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Determination and refinement of the crystal structure of turquois, $CuAl_6(PO_4)_4(OH)_8 \cdot 4H_2O$

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With 7 figures

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Auszug

Der Türkis hat die Raumgruppe $P\bar{1}$, die Gitterkonstanten $a = 7{,}424$ Å, $b = 7{,}629$ Å, $c = 9{,}910$ Å, $\alpha = 68{,}61°$, $\beta = 79{,}71°$, $\gamma = 65{,}08°$ und eine Formeleinheit in der Elementarzelle, so daß Cu an das Inversionszentrum gebunden ist. Die Reflex-Intensitäten wurden mit einem Proportionalzähler registriert und mit dem Lorentz-Polarisations-Faktor und auf Absorption korrigiert. Aus einer dreidimensionalen Patterson- und einer ebenfalls dreidimensionalen Elektronendichte-Funktion, beruhend allein auf den Vorzeichen der Cu-Beiträge, folgte ein Strukturvorschlag, der durch Fourier- und Ausgleichs-Methoden bis zu $R = 0{,}07$ verfeinert wurde.

Die Struktur kann beschrieben werden als aufgebaut aus Ebenen von O-Atomen in nahezu dichtester Kugelpackung parallel (001). Zwischen diesen Ebenen sind abwechselnd Schichten von Al in oktaedrischer Koordination und von Cu in (4+2)-Koordination eingelagert. Die oktaedrischen Aniongruppen um die Al-Atome sind einfach oder doppelt; zwei Tetraeder um Phosphoratome verbinden jede Doppelgruppe mit dazu identischen unter Bildung von Tetraeder-Oktaeder-Ketten parallel zur b-Achse. Die PO_4-Tetraeder ergeben zusammen mit den einfachen Oktaedern um Al-Atome zickzackförmige Ketten in Richtung der c-Achse. Es wurden vier Moleküle H_2O pro Zelle festgestellt.

Abstract

Turquois is triclinic, space group $P\bar{1}$, with cell dimensions $a = 7.424$ Å, $b = 7.629$ Å, $c = 9.910$ Å, $\alpha = 68.61°$, $\beta = 79.71°$, $\gamma = 65.08°$. The cell contains one formula of $CuAl_6(PO_4)_4(OH)_8 \cdot 4H_2O$, so the Cu atom is fixed in an inversion center. Three-dimensional intensity data were collected on a single-crystal diffractometer using a proportional counter as detector, and were corrected for Lorentz-polarization factors and absorption. The interpretation of a three-dimensional Patterson function and of a three-dimensional electron-density function based on signs due to the Cu contribution only, gave a trial

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structure that was refined by Fourier methods and then by least-squares methods to an R factor of 7%.

The structure can be described in terms of planes of approximately close-packed oxygen atoms oriented parallel to (001). Planes containing the Al in octahedral coordination and planes containing the Cu in a 4+2 octahedral coordination alternate between two oxygen layers. The octahedral groups of anions around the aluminum are single and double; two phosphorus tetrahedra link each double group to its translational equivalent, building a tetrahedra-octahedra chain parallel to the b axis. The PO_4 tetrahedra together with the simple aluminum octahedra constitute a zig-zag chain in the direction of the c axis. The water content has been determined to be four molecules per cell.

Introduction

The turquois group is one of the few examples of a well known mineral family whose crystal structures have not been worked out up to the present time. Two isomorphous series can be distinguished in this group. One is the turquois-chalcosiderite series, characterized by isomorphous substitution of Al_2O_3 by Fe_2O_3; this includes as members turquois[1], henwoodite[2], rashleighite[3], alumo-chalcosiderite[4], and chalcosiderite[5]. The other series is formed by isomorphous substitution of Cu by Zn and only the two end members, turquois and faustite[6], are known.

Of the whole group, single crystals suitable for x-ray structure determination have been reported only for chalcosiderite and turquois. A recent x-ray study of chalcosiderite crystals[7], has shown a curious feature that can be explained as a very thin epitaxial growth of turquois on all crystals examined. This fact made chalcosiderite an unfavorable case for structure determination.

For almost eighty centuries turquois had only been known to occur in the cryptocrystalline state. It was not until 1912 that the first single crystals of turquois were described by SCHALLER[1]. Crystals

[1] WALDEMAR T. SCHALLER, Crystallized turquois from Virginia. Amer. Jour. Sci. **33** (1912) 35—40.

[2] E. FISCHER, Henwoodit, ein Glied der Türkis-Chalkosiderit-Reihe. Chemie der Erde **21** (1961) 97—100.

[3] ARTHUR RUSSEL, On rashleighite, a new mineral from Cornwall, intermediate between turquois and chalcosiderite. Min. Mag. **28** (1948) 353—383.

[4] A. JAHN und E. GRUNER, Alumo-Chalkosiderit, ein neues Mineral vom Schneckenstein i.V. Mitt. Vogtld. Ges. Naturf. Nr. 8, 1933. (Taken from Ref. [2].)

[5] N. S. MASKELYNE, On andrewsite and chalcosiderite. Jour. Chem. Soc. [London] **28** (1875) 586—691.

[6] RICHARD C. ERD, MARGARET D. FOSTER and PAUL D. PROCTOR, Faustite, a new mineral, the zinc analogue of turquois. Amer. Min. **38** (1953) 964—971.

[7] HILDA CID-DRESDNER, X-ray study of chalcosiderite. Amer. Min. (in press).

from SCHALLER's original sample were kindly provided by Professor CLIFFORD FRONDEL, of Harvard University, and by Dr. GEORGE SWITZER, of the U. S. National Museum, for use in the crystal-structure determination reported here.

Unit cell and space group

Turquois is triclinic and the space group is $P\,\bar{1}$, as reported by SCHALLER[1] and GRAHAM[8]. The determination of the unit cell was based on data from two precession photographs, GRAHAM's a and b axes being the precession axes. As is customarily done for triclinic crystals, a reduced cell was chosen according to BUERGER's and BALASHOV's convention[9,10]. This convention uses the three shortest non-coplanar translations of the lattice as crystallographic axes and requires the interaxial angles to be all-acute or all-obtuse. The orientation of the set is completely defined by the condition $a < b < c$.

The relations of the chosen reduced cell to the previous work of SCHALLER and GRAHAM are given below. It should be noted that GRAHAM's cell is a reduced cell that satisfied PEACOCK's conventions for the setting of a triclinic crystal[11]. His set includes the three shortest non-coplanar translations of the lattice and satisfies the relations $a < c < b$; $\alpha, \beta > 90°$, $\gamma < 90°$.

	Direct transformation	Inverse transformation
SCHALLER to GRAHAM	$\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & 1 \end{bmatrix}$	$\begin{bmatrix} -1 & 1 & 0 \\ -1 & -1 & -1 \\ 0 & 0 & 1 \end{bmatrix}$
GRAHAM to CID-DRESDNER	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}$	$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & -1 & 0 \end{bmatrix}$
SCHALLER to CID-DRESDNER	$\begin{bmatrix} -\frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \\ 0 & 0 & -1 \\ \frac{1}{2} & -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}$	$\begin{bmatrix} -1 & 0 & 1 \\ -1 & 1 & -1 \\ 0 & -1 & 0 \end{bmatrix}$

[8] A. R. GRAHAM, X-ray study of chalcosiderite and turquois. Univ. Toronto, Stud. Geol. Soc. **52** (1948) 39–53.

[9] M. J. BUERGER, Reduced cells. Z. Kristallogr. **109** (1957) 42–60. — M. J. BUERGER, Note on reduced cells. Z. Kristallogr. **113** (1960) 52–56.

[10] V. BALASHOV, The choice of the unit cell in the triclinic system. Acta Crystallogr. **9** (1956) 319–320.

[11] M. A. PEACOCK, On the crystallography of axinite and the normal setting of triclinic crystals. Amer. Min. **22** (1937) 588–620, 987–989.

Final cell constants were obtained by refinement of data from three axial photographs taken with a precision back-reflection Weissenberg camera[12]. Five cycles of least-squares refinement using BURNHAM's LCLSQ 3 program[13] for the IBM 7094 computer yielded the lattice constants listed in Table 1, where they are compared with GRAHAM's values. The centro-symmetric space group was confirmed by a piezoelectric test.

Table 1. *Turquois cell constants*

	a	b	c	α	β	γ
GRAHAM's values for the all-acute cell	7.46 Å	7.65 Å	9.91 Å	68.35°	69.43°	64.62°
This work	7.424 ±.004 Å	7.629 ±.003 Å	9.910 ±.004 Å	68.61 ±.03°	69.71 ±.04°	65.08 ±.03°

The refined cell parameters of Table 1 and SCHALLER's analysis of crystalline turquois from Virginia[1] were used to determine the unit-cell contents. The original formula of turquois[1] was given as $CuAl_6(PO_4)_4O_4 \cdot 9H_2O$, since the chemical analysis reported 20 non-water oxygens. The values listed below have been normalized to 20 oxygens since the available values of the specific gravity[10] were not considered satisfactory.

Cu	0.94
P	4.02
Al	5.99
Fe	0.02
O	20.00
H_2O	9.33

This formula corresponds to the ideal composition $CuAl_6(PO_4)_4(OH)_8 \cdot (4H_2O + H_2O)$. Whether or not this extra water molecule belonged in the atomic arrangement of turquois was to be elucidated from the structure determination.

Intensity data

A small turquois crystal of average dimension 0.18 mm was selected for intensity measurements. The shape of the crystal was an irregular tetrahedron with truncated corners. Although this irregular

[12] M. J. BUERGER, The precision determination of the linear and angular lattice constants of single crystals. Z. Kristallogr. (A) **97** (1937) 433–468.

[13] CHARLES W. BURNHAM, Lattice constants refinement. Carnegie Inst. of Washington Ann. Rept. **61** (1962) 132–135.

shape precluded an accurate absorption correction, the choice of this particular crystal was made on account of its transparency, perfect extinction under the polarizing microscope, and the good shape of the x-ray diffraction spots that were obtained with it.

Of the 2600 reflections in the positive hemisphere of the Ewald sphere for CuK radiation, 1650 which were within the instrument limit, were measured on a single-crystal counter diffractometer. The instrument was based on equi-inclination, Weissenberg geometry[14], and the parameters Υ and φ as well as the Lorentz-polarization factor for each reflection were obtained using a program written by PREWITT[15] for the IBM 7094 computer. A proportional counter was used as a detector.

Counter-intensity data for each reflection consisted of the scan count [i.e., the total number of counts while the crystal was rotated through the maxima, from a position φ_1 to φ_2, where $\varphi_1 < \varphi\ (hkl) < \varphi_2$] and fixed-time background counts for the positions φ_1 and φ_2. The average background count from these last two measurements was subtracted from the total scan count.

The calibration of the absorbing foil was made in the following way. The integrated intensities of ten medium-sized reflections were measured twice; first with the Al foil and then without it. The ratio between the two measurements gave a good approximation of the factor by which the strongest reflection had been reduced. In addition, a separate scale factor for these reflections was allowed in the last cycles of refinement.

The calculation of the observed structure factors was made through two data-reduction programs[16] written for the IBM 7094 computer. The first computed the integrated intensities, allowing appropriate scaling adjustments for the reflections measured with Al foils; the second one applied Lorentz-polarization and absorption corrections to the integrated intensities. In this case an approximation to the absorption correction was made by applying a spherical-absorption correction since the lack of well-developed crystal faces made it impossible to use a prismatic correction[16]. Since the product

[14] M. J. BUERGER, New single-crystal counter-tube technique. Acta Crystallogr. **9** (1956) 834.

[15] C. T. PREWITT, The parameters Υ and φ for equi-inclination with application to the single crystal-counter diffractometer. Z. Kristallogr. **114** (1960) 355–360.

[16] CHARLES W. BURNHAM, The structures and crystal chemistry of the aluminum-silicate minerals. Ph. D. thesis (1961) Mass. Inst. of Technology, Cambridge, Mass.

of the linear-absorption coefficient and the average radius of the "sphere" was 0.835, the error introduced by this approximation was not expected to affect the results greatly, even if it showed up as a temperature effect.

Structure determination

a) Two-dimensional work

An attempt was made to solve the structure in projections. The three Patterson projections $P(xy)$, $P(xz)$ and $P(yz)$ were calculated with the FORTRAN program ERFR 2 on the IBM 7094 computer[17]. The

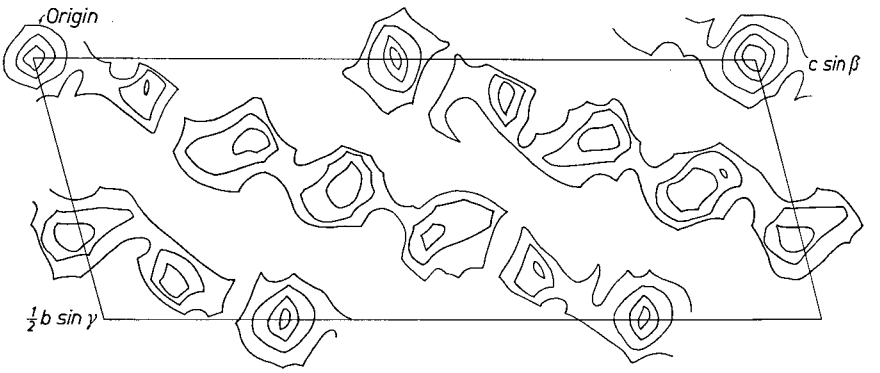

Fig. 1. Minimum function $M_4(yz)$

projection $P(yz)$ was studied first since it should show less superposition. The two strongest peaks were assumed to define the interatomic vectors from the copper atom to two other cations. Two minimum function $M_2(yz)$, based on the corresponding inversion peaks, were calculated and combined to produce the function $M_4(yz)$ which is illustrated in Fig. 1. The maxima from $M_4(yz)$ provided the coordinates y and z for a model structure, the x coordinates being obtained by correlation of $M_4(yz)$ with the other two Patterson projections. This model structure was refined independently in the three projections by successive Fourier syntheses followed by structure-factor calculations to discrepancy factors $R = 49.3\%$ for $\rho\,(xy)$, $R = 53.0\%$ for $\rho\,(xz)$, and $R = 36.5\%$ for $\rho\,(yz)$. At this stage the three projections

[17] W. G. SLY, D. P. SHOEMAKER and J. H. VAN DER HENDE, ERFR2, a two and three-dimensional crystallographic Fourier summation program for the IBM 7090 computer. Esso Research and Engineering Co., Lenden, N. J. Publication No. CBRL-22m-62.

could not be correlated any longer, and neither the Fourier refinement nor least-squares refinement succeeded in attaining further convergence. It was decided then that full three-dimensional data were necessary to solve the structure. Accordingly the model structure was discarded and a new start in three dimensions was made.

b) Three-dimensional work

A three-dimensional Patterson function, based on the 1600 intensities collected, was calculated. In the interpretation of the Patterson function the following features were taken into consideration:

1. Turquois can be treated as a structure composed of a heavy atom at the origin and a residual structure of atoms randomly distributed through the unit cell. The ratio of the contribution from the heavy atom and the maximum contribution of the residue is only 12%. Nevertheless the heavy atom is always making a maximum positive contribution. On the other hand, the contribution of residual atoms will never attain more than a fraction of their maximum value due to the fact that they are randomly distributed. Hence, in spite of the small ratio, the probabilities are that most of the structure-factor signs will be positive. If so, an electron-density function calculated with $|F_{o,hkl}|$ as coefficients will approximate the real structure.

