
| 14 | 13.5 | -14.0 |
| 15 | 26.9 | 27.3 |
| 16 | 5.6 | -5.6 |
| 17 | 2.8 | -2.4 |
| 18 | 10.7 | 10.6 |
| 19 | 11.0 | 11.4 |
| 20 | 2.0 | -2.1 |
| (H,2,6) | | |
| -22 | 5.6 | 5.5 |
| -21 | 8.6 | 8.4 |
| -20 | 7.5 | 7.1 |
| -19 | 9.7 | -9.4 |
| -18 | 14.7 | 14.5 |
| -17 | 1.5* | 0.8 |
| -16 | 9.3 | 9.4 |
| -15 | 8.9 | -8.7 |
| -14 | 2.0 | 0.0 |
| -13 | 6.3 | 6.2 |
| -12 | 21.8 | -21.8 |
| -11 | 11.9 | 13.0 |
| -10 | 8.9 | 9.2 |
| -9 | 24.6 | -24.0 |
| -8 | 39.2 | -38.5 |
| -7 | 34.9 | -34.4 |
| -6 | 31.0 | 30.9 |
| -5 | 23.8 | 23.8 |
| -4 | 18.6 | 18.6 |
| -3 | 20.1 | 19.2 |
| -2 | 23.9 | 24.3 |
| -1 | 5.2 | -4.9 |
| 0 | 13.1 | 12.7 |
| 1 | 32.5 | 32.9 |
| 2 | 10.3 | -11.3 |
| 3 | 1.5* | 0.9 |
| 4 | 53.6 | 53.9 |
| 5 | 2.8 | -2.2 |
| 6 | 1.6* | -1.6 |
| 7 | 13.8 | -13.7 |
| 8 | 27.8 | 28.3 |
| 9 | 1.6* | -1.5 |
| 10 | 5.0 | 5.7 |
| 11 | 3.8 | 3.5 |
| 12 | 47.1 | 47.6 |
| 13 | 2.8 | 2.9 |
| 14 | 22.4 | -22.6 |
| 15 | 23.0 | -22.4 |
| 16 | 1.6 | 1.4 |
| 17 | 7.6 | 7.5 |
| 18 | 2.5 | 1.9 |
| 19 | 6.5 | -6.7 |
| (H,3,6) | | |
| -21 | 13.2 | 13.3 |
| -20 | 2.6 | 2.4 |
| -19 | 14.1 | -14.2 |
| -18 | 2.1 | -2.4 |
| -17 | 27.6 | 27.6 |
| -16 | 4.3 | 4.5 |
| -15 | 1.5* | -0.2 |
| -14 | 10.9 | -11.0 |
| -13 | 33.7 | 33.3 |
| -12 | 13.2 | -13.2 |
| -11 | 2.9 | -2.6 |
| -10 | 20.6 | 21.0 |
| -9 | 6.7 | -7.3 |
| -8 | 18.4 | -18.5 |
| -7 | 17.4 | 16.8 |
| -6 | 7.4 | 6.7 |
| -5 | 47.5 | 48.8 |
| -4 | 10.7 | -10.5 |
| -3 | 29.8 | -30.5 |
| -2 | 1.6* | -0.5 |
| -1 | 2.1 | -1.1 |
| 0 | 8.2 | -8.3 |
| 1 | 49.3 | 50.2 |
| 2 | 2.7 | -1.5 |
| 3 | 19.3 | -20.0 |
| 4 | 7.3 | 6.9 |
| 5 | 10.6 | 10.1 |
| 6 | 29.7 | 31.0 |
| 7 | 20.1 | 19.7 |
| 8 | 14.9 | 14.7 |
| 9 | 6.7 | -6.2 |
| 10 | 14.3 | -14.3 |
| 11 | 15.5 | 15.0 |
| 12 | 3.9 | 4.4 |
| 13 | 19.9 | -19.2 |
| 14 | 10.4 | -10.5 |
| 15 | 9.5 | 10.3 |
| 16 | 9.5 | -9.9 |
| 17 | 1.1* | 0.4 |
| 18 | 2.9 | -3.3 |
| (H,4,6) | | |
| -20 | 3.4 | 3.3 |
| -19 | 9.7 | 9.8 |
| -18 | 1.1* | -0.3 |
| -17 | 16.0 | -16.0 |
| -16 | 17.3 | 17.7 |
| -15 | 8.4 | 8.2 |
| -14 | 5.6 | 5.9 |
| -13 | 9.5 | 9.7 |
| -12 | 6.1 | 6.1 |
| -11 | 3.5 | -3.8 |
| -10 | 27.2 | 27.3 |
| -9 | 10.3 | -10.4 |
| -8 | 40.9 | -40.1 |
| -7 | 3.2 | 1.0 |
| -6 | 32.7 | 33.5 |
| -5 | 9.6 | 9.4 |
| -4 | 7.9 | -8.2 |
| -3 | 8.7 | -7.7 |
| -2 | 18.9 | -19.7 |
| -1 | 3.3 | -1.9 |
| 0 | 22.7 | 23.1 |
| 1 | 4.9 | 5.1 |
| 2 | 9.4 | -9.6 |
| 3 | 5.9 | 4.9 |
| 4 | 27.3 | 26.7 |
| 5 | 4.3 | -3.8 |
| 6 | 17.7 | 18.8 |
| 7 | 5.2 | 5.3 |
| 8 | 14.2 | 14.6 |
| 9 | 18.8 | -19.1 |
| 10 | 8.1 | 7.3 |
| 11 | 14.9 | 15.0 |
| 12 | 24.0 | 23.7 |
| 13 | 4.2 | -4.4 |
| 14 | 3.7 | 3.9 |
| 15 | 3.0 | 2.7 |
| 16 | 3.3 | 3.1 |
| 17 | 2.8 | 3.0 |
| (H,5,6) | | |
| -17 | 19.5 | 19.4 |
| -16 | 1.0* | -1.6 |
| -15 | 4.3 | 4.5 |
| -14 | 4.0 | 4.1 |
| -13 | 8.1 | 8.0 |
| -12 | 18.0 | -18.3 |
| -11 | 10.7 | 10.5 |
| -10 | 2.6 | 1.5 |
| -9 | 2.5 | 1.8 |
| -8 | 20.1 | 20.7 |
| -7 | 17.0 | 17.4 |
| -6 | 4.8 | -4.9 |
| -5 | 2.8 | -2.3 |
| -4 | 9.4 | 8.5 |
| -3 | 16.4 | 16.2 |
| -2 | 4.3 | 4.9 |
| -1 | 14.5 | -14.7 |
| 0 | 1.6* | -0.8 |
| 1 | 29.9 | 29.9 |
| 2 | 3.7 | -3.6 |
| 3 | 17.3 | -17.5 |
| 4 | 9.3 | -9.0 |
| 5 | 18.5 | 18.9 |
| 6 | 15.5 | 16.0 |
| 7 | 1.5* | 1.1 |
| 8 | 8.4 | -9.2 |
| 9 | 2.9 | -3.2 |
| 10 | 15.5 | -15.0 |
| 11 | 21.9 | 21.1 |
| 12 | 7.0 | -7.0 |
| 13 | 12.6 | -12.0 |
| 14 | 16.5 | 15.8 |
| (H,6,6) | | |
| -14 | 9.6 | -9.6 |
| -13 | 9.8 | 9.9 |
| -12 | 3.1 | -2.6 |
| -11 | 3.0 | 3.0 |
| -10 | 12.9 | 12.6 |
| -9 | 2.4 | -1.8 |
| -8 | 13.9 | -14.4 |
| -7 | 5.0 | -4.9 |
| -6 | 11.2 | 11.1 |
| -5 | 6.5 | 6.0 |
| -4 | 11.3 | -11.2 |
| -3 | 9.5 | 9.1 |
| -2 | 9.2 | 9.2 |
| -1 | 18.6 | -17.9 |
| 0 | 17.9 | 18.3 |
| 1 | 1.4* | 0.2 |
| 2 | 5.0 | 5.2 |
| 3 | 12.1 | 11.5 |
| 4 | 14.7 | 14.2 |
| 5 | 13.5 | -13.2 |
| 6 | 13.4 | 13.4 |
| 7 | 8.7 | -8.7 |
| 8 | 14.9 | 14.5 |
| 9 | 6.4 | 6.3 |
| 10 | 7.4 | -7.4 |
| 11 | 6.3 | -6.3 |
| (H,7,6) | | |
| -8 | 5.2 | 5.3 |
| -7 | 4.7 | 4.7 |
| -6 | 6.7 | -6.6 |
| -5 | 4.8 | 5.2 |
| -4 | 3.4 | -3.5 |
| -3 | 10.1 | 10.2 |
| -2 | 2.4 | -1.5 |
| -1 | 3.9 | 3.7 |
| 0 | 11.3 | -10.6 |
| 1 | 15.5 | 15.3 |
| 2 | 12.2 | -12.3 |
| 3 | 12.4 | -12.1 |
| 4 | 7.0 | 6.5 |
| 5 | 6.9 | 6.7 |
| (H,0,7) | | |
| -21 | 20.6 | 20.1 |
| -19 | 8.9 | -8.5 |
| -17 | 5.5 | 5.1 |
| -15 | 20.9 | -21.6 |
| -13 | 26.8 | 27.6 |
| -11 | 10.1 | 10.3 |
| -9 | 40.3 | 40.7 |
| -7 | 15.7 | 16.7 |
| -5 | 27.6 | 27.8 |
| -3 | 30.6 | 30.8 |
| -1 | 38.3 | -39.1 |
| 1 | 47.8 | 48.8 |
| 3 | 21.5 | -22.1 |
| 5 | 22.6 | 22.8 |
| 7 | 25.4 | -24.9 |
| 9 | 7.1 | 7.1 |
| 11 | 35.2 | 33.9 |
| 13 | 21.3 | -21.4 |
| 15 | 22.9 | 22.2 |
| 17 | 23.8 | 23.8 |
| (H,1,7) | | |
| -22 | 5.4 | -5.4 |
| -21 | 4.1 | -3.9 |
| -20 | 22.1 | 21.9 |
| -19 | 13.4 | -13.0 |
| -18 | 6.3 | -6.0 |
| -17 | 1.4* | 0.5 |
| -16 | 12.3 | 11.9 |
| -15 | 16.5 | -16.4 |
| -14 | 14.6 | 14.8 |
| -13 | 5.9 | -5.4 |
| -12 | 5.2 | 5.8 |
| -11 | 4.2 | 4.0 |
| -10 | 26.6 | 25.9 |
| -9 | 1.6* | 0.9 |
| -8 | 9.2 | -9.1 |
| -7 | 3.4 | 3.6 |
| -6 | 19.7 | 19.7 |
| -5 | 11.6 | 11.5 |
| -4 | 19.2 | -19.7 |
| -3 | 7.1 | 6.7 |
| -2 | 14.2 | 14.6 |
| -1 | 22.5 | 22.3 |
| 0 | 19.0 | 18.9 |
| 1 | 3.3 | 3.3 |
| 2 | 32.8 | -32.7 |
| 3 | 7.0 | 6.6 |
| 4 | 3.9 | 3.0 |
| 5 | 30.0 | -28.8 |
| 6 | 10.1 | 9.5 |
| 7 | 16.2 | 16.7 |
| 8 | 8.4 | 8.2 |
| 9 | 11.3 | -10.8 |
| 10 | 4.5 | -4.8 |
| 11 | 14.7 | -15.7 |
| 12 | 37.7 | 37.7 |
| 13 | 1.5* | -0.8 |
| 14 | 7.3 | 8.1 |
| 15 | 7.2 | -7.5 |
| 16 | 20.2 | 20.9 |
| 17 | 2.5 | -2.5 |
| 18 | 4.6 | 4.8 |
| (H,2,7) | | |
| -21 | 7.9 | 7.9 |
| -20 | 5.4 | -4.7 |
| -19 | 7.5 | 7.5 |
| -18 | 5.3 | -5.4 |
| -17 | 4.0 | -4.2 |
| -16 | 1.4* | -1.1 |
| -15 | 1.5* | -2.1 |
| -14 | 1.6* | 1.1 |
| -13 | 22.7 | 22.5 |
| -12 | 8.9 | -9.4 |
| -11 | 6.5 | 6.3 |
| -10 | 4.5 | -5.1 |
| -9 | 6.8 | 6.3 |
| -8 | 14.1 | 15.0 |
| -7 | 10.0 | 9.9 |
| -6 | 1.6* | -0.9 |
| -5 | 2.5 | 2.0 |
| -4 | 5.8 | 5.3 |
| -3 | 16.8 | 16.6 |

