# Structure and Stability of Carboxylate Complexes. Part I. The Crystal and Molecular Structures of Copper(II) Glycollate, DL-Lactate, 2-Hydroxy-2-methylpropionate, Methoxyacetate, and Phenoxyacetate

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The crystal structures of bis(glycollato)copper(II), aquobis-(DL-lactato)copper(II) hemihydrate, diaquobis-(2-hydroxy-2-methylpropionato)copper(II), diaquobis(methoxyacetato)copper(II), and diaquobis(phenoxyacetato)copper(II) have been determined by three-dimensional *X*-ray structure analysis. All the complexes contain *trans*-chelate rings, which, apart from the bow-shaped lactate, are coplanar. The copper ions are in elongated tetragonally distorted octahedral environments with two exceptions: in the lactate, copper ions are in a nearly square-pyramidal five-co-ordinate environment; in the methoxyacetate, the octahedron is compressed. Details of the structures may be rationalised in terms of Jahn–Teller distortions and hydrogen-bonding.



MOST bis(monocarboxylato)copper(II) complexes in which the ligand is unequivocally unidentate have low magnetic moments (~ 1·45 B.M. at room temperature) in the solid state and in some non-aqueous solvents,[1] and may be assumed to have dimeric or polymeric structures. However, in aqueous solution the complexes are mononuclear,[2] up to a total copper ion concentration of at least 0·1M. The known crystal structures of aminocarboxylatocopper(II) complexes [3] indicate that 2- and 3-aminocarboxylates are invariably bidentate ligands in the solid state. The high thermodynamic stability and hydration [4] of these copper complexes give little reason to doubt that they are also chelates in aqueous solution. However, for 2- and 3-hydroxy, -alkoxy-, and -aryloxy-carboxylates the situation is less clear. No crystallographic information was available when the present programme was initiated. Copper complexes of the 2-substituted carboxylates $R^1R^2C(OR^3)CO_2^-$ have magnetic moments [5] of about 1·9 B.M. and are therefore monomeric, though not necessarily chelates. However, complexes of the analogous 3-substituted ligands have low magnetic moments,[5] indicative of the dimeric copper acetate structure.[6] Systematic studies of differential proton relaxation [7] in bound ligands indicate that 2- and 3-hydroxycarboxylates and 2-alkoxycarboxylates form chelates with copper(II) in aqueous solution, but that the 3-alkoxycarboxylates are unidentate ligands. Infrared data in heavy-water solution,[8] and thermodynamic data [2] are consistent with these deductions. There is a fine balance between the different structures of the complex and between the different functions of the ligand, and we have set out to investigate the structures of hydroxy- and alkoxy-carboxylates in the solid state. In aqueous solution, there is a good linear free-energy relationship [2] of the form

$$\log \beta_1 = a \log {}^{H}K_1 + b \qquad (1)$$

between the equilibrium constants for the reactions

$$Cu^{2+} + A^- \rightleftharpoons CuA^+ \quad \beta_1$$

and

$$H^+ + A^- \rightleftharpoons HA \quad {}^{H}K_1$$

with unequivocally unidentate ligands. In this paper we report the crystal structures of a series of complexes (phenoxyacetate, methoxyacetate, glycollate, lactate, and 2-hydroxy-2-methylpropionate) which are increasingly stabilised [2] in aqueous solution in terms of equation (1). Diaquobis(methoxyacetato)copper(II) dihydrate and bis(glycollato)copper(II) have been the subject of a preliminary communication.[9]

## RESULTS

All five structures were determined by three-dimensional *X*-ray techniques (see Experimental). In each compound the copper atom is surrounded by six oxygen atoms at the corners of a tetragonally distorted octahedron. However, in the lactate one of the copper–oxygen contacts is so long that it probably should not be regarded as a bond. The carboxylate ligands $O_2C{\cdot}C{\cdot}OR$ form two *trans*-five-membered chelate rings with the metal atom, and lie more or less in an equatorial plane of the co-ordination octahedron. The co-ordination sphere may be completed by two aquo-ligands (phenoxyacetate, methoxyacetate, 2-hydroxy-2-methylpropionate), two carboxyl oxygen atoms of neighbouring complexes (glycollate), or one aquo-ligand and one (carboxy-oxygen) lactate. In all crystals the complexes are bound together by a complex series of intermolecular hydrogen-bonds.

*Diaquobis(phenoxyacetato)copper*(II).—There are two crystallographically different units of the above composition in the crystal. One is located about copper atoms at inversion centres, and the other about copper atoms in general positions (Figure 1). Both units have approximately the same orientation in the crystal, and very similar geometries. Their best planes are parallel to within 1°.

[1] M. Kato, H. B. Jonassen, and J. C. Fanning, *Chem. Rev.*, 1964, **64**, 99.
[2] F. J. C. Rossotti, J. D. E. Carson, J. J. Clark, K. D. Dillon, D. L. Martin, and V. Moxham, unpublished work.
[3] H. C. Freeman, 'The Biochemistry of Copper,' ed. P. Aisen, W. Blumberg, and J. Peisach, Academic Press, New York, 1966, p. 77; *Adv. Protein Chem.*, 1967, **22**, 257.
[4] F. J. C. Rossotti and H. Sunshine, *Chem. Comm.*, 1968, 447.
[5] C. Lea, F. J. C. Rossotti, and D. H. Schärer, unpublished work.
[6] J. N. van Niekerk and F. R. L. Schoening, *Acta Cryst.*, 1953, **6**, 227; G. A. Barclay and C. H. L. Kennard, *J. Chem. Soc.*, 1961, 5244; F. Hanic, D. Stempelova, and K. Hanicova, *Acta Cryst.*, 1964, **17**, 633; B. H. O'Connor and E. N. Maslen, *ibid.*, 1966, **20**, 824.
[7] K. D. Dillon and F. J. C. Rossotti, *Chem. Comm.*, 1966, 768.
[8] F. J. C. Rossotti and A. Willson, unpublished work.
[9] J. G. Forrest, C. K. Prout, and F. J. C. Rossotti, *Chem. Comm.*, 1966, 658.

Each copper atom is co-ordinated to six oxygen atoms: two phenoxy-oxygen atoms at 2·46—2·50, two carboxy-oxygen atoms at 1·94—1·95, and two aquo-ligands at 1·97—1·99 Å. The copper atoms have therefore the elongated tetragonal distortion of the co-ordination octahedron generally observed. The four-fold axis is through a pair of bonds in the chelate ring, as also occurs in copper croconate.[10] In the centrosymmetric molecule, the angle O(1)CuO(3) of 73·6° in the chelate ring is, within experimental error, the same as the corresponding angles O(11)CuO(13) 74·3° and O(21)CuO(23) 75·1° in the other complex. However, in the latter complex the external angles O(13)CuO(21) 110·1° and O(11)CuO(23) 100·5° are different, a feature reflected by the differing behaviour of O(12) and O(22) with respect to intermolecular hydrogen-bonding. In both types of complex the aquo-ligands lie, to a very good approximation, along the perpendiculars to the chelate ring planes at the copper atom. Interatomic distances and interbond angles are summarized in Figure 2.

The configuration at the phenoxy-oxygen atom is approximately trigonal-planar. The plane of the phenyl groups in the three independent phenoxyacetate residues are inclined to the planes of the chelate rings (Figure 3). The angles of inclination are 8½° for the phenyl group at O(3), 6° for that at O(13), and 9° for that at O(23). In the complex, at a general position in the unit-cell the directions of tilt of the benzene rings are such that the near inversion centre is preserved. As the phenyl group turns out of plane, the carbon atom adjacent to the carbonyl group in the chelate ring is pushed up to 0·15 Å out of the plane in the same direction. Angular distortions at the phenoxy-oxygen and the phenyl ring carbon attached to it are consistent with overcrowding. Each water molecule forms two hydrogen-bonds to oxygen atoms of a carboxyl group. Hydrogen bonds O(4)O(2) of 2·67, O(12)O(24) of 2·70, and O(14)O(22) of 2·71 Å hold the molecules together in chains

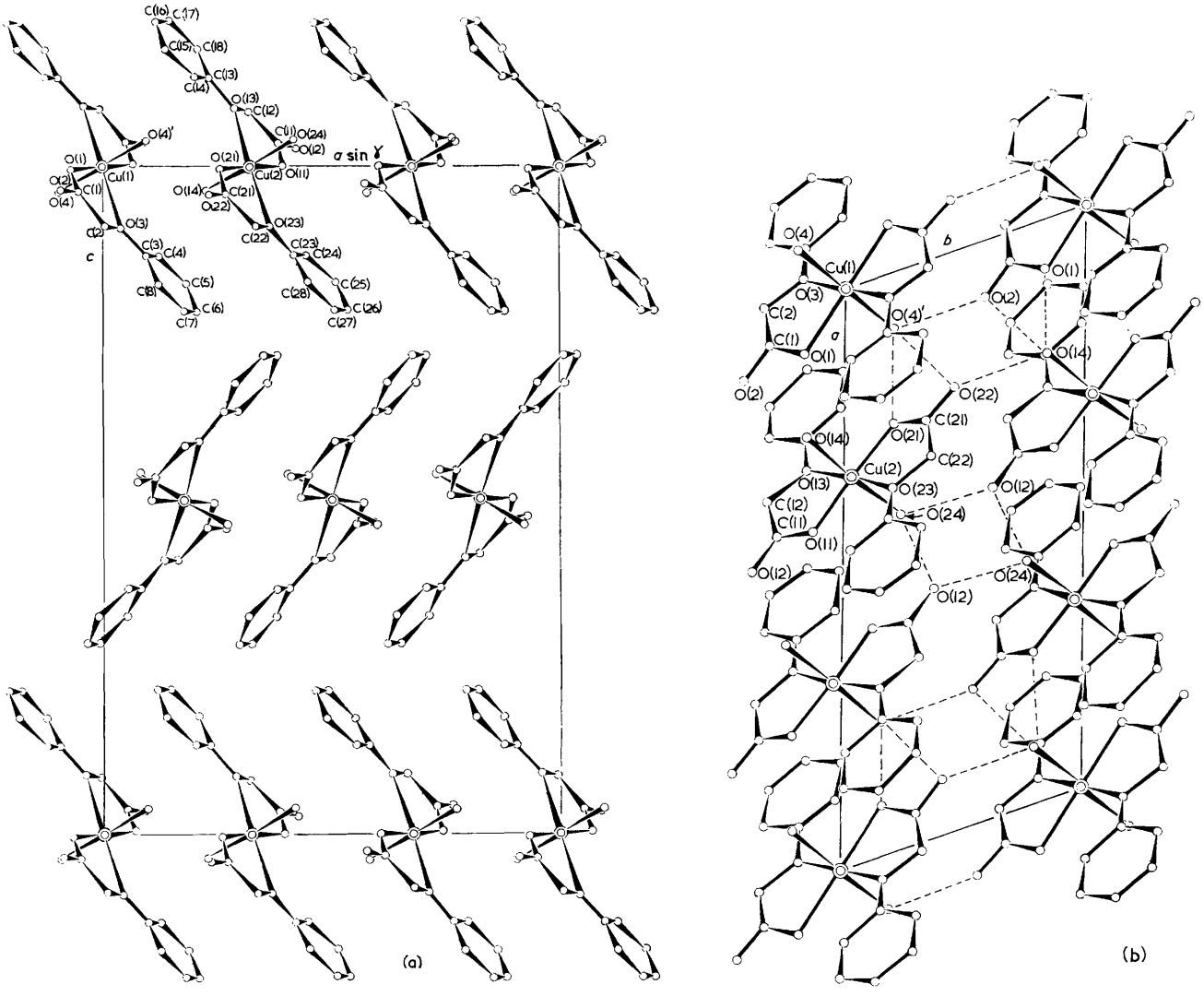


FIGURE 1 Diaquobis(phenoxyacetato)copper(II): (a) Projection of the structure along [010]; the molecules are hydrogen-bonded to give sheets parallel to [010]; (b) one of the sheets projected along [001]

[10] M. D. Glick, G. L. Downs, and L. F. Dahl, *Inorg. Chem.*, 1964, **3**, 1712.

parallel to *b*. The chains are linked to form sheets by the hydrogen-bonds O(4)O(21) of 2·87, O(14)O(1) of 2·84, and O(24)O(12) of 2·72 Å (Figure 1). These three hydrogen-bonds are coplanar with the carboxy-group at which they are formed. In contrast to the other structures described, there are two hydrogen-bonds to carboxy-oxygen atoms which are bound to the metal atoms. For each of these bonds the contacts to the neighbouring non-chelating atoms

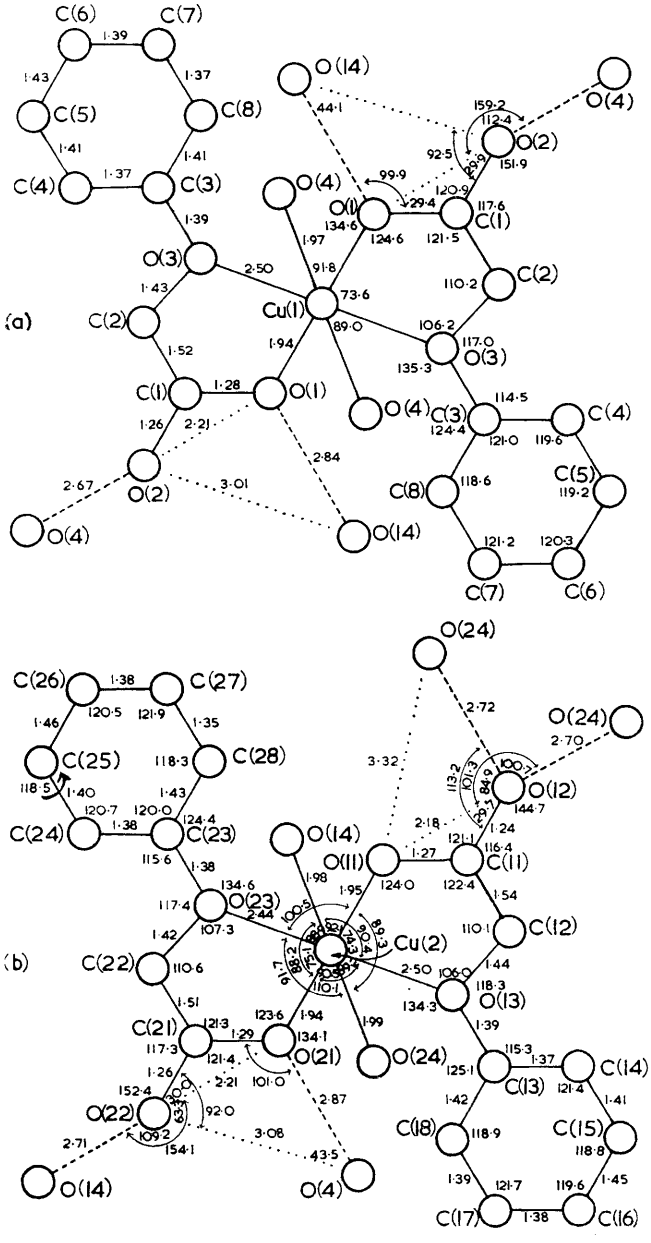


FIGURE 2 Diaquobis(phenoxyacetato)copper(II): interatomic distances and angles (a) in the centrosymmetric molecule about Cu(1); (b) in the molecule containing Cu(2)

[O(2)O(14) 3·01; O(4)O(22) 3·08 Å] suggests that these may be examples of bifurcated hydrogen-bonds. The arrangement of hydrogen-bonds at O(12) is more typical of the behaviour of the non-chelating carboxy-oxygen atom in the compounds described here.

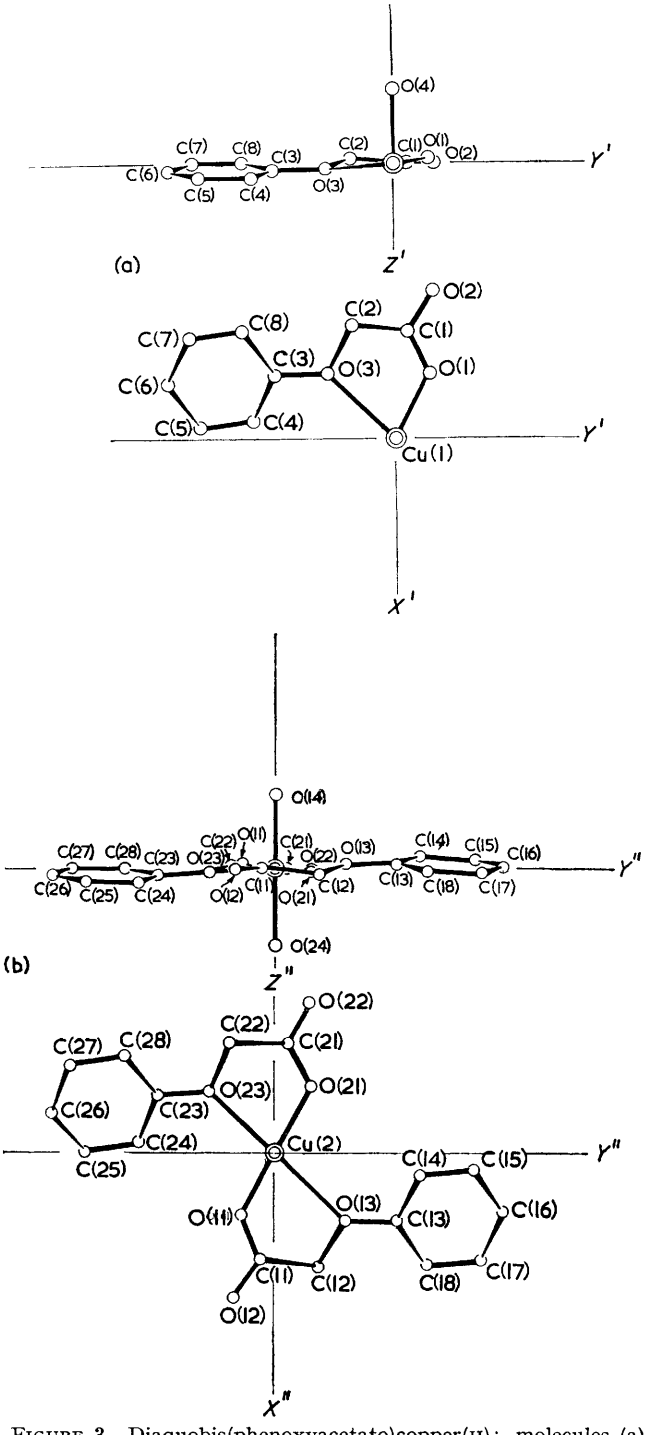


FIGURE 3 Diaquobis(phenoxyacetato)copper(II): molecules (a) about Cu(1), and (b) about Cu(2) projected parallel and perpendicular to the least-squares best planes through the atoms of their chelate rings. The transformation matrices from the orthogonal axes *a*, *b*, and *c** to the axes *X'Y'Z'* and *X''Y''Z''* are

| | | | | | |
|---|---|---|---|---|---|
| 0·502 | −0·754 | −0·425 | and | 0·519 | −0·749 | −0·412 |
| −0·653 | −0·008 | −0·757 | | −0·644 | −0·026 | −0·764 |
| 0·567 | 0·657 | −0·497 | | 0·561 | 0·662 | −0·496 |

*Diaquobis(methoxyacetato)copper*(II).—The crystals are built up from units of this composition located about copper atoms at inversion centres (Figure 4). The co-ordination is

superficially similar to that of the phenoxyacetate but there are interesting differences in the Cu–O contact distances (Figure 5). The co-ordination octahedron has two methoxy-oxygen atoms at 2·13, and two carboxy-oxygen

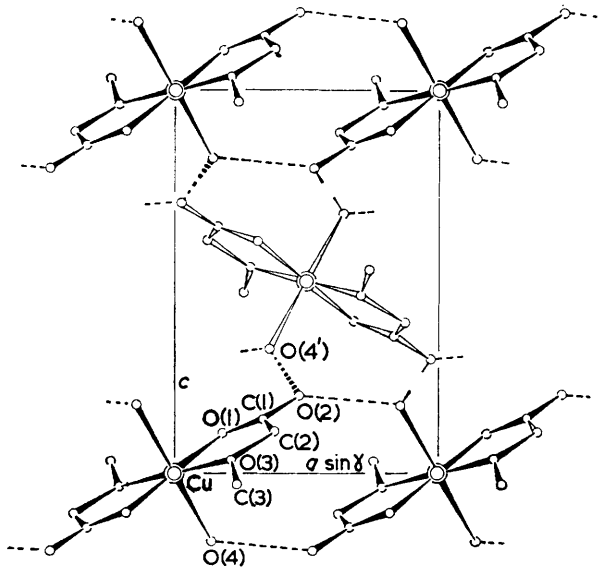


FIGURE 4 Diaquobis(methoxyacetato)copper(II): projection of the structure along [010]. Molecules with copper atoms at $y$ co-ordinates of 0 and 1 are represented by open and full lines respectively

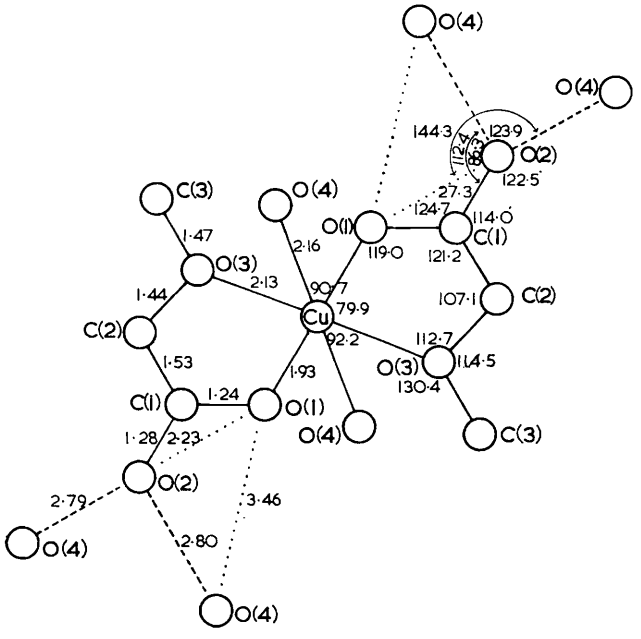


FIGURE 5 Diaquobis(methoxyacetato)copper(II): interatomic distances and angles

atoms at 1·93 Å in the chelate rings, and is completed by two aquo-ligands at 2·16 Å. The tetragonal distortion therefore takes on the unusual compressed form of four longer and two shorter bonds. The angle O(3)CuO(1) within the ring is 79·9°, and the water molecules lie very near to the perpendicular to the chelate ring plane at the copper atom. The atoms forming the two chelate rings have a maximum deviation of 0·027 and a mean deviation of 0·018 Å from their least-squares best plane. The methyl carbon C(3) is 0·29 Å above the plane and the oxygen O(2) 0·08 Å above it. As in the phenoxyacetate, the oxygen O(3) is nearly coplanar with C(2), C(3), and Cu, and the angle C(3)O(3)C(2) of 114·5° is greater than the expected angle (109°) at an ether oxygen. The bonded distance O(1)C(1) within the chelate ring is unexpectedly shorter than C(1)O(2), but this is without statistical significance. However, a similar short bond is found in bis-(methoxyacetato)nickel(II) dihydrate.[11] Other bonds have

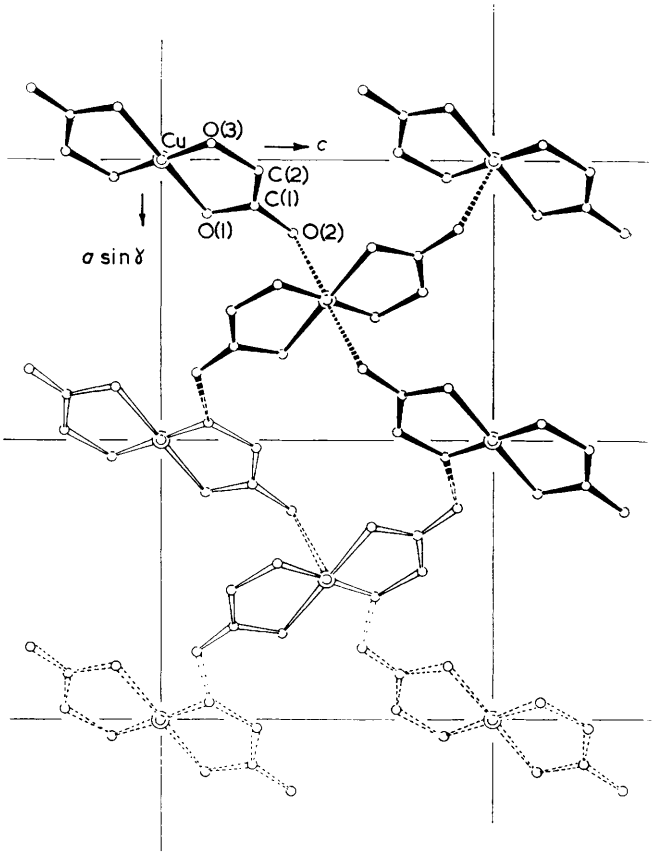


FIGURE 6 Bis(glycollato)copper(II): projection of the structure along [010]. Molecules with copper atoms at $y$ co-ordinates of 0, 1, and 2 are represented by dotted, open, and full lines respectively. Weak Cu–O(2) bonds join molecules at the same $y$ co-ordinates to form sheets perpendicular to [010], and hydrogen-bonds between O(2) and O(3) join the molecules to form sheets perpendicular to [110]

the expected lengths. The carboxyl oxygen O(2) not involved in co-ordination is hydrogen-bonded to two water molecules O(4) of neighbouring complexes (Figure 4). One of these water molecules is in the plane of O(2), C(1), O(1), and the hydrogen-bond 2·80 Å long is approximately parallel to the C(1)C(2) vector. The contact distance O(4)O(1) at 3·46 Å is too long to suggest any tendency to form a bifurcated hydrogen-bond. The second hydrogen-bond 2·79 Å long is also very close to the chelate ring plane, and approximately parallel to the bond C(1)O(1). Each water molecule O(4) has three near neighbours, the two

[11] C. K. Prout, F. J. C. Rossotti, and C. Walker, unpublished work.

hydrogen-bond oxygen atoms O(2) of two other complexes and the copper atom in its own complex, forming a shallow pyramid. There are no other intermolecular interactions other than van der Waals contacts.