2. In the absence of a substructure the strongest peaks in the Patterson map should correspond to vectors from the Cu atom to the Al and P atoms. The next highest peaks should be the Cu—O interactions of approximately the same height as an Al—P peak, but both about half of the Cu—Al peak. (Actually it was not expected that this would hold rigorously since structures based on oxygen are likely to show some kind of a substructure.)

3. The Cu is expected to be in a distorted octahedral coordination[18] with four oxygens at an approximate distance of 2 Å and the other two at a distance of 2.5 Å. The Al is expected to be in octahedral coordination with approximate Al—O distances of 1.9 Å, and the P will be surrounded by an oxygen tetrahedron with approximate P—O distances of 1.5 Å.

4. At least the peaks chosen as the cations in the structure should project as a peak in the old $M_4(yz)$ function.

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[18] F. Albert Cotton and G. Wilkinson, Advanced inorganic chemistry. Interscience Publishers (1962) 560—610.

An electron-density function, with all signs positive, was calculated, and from it a model structure which fulfilled all the preceding conditions was chosen. This model was refined by four successive electron-density functions followed by structure-factor calculations from the original discrepancy factor $R = 62\,\%$ to $R = 27\,\%$. In the course of the Fourier refinement five of the oxygens and one of the phosphorus atoms from the original model were found to be incorrect. The peak erroneously assumed to be a phosphorus was a substructure peak due to the superposition of the almost identical Al(1)—P(1) and Al(2)—P(2) vectors.

At this point the Fourier refinement had converged. The electron-density function whose atomic coordinates gave an R of $27\,\%$ showed round peaks of correct relative heights in the atomic locations and no spurious peaks. Consequently the structure was considered solved and the model was submitted to least-squares refinement. Only four water molecules were included in the structure, since no extra peak that could be attributed to the other oxygen had been found. On the other hand, the 28 oxygens per cell fulfilled the coordination requirements of all the cations, and if a fifth water molecule were to be placed in the unit cell it could not be attached to the cations in any of the usual ways.

Refinement of the structure

Least-squares refinement of the turquois structure was done on an IBM 7094 computer using the full-matrix program written by PREWITT[19]. Atomic scattering factors for Cu^{+2}, O, Al^{+1}, P, together with individual isotropic-temperature factors, were used in the first four cycles of least-squares refinement. The initial temperature coefficients were taken from the pseudomalachite structure[20], for Cu, O and P, and from the andalusite[21] structure for Al. These values were 0.5 for Cu, 0.15 for P, 0.6 for O and 0.25 for Al.

Only one scale factor for all reflections was used in the initial stages of the refinement. No rejection test was included, but, at this point, a special weighting scheme was used. The product of the discrepancy factor of a group of reflections and the weight of these reflections

[19] C. T. PREWITT, Structures and crystal chemistry of wollastonite and pectolite. Ph. D. thesis (1962) Mass. Inst. of Technology, Cambridge, Mass.

[20] SUBRATA GHOSE, The crystal structure of pseudomalachite, $Cu_5(PO_4)_2(OH)_4$. Acta Crystallogr. **16** (1963) 124—128.

[21] CHARLES W. BURNHAM and M. J. BUERGER, Refinement of the crystal structure of andalusite. Z. Kristallogr. **115** (1961) 269—290.

was maintained constant by this weighting scheme[22]. It was designed to give a larger weight to those structure factors that showed a better agreement, because this is desirable in the initial stages of the refinement.

One cycle of least-squares refinement, varying the atomic coordinates and the scale factor but not the temperature factors, improved the R factor from 27 % to 14.2 %. Three more cycles in the same conditions gave an R of 13.5 % and no movement in the atomic positions larger than the standard deviation was observed.

At this point the weighting scheme was changed. All reflections were given the same weight in order to allow more reflections to influence the refinement. Three more cycles of refinement only improved the R factor to 13.2 %.

Two scale factors, one for the reflections measured with an Al absorber and one for all the rest, were used from this point on. One cycle, varying isotropic temperature factors together with both scale factors, was run in order to study the interaction among these parameters. This was done through the Geller matrix coefficients[23] obtained from the least-squares refinement program. Rather large correlation coefficients were obtained for interactions between scale factor (1) and scale factor (2), and for interactions between scale factors and temperature factors. Accordingly, the scale factors and temperature factors were varied in consecutive independent cycles.

After three cycles of refinement of the isotropic temperature coefficients the discrepancy index R had attained 10 %. A three-dimensional difference-Fourier synthesis was calculated in order to see the hydrogen atoms. There are eight hydrogens in the asymmetric unit of turquois, four are attached to two water molecules and the other four belong to OH radicals. If those hydrogens were found, it would be the best way to differentiate an OH radical from an H_2O molecule.

The difference-synthesis maps showed two types of anomalies; these were, peaks in six out of the eight expected locations of the hydrogens, and also the characteristic combination of positive and negative peaks attributed to anisotropic motion of the atoms. Again,

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[22] BERNHARDT J. WUENSCH, The nature of the crystal structures of some sulfide minerals with substructures. Ph. D. thesis (1963) Mass. Inst. of Technology, Cambridge, Mass.

[23] S. GELLER, Parameter interaction in least-squares structure refinement. Acta Crystallogr. **14** (1961) 1026—1035.

no peak that could be interpreted as the fifth water molecule was found. When the six hydrogens were included, but not varied in a final cycle of isotropic refinement, the resulting R factor became 9.5%.

Four cycles of anisotropic refinement with the six hydrogens, included but not varied, converged to an R factor of 7.2%. During this refinement five oxygens did not maintain a definite positive character, even though their equivalent isotropic temperature factors

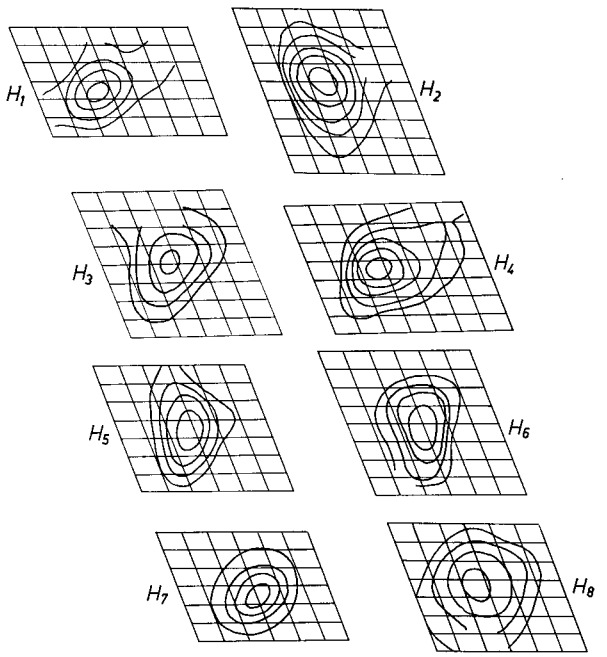

Fig. 2. The eight hydrogens of the turquois structure

were always positive. This was attributed to errors in the absorption correction due to the deviation of the shape of the crystal from a sphere.

A final three-dimensional difference-Fourier synthesis, using the results from the final cycle of anisotropic refinement, with the six hydrogens excluded, was calculated. The positions from the six hydrogens plus two others were recovered from it. The eight hydrogen peaks are shown in Fig. 2. When the hydrogen coordinates obtained from the last three-dimensional difference-Fourier synthesis were included in the refinement, a final discrepancy index of 7% was attained.