Table 2 (*cont.*)

| H | OBS | CALC |
|---|---|---|
| (H,2,7) | | |
| -2 | 12.7 | 12.9 |
| -1 | 1.6* | 0.6 |
| 0 | 20.5 | 20.2 |
| 1 | 29.7 | 29.4 |
| 2 | 13.6 | -13.6 |
| 3 | 9.0 | 8.5 |
| 4 | 11.3 | -11.5 |
| 5 | 43.9 | 46.5 |
| 6 | 12.2 | -11.8 |
| 7 | 8.5 | 8.6 |
| 8 | 12.2 | 12.4 |
| 9 | 4.2 | -4.9 |
| 10 | 4.9 | -4.7 |
| 11 | 11.5 | 12.6 |
| 12 | 9.1 | -9.1 |
| 13 | 22.5 | -22.8 |
| 14 | 5.9 | -5.8 |
| 15 | 8.0 | 7.7 |
| 16 | 5.7 | 5.6 |
| 17 | 0.9* | 0.2 |
| (H,3,7) | | |
| -20 | 16.5 | 16.9 |
| -19 | 4.6 | -4.4 |
| -18 | 3.8 | 3.3 |
| -17 | 2.5 | 2.3 |
| -16 | 10.0 | 9.7 |
| -15 | 4.4 | 4.9 |
| -14 | 21.8 | 21.7 |
| -13 | 8.3 | 7.9 |
| -12 | 23.5 | -22.8 |
| -11 | 1.6* | -0.2 |
| -10 | 26.1 | 25.6 |
| -9 | 11.4 | 12.1 |
| -8 | 12.1 | -11.6 |
| -7 | 9.9 | -9.9 |
| -6 | 6.5 | -6.1 |
| -5 | 13.2 | -13.2 |
| -4 | 1.6* | 0.8 |
| -3 | 10.8 | 10.5 |
| -2 | 39.6 | 39.7 |
| -1 | 6.0 | 5.8 |
| 0 | 15.9 | -16.4 |
| 1 | 6.2 | 6.1 |
| 2 | 9.1 | -9.4 |
| 3 | 10.5 | -10.8 |
| 4 | 20.9 | 20.4 |
| 5 | 4.7 | 4.7 |
| 6 | 6.8 | 7.1 |
| 7 | 21.1 | -20.8 |
| 8 | 25.0 | 24.7 |
| 9 | 1.6* | -1.5 |
| 10 | 9.6 | -9.2 |
| 11 | 1.4* | 2.2 |
| 12 | 12.8 | 13.3 |
| 13 | 7.8 | 7.2 |
| 14 | 6.1 | 5.9 |
| 15 | 4.3 | 4.5 |
| 16 | 11.4 | 11.4 |
| (H,4,7) | | |
| -18 | 11.4 | 11.6 |
| -17 | 4.1 | 4.0 |
| -16 | 3.5 | -3.6 |
| -15 | 7.5 | -7.6 |
| -14 | 8.9 | -8.9 |
| -13 | 22.1 | 22.1 |
| -12 | 1.4* | -0.4 |
| -11 | 28.2 | -28.4 |
| -10 | 1.5* | -1.5 |
| -9 | 29.0 | 29.2 |
| -8 | 4.8 | 5.1 |
| -7 | 1.6* | 0.5 |
| -6 | 10.2 | 10.0 |
| (H,4,7) | | |
| -5 | 11.9 | 11.8 |
| -4 | 4.9 | 4.6 |
| -3 | 47.3 | 48.4 |
| -2 | 8.9 | -9.1 |
| -1 | 5.0 | -4.6 |
| 0 | 8.0 | -8.3 |
| 1 | 14.5 | 14.4 |
| 2 | 9.0 | 9.4 |
| 3 | 1.6* | 2.7 |
| 4 | 18.2 | -18.2 |
| 5 | 10.7 | 10.4 |
| 6 | 6.4 | 5.3 |
| 7 | 4.0 | 3.1 |
| 8 | 14.5 | 14.1 |
| 9 | 4.1 | 4.0 |
| 10 | 2.4 | -2.1 |
| 11 | 9.1 | 9.1 |
| 12 | 9.1 | -9.0 |
| 13 | 13.9 | -14.2 |
| 14 | 1.3 | 1.7 |
| 15 | 13.3 | 12.6 |
| (H,5,7) | | |
| -16 | 3.5 | -3.5 |
| -15 | 7.1 | -7.3 |
| -14 | 13.2 | 13.3 |
| -13 | 7.3 | -6.5 |
| -12 | 7.3 | -7.1 |
| -11 | 7.6 | 7.8 |
| -10 | 6.1 | 6.4 |
| -9 | 3.2 | 3.0 |
| -8 | 1.6 | 1.2 |
| -7 | 5.5 | 5.4 |
| -6 | 9.1 | 8.9 |
| -5 | 7.6 | -7.1 |
| -4 | 11.0 | -11.2 |
| -3 | 8.1 | 8.3 |
| -2 | 17.9 | 17.6 |
| -1 | 3.3 | -3.6 |
| 0 | 4.3 | 4.1 |
| 1 | 7.2 | -7.2 |
| 2 | 3.9 | -3.4 |
| 3 | 18.8 | 19.0 |
| 4 | 20.3 | 20.2 |
| 5 | 2.0 | -2.5 |
| 6 | 3.9 | -4.0 |
| 7 | 4.8 | 5.0 |
| 8 | 15.6 | 15.8 |
| 9 | 14.8 | -14.6 |
| 10 | 12.1 | -11.5 |
| 11 | 6.2 | 5.8 |
| 12 | 12.8 | 12.8 |
| (H,6,7) | | |
| -12 | 13.5 | -13.7 |
| -11 | 2.2 | -2.0 |
| -10 | 0.9* | -0.1 |
| -9 | 2.3 | 1.9 |
| -8 | 6.4 | 6.4 |
| -7 | 7.9 | 7.8 |
| -6 | 3.4 | -3.5 |
| -5 | 7.0 | -6.9 |
| -4 | 9.3 | -9.5 |
| -3 | 14.0 | 14.5 |
| -2 | 3.0 | 2.5 |
| -1 | 2.6 | -2.7 |
| 0 | 1.2* | -1.8 |
| 1 | 31.9 | 31.1 |
| 2 | 2.2 | -1.5 |
| 3 | 8.4 | 8.2 |
| 4 | 1.2 | -1.3 |
| 5 | 16.8 | 16.6 |
| 6 | 6.0 | 5.9 |
| 7 | 6.4 | -6.2 |
| 8 | 6.7 | 6.9 |
| (H,0,8) | | |
| -20 | 20.0 | 19.2 |
| -18 | 10.2 | -10.2 |
| -16 | 19.0 | 19.0 |
| -14 | 3.1 | 3.3 |
| -12 | 9.5 | 9.0 |
| -10 | 37.3 | 37.9 |
| -8 | 14.1 | 14.7 |
| -6 | 8.4 | -8.6 |
| -4 | 13.5 | -14.0 |
| -2 | 31.4 | 31.8 |
| 0 | 17.1 | -17.5 |
| 2 | 22.9 | 23.0 |
| 4 | 2.4 | 2.2 |
| 6 | 19.2 | -19.5 |
| 8 | 19.0 | 18.1 |
| 10 | 24.0 | -23.9 |
| 12 | 27.2 | 27.1 |
| 14 | 5.7 | 6.3 |
| 16 | 0.9* | -0.4 |
| (H,1,8) | | |
| -20 | 6.0 | 5.5 |
| -19 | 1.0* | 1.3 |
| -18 | 12.3 | -12.1 |
| -17 | 10.7 | 10.2 |
| -16 | 6.5 | 6.7 |
| -15 | 2.4 | -1.8 |
| -14 | 9.0 | 8.1 |
| -13 | 6.3 | 6.2 |
| -12 | 1.6* | -3.2 |
| -11 | 13.6 | -14.1 |
| -10 | 1.6* | -1.3 |
| -9 | 33.9 | 34.4 |
| -8 | 2.9 | -2.9 |
| -7 | 4.4 | -4.6 |
| -6 | 20.5 | -20.5 |
| -5 | 2.8 | -3.1 |
| -4 | 18.0 | 18.4 |
| -3 | 22.6 | 22.7 |
| -2 | 9.5 | 9.1 |
| -1 | 34.0 | -34.2 |
| 0 | 2.4 | 2.2 |
| 1 | 42.5 | 43.3 |
| 2 | 1.6* | 0.2 |
| 3 | 6.3 | 6.3 |
| 4 | 12.8 | 13.0 |
| 5 | 13.4 | 13.2 |
| 6 | 28.6 | -28.7 |
| 7 | 17.0 | 17.3 |
| 8 | 1.6* | 0.2 |
| 9 | 24.6 | 24.5 |
| 10 | 7.1 | 7.0 |
| 11 | 1.4* | 5.1 |
| 12 | 4.0 | -4.0 |
| 13 | 7.5 | 7.5 |
| 14 | 3.0 | 2.8 |
| 15 | 6.7 | 6.8 |
| 16 | 4.7 | -4.8 |
| (H,2,8) | | |
| -19 | 2.2 | -2.2 |
| -18 | 12.5 | 12.6 |
| -17 | 12.9 | -12.3 |
| -16 | 20.4 | 19.9 |
| -15 | 4.0 | -4.3 |
| -14 | 14.9 | 14.7 |
| -13 | 23.6 | 23.1 |
| -12 | 11.8 | -12.0 |
| -11 | 1.5* | -0.8 |
| -10 | 27.2 | 26.5 |
| (H,2,8) | | |
| -9 | 7.0 | 7.2 |
| -8 | 12.4 | -12.0 |
| -7 | 6.3 | -7.0 |
| -6 | 2.0 | 1.6 |
| -5 | 5.9 | 5.9 |
| -4 | 14.0 | 14.7 |
| -3 | 2.0 | 2.0 |
| -2 | 4.2 | 3.8 |
| -1 | 11.4 | -11.7 |
| 0 | 1.6* | 0.9 |
| 1 | 1.6* | 1.2 |
| 2 | 14.7 | 15.1 |
| 3 | 9.8 | 9.9 |
| 4 | 7.3 | -7.5 |
| 5 | 18.1 | -18.4 |
| 6 | 15.6 | -15.5 |
| 7 | 3.6 | -4.0 |
| 8 | 34.0 | 35.0 |
| 9 | 1.5* | 0.5 |
| 10 | 4.8 | -5.1 |
| 11 | 1.4* | 0.4 |
| 12 | 14.9 | 15.3 |
| 13 | 12.1 | 11.7 |
| 14 | 1.0* | 2.0 |
| 15 | 3.1 | -3.6 |
| (H,3,8) | | |
| -18 | 3.9 | 4.2 |
| -17 | 4.6 | 4.9 |
| -16 | 5.7 | -5.4 |
| -15 | 2.0 | 1.4 |
| -14 | 11.6 | 11.6 |
| -13 | 15.7 | 15.9 |
| -12 | 3.2 | -3.5 |
| -11 | 24.9 | -24.9 |
| -10 | 3.9 | 3.5 |
| -9 | 14.6 | 14.2 |
| -8 | 16.0 | 15.7 |
| -7 | 8.1 | 7.9 |
| -6 | 5.7 | 6.0 |
| -5 | 12.2 | 11.8 |
| -4 | 4.1 | 3.9 |
| -3 | 11.3 | 11.4 |
| -2 | 1.6* | -1.5 |
| -1 | 3.4 | -3.0 |
| 0 | 24.0 | -25.0 |
| 1 | 26.4 | 26.3 |
| 2 | 5.3 | -5.3 |
| 3 | 1.6* | 1.2 |
| 4 | 16.4 | -16.9 |
| 5 | 10.4 | 10.0 |
| 6 | 6.1 | -5.9 |
| 7 | 13.9 | 14.0 |
| 8 | 13.0 | 13.0 |
| 9 | 11.6 | 11.4 |
| 10 | 2.6 | 1.5 |
| 11 | 16.1 | 15.6 |
| 12 | 13.4 | 13.9 |
| 13 | 14.2 | -13.8 |
| 14 | 0.8* | 0.2 |
| (H,4,8) | | |
| -16 | 10.6 | 10.4 |
| -15 | 8.7 | 8.1 |
| -14 | 4.7 | 4.5 |
| -13 | 3.6 | -3.6 |
| -12 | 2.5 | -2.2 |
| -11 | 1.3* | 1.5 |
| -10 | 21.6 | 21.7 |
| -9 | 3.9 | 4.0 |
| -8 | 1.4* | -0.6 |
| -7 | 10.9 | 10.7 |
| -6 | 32.1 | 32.0 |
| -5 | 7.3 | -7.1 |
| (H,4,8) | | |
| -4 | 9.5 | -9.4 |
| -3 | 2.2 | 2.7 |
| -2 | 27.4 | 27.2 |
| -1 | 9.4 | -9.5 |
| 0 | 4.0 | -4.3 |
| 1 | 6.7 | -7.0 |
| 2 | 13.1 | 12.8 |
| 3 | 17.0 | 16.8 |
| 4 | 6.0 | -6.0 |
| 5 | 3.1 | -3.1 |
| 6 | 7.9 | -7.7 |
| 7 | 5.7 | -5.6 |
| 8 | 7.5 | 7.7 |
| 9 | 1.1* | 0.4 |
| 10 | 19.3 | -18.3 |
| 11 | 4.2 | -4.6 |
| 12 | 2.7 | 3.1 |
| (H,5,8) | | |
| -13 | 0.7* | 0.2 |
| -12 | 8.9 | -8.9 |
| -11 | 1.0* | 0.1 |
| -10 | 12.9 | -13.2 |
| -9 | 9.3 | 9.0 |
| -8 | 1.1* | 0.3 |
| -7 | 3.5 | -3.7 |
| -6 | 4.4 | 4.5 |