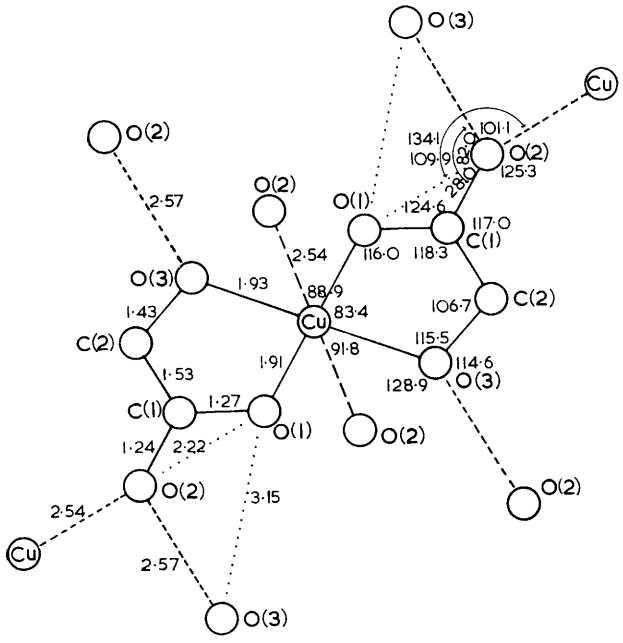


FIGURE 7 Bis(glycollato)copper(II): interatomic distances and angles

*Bis(glycollato)copper*(II).—Here also, the copper atoms at inversion centres are co-ordinated to two glycollate ligands forming coplanar chelate rings (Figure 6). The copper to hydroxy-oxygen contact CuO(3) is 1·93 and the copper carboxy-oxygen CuO(1) 1·91 Å, with the angle O(1)CuO(3) 83·4° (Figure 7). The copper atom and the atoms of both chelate rings are coplanar within experimental error. The maximum and mean deviations from the least-squares best plane are 0·013 and 0·008 Å respectively. The co-ordination octahedron is completed by the two carboxy-oxygens O(2) of two neighbouring complexes so that the Cu · · · O(2) vectors, 2·54 Å long, are perpendicular to the plane of the copper chelate containing the copper atom. In addition, each oxygen atom O(2) forms a remarkably short intermolecular hydrogen-bond 2·57 Å long to the hydroxy-group O(3) of a second neighbouring complex. This hydrogen-bond is coplanar with the chelate ring associated with O(2), and is approximately parallel to the C(1)C(2) bond of that ring. If the hydrogen-bond is linear, then O(3) has a trigonal-planar configuration. The CuO(2) contact rises 1·86 Å above the O(2)C(1)O(1)O(3)′ plane but is in a very similar direction to that of the second hydrogen-bond to the carboxy-oxygen in the methoxyacetate structure.

*Aquobis-*(DL-*lactato*)*copper*(II) *Hemihydrate*.—The crystals are formed from aquobis(lactato)copper(II) groups with the copper atom in general positions in the space-group *A*2, and isolated water molecules O(5) at general positions in the unit cell. These water molecules are located in channels parallel to *c*. There is space for each site to be occupied by water. In the crystal used for the *X*-ray analysis there were approximately half as many water molecules as sites. Analytical results and density measurements indicate that the amount of water varies with the age and previous handling of the crystals.

The copper co-ordination sphere has two crystallographically independent chelate rings, one formed from a D-lactate and the other from an L-lactate ligand. The absolute configuration has not been determined. The methyl groups on the 2-carbon atoms appear on opposite sides of the chelate rings (Figure 8). The co-ordination sphere is completed by a water molecule O(4) 2·30 Å from the copper at the apex of an approximately tetragonal prism (Figure 9). The copper atom is 0·15 Å above the best basal plane of the prism taken through the ring oxygen atoms (Figure 10). The oxygen atoms O(1) and O(11) are 0·05 Å above the plane, and the hydroxy-oxygen atoms O(3) and O(13) are 0·05 Å below the plane. The chelate rings as a whole are bent away from the water molecule O(4) in a bow shape. The individual rings are far less planar than those found in the methoxyacetate and glycollate complexes. In the ring containing O(1) the maximum

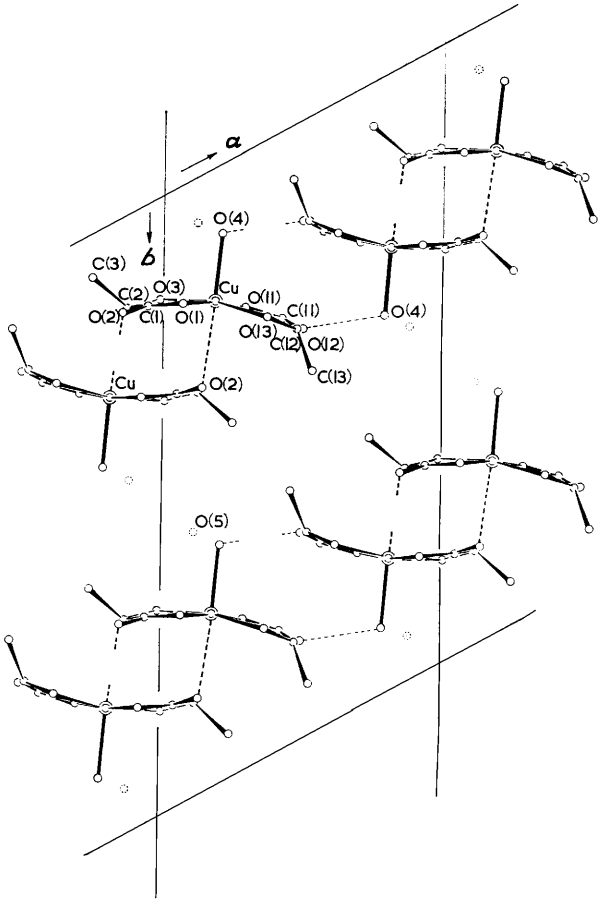


FIGURE 8 Aquobis-(DL-lacto)copper(II) hemihydrate: projection of the structure along [001]. The short contacts Cu–O(2) and O(4)–O(12) are shown by discontinuous dotted lines when they are to molecules at heights other than those drawn. The water molecule O(5), shown as a broken circle, has an occupation number of about 0·5

deviation from the best plane is 0·082 and the mean deviation 0·055 Å. For the ring containing O(11) the corresponding values are 0·070 and 0·046 Å. The aquobis(lactato)copper(II) complexes are joined by hydrogen-bonds

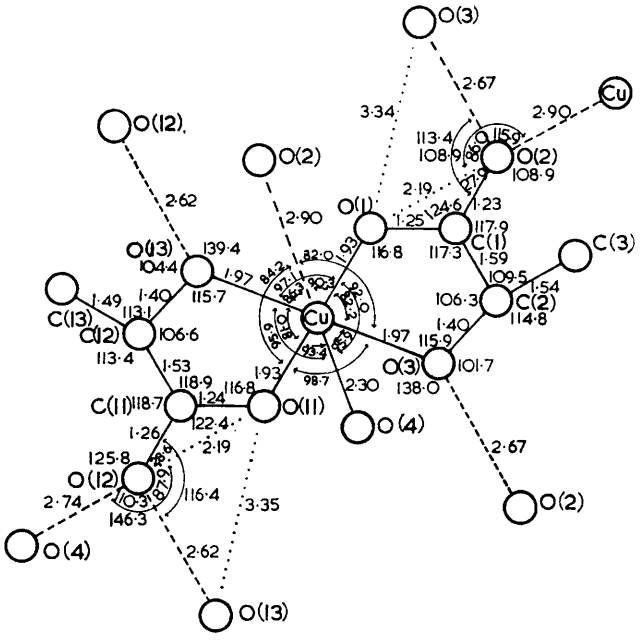


FIGURE 9 The aquobis-(DL-lactato)copper(II) molecule: interatomic distances and angles

to form ribbons parallel to *c*, and these ligands are associated in pairs by a weak interaction of the copper atoms and the non-chelating carboxy-oxygen atom O(2) at a separation of 2·9 Å (Figure 11). This oxygen atom O(2) forms one hydrogen-bond to the hydroxy-oxygen O(3) of a neighbouring complex, as well as the short contact to the copper atom in a complex related to that containing O(2) by rotation about a two-fold screw axis. The oxygen atom O(12) is involved in two hydrogen-bonds. One is to the hydroxy-group O(13) in another complex (Figure 11). The other is to the water molecules O(4) of a neighbouring complex and joins the double ribbons of complexes to form sheets (Figure 8). The hydrogen-bonds about O(12) are very similar to those about O(2) in the methoxyacetate. If it is assumed that the hydrogen-bonds are linear, the hydroxy-oxygen atoms O(3) and O(13) have a planar configuration.

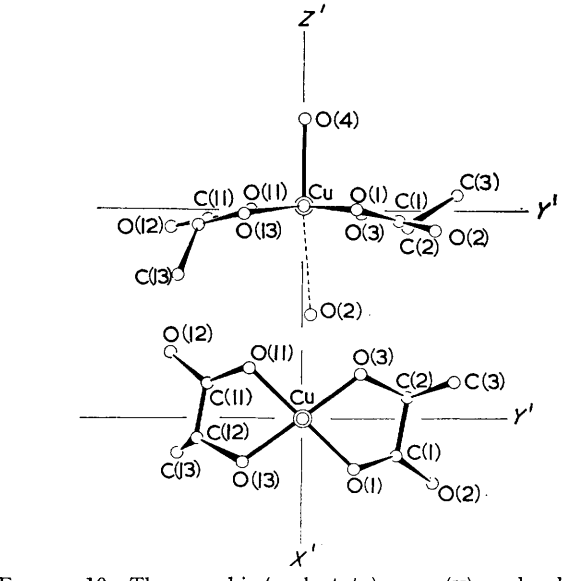


FIGURE 10 The aquobis-(DL-lactato)copper(II) molecules projected parallel and perpendicular to the least-squares best plane through O(1), O(3), O(11), and O(13). The transformation matrix from the orthogonal axes *a*, *b**, and *c* to the axes *X'*, *Y'*, and *Z'* is

| | | |
|---|---|---|
| 0·179 | 0·175 | 0·968 |
| 0·791 | 0·560 | −0·247 |
| −0·586 | 0·810 | −0·038 |

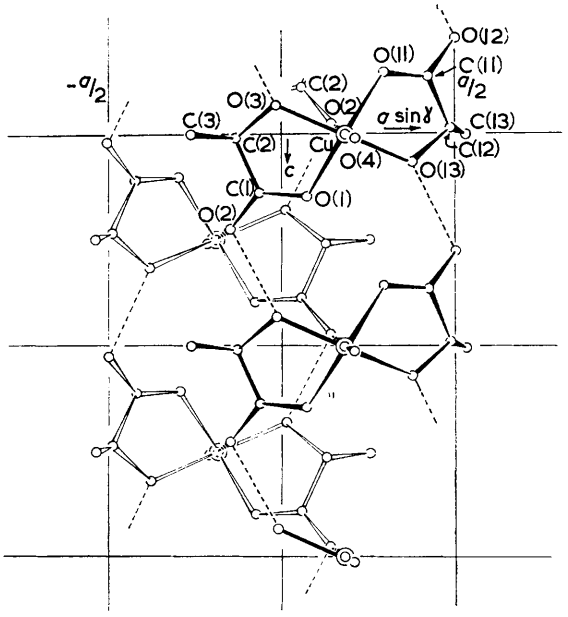


FIGURE 11 Aquobis-(DL-lactato)copper(II) hemihydrate: the double ribbon formation projected along [010]

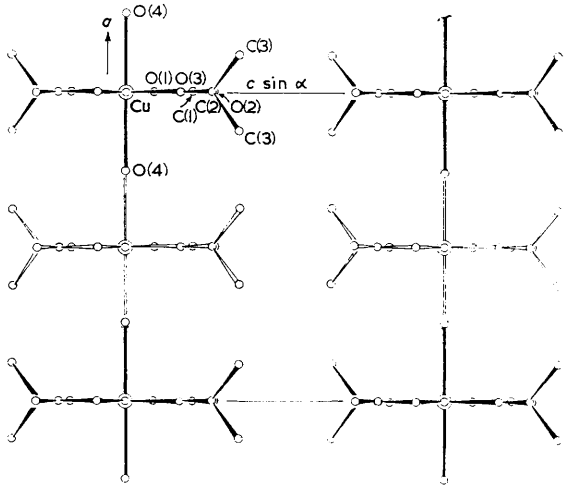


FIGURE 12 Diaquobis-(2-hydroxy-2-methylpropionato)-copper(II): projection of the structure along [010]

*Diaquobis-(2-hydroxy-2-methylpropionato)copper*(II).—This structure is the least well determined. In the isolated complex the copper atom appears to lie at a point of symmetry 2/*m* in a unit cell of space-group *C*2/*m*. The atoms of the chelate rings lie in the mirror plane (Figure 12). The co-ordination of the copper is distorted octahedral with the copper–water contact CuO(4) 2·56, copper–hydroxy-group CuO(3) 2·01, and the copper–carboxy-oxygen

CuO(1) 1·89 Å (Figure 13). The chelate rings and the copper atom are necessarily coplanar, but difference maps indicate a remarkably high anisotropic thermal motion along the O(4)CuO(4)′ vector. This appears better explained as a statistical distribution of copper atoms about the mirror plane (see Experimental) than as true anisotropic thermal

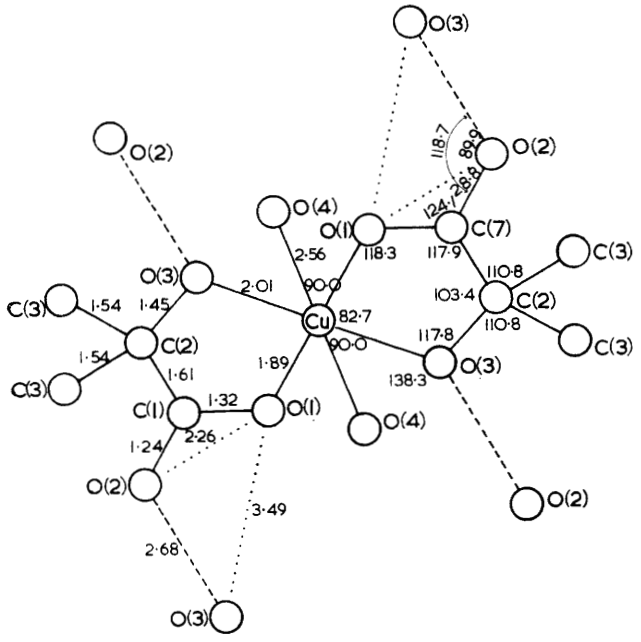


FIGURE 13 Diaquobis-(2-hydroxy-2-methylpropionato)-copper(II): interatomic distances and angles

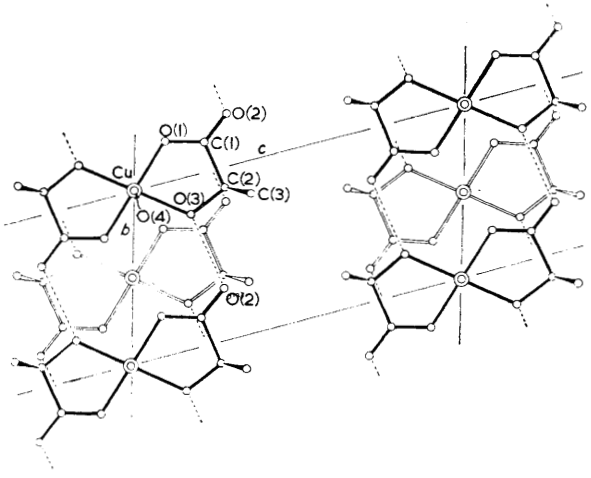


FIGURE 14 Diaquobis-(2-hydroxy-2-methylpropionato)copper-(II): projection of the structure along [100] showing the hydrogen-bonded ribbons

motion, and may represent a tendency to form a copper lactate-like structure. The structures of other modifications derived from the original triclinic twinned crystal may yield further information on this point. The complexes are joined together to form ribbons (Figure 14) by hydrogen-bonding of the hydroxy-group O(3) to O(2) of another molecule in the mirror plane, and the sheets are held together by hydrogen-bonding through the water molecules.

## DISCUSSION

The only other example of a hydroxycarboxylatocopper(II) structure in the literature appears to be that of the diaquobis(salicylato)-dihydrate.[12] The salicylate ligands, which may be regarded as 3-hydroxycarboxylates, are unidentate and bound to the copper ion through the carboxy-groups with Cu–O bonds of 1·91 Å. Chelation by the hydroxy-group is prevented by strong intramolecular hydrogen-bonding to the carboxylate oxygen unattached to copper. The copper ions are also co-ordinated to two aquo-ligands at a Cu–O distance of 1·95 Å, and form an asymmetric $[Cu(OH_2)_2]_n$ chain with longer Cu–O contacts of 2·8 Å. The interatomic distances in this compound have been calculated from a revised set of atomic parameters obtained from the data in the literature [12] by four cycles of least-squares refinement.

In Tables 1 and 2 the formally equivalent bond lengths and bond angles for the compounds reported here and for diaquobis(salicylato)copper(II) dihydrate are collected together. For all compounds each independent measurement of a particular bond is given. The mean values are the simple arithmetic means, and the standard deviations of the mean values were computed from the formula

$$\sigma_m = [\Sigma_i(d - d_i)^2/n(n-1)]^{\frac{1}{2}}$$

where $d_i$ is the $i$th of $n$ measurements for which $d$ is the mean value. In parentheses are the standard deviations of individual bond lengths and angles (for bond lengths $\sigma_i \times 10^2$) calculated from the standard deviations of atomic parameters in Table 3 and neglecting the covariances. Tables 1 and 2 are in the same form as the analogous Tables for copper-2-aminocarboxylates and copper peptides given by Freeman.[3]

The copper to carboxy-oxygen bond lengths represent a spread about a mean of 1·92 Å, which is somewhat shorter than the corresponding mean length of 1·97 Å found in the aminocarboxylate and peptide complexes [3] and in the copper carboxylate dimers.[6] The mean Cu–OR bond length is longer (2·16 Å), but the spread is much bigger, and the lengths increase in the order R = H < Me < Ph. The mean of the Cu–$OH_2$ bond lengths is also 2·16 Å, but again the spread is significantly larger than for the Cu–OOC bond lengths. As the bond length Cu–OR increases, so the Cu–$OH_2$ bond length decreases. It is noteworthy that the short Cu–$OH_2$ contact of 1·97 Å in the phenoxyacetate is equal to the mean short Cu–$OH_2$ contact in the hydroxycarboxylates. Similarly, the longer Cu–$OH_2$ contacts approximate to the longer Cu–OR contacts.

In the three diaquobiscarboxylate complexes, the $CuO_6$ co-ordination polyhedra all have symmetry $D_{2h}$, but may be considered to approximate to $D_{4h}$. In the 2-hydroxy-2-methylpropionate, the four-fold axis lies along the copper–water vector, and there are four short and two long bonds. In the methoxyacetate, the four-fold axis is along the copper to carboxylate oxygen bond,

[12] F. Hanic and J. Michalov, *Acta Cryst.*, 1959, **13**, 299.

and there are four long and two short contacts. In the phenoxyacetate, the four-fold axis is along the copper to phenoxy-oxygen bond, and there are four short and two long contacts. These tetragonal distortions may be attributed to the Jahn–Teller effect, provided that the oxygen atoms around the central copper atom neither have different radii nor have markedly different intrinsic donor powers due to their different chemical environments. We find [11] that diaquobis(methoxyacetato)-nickel(II), which is isomorphous with the copper complex, has three nearly equal independent pairs of Ni–O bonds (of which the Ni–OMe bond is the shortest at 1·99 Å).

TABLE 1

Collected bond lengths in the complexes (in Å) with standard deviations ($\times 10^2$) in parentheses

| | Organic ligand | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | $CO_2^-$ | | | | C–O–R | | | | | | | 'Axial' bonds | |
| Compound | C=O | C–O | Cu–O | O···O | C–O | Me–O | Ph–O | OH···O | Cu–O | O···O | C–C | Cu–$OH_2$ | Cu–O |
| (a) Diaquobis(phenoxyacetato)copper(II) | 1·26(2) | 1·28(2) | 1·94(1) | 2·21(2) | 1·43(2) | — | 1·39(2) | — | 2·50(1) | 2·84(3) | 1·52(2) | 1·97(1) | — |
| | 1·26(2) | 1·29(2) | 1·94(1) | 2·21(2) | 1·42(2) | — | 1·38(2) | — | 2·44(1) | 2·79(3) | 1·51(2) | 1·98(1) | — |
| | 1·24(2) | 1·27(2) | 1·94(1) | 2·18(2) | 1·44(2) | — | 1·39(2) | — | 2·50(1) | 2·76(3) | 1·54(2) | 1·99(1) | — |
| (b) Diaquobis(methoxyacetato(copper(II) | 1·28(2) | 1·24(2) | 1·93(1) | 2·23(2) | 1·44(2) | 1·47(2) | — | — | 2·13(1) | 2·61(2) | 1·42(2) | 2·16(1) | — |
| (c) Bis(glycollato)copper(II) | 1·24(2) | 1·27(2) | 1·91(1) | 2·22(2) | 1·43(2) | — | — | 2·57(2) | 1·93(1) | 2·57(2) | 1·53(2) | — | 2·54(1) |
| (d) Aquobis-(DL-lactato)copper(II) hemihydrate | 1·23(3) | 1·25(3) | 1·93(2) | 2·19(3) | 1·40(4) | — | — | 2·67(3) | 1·97(2) | 2·54(3) | 1·53(4) | 2·30(2) | 2·90(2) |
| | 1·26(3) | 1·24(3) | 1·93(2) | 2·19(3) | 1·40(4) | — | — | 2·62(3) | 1·97(2) | 2·56(3) | 1·59(4) | — | — |
| (e) Diaquobis(2-hydroxy-2-methylpropionato)-copper(II) | 1·24(4) | 1·32(4) | 1·89(2) | 2·26(4) | 1·45(4) | — | — | 2·68(3) | 2·01(2) | 2·58(3) | 1·61(4) | 2·56(3) | — |
| (f) Diaquobis(salicylato)copper(II) dihydrate | 1·27 | 1·28 | 1·91 | 2·22 | [1·32] | — | — | — | 1·95 ($Cu–OH_2$) | — | [1·43] | [2·80] | — |
| Mean | 1·254 | 1·271 | 1·924 | 2·212 | 1·426 | 1·47 | 1·39 | 2·64 | 2·160 | 2·656 | 1·545 | 2·160 | 2·72 |
| Standard deviation of the mean | 0·006 | 0·009 | 0·006 | 0·008 | 0·007 | — | 0·003 | 0·026 | 0·084 | 0·042 | 0·013 | 0·096 | — |
| Range | 1·23— 1·28 | 1·24— 1·32 | 1·89— 1·94 | 2·18— 2·26 | 1·40— 1·45 | 1·47 | 1·38— 1·39 | 2·57— 2·68 | 1·93— 2·50 | 2·54— 2·84 | 1·51— 1·61 | 1·97— 2·80 | 2·54— 2·90 |
| Number in sample | 9 | 9 | 9 | 9 | 8 | 1 | 3 | 4 | 9 | 8 | 9 | 7 | 2 |

TABLE 2

Collected bond angles in the complexes (in degrees) with standard deviations in parentheses

| | $CO_2^-$ | | | | | C–O–R | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Compound | O–Cu–O | Cu–O–C | O–C=O | O–C–C | O=C–C | C–C–OR | C–OH···O | C–O–R | Cu–O–C | Cu–O–R | Cu–OH···O |
| (a) Diaquobis(phenoxyacetato)copper(II) | 73·6(0·3) | 124·6(0·9) | 120·9(1·2) | 121·5(1·2) | 117·6(1·2) | 110·2(1·1) | — | 117·0(1·0) | 106·2(0·7) | 135·3(0·8) | — |
| | 75·1(0·3) | 123·6(0·9) | 121·4(1·2) | 121·3(1·2) | 117·3(1·2) | 110·6(1·2) | — | 117·4(1·0) | 107·3(0·7) | 134·6(0·7) | — |
| | 74·3(0·3) | 124·0(0·9) | 122·4(1·2) | 121·1(1·2) | 116·4(1·2) | 110·1(1·1) | — | 118·3(1·0) | 106·0(0·7) | 134·3(0·7) | — |
| (b) Diaquobis(methoxyacetato)copper(II) | 79·9(0·4) | 119·0(0·9) | 124·7(1·2) | 121·2(1·2) | 114·0(1·3) | 107·1(1·1) | — | 114·5(1·1) | 112·7(0·8) | 130·4(0·9) | — |
| (c) Bis(glycollato)copper(II) | 83·4(0·4) | 116·0(0·9) | 124·6(1·3) | 118·3(1·2) | 117·0(1·2) | 106·7(1·1) | 114·6(1·2) | — | 115·5(0·8) | — | 128·9(0·9) |
| (d) Aquobis-(DL-lactato)copper(II) hemi-hydrate | 82·2(0·4) | 116·8(1·5) | 124·6(2·2) | 117·3(2·1) | 117·9(2·2) | 106·3(2·2) | 101·7(2·0) | — | 115·9(1·5) | — | 138·0(1·9) |
| | 81·0(0·7) | 116·8(1·5) | 122·4(2·2) | 118·7(2·2) | 118·9(2·2) | 106·6(2·2) | 104·4(2·0) | — | 115·7(1·6) | — | 139·4(1·9) |
| (e) Diaquobis-(2-hydroxy-2-methylpropionato)-copper(II) | 82·7(0·8) | 118·3(1·7) | 124·1(2·8) | 117·9(2·5) | 118·1(2·2) | 103·4(2·2) | 104·3(2·8) | — | 117·8(1·8) | — | 138·3(1·8) |
| (f) Diaquobis(salicylato)copper(II) dihydrate | [88·5] | 121·8 | 121·4 | 121·2 | 117·4 | — | — | — | — | — | — |
| Mean | 79·0 | 120·1 | 122·9 | 119·9 | 117·1 | 107·6 | | 111·5 | 112·1 | | 134·9 |
| Standard deviation of the mean | 1·4° | 1·1 | 0·5 | 0·5 | 0·5 | 0·9 | | 2·4 | 1·6 | | 1·3 |
| Range | 73·6— 82·7 | 116·0— 124·6 | 120·9— 124·6 | 117·3— 121·5 | 114·0— 118·7 | 103·4— 110·6 | | 101·7— 118·3 | 106·0— 117·8 | | 128·9— 139·4 |
| Number in sample | 8 | 9 | 9 | 9 | 9 | 8 | | 8 | 8 | | 8 |

Accordingly, the tetragonal distortions do appear to be primarily due to the metal ion rather than to the ligands.