Table 2. *Observed and calculated structure factors of turquois*

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
1	0	0	19.71	20.21	0	8	0	16.93	15.26	-6	3	-1	17.59	17.28	-1	0	-2	25.39	24.89
2	0	0	-87.13	-82.18	1	8	0	5.43	4.31	-6	-3	-1	13.37	12.87	1	0	-2	24.70	27.28
3	0	0	35.48	34.94	2	8	0	22.88	20.86	6	-3	-1	- 9.16	-12.71	-2	0	-2	8.83	15.74
4	0	0	74.85	69.45	3	8	0	15.25	13.15	7	3	-1	- 1.38	- 1.30	2	0	-2	55.27	51.31
5	0	0	19.00	16.96	4	8	0	-20.23	-20.00	-7	-3	-1	-14.36	-14.61	-3	0	-2	32.15	30.25
7	0	0	14.35	13.97	5	8	0	15.70	14.52	-8	-3	-1	3.56	2.36	3	0	-2	- 8.63	- 5.85
8	0	0	12.73	12.13						0	4	-1	15.74	15.55	-4	0	-2	-44.33	-41.77
1	1	0	23.26	25.62	-2	0	-1	15.74	16.94	0	-4	-1	14.43	14.66	4	0	-2	-50.79	-43.11
1	-1	0	20.68	20.41	2	0	-1	45.78	44.50	1	4	-1	77.27	78.36	5	0	-2	35.47	34.50
2	1	0	93.48	100.02	-3	0	-1	10.80	14.03	-1	4	-1	2.37	1.47	-5	0	-2	12.25	12.86
2	-1	0	-15.77	- 5.93	3	0	-1	146.02	140.24	-1	-4	-1	50.00	47.46	-6	0	-2	66.27	67.90
3	1	0	13.44	15.70	-4	0	-1	33.93	33.27	1	-4	-1	65.15	61.94	6	0	-2	50.07	46.59
3	-1	0	41.23	41.33	4	0	-1	- 6.85	- 5.51	2	4	1	18.38	19.41	-7	0	-2	9.29	9.82
4	1	0	-40.00	-31.87	-5	0	-1	-12.45	-10.82	-2	4	-1	27.27	28.24	7	0	-2	- 7.71	- 8.78
-4	1	0	78.85	84.46	5	0	-1	24.90	24.13	-2	-4	-1	17.00	18.86	-8	0	-2	-24.97	-27.69
5	1	0	9.89	10.65	-6	0	-1	5.34	0.35	2	-4	-1	9.29	9.55	0	1	-2	-58.36	-53.16
5	-1	0	- 3.88	- 2.26	6	0	-1	21.48	19.88	3	4	-1	- 2.64	- 0.46	0	-1	-2	10.34	12.91
6	1	0	12.99	12.20	-7	0	-1	- 5.95	- 5.28	-3	4	-1	30.83	30.54	-1	1	-2	22.13	24.05
6	-1	0	-27.98	-27.96	7	0	-1	5.56	5.09	-3	-4	-1	- 6.65	- 1.86	1	1	-2	33.60	34.00
7	1	0	6.53	5.50	-8	0	-1	17.39	19.82	3	-4	-1	-37.55	-34.37	-1	-1	-2	26.55	26.73
7	-1	0	25.01	24.01	0	1	-1	20.22	22.24	4	4	-1	4.28	4.33	1	-1	-2	16.01	18.68
8	1	0	14.54	13.82	0	-1	-1	21.87	23.60	-4	4	-1	4.22	4.51	2	1	-2	20.49	24.04
0	2	0	7.17	8.82	1	1	-1	-11.53	- 8.88	-4	-4	-1	19.04	20.93	2	-1	-2	62.58	55.15
1	2	0	23.78	24.72	-1	-1	-1	53.36	51.27	4	-4	-1	11.40	12.12	-2	-1	-2	52.95	56.15
1	-2	0	24.10	24.15	1	-1	-1	49.41	46.23	5	4	-1	-21.94	-20.51	-2	1	-2	-69.77	-56.68
2	2	0	-43.17	-33.17	2	1	-1	19.50	20.58	-5	4	-1	-22.73	-24.20	-3	1	-2	- 5.53	- 3.43
2	-2	0	59.19	58.00	-2	1	-1	24.70	25.03	-5	-4	-1	37.29	37.18	-3	-1	-2	29.97	27.84
3	2	0	4.14	8.17	-2	-1	-1	23.65	26.07	5	-4	-1	33.40	33.98	3	-1	-2	16.93	16.48
3	-2	0	9.05	11.03	2	-1	-1	28.46	28.40	6	4	-1	27.67	29.13	3	1	-2	5.34	6.44
4	2	0	47.75	44.96	3	1	-1	36.17	34.71	-6	-4	-1	19.76	20.49	-4	1	-2	55.67	55.16
4	-2	0	-27.53	-25.40	-3	1	-1	-90.97	-85.52	7	4	-1	24.18	25.08	4	1	-2	46.90	42.01
5	2	0	32.25	32.03	-3	-1	-1	2.24	2.17	-7	-4	-1	24.44	24.59	-4	-1	-2	15.48	13.96
5	-2	0	8.08	6.46	3	-1	-1	67.00	63.27	-8	-4	-1	10.28	9.55	4	-1	-2	39.33	37.30
6	2	0	- 6.14	- 4.06	4	1	-1	28.33	28.67	0	5	-1	11.07	9.45	-5	1	-2	14.16	13.83
6	-2	0	- 6.01	- 4.96	-4	1	-1	22.60	22.87	0	-5	-1	12.38	11.99	5	1	-2	11.86	12.20
7	2	0	- 9.37	- 8.83	-4	-1	-1	5.99	7.35	1	5	-1	-51.25	-46.73	5	-1	-2	23.72	22.61
8	2	0	- 8.27	- 8.99	4	-1	-1	- 2.50	- 2.43	-1	5	-1	20.36	21.74	-5	-1	-2	23.72	24.33
0	3	0	48.92	47.46	5	1	-1	3.89	0.08	-1	-5	-1	56.46	56.33	-6	1	-2	-22.40	-22.91
-1	-3	0	18.16	19.24	-5	-1	-1	65.74	65.16	1	-5	-1	-71.21	-67.61	6	1	-2	- 6.65	- 4.01
1	-3	0	23.20	24.03	5	-1	-1	-58.37	-53.71	2	5	-1	22.07	21.95	-6	-1	-2	-32.35	-32.93
2	3	0	75.05	76.30	6	1	-1	1.91	1.60	-2	5	-1	5.80	6.24	6	-1	-2	10.28	13.53
2	-3	0	61.71	60.01	-6	1	-1	4.68	3.64	-2	-5	-1	20.95	22.73	-7	-1	-2	8.04	6.93
3	3	0	14.99	15.32	-6	-1	-1	25.36	25.50	2	-5	-1	19.76	18.94	-7	1	-2	- 7.91	- 8.69
3	-3	0	- 1.68	- 0.92	6	-1	-1	41.70	42.37	3	5	-1	43.28	41.27	7	1	-2	12.33	16.73
4	3	0	-68.56	-65.93	7	1	-1	19.83	22.14	-3	5	-1	14.76	13.91	7	-1	-2	-10.08	-10.96
4	-3	0	8.66	7.86	-7	1	-1	- 2.64	- 2.68	-3	-5	-1	-16.07	-16.61	-8	-1	-2	53.75	57.52
5	3	0	21.58	21.73	-7	-1	-1	8.37	7.72	3	-5	-1	58.43	60.06	0	2	-2	46.71	46.87
5	-3	0	27.92	27.14	7	-1	-1	51.25	55.81	4	5	-1	- 5.27	- 4.65	0	-2	-2	-28.85	-16.82
6	3	0	17.96	16.83	-8	-1	-1	- 3.23	- 3.50	-4	5	-1	5.73	5.73	1	2	-2	20.88	20.69
6	-3	0	48.72	48.52	0	2	-1	21.74	23.06	-4	-5	-1	12.32	13.43	-1	2	-2	7.77	9.92
7	3	0	15.12	14.55	0	-2	-1	25.16	26.55	4	-5	-1	3.69	4.26	-1	-2	-2	25.36	26.78
8	3	0	4.78	3.41	1	2	-1	94.81	95.39	5	5	-1	-21.08	-19.99	1	-2	-2	12.85	15.18
0	4	0	-31.60	-25.43	1	-2	-1	26.68	28.01	-5	-5	-1	27.60	27.76	2	2	-2	41.04	39.20
1	4	0	14.47	15.00	-1	-2	-1	12.78	15.90	6	5	-1	14.69	16.24	-2	2	-2	75.18	75.71
1	-4	0	18.03	19.47	-1	2	-1	-27.40	-32.39	-6	-5	-1	0.99	1.63	-2	-2	-2	-53.88	-46.18
2	4	0	3.04	0.91	2	2	-1	15.22	15.04	7	5	-1	-10.41	-11.03	2	-2	-2	6.59	7.21
2	-4	0	56.93	56.15	-2	2	-1	12.45	13.82	-7	-5	-1	-13.37	-13.31	3	2	-2	32.81	31.70
3	4	0	20.87	22.97	-2	-2	-1	26.02	28.21	-8	-5	-1	15.68	16.59	-3	2	-2	23.25	24.57
3	-4	0	5.88	4.64	2	-2	-1	3.43	1.50	0	6	-1	8.04	8.72	-3	-2	-2	8.70	9.51
4	4	0	66.04	64.27	3	2	-1	-36.89	-29.88	0	-6	-1	10.28	9.26	3	-2	-2	25.56	25.82
4	-4	0	19.45	19.57	-3	2	-1	45.13	46.51	1	6	-1	25.96	28.05	4	2	-2	45.45	42.82
5	4	0	- 1.49	- 0.41	-3	-2	-1	-20.55	- 9.64	-1	6	-1	45.32	44.08	-4	2	-2	-43.48	-42.86
5	-4	0	26.75	26.87	3	-2	-1	-15.42	-13.11	-1	-6	-1	-60.28	-59.47	4	-2	-2	6.26	6.07
6	4	0	-24.49	-21.25	4	2	-1	25.36	25.56	1	-6	-1	26.22	24.22	-4	-2	-2	71.71	73.09
7	4	0	16.41	15.98	-4	2	-1	14.30	13.76	-2	-6	-1	12.06	13.05	5	2	-2	- 2.70	- 1.79
8	4	0	36.25	33.81	-4	-2	-1	10.41	11.74	-2	6	-1	- 2.44	- 2.85	-5	2	-2	9.88	9.20
0	5	0	56.28	53.69	4	-2	-1	31.29	30.63	2	6	-1	9.09	8.25	5	-2	-2	- 8.43	- 4.20
1	5	0	14.09	12.19	5	2	-1	17.06	17.98	2	-6	-1	13.50	13.60	-5	-2	-2	6.85	5.20
1	-5	0	2.91	1.85	-5	2	-1	34.78	34.99	3	6	-1	-12.78	-12.77	6	2	-2	21.34	17.29
2	5	0	-38.71	-36.23	-5	-2	-1	-50.07	-47.59	-3	6	-1	5.80	5.68	-6	2	-2	19.30	18.87
2	-5	0	- 4.91	- 2.49	5	-2	-1	54.22	52.74	-3	-6	-1	18.45	19.71	-6	-2	-2	37.29	39.56
3	5	0	18.03	19.80	6	2	-1	4.41	3.76	3	-6	-1	- 4.28	- 3.96	6	-2	-2	7.44	6.90
3	-5	0	19.58	19.90	-6	2	-1	0.86	1.95	4	6	-1	12.25	13.32	-7	-2	-2	16.34	16.55
4	5	0	5.04	6.59	-6	-2	-1	9.55	9.64	-4	-6	-1	17.52	17.41	7	2	-2	30.04	29.98
4	-5	0	-24.56	-24.88	6	-2	-1	2.24	3.69	5	6	-1	33.66	33.84	-8	-2	-2	4.22	0.08
5	5	0	12.79	12.70	7	2	-1	-26.15	-28.10	-5	-6	-1	28.26	26.81	0	3	-2	114.64	117.17
6	5	0	26.95	25.40	-7	-2	-1	31.55	33.50	6	6	-1	9.42	8.72	0	-3	-2	11.33	17.77
7	5	0	9.05	8.33	-8	-2	-1	2.31	1.64	-6	-6	-1	2.31	0.13	1	3	-2	12.12	13.60
8	5	0	- 2.07	- 1.12	0	3	-1	17.85	18.58	-7	-6	-1	15.22	16.14	-1	3	-2	23.98	24.22
0	6	0	14.09	12.86	0	-3	-1	15.81	16.84	0	7	-1	5.80	5.61	-1	-3	-2	21.15	22.23
1	6	0	8.47	7.70	1	3	-1	91.94	90.21	0	-7	-1	12.12	12.59	1	-3	-2	13.37	13.70
1	-6	0	6.72	5.23	-1	3	-1	- 3.82	- 0.82	1	7	-1	23.85	23.78	2	3	-2	-50.26	-43.00
2	6	0	17.90	16.35	-1	-3	-1	-57.71	-52.15	-1	7	-1	17.33	17.35	-2	3	-2	-78.79	-76.89
2	-6	0	-21.71	-19.91	2	3	-1	10.67	10.12	-1	-7	-1	15.68	17.21	2	-3	-2	-44.60	-41.59
3	6	0	13.12	12.08	-2	3	-1	29.58	29.91	1	-7	-1	5.93	8.34	3	3	-2	28.66	29.04
3	-6	0	6.91	7.03	-2	-3	-1	18.64	20.17	2	7	-1	9.88	9.02	-3	3	-2	22.66	23.84
4	6	0	-20.94	-21.69	2	-3	-1	4.81	5.29	-2	-7	-1	9.88	11.16	-3	-3	-2	29.45	29.07
5	6	0	9.31	10.47	3	3	-1	21.21	19.69	3	7	-1	10.41	9.92	3	-3	-2	13.57	15.06
6	6	0	-23.59	-22.83	-3	3	-1	62.58	61.66	-3	-7	-1	- 5.01	- 3.24	-4	3	-2	60.47	61.91
7	6	0	14.41	12.91	-3	-3	-1	-15.74	- 7.80	4	7	-1	9.29	10.99	4	3	-2	85.64	83.73
0	7	0	-33.28	-34.36	3	-3	-1	49.41	48.72	-4	-7	-1	11.79	12.30	4	-3	-2	8.50	8.61
1	7	0	9.37	8.93	4	3	-1	33.47	32.94	5	7	-1	-15.48	-15.01	-4	-3	-2	-25.63	-22.00
1	-7	0	6.85	6.03	-4	3	-1	7.44	6.67	-5	-7	-1	5.93	6.57	5	3	-2	- 2.64	- 0.42
2	7	0	17.90	17.94	-4	-3	-1	17.26	18.42	-6	-7	-1	17.92	17.24	-5	3	-2	6.72	6.10
2	-7	0	48.85	51.57	4	-3	-1	17.65	17.73	0	-8	-1	16.34	16.73	5	-3	-2	2.17	0.48
3	7	0	12.34	11.91	5	3	-1	65.28	62.51	-1	-8	-1	-31.03	-33.47	-5	-3	-2	8.30	8.01
4	7	0	13.18	12.22	-5	3	-1	-31.36	-35.66	-2	-8	-1	8.04	8.50	6	3	-2	-36.76	-35.43
5	7	0	7.43	7.14	-5	-3	-1	31.75	31.25	-3	-8	-1	60.14	65.11	-6	-3	-2	21.81	22.59
6	7	0	47.88	46.46	5	-3	-1	8.30	9.37	-4	-8	-1	8.63	9.28	-6	3	-2	- 4.81	- 2.23
7	7	0	7.82	6.90	6	3	-1	- 3.56	- 1.11	-5	-8	-1	-18.05	-20.02	6	-3	-2	1.45	1.26