| -5 | 11.5 | 11.5 |
| -4 | 5.2 | -5.4 |
| -3 | 22.9 | 22.7 |
| -2 | 6.4 | 6.4 |
| -1 | 11.1 | -11.1 |
| 0 | 8.0 | 7.8 |
| 1 | 32.1 | 32.0 |
| 2 | 1.2* | 1.5 |
| 3 | 1.2* | -1.2 |
| 4 | 3.5 | 4.0 |
| 5 | 8.9 | 9.4 |
| 6 | 2.0 | 2.2 |
| 7 | 2.2 | -2.0 |
| 8 | 4.5 | -4.2 |
| 9 | 7.4 | 7.2 |
| (H,6,8) | | |
| -7 | 7.3 | 7.7 |
| -6 | 0.8* | -0.6 |
| -5 | 2.6 | -2.4 |
| -4 | 5.7 | 5.7 |
| -3 | 6.7 | -6.3 |
| -2 | 5.6 | 5.6 |
| -1 | 2.5 | -2.0 |
| 0 | 0.8* | 1.8 |
| 1 | 12.2 | 11.8 |
| 2 | 4.2 | -3.7 |
| 3. | 6.0 | 5.9 |
| (H,0,9) | | |
| -17 | 11.7 | 12.2 |
| -15 | 23.3 | -22.9 |
| -13 | 25.8 | 25.8 |
| -11 | 23.1 | -22.4 |
| -9 | 1.5* | -0.1 |
| -7 | 9.9 | -9.8 |
| -5 | 35.5 | 35.7 |
| -3 | 1.6 | 0.9 |
| -1 | 16.0 | -16.0 |
| 1 | 37.0 | 37.4 |
| 3 | 2.5 | -1.9 |
| 5 | 16.0 | 16.3 |
| 7 | 6.6 | -6.6 |
| 9 | 22.3 | 22.0 |
| 11 | 1.2* | -1.1 |
| 13 | 16.4 | 16.4 |
| (H,1,9) | | |
| -18 | 7.9 | -8.0 |
| -17 | 3.1 | 2.6 |
| -16 | 11.6 | 11.2 |
| -15 | 12.8 | -12.5 |
| -14 | 8.1 | 7.9 |
| -13 | 10.1 | 10.1 |
| -12 | 4.8 | 5.3 |
| -11 | 7.1 | -7.4 |
| -10 | 4.6 | 4.4 |
| -9 | 5.0 | 5.5 |
| -8 | 8.2 | 8.2 |
| -7 | 6.4 | -5.9 |
| -6 | 11.1 | 10.8 |
| -5 | 1.6* | -1.5 |
| -4 | 12.3 | -12.6 |
| -3 | 19.3 | -18.7 |
| -2 | 24.1 | 23.6 |
| -1 | 20.9 | 21.0 |
| 0 | 14.1 | 14.1 |
| 1 | 12.8 | -13.0 |
| 2 | 17.7 | 17.5 |
| 3 | 6.0 | -6.1 |
| 4 | 11.3 | 11.5 |
| 5 | 15.0 | 15.2 |
| 6 | 1.5* | 0.5 |
| 7 | 12.9 | 13.2 |
| 8 | 15.7 | 15.2 |
| 9 | 6.6 | -6.7 |
| 10 | 25.5 | -25.5 |
| 11 | 14.0 | 14.0 |
| 12 | 19.0 | 18.8 |
| 13 | 7.7 | -7.8 |
| (H,2,9) | | |
| -17 | 3.8 | 4.4 |
| -16 | 3.3 | 3.0 |
| -15 | 4.8 | -4.3 |
| -14 | 4.6 | 5.4 |
| -13 | 24.9 | 24.3 |
| -12 | 6.7 | 6.4 |
| -11 | 1.4* | -0.3 |
| -10 | 1.4* | 0.6 |
| -9 | 1.4* | -1.8 |
| -8 | 9.7 | -9.4 |
| -7 | 2.4 | 2.5 |
| -6 | 2.7 | 2.5 |
| -5 | 1.5* | -1.9 |
| -4 | 17.0 | -17.3 |
| -3 | 14.0 | 14.4 |
| -2 | 7.2 | 7.1 |
| -1 | 27.2 | -26.7 |
| 0 | 7.8 | 7.9 |
| 1 | 3.6 | 3.1 |
| 2 | 14.4 | -14.5 |
| 3 | 9.8 | 10.0 |
| 4 | 3.2 | -2.1 |
| 5 | 20.7 | 20.0 |
| 6 | 1.4* | -2.3 |
| 7 | 9.7 | 9.5 |
| 8 | 9.1 | 9.1 |
| 9 | 6.3 | 6.3 |
| 10 | 8.7 | 8.5 |
| 11 | 21.3 | 21.8 |
| 12 | 0.9* | 0.9 |
| 13 | 0.7* | 1.6 |
| (H,3,9) | | |
| -16 | 7.4 | 7.6 |
| -15 | 5.2 | -5.0 |
| -14 | 1.6 | 1.6 |
| -13 | 1.1* | 1.0 |
| -12 | 13.4 | 12.5 |
| -11 | 24.2 | 23.6 |
| -10 | 14.0 | 13.5 |
| (H,3,9) | | |
| -9 | 6.6 | -6.4 |
| -8 | 10.7 | -10.4 |
| -7 | 1.4* | 1.8 |
| -6 | 33.0 | 32.6 |
| -5 | 12.1 | -11.8 |
| -4 | 8.9 | -8.2 |
| -3 | 1.5* | -0.3 |
| -2 | 28.8 | 28.5 |
| -1 | 1.5* | 1.3 |
| 0 | 6.1 | -5.5 |
| 1 | 15.3 | -15.2 |
| 2 | 8.8 | 8.5 |
| 3 | 1.4* | 0.8 |
| 4 | 6.4 | -6.2 |
| 5 | 8.3 | 9.1 |
| 6 | 9.7 | 9.8 |
| 7 | 8.2 | -8.1 |
| 8 | 9.2 | 8.8 |
| 9 | 1.0* | 0.6 |
| 10 | 19.6 | -19.3 |
| 11 | 0.8* | -1.1 |
| (H,4,9) | | |
| -13 | 16.1 | 16.3 |
| -12 | 10.0 | 9.7 |
| -11 | 4.3 | -4.1 |
| -10 | 15.6 | -15.4 |
| -9 | 1.1* | -0.3 |
| -8 | 1.9 | 2.1 |
| -7 | 1.2* | -0.3 |
| -6 | 8.4 | 8.5 |
| -5 | 22.0 | 22.4 |
| -4 | 1.3* | -1.3 |
| -3 | 14.1 | 14.1 |
| -2 | 1.9 | -1.7 |
| -1 | 3.7 | -2.9 |
| 0 | 7.0 | 6.8 |
| 1 | 9.0 | 9.1 |
| 2 | 7.4 | -7.7 |
| 3 | 13.9 | -14.1 |
| 4 | 5.8 | -5.5 |
| 5 | 13.6 | 13.4 |
| 6 | 3.0 | 3.2 |
| 7 | 10.5 | -10.4 |
| 8 | 2.5 | -2.5 |
| 9 | 5.6 | 5.9 |
| (H,5,9) | | |
| -9 | 3.2 | 3.2 |
| -8 | 11.9 | 12.0 |
| -7 | 5.4 | -5.1 |
| -6 | 16.0 | 16.4 |
| -5 | 2.5 | 2.1 |
| -4 | 1.8 | -1.4 |
| -3 | 9.4 | 9.7 |
| -2 | 14.5 | 14.8 |
| -1 | 13.4 | -12.7 |
| 0 | 2.7 | 2.7 |
| 1 | 3.4 | -3.6 |
| 2 | 0.9* | 1.0 |
| 3 | 9.2 | 8.7 |
| 4 | 5.6 | 5.6 |
| (H,0,10) | | |
| -16 | 13.0 | -13.4 |
| -14 | 8.9 | -9.2 |
| -12 | 10.3 | 10.1 |
| -10 | 5.2 | 4.8 |
| -8 | 10.5 | 10.7 |
| -6 | 10.9 | 10.1 |
| -4 | 20.8 | -20.3 |
| -2 | 38.5 | 38.5 |
| 0 | 3.9 | 3.2 |
| (H,0,10) | | |
| 2 | 21.4 | 21.9 |
| 4 | 30.5 | 31.4 |
| 6 | 5.5 | -4.9 |
| 8 | 7.0 | 6.7 |
| 10 | 5.5 | -5.6 |
| (H,1,10) | | |
| -15 | 19.7 | -18.8 |
| -14 | 2.0 | 1.6 |
| -13 | 18.7 | 18.6 |
| -12 | 9.7 | 9.8 |
| -11 | 6.8 | -6.4 |
| -10 | 3.0 | -2.7 |
| -9 | 11.2 | 11.0 |
| -8 | 20.8 | -20.5 |
| -7 | 4.0 | 3.9 |
| -6 | 5.3 | -5.4 |
| -5 | 1.4* | -0.9 |
| -4 | 5.7 | -5.6 |
| -3 | 13.6 | 13.3 |
| -2 | 1.4* | -0.3 |
| -1 | 18.5 | 18.8 |
| 0 | 1.4* | -1.3 |
| 1 | 10.6 | -10.4 |
| 2 | 27.4 | 27.0 |
| 3 | 5.7 | -5.6 |
| 4 | 5.8 | -5.8 |
| 5 | 24.1 | 23.8 |
| 6 | 1.4 | -1.2 |
| 7 | 16.6 | -16.7 |
| 8 | 6.4 | 6.4 |
| 9 | 8.4 | 8.5 |
| 10 | 2.1 | 2.3 |
| (H,2,10) | | |
| -14 | 0.8* | 0.6 |
| -13 | 0.9* | 0.6 |
| -12 | 13.5 | 13.7 |
| -11 | 2.2 | -1.7 |
| -10 | 6.4 | -6.3 |
| -9 | 1.9 | -1.9 |
| -8 | 5.6 | 4.8 |
| -7 | 2.6 | -2.4 |
| -6 | 20.9 | 20.8 |
| -5 | 4.3 | -3.7 |
| -4 | 20.9 | -21.0 |
| -3 | 8.1 | -8.1 |
| -2 | 24.8 | 24.5 |
| -1 | 2.8 | 2.1 |
| 0 | 8.4 | 8.5 |
| 1 | 1.3* | 1.8 |
| 2 | 3.2 | 2.7 |
| 3 | 4.2 | 4.5 |
| 4 | 5.0 | 5.4 |
| 5 | 1.6 | 0.9 |
| 6 | 3.3 | -2.9 |
| 7 | 6.9 | 6.5 |
| 8 | 22.8 | 21.7 |
| 9 | 2.0 | 2.3 |
| (H,3,10) | | |
| -12 | 6.8 | -6.5 |
| -11 | 5.5 | -5.2 |
| -10 | 2.5 | 2.7 |
| -9 | 17.6 | 17.2 |
| -8 | 2.7 | -2.8 |
| -7 | 1.1* | -1.2 |
| -6 | 3.7 | 3.7 |
| -5 | 2.9 | -2.5 |
| -4 | 3.5 | 3.4 |
| -3 | 17.4 | 16.8 |
| -2 | 3.4 | -3.0 |
| -1 | 6.3 | -6.1 |
| (H,3,10) | | |
| 0 | 7.7 | 7.9 |
| 1 | 1.1* | 0.0 |
| 2 | 5.0 | -5.0 |
| 3 | 11.8 | -12.1 |
| 4 | 2.2 | 2.1 |
| 5 | 9.8 | 9.8 |
| 6 | 8.0 | -8.3 |
| 7 | 6.1 | -6.3 |
| (H,4,10) | | |
| -8 | 4.3 | 4.4 |
| -7 | 6.1 | 6.0 |
| -6 | 9.2 | 9.7 |
| -5 | 1.1 | 0.0 |
| -4 | 9.0 | -9.1 |
| -3 | 4.8 | -5.3 |
| -2 | 17.1 | 17.0 |
| -1 | 0.9* | -0.2 |
| 0 | 6.1 | -6.4 |
| 1 | 2.1 | 2.0 |
| 2 | 19.0 | 19.4 |
| 3 | 5.5 | -5.6 |
| (H,0,11) | | |
| -11 | 11.5 | -11.0 |
| -9 | 13.1 | 12.8 |
| -7 | 1.0* | 0.3 |
| -5 | 19.9 | 20.7 |
| -3 | 1.1* | 1.6 |
| -1 | 13.5 | 13.6 |
| 1 | 18.4 | 18.2 |
| 3 | 6.8 | -6.4 |
| 5 | 0.8* | -1.3 |
| (H,1,11) | | |
| -11 | 0.7* | -0.9 |
| -10 | 13.3 | 13.2 |
| -9 | 7.5 | 7.5 |
| -8 | 2.6 | 2.4 |
| -7 | 9.7 | -9.6 |
| -6 | 14.3 | 14.6 |
| -5 | 2.6 | 2.1 |
| -4 | 6.1 | -6.6 |
| -3 | 1.1* | 0.6 |
| -2 | 1.5 | 1.2 |
| -1 | 5.8 | 5.7 |
| 0 | 1.0* | -1.2 |
| 1 | 10.9 | -11.3 |
| 2 | 20.4 | 19.7 |
| 3 | 2.6 | 2.5 |
| 4 | 0.8* | 1.1 |
| 5 | 4.3 | 4.4 |
| (H,2,11) | | |
| -9 | 15.5 | 15.9 |
| -8 | 11.3 | -11.5 |
| -7 | 5.9 | -5.9 |
| -6 | 0.9* | -1.2 |
| -5 | 19.2 | 19.3 |
| -4 | 0.9* | 0.0 |
| -3 | 4.4 | 4.6 |
| -2 | 2.7 | 2.7 |
| -1 | 6.9 | -7.2 |
| 0 | 7.9 | 7.9 |
| 1 | 6.3 | 6.4 |
| 2 | 6.3 | 6.5 |
| 3 | 3.6 | -3.4 |