It is widely believed that the $CuF_6$ polyhedron shows compressed tetragonal distortion in $KCuF_3$ and $K_2CuF_4$. However, the earlier report [13] of four long and two short Cu–F bonds in $KCuF_3$ appears to have been erroneous.[14] Similarly, the original structure [15] of $K_2CuF_4$ has been questioned.[16] Our diaquobis(methoxyacetato)copper(II) complex appears to be a rare example of the compressed tetragonal distortion. Although Liehr and Ballhausen's electrostatic model [17] for $CuF_6$ suggested that the compressed octahedron is more stable than the elongated form, a later [18] MO treatment predicts a difference of about 0·2 Å between the shorter and longer Cu–F bonds, but is unable to define the direction of the distortion, which appears to be very sensitive to the amount of covalency in the bonds.[19] In the present $CuO_6$ polyhedra, the three pairs of oxygen donors are nearly, but not quite, equivalent. The free energies [2] and enthalpies [20] of the copper complexes in solution indicate that the strengths of the bonds from Cu to $CO_2^-$, OH, OMe, and OPh differ remarkably little from the strength of the copper–water bonds, but decrease in that order, which is also the order of increasing bond lengths. It appears that the four-fold axis lies along the two bonds that differ most in strength from the remaining four, *i.e.*, along the weak Cu–$OH_2$ bonds in the 2-hydroxy-2-methylpropionate, and along the weak Cu–OPh bonds in the phenoxyacetate, but along the strong Cu–OOC bonds in the methoxyacetate.

In accommodating the varying Cu–OR bond lengths, distortions in the chelate ring are necessary. Equivalent bonds within the various ligands have lengths randomly spread about their means which are acceptable values for each particular type of bond. The separation between the two ring oxygen atoms increases as R is changed

[13] A. J. Edwards and R. D. Peacock, *J. Chem. Soc.*, 1959, 4126.
[14] A. Okazaki and Y. Suemune, *J. Phys. Soc. Japan*, 1961, **16**, 176.
[15] K. Knox, *J. Chem. Phys.*, 1959, **30**, 991.
[16] K. Oelkrug, *Z. phys. Chem. (Leipzig)*, 1967, **56**, 325; D. Babel, *Structure and Bonding*, 1967, **3**, 1.
[17] A. D. Liehr and C. J. Ballhausen, *Ann. Phys.*, 1958, **3**, 304.
[18] C. J. Ballhausen and H. Johansen, *Mol. Phys.*, 1966, **10**, 183.
[19] M. H. L. Pryce, K. P. Sinha, and Y. Tanabe, *Mol. Phys.*, 1965, **9**, 33.
[20] J. D. Pocock and F. J. C. Rossotti, unpublished work.

from H to Me to Ph with a concommitant opening of the angles at the carbon atoms. The angle C–C–OR is less than the tetrahedral angle for R = H, and greater for R = Ph. The angles at the carboxy-group are symmetrical with respect to the C–C bond for R = H, but unsymmetrical for R = Me and Ph. If it is assumed that the hydrogen-bonds formed by the hydroxy-groups in the hydroxycarboxylates are linear, the oxygen atom of all Cu–O(R)–C groups appears to be trigonal-planar to a high degree of approximation, although the angles about the oxygen may deviate widely from 120°. By contrast, oxygen atoms in bridging hydroxy-groups [21] or

TABLE 3

Atomic co-ordinates ($\times 10^4$) and their estimated standard deviations ($\times 10^4$)

| | $x/a$ | $\sigma(x/a)$ | $y/b$ | $\sigma(y/b)$ | $z/c$ | $\sigma(z/c)$ | $U_{iso}$ | $\sigma(U_{iso})$ |
|---|---|---|---|---|---|---|---|---|
| | (a) *Diaquobis(phenoxyacetato)copper*(II) | | | | | | | |
| Cu(1) | 0 | 0 | 0 | 0 | 0 | 0 | 351 | 7 |
| O(1) | 681 | 5 | −1738 | 10 | −51 | 3 | 363 | 18 |
| O(2) | −929 | 6 | 4345 | 11 | 363 | 3 | 416 | 21 |
| O(3) | 414 | 5 | 1788 | 10 | 904 | 3 | 309 | 17 |
| O(4) | −968 | 5 | −2018 | 10 | 384 | 3 | 321 | 17 |
| C(1) | −530 | 8 | 3147 | 16 | 397 | 4 | 324 | 25 |
| C(2) | 131 | 8 | 3440 | 15 | 867 | 4 | 289 | 24 |
| C(3) | 961 | 8 | 1754 | 14 | 1344 | 4 | 300 | 25 |
| C(4) | 1246 | 9 | 196 | 16 | 1350 | 5 | 378 | 28 |
| C(5) | 1858 | 10 | 56 | 18 | 1762 | 5 | 465 | 33 |
| C(6) | 2110 | 11 | 1478 | 20 | 2175 | 5 | 541 | 36 |
| C(7) | 1820 | 10 | 3040 | 20 | 2171 | 5 | 520 | 35 |
| C(8) | 1237 | 9 | 3214 | 16 | 1757 | 4 | 363 | 27 |
| Cu(2) | 3292 | 1 | 344 | 2 | 4 | 1 | 371 | 5 |
| O(11) | 4004 | 6 | −1330 | 11 | 5 | 4 | 447 | 20 |
| O(12) | 4312 | 6 | −3870 | 11 | −272 | 3 | 368 | 19 |
| O(13) | 2922 | 5 | 1588 | 10 | −889 | 3 | 297 | 17 |
| O(14) | 2316 | 6 | −1673 | 10 | 389 | 3 | 329 | 18 |
| C(11) | 3892 | 8 | −2747 | 15 | −325 | 4 | 300 | 25 |
| C(12) | 3240 | 8 | −3182 | 14 | −817 | 4 | 283 | 24 |
| C(13) | 2370 | 8 | −1653 | 14 | −1327 | 4 | 277 | 23 |
| C(14) | 2049 | 9 | −155 | 17 | −1350 | 5 | 392 | 28 |
| C(15) | 1403 | 10 | −114 | 18 | 1763 | 5 | 483 | 33 |
| C(16) | 1165 | 11 | −1569 | 20 | −2162 | 6 | 542 | 36 |
| C(17) | 1507 | 11 | −3070 | 21 | −2146 | 6 | 551 | 36 |
| C(18) | 2112 | 9 | −3150 | 17 | −1729 | 5 | 409 | 29 |
| O(21) | 2626 | 5 | 2098 | 10 | 55 | 3 | 364 | 18 |
| O(22) | 2369 | 6 | 4648 | 12 | 415 | 3 | 471 | 22 |
| O(23) | 3725 | 5 | 2034 | 10 | 890 | 3 | 327 | 18 |
| O(24) | 4251 | 6 | 2392 | 10 | −393 | 3 | 353 | 17 |
| C(21) | 2774 | 9 | 3453 | 16 | 426 | 4 | 352 | 27 |
| C(22) | 3414 | 8 | 3634 | 15 | 897 | 4 | 305 | 24 |
| C(23) | 4266 | 8 | 1920 | 14 | 1320 | 4 | 283 | 23 |
| C(24) | 4544 | 9 | 341 | 17 | 1302 | 5 | 417 | 29 |
| C(25) | 5173 | 10 | 150 | 19 | 1709 | 5 | 485 | 34 |
| C(26) | 5431 | 10 | 1510 | 20 | 2134 | 5 | 529 | 35 |
| C(27) | 5154 | 10 | 3060 | 20 | 2149 | 6 | 551 | 37 |
| C(28) | 4556 | 9 | 3310 | 18 | 1744 | 5 | 437 | 31 |
| H(1) | 691 | | 4738 | | 782 | | 400 | |
| H(2) | −163 | | 3622 | | 1252 | | 400 | |
| H(3) | −954 | | −3382 | | 376 | | 400 | |
| H(4) | 1008 | | −962 | | 1037 | | 400 | |
| H(5) | 2114 | | −1127 | | 1752 | | 400 | |
| H(6) | 2553 | | 1365 | | 2504 | | 400 | |
| H(7) | 2038 | | 4148 | | 2493 | | 400 | |
| H(8) | 1013 | | 4448 | | 1757 | | 400 | |
| H(9) | −1520 | | −2505 | | 159 | | 400 | |
| H(11) | 3569 | | −3337 | | −1192 | | 400 | |
| H(12) | 2702 | | −4500 | | −735 | | 400 | |
| H(13) | 2334 | | −3034 | | 397 | | 400 | |
| H(14) | 2277 | | 1028 | | −1048 | | 400 | |
| H(15) | 1126 | | 1031 | | −1755 | | 400 | |
| H(16) | 702 | | 1539 | | 2487 | | 400 | |
| H(17) | 1303 | | −4211 | | −2461 | | 400 | |
| H(18) | 2363 | | −4338 | | −1726 | | 400 | |
| H(19) | 1759 | | −2175 | | 169 | | 400 | |
| H(21) | 3955 | | 4970 | | 850 | | 400 | |
| H(22) | 3087 | | 3636 | | 1285 | | 400 | |
| H(23) | 4271 | | 3765 | | −349 | | 400 | |
| H(24) | 4300 | | −762 | | 981 | | 400 | |
| H(25) | 5429 | | −1041 | | 1678 | | 400 | |
| H(26) | 5469 | | 1341 | | 2459 | | 400 | |
| H(27) | 5401 | | 4140 | | 2477 | | 400 | |
| H(28) | 4333 | | 4542 | | 1769 | | 400 | |
| H(29) | 4776 | | 2929 | | −149 | | 400 | |

TABLE 3 (*Continued*)

| | $x/a$ | $\sigma(x/a)$ | $y/b$ | $\sigma(y/b)$ | $z/c$ | $\sigma(z/c)$ | $U_{iso}$ | $\sigma(U_{iso})$ |
|---|---|---|---|---|---|---|---|---|
| | (b) *Diaquobis(methoxyacetato)copper*(II) | | | | | | | |
| Cu | 0 | 0 | 0 | 0 | 0 | 0 | 376 | 7 |
| O(1) | 1842 | 14 | −1154 | 11 | 1051 | 7 | 345 | 19 |
| O(2) | 4731 | 14 | −837 | 11 | 2039 | 8 | 365 | 19 |
| O(3) | 2096 | 14 | 2341 | 12 | 353 | 7 | 346 | 19 |
| O(4) | 1423 | 16 | −708 | 13 | −1794 | 8 | 435 | 22 |
| C(1) | 3356 | 19 | −205 | 15 | 1411 | 10 | 268 | 22 |
| C(2) | 3739 | 21 | 1866 | 16 | 1082 | 11 | 337 | 26 |
| C(3) | 2398 | 25 | 4157 | 20 | −312 | 13 | 472 | 34 |
| | (c) *Bis(glycollato)copper*(II) | | | | | | | |
| Cu | 0 | 0 | 0 | 0 | 0 | 0 | 273 | 8 |
| O(1) | 1575 | 12 | 2063 | 18 | 1604 | 12 | 207 | 20 |
| O(2) | 2572 | 12 | 1676 | 19 | 3954 | 12 | 217 | 21 |
| O(3) | −614 | 12 | −3055 | 18 | 1469 | 11 | 203 | 20 |
| C(1) | 1612 | 17 | 681 | 25 | 2809 | 17 | 186 | 26 |
| C(2) | 335 | 18 | −2403 | 26 | 2907 | 17 | 209 | 28 |
| | (d) *Aquobis(lactato)copper*(II) *hemihydrate* | | | | | | | |
| Cu | 1816 | 2 | 2158 | 1 | 0 | 0 | 436 | 8 |
| O(1) | 736 | 13 | 1906 | 7 | 2923 | 29 | 405 | 30 |
| O(2) | −1418 | 15 | 1548 | 7 | 4455 | 32 | 500 | 35 |
| O(3) | −154 | 12 | 1647 | 6 | −1362 | 32 | 371 | 27 |
| O(4) | 2090 | 13 | 1118 | 6 | 198 | 40 | 465 | 29 |
| O(5) | 1184 | 29 | 5713 | 15 | 270 | 79 | 606 | 115 |
| C(1) | −606 | 17 | 1652 | 9 | 2769 | 41 | 320 | 35 |
| C(2) | −1292 | 18 | 1493 | 9 | 198 | 56 | 416 | 38 |
| C(3) | −2576 | 20 | 688 | 10 | 75 | 72 | 546 | 44 |
| C(11) | 4186 | 18 | 3027 | 9 | −2722 | 42 | 339 | 37 |
| C(12) | 4808 | 17 | 3313 | 8 | −265 | 51 | 356 | 35 |
| C(13) | 5290 | 19 | 4118 | 10 | 68 | 66 | 524 | 43 |
| O(11) | 2918 | 12 | 2505 | 4 | −2896 | 28 | 367 | 28 |
| O(12) | 4967 | 14 | 3336 | 7 | −4502 | 32 | 473 | 34 |
| O(13) | 3745 | 14 | 2855 | 7 | 1355 | 34 | 431 | 31 |

[The occupation number of O(5) is 0·503 with an e.s.d. of 0·053.]

(e) *Diaquobis-(2-hydroxy-2-methylpropionato(copper*(II)

(i) With anisotropic temperature factors for the copper atom giving $R = 0{\cdot}169$.

| | $x/a$ | $\sigma(x/a)$ | $y/b$ | $\sigma(y/b)$ | $z/c$ | $\sigma(z/c)$ | $U_{iso}$ | $\sigma(U_{iso})$ |
|---|---|---|---|---|---|---|---|---|
| Cu | 0 | 0 | 0 | 0 | 0 | 0 | — | — |
| O(1) | 0 | 0 | −2364 | 35 | 882 | 16 | 378 | 46 |
| O(2) | 0 | 0 | −3069 | 40 | 2775 | 18 | 509 | 56 |
| O(3) | 0 | 0 | 2295 | 34 | 1712 | 15 | 351 | 45 |
| O(4) | 2534 | 27 | 0 | 0 | 0 | 0 | 736 | 69 |
| C(1) | 0 | 0 | −1656 | 55 | 2128 | 24 | 398 | 69 |
| C(2) | 0 | 0 | 1297 | 52 | 2750 | 22 | 334 | 63 |
| C(3) | 1236 | 25 | 1954 | 41 | 3545 | 19 | 554 | 60 |

The anisotropic temperature factors ($\times 10^4$) for the copper atom with their e.s.d. in parentheses are $U_{11}$, 879(44); $U_{22}$, 260(37); $U_{33}$, 71(18); $U_{12}$, 0(0); $U_{13}$, 0(0); $U_{23}$, 47(35).

(ii) With disordered copper atoms giving $R = 0{\cdot}129$.

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Cu(1) | 0 | 0 | 0 | 0 | 0 | 0 | 156 | — |
| Cu(2) | 550 | — | 0 | 0 | 0 | 0 | 156 | — |
| O(1) | 0 | 0 | −2353 | 29 | 881 | 13 | 439 | 38 |
| O(2) | 0 | 0 | −3007 | 30 | 2774 | 13 | 467 | 41 |
| O(3) | 0 | 0 | 2261 | 27 | 1714 | 12 | 366 | 36 |
| O(4) | 2520 | 22 | 0 | 0 | 0 | 0 | 771 | 56 |
| C(1) | 0 | 0 | −1631 | 41 | 2098 | 19 | 364 | 51 |
| C(2) | 0 | 0 | 1209 | 38 | 2749 | 16 | 281 | 44 |
| C(3) | 1229 | 20 | 1946 | 33 | 3545 | 15 | 573 | 47 |

The occupation numbers of Cu(1) and Cu(2) are 0·702 and 0·149 respectively. Parameters for which there are no e.s.d.'s were not refined in the final cycles.

[21] C. K. Prout, *J. Chem. Soc.*, 1962, 4429.