Table 2. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
-7 -3 -2	16.67	17.75	-4 -8 -2	23.81	24.64	-5 -3 -3	17.07	16.24	-4 -9 -3	- 2.16	- 1.37
7 3 -2	19.24	17.98	-5 -8 -2	2.97	2.90	5 -3 -3	8.77	7.40			
-8 -3 -2	23.25	23.61	-6 -8 -2	21.18	21.37	6 3 -3	21.18	20.26	0 0 -4	-25.03	-14.08
0 4 -2	0.99	1.89	-2 -9 -2	7.02	7.03	-6 3 -3	- 1.75	- 2.01	-1 0 -4	15.24	16.09
0 -4 -2	-33.82	-31.09	-3 -9 -2	4.25	3.00	-6 -3 -3	- 6.00	- 4.29	1 0 -4	22.66	21.34
1 4 -2	19.70	20.24	-4 -9 -2	32.04	32.94	7 3 -3	11.74	11.79	-2 0 -4	- 9.98	- 9.83
-1 4 -2	12.91	12.56				-7 -3 -3	- 9.85	- 9.53	2 0 -4	17.47	15.37
-1 -4 -2	21.94	22.87	0 0 -3	20.44	19.92	-8 -3 -3	4.59	4.36	-3 0 -4	7.08	7.74
1 4 -2	17.33	17.91	-1 0 -3	21.99	23.62	0 -4 -3	20.24	21.55	3 0 -4	15.72	16.13
2 4 -2	11.00	11.85	1 0 -3	-75.52	-59.98	0 4 -3	11.40	11.43	-4 0 -4	62.19	65.17
-2 4 -2	- 8.70	- 8.83	-2 0 -3	27.39	25.18	1 4 -3	- 9.85	- 8.27	4 0 -4	-28.13	-23.41
-2 -4 -2	48.81	48.81	2 0 -3	26.78	26.47	-1 4 -3	9.11	7.82	-5 0 -4	- 1.01	- 1.23
2 -4 -2	57.11	56.87	-3 0 -3	6.68	8.49	-1 -4 -3	43.51	40.10	5 0 -4	5.06	4.30
-3 4 -2	17.59	16.63	3 0 -3	27.12	23.49	1 -4 -3	8.50	8.86	-6 0 -4	23.14	23.22
3 4 -2	14.23	13.88	-4 0 -3	6.75	5.55	2 4 -3	15.38	14.47	6 0 -4	-16.53	-15.34
-3 -4 -2	25.56	26.64	4 0 -3	21.05	20.18	-2 4 -3	4.38	4.68	-7 0 -4	6.81	6.66
-4 4 -2	10.67	10.02	-5 0 -3	-19.43	-18.10	-2 -4 -3	25.68	23.53	-8 0 -4	4.79	5.29
4 4 -2	30.83	29.76	5 0 -3	37.84	33.41	2 -4 -3	8.30	7.89	0 1 -4	8.23	6.83
4 -4 -2	20.95	19.11	-6 0 -3	17.81	19.35	3 4 -3	29.27	28.41	0 -1 -4	62.93	58.41
-4 -4 -2	16.34	15.74	6 0 -3	-13.90	-12.40	-3 4 -3	-22.53	-21.05	-1 1 -4	20.84	21.49
5 4 -2	15.42	16.90	7 0 -3	-14.91	-13.19	-3 -4 -3	-31.77	-27.64	1 1 -4	15.04	16.24
-5 -4 -2	14.30	13.29	-7 0 -3	4.25	2.38	3 -4 -3	- 7.42	-14.09	-1 -1 -4	37.77	36.59
-5 4 -2	- 4.94	- 3.04	-8 0 -3	- 9.11	-14.05	4 4 -3	8.63	7.88	1 -1 -4	7.02	8.16
5 -4 -2	- 5.27	- 5.61	0 1 -3	23.54	24.39	-4 4 -3	6.48	5.53	-2 1 -4	61.11	65.79
6 4 -2	35.77	32.02	0 -1 -3	43.98	41.37	-4 -4 -3	6.61	6.27	2 1 -4	17.74	18.51
-6 -4 -2	- 4.81	- 1.26	-1 1 -3	19.36	21.44	4 -4 -3	13.63	12.74	-2 -1 -4	55.45	53.87
-7 -4 -2	5.86	5.57	1 1 -3	55.78	55.78	5 4 -3	-45.60	-41.43	2 -1 -4	-16.12	-11.72
7 4 -2	- 3.10	- 4.40	-1 -1 -3	-58.36	-57.37	-5 4 -3	43.10	44.89	-3 1 -4	20.37	22.06
-8 -4 -2	- 5.47	- 4.28	1 -1 -3	34.64	38.59	-5 -4 -3	48.57	49.72	3 1 -4	31.43	28.28
0 5 -2	50.00	50.31	-2 1 -3	6.01	6.47	5 -4 -3	-11.47	- 8.53	-3 -1 -4	18.75	21.20
0 -5 -2	30.76	28.59	2 1 -3	- 4.76	- 3.92	6 4 -3	8.84	8.08	3 -1 -4	30.56	28.31
-1 5 -2	11.59	9.79	-2 -1 -3	25.65	24.36	-6 -4 -3	21.32	20.47	-4 1 -4	28.47	26.46
1 5 -2	13.24	12.86	2 -1 -3	10.66	12.35	-7 -4 -3	21.38	21.54	4 1 -4	52.95	48.91
-1 -5 -2	13.90	15.03	-3 1 -3	18.80	19.40	-8 -4 -3	- 4.25	- 3.27	-4 -1 -4	-15.85	-14.88
1 -5 -2	25.10	25.12	3 1 -3	-63.91	-57.68	0 5 -3	9.98	9.28	4 -1 -4	-15.18	-13.81
-2 5 -2	15.42	10.07	-3 -1 -3	37.74	35.87	0 -5 -3	17.54	17.99	-5 1 -4	2.56	0.59
2 5 -2	33.73	32.44	3 -1 -3	- 3.23	- 0.11	1 5 -3	9.51	7.10	5 1 -4	- 4.99	- 3.41
2 -5 -2	9.49	7.91	-4 1 -3	15.70	17.74	-1 5 -3	- 7.15	- 2.82	-5 -1 -4	21.38	22.57
-2 -5 -2	8.23	8.22	4 1 -3	34.77	34.08	-1 -5 -3	15.31	17.06	5 -1 -4	7.15	6.51
3 5 -2	- 0.99	- 1.64	-4 -1 -3	15.38	15.76	1 -5 -3	43.37	40.84	-6 1 -4	- 8.57	-10.03
-3 5 -2	8.89	8.69	4 -1 -3	10.21	10.33	2 5 -3	12.95	11.90	6 1 -4	4.79	4.26
3 -5 -2	- 0.92	- 2.08	-5 1 -3	23.72	24.54	-2 5 -3	12.48	11.40	-6 -1 -4	13.49	13.66
-3 -5 -2	12.25	13.36	5 1 -3	12.41	12.56	-2 -5 -3	9.78	11.46	6 -1 -4	33.66	32.52
4 5 -2	-23.19	-21.25	-5 -1 -3	55.96	57.25	2 -5 -3	15.85	13.99	-7 1 -4	23.34	25.81
-4 -5 -2	27.67	30.13	5 -1 -3	19.58	18.21	3 5 -3	26.17	27.92	-7 -1 -4	2.56	1.03
-4 5 -2	- 2.83	- 4.22	-6 1 -3	5.56	5.20	-3 5 -3	30.29	27.46	0 2 -4	45.19	44.94
4 -5 -2	-12.85	-12.79	6 1 -3	4.07	3.59	-3 -5 -3	122.32	127.85	0 -2 -4	7.89	8.70
5 5 -2	30.11	29.84	-6 -1 -3	11.44	12.58	3 -5 -3	- 3.37	- 3.39	-1 2 -4	27.32	28.78
-5 -5 -2	19.85	19.93	6 -1 -3	6.40	5.14	4 5 -3	20.44	19.56	1 2 -4	12.28	15.80
-6 -5 -2	85.90	88.37	-7 1 -3	41.68	46.41	-4 5 -3	5.33	3.51	-1 -2 -4	20.24	21.68
6 5 -2	7.77	5.64	7 1 -3	25.00	20.77	-4 -5 -3	24.76	24.07	1 -2 -4	37.50	34.60
-7 -5 -2	- 2.37	- 3.74	-7 -1 -3	- 2.07	- 0.66	4 -5 -3	16.80	16.04	-2 2 -4	19.02	18.91
7 5 -2	- 6.26	- 6.39	-8 -1 -3	20.10	21.31	5 5 -3	64.74	64.30	2 2 -4	4.25	5.08
-8 -5 -2	-24.51	-25.02	0 2 -3	22.10	23.90	-5 -5 -3	-88.03	-89.96	-2 -2 -4	77.85	71.44
0 6 -2	-31.16	-33.67	0 -2 -3	12.54	11.52	6 5 -3	-10.93	-11.73	2 -2 -4	44.92	43.06
0 -6 -2	-20.82	-20.68	1 2 -3	-45.23	-40.56	-6 -5 -3	14.70	15.41	-3 2 -4	9.98	9.52
1 6 -2	17.19	16.30	-1 2 -3	3.42	4.06	-7 -5 -3	56.05	58.54	3 2 -4	10.99	10.35
-1 6 -2	14.10	13.55	1 -2 -3	-10.32	- 6.60	-8 -5 -3	4.79	4.49	-3 -2 -4	20.98	22.26
1 -6 -2	18.25	17.78	2 2 -3	25.16	24.34	0 6 -3	15.58	15.20	3 -2 -4	15.18	14.39
-1 -6 -2	11.92	12.22	-2 2 -3	20.98	21.37	0 -6 -3	31.91	31.91	-4 2 -4	13.69	13.87
2 6 -2	66.14	64.40	-2 -2 -3	34.87	32.64	1 6 -3	70.15	66.06	4 2 -4	-40.00	-33.87
2 -6 -2	4.22	2.89	2 -2 -3	23.14	23.08	-1 6 -3	7.76	6.32	-4 -2 -4	-12.41	- 7.51
-2 6 -2	39.92	38.92	3 2 -3	114.18	112.42	-1 -6 -3	-47.35	-43.81	4 -2 -4	59.56	54.58
-2 -6 -2	91.01	91.51	-3 2 -3	5.19	5.48	1 -6 -3	53.13	49.45	-5 2 -4	24.55	27.14
3 6 -2	1.78	0.53	-3 -2 -3	14.84	10.76	2 6 -3	1.89	1.21	5 2 -4	26.44	24.56
-3 -6 -2	17.92	18.46	3 -2 -3	6.00	6.72	-2 6 -3	20.03	18.65	-5 -2 -4	17.74	21.08
-3 6 -2	7.64	7.40	4 2 -3	- 4.32	- 3.45	-2 -6 -3	6.21	2.37	5 -2 -4	8.84	7.38
3 -6 -2	5.86	4.37	-4 2 -3	6.88	8.05	2 -6 -3	4.63	4.26	-6 2 -4	8.90	8.65
4 6 -2	7.91	6.70	-4 -2 -3	26.78	27.59	3 6 -3	-32.24	-29.76	6 2 -4	51.13	50.10
-4 -6 -2	-46.44	-46.07	4 -2 -3	14.64	13.85	-3 -6 -3	44.79	44.22	-6 -2 -4	36.90	36.56
5 6 -2	11.00	10.54	5 2 -3	-24.82	-19.31	3 -6 -3	8.16	5.65	6 -2 -4	-25.16	-23.62
-5 -6 -2	10.28	9.45	-5 2 -3	45.17	45.01	4 6 -3	26.04	25.04	-7 -2 -4	4.11	0.99
-6 -6 -2	26.94	27.27	-5 -2 -3	60.84	56.88	-4 -6 -3	2.16	1.12	-8 -2 -4	-31.97	-34.46
6 6 -2	1.52	2.18	5 -2 -3	3.24	1.67	5 6 -3	37.37	37.67	0 3 -4	-80.79	-82.46
-7 -6 -2	8.17	7.96	6 2 -3	30.83	28.59	-5 -6 -3	37.37	36.70	0 -3 -4	-16.59	-12.54
-8 -6 -2	11.00	10.56	-6 2 -3	14.17	15.21	-6 -6 -3	9.71	9.69	1 3 -4	27.86	27.92
0 -7 -2	3.84	0.36	-6 -2 -3	5.06	4.85	-7 -6 -3	-19.49	-19.29	-1 3 -4	4.72	2.50
0 7 -2	22.80	22.08	6 -2 -3	8.23	8.60	-8 -6 -3	2.29	1.40	-1 -3 -4	1.55	0.73
-1 -7 -2	14.50	14.76	7 2 -3	46.95	44.14	0 7 -3	11.40	9.45	1 -3 -4	33.12	31.85
1 7 -2	6.68	4.64	-7 -2 -3	3.31	3.64	0 -7 -3	6.27	6.78	2 3 -4	51.67	49.50
-1 7 -2	16.12	14.54	-8 -2 -3	21.99	23.45	1 7 -3	21.72	21.16	-2 3 -4	23.54	24.87
1 -7 -2	11.53	10.69	0 3 -3	20.78	21.22	-1 -7 -3	38.31	37.41	-2 -3 -4	99.89	102.59
-2 -7 -2	-29.07	-26.83	0 -3 -3	27.72	26.12	1 -7 -3	11.13	9.31	2 -3 -4	57.47	55.26
2 7 -2	-19.56	-16.91	1 3 -3	-21.45	-19.46	2 7 -3	12.41	12.27	3 3 -4	4.65	4.49
2 -7 -2	12.75	11.65	-1 3 -3	49.65	48.03	-2 -7 -3	12.95	11.23	-3 3 -4	10.39	9.66
-3 -7 -2	6.75	6.99	-1 -3 -3	-49.98	-42.47	2 -7 -3	3.78	3.22	-3 -3 -4	12.95	13.78
3 7 -2	16.53	16.46	1 -3 -3	15.24	12.08	3 7 -3	22.46	19.68	3 -3 -4	1.01	0.54
-4 -7 -2	58.62	56.70	2 3 -3	27.12	26.11	-3 -7 -3	-19.56	-18.36	4 3 -4	-26.85	-24.09
4 7 -2	42.90	40.88	-2 3 -3	11.40	12.77	-4 -7 -3	7.55	6.85	-4 3 -4	- 3.78	- 1.54
-5 -7 -2	7.28	5.35	-2 -3 -3	14.91	14.16	-5 -7 -3	9.31	10.77	-4 -3 -4	-24.82	-20.45
5 7 -2	- 0.67	- 0.65	2 -3 -3	35.01	34.00	-6 -7 -3	- 0.94	- 1.90	4 -3 -4	-61.38	-57.38
-6 -7 -2	-33.12	-33.14	3 3 -3	23.74	25.18	-7 -7 -3	17.00	15.65	5 3 -4	16.26	14.74
-7 -7 -2	6.54	5.75	-3 3 -3	-25.09	-23.88	0 -8 -3	- 2.90	- 3.37	-5 3 -4	1.48	0.64
0 -8 -2	44.99	45.58	-3 -3 -3	54.17	54.57	-1 -8 -3	32.38	33.58	-5 -3 -4	6.95	8.56
-1 -8 -2	12.14	12.72	4 3 -3	6.48	3.76	-2 -8 -3	9.71	9.60	5 -3 -4	31.57	30.30
1 -8 -2	0.67	4.03	-4 3 -3	21.05	21.19	-3 -8 -3	8.84	8.66	6 3 -4	11.40	11.77
2 8 -2	7.28	5.92	-4 -3 -3	17.27	18.07	-4 -8 -3	11.26	10.79	-6 3 -4	37.44	37.52
-2 -8 -2	2.50	3.26	4 -3 -3	- 8.50	- 6.83	-5 -8 -3	3.37	0.04	-6 -3 -4	63.61	67.75
-3 -8 -2	5.26	5.06	5 3 -3	38.72	34.46	-6 -8 -3	3.37	2.08	-8 -3 -4	- 2.09	- 0.22
3 8 -2	8.23	7.79	-5 3 -3	-14.70	-16.05	-3 -9 -3	- 8.57	-12.96	0 4 -4	35.55	34.77