factors on the Mg, O and C atoms, the structure refined to an $R$ value of 0·091 ($R'=0·096$)*. All fifteen hydrogen atoms were found from a three-dimensional difference Fourier synthesis. An $R$ value of 0·074 was obtained using individual isotropic temperature factors on the non-hydrogen atoms, with the hydrogens taking the temperature factor of their covalent bonded neighbor.

Anisotropic temperature factors in the form

$$\exp\left(-b_{11}h^2-b_{22}k^2-b_{33}l^2-b_{12}hk-b_{23}kl-b_{13}hl\right) \quad (3)$$

were then applied to the non-hydrogen atoms. Several cycles of least-squares refinement followed in which the 20 heavy atoms were refined with these factors. The 15 hydrogen atoms were simultaneously refined with isotropic temperature factors. An $R$ value of 0·036 was realized on the entire 2725 data.

The extinction test described by Vand (1955) was applied and clearly indicated that effects characteristic of extinction were present. It was checked that these effects were not produced by an erroneous X-ray attenuation-filter constant or by incorrect over-all scale and temperature factors. Since it was not possible to separate primary and secondary extinction effects, a correction for secondary extinction alone was applied to the entire set of intensity data by multiplying each observed intensity by $\exp[\alpha(KF_o)^2\{(1+\cos^2 2\theta)/\sin 2\theta\}]$. $\alpha$ was determined to be $2\times10^{-6}$. The magnitudes of 31 structure factors were increased by 1 to 2% and 10 others were increased 2 to 4%. The largest changes were $(\bar{3}12)$ and $(\bar{3}01)$, which were increased 6·5% and 14·6% respectively.

Two cycles of block-diagonal least-squares refinement using the extinction corrected data with the unobserved structure factors excluded yielded a reliability

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* An adjusted agreement ratio $R'$ defined as

$$R'=[2/\pi\ \Sigma w|F_o-F_c|^2/\Sigma w(F_o)^2]^{\frac{1}{2}}$$

is an indicator which reflects the progress of least-squares refinement and still maintains a numerical value comparable with the classical reliability index

$$R=\Sigma|F_o-F_c|/\Sigma|F_o|\ .$$

The $(2/\pi)^{\frac{1}{2}}$ factor takes account of the fact that the *mean deviation* for a normal distribution is $(2/\pi)^{\frac{1}{2}}$ times the *standard deviation*. Note the close correspondence between these two indicators in Table 1.

index for the complete set of data, including unobserved, of $R=0·034$. With the unobserved reflections omitted, $R$ becomes 0·030. All parameters converged, including the positional and isotropic temperature parameters of the hydrogens. The values of $F_o$ with extinction corrections and of $F_c$ from parameters derived by this refinement are given in Table 2.

Additional refinement with full-matrix least squares was done at the Oak Ridge National Laboratory. Several cycles of refinement were performed, up to 190 parameters being adjusted per cycle. The temperature factor of each hydrogen atom was included as anisotropic, during this refinement, and was set equal to that of the heavier covalently bonded neighbor atom. An atom multiplier (occupancy factor) for each hydrogen was adjusted during the refinement [see *Description of the structure* (*c*)]. The final $R$ is 0·031 for the entire data set and 0·028 for the measurable data alone while $R'$ is 0·036 in both cases. Parameters resulting from the full matrix refinement are given in Tables 3 and 4.

The atomic scattering factors of Berghuis, Haanappel, Potters, Loopstra, MacGillavry & Veenendaal (1955) were used for C, O and $Mg^{2+}$, and those of Ibers (1962) were used for H. Allowance was made for the ionization of the carboxyl oxygen atoms by averaging the tabulated atomic scattering factor for O and $O^-$ given by Ibers (1962). The anomalous dispersion correction for Mg is small with $\Delta f'=0·1$ and $\Delta f''=0·2-0·3$ for Cu radiation (Templeton, 1962). This cor-

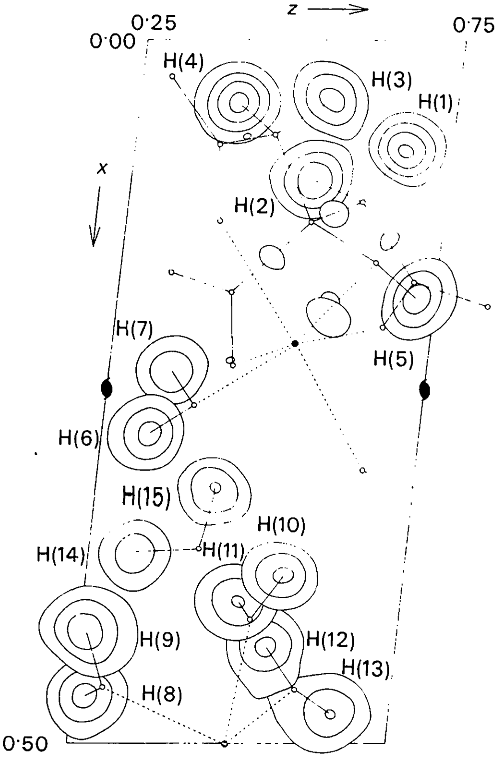

Fig. 1. Composite three-dimensional difference Fourier synthesis showing hydrogen atoms. Viewed along $b$ axis. The first contour is at 0·2 e.Å$^{-3}$. Contour interval: 0·2 e.Å$^{-3}$.

Table 3. *Final atomic positional parameters* (*fractional*) *and anisotropic temperature factor parameters from full-matrix least-squares refinement*

The standard error in parenthesis after each parameter is for the last decimal place given and is derived from the full-matrix refinement. The $b_{ij}$ coefficients are defined in expression (3).