TABLE 4

Observed structure amplitudes and calculated structure factors for diaquobis(phenoxyacetato)copper(II)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 0 | 0 | 8 | 566 | 635 |
| 0 | 0 | 10 | 667 | 701 |
| 0 | 0 | 12 | 414 | 392 |
| 0 | 0 | 14 | 391 | 322 |
| 0 | 0 | 16 | 78 | 56 |
| 0 | 0 | 18 | 235 | 183 |
| 0 | 0 | 20 | 182 | 149 |
| 0 | 0 | 22 | 599 | 682 |
| 0 | 0 | 24 | 505 | 568 |
| 0 | 0 | 26 | 61 | 104 |
| 0 | 0 | 28 | 226 | 245 |
| 0 | 0 | 30 | 134 | 165 |
| 0 | 1 | 4 | 254 | 199 |
| 0 | 1 | 5 | 626 | 710 |
| 0 | 1 | 6 | 171 | -136 |
| 0 | 1 | 7 | 820 | 1112 |
| 0 | 1 | 8 | 613 | 552 |
| 0 | 1 | 9 | 739 | 928 |
| 0 | 1 | 10 | 78 | -41 |
| 0 | 1 | 11 | 652 | 671 |
| 0 | 1 | 12 | 42 | -51 |
| 0 | 1 | 13 | 650 | 693 |
| 0 | 1 | 14 | 341 | -317 |
| 0 | 1 | 15 | 636 | 680 |
| 0 | 1 | 16 | 259 | -250 |
| 0 | 1 | 17 | 441 | 483 |
| 0 | 1 | 18 | 23 | -27 |
| 0 | 1 | 19 | 268 | 292 |
| 0 | 1 | 20 | 76 | 70 |
| 0 | 1 | 21 | 299 | 311 |
| 0 | 1 | 22 | 197 | 161 |
| 0 | 1 | 23 | 304 | 316 |
| 0 | 1 | 24 | 231 | -225 |
| 0 | 1 | 25 | 122 | 118 |
| 0 | 1 | 26 | 48 | -71 |
| 0 | 1 | 27 | 102 | 90 |
| 0 | 1 | 28 | 26 | 33 |
| 0 | 1 | 29 | 153 | 153 |
| 0 | 2 | 0 | 228 | -147 |
| 0 | 2 | 2 | 222 | 239 |
| 0 | 2 | 3 | 299 | 227 |
| 0 | 2 | 4 | 180 | 220 |
| 0 | 2 | 5 | 522 | 455 |
| 0 | 2 | 6 | 797 | 799 |
| 0 | 2 | 7 | 762 | 684 |
| 0 | 2 | 8 | 575 | 543 |
| 0 | 2 | 9 | 205 | 142 |
| 0 | 2 | 10 | 231 | 247 |
| 0 | 2 | 12 | 452 | 451 |
| 0 | 2 | 13 | 235 | 189 |
| 0 | 2 | 14 | 290 | 301 |
| 0 | 2 | 15 | 200 | -192 |
| 0 | 2 | 16 | 571 | 547 |
| 0 | 2 | 17 | 219 | -215 |
| 0 | 2 | 18 | 288 | 311 |
| 0 | 2 | 19 | 76 | -81 |
| 0 | 2 | 20 | 214 | 200 |
| 0 | 2 | 21 | 85 | -101 |
| 0 | 2 | 22 | 100 | 100 |
| 0 | 2 | 23 | 149 | -127 |
| 0 | 2 | 24 | 56 | 45 |
| 0 | 2 | 25 | 79 | -89 |
| 0 | 2 | 26 | 102 | 98 |
| 0 | 2 | 28 | 81 | 91 |
| 0 | 2 | 29 | 60 | 56 |
| 0 | 3 | 1 | 226 | 259 |
| 0 | 3 | 2 | 164 | -112 |
| 0 | 3 | 3 | 142 | -27 |
| 0 | 3 | 4 | 264 | -211 |
| 0 | 3 | 5 | 536 | 547 |
| 0 | 3 | 6 | 289 | -206 |
| 0 | 3 | 7 | 417 | 408 |
| 0 | 3 | 8 | 320 | -282 |
| 0 | 3 | 9 | 42 | 67 |
| 0 | 3 | 10 | 170 | -156 |
| 0 | 3 | 11 | 412 | 412 |
| 0 | 3 | 12 | 36 | -27 |
| 0 | 3 | 13 | 231 | 243 |
| 0 | 3 | 14 | 104 | 61 |
| 0 | 3 | 15 | 165 | 168 |
| 0 | 3 | 16 | 81 | 69 |
| 0 | 3 | 17 | 317 | 339 |
| 0 | 3 | 18 | 80 | 60 |
| 0 | 3 | 19 | 115 | 109 |
| 0 | 3 | 20 | 94 | 83 |
| 0 | 3 | 23 | 130 | 123 |
| 0 | 3 | 24 | 30 | 34 |
| 0 | 3 | 25 | 80 | 55 |
| 0 | 3 | 27 | 81 | 85 |
| 0 | 4 | 0 | 309 | 282 |
| 0 | 4 | 1 | 87 | -55 |
| 0 | 4 | 2 | 311 | 318 |
| 0 | 4 | 3 | 132 | 109 |
| 0 | 4 | 4 | 290 | 251 |
| 0 | 4 | 6 | 436 | 479 |
| 0 | 4 | 7 | 289 | -270 |
| 0 | 4 | 8 | 242 | 259 |
| 0 | 4 | 10 | 98 | 116 |
| 0 | 4 | 12 | 165 | 164 |
| 0 | 4 | 14 | 149 | 141 |
| 0 | 4 | 15 | 137 | 120 |
| 0 | 4 | 16 | 246 | 266 |
| 0 | 4 | 17 | 98 | 113 |
| 0 | 4 | 18 | 163 | 179 |
| 0 | 4 | 20 | 97 | 114 |
| 0 | 4 | 21 | 68 | 64 |
| 0 | 4 | 22 | 132 | 124 |
| 0 | 4 | 23 | 73 | 75 |
| 0 | 4 | 24 | 86 | 90 |
| 0 | 4 | 25 | 38 | 35 |
| 0 | 4 | 26 | 91 | 87 |
| 0 | 5 | 1 | 469 | 490 |
| 0 | 5 | 2 | 167 | 172 |
| 0 | 5 | 3 | 265 | 263 |
| 0 | 5 | 5 | 155 | 132 |
| 0 | 5 | 6 | 23 | 16 |
| 0 | 5 | 7 | 377 | 382 |
| 0 | 5 | 8 | 179 | -198 |
| 0 | 5 | 9 | 271 | 229 |
| 0 | 5 | 10 | 59 | -54 |
| 0 | 5 | 11 | 182 | 175 |
| 0 | 5 | 13 | 170 | 146 |
| 0 | 5 | 14 | 109 | 96 |
| 0 | 5 | 15 | 159 | 172 |
| 0 | 5 | 16 | 34 | 56 |
| 0 | 5 | 17 | 100 | 85 |
| 0 | 5 | 18 | 39 | -34 |
| 0 | 5 | 19 | 22 | 21 |
| 0 | 5 | 21 | 154 | 172 |
| 0 | 5 | 22 | 44 | -46 |
| 0 | 5 | 23 | 132 | 140 |
| 0 | 5 | 24 | 86 | 76 |
| 0 | 6 | 0 | 482 | 556 |
| 0 | 6 | 2 | 142 | 104 |
| 0 | 6 | 3 | 65 | -95 |
| 0 | 6 | 5 | 149 | 145 |
| 0 | 6 | 6 | 115 | 136 |
| 0 | 6 | 7 | 141 | 129 |
| 0 | 6 | 8 | 112 | 99 |
| 0 | 6 | 10 | 166 | 171 |
| 0 | 6 | 12 | 174 | 156 |
| 0 | 6 | 13 | 33 | -50 |
| 0 | 6 | 14 | 130 | 149 |
| 0 | 6 | 15 | 58 | -42 |
| 0 | 6 | 16 | 73 | 71 |
| 0 | 6 | 17 | 122 | -125 |
| 0 | 7 | 2 | 179 | -223 |
| 0 | 7 | 5 | 125 | 156 |
| 0 | 7 | 7 | 87 | 72 |
| 0 | 7 | 9 | 65 | 75 |
| 0 | 8 | 0 | 60 | -66 |
| 0 | 8 | 6 | 38 | 51 |
| 0 | 8 | 9 | 36 | -51 |
| 0 | 8 | 12 | 35 | 36 |
| 1 | 0 | 4 | 31 | -36 |
| 1 | 0 | 7 | 54 | -51 |
| 1 | 0 | 8 | 34 | 21 |
| 1 | 0 | 9 | 59 | -55 |
| 1 | 0 | 11 | 56 | -47 |
| 1 | 0 | 13 | 18 | -20 |
| 1 | 0 | 14 | 33 | 33 |
| 1 | 0 | 16 | 63 | 58 |
| 1 | 0 | 21 | 74 | 82 |
| 1 | 0 | 22 | 49 | -59 |
| 1 | 0 | 23 | 35 | 47 |
| 1 | 0 | 24 | 72 | -79 |
| 1 | 0 | 26 | 27 | -39 |
| 1 | 0 | 27 | 25 | 37 |
| 1 | 0 | 28 | 29 | -34 |
| 1 | 1 | 0 | 62 | -61 |
| 1 | 1 | 1 | 45 | 40 |
| 1 | 1 | 2 | 78 | -82 |
| 1 | 1 | 3 | 90 | 92 |
| 1 | 1 | 4 | 54 | -50 |
| 1 | 1 | 5 | 11 | -6 |
| 1 | 1 | 7 | 40 | -29 |
| 1 | 1 | 8 | 87 | -76 |
| 1 | 1 | 9 | 62 | -48 |
| 1 | 1 | 10 | 48 | -42 |
| 1 | 1 | 12 | 43 | -37 |
| 1 | 1 | 14 | 48 | -45 |
| 1 | 1 | 16 | 68 | -66 |
| 1 | 1 | 18 | 98 | -111 |
| 1 | 1 | 20 | 75 | -93 |
| 1 | 1 | 22 | 67 | -73 |
| 1 | 1 | 24 | 56 | -57 |
| 1 | -1 | 1 | 42 | 39 |
| 1 | -1 | 2 | 59 | 60 |
| 1 | -1 | 3 | 67 | 64 |
| 1 | -1 | 4 | 68 | 77 |
| 1 | -1 | 5 | 19 | 15 |
| 1 | -1 | 6 | 107 | 106 |
| 1 | -1 | 7 | 75 | -58 |
| 1 | -1 | 8 | 154 | 145 |
| 1 | -1 | 9 | 82 | -80 |
| 1 | -1 | 10 | 132 | 126 |
| 1 | -1 | 11 | 92 | -89 |
| 1 | -1 | 12 | 96 | 95 |
| 1 | -1 | 13 | 54 | -52 |
| 1 | -1 | 14 | 70 | 69 |
| 1 | -1 | 15 | 48 | -51 |
| 1 | -1 | 16 | 66 | 70 |
| 1 | -1 | 17 | 61 | -67 |
| 1 | -1 | 18 | 43 | 54 |
| 1 | -1 | 19 | 48 | -48 |
| 1 | -1 | 20 | 67 | 73 |
| 1 | -1 | 22 | 82 | 86 |
| 1 | -1 | 23 | 52 | 65 |
| 1 | -1 | 24 | 24 | -22 |
| 1 | -1 | 25 | 36 | 55 |
| 1 | -1 | 26 | 16 | -14 |
| 1 | -1 | 27 | 32 | 38 |
| 1 | 2 | 1 | 69 | 54 |
| 1 | 2 | 2 | 37 | -25 |
| 1 | 2 | 3 | 61 | -69 |
| 1 | 2 | 4 | 57 | -49 |
| 1 | 2 | 5 | 151 | -145 |
| 1 | 2 | 6 | 100 | -82 |
| 1 | 2 | 7 | 172 | -176 |
| 1 | 2 | 8 | 77 | -67 |
| 1 | 2 | 9 | 154 | -172 |
| 1 | 2 | 10 | 35 | -36 |
| 1 | 2 | 11 | 126 | -139 |
| 1 | 2 | 12 | 41 | -40 |
| 1 | 2 | 13 | 138 | -153 |
| 1 | 2 | 14 | 45 | -44 |
| 1 | 2 | 15 | 81 | -96 |
| 1 | 2 | 16 | 28 | -26 |
| 1 | 2 | 17 | 81 | -92 |
| 1 | 2 | 19 | 62 | -58 |
| 1 | -2 | 1 | 108 | 106 |
| 1 | -2 | 2 | 110 | -90 |
| 1 | -2 | 3 | 161 | 158 |
| 1 | -2 | 4 | 160 | -142 |
| 1 | -2 | 5 | 175 | 187 |
| 1 | -2 | 6 | 193 | -182 |
| 1 | -2 | 7 | 193 | 165 |
| 1 | -2 | 8 | 119 | -108 |
| 1 | -2 | 9 | 99 | 110 |
| 1 | -2 | 11 | 54 | 57 |
| 1 | -2 | 12 | 42 | 39 |
| 1 | -2 | 13 | 69 | 75 |
| 1 | -2 | 14 | 109 | 117 |
| 1 | -2 | 15 | 106 | 99 |
| 1 | -2 | 16 | 108 | 105 |
| 1 | -2 | 17 | 49 | 39 |
| 1 | -2 | 18 | 78 | 84 |
| 1 | -2 | 20 | 52 | 65 |
| 1 | -2 | 22 | 76 | 80 |
| 1 | -2 | 24 | 44 | 46 |
| 1 | -2 | 25 | 35 | 28 |
| 1 | -2 | 26 | 21 | -19 |
| 1 | -2 | 27 | 57 | 6 |
| 1 | 3 | 0 | 138 | -139 |
| 1 | 3 | 1 | 33 | 15 |
| 1 | 3 | 2 | 134 | -139 |
| 1 | 3 | 3 | 39 | 20 |
| 1 | 3 | 4 | 126 | -141 |
| 1 | 3 | 5 | 71 | 65 |
| 1 | 3 | 6 | 88 | -99 |
| 1 | 3 | 7 | 109 | 107 |
| 1 | 3 | 8 | 69 | -84 |
| 1 | 3 | 9 | 83 | 82 |
| 1 | 3 | 10 | 35 | -41 |
| 1 | 3 | 11 | 33 | 33 |
| 1 | 3 | 12 | 45 | -41 |
| 1 | 3 | 14 | 32 | -29 |
| 1 | 3 | 16 | 29 | -22 |
| 1 | 3 | 18 | 65 | -59 |
| 1 | -3 | 0 | 87 | -40 |
| 1 | -3 | 2 | 57 | -19 |
| 1 | -3 | 3 | 106 | 87 |
| 1 | -3 | 4 | 57 | 67 |
| 1 | -3 | 5 | 115 | 102 |
| 1 | -3 | 6 | 118 | 122 |
| 1 | -3 | 7 | 91 | 74 |
| 1 | -3 | 8 | 112 | 109 |
| 1 | -3 | 9 | 63 | 66 |
| 1 | -3 | 10 | 167 | 158 |
| 1 | -3 | 12 | 154 | 164 |
| 1 | -3 | 13 | 34 | -18 |
| 1 | -3 | 14 | 166 | 181 |
| 1 | -3 | 16 | 160 | 182 |
| 1 | -3 | 17 | 17 | -14 |
| 1 | -3 | 18 | 115 | 127 |
| 1 | -3 | 19 | 39 | -37 |
| 1 | -3 | 20 | 89 | 99 |
| 1 | -3 | 21 | 25 | -30 |
| 1 | -3 | 22 | 74 | 79 |
| 1 | -3 | 23 | 40 | -38 |
| 1 | -3 | 24 | 54 | 56 |
| 1 | -3 | 25 | 33 | -29 |
| 1 | -3 | 26 | 44 | 43 |
| 1 | -3 | 28 | 40 | 38 |
| 1 | 4 | 1 | 103 | -99 |
| 1 | 4 | 3 | 112 | -108 |
| 1 | 4 | 5 | 75 | -73 |
| 1 | 4 | 6 | 36 | 39 |
| 1 | 4 | 7 | 75 | -81 |
| 1 | 4 | 8 | 46 | 48 |
| 1 | 4 | 9 | 70 | -85 |
| 1 | 4 | 10 | 23 | 29 |
| 1 | 4 | 11 | 23 | -29 |
| 1 | 4 | 13 | 38 | -41 |
| 1 | 4 | 15 | 46 | -45 |
| 1 | 4 | 16 | 49 | -38 |
| 1 | 4 | 17 | 55 | -57 |
| 1 | 4 | 19 | 51 | -60 |
| 1 | 4 | 21 | 48 | -54 |
| 1 | 4 | 23 | 49 | -54 |
| 1 | 4 | 25 | 42 | -44 |
| 1 | 4 | 1 | 221 | 231 |
| 1 | 4 | 2 | 35 | -24 |
| 1 | 4 | 3 | 269 | 286 |
| 1 | 4 | 5 | 341 | 363 |
| 1 | 4 | 6 | 85 | 77 |
| 1 | 4 | 7 | 303 | 303 |
| 1 | 4 | 8 | 64 | 57 |
| 1 | 4 | 9 | 250 | 249 |
| 1 | 4 | 11 | 204 | 203 |
| 1 | 4 | 13 | 175 | 169 |
| 1 | 4 | 14 | 65 | -55 |
| 1 | 4 | 15 | 181 | 181 |
| 1 | 4 | 16 | 87 | -81 |
| 1 | 4 | 17 | 167 | 166 |
| 1 | 4 | 18 | 87 | -71 |
| 1 | 4 | 19 | 130 | 124 |
| 1 | 4 | 20 | 58 | -52 |
| 1 | 4 | 21 | 102 | 96 |
| 1 | 4 | 22 | 41 | -36 |
| 1 | 4 | 23 | 63 | 58 |
| 1 | 4 | 24 | 36 | -27 |
| 1 | 4 | 25 | 43 | 36 |
| 1 | 4 | 27 | 56 | 60 |
| 1 | 5 | 0 | 175 | -192 |
| 1 | 5 | 2 | 163 | -173 |
| 1 | 5 | 3 | 54 | -48 |
| 1 | 5 | 4 | 108 | -106 |
| 1 | 5 | 5 | 41 | -35 |
| 1 | 5 | 6 | 102 | -87 |
| 1 | 5 | 7 | 24 | -21 |
| 1 | 5 | 8 | 108 | -99 |
| 1 | 5 | 10 | 86 | -84 |
| 1 | 5 | 12 | 74 | -68 |
| 1 | 5 | 13 | 35 | -26 |
| 1 | 5 | 14 | 69 | -68 |
| 1 | 5 | 16 | 51 | -51 |
| 1 | 5 | 18 | 45 | -38 |
| 1 | 5 | 20 | 43 | -34 |
| 1 | 5 | 22 | 35 | -44 |
| 1 | 5 | 24 | 49 | -62 |
| 1 | -5 | 4 | 334 | 334 |
| 1 | -5 | 5 | 88 | 80 |
| 1 | -5 | 6 | 316 | 289 |
| 1 | -5 | 7 | 160 | 140 |
| 1 | -5 | 8 | 306 | 285 |
| 1 | -5 | 9 | 115 | 95 |
| 1 | -5 | 10 | 271 | 247 |
| 1 | -5 | 11 | 30 | 30 |
| 1 | -5 | 12 | 224 | 209 |
| 1 | -5 | 13 | 60 | -51 |
| 1 | -5 | 14 | 210 | 226 |
| 1 | -5 | 15 | 87 | -82 |
| 1 | -5 | 16 | 186 | 179 |
| 1 | -5 | 17 | 70 | -68 |
| 1 | -5 | 18 | 138 | 130 |
| 1 | -5 | 19 | 23 | -20 |
| 1 | -5 | 20 | 143 | 152 |
| 1 | -5 | 22 | 129 | 146 |
| 1 | -5 | 23 | 30 | -31 |
| 1 | -5 | 24 | 117 | 126 |
| 1 | 6 | 1 | 91 | -103 |
| 1 | 6 | 2 | 39 | 37 |
| 1 | 6 | 3 | 68 | -70 |
| 1 | 6 | 5 | 39 | -34 |
| 1 | 6 | 6 | 58 | -50 |
| 1 | 6 | 7 | 55 | -62 |
| 1 | 6 | 8 | 30 | -31 |
| 1 | 6 | 9 | 81 | -87 |
| 1 | 6 | 11 | 100 | -118 |
| 1 | 6 | 13 | 79 | -95 |
| 1 | 6 | 15 | 57 | -66 |
| 1 | 6 | 16 | 33 | 40 |
| 1 | 6 | 17 | 39 | -39 |
| 1 | 6 | 18 | 26 | 32 |
| 1 | 6 | 19 | 39 | -39 |
| 1 | -6 | 8 | 195 | -151 |
| 1 | -6 | 9 | 237 | 231 |
| 1 | -6 | 10 | 115 | -94 |
| 1 | -6 | 11 | 213 | 214 |
| 1 | -6 | 12 | 66 | -44 |
| 1 | -6 | 13 | 177 | 173 |
| 1 | -6 | 14 | 17 | 26 |
| 1 | -6 | 15 | 137 | 122 |
| 1 | -6 | 16 | 85 | 80 |
| 1 | -6 | 17 | 84 | 65 |
| 1 | -6 | 18 | 35 | 45 |
| 1 | -6 | 19 | 101 | 76 |
| 1 | -6 | 20 | 45 | 48 |
| 1 | 7 | 2 | 46 | -50 |
| 1 | 7 | 3 | 48 | 49 |
| 1 | 7 | 4 | 58 | -79 |
| 1 | 7 | 6 | 52 | -60 |
| 1 | 7 | 7 | 38 | -28 |
| 1 | 7 | 8 | 43 | -49 |
| 1 | 7 | 9 | 30 | -23 |
| 1 | 7 | 10 | 38 | -41 |
| 1 | 8 | 4 | 20 | 58 |
| 1 | 8 | 6 | 31 | 14 |
| 2 | 0 | 6 | 61 | 8 |
| 2 | 0 | 7 | 19 | -4 |
| 2 | 0 | 8 | 52 | 60 |
| 2 | 0 | 10 | 61 | 69 |
| 2 | 0 | 11 | 33 | 34 |
| 2 | 0 | 14 | 42 | -37 |
| 2 | 0 | 15 | 41 | -34 |
| 2 | 0 | 16 | 52 | -52 |
| 2 | 0 | 17 | 24 | -24 |
| 2 | 0 | 18 | 35 | -38 |
| 2 | 0 | 20 | 26 | -34 |
| 2 | 0 | 22 | 50 | -56 |
| 2 | 0 | 23 | 26 | 35 |
| 2 | 0 | 25 | 50 | 56 |
| 2 | 0 | 27 | 38 | 43 |
| 2 | 1 | 1 | 69 | 65 |
| 2 | 1 | 2 | 89 | -82 |
| 2 | 1 | 3 | 54 | 50 |
| 2 | 1 | 4 | 43 | -35 |
| 2 | 1 | 5 | 31 | 28 |
| 2 | 1 | 6 | 10 | -8 |
| 2 | 1 | 7 | 52 | 48 |
| 2 | 1 | 9 | 37 | 32 |
| 2 | 1 | 10 | 18 | -18 |
| 2 | 1 | 11 | 26 | 25 |
| 2 | 1 | 12 | 28 | -19 |
| 2 | 1 | 13 | 49 | 46 |
| 2 | 1 | 15 | 72 | 72 |
| 2 | 1 | 17 | 106 | 122 |
| 2 | 1 | 18 | 84 | 97 |
| 2 | 1 | 19 | 131 | 155 |
| 2 | 1 | 20 | 56 | 64 |
| 2 | 1 | 21 | 63 | 82 |
| 2 | 1 | 23 | 62 | 71 |
| 2 | 1 | 25 | 55 | 59 |
| 2 | -1 | 5 | 81 | -75 |
| 2 | -1 | 6 | 26 | 24 |
| 2 | -1 | 7 | 83 | -93 |
| 2 | -1 | 8 | 52 | 49 |
| 2 | -1 | 9 | 106 | -101 |
| 2 | -1 | 10 | 89 | 86 |
| 2 | -1 | 11 | 68 | -64 |
| 2 | -1 | 12 | 101 | 95 |
| 2 | -1 | 13 | 32 | -31 |
| 2 | -1 | 14 | 15 | 20 |
| 2 | -1 | 15 | 47 | -39 |
| 2 | -1 | 16 | 49 | 49 |
| 2 | -1 | 17 | 30 | -24 |
| 2 | -1 | 18 | 56 | 54 |
| 2 | -1 | 19 | 26 | -24 |
| 2 | -1 | 20 | 26 | 29 |
| 2 | -1 | 21 | 63 | -61 |
| 2 | -1 | 23 | 53 | -42 |
| 2 | 2 | 0 | 48 | -25 |
| 2 | 2 | 2 | 30 | 43 |
| 2 | 2 | 3 | 28 | 21 |
| 2 | 2 | 4 | 153 | 155 |
| 2 | 2 | 5 | 48 | 38 |
| 2 | 2 | 6 | 219 | 221 |
| 2 | 2 | 7 | 39 | 32 |
| 2 | 2 | 8 | 214 | 224 |
| 2 | 2 | 9 | 33 | 31 |
| 2 | 2 | 10 | 189 | 208 |
| 2 | 2 | 11 | 41 | 45 |
| 2 | 2 | 12 | 203 | 227 |
| 2 | 2 | 13 | 61 | 67 |
| 2 | 2 | 14 | 150 | 175 |
| 2 | 2 | 15 | 48 | 48 |
| 2 | 2 | 16 | 136 | 153 |
| 2 | 2 | 17 | 40 | 42 |
| 2 | 2 | 18 | 93 | 101 |
| 2 | 2 | 20 | 27 | -25 |
| 2 | 2 | 21 | 38 | -42 |
| 2 | 2 | 22 | 26 | -36 |
| 2 | 2 | 23 | 26 | -27 |
| 2 | 2 | 25 | 40 | -42 |
| 2 | 2 | 26 | 34 | 25 |
| 2 | -2 | 0 | 131 | -136 |
| 2 | -2 | 1 | 39 | 32 |
| 2 | -2 | 2 | 140 | -145 |
| 2 | -2 | 3 | 95 | 78 |
| 2 | -2 | 4 | 172 | -163 |
| 2 | -2 | 5 | 109 | 106 |
| 2 | -2 | 6 | 115 | -122 |
| 2 | -2 | 7 | 121 | 114 |
| 2 | -2 | 8 | 81 | -85 |
| 2 | -2 | 9 | 58 | 49 |
| 2 | -2 | 10 | 41 | -43 |
| 2 | -2 | 11 | 19 | 8 |
| 2 | -2 | 13 | 50 | -47 |
| 2 | -2 | 14 | 47 | -43 |
| 2 | -2 | 15 | 78 | -83 |
| 2 | -2 | 16 | 74 | -69 |
| 2 | -2 | 17 | 53 | -60 |
| 2 | -2 | 19 | 32 | -34 |
| 2 | -2 | 21 | 27 | -26 |
| 2 | -2 | 22 | 32 | -24 |
| 2 | -2 | 23 | 32 | -29 |
| 2 | 3 | 1 | 273 | 273 |
| 2 | 3 | 2 | 23 | -15 |
| 2 | 3 | 3 | 247 | 253 |