Table 2. *(Continued)*

h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c	h	k	l	F_o	F_c
0	-4	-4	46.75	46.12	0	-1	-5	15.11	15.92	-8	-4	-5	18.35	19.18	-7	1	-6	- 0.90	- 0.64
1	4	-4	7.15	3.93	-1	1	-5	52.75	52.33	-9	-4	-5	- 5.80	- 7.04	-7	-1	-6	11.24	11.32
-1	4	-4	12.88	12.78	1	1	-5	43.24	41.20	0	5	-5	3.84	4.59	-8	-1	-6	28.56	35.01
-1	-4	-4	17.74	18.85	-1	-1	-5	-18.89	-17.05	0	-5	-5	-15.38	-15.26	0	2	-6	44.39	42.98
1	-4	-4	15.72	16.17	1	-1	-5	1.48	1.64	1	5	-5	-46.21	-43.90	0	-2	-6	- 9.18	- 5.21
2	4	-4	-28.80	-26.41	-2	1	-5	22.73	24.41	-1	5	-5	49.31	47.73	-1	2	-6	22.62	22.32
-2	4	-4	15.72	15.92	2	1	-5	18.62	17.58	-1	-5	-5	67.99	69.87	1	2	-6	- 6.53	- 5.61
-2	-4	-4	4.92	5.40	-2	-1	-5	12.68	14.34	1	-5	-5	-35.21	-33.81	-1	-2	-6	10.47	14.07
2	-4	-4	-23.68	-21.78	2	-1	-5	38.11	34.09	2	5	-5	21.18	21.49	1	-2	-6	8.98	8.87
3	4	-4	11.74	11.37	-3	1	-5	-35.08	-35.25	-2	5	-5	14.91	14.17	-2	2	-6	-10.15	-10.45
-3	4	-4	2.63	2.44	3	1	-5	7.35	6.91	-2	-5	-5	20.30	21.40	2	2	-6	- 7.04	- 7.36
-3	-4	-4	12.55	7.48	-3	-1	-5	9.11	10.21	2	-5	-5	21.99	23.10	2	-2	-6	24.30	23.52
3	-4	-4	17.20	16.70	3	-1	-5	63.00	55.96	3	5	-5	52.41	50.58	-3	2	-6	- 2.39	- 1.86
4	4	-4	40.88	36.75	-4	1	-5	10.99	11.92	-3	5	-5	2.23	0.38	3	2	-6	20.23	21.05
-4	4	-4	9.58	7.38	4	1	-5	11.33	10.94	-3	-5	-5	-35.28	-35.51	-3	-2	-6	26.04	26.86
-4	-4	-4	42.77	42.57	-4	-1	-5	1.55	0.44	3	-5	-5	10.25	11.44	3	-2	-6	22.29	22.12
4	-4	-4	39.12	35.43	4	-1	-5	1.42	0.67	4	5	-5	7.35	6.94	-4	2	-6	-14.47	-15.81
5	4	-4	14.91	14.43	5	1	-5	- 7.76	- 6.20	-4	-5	-5	13.96	14.25	4	2	-6	-22.81	-22.03
-5	-4	-4	15.11	15.49	-5	-1	-5	0.88	2.51	5	5	-5	- 4.99	- 5.57	-4	-2	-6	13.96	15.68
6	4	-4	9.31	9.45	-5	1	-5	67.12	83.30	-5	-5	-5	5.06	2.92	4	-2	-6	37.16	37.01
-6	-4	-4	-70.42	-75.45	5	-1	-5	-26.51	-23.01	-6	-5	-5	14.91	15.38	-5	2	-6	2.07	0.61
-7	-4	-4	7.96	7.08	-6	1	-5	10.66	10.82	-7	-5	-5	- 3.51	- 0.65	5	2	-6	12.21	10.82
-8	-4	-4	33.59	36.48	6	1	-5	18.41	16.44	-8	-5	-5	4.18	3.04	-5	-2	-6	6.20	5.10
0	5	-4	18.68	16.63	-6	-1	-5	9.71	7.60	0	6	-5	9.51	8.23	5	-2	-6	- 2.97	- 3.52
0	-5	-4	28.67	28.22	6	-1	-5	14.17	13.49	0	-6	-5	3.64	2.03	-6	2	-6	44.78	50.45
1	5	-4	18.15	17.90	-7	1	-5	-18.08	-21.27	1	6	-5	- 2.23	- 0.60	-6	-2	-6	-38.51	-44.17
-1	5	-4	7.96	7.71	-7	-1	-5	- 5.67	- 6.00	-1	6	-5	23.27	21.68	-7	-2	-6	10.73	10.96
-1	-5	-4	21.11	21.84	-8	-1	-5	- 7.55	- 8.73	-1	-6	-5	9.11	8.80	-8	-2	-6	8.79	8.71
1	-5	-4	9.78	11.29	0	2	-5	35.35	32.87	1	-6	-5	4.45	5.43	0	3	-6	14.28	15.21
2	5	-4	26.71	25.16	0	-2	-5	33.12	28.99	2	6	-5	2.50	1.39	0	-3	-6	84.93	85.91
-2	5	-4	- 5.26	- 5.69	-1	2	-5	-37.17	-35.23	-2	-6	-5	15.18	14.77	-1	3	-6	13.69	13.34
-2	-5	-4	-44.86	-41.77	1	2	-5	26.14	26.88	2	-6	-5	21.85	21.72	1	3	-6	7.82	7.99
2	-5	-4	39.66	37.17	-1	-2	-5	-33.66	-30.53	3	6	-5	-20.98	-20.26	-1	-3	-6	37.98	40.98
3	5	-4	6.21	5.67	1	-2	-5	95.51	90.77	-3	-6	-5	14.77	14.09	1	-3	-6	-13.42	-11.70
-3	5	-4	12.68	12.21	-2	2	-5	5.80	5.85	3	-6	-5	52.55	52.28	-2	3	-6	- 4.86	- 6.54
-3	-5	-4	8.50	9.47	2	2	-5	13.02	13.04	-4	-6	-5	13.22	14.81	2	3	-6	32.31	33.15
3	-5	-4	10.32	9.46	-2	-2	-5	2.16	5.60	-5	-6	-5	2.90	1.73	-2	-3	-6	-85.40	-92.78
4	5	-4	-14.64	-12.42	2	-2	-5	6.14	5.91	-6	-6	-5	15.72	16.42	2	-3	-6	-12.34	- 8.70
-4	5	-4	15.04	15.33	-3	2	-5	51.74	54.69	-7	-6	-5	- 6.27	- 8.12	-3	3	-6	- 0.81	- 0.70
-4	-5	-4	36.90	38.71	3	2	-5	17.74	15.87	-8	-6	-5	7.02	6.95	3	3	-6	18.35	17.90
5	5	-4	4.05	2.99	-3	-2	-5	73.65	77.59	0	-7	-5	11.74	11.17	3	-3	-6	27.99	26.56
-5	-5	-4	- 3.17	- 1.87	3	-2	-5	-50.46	-43.28	-1	-7	-5	5.53	3.79	-4	3	-6	46.75	49.06
6	5	-4	20.03	19.80	-4	2	-5	19.63	20.48	1	-7	-5	11.06	8.49	4	3	-6	33.25	29.79
-6	-5	-4	- 1.08	- 1.03	4	2	-5	21.72	20.45	-2	-7	-5	5.80	3.98	-4	-3	-6	49.24	48.22
-7	-5	-4	21.79	23.17	-4	-2	-5	20.71	21.97	-3	-7	-5	- 3.71	- 2.20	4	-3	-6	31.97	30.70
-8	-5	-4	-14.50	-15.11	4	-2	-5	20.03	17.65	-4	-7	-5	9.11	7.86	-5	3	-6	11.67	12.29
0	6	-4	5.60	2.69	-5	2	-5	-13.15	-15.83	-5	-7	-5	8.43	9.31	5	3	-6	- 7.42	- 7.65
0	-6	-4	90.25	88.58	5	2	-5	26.10	23.66	-6	-7	-5	6.88	6.34	-5	-3	-6	25.83	24.35
1	6	-4	11.94	11.89	-5	-2	-5	-60.71	-61.34	-7	-7	-5	49.31	52.72	-6	-3	-6	15.99	16.59
-1	6	-4	7.02	5.82	5	-2	-5	34.60	32.91	-8	-7	-5	8.03	7.73	-7	-3	-6	5.40	3.82
-1	-6	-4	20.84	20.72	-6	2	-5	- 3.44	- 6.29	0	-8	-5	13.15	13.32	-8	-3	-6	10.59	8.94
1	-6	-4	-16.73	-16.19	6	2	-5	- 5.46	- 5.75	-1	-8	-5	-16.93	-17.65	0	4	-6	32.11	32.53
2	6	-4	-31.64	-31.02	-6	-2	-5	17.67	18.12	-2	-8	-5	- 2.83	- 0.88	0	-4	-6	3.91	1.36
-2	6	-4	-25.16	-24.93	-7	-2	-5	59.49	65.34	-3	-8	-5	38.18	38.66	1	4	-6	1.96	2.85
-2	-6	-4	- 1.96	- 3.06	-8	-2	-5	7.08	6.61	-4	-8	-5	18.80	17.86	-1	4	-6	12.61	11.71
2	-6	-4	-38.45	-37.32	0	3	-5	2.23	2.22	-5	-8	-5	-20.84	-22.79	-1	-4	-6	-13.42	-12.90
3	6	-4	24.89	24.30	0	-3	-5	28.40	29.38	-6	-8	-5	10.05	9.79	1	-4	-6	8.97	8.32
-3	-6	-4	4.32	2.85	1	3	-5	- 4.92	- 2.52	-7	-8	-5	- 1.75	- 1.14	-2	4	-6	41.89	43.37
3	-6	-4	30.29	30.19	-1	3	-5	58.62	59.52	-2	-9	-5	14.10	14.44	-2	-4	-6	78.92	85.55
4	6	-4	72.31	74.04	-1	-3	-5	16.59	19.77	-3	-9	-5	-34.47	-37.89	2	-4	-6	-16.86	-15.29
-4	-6	-4	29.61	31.67	1	-3	-5	53.02	51.29	-4	-9	-5	3.04	1.79	3	4	-6	17.13	16.22
-5	-6	-4	17.13	18.28	2	3	-5	4.32	5.61	-5	-9	-5	44.25	47.21	-3	4	-6	23.47	23.86
-6	-6	-4	- 3.31	- 0.79	-2	3	-5	15.45	16.07						-3	-4	-6	34.74	33.89
-7	-6	-4	4.72	4.90	-2	-3	-5	9.11	11.51	0	0	-6	-42.97	-35.72	3	-4	-6	13.90	14.36
-8	-6	-4	27.93	29.73	2	-3	-5	- 6.41	- 5.04	1	0	-6	55.92	50.07	4	4	-6	1.55	1.22
0	-7	-4	-19.36	-17.88	3	3	-5	-28.47	-26.61	-1	0	-6	2.23	1.93	-4	4	-6	- 7.89	-10.16
-1	-7	-4	- 5.13	- 1.61	-3	3	-5	8.36	8.84	-2	0	-6	22.73	23.80	-4	-4	-6	-37.64	-36.00
1	-7	-4	13.49	12.80	4	3	-5	20.51	18.59	2	0	-6	119.78	116.30	4	-4	-6	25.03	22.67
-2	-7	-4	32.85	31.74	-4	3	-5	- 3.84	- 5.82	-3	0	-6	7.35	8.44	-5	-4	-6	6.48	4.39
2	-7	-4	20.37	20.84	-4	-3	-5	13.02	13.85	3	0	-6	-21.52	-20.10	-6	-4	-6	40.67	40.48
-3	-7	-4	14.30	12.53	4	-3	-5	32.38	30.58	-4	0	-6	10.66	10.49	-7	-4	-6	17.94	19.63
-4	-7	-4	-15.04	-15.64	5	3	-5	2.70	0.05	4	0	-6	-17.74	-17.28	-8	-4	-6	13.63	12.06
-5	-7	-4	9.24	9.67	-5	3	-5	1.82	1.10	-5	0	-6	14.64	15.38	0	5	-6	- 2.97	- 1.85
-6	-7	-4	6.54	5.91	5	-3	-5	29.14	27.81	5	0	-6	22.46	26.94	0	-5	-6	-36.76	-37.30
-7	-7	-4	- 6.34	- 0.77	6	3	-5	3.71	3.74	-6	0	-6	13.29	15.18	1	5	-6	15.31	15.85
-8	-7	-4	-18.21	-21.05	-6	-3	-5	21.65	23.27	-7	0	-6	6.34	5.55	-1	5	-6	16.19	14.93
0	-8	-4	4.92	3.92	-7	-3	-5	-24.42	-27.68	0	1	-6	- 4.05	- 2.30	-1	-5	-6	4.86	2.50
-1	-8	-4	- 0.88	- 0.93	-8	-3	-5	5.87	4.58	0	-1	-6	86.80	81.77	1	-5	-6	33.93	34.79
-2	-8	-4	-16.12	-16.00	0	-4	-5	10.05	11.74	-1	1	-6	2.00	2.80	2	5	-6	17.61	24.50
-3	-8	-4	6.48	4.65	0	4	-5	23.95	23.50	1	1	-6	20.61	20.76	-2	5	-6	-14.37	-15.33
-5	-8	-4	7.35	7.32	1	4	-5	42.02	39.92	-1	-1	-6	17.45	20.37	-2	-5	-6	-15.58	-12.70
-6	-8	-4	19.43	19.69	-1	4	-5	-28.13	-26.26	1	-1	-6	- 8.47	- 6.83	2	-5	-6	45.13	44.10
-2	-9	-4	38.79	40.15	-1	-4	-5	-22.80	-20.69	-2	1	-6	84.01	93.25	3	5	-6	- 2.02	- 1.95
					1	-4	-5	40.74	38.44	2	1	-6	11.83	12.50	-3	-5	-6	11.53	12.41
0	0	-5	- 7.96	- 4.07	2	4	-5	2.90	3.58	-2	-1	-6	-26.43	-26.06	3	-5	-6	-18.48	-18.62
1	0	-5	17.54	14.10	-2	4	-5	- 3.31	- 3.26	2	-1	-6	-50.86	-47.29	-4	-5	-6	30.42	27.17
-1	0	-5	93.34	101.82	-2	-4	-5	10.19	11.65	-3	1	-6	27.79	31.52	-5	-5	-6	16.05	14.89
-2	0	-5	17.47	20.06	2	-4	-5	6.34	5.88	3	1	-6	24.04	24.81	-6	-5	-6	-15.31	-17.62
2	0	-5	30.69	29.14	3	4	-5	2.63	1.65	-3	-1	-6	- 3.62	- 3.55	-7	-5	-6	- 4.32	- 6.54
-3	0	-5	34.74	31.92	-3	4	-5	32.78	33.09	3	-1	-6	8.59	8.55	-8	-5	-6	9.71	8.37
3	0	-5	3.44	0.44	-3	-4	-5	-32.11	-29.40	-4	1	-6	-46.98	-54.06	0	-6	-6	2.50	12.46
-4	0	-5	16.19	18.13	3	-4	-5	3.37	3.70	4	1	-6	51.31	49.22	-1	-6	-6	16.39	16.33
4	0	-5	7.08	7.64	4	4	-5	10.99	9.80	-4	-1	-6	23.26	24.67	1	-6	-6	6.27	6.04
-5	0	-5	-14.23	-13.47	-4	4	-5	11.33	10.75	4	-1	-6	16.16	15.26	-2	-6	-6	-10.86	-10.80
5	0	-5	20.91	25.60	-4	-4	-5	4.72	3.41	-5	1	-6	15.51	16.77	2	-6	-6	7.15	5.35
-6	0	-5	4.79	4.87	4	-4	-5	17.47	17.67	5	1	-6	3.23	1.45	-3	-6	-6	13.02	13.01
6	0	-5	17.61	16.50	5	4	-5	4.79	5.09	-5	-1	-6	4.52	5.24	-4	-6	-6	- 7.69	- 7.20
-7	0	-5	12.41	14.24	-5	-4	-5	40.20	40.60	5	-1	-6	28.95	29.59	-5	-6	-6	7.42	8.12
-8	0	-5	7.55	7.37	-6	-4	-5	- 8.23	- 9.30	-6	1	-6	5.36	0.44	-6	-6	-6	34.27	35.46
0	1	-5	21.25	18.12	-7	-4	-5	11.67	11.12	-6	-1	-6	- 1.74	- 0.26	-7	-6	-6	12.68	11.17