| Atom | $x$ | $y$ | $z$ | $b_{11}$ | $b_{22}$ | $b_{33}$ | $b_{12}$ | $b_{23}$ | $b_{13}$ |
|---|---|---|---|---|---|---|---|---|---|
| Mg(1) | 0·00000 | 0·00000 | 0·00000 | 0·00084 (2) | 0·00730 (15) | 0·00449 (9) | +0·00009 (8) | −0·00046 (17) | +0·00004 (6) |
| Mg(2) | 0·21788 (3) | 0·50189 (8) | 0·53903 (6) | 0·00077 (1) | 0·00674 (10) | 0·00367 (6) | −0·00050 (5) | −0·00058 (12) | −0·00016 (4) |
| O(1) | 0·19066 (6) | −0·0273 (2) | 0·8340 (1) | 0·00094 (3) | 0·0095 (2) | 0·0043 (1) | +0·0004 (1) | −0·0022 (3) | −0·00024 (8) |
| O(2) | 0·20762 (7) | −0·2632 (2) | 0·6734 (1) | 0·00155 (3) | 0·0109 (3) | 0·0066 (1) | +0·0025 (2) | −0·0055 (3) | −0·00068 (10) |
| O(3) | 0·02617 (7) | 0·4971 (2) | 0·2942 (2) | 0·00122 (3) | 0·0103 (3) | 0·0081 (2) | +0·0001 (1) | +0·0036 (3) | −0·00251 (11) |
| O(4) | 0·12989 (6) | 0·5318 (2) | 0·3982 (1) | 0·00106 (3) | 0·0109 (3) | 0·0066 (1) | −0·0013 (1) | +0·0048 (3) | −0·00112 (10) |
| O(5) | 0·23356 (6) | 0·2266 (2) | 0·4425 (1) | 0·00089 (3) | 0·0108 (3) | 0·0071 (1) | −0·0011 (1) | −0·0055 (3) | +0·00146 (9) |
| O(6) | 0·16724 (6) | −0·0037 (2) | 0·3287 (1) | 0·00129 (3) | 0·0115 (3) | 0·0051 (1) | −0·0014 (1) | −0·0052 (3) | +0·00076 (10) |
| O(7) | 0·16006 (6) | 0·3011 (2) | 0·6502 (1) | 0·00108 (3) | 0·0074 (2) | 0·0036 (1) | −0·0002 (1) | −0·0007 (2) | −0·00007 (8) |
| O(8) | 0·26173 (6) | 0·6641 (2) | 0·3893 (1) | 0·00140 (3) | 0·0121 (3) | 0·0054 (1) | −0·0002 (1) | +0·0030 (3) | +0·00120 (10) |
| O(9) | 0·03990 (6) | −0·1129 (2) | 0·2039 (1) | 0·00123 (3) | 0·0097 (2) | 0·0058 (1) | −0·0006 (1) | +0·0021 (3) | −0·00097 (10) |
| O(10) | 0·08787 (6) | 0·1547 (2) | −0·0182 (2) | 0·00109 (3) | 0·0120 (3) | 0·0094 (2) | −0·0016 (1) | −0·0042 (3) | +0·00162 (11) |
| O(11) | −0·04031 (7) | 0·2409 (2) | 0·0987 (2) | 0·00143 (3) | 0·0107 (3) | 0·0069 (1) | +0·0019 (1) | −0·0042 (3) | −0·00085 (10) |
| O(12) | 0·13837 (7) | 0·5501 (2) | 0·0763 (2) | 0·00124 (3) | 0·0158 (3) | 0·0092 (2) | +0·0002 (2) | +0·0006 (4) | +0·00092 (12) |
| C(1) | 0·17481 (7) | −0·1204 (2) | 0·7143 (2) | 0·00086 (3) | 0·0066 (3) | 0·0040 (2) | −0·0006 (2) | +0·0014 (3) | +0·00019 (11) |
| C(2) | 0·11485 (8) | −0·0411 (2) | 0·6162 (2) | 0·00083 (3) | 0·0081 (3) | 0·0046 (2) | −0·0006 (2) | +0·0016 (3) | −0·00018 (11) |
| C(3) | 0·13136 (7) | 0·1575 (2) | 0·5431 (2) | 0·00081 (3) | 0·0067 (3) | 0·0037 (2) | −0·0001 (2) | −0·0002 (3) | +0·00014 (10) |
| C(4) | 0·06670 (7) | 0·2499 (2) | 0·4681 (2) | 0·00075 (3) | 0·0088 (3) | 0·0054 (2) | +0·0002 (2) | +0·0015 (4) | +0·00031 (11) |
| C(5) | 0·07520 (8) | 0·4397 (2) | 0·3811 (2) | 0·00092 (3) | 0·0076 (3) | 0·0046 (2) | +0·0008 (2) | −0·0004 (3) | −0·00037 (12) |
| C(6) | 0·18128 (7) | 0·1223 (2) | 0·4288 (2) | 0·00081 (3) | 0·0073 (3) | 0·0040 (2) | +0·0006 (1) | +0·0006 (3) | +0·00015 (10) |

rection was not applied. Fig. 1 is a composite drawing of a three-dimensional difference Fourier synthesis computed before full-matrix refinement with hydrogen atoms omitted from the $F_c$ component. The peak heights of the hydrogen atoms appearing in this difference Fourier range from 0·5 to 0·8 e.Å$^{-3}$.

### Assessment of precision

Three methods, each based on least-squares refinement, were utilized during the error analysis of the positional and thermal parameters. This approach was followed in order to compare the standard errors derived by the partial data refinement method, the block diagonal inverted matrix method and the more rigorous full inverted matrix method.

A technique used by Nordman (1962) was employed first. The data (with extinction corrections) were randomly divided into five groups and several cycles of block-diagonal least-squares refinement were performed with each segment of data. Three to five cycles were required with each segment. The mean, $\bar{x}$, and the standard error of the mean, $s_{\bar{x}}$

$$s_{\bar{x}} = \left[ \frac{\sum_i (x_i - \bar{x})^2}{n(n-1)} \right]^{\frac{1}{2}} \tag{4}$$

were computed for each parameter from the five values obtained with the separate least-squares refinements. Unobserved reflections were excluded from the refinement. There were 239 parameters to be fitted. The five segments contained 514, 491, 479, 501 and 499 data respectively. The final $R$ values were 0·024, 0·024, 0·028, 0·028 and 0·026. The corresponding $R'$ values were 0·024, 0·024, 0·030, 0·028 and 0·026. The other two methods utilized the diagonal elements of the inverted matrices from the block diagonal and from the full-matrix refinements. The block size used in the IBM 1620 computer program was 3 × 3 for positional, 6 × 6 for anisotropic temperature and 2 × 2 for over-all scale and temperature factor.

Table 4. *Hydrogen parameters from full-matrix least-squares refinement*

Standard errors are for the last decimal place of each parameter obtained from full-matrix least-squares. Positional parameters are fractional.

| Atom | Bonded to | $x$ | $y$ | $z$ | Multiplier |
|---|---|---|---|---|---|
| H(1) | C(2) | 0·077 (1) | −0·015 (4) | 0·675 (3) | 1·11 (5) |
| H(2) | | 0·099 (1) | −0·136 (4) | 0·536 (3) | 1·19 (5) |
| H(3) | C(4) | 0·039 (1) | 0·285 (4) | 0·545 (3) | 1·07 (5) |
| H(4) | | 0·041 (1) | 0·150 (4) | 0·401 (3) | 1·23 (5) |
| H(5) | O(7) | 0·184 (1) | 0·243 (4) | 0·717 (3) | 1·04 (5) |
| H(6) | O(8) | 0·282 (2) | 0·610 (5) | 0·324 (3) | 0·99 (6) |
| H(7) | | 0·236 (2) | 0·758 (5) | 0·352 (4) | 0·91 (6) |
| H(8) | O(9) | 0·034 (2) | −0·232 (5) | 0·231 (4) | 0·91 (6) |
| H(9) | | 0·078 (2) | −0·087 (4) | 0·238( 3) | 1·10 (6) |
| H(10) | O(10) | 0·120 (1) | 0·097 (5) | −0·057 (3) | 1·09 (6) |
| H(11) | | 0·101 (1) | 0·256 (5) | 0·007 (3) | 1·06 (7) |
| H(12) | O(11) | −0·068 (1) | 0·299 (4) | 0·051 (3) | 1·10 (6) |
| H(13) | | −0·024 (2) | 0·320 (5) | 0·163 (4) | 0·99 (5) |
| H(14) | O(12) | 0·135 (2) | 0·563 (6) | 0·169 (4) | 0·93 (7) |
| H(15) | | 0·175 (2) | 0·590 (5) | 0·065 (3) | 1·11 (6) |

Table 5. *Average standard errors and their r.m.s. dispersion for each type of atom*

(*a*) Determined from inverted full matrix.
(*b*) Determined from inverted block-diagonal matrix.
(*c*) Determined from five partial-data refinements.

| Type of atom | Number of atoms | Method | $\sigma(x)$ | $\sigma(y)$ | $\sigma(z)$ |
|---|---|---|---|---|---|
| Mg | 1 | *a* | 0·0005 Å | 0·0005 Å | 0·0005 Å |
| | | *b* | 0·0004 | 0·0004 | 0·0005 |
| | | *c* | 0·0000 | 0·0005 | 0·0011 |
| O | 12 | *a* | 0·0013 (2) | 0·0013 (1) | 0·0013 (1) |
| | | *b* | 0·0011 (1) | 0·0011 (1) | 0·0011 (1) |
| | | *c* | 0·0012 (4) | 0·0011 (3) | 0·0011 (4) |
| C | 6 | *a* | 0·0015 (< 1) | 0·0015 (< 1) | 0·0015 (< 1) |
| | | *b* | 0·0013 (< 1) | 0·0011 (< 1) | 0·0013 (1) |
| | | *c* | 0·0014 (2) | 0·0011 (5) | 0·0016 (4) |
| H | 15 | *a* | 0·030 (4) | 0·031 (4) | 0·030 (4) |
| | | *b* | 0·024 (3) | 0·024 (3) | 0·024 (3) |
| | | *c* | 0·032 (10) | 0·028 (11) | 0·026 (7) |

There is good relative agreement among the results of these three methods both with respect to the parameter values and the magnitudes of the standard errors. The results of the full matrix refinement are given in Tables 3 and 4.

Average standard errors determined by the three methods for the Mg, O, C and H positional parameters, and the r.m.s. dispersion of the average standard errors are given in Table 5. On the basis of maximum isotropic standard error values and the estimated uncertainty for the unit-cell dimensions, the standard errors in the bond lengths are: $\sigma(\text{Mg}-\text{O})=0{\cdot}001$ Å, $\sigma(\text{C}-\text{O})=0{\cdot}002$ Å, $\sigma(\text{C}-\text{C})=0{\cdot}002$ Å, $\sigma(C-\text{H})=0{\cdot}02$ Å and $\sigma(\text{O}-\text{H})=0{\cdot}02$ Å.

## Analysis of thermal anisotropy

A method derived by Patterson (1962) was used to obtain principal axes from the anisotropic temperature factor coefficients. The Debye–Waller temperature factor utilized in the least-squares refinement for anisotropic temperature factors may be expressed in reciprocal lattice parameters $\mathbf{h}$ as $\exp(-2\pi^2\tilde{\mathbf{h}}\boldsymbol{\beta}\mathbf{h})$. This expression in terms of the parameters $\mathbf{X}_e$ in the unique orthonormal $\mathbf{E}$ coordinate system described by Patterson (1952) becomes $\exp(-2\pi^2\tilde{\mathbf{X}}_e\boldsymbol{\gamma\beta\gamma}\mathbf{X}_e)$ where $\gamma$ is the square root of the metric tensor $\mathbf{g}$. The eigenvalues and eigenvectors of the symmetric matrix $(\boldsymbol{\gamma\beta\gamma})$ give the principal axes of thermal motion in Å$^2$ referred to the $\mathbf{E}$ coordinate system. A pure rotation may then be used to express the principal axis in terms of any other orthogonal coordinate system.

The $\gamma$ matrix for the present monoclinic crystal is

$$\gamma=\begin{bmatrix} 20{\cdot}20799 & 0 & -0{\cdot}75275 \\ 0 & 6{\cdot}68600 & 0 \\ -0{\cdot}75275 & 0 & 9{\cdot}10393 \end{bmatrix}$$

A rotation of 34·05° about the $b$ axis was chosen so that $X$ is perpendicular to the $(30\bar{1})$ cleavage plane and $Y$ is perpendicular to the (010) plane. The eigenfunctions were determined by the Jacobi method (see, *e.g.*, Greenstadt, 1960). The results derived from the full-matrix parameters are tabulated in Table 6 in terms of the root mean square displacement. A complete set of principal axes was derived from each of the five partial-data refinements. The first set of standard errors listed in Table 6 were estimated by a standard error of the mean calculation (equation 4) using the five different sets of principal axis parameters. The second set of standard errors listed was obtained from the inverted full matrix with the 7090 Function and Error Program, ORFFE, which utilizes numerical differentiation.

Figs. 2 and 3 are drawings of the structure viewed along the crystallographic $b$ axis with the pronounced $(30\bar{1})$ cleavage plane horizontal. A projected ellipsoid representation of thermal motion is centered on each atomic site. The ellipsoid axes are drawn proportional to the r.m.s. component of thermal displacement determined by the principal axis transformation of the least-squares anisotropic temperature factor coefficients. The projected axes, principal plane curves, boundary curves, shading details and tapered bonds were drawn by a digital $X-Y$ plotter*. The axial dimensions on the ellipsoids in Fig. 2 are enlarged by a scale factor of 2 over the actual r.m.s. displacement values. In Fig. 3 this scale factor is 1·5 and hydrogens are included with the assumption that they have the same temperature motion as their parent atoms.