TABLE 4 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 2 | 3 | 4 | 56 | -42 |
| 2 | 3 | 5 | 172 | 183 |
| 2 | 3 | 6 | 137 | -122 |
| 2 | 3 | 7 | 123 | 126 |
| 2 | 3 | 8 | 135 | -134 |
| 2 | 3 | 9 | 46 | 51 |
| 2 | 3 | 10 | 86 | -91 |
| 2 | 3 | 11 | 16 | 23 |
| 2 | 3 | 12 | 69 | -72 |
| 2 | 3 | 14 | 50 | -54 |
| 2 | 3 | 17 | 57 | 48 |
| 2 | 3 | 18 | 50 | -53 |
| 2 | 3 | 19 | 46 | 43 |
| 2 | 3 | 21 | 52 | 48 |
| 2 | 3 | 22 | 40 | 36 |
| 2 | 3 | 23 | 59 | 73 |
| 2 | 3 | 24 | 36 | 37 |
| 2 | 3 | 25 | 74 | 82 |
| 2 | 3 | 26 | 19 | 22 |
| 2 | 3 | 27 | 47 | 0 |
| 2 | -3 | 1 | 41 | 9 |
| 2 | -3 | 3 | 26 | -35 |
| 2 | -3 | 4 | 40 | -34 |
| 2 | -3 | 5 | 103 | -109 |
| 2 | -3 | 7 | 110 | -118 |
| 2 | -3 | 9 | 117 | -119 |
| 2 | -3 | 11 | 126 | 123 |
| 2 | -3 | 12 | 44 | 18 |
| 2 | -3 | 13 | 112 | -110 |
| 2 | -3 | 15 | 121 | -117 |
| 2 | -3 | 17 | 86 | -94 |
| 2 | -3 | 19 | 63 | -66 |
| 2 | -3 | 21 | 57 | -53 |
| 2 | -3 | 23 | 31 | -25 |
| 2 | 4 | 0 | 165 | 138 |
| 2 | 4 | 2 | 161 | 151 |
| 2 | 4 | 4 | 136 | 111 |
| 2 | 4 | 6 | 121 | 111 |
| 2 | 4 | 7 | 41 | -42 |
| 2 | 4 | 8 | 125 | 116 |
| 2 | 4 | 9 | 52 | -35 |
| 2 | 4 | 10 | 69 | 61 |
| 2 | 4 | 12 | 55 | 50 |
| 2 | 4 | 14 | 70 | 67 |
| 2 | 4 | 15 | 42 | 47 |
| 2 | 4 | 16 | 69 | 78 |
| 2 | 4 | 17 | 53 | 34 |
| 2 | 4 | 18 | 79 | 100 |
| 2 | 4 | 20 | 85 | 106 |
| 2 | 4 | 22 | 76 | 83 |
| 2 | 4 | 24 | 67 | 78 |
| 2 | 4 | 26 | 50 | 53 |
| 2 | -4 | 2 | 133 | -139 |
| 2 | -4 | 4 | 205 | -199 |
| 2 | -4 | 5 | 41 | -36 |
| 2 | -4 | 6 | 231 | -241 |
| 2 | -4 | 7 | 63 | -51 |
| 2 | -4 | 8 | 159 | -165 |
| 2 | -4 | 9 | 28 | -29 |
| 2 | -4 | 10 | 144 | -156 |
| 2 | -4 | 12 | 122 | -132 |
| 2 | -4 | 14 | 108 | -113 |
| 2 | -4 | 16 | 115 | -119 |
| 2 | -4 | 17 | 46 | 40 |
| 2 | -4 | 18 | 85 | -96 |
| 2 | -4 | 19 | 38 | 21 |
| 2 | -4 | 20 | 78 | -84 |
| 2 | -4 | 22 | 39 | -34 |
| 2 | 5 | 1 | 296 | 299 |
| 2 | 5 | 2 | 81 | 71 |
| 2 | 5 | 3 | 234 | 207 |
| 2 | 5 | 4 | 106 | 101 |
| 2 | 5 | 5 | 177 | 161 |
| 2 | 5 | 6 | 118 | 108 |
| 2 | 5 | 7 | 163 | 157 |
| 2 | 5 | 8 | 42 | 28 |
| 2 | 5 | 9 | 173 | 162 |
| 2 | 5 | 11 | 163 | 161 |
| 2 | 5 | 12 | 57 | 49 |
| 2 | 5 | 13 | 151 | 138 |
| 2 | 5 | 14 | 53 | 34 |
| 2 | 5 | 15 | 118 | 96 |
| 2 | 5 | 17 | 86 | 77 |
| 2 | 5 | 19 | 77 | 61 |
| 2 | 5 | 21 | 71 | 69 |
| 2 | 5 | 23 | 81 | 90 |
| 2 | -5 | 5 | 133 | -137 |
| 2 | -5 | 6 | 92 | -85 |
| 2 | -5 | 7 | 136 | -139 |
| 2 | -5 | 8 | 98 | -97 |
| 2 | -5 | 9 | 125 | -136 |
| 2 | -5 | 10 | 41 | -41 |
| 2 | -5 | 11 | 130 | -128 |
| 2 | -5 | 12 | 19 | -21 |
| 2 | -5 | 13 | 105 | -106 |
| 2 | -5 | 15 | 111 | -114 |
| 2 | -5 | 17 | 74 | -75 |
| 2 | -5 | 18 | 26 | 28 |
| 2 | -5 | 19 | 39 | -54 |
| 2 | -5 | 20 | 24 | -23 |
| 2 | -5 | 21 | 77 | -79 |
| 2 | -5 | 22 | 31 | -29 |
| 2 | -5 | 23 | 56 | -58 |
| 2 | 6 | 0 | 207 | 194 |
| 2 | 6 | 1 | 27 | -49 |
| 2 | 6 | 2 | 189 | 156 |
| 2 | 6 | 4 | 166 | 139 |
| 2 | 6 | 5 | 63 | 58 |
| 2 | 6 | 6 | 173 | 147 |
| 2 | 6 | 7 | 90 | 82 |
| 2 | 6 | 8 | 213 | 205 |
| 2 | 6 | 9 | 83 | 71 |
| 2 | 6 | 10 | 256 | 283 |
| 2 | 6 | 11 | 54 | 49 |
| 2 | 6 | 12 | 255 | 273 |
| 2 | 6 | 14 | 202 | 208 |
| 2 | 6 | 16 | 144 | 146 |
| 2 | 6 | 18 | 126 | 124 |
| 2 | 6 | 20 | 110 | 103 |
| 2 | -6 | 10 | 57 | -69 |
| 2 | -6 | 11 | 38 | 24 |
| 2 | -6 | 12 | 53 | -59 |
| 2 | -6 | 14 | 51 | -57 |
| 2 | -6 | 16 | 38 | -36 |
| 2 | 7 | 1 | 180 | 141 |
| 2 | 7 | 2 | 59 | -69 |
| 2 | 7 | 3 | 212 | 228 |
| 2 | 7 | 4 | 23 | -38 |
| 2 | 7 | 5 | 213 | 240 |
| 2 | 7 | 7 | 206 | 192 |
| 2 | 7 | 8 | 27 | 28 |
| 2 | 7 | 9 | 174 | 159 |
| 2 | 7 | 11 | 130 | 117 |
| 2 | 7 | 13 | 103 | 100 |
| 2 | 7 | 15 | 119 | 111 |
| 2 | 8 | 0 | 86 | 59 |
| 2 | 8 | 2 | 107 | 94 |
| 2 | 8 | 3 | 35 | -26 |
| 2 | 8 | 4 | 138 | 138 |
| 2 | 8 | 5 | 76 | -79 |
| 2 | 8 | 6 | 130 | 125 |
| 2 | 8 | 7 | 98 | -104 |
| 2 | 8 | 8 | 106 | 82 |
| 2 | 8 | 9 | 109 | -98 |
| 3 | 0 | 4 | 512 | 524 |
| 3 | 0 | 5 | 350 | -274 |
| 3 | 0 | 7 | 416 | 482 |
| 3 | 0 | 8 | 533 | 705 |
| 3 | 0 | 9 | 571 | 756 |
| 3 | 0 | 10 | 556 | 642 |
| 3 | 0 | 12 | 206 | 179 |
| 3 | 0 | 13 | 588 | 698 |
| 3 | 0 | 14 | 30 | -28 |
| 3 | 0 | 15 | 405 | 412 |
| 3 | 0 | 16 | 275 | -266 |
| 3 | 0 | 17 | 183 | 165 |
| 3 | 0 | 18 | 302 | -279 |
| 3 | 0 | 19 | 306 | 283 |
| 3 | 0 | 20 | 109 | 51 |
| 3 | 0 | 21 | 455 | 440 |
| 3 | 0 | 23 | 127 | 166 |
| 3 | 0 | 24 | 134 | -156 |
| 3 | 0 | 25 | 302 | 308 |
| 3 | 0 | 26 | 66 | -63 |
| 3 | 0 | 27 | 122 | 120 |
| 3 | 0 | 28 | 116 | 123 |
| 3 | 1 | 0 | 154 | 206 |
| 3 | 1 | 1 | 241 | 196 |
| 3 | 1 | 2 | 673 | 896 |
| 3 | 1 | 5 | 416 | -433 |
| 3 | 1 | 6 | 675 | 758 |
| 3 | 1 | 7 | 281 | 252 |
| 3 | 1 | 8 | 793 | 895 |
| 3 | 1 | 9 | 236 | -262 |
| 3 | 1 | 10 | 705 | 865 |
| 3 | 1 | 11 | 81 | -84 |
| 3 | 1 | 12 | 482 | 557 |
| 3 | 1 | 13 | 159 | -145 |
| 3 | 1 | 14 | 552 | 623 |
| 3 | 1 | 16 | 339 | 386 |
| 3 | 1 | 17 | 119 | -88 |
| 3 | 1 | 18 | 499 | 537 |
| 3 | 1 | 19 | 375 | 374 |
| 3 | 1 | 20 | 417 | 414 |
| 3 | 1 | 21 | 154 | 147 |
| 3 | 1 | 22 | 65 | 53 |
| 3 | 1 | 24 | 129 | 111 |
| 3 | 1 | 26 | 249 | 251 |
| 3 | 1 | 27 | 113 | -112 |
| 3 | 1 | 28 | 184 | 173 |
| 3 | 1 | 29 | 89 | 64 |
| 3 | -1 | 3 | 424 | 376 |
| 3 | -1 | 4 | 85 | 117 |
| 3 | -1 | 5 | 229 | 208 |
| 3 | -1 | 6 | 272 | 317 |
| 3 | -1 | 7 | 101 | -67 |
| 3 | -1 | 8 | 293 | 345 |
| 3 | -1 | 9 | 510 | -515 |
| 3 | -1 | 10 | 330 | 389 |
| 3 | -1 | 11 | 291 | -255 |
| 3 | -1 | 12 | 325 | 340 |
| 3 | -1 | 13 | 452 | 439 |
| 3 | -1 | 14 | 217 | 209 |
| 3 | -1 | 15 | 92 | 66 |
| 3 | -1 | 16 | 279 | 264 |
| 3 | -1 | 18 | 136 | 142 |
| 3 | -1 | 19 | 110 | -64 |
| 3 | -1 | 20 | 253 | 249 |
| 3 | -1 | 21 | 46 | 34 |
| 3 | -1 | 22 | 271 | 287 |
| 3 | -1 | 24 | 179 | 197 |
| 3 | -1 | 26 | 117 | 112 |
| 3 | -1 | 27 | 127 | 124 |
| 3 | -1 | 28 | 43 | 57 |
| 3 | 2 | 1 | 180 | -70 |
| 3 | 2 | 2 | 90 | 70 |
| 3 | 2 | 3 | 482 | 504 |
| 3 | 2 | 4 | 80 | -73 |
| 3 | 2 | 6 | 342 | -334 |
| 3 | 2 | 7 | 432 | 464 |
| 3 | 2 | 8 | 225 | -179 |
| 3 | 2 | 9 | 671 | 781 |
| 3 | 2 | 10 | 248 | -241 |
| 3 | 2 | 11 | 620 | 656 |
| 3 | 2 | 12 | 73 | -58 |
| 3 | 2 | 13 | 587 | 657 |
| 3 | 2 | 15 | 476 | 529 |
| 3 | 2 | 16 | 91 | 43 |
| 3 | 2 | 17 | 504 | 563 |
| 3 | 2 | 18 | 124 | 66 |
| 3 | 2 | 19 | 487 | 520 |
| 3 | 2 | 20 | 71 | -52 |
| 3 | 2 | 21 | 96 | 89 |
| 3 | 2 | 23 | 104 | 72 |
| 3 | 2 | 24 | 54 | 33 |
| 3 | 2 | 25 | 75 | 84 |
| 3 | 2 | 26 | 46 | 28 |
| 3 | 2 | 27 | 184 | 175 |
| 3 | -2 | 1 | 562 | 686 |
| 3 | -2 | 2 | 119 | 70 |
| 3 | -2 | 3 | 798 | 856 |
| 3 | -2 | 5 | 434 | 492 |
| 3 | -2 | 6 | 134 | -145 |
| 3 | -2 | 7 | 311 | 367 |
| 3 | -2 | 8 | 112 | -101 |
| 3 | -2 | 9 | 351 | 383 |
| 3 | -2 | 10 | 431 | -440 |
| 3 | -2 | 11 | 307 | -217 |
| 3 | -2 | 12 | 174 | 163 |
| 3 | -2 | 14 | 219 | 170 |
| 3 | -2 | 15 | 185 | 201 |
| 3 | -2 | 16 | 111 | -82 |
| 3 | -2 | 17 | 50 | 53 |
| 3 | -2 | 18 | 68 | 65 |
| 3 | -2 | 19 | 188 | 182 |
| 3 | -2 | 21 | 192 | 189 |
| 3 | -2 | 23 | 167 | 162 |
| 3 | -2 | 24 | 62 | 59 |
| 3 | -2 | 25 | 142 | 156 |
| 3 | -2 | 27 | 139 | 131 |
| 3 | -2 | 28 | 68 | -59 |
| 3 | -2 | 29 | 94 | 111 |
| 3 | 3 | 0 | 535 | 506 |
| 3 | 3 | 2 | 724 | 808 |
| 3 | 3 | 3 | 268 | 253 |
| 3 | 3 | 4 | 652 | 659 |
| 3 | 3 | 5 | 61 | -43 |
| 3 | 3 | 6 | 222 | 208 |
| 3 | 3 | 7 | 164 | -153 |
| 3 | 3 | 8 | 304 | 326 |
| 3 | 3 | 10 | 169 | 151 |
| 3 | 3 | 12 | 34 | 47 |
| 3 | 3 | 13 | 56 | 45 |
| 3 | 3 | 14 | 177 | 151 |
| 3 | 3 | 15 | 36 | 37 |
| 3 | 3 | 16 | 124 | 93 |
| 3 | 3 | 17 | 113 | 74 |
| 3 | 3 | 18 | 111 | 106 |
| 3 | 3 | 19 | 122 | -93 |
| 3 | 3 | 20 | 218 | 227 |
| 3 | 3 | 22 | 181 | 144 |
| 3 | 3 | 24 | 176 | 171 |
| 3 | 3 | 26 | 196 | 206 |
| 3 | -3 | 0 | 342 | -189 |
| 3 | -3 | 1 | 92 | -70 |
| 3 | -3 | 2 | 465 | 509 |
| 3 | -3 | 3 | 98 | 85 |
| 3 | -3 | 4 | 447 | 469 |
| 3 | -3 | 5 | 227 | -196 |
| 3 | -3 | 6 | 218 | 245 |
| 3 | -3 | 7 | 400 | -341 |
| 3 | -3 | 8 | 501 | 525 |
| 3 | -3 | 9 | 249 | -245 |
| 3 | -3 | 10 | 332 | 387 |
| 3 | -3 | 11 | 95 | -68 |
| 3 | -3 | 12 | 280 | 275 |
| 3 | -3 | 14 | 442 | 483 |
| 3 | -3 | 15 | 96 | 81 |
| 3 | -3 | 16 | 299 | 322 |
| 3 | -3 | 17 | 45 | 55 |
| 3 | -3 | 18 | 205 | 205 |
| 3 | -3 | 20 | 226 | 256 |
| 3 | -3 | 22 | 82 | 87 |
| 3 | -3 | 24 | 93 | 102 |
| 3 | -3 | 26 | 181 | 184 |
| 3 | -3 | 28 | 54 | 57 |
| 3 | 4 | 1 | 276 | 246 |
| 3 | 4 | 2 | 148 | 136 |
| 3 | 4 | 3 | 324 | 342 |
| 3 | 4 | 4 | 66 | -53 |
| 3 | 4 | 5 | 163 | 142 |
| 3 | 4 | 6 | 42 | 25 |
| 3 | 4 | 7 | 174 | 159 |
| 3 | 4 | 9 | 218 | 249 |
| 3 | 4 | 10 | 120 | -133 |
| 3 | 4 | 11 | 69 | 45 |
| 3 | 4 | 12 | 95 | 78 |
| 3 | 4 | 13 | 103 | 103 |
| 3 | 4 | 14 | 76 | 63 |
| 3 | 4 | 15 | 165 | 143 |
| 3 | 4 | 16 | 71 | -78 |
| 3 | 4 | 19 | 121 | 119 |
| 3 | 4 | 21 | 111 | 127 |
| 3 | 4 | 23 | 87 | 77 |
| 3 | 4 | 24 | 71 | 60 |
| 3 | 4 | 25 | 118 | 98 |
| 3 | -4 | 1 | 75 | 106 |
| 3 | -4 | 2 | 143 | -122 |
| 3 | -4 | 3 | 527 | 530 |
| 3 | -4 | 4 | 254 | 206 |
| 3 | -4 | 5 | 704 | 751 |
| 3 | -4 | 7 | 434 | 419 |
| 3 | -4 | 8 | 144 | 118 |
| 3 | -4 | 9 | 401 | 396 |
| 3 | -4 | 10 | 57 | -51 |
| 3 | -4 | 11 | 327 | 329 |
| 3 | -4 | 13 | 326 | 315 |
| 3 | -4 | 15 | 301 | 282 |
| 3 | -4 | 16 | 92 | -39 |
| 3 | -4 | 17 | 316 | 331 |
| 3 | -4 | 18 | 27 | -16 |
| 3 | -4 | 19 | 306 | 280 |
| 3 | -4 | 20 | 45 | -52 |
| 3 | -4 | 21 | 36 | 38 |
| 3 | -4 | 24 | 78 | -64 |
| 3 | -4 | 25 | 74 | 72 |
| 3 | -4 | 27 | 125 | 133 |
| 3 | 5 | 0 | 230 | 232 |
| 3 | 5 | 2 | 186 | 183 |
| 3 | 5 | 3 | 123 | 109 |
| 3 | 5 | 4 | 141 | 118 |
| 3 | 5 | 5 | 129 | 102 |
| 3 | 5 | 6 | 109 | 88 |
| 3 | 5 | 7 | 125 | 114 |
| 3 | 5 | 8 | 126 | 104 |
| 3 | 5 | 10 | 252 | 236 |
| 3 | 5 | 12 | 215 | 228 |
| 3 | 5 | 13 | 177 | 166 |
| 3 | 5 | 14 | 107 | 101 |
| 3 | 5 | 16 | 66 | 47 |
| 3 | 5 | 18 | 100 | 86 |
| 3 | 5 | 20 | 94 | 90 |
| 3 | 5 | 22 | 95 | 103 |
| 3 | -5 | 3 | 306 | -283 |
| 3 | -5 | 4 | 389 | 413 |
| 3 | -5 | 5 | 86 | 72 |
| 3 | -5 | 6 | 180 | 157 |
| 3 | -5 | 7 | 311 | 311 |
| 3 | -5 | 8 | 270 | 264 |
| 3 | -5 | 9 | 119 | 69 |
| 3 | -5 | 10 | 370 | 382 |
| 3 | -5 | 11 | 58 | 64 |
| 3 | -5 | 12 | 216 | 195 |
| 3 | -5 | 13 | 96 | 81 |
| 3 | -5 | 14 | 299 | 313 |
| 3 | -5 | 15 | 66 | -66 |
| 3 | -5 | 16 | 133 | 108 |
| 3 | -5 | 17 | 87 | -69 |
| 3 | -5 | 18 | 218 | 244 |
| 3 | -5 | 19 | 188 | 160 |
| 3 | -5 | 20 | 182 | 174 |
| 3 | -5 | 21 | 105 | 96 |
| 3 | -5 | 22 | 64 | 53 |
| 3 | -5 | 23 | 39 | -31 |
| 3 | -5 | 24 | 65 | 59 |
| 3 | -5 | 25 | 71 | -72 |
| 3 | 6 | 1 | 84 | 56 |
| 3 | 6 | 2 | 125 | -131 |
| 3 | 6 | 3 | 211 | 238 |
| 3 | 6 | 5 | 45 | 25 |
| 3 | 6 | 6 | 59 | 44 |
| 3 | 6 | 7 | 78 | 78 |
| 3 | 6 | 8 | 73 | 63 |
| 3 | 6 | 9 | 171 | 123 |
| 3 | 6 | 11 | 258 | 273 |
| 3 | 6 | 13 | 168 | 177 |
| 3 | 6 | 14 | 50 | -53 |
| 3 | 6 | 15 | 87 | 76 |
| 3 | 6 | 16 | 34 | -48 |
| 3 | 6 | 17 | 74 | 61 |
| 3 | 6 | 19 | 78 | 77 |
| 3 | -6 | 8 | 123 | -132 |
| 3 | -6 | 9 | 154 | 171 |
| 3 | -6 | 11 | 60 | 53 |
| 3 | -6 | 13 | 79 | 82 |
| 3 | -6 | 14 | 36 | 42 |
| 3 | -6 | 15 | 44 | 58 |
| 3 | -6 | 16 | 81 | -55 |
| 3 | -6 | 17 | 97 | -81 |
| 3 | -6 | 18 | 96 | -96 |
| 3 | -6 | 19 | 64 | 42 |
| 3 | -6 | 20 | 99 | 106 |
| 3 | -6 | 21 | 141 | 150 |
| 3 | 7 | 0 | 69 | -114 |
| 3 | 7 | 1 | 39 | 73 |
| 3 | 7 | 2 | 92 | 109 |
| 3 | 7 | 3 | 72 | -93 |
| 3 | 7 | 4 | 170 | 191 |
| 3 | 7 | 5 | 49 | -57 |
| 3 | 7 | 6 | 87 | 70 |
| 3 | 7 | 7 | 37 | 38 |
| 3 | 7 | 8 | 36 | 43 |
| 3 | 8 | 0 | 0 | 35 |
| 3 | 8 | 6 | 58 | -40 |
| 4 | 1 | 1 | 111 | -109 |
| 4 | 1 | 3 | 95 | -89 |
| 4 | 1 | 5 | 110 | -101 |
| 4 | 1 | 7 | 104 | -84 |
| 4 | 1 | 8 | 61 | -43 |
| 4 | 1 | 11 | 50 | -37 |
| 4 | 1 | 12 | 85 | 70 |
| 4 | 1 | 14 | 62 | 55 |
| 4 | 1 | 19 | 51 | -37 |
| 4 | 1 | 21 | 63 | -50 |
| 4 | -1 | 3 | 103 | 108 |
| 4 | -1 | 4 | 73 | 59 |
| 4 | -1 | 5 | 102 | 97 |
| 4 | -1 | 6 | 61 | 55 |
| 4 | -1 | 7 | 140 | 135 |
| 4 | -1 | 9 | 161 | 149 |
| 4 | -1 | 11 | 163 | 154 |
| 4 | -1 | 12 | 59 | 56 |
| 4 | -1 | 13 | 74 | 57 |
| 4 | -1 | 14 | 36 | 37 |
| 4 | -1 | 19 | 35 | 35 |
| 4 | 2 | 0 | 42 | -35 |
| 4 | 2 | 2 | 74 | -63 |
| 4 | 2 | 3 | 51 | 39 |
| 4 | 2 | 4 | 145 | -119 |
| 4 | 2 | 5 | 74 | 56 |
| 4 | 2 | 6 | 190 | -159 |
| 4 | 2 | 7 | 115 | 94 |
| 4 | 2 | 8 | 110 | -84 |
| 4 | 2 | 9 | 28 | 21 |
| 4 | 2 | 10 | 99 | -78 |
| 4 | 2 | 12 | 102 | -87 |
| 4 | 2 | 13 | 51 | -35 |
| 4 | 2 | 14 | 105 | -94 |
| 4 | 2 | 15 | 93 | -90 |
| 4 | 2 | 16 | 126 | -123 |
| 4 | 2 | 17 | 91 | -80 |
| 4 | 2 | 18 | 89 | -81 |
| 4 | 2 | 19 | 68 | -49 |
| 4 | 2 | 20 | 73 | -73 |
| 4 | 2 | 22 | 66 | -53 |
| 4 | -2 | 0 | 314 | 319 |
| 4 | -2 | 1 | 40 | 31 |
| 4 | -2 | 2 | 285 | 304 |
| 4 | -2 | 3 | 37 | 20 |
| 4 | -2 | 4 | 220 | 229 |
| 4 | -2 | 6 | 143 | 160 |
| 4 | -2 | 9 | 50 | -28 |
| 4 | -2 | 11 | 74 | 70 |
| 4 | -2 | 13 | 87 | 79 |
| 4 | -2 | 14 | 30 | 32 |
| 4 | -2 | 16 | 62 | 61 |
| 4 | -2 | 18 | 82 | 85 |
| 4 | -2 | 20 | 93 | 93 |
| 4 | -2 | 22 | 81 | 88 |
| 4 | -2 | 24 | 84 | 101 |
| 4 | -2 | 26 | 68 | 93 |
| 4 | -2 | 28 | 57 | 80 |
| 4 | 3 | 1 | 245 | -207 |
| 4 | 3 | 2 | 114 | -85 |
| 4 | 3 | 3 | 215 | -163 |
| 4 | 3 | 4 | 117 | -89 |
| 4 | 3 | 5 | 175 | -137 |
| 4 | 3 | 6 | 75 | -54 |
| 4 | 3 | 7 | 129 | -108 |
| 4 | 3 | 8 | 53 | -37 |
| 4 | 3 | 9 | 116 | -97 |
| 4 | 3 | 10 | 65 | -52 |
| 4 | 3 | 11 | 78 | -75 |
| 4 | 3 | 13 | 55 | -50 |
| 4 | 3 | 14 | 56 | -34 |
| 4 | 3 | 15 | 72 | -59 |
| 4 | 3 | 17 | 45 | -31 |
| 4 | 3 | 21 | 59 | -47 |
| 4 | 3 | 23 | 37 | -37 |
| 4 | -3 | 1 | 319 | 333 |
| 4 | -3 | 3 | 336 | 354 |
| 4 | -3 | 4 | 129 | -125 |
| 4 | -3 | 5 | 302 | 313 |
| 4 | -3 | 6 | 206 | -195 |
| 4 | -3 | 7 | 290 | 307 |
| 4 | -3 | 8 | 218 | -215 |
| 4 | -3 | 9 | 243 | 270 |
| 4 | -3 | 10 | 162 | -174 |
| 4 | -3 | 11 | 223 | 229 |
| 4 | -3 | 12 | 77 | -74 |