Table 2. *(Continued)*

h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c	h k l	F_o	F_c
-8 -6 -6	13.36	13.65	1 3 -7	18.62	18.78	3 0 -8	20.91	25.47	-3 -7 -8	17.34	17.98
0 -7 -6	15.78	16.55	-1 -3 -7	33.46	36.04	-4 0 -8	46.95	53.40	-4 -7 -8	-29.68	-28.93
-1 -7 -6	13.49	11.27	1 -3 -7	-39.93	-36.43	4 0 -8	39.06	46.75	-6 -7 -8	17.07	17.50
1 -7 -6	3.98	1.08	-2 3 -7	15.72	15.54	-5 0 -8	19.97	22.04	-2 -8 -8	8.70	7.48
-2 -7 -6	20.37	20.33	2 3 -7	14.77	16.17	-6 0 -8	-19.22	-25.08	-3 -8 -8	8.23	6.27
-3 -7 -6	12.28	12.04	-2 -3 -7	19.49	19.67	0 1 -8	9.98	8.29	-4 -8 -8	14.97	15.30
-4 -7 -6	49.04	47.87	2 -3 -7	24.82	23.53	0 -1 -8	9.98	6.31	-5 -8 -8	9.17	9.55
-5 -7 -6	20.51	21.20	-3 3 -7	-11.40	-13.18	-1 1 -8	- 1.89	- 0.70	-6 -8 -8	15.78	12.28
-6 -7 -6	-27.18	-28.89	3 3 -7	2.90	2.39	1 1 -8	- 6.00	- 7.37			
-7 -7 -6	8.84	8.25	-3 -3 -7	34.20	34.00	1 -1 -8	21.45	19.25	0 0 -9	10.19	10.18
-8 -7 -6	32.72	34.24	3 -3 -7	21.18	20.45	-2 1 -8	17.27	17.67	-1 0 -9	11.20	17.03
0 -8 -6	4.18	0.84	-4 3 -7	9.38	8.55	2 1 -8	-30.76	-29.95	1 0 -9	- 3.24	- 4.76
-1 -8 -6	23.47	23.82	4 3 -7	- 1.82	- 0.50	-2 -1 -8	28.47	30.52	-2 0 -9	4.86	9.98
-2 -8 -6	-16.93	-17.79	-4 -3 -7	31.30	31.71	2 -1 -8	10.66	9.84	2 0 -9	9.31	7.66
-3 -8 -6	3.31	2.91	4 -3 -7	- 3.64	- 3.85	3 1 -8	22.33	21.98	-3 0 -9	- 7.28	-11.43
-4 -8 -6	14.23	11.92	-5 -3 -7	-20.64	-22.66	-3 -1 -8	31.30	32.67	3 0 -9	- 6.00	-18.18
-5 -8 -6	2.63	1.21	-6 -3 -7	7.69	5.02	-3 1 -8	11.94	15.01	-4 0 -9	4.05	5.99
-6 -8 -6	29.21	29.85	-7 -3 -7	14.97	17.16	-4 1 -8	5.87	3.51	-5 0 -9	13.09	9.17
-7 -8 -6	4.38	3.48	-8 -3 -7	13.76	17.43	-4 -1 -8	-21.85	-23.88	-6 0 -9	- 6.81	-12.70
-3 -9 -6	12.01	12.99	0 4 -7	6.61	7.41	-5 -1 -8	- 9.11	-12.69	0 -1 -9	12.14	11.40
-4 -9 -6	- 8.43	- 8.91	0 -4 -7	10.99	12.08	-6 -1 -8	55.65	62.19	1 1 -9	-11.33	-11.04
-5 -9 -6	3.71	2.85	1 4 -7	2.02	1.95	-7 -1 -8	19.97	23.49	1 -1 -9	-17.20	-13.39
			-1 4 -7	12.61	11.32	0 2 -8	31.37	33.86	-1 -1 -9	30.76	30.23
0 0 -7	17.00	15.07	-1 -4 -7	-17.00	-17.43	0 -2 -8	-11.47	-11.66	2 1 -9	23.07	21.48
-1 0 -7	29.68	28.27	1 -4 -7	30.22	30.10	-1 2 -8	21.52	22.56	-2 1 -9	9.63	9.81
1 0 -7	23.54	21.13	2 4 -7	24.15	23.58	1 2 -8	2.29	0.34	2 -1 -9	21.99	19.28
-2 0 -7	21.92	22.89	-2 4 -7	18.62	17.79	-1 -2 -8	-12.88	- 5.30	3 -1 -9	32.51	30.12
2 0 -7	-17.00	-15.63	-2 -4 -7	8.09	7.65	1 -2 -8	23.20	21.76	-3 -1 -9	33.39	35.54
-3 0 -7	7.55	7.67	2 -4 -7	6.21	5.66	-2 2 -8	-43.17	-44.43	-4 -1 -9	20.30	20.95
3 0 -7	-15.11	-13.61	3 4 -7	43.84	43.30	2 -2 -8	- 1.21	- 0.04	-5 1 -9	39.33	39.85
-4 0 -7	12.01	12.11	-3 4 -7	-25.09	-25.77	-3 -2 -8	10.12	8.94	-6 -1 -9	17.13	19.01
4 0 -7	43.71	43.33	-3 -4 -7	25.36	23.67	-4 2 -8	27.99	27.13	0 2 -9	- 5.80	- 5.28
-5 0 -7	- 4.52	- 4.20	3 -4 -7	41.75	41.44	-4 -2 -8	43.31	43.02	0 -2 -9	36.22	34.99
5 0 -7	31.30	35.82	-4 -4 -7	21.32	19.91	-5 -2 -8	22.33	24.12	-1 2 -9	28.13	27.60
-6 0 -7	13.90	16.69	-5 -4 -7	35.95	34.57	-6 -2 -8	-18.82	-22.55	1 -2 -9	56.19	49.56
-7 0 -7	21.11	20.30	-6 -4 -7	14.37	13.45	-7 -2 -8	- 9.04	-12.62	2 2 -9	13.15	12.38
0 1 -7	40.34	38.22	-7 -4 -7	- 2.90	- 2.77	0 3 -8	-23.41	-28.04	-2 2 -9	13.42	13.37
0 -1 -7	11.06	4.32	-8 -4 -7	- 0.67	- 1.29	0 -3 -8	3.10	0.60	2 -2 -9	-12.21	-12.94
-1 1 -7	-80.74	-83.14	0 5 -7	11.26	10.51	1 3 -8	31.30	31.37	-3 2 -9	26.91	28.24
1 1 -7	68.40	66.92	0 -5 -7	21.45	23.03	-1 -3 -8	24.15	26.44	-5 -2 -9	17.27	15.86
-1 -1 -7	- 8.57	- 8.01	1 5 -7	27.12	26.67	1 -3 -8	24.76	22.67	-7 -2 -9	20.91	21.58
1 -1 -7	26.31	23.20	-1 -5 -7	11.94	9.68	-2 3 -8	32.78	32.34	0 3 -9	16.32	21.44
-2 -1 -7	9.51	11.24	1 -5 -7	16.73	16.06	2 3 -8	43.84	43.63	0 -3 -9	- 3.24	- 4.88
2 1 -7	- 2.23	- 1.18	-2 -5 -7	8.16	6.75	-2 -3 -8	-18.62	-20.48	1 -3 -9	-27.32	-26.00
-2 1 -7	- 1.15	- 1.34	2 -5 -7	-15.85	-17.68	2 -3 -8	33.19	31.13	-1 -3 -9	41.75	37.61
2 -1 -7	17.20	15.87	-3 -5 -7	6.21	3.88	-3 3 -8	13.29	13.68	2 -3 -9	15.04	13.99
-3 1 -7	25.23	24.39	-4 -5 -7	4.79	3.36	-3 -3 -8	10.59	7.58	-3 -3 -9	16.26	13.01
3 1 -7	- 8.70	- 7.86	-5 -5 -7	15.58	15.50	3 -3 -8	- 5.33	- 6.38	-7 -3 -9	11.53	13.64
-3 -1 -7	31.43	32.49	-6 -5 -7	3.98	3.26	-4 -3 -8	7.28	5.97	0 -4 -9	19.49	22.89
3 -1 -7	34.06	31.69	-7 -5 -7	48.03	49.75	-5 -3 -8	- 3.10	- 0.69	1 -4 -9	27.66	28.02
-4 1 -7	1.96	1.94	-8 -5 -7	4.72	3.06	-6 -3 -8	31.91	32.35	-1 -4 -9	-12.41	-11.93
4 1 -7	6.54	6.84	0 -6 -7	4.11	2.85	-7 -3 -8	9.58	6.96	2 -4 -9	13.29	13.19
-4 -1 -7	21.05	19.88	-1 -6 -7	23.88	25.89	-8 -3 -8	-24.15	-28.73	-3 -4 -9	24.96	25.16
4 -1 -7	4.52	5.11	1 -6 -7	-33.12	-34.93	0 4 -8	- 2.97	- 2.55	-4 -4 -9	13.90	13.98
-5 1 -7	-15.31	-13.70	-2 -6 -7	15.51	17.95	0 -4 -8	27.45	27.40	-5 -4 -9	23.14	19.92
-5 -1 -7	11.33	9.50	2 -6 -7	14.50	14.45	-1 -4 -8	16.53	16.98	-6 -4 -9	14.37	13.92
-6 1 -7	7.02	5.90	-3 -6 -7	16.19	16.93	1 -4 -8	1.75	0.24	-7 -4 -9	-47.82	-50.24
-6 -1 -7	3.78	3.94	-4 -6 -7	14.03	13.50	-2 -4 -8	25.70	28.72	0 -5 -9	- 1.96	- 2.97
-7 -1 -7	- 5.26	- 9.62	-5 -6 -7	8.16	11.30	2 -4 -8	-22.26	-22.05	-1 -5 -9	56.73	56.49
0 2 -7	- 5.53	- 5.38	-6 -6 -7	9.24	10.22	-3 4 -8	18.21	17.75	-2 -5 -9	34.67	34.90
0 -2 -7	- 1.69	- 1.51	-7 -6 -7	-25.83	-27.87	-4 -4 -8	9.38	6.68	-3 -5 -9	-52.61	-54.91
-1 2 -7	16.93	16.70	-8 -6 -7	- 1.89	- 1.72	-5 -4 -8	6.00	8.05	-4 -5 -9	-17.00	-17.05
1 2 -7	- 9.24	- 8.79	0 -7 -7	14.44	17.23	-6 -4 -8	4.25	0.63	-5 -5 -9	50.12	46.15
-1 -2 -7	26.31	26.23	-1 -7 -7	- 5.46	- 7.50	-7 -4 -8	7.35	7.53	-6 -5 -9	12.21	9.13
1 -2 -7	-25.70	-24.52	-2 -7 -7	12.75	13.60	-8 -4 -8	43.91	46.00	0 -6 -9	- 2.09	- 8.96
-2 2 -7	5.60	4.27	-3 -7 -7	- 5.60	- 4.10	0 -5 -8	- 2.63	- 2.42	-3 -6 -9	50.19	51.97
2 2 -7	24.01	24.06	-4 -7 -7	6.95	7.02	-1 -5 -8	14.23	12.86	-4 -6 -9	18.68	18.78
2 -2 -7	21.18	21.98	-5 -7 -7	32.04	30.28	1 -5 -8	7.62	6.23	-5 -6 -9	-27.18	-28.54
-3 2 -7	34.60	34.42	-6 -7 -7	4.38	2.64	-2 -5 -8	29.41	32.20	-7 -6 -9	22.73	21.41
3 2 -7	37.64	35.10	-7 -7 -7	3.64	0.21	2 -5 -8	29.54	28.87	-1 -7 -9	-13.83	-14.21
-3 -2 -7	-64.89	-67.56	-1 -8 -7	52.88	56.05	-3 -5 -8	0.74	2.51	-6 -7 -9	13.83	13.73
3 -2 -7	9.98	10.22	-2 -8 -7	17.40	17.77	-4 -5 -8	57.54	55.52	-4 -8 -9	16.66	14.35
-4 2 -7	8.36	9.24	-3 -8 -7	- 6.21	- 6.38	-5 -5 -8	21.72	19.72			
4 2 -7	- 5.33	- 5.86	-4 -8 -7	- 4.32	- 5.11	-6 -5 -8	-21.85	-22.18	0 0 -10	-20.94	-20.44
-4 -2 -7	- 8.43	-12.21	-5 -8 -7	34.53	34.02	0 -6 -8	20.91	21.23	-1 0 -10	-19.27	-12.11
4 -2 -7	- 7.49	- 8.84	-6 -8 -7	11.26	10.29	-1 -6 -8	19.83	20.72	1 0 -10	12.99	16.27
-5 2 -7	-24.76	-27.99	-7 -8 -7	- 7.82	- 7.25	-2 -6 -8	-22.53	-24.73	-3 0 -10	13.25	13.05
-5 -2 -7	52.01	56.05				-3 -6 -8	- 0.81	- 0.63	-4 0 -10	4.85	1.18
-6 -2 -7	9.65	9.28	0 0 -8	34.27	33.60	-4 -6 -8	- 2.43	- 0.44	0 1 -10	29.47	32.00
-7 -2 -7	15.38	14.46	-1 0 -8	27.93	31.93	-5 -6 -8	- 6.41	- 8.43	0 -1 -10	22.62	21.49
-8 -2 -7	- 1.48	- 1.55	1 0 -8	6.81	5.83	-6 -6 -8	29.88	28.06	0 -2 -10	21.52	17.40
0 3 -7	- 2.70	- 2.44	-2 0 -8	-33.93	-47.51	0 -7 -8	-12.68	-23.98	0 -3 -10	18.48	17.02
0 -3 -7	- 0.94	- 0.71	2 0 -8	-11.80	-10.74	-1 -7 -8	- 6.34	- 6.91	0 -4 -10	- 3.30	- 3.21
-1 3 -7	36.56	36.44	-3 0 -8	1.48	1.74	-2 -7 -8	60.57	61.85	0 -5 -10	- 2.26	- 9.56

Results from the refinement

Table 3 lists the discrepancy indices R as obtained at the various stages of the refinement. These values were obtained from the relation

$$R = \frac{\Sigma \| F_o | - | F_c \|}{\Sigma | F_o |} .$$

Table 3. *Discrepancy index R for the different stages of determination and refinement of the structure of turquois*

	R
Originial coordinates	62%
Results of Fourier refinement	27%
Least-squares isotropic refinement	9.5%
Least-squares anisotropic refinement	7%

Table 4. *Coordinates for the non-hydrogen atoms of turquois*

Atom	x	$\sigma(x)$	y	$\sigma(y)$	z	$\sigma(z)$
Cu	0		0		0	
P_1	0.3504	0.0006	0.3867	0.0006	0.9429	0.0004
P_2	0.8423	0.0006	0.3866	0.0005	0.4570	0.0004
Al_1	0.2843	0.0006	0.1766	0.0006	0.7521	0.0005
Al_2	0.7520	0.0006	0.1862	0.0006	0.2736	0.0005
Al_3	0.2448	0.0007	0.5023	0.0007	0.2438	0.0005
O_1	0.0675	0.0014	0.3633	0.0014	0.3841	0.0011
O_2	0.8058	0.0014	0.3435	0.0014	0.6262	0.0011
O_3	0.2757	0.0014	0.3554	0.0014	0.1129	0.0011
O_4	0.0663	0.0015	0.0639	0.0015	0.1973	0.0011
O_5	0.2375	0.0015	0.0739	0.0015	0.6287	0.0012
O_6	0.7334	0.0014	0.0857	0.0014	0.1243	0.0011
O_7	0.2978	0.0015	0.4016	0.0014	0.6060	0.0011
O_8	0.3249	0.0014	0.2227	0.0014	0.9049	0.0011
O_9	0.9857	0.0014	0.2807	0.0014	0.8471	0.0011
O_{10}	0.5756	0.0016	0.0467	0.0015	0.6855	0.0012
O_{11}	0.7866	0.0014	0.4067	0.0015	0.1319	0.0011
O_{12}	0.4630	0.0014	0.2950	0.0014	0.3277	0.0011
O_{13}	0.7864	0.0014	0.2281	0.0014	0.4323	0.0011
O_{14}	0.5779	0.0014	0.3660	0.0014	0.8987	0.0011

In Table 4 are listed the final refined coordinates for the non-hydrogen atoms in turquois together with the standard deviations as given by the least-squares program. Table 5 lists the refined anisotropic coefficients β_{ij} for the non-hydrogen atoms together with the equivalent isotropic temperature factor as calculated from HAMILTON's formula[24]

$$B = \frac{4}{3} \sum_i \sum_j \beta_{ij} (\mathbf{a}_i \cdot \mathbf{a}_j) \ .$$

Values marked with a star correspond to those coefficients responsible for the non-definitive positive character of the temperature vibration.

[24] W. C. HAMILTON, On the isotropic temperature factor equivalent to a given anisotropic temperature factor. Acta Crystallogr. **12** (1959) 609—610.

Table 5. *Anisotropic temperature coefficients*

Atom		β_{ij}	B	Atom		β_{ij}	B
Cu				O_1			
	β_{11}	0.0076	1.6		β_{11}	0.0009	0.74
	β_{22}	0.0079			β_{22}	0.0042	
	β_{33}	0.0047			β_{33}	0.0014	
	β_{12}	− 0.0027			β_{12}	− 0.0012	
	β_{13}	0.0012			β_{13}	0.0025	
	β_{23}	− 0.0012			β_{33}	0.0001	
P_1				O_2			
	β_{11}	0.0015	0.26		β_{11}	0.0038	0.56
	β_{22}	0.0015			β_{22}	0.0036	
	β_{33}	0.0008			β_{33}	0.0007*	
	β_{12}	− 0.0005			β_{12}	− 0.0032*	
	β_{13}	− 0.0003			β_{13}	0.0016	
	β_{23}	− 0.0003			β_{23}	0.0001	
P_2				O_3			
	β_{11}	0.0012	0.21		β_{11}	0.0032	0.62
	β_{22}	0.0012			β_{22}	0.0040	
	β_{33}	0.0006			β_{33}	0.0011	
	β_{12}	− 0.0004			β_{12}	− 0.0027	
	β_{13}	− 0.0002			β_{13}	0.0019	
	β_{23}	− 0.0002			β_{23}	− 0.0003	
Al_1				O_4			
	β_{11}	0.0028	0.40		β_{11}	0.0058	0.82
	β_{22}	0.0008			β_{22}	0.0029	
	β_{33}	0.0012			β_{33}	0.0024	
	β_{12}	− 0.0012			β_{12}	− 0.0016	
	β_{13}	0.0010			β_{13}	− 0.0008	
	β_{23}	− 0.0002			β_{23}	0.0002	
Al_2				O_5			
	β_{11}	0.0016	0.39		β_{11}	0.0048	0.68
	β_{22}	0.0005			β_{22}	0.0011	
	β_{33}	0.0016			β_{33}	0.0027	
	β_{12}	− 0.0006			β_{12}	− 0.0012	
	β_{13}	0.0012			β_{13}	− 0.0003	
	β_{23}	− 0.0003			β_{23}	− 0.0002	
Al_3				O_6			
	β_{11}	0.0012	0.25		β_{11}	0.0031	0.66
	β_{22}	0.0012			β_{22}	0.0020	
	β_{33}	0.0007			β_{33}	0.0026	
	β_{12}	− 0.0004			β_{12}	− 0.0011	
	β_{13}	− 0.0002			β_{13}	0.0002	
	β_{23}	− 0.0002			β_{23}	− 0.0001	

Table 5. *(Continued)*

Atom		β_{ij}	B	Atom		β_{ij}	B
O_7				O_{11}			
	β_{11}	0.0037	0.86		β_{11}	0.0054	0.66
	β_{22}	0.0012			β_{22}	0.0018	
	β_{33}	0.0041			β_{33}	0.0021	
	β_{12}	− 0.0016			β_{12}	− 0.0016	
	β_{13}	0.0014			β_{13}	0.0008	
	β_{23}	− 0.0005			β_{23}	− 0.0001	
O_8				O_{12}			
	β_{11}	0.0075	0.74		β_{11}	0.0016	0.61
	β_{22}	0.0037			β_{22}	0.0026	
	β_{33}	0.0013			β_{33}	0.0025	
	β_{12}	− 0.0040			β_{12}	− 0.0003	
	β_{13}	− 0.0003			β_{13}	0.0012	
	β_{23}	0.0001			β_{23}	− 0.0010	
O_9				O_{13}			
	β_{11}	0.0048	0.61		β_{11}	0.0025	0.59
	β_{22}	0.0033			β_{22}	0.0038	
	β_{33}	0.0009			β_{33}	0.0015	
	β_{12}	− 0.0025			β_{12}	− 0.0026	
	β_{13}	0.0006			β_{13}	0.0009	
	β_{23}	0.0001			β_{23}	0.0003	
O_{10}				O_{14}			
	β_{11}	0.0043	0.95		β_{11}	0.0007*	0.41
	β_{22}	0.0016			β_{22}	0.0042	
	β_{33}	0.0043			β_{33}	0.0002*	
	β_{12}	− 0.0011			β_{12}	− 0.0015	
	β_{13}	0.0002			β_{13}	0.0024	
	β_{23}	0.0001			β_{23}	− 0.0008	

Usually an arbitrary change of approximately half of the standard deviation will give a positive character.