## Description of the structure

### (*a*) *Coordination octahedra*

Each magnesium ion is coordinated to six oxygen atoms and there are no shared edges or corners between the two coordination octahedra. The magnesium

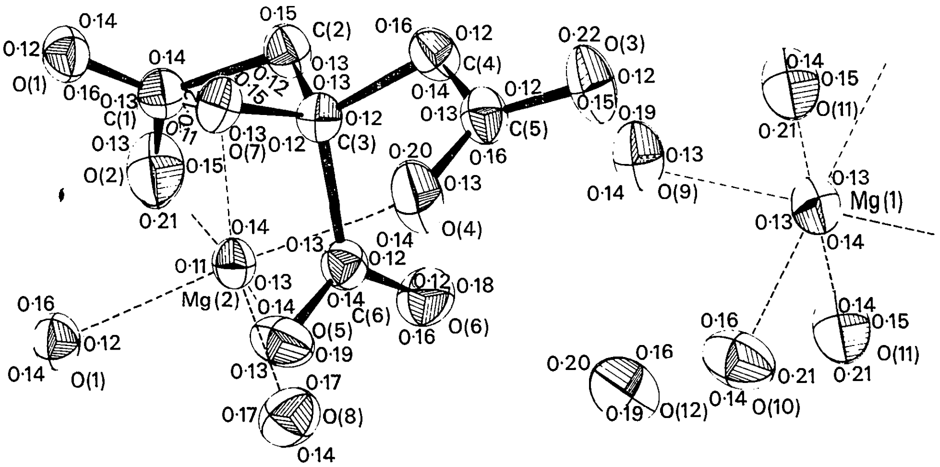

Fig. 2. Drawing of asymmetric unit viewed among the $b$ axis. The $(30\bar{1})$ plane is horizontal. The r.m.s. thermal displacement ellipsoids at double scale are centered on the atomic positions (see text). The r.m.s. displacements in Å along each principal axis are also given.

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* A model 580 Magnetic Tape Plotting System, manufactured by California Computer Products, Inc., Downey, California, was used at the Oak Ridge National Laboratory Computing Center.

at the center of symmetry, Mg(1), is a completely hydrated cation $[Mg(H_2O)_6]^{2+}$ and does not coordinate with the citrate oxygen atoms. The citrate ion is chelated to Mg(2) in a tridentate manner with the hydroxyl oxygen atom O(7) and two carboxyl oxygen atoms, one [O(4)] from an end carboxyl and one [O(5)] from the central carboxyl, forming the three points of attachment. The remaining three oxygen atoms of the second octahedron are a water oxygen atom [O(8)] and two carboxyl oxygen atoms [O(2′) and O(1″)] of two

Table 6. *Principal axes of anisotropic temperature factors, referred to orthogonal axes XYZ*

$X$ is the normal to the $(30\bar{1})$ cleavage plane and $Y$ is along the crystallographic $b$ axis. The r.m.s. displacements $\bar{\mu}_i$ are in Å and the direction angles, $\theta$, are in degrees. The first set of standard errors was derived from the five partial-data refinements, and the second was obtained by numerical differentiation from the results of the full matrix refinement.

| Atom | $i$ | $\bar{\mu}_i$ | $\theta_{(X)}$ | $\theta_{(Y)}$ | $\theta_{(Z)}$ |
|---|---|---|---|---|---|
| Mg(1) | 1 | 0·143 (1) (1) | 24 (3) (4) | 78 (2) (4) | 110 (2) (3) |
| | 2 | 0·128 (1) (1) | 105 (6) (12) | 17 (6) (26) | 97 (12) (34) |
| | 3 | 0·126 (1) (1) | 72 (4) (11) | 78 (13) (35) | 22 (3) (13) |
| Mg(2) | 1 | 0·137 (1) (1) | 14 (2) (3) | 104 (2) (4) | 92 (1) (3) |
| | 2 | 0·127 (1) (1) | 80 (2) (4) | 34 (2) (3) | 122 (1) (3) |
| | 3 | 0·111 (1) (1) | 81 (1) (2) | 60 (1) (3) | 32 (1) (3) |
| O(1) | 1 | 0·160 (2) (2) | 43 (2) (4) | 49 (2) (3) | 100 (1) (2) |
| | 2 | 0·138 (1) (2) | 133 (2) (4) | 48 (2) (4) | 107 (3) (6) |
| | 3 | 0·123 (1) (2) | 94 (3) (4) | 71 (2) (5) | 20 (2) (5) |
| O(2) | 1 | 0·213 (1) (2) | 32 (1) (1) | 58 (1) (1) | 93 (1) (1) |
| | 2 | 0·154 (1) (2) | 79 (2) (2) | 101 (3) (3) | 15 (3) (4) |
| | 3 | 0·129 (2) (2) | 60 (1) (1) | 146 (1) (2) | 105 (3) (4) |
| O(3) | 1 | 0·219 (1) (2) | 21 (1) (1) | 100 (0) (1) | 108 (1) (1) |
| | 2 | 0·154 (1) (2) | 74 (0) (1) | 24 (2) (2) | 73 (2) (3) |
| | 3 | 0·118 (2) (2) | 76 (1) (1) | 111 (2) (3) | 25 (1) (2) |
| O(4) | 1 | 0·200 (2) (2) | 36 (3) (1) | 121 (1) (1) | 107 (2) (1) |
| | 2 | 0·139 (3) (2) | 58 (2) (4) | 32 (2) (3) | 92 (6) (9) |
| | 3 | 0·130 (3) (2) | 74 (3) (6) | 97 (6) (9) | 17 (2) (2) |
| O(5) | 1 | 0·192 (3) (2) | 76 (2) (1) | 54 (1) (1) | 141 (1) (1) |
| | 2 | 0·135 (2) (2) | 120 (16) (11) | 41 (3) (6) | 66 (8) (6) |
| | 3 | 0·127 (2) (2) | 34 (8) (11) | 73 (9) (9) | 62 (6) (6) |
| O(6) | 1 | 0·184 (1) (2) | 83 (2) (3) | 137 (2) (2) | 48 (1) (1) |
| | 2 | 0·157 (1) (2) | 18 (2) (3) | 74 (2) (3) | 82 (2) (3) |
| | 3 | 0·122 (1) (2) | 108 (2) (3) | 52 (1) (2) | 43 (1) (1) |
| O(7) | 1 | 0·153 (1) (2) | 19 (2) (3) | 94 (3) (4) | 72 (2) (3) |
| | 2 | 0·131 (1) (2) | 80 (3) (4) | 22 (1) (7) | 109 (1) (6) |
| | 3 | 0·118 (1) (2) | 104 (1) (3) | 68 (1) (7) | 27 (1) (5) |
| O(8) | 1 | 0·174 (1) (2) | 95 (5) (15) | 38 (3) (13) | 53 (4) (16) |
| | 2 | 0·170 (1) (2) | 45 (2) (3) | 112 (3) (18) | 54 (3) (16) |
| | 3 | 0·136 (1) (2) | 45 (2) (3) | 62 (2) (2) | 122 (2) (3) |
| O(9) | 1 | 0·186 (2) (2) | 20 (1) (2) | 108 (0) (2) | 99 (1) (2) |
| | 2 | 0·145 (2) (2) | 70 (1) (2) | 23 (6) (6) | 78 (8) (8) |
| | 3 | 0·134 (1) (2) | 86 (3) (3) | 104 (8) (8) | 15 (7) (7) |
| O(10) | 1 | 0·208 (1) (2) | 73 (1) (2) | 65 (1) (2) | 149 (1) (1) |
| | 2 | 0·162 (1) (2) | 130 (2) (3) | 41 (1) (3) | 81 (2) (2) |
| | 3 | 0·137 (2) (2) | 45 (2) (3) | 60 (2) (3) | 61 (1) (1) |
| O(11) | 1 | 0·206 (2) (2) | 29 (1) (1) | 62 (1) (1) | 98 (1) (1) |
| | 2 | 0·150 (1) (2) | 79 (4) (4) | 93 (6) (7) | 11 (3) (6) |
| | 3 | 0·138 (1) (2) | 63 (2) (2) | 152 (2) (1) | 97 (1) (8) |
| O(12) | 1 | 0·196 (1) (2) | 59 (4) (4) | 108 (10) (11) | 143 (3) (5) |
| | 2 | 0·188 (1) (2) | 78 (9) (6) | 29 (5) (11) | 103 (5) (9) |
| | 3 | 0·159 (1) (2) | 34 (2) (2) | 93 (5) (3) | 57 (2) (2) |
| C(1) | 1 | 0·142 (2) (2) | 31 (2) (4) | 120 (2) (4) | 94 (4) (7) |
| | 2 | 0·127 (1) (3) | 80 (6) (8) | 83 (4) (9) | 12 (3) (10) |
| | 3 | 0·114 (1) (3) | 119 (2) (4) | 149 (2) (5) | 79 (7) (10) |
| C(2) | 1 | 0·154 (1) (2) | 37 (3) (4) | 123 (3) (4) | 105 (3) (4) |
| | 2 | 0·127 (3) (3) | 112 (11) (15) | 142 (8) (14) | 63 (14) (27) |
| | 3 | 0·123 (1) (3) | 117 (7) (12) | 107 (10) (24) | 147 (15) (25) |
| C(3) | 1 | 0·133 (1) (2) | 9 (3) (12) | 99 (8) (11) | 91 (6) (10) |
| | 2 | 0·123 (2) (3) | 81 (10) (12) | 14 (11) (78) | 101 (15) (102) |
| | 3 | 0·122 (3) (3) | 87 (11) (18) | 80 (13) (102) | 11 (9) (102) |
| C(4) | 1 | 0·156 (4) (2) | 49 (9) (5) | 116 (10) (6) | 128 (3) (3) |
| | 2 | 0·139 (3) (3) | 60 (7) (7) | 31 (9) (7) | 94 (10) (6) |
| | 3 | 0·121 (2) (3) | 56 (3) (5) | 105 (4) (6) | 38 (1) (3) |
| C(5) | 1 | 0·156 (1) (2) | 21 (2) (4) | 71 (3) (4) | 97 (3) (4) |
| | 2 | 0·131 (2) (3) | 101 (4) (5) | 41 (4) (10) | 52 (9) (11) |
| | 3 | 0·120 (2) (3) | 72 (4) (4) | 123 (9) (10) | 39 (6) (11) |
| C(6) | 1 | 0·137 (2) (2) | 38 (14) (19) | 55 (5) (14) | 77 (15) (15) |
| | 2 | 0·132 (4) (3) | 124 (14 )(20) | 58 (11) (15) | 51 (9) (10) |
| | 3 | 0·118 (3) (3) | 76 (6) (7) | 129 (8) (7) | 42 (7) (8) |

other citrate ions. These are related to the first by a *b*-lattice translation and by a twofold screw operation respectively. Only one water molecule [O(12)] is not coordinated to a magnesium.

Some data on the two octahedra are given in Table 7. The shortest octahedron edge is the citrate intramolecular distance 2·595 Å between the hydroxyl oxygen O(7) and the central carboxyl oxygen O(5). The associated Mg(2)–O(7) and Mg(2)–O(5) distances of 2·118 and 2·081 Å are the longest of this type in the structure. The completely hydrated $[Mg(H_2O)_6]^{2+}$ cation forms a nearly perfect octahedron. $[Mg(H_2O)_6]^{2+}$ ions have been demonstrated in several recent crystal structure determinations with Mg–O distances as follows: magnesium benzenesulphonate hexahydrate (Broomhead & Nicol, 1948) 2·04 Å; magnesium phosphate hexahydrate (Corbridge, 1956) 2·10 Å; magnesium thiosulphate hexahydrate (Nardelli, Fava & Giraldi, 1962) 2·08 Å; and magnesium ammonium sulfate hexahydrate (Margulis & Templeton, 1962) 2·07 Å. These values are in essential agreement with the average value of 2·074 Å found in the present $[Mg(H_2O)_6]^{2+}$ ion.