TABLE 4 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 4 | -3 | 13 | 223 | 243 |
| 4 | -3 | 14 | 51 | -41 |
| 4 | -3 | 15 | 171 | 186 |
| 4 | -3 | 17 | 130 | 145 |
| 4 | -3 | 19 | 132 | 138 |
| 4 | -3 | 21 | 99 | 100 |
| 4 | -3 | 23 | 90 | 89 |
| 4 | -3 | 25 | 83 | 92 |
| 4 | -3 | 27 | 58 | 56 |
| 4 | 4 | 0 | 165 | -150 |
| 4 | 4 | 2 | 126 | -98 |
| 4 | 4 | 4 | 105 | -74 |
| 4 | 4 | 6 | 96 | -68 |
| 4 | 4 | 8 | 69 | -52 |
| 4 | 4 | 10 | 43 | -46 |
| 4 | 4 | 12 | 51 | -34 |
| 4 | -4 | 2 | 323 | 307 |
| 4 | -4 | 3 | 68 | 26 |
| 4 | -4 | 4 | 444 | 443 |
| 4 | -4 | 6 | 438 | 458 |
| 4 | -4 | 7 | 41 | -32 |
| 4 | -4 | 8 | 327 | 386 |
| 4 | -4 | 10 | 284 | 328 |
| 4 | -4 | 12 | 270 | 319 |
| 4 | -4 | 14 | 235 | 285 |
| 4 | -4 | 16 | 231 | 277 |
| 4 | -4 | 18 | 215 | 268 |
| 4 | -4 | 20 | 156 | 175 |
| 4 | -4 | 22 | 78 | 82 |
| 4 | -4 | 24 | 59 | 70 |
| 4 | -4 | 26 | 61 | 69 |
| 4 | 5 | 1 | 36 | -33 |
| 4 | 5 | 4 | 36 | -31 |
| 4 | 5 | 5 | 51 | -38 |
| 4 | 5 | 6 | 36 | -25 |
| 4 | 5 | 7 | 45 | -33 |
| 4 | 5 | 9 | 86 | -62 |
| 4 | 5 | 11 | 115 | -92 |
| 4 | 5 | 13 | 109 | -92 |
| 4 | 5 | 15 | 67 | -54 |
| 4 | 5 | 17 | 49 | -41 |
| 4 | -5 | 3 | 257 | 261 |
| 4 | -5 | 4 | 124 | -87 |
| 4 | -5 | 5 | 263 | 331 |
| 4 | -5 | 7 | 279 | 322 |
| 4 | -5 | 8 | 96 | 88 |
| 4 | -5 | 9 | 291 | 334 |
| 4 | -5 | 11 | 288 | 392 |
| 4 | -5 | 13 | 295 | 351 |
| 4 | -5 | 14 | 106 | -85 |
| 4 | -5 | 15 | 213 | 264 |
| 4 | -5 | 16 | 73 | -72 |
| 4 | -5 | 17 | 205 | 250 |
| 4 | -5 | 19 | 155 | 173 |
| 4 | -5 | 20 | 52 | 55 |
| 4 | -5 | 21 | 89 | 81 |
| 4 | -5 | 23 | 57 | 54 |
| 4 | 6 | 0 | 71 | -53 |
| 4 | 6 | 2 | 79 | -53 |
| 4 | 6 | 4 | 83 | -63 |
| 4 | 6 | 6 | 70 | -38 |
| 4 | 6 | 8 | 72 | -44 |
| 4 | 6 | 10 | 103 | -77 |
| 4 | 6 | 12 | 97 | -81 |
| 4 | 6 | 14 | 67 | -55 |
| 4 | 6 | 16 | 35 | -24 |
| 4 | -6 | 7 | 149 | 145 |
| 4 | -6 | 8 | 129 | 122 |
| 4 | -6 | 9 | 82 | 78 |
| 4 | -6 | 10 | 139 | 147 |
| 4 | -6 | 11 | 45 | 46 |
| 4 | -6 | 12 | 131 | 133 |
| 4 | -6 | 13 | 36 | 48 |
| 4 | -6 | 14 | 56 | 52 |
| 4 | 7 | 1 | 29 | -17 |
| 4 | 7 | 3 | 54 | -46 |
| 4 | 7 | 5 | 69 | -71 |
| 4 | 7 | 7 | 53 | -53 |
| 5 | 0 | 10 | 39 | 45 |
| 5 | 0 | 11 | 47 | -37 |
| 5 | 0 | 12 | 44 | 47 |
| 5 | 0 | 13 | 46 | -44 |
| 5 | 0 | 14 | 59 | 9 |
| 5 | 0 | 15 | 50 | -42 |
| 5 | 0 | 16 | 46 | 44 |
| 5 | 1 | 0 | 72 | 87 |
| 5 | 1 | 2 | 84 | 90 |
| 5 | 1 | 4 | 113 | 122 |
| 5 | 1 | 5 | 23 | 19 |
| 5 | 1 | 6 | 82 | 81 |
| 5 | 1 | 7 | 55 | 49 |
| 5 | 1 | 8 | 27 | 37 |
| 5 | 1 | 9 | 28 | -29 |
| 5 | 1 | 11 | 77 | -66 |
| 5 | 1 | 12 | 33 | -30 |
| 5 | 1 | 13 | 81 | -77 |
| 5 | -1 | 3 | 51 | -45 |
| 5 | -1 | 4 | 67 | -84 |
| 5 | -1 | 5 | 62 | -69 |
| 5 | -1 | 6 | 87 | 102 |
| 5 | -1 | 7 | 32 | -38 |
| 5 | -1 | 8 | 47 | -81 |
| 5 | -1 | 10 | 92 | -103 |
| 5 | -1 | 11 | 49 | -45 |
| 5 | -1 | 12 | 101 | -103 |
| 5 | -1 | 14 | 41 | -39 |
| 5 | 2 | 1 | 84 | 80 |
| 5 | 2 | 3 | 133 | 117 |
| 5 | 2 | 4 | 39 | -43 |
| 5 | 2 | 5 | 151 | 142 |
| 5 | 2 | 6 | 95 | -88 |
| 5 | 2 | 7 | 91 | 87 |
| 5 | 2 | 8 | 59 | -50 |
| 5 | 2 | 9 | 100 | 92 |
| 5 | 2 | 11 | 99 | 86 |
| 5 | 2 | 12 | 45 | 36 |
| 5 | 2 | 13 | 121 | 120 |
| 5 | 2 | 14 | 115 | 113 |
| 5 | 2 | 15 | 150 | 176 |
| 5 | 2 | 16 | 117 | 116 |
| 5 | 2 | 17 | 96 | 111 |
| 5 | 2 | 18 | 59 | 56 |
| 5 | 2 | 19 | 82 | 91 |
| 5 | 2 | 20 | 40 | 47 |
| 5 | 2 | 21 | 63 | 76 |
| 5 | 2 | 23 | 46 | 56 |
| 5 | 2 | 25 | 46 | 54 |
| 5 | 2 | 27 | 42 | 49 |
| 5 | -2 | 1 | 218 | -231 |
| 5 | -2 | 2 | 66 | -57 |
| 5 | -2 | 3 | 149 | -168 |
| 5 | -2 | 4 | 59 | -51 |
| 5 | -2 | 5 | 135 | -149 |
| 5 | -2 | 6 | 59 | -65 |
| 5 | -2 | 7 | 79 | -91 |
| 5 | -2 | 8 | 25 | -23 |
| 5 | -2 | 11 | 47 | -42 |
| 5 | -2 | 12 | 50 | -47 |
| 5 | -2 | 13 | 58 | -55 |
| 5 | -2 | 15 | 45 | -46 |
| 5 | -2 | 17 | 67 | -58 |
| 5 | -2 | 19 | 70 | -68 |
| 5 | -2 | 21 | 41 | -49 |
| 5 | -2 | 23 | 63 | -73 |
| 5 | -2 | 25 | 72 | -78 |
| 5 | 3 | 0 | 274 | 266 |
| 5 | 3 | 1 | 65 | 54 |
| 5 | 3 | 2 | 264 | 249 |
| 5 | 3 | 3 | 140 | 121 |
| 5 | 3 | 4 | 212 | 211 |
| 5 | 3 | 5 | 136 | 105 |
| 5 | 3 | 6 | 178 | 178 |
| 5 | 3 | 7 | 122 | 106 |
| 5 | 3 | 8 | 175 | 182 |
| 5 | 3 | 9 | 138 | 90 |
| 5 | 3 | 12 | 118 | 105 |
| 5 | 3 | 13 | 49 | 48 |
| 5 | 3 | 14 | 111 | 95 |
| 5 | 3 | 17 | 59 | -76 |
| 5 | 3 | 19 | 56 | -69 |
| 5 | 3 | 20 | 47 | 41 |
| 5 | 3 | 21 | 46 | -53 |
| 5 | 3 | 22 | 50 | 43 |
| 5 | -3 | 0 | 269 | -298 |
| 5 | -3 | 1 | 49 | -34 |
| 5 | -3 | 2 | 278 | -304 |
| 5 | -3 | 4 | 254 | -257 |
| 5 | -3 | 5 | 87 | 76 |
| 5 | -3 | 6 | 207 | -226 |
| 5 | -3 | 7 | 90 | 90 |
| 5 | -3 | 8 | 163 | -178 |
| 5 | -3 | 9 | 104 | 100 |
| 5 | -3 | 10 | 128 | -137 |
| 5 | -3 | 11 | 33 | 34 |
| 5 | -3 | 12 | 103 | -116 |
| 5 | -3 | 14 | 104 | -104 |
| 5 | -3 | 16 | 104 | -100 |
| 5 | -3 | 18 | 87 | -86 |
| 5 | -3 | 20 | 77 | -75 |
| 5 | -3 | 22 | 63 | -60 |
| 5 | -3 | 24 | 63 | -65 |
| 5 | -3 | 26 | 49 | -51 |
| 5 | 4 | 1 | 166 | 159 |
| 5 | 4 | 3 | 138 | 123 |
| 5 | 4 | 5 | 114 | 106 |
| 5 | 4 | 7 | 105 | 90 |
| 5 | 4 | 9 | 86 | 80 |
| 5 | 4 | 11 | 82 | 75 |
| 5 | 4 | 13 | 72 | 57 |
| 5 | 4 | 15 | 58 | 49 |
| 5 | 4 | 16 | 49 | -47 |
| 5 | 4 | 17 | 73 | 65 |
| 5 | 4 | 19 | 77 | 76 |
| 5 | 4 | 21 | 78 | 94 |
| 5 | 4 | 23 | 66 | 72 |
| 5 | -4 | 1 | 90 | -98 |
| 5 | -4 | 2 | 36 | -29 |
| 5 | -4 | 3 | 214 | -208 |
| 5 | -4 | 5 | 250 | -262 |
| 5 | -4 | 7 | 240 | -240 |
| 5 | -4 | 9 | 182 | -180 |
| 5 | -4 | 11 | 144 | -153 |
| 5 | -4 | 13 | 139 | -150 |
| 5 | -4 | 15 | 110 | -118 |
| 5 | -4 | 17 | 137 | -152 |
| 5 | -4 | 19 | 116 | -127 |
| 5 | -4 | 21 | 55 | -64 |
| 5 | 5 | 6 | 50 | 40 |
| 5 | 5 | 8 | 109 | 87 |
| 5 | 5 | 10 | 152 | 155 |
| 5 | 5 | 12 | 174 | 176 |
| 5 | 5 | 14 | 127 | 130 |
| 5 | 5 | 16 | 99 | 92 |
| 5 | 5 | 18 | 62 | 56 |
| 5 | 5 | 20 | 51 | 46 |
| 5 | -5 | 3 | 112 | 91 |
| 5 | -5 | 4 | 122 | -133 |
| 5 | -5 | 5 | 96 | 70 |
| 5 | -5 | 6 | 116 | -127 |
| 5 | -5 | 8 | 89 | -101 |
| 5 | -5 | 10 | 100 | -121 |
| 5 | -5 | 12 | 140 | -159 |
| 5 | -5 | 14 | 88 | -104 |
| 5 | -5 | 15 | 59 | 56 |
| 5 | -5 | 16 | 65 | -69 |
| 5 | -5 | 18 | 116 | -112 |
| 5 | -5 | 20 | 74 | -64 |
| 5 | 6 | 1 | 114 | 98 |
| 5 | 6 | 2 | 39 | -52 |
| 5 | 6 | 3 | 134 | 128 |
| 5 | 6 | 4 | 90 | -91 |
| 5 | 6 | 5 | 121 | 93 |
| 5 | 6 | 7 | 123 | 94 |
| 5 | 6 | 9 | 132 | 112 |
| 5 | 6 | 11 | 131 | 122 |
| 5 | 6 | 13 | 107 | 104 |
| 5 | 6 | 15 | 79 | 67 |
| 5 | 6 | 17 | 61 | 54 |
| 5 | -6 | 6 | 64 | -66 |
| 5 | -6 | 8 | 41 | -44 |
| 5 | -6 | 9 | 41 | -48 |
| 5 | -6 | 11 | 88 | -90 |
| 5 | -6 | 13 | 76 | -66 |
| 5 | -6 | 16 | 66 | 54 |
| 5 | 7 | 0 | 148 | 105 |
| 5 | 7 | 2 | 157 | 124 |
| 5 | 7 | 4 | 168 | 175 |
| 5 | 7 | 6 | 169 | 179 |
| 5 | 7 | 8 | 133 | 111 |
| 5 | 7 | 10 | 74 | 50 |
| 6 | 0 | 0 | 128 | -71 |
| 6 | 0 | 1 | 235 | -256 |
| 6 | 0 | 2 | 316 | -225 |
| 6 | 0 | 5 | 494 | -602 |
| 6 | 0 | 6 | 107 | 153 |
| 6 | 0 | 7 | 103 | 89 |
| 6 | 0 | 8 | 245 | 242 |
| 6 | 0 | 9 | 454 | 431 |
| 6 | 0 | 10 | 647 | 779 |
| 6 | 0 | 11 | 91 | -63 |
| 6 | 0 | 12 | 691 | 772 |
| 6 | 0 | 13 | 143 | -156 |
| 6 | 0 | 14 | 483 | 533 |
| 6 | 0 | 15 | 281 | -253 |
| 6 | 0 | 16 | 237 | 282 |
| 6 | 0 | 17 | 211 | 205 |
| 6 | 0 | 18 | 346 | 330 |
| 6 | 0 | 19 | 125 | 112 |
| 6 | 0 | 20 | 170 | 165 |
| 6 | 0 | 22 | 200 | 102 |
| 6 | 0 | 23 | 109 | 46 |
| 6 | 0 | 24 | 144 | 87 |
| 6 | 0 | 26 | 174 | 45 |
| 6 | 0 | 28 | 151 | 29 |
| 6 | 1 | 1 | 702 | 738 |
| 6 | 1 | 2 | 125 | -119 |
| 6 | 1 | 3 | 692 | 771 |
| 6 | 1 | 4 | 43 | 31 |
| 6 | 1 | 5 | 817 | 966 |
| 6 | 1 | 6 | 415 | -413 |
| 6 | 1 | 7 | 834 | 974 |
| 6 | 1 | 8 | 298 | 281 |
| 6 | 1 | 9 | 125 | -81 |
| 6 | 1 | 10 | 374 | 364 |
| 6 | 1 | 11 | 214 | 229 |
| 6 | 1 | 12 | 75 | -95 |
| 6 | 1 | 14 | 178 | -168 |
| 6 | 1 | 15 | 184 | 181 |
| 6 | 1 | 16 | 253 | 207 |
| 6 | 1 | 17 | 509 | 492 |
| 6 | 1 | 18 | 255 | 168 |
| 6 | 1 | 19 | 176 | 182 |
| 6 | 1 | 21 | 206 | 189 |
| 6 | 1 | 22 | 116 | 101 |
| 6 | 1 | 23 | 155 | 150 |
| 6 | 1 | 25 | 178 | 175 |
| 6 | 1 | 27 | 161 | 186 |
| 6 | 1 | 28 | 54 | -70 |
| 6 | -1 | 3 | 272 | 396 |
| 6 | -1 | 4 | 297 | 321 |
| 6 | -1 | 5 | 313 | 351 |
| 6 | -1 | 6 | 66 | -34 |
| 6 | -1 | 7 | 182 | -90 |
| 6 | -1 | 8 | 201 | -171 |
| 6 | -1 | 9 | 436 | 499 |
| 6 | -1 | 10 | 225 | 169 |
| 6 | -1 | 11 | 522 | 546 |
| 6 | -1 | 12 | 149 | -142 |
| 6 | -1 | 13 | 415 | 443 |
| 6 | -1 | 14 | 76 | -73 |
| 6 | -1 | 15 | 124 | 139 |
| 6 | -1 | 16 | 83 | 84 |
| 6 | -1 | 17 | 70 | 77 |
| 6 | -1 | 18 | 108 | -113 |
| 6 | -1 | 19 | 253 | 247 |
| 6 | -1 | 20 | 64 | -70 |
| 6 | -1 | 21 | 123 | 130 |
| 6 | -1 | 23 | 124 | 120 |
| 6 | -1 | 25 | 69 | 87 |
| 6 | -1 | 27 | 86 | 74 |
| 6 | -1 | 28 | 34 | 31 |
| 6 | 2 | 0 | 645 | 594 |
| 6 | 2 | 1 | 222 | 196 |
| 6 | 2 | 2 | 707 | 767 |
| 6 | 2 | 3 | 64 | 54 |
| 6 | 2 | 4 | 596 | 614 |
| 6 | 2 | 5 | 149 | -106 |
| 6 | 2 | 6 | 708 | 803 |
| 6 | 2 | 7 | 576 | -594 |
| 6 | 2 | 8 | 644 | 695 |
| 6 | 2 | 9 | 217 | -218 |
| 6 | 2 | 10 | 239 | 215 |
| 6 | 2 | 12 | 279 | 239 |
| 6 | 2 | 13 | 198 | -201 |
| 6 | 2 | 14 | 338 | 305 |
| 6 | 2 | 15 | 340 | 291 |
| 6 | 2 | 16 | 454 | 448 |
| 6 | 2 | 17 | 160 | 132 |
| 6 | 2 | 18 | 172 | 204 |
| 6 | 2 | 20 | 216 | 216 |
| 6 | 2 | 22 | 185 | 204 |
| 6 | 2 | 23 | 59 | 71 |
| 6 | 2 | 24 | 177 | 158 |
| 6 | 2 | 25 | 136 | 117 |
| 6 | 2 | 26 | 161 | 153 |
| 6 | 2 | 27 | 48 | 32 |
| 6 | -2 | 0 | 646 | 928 |
| 6 | -2 | 1 | 132 | -113 |
| 6 | -2 | 2 | 388 | 486 |
| 6 | -2 | 3 | 303 | 270 |
| 6 | -2 | 4 | 330 | 394 |
| 6 | -2 | 5 | 349 | 330 |
| 6 | -2 | 6 | 620 | 662 |
| 6 | -2 | 7 | 48 | 41 |
| 6 | -2 | 8 | 222 | 270 |
| 6 | -2 | 9 | 138 | 111 |
| 6 | -2 | 10 | 398 | 442 |
| 6 | -2 | 11 | 194 | 148 |
| 6 | -2 | 12 | 467 | 485 |
| 6 | -2 | 13 | 53 | -57 |
| 6 | -2 | 14 | 137 | 163 |
| 6 | -2 | 15 | 41 | 29 |
| 6 | -2 | 16 | 238 | 255 |
| 6 | -2 | 17 | 123 | -127 |
| 6 | -2 | 18 | 326 | 310 |
| 6 | -2 | 19 | 159 | -172 |
| 6 | -2 | 20 | 166 | 186 |
| 6 | -2 | 22 | 252 | 274 |
| 6 | -2 | 24 | 185 | 200 |
| 6 | -2 | 25 | 55 | -59 |
| 6 | -2 | 26 | 75 | 85 |
| 6 | -2 | 27 | 32 | 17 |
| 6 | -2 | 28 | 138 | 128 |
| 6 | 3 | 1 | 691 | 624 |
| 6 | 3 | 2 | 334 | 289 |
| 6 | 3 | 3 | 299 | 232 |
| 6 | 3 | 4 | 298 | 215 |
| 6 | 3 | 5 | 345 | 321 |
| 6 | 3 | 6 | 350 | 271 |
| 6 | 3 | 7 | 383 | 347 |
| 6 | 3 | 8 | 137 | 82 |
| 6 | 3 | 9 | 461 | 443 |
| 6 | 3 | 10 | 151 | 109 |
| 6 | 3 | 11 | 341 | 320 |
| 6 | 3 | 12 | 26 | 19 |
| 6 | 3 | 13 | 423 | 375 |
| 6 | 3 | 15 | 381 | 341 |
| 6 | 3 | 16 | 120 | -96 |
| 6 | 3 | 17 | 217 | 194 |
| 6 | 3 | 18 | 144 | -173 |
| 6 | 3 | 19 | 187 | 155 |
| 6 | 3 | 20 | 101 | -140 |
| 6 | 3 | 21 | 176 | 197 |
| 6 | 3 | 22 | 95 | -125 |
| 6 | 3 | 23 | 249 | 262 |
| 6 | 3 | 25 | 112 | 111 |
| 6 | -3 | 1 | 943 | 1172 |
| 6 | -3 | 2 | 296 | 341 |
| 6 | -3 | 3 | 525 | 571 |
| 6 | -3 | 4 | 61 | 47 |
| 6 | -3 | 5 | 682 | 741 |
| 6 | -3 | 6 | 217 | -167 |
| 6 | -3 | 7 | 417 | 440 |
| 6 | -3 | 8 | 203 | -142 |
| 6 | -3 | 9 | 360 | 403 |
| 6 | -3 | 10 | 10 | -99 |
| 6 | -3 | 11 | 269 | 277 |
| 6 | -3 | 13 | 250 | 271 |
| 6 | -3 | 14 | 75 | 64 |
| 6 | -3 | 15 | 245 | 213 |
| 6 | -3 | 17 | 194 | 199 |
| 6 | -3 | 19 | 170 | 165 |
| 6 | -3 | 20 | 91 | -82 |
| 6 | -3 | 21 | 173 | 186 |
| 6 | -3 | 23 | 264 | 316 |
| 6 | -3 | 24 | 102 | 96 |
| 6 | -3 | 25 | 139 | 162 |
| 6 | -3 | 27 | 111 | 133 |
| 6 | 4 | 0 | 482 | 448 |
| 6 | 4 | 1 | 94 | -89 |
| 6 | 4 | 2 | 247 | 196 |
| 6 | 4 | 4 | 224 | 194 |
| 6 | 4 | 5 | 63 | 63 |
| 6 | 4 | 6 | 281 | 284 |
| 6 | 4 | 8 | 201 | 172 |
| 6 | 4 | 9 | 58 | 36 |
| 6 | 4 | 10 | 224 | 217 |
| 6 | 4 | 12 | 232 | 234 |
| 6 | 4 | 14 | 118 | 100 |
| 6 | 4 | 16 | 124 | 121 |
| 6 | 4 | 18 | 154 | 132 |
| 6 | 4 | 19 | 61 | -66 |
| 6 | 4 | 20 | 58 | 60 |
| 6 | 4 | 22 | 132 | 122 |
| 6 | -4 | 0 | 98 | 136 |
| 6 | -4 | 1 | 289 | 307 |
| 6 | -4 | 2 | 237 | 240 |
| 6 | -4 | 3 | 154 | 86 |
| 6 | -4 | 4 | 515 | 512 |
| 6 | -4 | 6 | 580 | 577 |
| 6 | -4 | 7 | 196 | -207 |
| 6 | -4 | 8 | 484 | 466 |
| 6 | -4 | 9 | 44 | 40 |
| 6 | -4 | 10 | 313 | 273 |
| 6 | -4 | 11 | 176 | 144 |
| 6 | -4 | 12 | 186 | 206 |
| 6 | -4 | 13 | 121 | -118 |
| 6 | -4 | 14 | 336 | 337 |
| 6 | -4 | 15 | 245 | 263 |
| 6 | -4 | 16 | 332 | 340 |
| 6 | -4 | 17 | 166 | 132 |
| 6 | -4 | 18 | 220 | 256 |
| 6 | -4 | 20 | 120 | 131 |
| 6 | -4 | 21 | 70 | -51 |
| 6 | -4 | 22 | 48 | 43 |
| 6 | -4 | 23 | 39 | 27 |
| 6 | -4 | 24 | 58 | 43 |
| 6 | -4 | 25 | 84 | 83 |
| 6 | -4 | 26 | 76 | 85 |
| 6 | 5 | 1 | 59 | 72 |
| 6 | 5 | 2 | 53 | -56 |
| 6 | 5 | 3 | 74 | 78 |
| 6 | 5 | 5 | 74 | 55 |
| 6 | 5 | 6 | 82 | -60 |
| 6 | 5 | 7 | 82 | 56 |
| 6 | 5 | 8 | 85 | -82 |
| 6 | 5 | 9 | 171 | 168 |
| 6 | 5 | 11 | 210 | 205 |
| 6 | 5 | 12 | 68 | -78 |
| 6 | 5 | 13 | 156 | 167 |
| 6 | 5 | 15 | 95 | 82 |
| 6 | 5 | 16 | 85 | 85 |
| 6 | 5 | 17 | 58 | 52 |
| 6 | 5 | 19 | 82 | 84 |
| 6 | 5 | 20 | 48 | 19 |
| 6 | -5 | 2 | 174 | -139 |
| 6 | -5 | 3 | 175 | 187 |
| 6 | -5 | 4 | 270 | -211 |
| 6 | -5 | 5 | 253 | 249 |
| 6 | -5 | 6 | 248 | -207 |
| 6 | -5 | 7 | 261 | 302 |
| 6 | -5 | 9 | 104 | -91 |
| 6 | -5 | 10 | 194 | 207 |
| 6 | -5 | 11 | 237 | 286 |
| 6 | -5 | 12 | 177 | -185 |
| 6 | -5 | 13 | 45 | 67 |
| 6 | -5 | 14 | 203 | -167 |
| 6 | -5 | 15 | 59 | 49 |
| 6 | -5 | 16 | 141 | 129 |
| 6 | -5 | 17 | 297 | 299 |
| 6 | -5 | 18 | 119 | 114 |
| 6 | -5 | 19 | 125 | 136 |
| 6 | -5 | 20 | 91 | 96 |
| 6 | -5 | 21 | 104 | 105 |
| 6 | -5 | 22 | 72 | 75 |
| 6 | -5 | 23 | 32 | 21 |
| 6 | -5 | 24 | 48 | 37 |
| 6 | -5 | 25 | 82 | 64 |
| 6 | 6 | 0 | 132 | 126 |
| 6 | 6 | 2 | 95 | 68 |
| 6 | 6 | 3 | 53 | -46 |
| 6 | 6 | 4 | 96 | 108 |
| 6 | 6 | 5 | 98 | -107 |
| 6 | 6 | 6 | 72 | 57 |
| 6 | 6 | 8 | 79 | 64 |
| 6 | 6 | 9 | 80 | 99 |
| 6 | 6 | 10 | 85 | 86 |
| 6 | 6 | 12 | 68 | 45 |
| 6 | 6 | 13 | 59 | -70 |
| 6 | 6 | 14 | 86 | 94 |