In regard to the fact that the absorption correction was not accurate enough, no attempt was made to interpret the vibration ellipsoids of the atoms. The only remark that can be made is that the Cu vibration is in the direction of the longer bond (Cu—H_2O) which is approximately perpendicular to the plane of the square arrangement of OH radicals.

Table 6 gives the hydrogen coordinates unrefined, as obtained from the last three-dimensional electron-density difference function using $F_o - F_c$ as coefficients. An arbitrary isotropic temperature

Table 6. *Atomic coordinates of the hydrogen atoms in turquois*

Atom	x	y	z
H_1	0.8667	0.0333	0.7533
H_2	0.1500	0.1567	0.1500
H_3	0.6333	0.1433	0.5900
H_4	0.3933	0.0833	0.2900
H_5	0.1433	0.1167	0.5933
H_6	0.6500	0.1433	0.1000
H_7	0.9800	0.3500	0.9000
H_8	0.4500	0.2767	0.4233

coefficient of 2.0 was assigned to all hydrogens when included in the refinement, but no attempt was made to change it.

The largest O—H distance is 1.17 Å and the shortest 0.72 Å. Taking the average value 0.95 Å as the normal O—H distance, a standard deviation of the hydrogen coordinates can be estimated in 0.2 Å. All 8 hydrogen atoms seem to be involved in hydrogen bonding. Table 7 gives the relation between them and the atoms they contribute to bind.

Table 7. *Distances in hydrogen bonds*

O_i—H_j $\cdots$ O_k	O_i—H_j	O_k—H_j	O_i—O_k
O_4—H_1 $\cdots$ O_2	0.869 Å	2.067 Å	2.871 Å
O_4—H_2 $\cdots$ O_3	1.150	0.901	2.950
O_{10}—H_3 $\cdots$ O_{13}	1.172	1.567	2.688
O_{10}—H_4 $\cdots$ O_{12}	1.004	1.881	2.780
O_5—H_5 $\cdots$ O_1	0.743	2.292	2.883
O_6—H_6 $\cdots$ O_{14}	0.716	2.062	2.670
O_9—H_7 $\cdots$ O_{11}	0.844	2.220	2.970
O_{12}—H_8 $\cdots$ O_7	0.725	2.173	2.862

Interatomic distances and bond angles were computed with SHOEMAKER's program DISTAN [25]. Interatomic distances are listed on Table 8 and bond angles on Table 9. In both tables the atoms designated with a single prime represent the centrosymmetrical equivalent of the unprimed atom whose coordinates are listed on Table 4, plus or minus a cell translation. The short distance O_5—O_6 corresponds to the share edge of the Al_1 and Al_2 octahedra.

[25] DAVID P. SHOEMAKER, DISTAN, crystallographic bond distance, bond angle and dihedral angle computer program. Internal publication of the Chemistry Department (1963) Mass. Inst. of Technology, Cambridge, Mass.

Table 8. *The interatomic distances in the turquois structure*

Atom pair	Multiplicity	Distance	Atom pair	Multiplicity	Distance
Cu pseudo octahedron			O_5'—O_{13}	1	2.676
Cu—$O_4(H_2O)$	2	2.422 Å	O_6—O_{11}	1	2.669
Cu—O_6(OH)	2	1.915	O_6—O_{12}	1	2.725
Cu—O_9(OH)	2	2.109	O_{11}—O_{12}	1	2.759
O_4—O_6	2	2.748	O_{11}—O_{13}	1	2.752
O_4—O_6'	2	3.420	O_{12}—O_{13}	1	2.720
O_4—O_9	2	3.420			
O_4—O_9'	2	3.029	Al_3 octahedron		
O_6—O_9	2	2.690	Al_3—O_1	1	1.903
O_6—O_9'	2	3.025	Al_3—O_2'	1	1.893
			Al_3—O_3	1	1.904
Al_1 octahedron			Al_3—O_9'(OH)	1	2.164
Al_1—O_5(OH)	1	1.858	Al_3—O_{12}(OH)	1	1.906
Al_1—O_6'(OH)	1	1.963	Al_3—O_{14}	1	1.878
Al_1—O_7	1	1.812	O_1—O_2'	1	2.734
Al_1—O_8	1	1.817	O_1—O_3	1	2.593
Al_1—O_9'(OH)	1	2.011	O_1—O_9	1	2.811
Al_1—$O_{10}(H_2O)$	1	1.943	O_2—O_9	1	2.797
O_5—O_6'	1	2.340*	O_9'—O_{14}'	1	2.702
O_5—O_7	1	2.623	O_9'—O_3	1	2.702
O_5—O_9'	1	2.808	O_{12}—O_1	1	2.647
O_5—O_{10}	1	2.668	O_{12}—O_3	1	2.730
O_6'—O_8	1	2.699	O_{12}—O_2	1	2.730
O_6'—O_{10}	1	2.722	O_{12}—O_{14}	1	2.729
O_6'—O_9	1	2.690	O_{14}—O_3	1	2.709
O_7—O_8	1	2.834	O_{14}'—O_2'	1	2.667
O_7—O_{10}	1	2.675			
O_7—O_9	1	2.875	P_1 tetrahedron		
O_8—O_{10}	1	2.704	P_1—O_3'	1	1.541
O_8—O_9	1	2.584	P_1—O_8	1	1.521
			P_1—O_{11}'	1	1.539
Al_2 octahedron			P_1—O_{14}	1	1.556
Al_2—$O_4'(H_2O)$	1	2.084	O_3'—O_8	1	2.458
Al_2—O_5'(OH)	1	1.844	O_3'—O_{11}'	1	2.489
Al_2—O_6(OH)	1	1.963	O_3—O_{14}	1	2.501
Al_2—O_{11}	1	1.805	O_8—O_{11}	1	2.504
Al_2—O_{12}(OH)	1	1.899	O_8—O_{14}	1	2.531
Al_2—O_{13}	1	1.832	O_{11}'—O_{14}	1	2.591
O_4'—O_5'	1	2.681			
O_4'—O_6	1	2.748	P_2 tetrahedron		
O_4'—O_{11}	1	2.606	P_2—O_1'	1	1.534
O_4'—O_{13}	1	2.815	P_2—O_2	1	1.533
O_5'—O_6	1	2.340*	P_2—O_7'	1	1.543
O_5'—O_{12}	1	2.752	P_2—O_{13}	1	1.550

Table 8. *(Continued)*

Atom pair	Multiplicity	Distance	Atom pair	Multiplicity	Distance
O_1'—O_2	1	2.527	O_2—O_7'	1	2.507
O_1'—O_7	1	2.524	O_2—O_{13}	1	2.470
O_1'—O_{13}	1	2.528	O_7—O_{13}	1	2.538

* Shared edge.

A maximum error of 0.005 can be assumed on all distances

Table 9. *Bond angles in the turquois structure*

Atoms	Multiplicity	Angle	
Cu pseudo octahedron			
O_6'—Cu—$O_4(H_2O)$	2	77.4°	
O_6'—Cu—$O_4'(H_2O)$	2	102.6°	
O_9'—Cu—$O_4(H_2O)$	2	96.7°	
O_9'—Cu—$O_4'(H_2O)$	2	83.3°	
O_6—Cu—O_9'	2	96.5°	
O_6'—Cu—O_9'	2	83.5°	
Al_1 octahedron			
O_5—Al_1—O_6'	1	75.6°	(shared edge)
O_5—Al_1—O_7	1	91.4°	
O_6—Al_1—O_8	1	90.8°	
O_7—Al_1—O_8	1	102.2°	
O_5—Al_1—O_9	1	93.3°	
O_6'—Al_1—O_9	1	85.2°	
O_7—Al_1—O^9	1	97.3°	
O_8—Al_1—O_9	1	84.6°	
O_5—Al_1—$O_{10}(H_2O)$	1	89.0°	
O_6'—Al_1—$O_{10}(H_2O)$	1	88.0°	
O_7—Al_1—$O_{10}(H_2O)$	1	90.3°	
O_8—Al_1—$O_{10}(H_2O)$	1	91.3°	
O_9'—Al_1—$O_{10}(H_2O)$	1	172.0°	
O_6'—Al_1—O_7	1	166.9°	
O_5—Al_1—O_8	1	166.4°	
Al_2 octahedron			
O_4—Al_2—O_5'	1	85.3°	
O_4—Al_2—O_6	1	85.2°	
O_5—Al_2—O_6	1	75.7°	(shared edge)
O_4—Al_2—O_{11}	1	83.2°	
O_6—Al_2—O_{11}	1	90.0°	
O_5'—Al_2—O_{12}	1	94.4°	
O_6—Al_2—O_{12}	1	89.9°	

Table 9. *(Continued)*

Atoms	Multiplicity	Angle
O_{11}—Al_2—O_{12}	1	96.0°
O_4—Al_2—O_{13}	1	91.3°
O_5—Al_2—O_{13}	1	93.4°
O_{11}—Al_2—O_{13}	1	100.2°
O_{12}—Al_2—O_{13}	1	93.7°
O_5'—Al_2—O_{11}	1	162.4°
O_4—Al_2—O_{12}	1	175.0°
O_6—Al_2—O_{13}	1	168.8°
Al_3 octahedron		
O_1—Al_3—O_2'	1	92.4°
O_1—Al_3—O_3	1	85.9°
O_1—Al_3—O_9'	1	91.8°
O_2'—Al_3—O'_9	1	89.4°
O_3—Al_3—O_9'	1	87.2°
O_1—Al_3—O_{12}	1	88.1°
O_2'—Al_3—O_{12}	1	92.0°
O_3—Al_3—O_{12}	1	91.5°
O_2'—Al_3—O_{14}'	1	90.2°
O_3—Al_3—O_{14}'	1	91.5°
O_9'—Al_3—O_{14}'	1	88.0°
O_{12}—Al_3—O_{14}'	1	92.1°
O_2'—Al_3—O_3	1	176.1°
O_9'—Al_3—O_{12}	1	178.6°
O_1—Al_3—O_{14}'	1	177.4°
P_1 tetrahedron		
O_3'—P_1—O_8	1	106.8°
O_3'—P_1—O_{11}'	1	107.8°
O_8—P_1—O_{11}'	1	109.8°
O_3'—P_1—O_{14}	1	107.7°
O_8—P_1—O_{14}	1	110.7°
O_{11}'—P_1—O_{14}	1	113.7°
P_2 tetrahedron		
O_1'—P_2—O_2	1	110.6°
O_1'—P_2—O_7'	1	110.7°
O_2—P_2—O_7'	1	109.7°
O_1'—P_2—O_{13}	1	110.0°
O_2—P_2—O_{13}	1	105.6°
O_7'—P_2—O_{13}	1	110.1°
Oxygen coordination angle		
P_2'—O_1—Al_3	1	143.4°
P_2—O_2—Al_3'	1	134.1°
P_1'—O_3—Al_3	1	133.2°

Table 9. *(Continued)*

Atoms	Multiplicity	Angle	
$Cu—O_4—Al_2$	1	88.2°	(H_2O coordination angle)
$Al_1—O_5—Al_2'$	1	108.1°	
$Cu'—O_6—Al_1$	1	98.6°	
$Cu'—O_6—Al_2'$	1	108.4°	
$Al_1'—O_6—Al_2$	1	99.8°	
$P_2'—O_7—Al_1$	1	140.1°	
$P_1—O_8—Al_1$	1	140.2°	
$Cu'—O_9'—Al_1$	1	91.3°	
$Cu'—O_9—Al_3'$	1	130.9°	
$Al_1—O_9'—Al_3'$	1	129.9°	
$—O_{10}—Al_1$	1	—	(H_2O single-coordinated)
$P_1'—O_{11}—Al_2$	1	137.3°	
$Al_2—O_{12}—Al_3$	1	138.8°	
$P_2—O_{13}—Al_2$	1	135.7°	
$P_1—O_{14}—Al_3'$	1	139.6°	

Description and discussion of the structure

A final three-dimensional electron-density function was calculated after the last cycle of refinement of the turquois structure. A composite of sections of the structure which contains maxima, as seen looking down the a axis, is shown in Fig. 3. If this composite section is compared to the minimum function $M_4(yz)$ of Fig. 1, a close correspondence can be recognized. The false peak on $M_4(yz)$, that projects on the inversion center $0, \frac{1}{2}$, is due to the pseudosymmetry $C\,\bar{1}$ of the crystal. In a first approximation turquois can be described as a C-centered structure with a Cu deficiency in the inversion center $\frac{1}{2}, 0, \frac{1}{2}$. Actually the biggest hole in the structure corresponds to this location, as can be seen from Figs. 4 to 7.

Figure 4 is the interpretation of the three-dimensional electron-density function projected parallel to the a axis. Fig. 5 and 6 are views of the structure represented as linked polyhedra as seen looking in the direction of the a axis. For simplicity, the structure has been divided into two parts, centrosymmetrically related. The first half of the structure, considered from $x = 0$ to $x = \frac{1}{2}$ is represented on Fig. 5; the second half, from $x = \frac{1}{2}$ to $x = 1$ is represented in Fig. 6.

The structure can be described in terms of single and double octahedral groups of oxygen atoms, OH radicals, and water around the aluminum atoms. The double group consists of two Al octahedra sharing an edge. It is linked by four PO_4 tetrahedra to the two trans-

lational-equivalent groups in the direction of the b axis. These tetrahedra are attached to the four free corners of the square sections with the common edge, as shown in Figs. 5 to 7.