Table 7. *Coordination octahedra in* $[Mg(H_2O)_6]\,[MgC_6H_5O_7(H_2O)]_2\,.\,2H_2O$

| | | | | | |
|---|---|---|---|---|---|
| Mg–O distances | | | | | |
| Mg(1)–O(9) | 2·081 Å | (0·001) | Mg(2)–O(2″) | 2·019 Å | (0·001) |
| | | | Mg(2)–O(5) | 2·081 | (0·001) |
| Mg(1)–O(10) | 2·080 | (0·001) | Mg(2)–O(1′) | 2·072 | (0·001) |
| | | | Mg(2)–O(4) | 2·077 | (0·001) |
| Mg(1)–O(11) | 2·061 | (0·001) | Mg(2)–O(8) | 2·031 | (0·001) |
| | | | Mg(2)–O(7) | 2·118 | (0·001) |
| average | 2·074 Å | | average | 2·066 Å | |
| Shortest edge | | | | | |
| O(10)–O(11′) | 2·879 Å | (0·001) | O(5)–O(7) | 2·595 Å | (0·001) |
| Longest edge | | | | | |
| O(10)–O(11) | 2·976 Å | (0·001) | O(1′)–O(7) | 3·216 Å | (0·001) |
| Smallest angle | | | | | |
| O(10′)–Mg(1)–O(11) | 88·12° | (0·05) | O(5)–Mg(2)–O(7) | 76·32° | (0·05) |
| Largest angle | | | | | |
| O(10‴)–Mg(1)–O(11″) | 91·88° | (0·05) | O(1′)–Mg(2)–O(7) | 100·30° | (0·05) |

(Standard errors in parentheses).

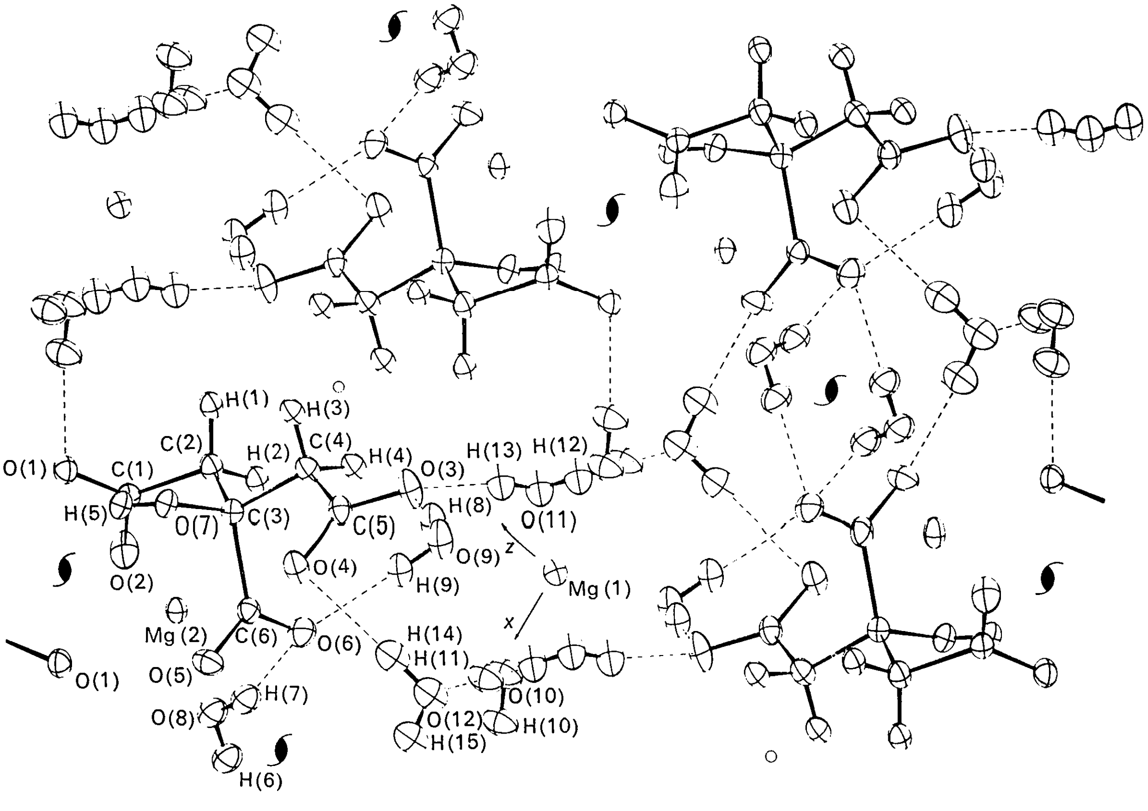

Fig. 3. Hydrogen bonding and molecular packing in $[Mg(H_2O)_6][MgC_6H_5O_7(H_2O)]_2\,.\,2H_2O$ viewed along the *b* axis. The (301) plane is horizontal

The angle between the line bisecting the angle between two hydrogen atoms of a water molecule and the metal to water oxygen coordinate bond varies from 173° for O(10) to 143° for O(8). O(11) and O(9) display corresponding angles of 157° and 150° respectively. The smallest Mg--O–H angle is 112° for Mg(2)--O(8)–H(7) and the largest angle is 134° for Mg(1)--O(10)–H(11).

### (*b*) *The citrate ion*

Intramolecular distances and angles for the triionized citrate ion are given in Tables 8 and 9. The chemically equivalent covalent bonds are (*a*) C(1)–C(2) and C(4)–C(5), (*b*) C(2)–C(3) and C(3)–C(4), and (*c*) the 6 C–O bonds of the 3 carboxyl groups. The equivalent C–C bond lengths uncorrected for thermal motion differ in length by (*a*) 0·003 Å and (*b*) 0·009 Å. The two C–O bonds in the individual carboxyl groups differ by 0·020. 0·005 and 0·010 Å for groups C(1), C(5) and C(6) respectively.

The marked asymmetry of C(1)–O(1) (1·266 Å) and C(1)–O(2) (1·246 Å) has a possible physical explanation in terms of thermal motion. The interatomic distance correction for thermal motion suggested by Busing & Levy (1964) was applied to the C–O carboxyl distances. The assumption involved is that the carboxyl oxygen atoms are 'riding' on the carboxyl carbon atoms of the citrate ion. The correction for 'riding' adds 0·015 Å to C(1)–O(2) but only 0·004 Å to C(1)–O(1). The corrected carboxyl C–O lengths for O(1) through O(6) are 1·270, 1·261, 1·266, 1·268, 1·270 and 1·261 Å respectively.

Table 8. *Citrate intramolecular distances*

| Type of atom | | Distance | |
|---|---|---|---|
| Terminal carboxyl C–C | | | |
| | C(1)–C(2) | 1·515 Å | (0·002) |
| | C(4)–C(5) | 1·518 | (0·002) |
| Middle carboxyl C–C | | | |
| | C(3)–C(6) | 1·555 | (0·002) |
| Other C–C | | | |
| | C(2)–C(3) | 1·541 | (0·002) |
| | C(3)–C(4) | 1·532 | (0·002) |
| Carboxyl O–O | | | |
| | O(1)–O(2) | 2·209 | (0·002) |
| | O(3)–O(4) | 2·209 | (0·002) |
| | O(5)–O(6) | 2·218 | (0·002) |
| Carboxyl C–O | | | |
| | C(1)–O(1) | 1·266 | (0·002) |
| | C(1)–O(2) | 1·246 | (0·002) |
| | C(5)–O(3) | 1·254 | (0·002) |
| | C(5)–O(4) | 1·259 | (0·002) |
| | C(6)–O(5) | 1·260 | (0·002) |
| | C(6)–O(6) | 1·250 | (0·002) |
| Hydroxyl C–O | | | |
| | C(3)–O(7) | 1·443 | (0·002) |
| Hydrogen | | | |
| | C(2)–H(1) | 1·00 | (0·02) |
| | C(2)–H(2) | 0·09 | (0·02) |
| | C(4)–H(3) | 0·98 | (0·02) |
| | C(4)–H(4) | 1·00 | (0·02) |
| | O(7)–H(5) | 0·83 | (0·02) |

(Standard errors in parentheses)

Distances from the least-squares best plane fitted to the nearly coplanar backbone carbon atoms C(1), C(2), C(3), C(4), C(5) are 0·06, −0·06, −0·05, 0·06 and −0·01 Å respectively. The equation for the backbone plane in terms of fractional coordinates along the unit cell axes is

$$-5{\cdot}616x+3{\cdot}203y+7{\cdot}249z=3{\cdot}754$$

where the constant on the right hand side of the equation is the perpendicular distance in Å from the origin to the plane. The terminal carboxyl oxygen atoms O(1), O(2), O(3), O(4) are removed from the plane by 1·13, −0·88, 0·18 and −0·11 Å. This finding is in concurrence with the structural results obtained for citric acid (Nordman, Weldon & Patterson, 1960*b*) and sodium dihydrogen citrate (Glusker, van der Helm, Love, Dornberg, Minkin, Johnson & Patterson, 1961). In each case, one terminal carboxyl is in the plane of the backbone and the oxygens of the other terminal carboxyl are out of this plane. Rubidium dihydrogen citrate, on the other hand, displays considerable departure from this planarity (Nordman, Weldon & Patterson, 1960*a*).

A characteristic feature of the citrate molecule is the coplanarity of the middle carboxyl group with its α-hydroxyl oxygen atom (Nordman *et al.*, 1960 *a*, *b*). This feature is common to many α-hydroxyacids (see *e.g.* Jeffrey & Parry, 1954). The equation of the least-

Table 9. *Citrate intramolecular angles*

| Type of atom | | Angle | |
|---|---|---|---|
| Carboxyl O–C–O | | | |
| | O(1)–C(1)–O(2) | 123·2° | (0·1) |
| | O(3)–C(5)–O(4) | 123·0 | (0·1) |
| | O(5)–C(6)–O(6) | 124·1 | (0·1) |
| Carboxyl O–C–C | | | |
| | O(1)–C(1)–C(2) | 116·2 | (0·1) |
| | O(2)–C(1)–C(2) | 120·5 | (0·1) |
| | O(3)–C(5)–C(4) | 117·2 | (0·1) |
| | O(4)–C(5)–C(4) | 119·8 | (0·1) |
| | O(5)–C(6)–C(3) | 117·0 | (0·1) |
| | O(6)–C(6)–C(3) | 118·9 | (0·1) |
| Hydroxyl O–C–C | | | |
| | O(7)–C(3)–C(2) | 111·7 | (0·1) |
| | O(7)–C(3)–C(4) | 106·7 | (0·1) |
| | O(7)–C(3)–C(6) | 108·4 | (0·1) |
| Carbon C–C–C | | | |
| | C(1)–C(2)–C(3) | 111·0 | (0·1) |
| | C(3)–C(4)–C(5) | 115·3 | (0·1) |
| | C(2)–C(3)–C(6) | 110·6 | (0·1) |
| | C(4)–C(3)–C(6) | 110·4 | (0·1) |
| | C(2)–C(3)–C(4) | 108·9 | (0·1) |
| Hydrogen H–C–C | | | |
| | H(1)–C(2)–C(1) | 111 | (1) |
| | H(1)–C(2)–C(3) | 107 | (1) |
| | H(2)–C(2)–C(1) | 112 | (1) |
| | H(2)–C(2)–C(3) | 107 | (1) |
| | H(3)–C(4)–C(3) | 107 | (1) |
| | H(3)–C(4)–C(5) | 107 | (1) |
| Hydrogen H–C–H | | | |
| | H(1)–C(2)–H(2) | 108 | (2) |
| | H(3)–C(4)–H(4) | 108 | (2) |
| Hydroxyl hydrogen C–O–H | | | |
| | C(3)–O(7)–H(5) | 110 | (2) |

(Standard errors in parentheses)

squares best plane fitted to O(7), C(3), C(6), O(5), O(6) of the present structure is $8{\cdot}509x-5{\cdot}058y+4{\cdot}999z=3{\cdot}067$ and the distances from the plane to the five respective atoms are 0·02, −0·03, 0·00, −0·01 and 0·02 Å. The angle between the plane just discussed and the backbone plane is 86·4°.