TABLE 4 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 6 | 6 | 16 | 35 | 33 |
| 6 | -6 | 6 | 63 | 61 |
| 6 | -6 | 7 | 176 | 147 |
| 6 | -6 | 8 | 79 | -71 |
| 6 | -6 | 9 | 168 | 175 |
| 6 | -6 | 10 | 182 | 177 |
| 6 | -6 | 12 | 257 | 286 |
| 6 | -6 | 14 | 68 | -59 |
| 6 | -6 | 15 | 162 | -160 |
| 6 | -6 | 16 | 48 | -36 |
| 6 | -6 | 19 | 52 | -36 |
| 6 | 7 | 1 | 80 | 72 |
| 6 | 7 | 3 | 55 | 27 |
| 6 | 7 | 5 | 107 | 119 |
| 6 | 7 | 7 | 120 | 139 |
| 7 | 0 | 5 | 55 | 63 |
| 7 | 0 | 7 | 63 | 82 |
| 7 | 0 | 9 | 75 | 80 |
| 7 | 0 | 11 | 83 | 86 |
| 7 | 0 | 12 | 78 | -63 |
| 7 | 0 | 15 | 83 | 77 |
| 7 | 1 | 5 | 30 | -31 |
| 7 | 1 | 7 | 54 | -56 |
| 7 | 1 | 8 | 62 | -55 |
| 7 | 2 | 1 | 113 | -107 |
| 7 | 2 | 3 | 112 | -113 |
| 7 | 2 | 5 | 92 | -88 |
| 7 | 2 | 7 | 56 | -53 |
| 7 | 2 | 10 | 53 | 67 |
| 7 | 3 | 0 | 67 | -63 |
| 7 | 3 | 2 | 74 | -67 |
| 7 | 3 | 4 | 43 | -30 |
| 7 | 3 | 6 | 77 | -61 |
| 7 | 3 | 8 | 107 | -101 |
| 7 | 3 | 10 | 124 | -126 |
| 7 | 3 | 12 | 127 | -140 |
| 7 | 3 | 13 | 59 | -64 |
| 7 | 3 | 14 | 103 | -104 |
| 7 | 3 | 16 | 59 | -72 |
| 7 | 3 | 18 | 46 | -52 |
| 7 | 4 | 1 | 106 | -108 |
| 7 | 4 | 3 | 101 | -105 |
| 7 | 4 | 5 | 96 | -83 |
| 7 | 4 | 6 | 47 | -49 |
| 7 | 4 | 7 | 91 | -86 |
| 7 | 4 | 9 | 91 | -78 |
| 7 | 4 | 11 | 90 | -88 |
| 7 | 4 | 13 | 81 | -64 |
| 7 | 4 | 15 | 45 | -34 |
| 7 | -1 | 4 | 54 | 58 |
| 7 | -1 | 5 | 46 | -32 |
| 7 | -1 | 6 | 43 | 50 |
| 7 | -1 | 8 | 120 | 133 |
| 7 | -1 | 9 | 38 | 39 |
| 7 | -1 | 10 | 145 | 156 |
| 7 | -1 | 12 | 113 | 116 |
| 7 | -1 | 14 | 72 | 73 |
| 7 | -1 | 16 | 64 | 61 |
| 7 | -1 | 18 | 67 | 69 |
| 7 | -1 | 20 | 60 | 63 |
| 7 | -1 | 22 | 58 | 60 |
| 7 | -2 | 1 | 216 | 246 |
| 7 | -2 | 2 | 41 | 31 |
| 7 | -2 | 3 | 223 | 235 |
| 7 | -2 | 4 | 112 | 104 |
| 7 | -2 | 5 | 214 | 215 |
| 7 | -2 | 6 | 38 | 30 |
| 7 | -2 | 7 | 201 | 211 |
| 7 | -2 | 8 | 38 | 35 |
| 7 | -2 | 9 | 239 | 254 |
| 7 | -2 | 10 | 35 | 25 |
| 7 | -2 | 11 | 196 | 222 |
| 7 | -2 | 12 | 38 | -47 |
| 7 | -2 | 13 | 183 | 191 |
| 7 | -2 | 14 | 51 | -56 |
| 7 | -2 | 15 | 152 | 166 |
| 7 | -2 | 16 | 79 | -88 |
| 7 | -2 | 17 | 151 | 150 |
| 7 | -2 | 18 | 117 | -122 |
| 7 | -2 | 19 | 113 | 106 |
| 7 | -2 | 20 | 60 | -73 |
| 7 | -2 | 21 | 102 | 89 |
| 7 | -2 | 23 | 91 | 76 |
| 7 | -2 | 25 | 70 | 63 |
| 7 | -2 | 27 | 65 | 59 |
| 7 | -3 | 0 | 600 | 687 |
| 7 | -3 | 1 | 46 | 32 |
| 7 | -3 | 2 | 499 | 574 |
| 7 | -3 | 3 | 110 | 92 |
| 7 | -3 | 4 | 405 | 440 |
| 7 | -3 | 5 | 83 | 71 |
| 7 | -3 | 6 | 302 | 351 |
| 7 | -3 | 8 | 277 | 283 |
| 7 | -3 | 10 | 221 | 230 |
| 7 | -3 | 12 | 172 | 164 |
| 7 | -3 | 14 | 174 | 147 |
| 7 | -3 | 16 | 178 | 151 |
| 7 | -3 | 18 | 128 | 122 |
| 7 | -3 | 20 | 136 | 133 |
| 7 | -3 | 22 | 165 | 176 |
| 7 | -3 | 24 | 130 | 139 |
| 7 | -3 | 26 | 94 | 105 |
| 7 | -4 | 1 | 263 | 280 |
| 7 | -4 | 2 | 98 | 66 |
| 7 | -4 | 3 | 292 | 314 |
| 7 | -4 | 5 | 338 | 362 |
| 7 | -4 | 6 | 116 | -103 |
| 7 | -4 | 7 | 361 | 380 |
| 7 | -4 | 8 | 109 | -107 |
| 7 | -4 | 9 | 301 | 317 |
| 7 | -4 | 10 | 51 | -59 |
| 7 | -4 | 11 | 201 | 189 |
| 7 | -4 | 13 | 202 | 201 |
| 7 | -4 | 14 | 33 | 32 |
| 7 | -4 | 15 | 238 | 254 |
| 7 | -4 | 16 | 68 | 46 |
| 7 | -4 | 17 | 222 | 225 |
| 7 | -4 | 19 | 175 | 170 |
| 7 | -4 | 21 | 149 | 140 |
| 7 | -4 | 23 | 110 | 104 |
| 7 | -4 | 24 | 59 | 62 |
| 7 | -4 | 25 | 71 | 75 |
| 7 | -5 | 2 | 262 | 244 |
| 7 | -5 | 3 | 217 | -188 |
| 7 | -5 | 4 | 310 | 307 |
| 7 | -5 | 5 | 265 | -232 |
| 7 | -5 | 6 | 293 | 310 |
| 7 | -5 | 7 | 182 | -170 |
| 7 | -5 | 8 | 239 | 238 |
| 7 | -5 | 10 | 147 | 143 |
| 7 | -5 | 12 | 89 | 88 |
| 7 | -5 | 13 | 84 | -66 |
| 7 | -5 | 14 | 149 | 142 |
| 7 | -5 | 15 | 49 | 53 |
| 7 | -5 | 16 | 170 | 170 |
| 7 | -5 | 17 | 100 | 114 |
| 7 | -5 | 18 | 113 | 114 |
| 7 | -5 | 19 | 90 | 112 |
| 7 | -5 | 20 | 68 | 53 |
| 7 | -5 | 21 | 95 | 95 |
| 7 | -5 | 22 | 38 | 33 |
| 7 | -5 | 24 | 64 | 58 |
| 7 | -6 | 5 | 82 | 77 |
| 7 | -6 | 6 | 158 | 130 |
| 7 | -6 | 7 | 96 | 79 |
| 7 | -6 | 8 | 229 | 201 |
| 7 | -6 | 9 | 196 | 171 |
| 7 | -6 | 10 | 161 | 152 |
| 7 | -6 | 11 | 254 | 263 |
| 7 | -6 | 13 | 197 | 194 |
| 7 | -6 | 14 | 81 | -72 |
| 7 | -6 | 15 | 149 | 148 |
| 7 | -6 | 17 | 129 | 120 |
| 7 | -6 | 19 | 91 | 94 |
| 7 | -6 | 22 | 70 | -57 |
| 8 | 0 | 0 | 43 | -72 |
| 8 | 0 | 1 | 80 | -24 |
| 8 | 0 | 2 | 82 | -82 |
| 8 | 0 | 4 | 88 | -68 |
| 8 | 0 | 8 | 82 | -76 |
| 8 | 0 | 10 | 64 | -53 |
| 8 | 2 | 0 | 121 | 109 |
| 8 | 2 | 2 | 118 | 108 |
| 8 | 2 | 4 | 84 | 74 |
| 8 | 2 | 6 | 61 | 48 |
| 8 | 3 | 1 | 82 | 65 |
| 8 | 3 | 5 | 84 | 66 |
| 8 | 3 | 6 | 63 | 47 |
| 8 | 3 | 7 | 131 | 105 |
| 8 | 3 | 9 | 152 | 157 |
| 8 | 3 | 10 | 66 | 78 |
| 8 | 3 | 11 | 183 | 204 |
| 8 | 3 | 12 | 103 | 92 |
| 8 | 3 | 13 | 151 | 165 |
| 8 | 3 | 15 | 105 | 114 |
| 8 | 3 | 17 | 88 | 94 |
| 8 | 3 | 19 | 72 | 70 |
| 8 | 3 | 21 | 55 | 55 |
| 8 | 4 | 0 | 173 | 173 |
| 8 | 4 | 2 | 173 | 163 |
| 8 | 4 | 4 | 157 | 161 |
| 8 | 4 | 6 | 152 | 140 |
| 8 | 4 | 8 | 142 | 127 |
| 8 | 4 | 10 | 131 | 126 |
| 8 | 4 | 12 | 98 | 85 |
| 8 | 4 | 14 | 60 | 55 |
| 8 | 4 | 16 | 56 | 40 |
| 8 | 4 | 18 | 59 | 49 |
| 8 | 4 | 20 | 51 | 48 |
| 8 | 5 | 1 | 128 | 94 |
| 8 | 5 | 3 | 102 | 85 |
| 8 | 5 | 4 | 80 | -77 |
| 8 | 5 | 5 | 88 | 66 |
| 8 | 5 | 6 | 96 | -90 |
| 8 | 5 | 7 | 72 | 47 |
| 8 | 5 | 8 | 76 | -72 |
| 8 | 5 | 9 | 79 | 64 |
| 8 | 5 | 10 | 63 | -52 |
| 8 | 5 | 11 | 61 | 61 |
| 8 | 5 | 13 | 65 | 73 |
| 8 | 5 | 15 | 53 | 65 |
| 8 | 5 | 17 | 48 | 53 |
| 8 | 6 | 0 | 86 | 82 |
| 8 | 6 | 2 | 79 | 63 |
| 8 | 6 | 4 | 67 | 63 |
| 8 | 6 | 6 | 74 | 76 |
| 8 | 6 | 8 | 60 | 53 |
| 8 | 6 | 10 | 40 | 32 |
| 8 | -1 | 3 | 71 | -86 |
| 8 | -1 | 5 | 45 | -45 |
| 8 | -1 | 7 | 86 | -83 |
| 8 | -1 | 9 | 125 | -123 |
| 8 | -1 | 11 | 110 | -108 |
| 8 | -1 | 13 | 76 | -80 |
| 8 | -1 | 15 | 82 | -76 |
| 8 | -1 | 17 | 58 | -57 |
| 8 | -1 | 21 | 65 | -61 |
| 8 | -2 | 0 | 153 | -159 |
| 8 | -2 | 2 | 168 | -183 |
| 8 | -2 | 4 | 138 | -150 |
| 8 | -2 | 6 | 134 | -140 |
| 8 | -2 | 8 | 166 | -186 |
| 8 | -2 | 10 | 178 | -182 |
| 8 | -2 | 12 | 152 | -166 |
| 8 | -2 | 14 | 128 | -133 |
| 8 | -2 | 16 | 106 | -103 |
| 8 | -2 | 17 | 41 | 53 |
| 8 | -2 | 18 | 60 | -55 |
| 8 | -2 | 20 | 42 | -46 |
| 8 | -2 | 22 | 64 | -52 |
| 8 | -3 | 1 | 281 | -320 |
| 8 | -3 | 2 | 80 | -72 |
| 8 | -3 | 3 | 230 | -239 |
| 8 | -3 | 4 | 138 | -118 |
| 8 | -3 | 5 | 163 | -167 |
| 8 | -3 | 6 | 94 | -79 |
| 8 | -3 | 7 | 164 | -168 |
| 8 | -3 | 8 | 61 | -53 |
| 8 | -3 | 9 | 170 | -162 |
| 8 | -3 | 11 | 119 | -115 |
| 8 | -3 | 13 | 128 | -122 |
| 8 | -3 | 14 | 68 | -41 |
| 8 | -3 | 15 | 120 | -113 |
| 8 | -3 | 17 | 88 | -95 |
| 8 | -3 | 21 | 64 | -74 |
| 8 | -3 | 23 | 74 | -81 |
| 8 | -4 | 0 | 90 | -98 |
| 8 | -4 | 2 | 85 | -105 |
| 8 | -4 | 4 | 125 | -131 |
| 8 | -4 | 6 | 143 | -159 |
| 8 | -4 | 7 | 72 | 66 |
| 8 | -4 | 8 | 152 | -170 |
| 8 | -4 | 9 | 35 | 41 |
| 8 | -4 | 10 | 83 | -86 |
| 8 | -4 | 11 | 47 | 44 |
| 8 | -4 | 14 | 82 | -85 |
| 8 | -4 | 15 | 59 | -39 |
| 8 | -4 | 16 | 111 | 124 |
| 8 | -4 | 18 | 84 | -85 |
| 8 | -5 | 1 | 117 | -109 |
| 8 | -5 | 2 | 72 | 51 |
| 8 | -5 | 3 | 116 | -123 |
| 8 | -5 | 4 | 94 | 85 |
| 8 | -5 | 5 | 112 | -124 |
| 8 | -5 | 6 | 76 | 85 |
| 8 | -5 | 7 | 98 | -113 |
| 8 | -5 | 9 | 57 | -65 |
| 8 | -5 | 10 | 41 | -36 |
| 8 | -5 | 12 | 42 | 44 |
| 8 | -5 | 14 | 51 | 56 |
| 8 | -6 | 9 | 89 | -84 |
| 8 | -6 | 10 | 89 | -89 |
| 8 | -6 | 11 | 42 | -41 |
| 8 | -6 | 12 | 72 | -89 |
| 9 | 0 | 1 | 549 | 569 |
| 9 | 0 | 2 | 242 | -195 |
| 9 | 0 | 3 | 206 | 212 |
| 9 | 0 | 4 | 538 | -512 |
| 9 | 0 | 5 | 305 | 367 |
| 9 | 0 | 6 | 144 | -124 |
| 9 | 0 | 7 | 410 | 420 |
| 9 | 0 | 8 | 201 | -145 |
| 9 | 0 | 9 | 240 | 224 |
| 9 | 0 | 11 | 97 | 84 |
| 9 | 0 | 12 | 162 | -158 |
| 9 | 0 | 13 | 138 | 148 |
| 9 | 0 | 14 | 145 | -125 |
| 9 | 0 | 15 | 251 | 235 |
| 9 | 0 | 17 | 179 | 180 |
| 9 | 0 | 18 | 120 | 102 |
| 9 | 0 | 19 | 87 | 61 |
| 9 | 0 | 20 | 179 | 172 |
| 9 | 0 | 21 | 125 | 120 |
| 9 | 0 | 23 | 157 | 193 |
| 9 | 0 | 25 | 71 | 86 |
| 9 | 0 | 26 | 62 | -62 |
| 9 | 1 | 0 | 325 | 269 |
| 9 | 1 | 2 | 136 | 108 |
| 9 | 1 | 3 | 122 | 111 |
| 9 | 1 | 4 | 407 | 383 |
| 9 | 1 | 5 | 329 | 249 |
| 9 | 1 | 6 | 332 | 363 |
| 9 | 1 | 7 | 343 | 276 |
| 9 | 1 | 8 | 399 | 426 |
| 9 | 1 | 9 | 108 | 58 |
| 9 | 1 | 11 | 63 | 72 |
| 9 | 1 | 12 | 290 | -273 |
| 9 | 1 | 13 | 129 | 110 |
| 9 | 1 | 14 | 334 | 349 |
| 9 | 1 | 16 | 253 | 240 |
| 9 | 1 | 17 | 148 | -145 |
| 9 | 1 | 18 | 199 | 207 |
| 9 | 1 | 20 | 140 | 136 |
| 9 | 1 | 22 | 113 | 107 |
| 9 | 1 | 24 | 97 | 100 |
| 9 | 1 | 26 | 64 | 87 |
| 9 | 2 | 1 | 492 | 486 |
| 9 | 2 | 2 | 158 | 156 |
| 9 | 2 | 3 | 485 | 399 |
| 9 | 2 | 4 | 270 | 220 |
| 9 | 2 | 5 | 386 | 356 |
| 9 | 2 | 6 | 117 | 103 |
| 9 | 2 | 7 | 371 | 340 |
| 9 | 2 | 9 | 254 | 269 |
| 9 | 2 | 10 | 313 | -367 |
| 9 | 2 | 11 | 124 | 115 |
| 9 | 2 | 12 | 283 | 275 |
| 9 | 2 | 13 | 174 | 141 |
| 9 | 2 | 14 | 264 | 270 |
| 9 | 2 | 15 | 163 | 177 |
| 9 | 2 | 16 | 68 | -95 |
| 9 | 2 | 17 | 128 | 114 |
| 9 | 2 | 19 | 117 | 108 |
| 9 | 2 | 21 | 116 | 135 |
| 9 | 2 | 23 | 126 | 140 |
| 9 | 3 | 0 | 196 | 191 |
| 9 | 3 | 2 | 275 | 256 |
| 9 | 3 | 4 | 146 | 98 |
| 9 | 3 | 6 | 254 | 209 |
| 9 | 3 | 8 | 305 | 273 |
| 9 | 3 | 9 | 123 | -129 |
| 9 | 3 | 10 | 441 | 446 |
| 9 | 3 | 12 | 539 | 584 |
| 9 | 3 | 13 | 86 | 90 |
| 9 | 3 | 14 | 281 | 265 |
| 9 | 3 | 16 | 260 | 246 |
| 9 | 3 | 18 | 153 | 138 |
| 9 | 3 | 20 | 141 | 129 |
| 9 | 3 | 21 | 85 | 60 |
| 9 | 3 | 22 | 104 | 116 |
| 9 | 4 | 1 | 249 | 187 |
| 9 | 4 | 3 | 336 | 308 |
| 9 | 4 | 5 | 251 | 185 |
| 9 | 4 | 6 | 62 | 67 |
| 9 | 4 | 7 | 180 | 164 |
| 9 | 4 | 9 | 218 | 209 |
| 9 | 4 | 11 | 198 | 195 |
| 9 | 4 | 13 | 145 | 169 |
| 9 | 4 | 15 | 143 | 135 |
| 9 | 4 | 17 | 124 | 118 |
| 9 | 4 | 19 | 169 | 169 |
| 9 | 4 | 20 | 45 | 33 |
| 9 | 5 | 0 | 217 | 179 |
| 9 | 5 | 2 | 216 | 176 |
| 9 | 5 | 4 | 190 | 153 |
| 9 | 5 | 5 | 116 | -119 |
| 9 | 5 | 6 | 135 | 110 |
| 9 | 5 | 8 | 142 | 109 |
| 9 | 5 | 10 | 84 | 83 |
| 9 | 5 | 12 | 71 | 61 |
| 9 | 5 | 14 | 61 | 55 |
| 9 | 6 | 1 | 85 | 86 |
| 9 | 6 | 3 | 41 | 26 |
| 9 | 6 | 5 | 61 | 70 |
| 9 | 6 | 6 | 45 | 45 |
| 9 | 6 | 7 | 65 | 101 |
| 9 | -1 | 2 | 347 | 525 |
| 9 | -1 | 3 | 156 | -153 |
| 9 | -1 | 4 | 300 | 321 |
| 9 | -1 | 5 | 322 | -313 |
| 9 | -1 | 6 | 335 | 375 |
| 9 | -1 | 7 | 161 | 120 |
| 9 | -1 | 8 | 447 | 487 |
| 9 | -1 | 9 | 83 | -79 |
| 9 | -1 | 10 | 438 | 478 |
| 9 | -1 | 11 | 96 | -91 |
| 9 | -1 | 12 | 452 | 468 |
| 9 | -1 | 13 | 61 | 44 |
| 9 | -1 | 14 | 319 | 369 |
| 9 | -1 | 15 | 41 | -47 |
| 9 | -1 | 16 | 273 | 294 |
| 9 | -1 | 17 | 86 | 73 |
| 9 | -1 | 18 | 180 | 189 |
| 9 | -1 | 19 | 157 | 154 |
| 9 | -1 | 20 | 183 | 207 |
| 9 | -1 | 22 | 158 | 184 |
| 9 | -1 | 24 | 115 | 128 |
| 9 | -1 | 26 | 83 | 98 |
| 9 | -2 | 1 | 379 | 504 |
| 9 | -2 | 2 | 91 | -75 |
| 9 | -2 | 3 | 545 | 629 |
| 9 | -2 | 4 | 186 | -161 |
| 9 | -2 | 5 | 296 | 351 |
| 9 | -2 | 6 | 104 | 85 |
| 9 | -2 | 7 | 360 | 415 |
| 9 | -2 | 9 | 589 | 686 |
| 9 | -2 | 11 | 459 | 468 |
| 9 | -2 | 13 | 455 | 460 |
| 9 | -2 | 15 | 370 | 371 |
| 9 | -2 | 16 | 60 | -74 |
| 9 | -2 | 17 | 183 | 195 |
| 9 | -2 | 19 | 269 | 301 |
| 9 | -2 | 20 | 86 | 64 |
| 9 | -2 | 21 | 223 | 250 |
| 9 | -2 | 23 | 109 | 116 |
| 9 | -2 | 25 | 123 | 133 |
| 9 | -2 | 27 | 81 | 94 |
| 9 | -3 | 0 | 512 | 507 |
| 9 | -3 | 1 | 102 | 110 |
| 9 | -3 | 2 | 561 | 617 |
| 9 | -3 | 3 | 183 | 151 |
| 9 | -3 | 4 | 205 | 208 |
| 9 | -3 | 5 | 434 | 445 |
| 9 | -3 | 6 | 268 | 300 |
| 9 | -3 | 7 | 277 | 225 |
| 9 | -3 | 8 | 367 | 399 |
| 9 | -3 | 9 | 24 | 31 |
| 9 | -3 | 10 | 387 | 414 |
| 9 | -3 | 11 | 164 | 154 |
| 9 | -3 | 12 | 469 | 488 |
| 9 | -3 | 13 | 167 | 157 |
| 9 | -3 | 14 | 244 | 244 |
| 9 | -3 | 15 | 85 | 47 |
| 9 | -3 | 16 | 213 | 215 |
| 9 | -3 | 17 | 160 | -174 |
| 9 | -3 | 18 | 87 | 64 |
| 9 | -3 | 19 | 106 | -99 |
| 9 | -3 | 20 | 148 | 140 |
| 9 | -3 | 22 | 160 | 181 |
| 9 | -3 | 24 | 119 | 126 |
| 9 | -3 | 26 | 86 | 74 |
| 9 | -4 | 1 | 125 | 169 |
| 9 | -4 | 2 | 95 | 106 |
| 9 | -4 | 3 | 154 | 162 |
| 9 | -4 | 4 | 99 | 76 |
| 9 | -4 | 5 | 119 | 117 |
| 9 | -4 | 6 | 85 | -68 |
| 9 | -4 | 7 | 369 | 420 |
| 9 | -4 | 8 | 110 | -77 |
| 9 | -4 | 9 | 114 | 96 |
| 9 | -4 | 10 | 387 | -374 |
| 9 | -4 | 12 | 189 | 199 |
| 9 | -4 | 13 | 126 | 91 |
| 9 | -4 | 14 | 249 | 239 |
| 9 | -4 | 15 | 251 | 276 |
| 9 | -4 | 17 | 216 | 212 |
| 9 | -4 | 21 | 141 | 146 |
| 9 | -4 | 23 | 94 | 97 |
| 9 | -4 | 25 | 86 | 82 |
| 9 | -5 | 0 | 223 | 215 |
| 9 | -5 | 1 | 92 | -75 |
| 9 | -5 | 2 | 188 | 161 |
| 9 | -5 | 4 | 229 | 236 |
| 9 | -5 | 5 | 104 | -116 |
| 9 | -5 | 6 | 176 | 190 |
| 9 | -5 | 7 | 81 | 55 |
| 9 | -5 | 8 | 285 | 295 |
| 9 | -5 | 10 | 134 | -91 |
| 9 | -5 | 11 | 129 | -100 |
| 9 | -5 | 12 | 314 | -337 |
| 9 | -5 | 14 | 148 | 161 |
| 9 | -5 | 15 | 153 | -154 |
| 9 | -5 | 16 | 52 | 75 |
| 9 | -5 | 22 | 45 | 47 |
| 9 | -6 | 3 | 61 | -48 |
| 9 | -6 | 4 | 96 | -97 |
| 9 | -6 | 7 | 97 | 67 |
| 9 | -6 | 8 | 97 | 55 |
| 9 | -6 | 9 | 180 | 190 |
| 9 | -6 | 10 | 154 | 160 |
| 9 | -6 | 11 | 44 | 49 |
| 9 | -6 | 12 | 44 | -49 |
| 9 | -6 | 13 | 135 | 137 |
| 9 | -6 | 15 | 119 | 136 |
| 10 | 0 | 0 | 110 | 97 |
| 10 | 0 | 1 | 72 | -17 |
| 10 | 0 | 2 | 70 | 62 |
| 10 | 0 | 3 | 46 | -34 |
| 10 | 0 | 4 | 91 | 76 |
| 10 | 0 | 6 | 93 | 79 |
| 10 | 0 | 8 | 66 | 48 |
| 10 | 1 | 1 | 69 | 58 |
| 10 | 4 | 0 | 53 | -35 |
| 10 | 4 | 2 | 53 | -49 |
| 10 | 4 | 4 | 65 | -59 |
| 10 | 4 | 6 | 63 | -50 |
| 10 | 4 | 8 | 72 | -62 |
| 10 | 4 | 10 | 60 | -70 |
| 10 | 4 | 12 | 57 | -58 |
| 10 | 5 | 1 | 85 | -88 |
| 10 | 5 | 3 | 78 | -84 |
| 10 | 5 | 5 | 69 | -68 |
| 10 | 5 | 7 | 52 | -54 |
| 10 | -1 | 2 | 46 | -40 |
| 10 | -1 | 3 | 141 | 116 |
| 10 | -1 | 4 | 87 | -78 |
| 10 | -1 | 5 | 69 | 149 |
| 10 | -1 | 6 | 41 | -41 |
| 10 | -1 | 7 | 151 | 132 |
| 10 | -1 | 8 | 53 | -59 |