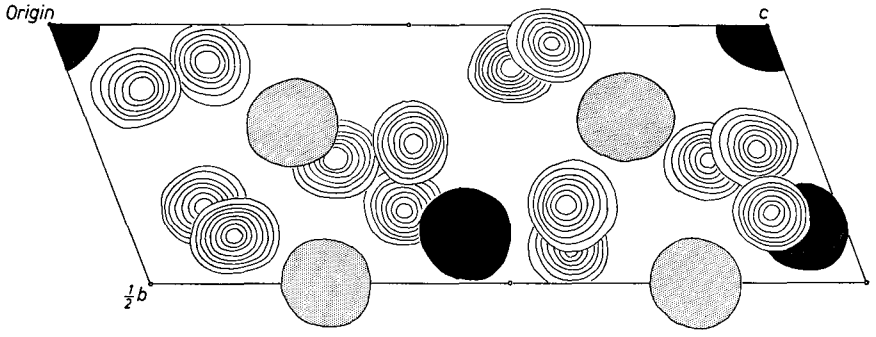

Fig. 3. Composite of sections from the final electron-density function

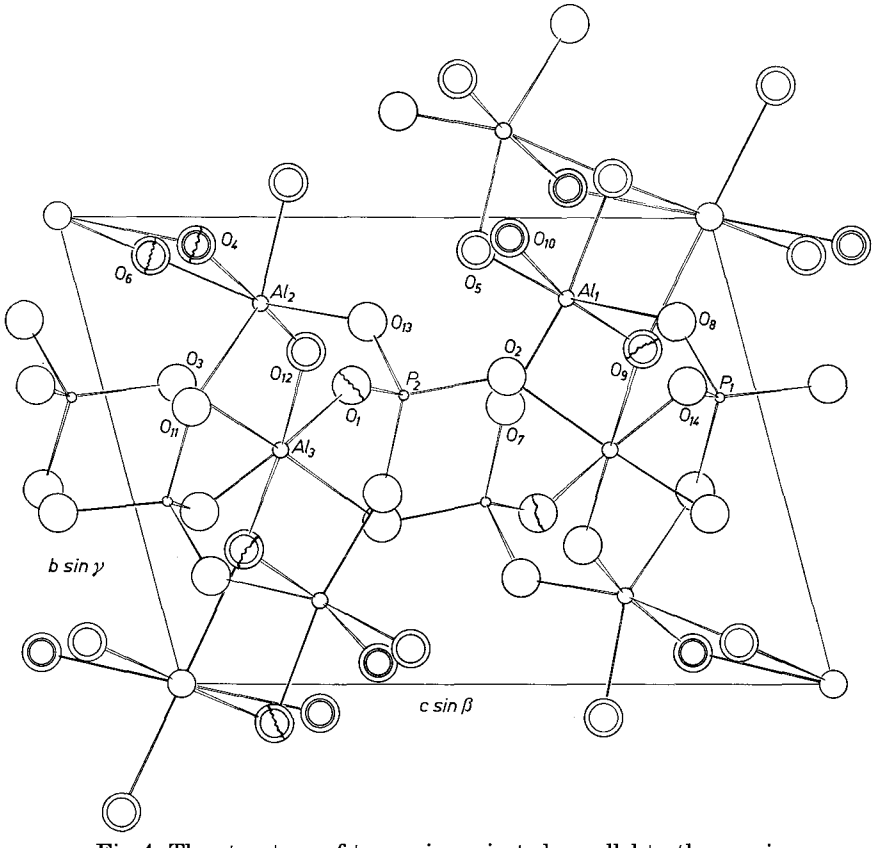

Fig. 4. The structure of turquois projected parallel to the a axis

The single aluminum octahedron shares the four oxygens at the corners of a square section with four PO_4 tetrahedra. Of the two remaining vertices, one is shared with the double octahedral group, and the other is also common to an octahedron of the double group and to the Cu octahedron. There are only two OH radicals in the asym-

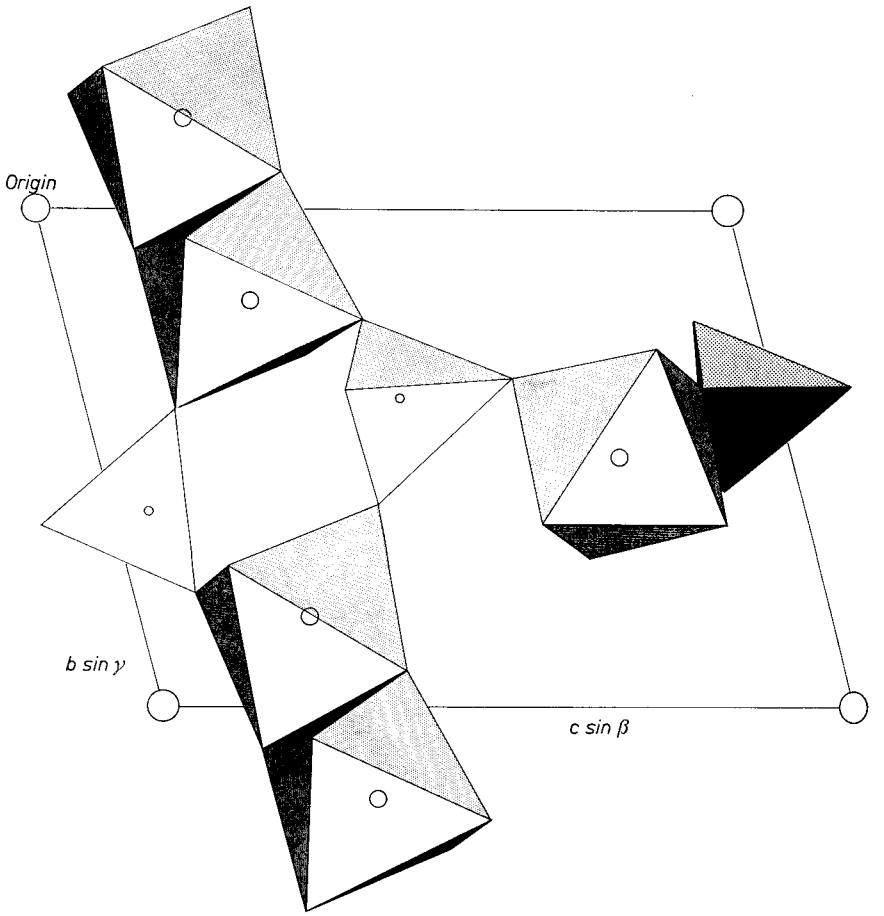

Fig. 5. Polyhedral chains, view parallel to the a axis, sections from $x = 0$ to $x = \frac{1}{2}$

metric unit that are common to the coordination polyhedra of three cations. One is OH(6), in the shared edge of the double group which also belongs to the Cu polyhedron. The other is OH(9), common to one single octahedral group, to a double octahedral group, and to the Cu octahedron.

The Cu octahedron has the expected $4 + 2$ coordination predicted by the Jahn-Teller effect[18]. The square coordination is formed by two OH radicals and their centrosymmetrical equivalents. The two long bonds are directed to two water molecules, related by an inversion center, which also complete the Al(2) octahedron.

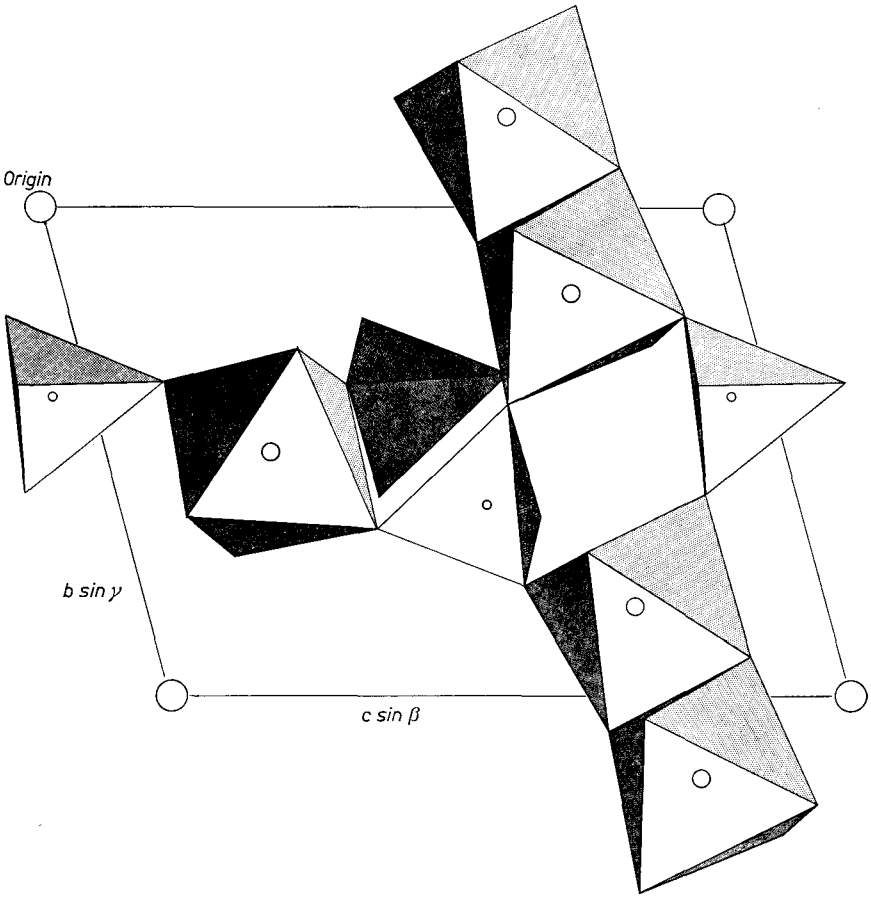

Fig. 6. Polyhedral chains, view parallel to the a axis, sections from $x = \frac{1}{2}$ to $x = 1$

The location of the water molecules in the Cu coordination agrees with the distribution found in eucroite[26] and liroconite[27]. However,

[26] GUISEPPE GUISEPPETTI, La struttura cristallina del'eucroite $Cu_2(AsO_4)(OH) \cdot 3H_2O$. Periodico Mineral. **32** (1963) 131—156.

[27] G. GUISEPPETTI, A. CODA, F. MAZZI e C. TADINI, La struttura cristallina della liroconite, $Cu_2Al(As,P)O_4(OH)_4 \cdot 4H_2O$. Periodico Mineral. **31** (1962) 19—42.

the results reported for kröhnkite[28] place the H_2O molecules as completing the square coordination of the Cu.

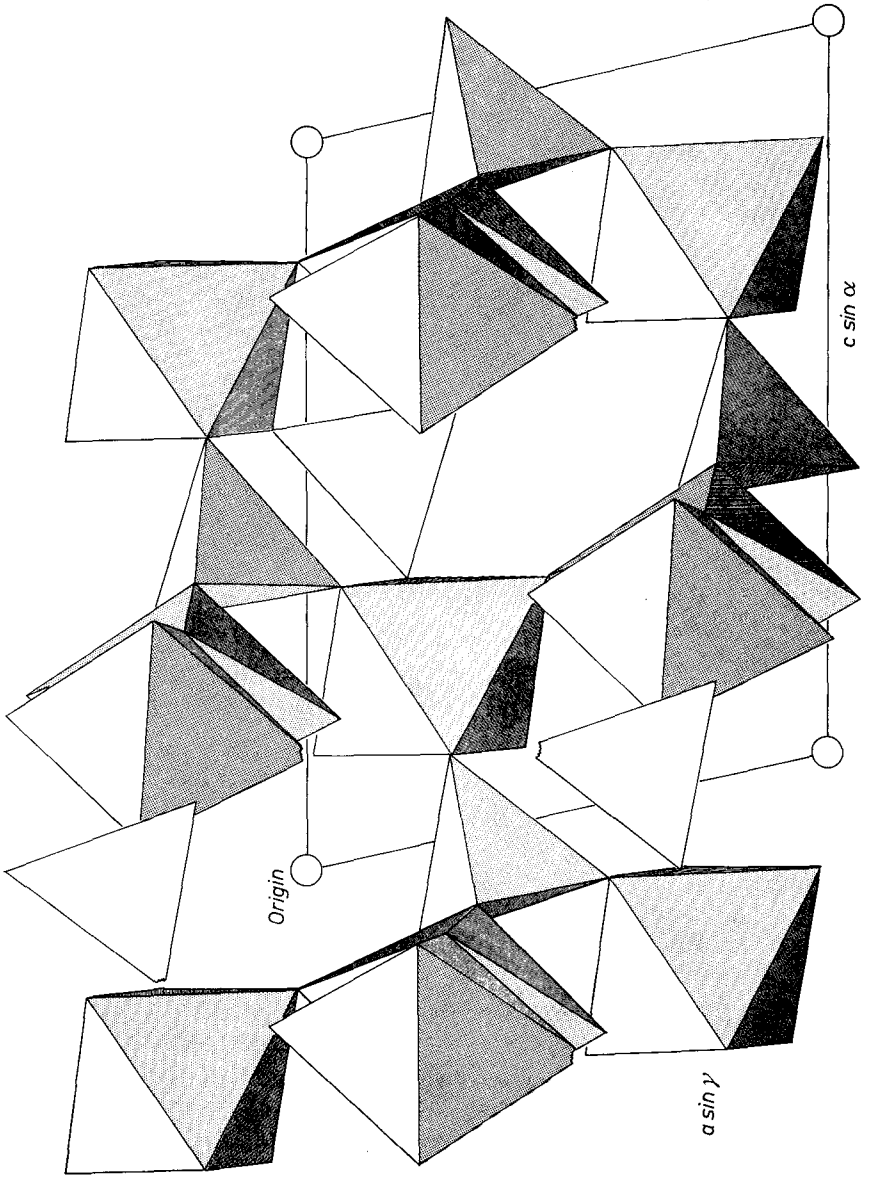

Fig. 7. Polyhedral chains in turquois, view parallel to the *b* axis

[28] B. RAMA RAO, Die Verfeinerung der Kristallstruktur von Kröhnkit, $Na_2Cu(SO_4)_2 \cdot 2H_2O$. Acta Crystallogr. **14** (1961) 738—743.

The values of the interatomic distances and angles for the PO_4 tetrahedra agree well with the reported values in related compounds. The single Al octahedron is also regular, the average Al—O distance is 1.94 Å, the longest value is 2.164 Å and the shortest value is 1.878 Å. The average octahedral angle for the single octahedron is 90.01° with values ranging from 85.9° to 92.5°.

The largest departures from regularity are found in the interatomic distances and angles of the double octahedral group. The shared edge O_5—O_6 shows an extremely short bond distance of 2.34 Å, coupled with octahedral angles 75.7° (O_5—Al_2—O_6) and 75.6° (O_5—Al_1—O_6). Bonds of 2.43 Å had been reported for shared octahedral edges in andalusite[21] and in anatase and rutile[29], but they are seldom found. A possible reason for this rather remarkable distortion is that the double octahedral group also has two edges (one from each octahedron) in common with the Cu pseudo octahedron. These edges are O_6—O_4 of the Al_2 octahedron and O_6—O_9 of the Al_2 octahedron. One of the OH radicals (O_6) belonging to the share edge also completes the Cu square coordination, thus becoming one of the two anions actually bonded to three cations. The second negative ion coordinated to three cations is O_9. It can be observed from Table 9, that the oxygen-bond angles which agree the least with the ideal values are the ones including O_6 and O_9. The only exception is the value 88.2° for one of the water molecules, in the coordination angle Cu—O_4—Al_2.

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[29] Ralph W. G. Wyckoff, Crystal structures, vol. 1. Interscience Publishers, 2d ed. (1963) 252–255.