### (*c*) *Hydrogen positions*

The positional parameters of all 15 hydrogen atoms listed in Table 4 were refined by least squares and converged satisfactorily. An atom multiplier (occupancy factor) for each hydrogen atom was refined during the full-matrix refinement and the temperature factor for each hydrogen was set equal to that of the heavier covalently bonded neighbor atom. This approach was adopted because the isotropic temperature factors obtained during the block-diagonal least-squares refinement seemed unrealistic ($B=0{\cdot}1\text{–}1{\cdot}5$) for the hydrogen atoms attached to carbon. The hydrogen atoms attached to oxygen had isotropic temperature factors ranging from 1·7 to 3·1. The refined hydrogen multipliers listed in Table 4 show anomalies similar to those found for the isotropic temperature factors. Substantially the same results for the standard errors were obtained from the full matrix and the block-diagonal matrix refinements.

The C–H distances are 1·00, 0·99, 0·98 and 1·00 Å for hydrogen atoms (1) through (4) respectively with a standard deviation of 0·02 Å. The H(1)–H(2) and H(2)–H(3) separations are 1·61 and 1·60 Å respectively. The O–H distances are given in Table 10 along with H--O and O---O hydrogen bond distances. The mean of the 11 O–H lengths is 0·83 Å and σ(O–H) determined from the error analysis is 0·03 Å. The mean O–H distance is 6σ shorter than the O–D internuclear separation of 1·01 Å found in heavy water by neutron diffraction (Peterson & Levy, 1957). The comparison is complicated by the fact that the effective X-ray scattering center of a bonded hydrogen atom is not well established and that thermal corrections have not been applied to the present distances. The intramolecular H–H distances of the water molecules are 1·40, 1·32, 1·29, 1·28 and 1·33 Å respectively for the water oxygen atoms O(8)–O(12). On the other hand, the interproton separation in hydrated crystals is found by proton magnetic resonance to lie in the range 1·56 to 1·61 Å (McGrath & Silvidi, 1961; Chidambaram, 1962).

Table 10. *Hydrogen bonds in* $[Mg(H_2O)_6]\,[MgC_6H_5O_7(H_2O)]_2\,.\,2H_2O$

| | Hydrogen Bond Donor(d) | Acceptor(a) at (x,y,z) | $O_d$----$O_a$ (Å) | $O_d$—H (Å) | H----$O_a$ (Å) | <H—$O_d$---$O_a$ (degrees) (s.d.=2°) | <H—$O_d$—H in water (degrees) (s.d.=3°) |
|---|---|---|---|---|---|---|---|
| **Hydroxyl** | | | | | | | |
| (½-x, -½+y, 3/2-z) | O(7)—H(5) | (?) O(2) 'bifurcated' | 2.985 | 0.84 | 2.29 | 29 | |
| ( x, y, z) | O(7)—H(5) | (?) O(1) | 2.788 | | 2.09 | 29 | |
| **Water** | | | | | | | |
| ( x, y, 1+z) | O(10)—H(10) | O(1) | 2.880 | 0.86 | 2.02 | 4 | 106 |
| ( x, y, z) | O(10)—H(11) | *O(12) | 2.927 | 0.75 | 2.18 | 1 | |
| **Water** | | | | | | | |
| ( x, y, z) | *O(12)—H(14) | O(4) | 2.968 | 0.86 | 2.12 | 8 | 105 |
| (½-x, -½+y, ½-z) | O(12)—H(15) | O(5) | 2.870 | 0.81 | 2.07 | 6 | |
| **Water** | | | | | | | |
| ( -x, 1-y, -z) | O(11)—H(12) | O(12) | 2.772 | 0.77 | 2.00 | 1 | 106 |
| ( x, y, z) | O(11)—H(13) | *O(3) | 2.713 | 0.83 | 1.89 | 7 | |
| **Water** | | | | | | | |
| ( -x, 1-y, -z) | O(9)—H(8) | *O(3) | 2.759 | 0.85 | 1.91 | 3 | 105 |
| ( x, y, z) | O(9)—H(9) | *O(6) | 2.786 | 0.82 | 1.97 | 4 | |
| **Water** | | | | | | | |
| (½-x, -½+y, ½-z) | O(8)—H(6) | *O(6) | 2.823 | 0.85 | 1.98 | 2 | 110 |
| ( x, -1+y, z) | O(8)—H(7) | *O(6) | 2.939 | 0.86 | 2.11 | 13 | |

*Not coordinated with a Mg.

## Molecular packing

### (*a*) *Chelation*

The molecular packing is based on the chelation pattern of the citrate ligand. Fig. 4 illustrates the fact that each citrate ligand bridges three magnesium atoms which are in equivalent crystallographic general positions about a twofold screw. Pairs of central atoms are doubly bridged together by different bridging elements of two citrate ligands. This leads to an infinite, ribbon-like, chelated system parallel to the $(30\bar{1})$ plane and extending along a twofold screw axis. Between the extended ribbons are columns of hexaaquomagnesium ions, $[Mg(H_2O)_6]^{2+}$, with their magnesium atoms on symmetry centers. Hydrogen bonding holds the ribbons and columns together to form a sheet parallel to $(30\bar{1})$. Adjacent sheets are 5·72 Å apart and related one to another by crystallographic symmetry centers and twofold screw axes.

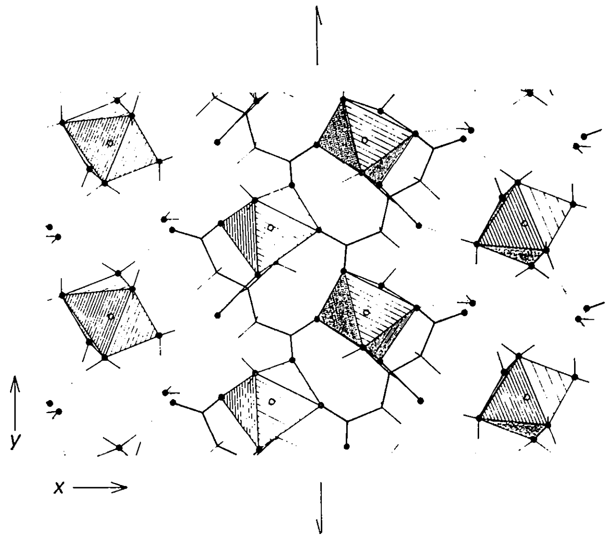

Fig. 4. Coordination octahedra and hydrogen bonding in the $(30\bar{1})$ sheet of $[Mg(H_2O)_6][MgC_6H_5O_7(H_2O)]_2 . 2H_2O$. The *b* axis is vertical.

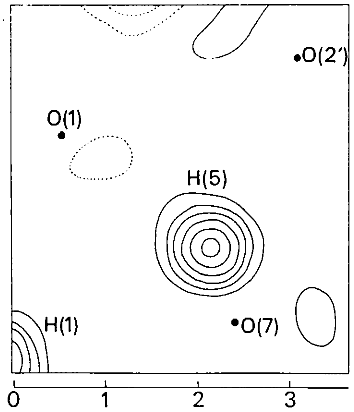

Fig. 5. Difference Fourier synthesis showing hydrogen H(5) of the bifurcated hydrogen bonding system. Least-squares best plane through O(7), H(5), O(1), O(2'). Contour interval 0·1 e.Å$^{-3}$. Negative contours are broken. Zero contour is omitted.

### (*b*) *Hydrogen bonds*

The direct intrasheet hydrogen bonds are O(11)–H(13) · · · O(3), O(9)–H(8) · · · O(6), O(9)–H(9) · · · O(6), and O(8)–H(7)· · ·O(6). The first three are between the chelated ribbon and the column of $[Mg(H_2O)_6]^{2+}$ ions, and the fourth is along the chelated ribbon. The direct intersheet hydrogen bonds are O(10)–H(10)· · ·O(1), and O(8)–H(6)· · ·O(6). Additional hydrogen bonding systems extend through the single water oxygen atom [O(12)] which does not coordinate to a metal. These bonds are O(10) – H(11)· · ·O(12), O(9)–H(8)· · ·O(12), O(12)–H(14) · · · O(4), and O(12)–H(15) · · · O(5). The first three lie within the sheet while the fourth may be considered to be an intersheet hydrogen bond. The arrangement of hydrogen bonds about O(12) is very nearly tetrahedral. The O–H · · · O angles and the associated distances for all hydrogen bonds are given in Table 10.

The hydroxyl hydrogen atom H(5) is so situated that it cannot form a linear hydrogen bond. A bifurcation exists between the citrate intramolecular hydrogen bond possibility O(7)–H(5) · · · O(1) and the possible intermolecular hydrogen bond O(7)–H(5) · · · O(2). The C(3)–O(7)–H(5) angle is 110°, while the C(3)–O(7) · · · O(1) and C(3)–O(7) · · · O(2) angles are 85·8° and 122·2° respectively. A general plane difference Fourier synthesis with hydrogen atoms omitted from the $F_c$ component was computed on the least-squares best plane for the nearly coplanar set of atoms O(7), H(5), O(1), O(2'). This difference Fourier synthesis is shown in Fig. 5. It suggests that H(5) is stably situated at the branch point of the bifurcation.

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# Concerning the Evidence for the Molecular Symmetry of $IF_7$

BY JERRY DONOHUE

*Department of Chemistry, University of Southern California, Los Angeles, California, U.S.A.*

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Additional refinements on the partial data from orthorhombic $IF_7$ show that it is not possible at the present time to demonstrate that the molecular symmetry is different from $D_{5h}$.

## Introduction

In the most recent paper on the crystal structure of $IF_7$ (Burbank, 1962) it was stated that need for further discussion of the regular pentagonal bipyramidal ($D_{5h}$) structure for the molecule was obviated by certain evidence presented therein. The history of the crystal structure of this compound is as follows:

(1) In a short note, Burbank & Bensey (1957) stated at the outset, 'The crystal structure analysis of iodine heptafluoride is obscured by the possibility of systematic error and an inadequate treatment of thermal motion.' This note also included the statement regarding the space group that 'No evidence was found for the type of disorder which would give rise to *Abam* and *Aba*2 was accepted as the correct space group.' In addition, refined positional and thermal parameters as obtained from a series of six three-dimensional Fourier difference syntheses were presented, and the resulting molecule was described as having an idealized description of 'five F atoms forming a tetragonal pyramid with the I atom situated *below* the base of the pyramid to which are added two more F atoms lying below the I atom',* a result which was stated to be 'in sharp contrast to the pentagonal bipyramid arrangement proposed by Lord *et al.* (1950) from a study of infrared and Raman spectra'. Standard errors in the bond distances were said to average 0·04 Å, with the effect of systematic errors unknown.

(2) In Donohue (1959) it was then pointed out that the data (*i.e.* the positional parameters) given by Burbank & Bensey did in fact give a molecule which closely approximated a pentagonal bipyramid; it was shown that the parameters corresponded to bond angles which did not differ significantly from those for the ideal molecule, and that the seven I–F bond distances were all equal, within experimental error.

(3) Next, Burbank (1959), in commenting on (2), above, included extensive quotations from a U.S.A.E.C. Technical Report, the existence of which had not been mentioned in the previous note. It was stated that in the Technical Report the pentagonal bipyramidal model had in fact been considered, but rejected, in large part because the refinement led to an I–F(1) bond distance which was shorter than the other six bonds. This information was, of course, in sharp contrast to the discussion of (1).

(4) Lohr & Lipscomb (1962) then published the results of their least-squares refinement of the crystallographic data contained in the Technical Report. They stated that their results supported the position taken in (2), above, and 'that the X-ray data do not eliminate the pentagonal bipyramidal arrangement'. They further stated, on the basis of a statistical analysis, that 'the various sources of error, chiefly those in the intensity estimates, are nearly random.'

(5) Burbank (1962) then reported the results of still more refinement of the original data, this time by least squares. In the introduction to this paper, Burbank included the following: 'Donohue (1959) made the

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* This description is, of course, ambiguous.