TABLE 4 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 10 | -1 | 9 | 140 | 124 |
| 10 | -1 | 10 | 60 | -67 |
| 10 | -1 | 11 | 135 | 126 |
| 10 | -1 | 13 | 110 | 102 |
| 10 | -1 | 15 | 82 | 77 |
| 10 | -1 | 17 | 76 | 72 |
| 10 | -1 | 19 | 76 | 77 |
| 10 | -1 | 23 | 55 | 68 |
| 10 | -2 | 2 | 207 | 229 |
| 10 | -2 | 3 | 81 | -84 |
| 10 | -2 | 4 | 242 | 234 |
| 10 | -2 | 5 | 48 | -64 |
| 10 | -2 | 6 | 258 | 246 |
| 10 | -2 | 8 | 250 | 247 |
| 10 | -2 | 10 | 245 | 249 |
| 10 | -2 | 12 | 233 | 241 |
| 10 | -2 | 14 | 186 | 200 |
| 10 | -2 | 16 | 130 | 145 |
| 10 | -2 | 18 | 126 | 125 |
| 10 | -2 | 20 | 98 | 96 |
| 10 | -2 | 22 | 69 | 59 |
| 10 | -3 | 1 | 228 | 216 |
| 10 | -3 | 2 | 72 | 62 |
| 10 | -3 | 3 | 183 | 183 |
| 10 | -3 | 4 | 149 | 136 |
| 10 | -3 | 5 | 161 | 159 |
| 10 | -3 | 6 | 185 | 181 |
| 10 | -3 | 7 | 179 | 190 |
| 10 | -3 | 8 | 105 | 95 |
| 10 | -3 | 9 | 234 | 238 |
| 10 | -3 | 10 | 46 | 42 |
| 10 | -3 | 11 | 270 | 300 |
| 10 | -3 | 12 | 34 | 26 |
| 10 | -3 | 13 | 257 | 276 |
| 10 | -3 | 15 | 190 | 194 |
| 10 | -3 | 17 | 132 | 147 |
| 10 | -3 | 19 | 130 | 145 |
| 10 | -3 | 21 | 110 | 119 |
| 10 | -3 | 23 | 87 | 93 |
| 10 | -3 | 25 | 60 | 65 |
| 10 | -4 | 0 | 212 | 233 |
| 10 | -4 | 2 | 196 | 211 |
| 10 | -4 | 3 | 39 | 48 |
| 10 | -4 | 4 | 212 | 212 |
| 10 | -4 | 5 | 41 | 49 |
| 10 | -4 | 6 | 236 | 260 |
| 10 | -4 | 7 | 31 | -38 |
| 10 | -4 | 8 | 179 | 194 |
| 10 | -4 | 9 | 162 | -133 |
| 10 | -4 | 10 | 143 | -147 |
| 10 | -4 | 12 | 132 | 129 |
| 10 | -4 | 13 | 91 | 91 |
| 10 | -4 | 14 | 93 | 89 |
| 10 | -4 | 16 | 85 | 90 |
| 10 | -4 | 18 | 91 | 76 |
| 10 | -4 | 20 | 85 | 80 |
| 10 | -4 | 22 | 69 | 70 |
| 10 | -4 | 24 | 62 | 2 |
| 10 | -5 | 1 | 290 | 313 |
| 10 | -5 | 3 | 282 | 297 |
| 10 | -5 | 5 | 281 | 288 |
| 10 | -5 | 6 | 100 | 83 |
| 10 | -5 | 7 | 225 | 227 |
| 10 | -5 | 8 | 96 | 70 |
| 10 | -5 | 11 | 130 | -103 |
| 10 | -5 | 12 | 93 | 84 |
| 10 | -5 | 15 | 65 | 77 |
| 10 | -5 | 17 | 102 | 94 |
| 10 | -5 | 19 | 88 | 87 |
| 10 | -5 | 21 | 83 | 94 |
| 10 | -5 | 23 | 76 | 99 |
| 10 | -6 | 2 | 118 | 117 |
| 10 | -6 | 3 | 124 | -108 |
| 10 | -6 | 4 | 119 | 105 |
| 10 | -6 | 5 | 106 | -92 |
| 10 | -6 | 6 | 200 | 179 |
| 10 | -6 | 8 | 228 | 234 |
| 10 | -6 | 10 | 224 | 201 |
| 10 | -6 | 11 | 53 | -62 |
| 10 | -6 | 12 | 224 | 228 |
| 10 | -6 | 13 | 63 | -81 |
| 10 | -6 | 14 | 224 | 249 |
| 10 | -6 | 16 | 184 | 186 |
| 10 | -6 | 18 | 113 | 118 |
| 10 | -6 | 20 | 81 | 87 |
| 10 | -7 | 6 | 117 | -89 |
| 10 | -7 | 7 | 232 | 233 |
| 10 | -7 | 8 | 63 | -61 |
| 10 | -7 | 9 | 214 | 229 |
| 10 | -7 | 10 | 70 | -55 |
| 10 | -7 | 11 | 202 | 231 |
| 10 | -7 | 13 | 181 | 195 |
| 10 | -7 | 15 | 141 | 141 |
| 10 | -7 | 17 | 120 | 121 |
| 11 | -1 | 2 | 125 | -119 |
| 11 | -1 | 4 | 118 | -113 |
| 11 | -1 | 5 | 43 | 40 |
| 11 | -1 | 6 | 124 | -116 |
| 11 | -1 | 8 | 96 | -88 |
| 11 | -1 | 10 | 90 | -67 |
| 11 | -1 | 12 | 90 | -64 |
| 11 | -2 | 3 | 131 | -146 |
| 11 | -2 | 4 | 30 | 37 |
| 11 | -2 | 5 | 140 | -152 |
| 11 | -2 | 7 | 114 | -110 |
| 11 | -2 | 9 | 134 | -123 |
| 11 | -2 | 11 | 148 | -143 |
| 11 | -2 | 13 | 130 | -126 |
| 11 | -2 | 15 | 88 | -80 |
| 11 | -2 | 17 | 69 | -56 |
| 11 | -2 | 19 | 68 | -58 |
| 11 | -3 | 0 | 59 | -62 |
| 11 | -3 | 2 | 40 | -42 |
| 11 | -3 | 4 | 43 | -49 |
| 11 | -3 | 5 | 71 | -68 |
| 11 | -3 | 6 | 57 | -57 |
| 11 | -3 | 8 | 55 | -57 |
| 11 | -3 | 10 | 143 | -156 |
| 11 | -3 | 12 | 158 | -184 |
| 11 | -3 | 14 | 117 | -134 |
| 11 | -3 | 16 | 69 | -70 |
| 11 | -4 | 1 | 79 | -84 |
| 11 | -4 | 3 | 80 | -76 |
| 11 | -4 | 4 | 107 | -119 |
| 11 | -4 | 7 | 91 | -98 |
| 11 | -4 | 8 | 93 | 75 |
| 11 | -4 | 10 | 99 | 85 |
| 11 | -5 | 2 | 71 | -79 |
| 11 | -5 | 4 | 90 | -94 |
| 11 | -5 | 5 | 52 | -55 |
| 11 | -5 | 6 | 118 | -125 |
| 11 | -5 | 7 | 100 | -81 |
| 11 | -5 | 8 | 95 | -78 |
| 12 | 0 | 1 | 310 | -165 |
| 12 | 0 | 2 | 707 | 485 |
| 12 | 0 | 4 | 454 | 459 |
| 12 | 0 | 5 | 185 | 152 |
| 12 | 0 | 6 | 382 | 340 |
| 12 | 0 | 7 | 142 | 90 |
| 12 | 0 | 8 | 357 | 338 |
| 12 | 0 | 9 | 125 | 105 |
| 12 | 0 | 10 | 200 | 197 |
| 12 | 0 | 12 | 160 | 157 |
| 12 | 0 | 14 | 165 | 215 |
| 12 | 0 | 16 | 211 | 208 |
| 12 | 0 | 18 | 156 | 150 |
| 12 | 0 | 20 | 165 | 170 |
| 12 | 1 | 3 | 378 | 242 |
| 12 | 1 | 5 | 262 | 274 |
| 12 | 1 | 6 | 151 | 121 |
| 12 | 1 | 7 | 257 | 290 |
| 12 | 1 | 9 | 131 | 151 |
| 12 | 1 | 11 | 251 | 281 |
| 12 | 1 | 13 | 165 | 182 |
| 12 | 1 | 15 | 160 | 170 |
| 12 | 1 | 17 | 217 | 268 |
| 12 | 1 | 19 | 142 | 176 |
| 12 | 3 | 1 | 286 | 226 |
| 12 | 3 | 5 | 131 | 131 |
| 12 | 3 | 6 | 160 | -209 |
| 12 | 3 | 9 | 156 | 225 |
| 12 | -1 | 1 | 727 | 516 |
| 12 | -1 | 2 | 312 | -186 |
| 12 | -1 | 3 | 425 | 440 |
| 12 | -1 | 5 | 477 | 479 |
| 12 | -1 | 7 | 439 | 390 |
| 12 | -1 | 9 | 291 | 239 |
| 12 | -1 | 11 | 278 | 237 |
| 12 | -1 | 13 | 207 | 199 |
| 12 | -1 | 15 | 214 | 201 |
| 12 | -1 | 17 | 251 | 241 |
| 12 | -1 | 19 | 156 | 179 |
| 12 | -1 | 21 | 165 | 174 |
| 12 | -1 | 23 | 193 | 200 |
| 12 | -2 | 4 | 321 | 375 |
| 12 | -2 | 5 | 100 | -102 |
| 12 | -2 | 6 | 374 | 379 |
| 12 | -2 | 8 | 278 | 237 |
| 12 | -2 | 9 | 248 | 173 |
| 12 | -2 | 10 | 273 | 247 |
| 12 | -2 | 12 | 357 | 286 |
| 12 | -2 | 16 | 137 | 151 |
| 12 | -2 | 18 | 161 | 157 |
| 12 | -2 | 20 | 125 | 137 |
| 12 | -2 | 32 | 136 | 115 |
| 12 | -3 | 4 | 85 | 88 |
| 12 | -3 | 6 | 200 | -151 |
| 12 | -3 | 9 | 347 | 339 |
| 12 | -3 | 11 | 433 | 460 |
| 12 | -3 | 13 | 384 | 381 |
| 12 | -3 | 15 | 136 | 138 |
| 12 | -3 | 19 | 181 | 175 |
| 12 | -4 | 0 | 227 | 216 |
| 12 | -4 | 3 | 107 | 95 |
| 12 | -4 | 4 | 295 | 304 |
| 12 | -4 | 5 | 207 | 182 |
| 12 | -4 | 7 | 265 | -239 |
| 12 | -4 | 9 | 233 | -212 |
| 12 | -4 | 10 | 131 | 156 |
| 12 | -4 | 15 | 136 | 140 |
| 12 | -4 | 18 | 156 | 167 |
| 12 | -4 | 19 | 120 | -121 |
| 12 | -5 | 5 | 283 | 276 |
| 12 | -5 | 6 | 273 | 268 |
| 12 | -5 | 7 | 227 | 191 |
| 12 | -5 | 18 | 120 | -129 |

in aquo-ligands appear to be pyramidal. In the chelate ring, there is a steady decrease in the angle Cu–OR–C for R = H, Me, Ph, accompanied by an increase in CuOC angle at the carboxylate oxygen. The C–O–R angles follow a pattern consistent with expected intramolecular repulsions for the phenoxyacetate, methoxyacetate, and glycollate, but have widely different values for the lactate and 2-hydroxy-2-methylpropionate, and these variations are necessarily reflected in the variations in the CuOR angle.

In the three 2-hydroxycarboxylates, each hydroxy-group is not only bound to the copper atom, but is also hydrogen-bonded to the non-chelated carboxylate oxygen atom of another complex. Although variations in the O–Cu and O–H bond lengths could be attributed to experimental error, it is noteworthy that the hydrogen bonds appear to shorten as the Cu–OH bonds shorten. A similar effect is observable for the water molecules in the hexa-aquocopper(II) ion in Tutton's salt.[22] Such a co-operative strengthening of bonds would be expected from an electronic viewpoint.

The carboxylate group usually forms hydrogen-bonds only at the non-chelating oxygen atom. When this happens there is one hydrogen-bond approximately parallel to the carbon–carbon bond of the chelate ring and coplanar with it. Some non-chelating oxygen atoms (in phenoxyacetate, methoxyacetate, and lactate) form a second hydrogen-bond which is near to the carboxylate plane and roughly parallel to the O · · · O vector in the carboxylate group, but others (in lactate and glycollate) form a long contact to a copper atom in another molecule.

The hydration of the 2-hydroxycarboxylate complexes increases from 0 to 1 to 2 in the sequence glycollate, lactate, 2-hydroxy-2-methylpropionate, *i.e.*, in parallel with the substitution of methyl groups on the 2-carbon atom. In the 2-hydroxy-2-methylpropionate, adjacent chelate rings are linked into a ribbon structure by hydrogen-bonds from O(2) to O(3). The carboxy-group does not form a second hydrogen-bond (see above). The inclination of the two methyl substituents in each chelate ring keeps superimposed planes of chelate rings sufficiently far apart to accommodate two *trans* water molecules on each copper ion (see Figure 12). The hypothetical conversion of the 2-hydroxy-2-methylpropionate into the lactate involves the removal of one methyl group from each chelate ring, and the formation of large holes in the structure. The consequent closer approach of superimposed planes of chelate rings is such that there is now only room for one aquo-ligand on each copper ion. One lactate ligand only of each complex forms the second type of hydrogen-bond (see above), and a double hydrogen-bond ribbon is formed. The hypothetical conversion of lactate into glycollate involves the removal of the remaining two methyl substituents from the rings, and again the formation of holes. If the original ribbon structure were to be retained, a reasonably close packed structure could not be formed with axial Cu–O contacts of less than about 2·9 Å. The original O(2) · · · O(3) two-dimensional sheet with shorter Cu–O(2) contacts of 2·54 Å results.

The formation of two hydrogen-bonds by the non-chelating oxygen atom suggests $sp^2$ hybridisation of the

[22] H. Montgomery and E. C. Lingafelter, *Acta Cryst.*, 1966, **20**, 659.

TABLE 5

Observed structure amplitudes and calculated structure factors for diaquobis(methoxyacetato)copper(II)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 0 | 0 | 2 | 263 | 300 |
| 0 | 0 | 4 | 122 | 127 |
| 0 | 0 | 6 | 186 | 204 |
| 0 | 0 | 8 | 92 | 96 |
| 0 | 0 | 10 | 84 | 96 |
| 0 | 0 | 12 | 10 | 5 |
| 0 | 1 | 2 | 54 | -32 |
| 0 | 1 | 3 | 156 | -111 |
| 0 | 1 | 4 | 49 | -54 |
| 0 | 1 | 5 | 195 | 187 |
| 0 | 1 | 6 | 36 | -31 |
| 0 | 1 | 7 | 114 | 111 |
| 0 | 1 | 8 | 41 | -48 |
| 0 | 1 | 9 | 89 | 105 |
| 0 | 1 | 11 | 43 | 62 |
| 0 | 2 | 0 | 298 | 333 |
| 0 | 2 | 1 | 39 | 52 |
| 0 | 2 | 2 | 39 | 41 |
| 0 | 2 | 3 | 45 | -21 |
| 0 | 2 | 4 | 128 | 131 |
| 0 | 2 | 5 | 29 | -17 |
| 0 | 2 | 6 | 192 | 193 |
| 0 | 2 | 7 | 67 | -69 |
| 0 | 2 | 8 | 78 | 80 |
| 0 | 2 | 9 | 25 | -28 |
| 0 | 2 | 10 | 47 | 62 |
| 0 | 2 | 12 | 27 | 42 |
| 0 | 3 | 1 | 120 | 131 |
| 0 | 3 | 2 | 194 | 151 |
| 0 | 3 | 3 | 125 | 138 |
| 0 | 3 | 4 | 123 | 103 |
| 0 | 3 | 5 | 194 | 196 |
| 0 | 3 | 6 | 59 | 46 |
| 0 | 3 | 7 | 117 | 126 |
| 0 | 3 | 9 | 28 | 35 |
| 0 | 3 | 10 | 50 | 56 |
| 0 | 3 | 11 | 19 | 27 |
| 0 | 3 | 12 | 13 | 16 |
| 0 | 4 | 0 | 147 | 128 |
| 0 | 4 | 1 | 58 | 52 |
| 0 | 4 | 2 | 209 | 203 |
| 0 | 4 | 3 | 37 | 34 |
| 0 | 4 | 4 | 181 | 159 |
| 0 | 4 | 6 | 132 | 133 |
| 0 | 4 | 7 | 51 | -47 |
| 0 | 4 | 8 | 73 | 77 |
| 0 | 4 | 11 | 18 | 22 |
| 0 | 5 | 1 | 170 | 152 |
| 0 | 5 | 2 | 26 | -18 |
| 0 | 5 | 3 | 202 | 180 |
| 0 | 5 | 4 | 24 | -20 |
| 0 | 5 | 5 | 80 | 69 |
| 0 | 5 | 6 | 25 | -21 |
| 0 | 5 | 7 | 105 | 109 |
| 0 | 5 | 8 | 13 | -14 |
| 0 | 5 | 9 | 39 | 37 |
| 0 | 5 | 10 | 9 | 8 |
| 0 | 6 | 1 | 42 | -34 |
| 0 | 6 | 2 | 96 | 89 |
| 0 | 6 | 3 | 43 | -40 |
| 0 | 6 | 4 | 35 | 26 |
| 0 | 6 | 5 | 14 | -13 |
| 0 | 6 | 6 | 43 | 40 |
| 0 | 6 | 7 | 13 | 9 |
| 0 | 6 | 8 | 65 | 79 |
| 0 | 6 | 9 | 16 | 12 |
| 0 | 7 | 1 | 73 | 60 |
| 0 | 7 | 2 | 34 | -24 |
| 0 | 7 | 3 | 89 | 81 |
| 0 | 7 | 5 | 25 | 19 |
| 0 | 7 | 7 | 56 | 60 |
| 0 | 7 | 8 | 31 | 35 |
| 0 | 8 | 0 | 54 | 46 |
| 0 | 8 | 2 | 68 | 68 |
| 0 | 8 | 3 | 19 | 18 |
| 0 | 8 | 4 | 39 | 37 |
| 0 | 8 | 6 | 29 | 28 |
| 0 | 9 | 1 | 52 | 50 |
| 0 | 9 | 2 | 12 | 17 |
| 1 | 0 | 2 | 175 | -212 |
| 1 | 0 | 3 | 281 | 300 |
| 1 | 0 | 4 | 129 | -127 |
| 1 | 0 | 5 | 146 | 155 |
| 1 | 0 | 6 | 84 | 76 |
| 1 | 0 | 7 | 143 | 146 |
| 1 | 0 | 8 | 30 | 26 |
| 1 | 0 | 9 | 44 | 50 |
| 1 | 0 | 10 | 34 | -44 |
| 1 | 0 | 11 | 46 | 64 |
| 1 | -1 | 2 | 417 | 475 |
| 1 | -1 | 3 | 246 | -257 |
| 1 | -1 | 4 | 235 | 272 |
| 1 | -1 | 6 | 153 | 158 |
| 1 | -1 | 7 | 113 | 109 |
| 1 | -1 | 8 | 95 | 97 |
| 1 | -1 | 9 | 40 | -41 |
| 1 | -1 | 10 | 41 | 38 |
| 1 | -1 | 11 | 21 | -25 |
| 1 | -1 | 12 | 30 | 39 |
| 1 | -2 | 1 | 66 | 71 |
| 1 | -2 | 2 | 112 | 85 |
| 1 | -2 | 3 | 250 | 267 |
| 1 | -2 | 4 | 87 | -56 |
| 1 | -2 | 5 | 107 | 111 |
| 1 | -2 | 6 | 183 | 172 |
| 1 | -2 | 7 | 110 | 116 |
| 1 | -2 | 8 | 31 | 39 |
| 1 | -2 | 9 | 69 | 72 |
| 1 | -2 | 10 | 13 | -0 |
| 1 | -2 | 11 | 52 | 57 |
| 1 | -2 | 12 | 17 | 23 |
| 1 | -3 | 0 | 63 | -30 |
| 1 | -3 | 1 | 204 | 169 |
| 1 | -3 | 2 | 218 | 193 |
| 1 | -3 | 3 | 24 | -23 |
| 1 | -3 | 4 | 223 | 219 |
| 1 | -3 | 6 | 97 | 103 |
| 1 | -3 | 7 | 23 | 15 |
| 1 | -3 | 8 | 76 | 83 |
| 1 | -3 | 9 | 44 | -46 |
| 1 | -3 | 10 | 51 | 55 |
| 1 | -3 | 11 | 24 | 29 |
| 1 | -3 | 12 | 29 | 41 |
| 1 | -4 | 1 | 15 | 18 |
| 1 | -4 | 2 | 84 | 78 |
| 1 | -4 | 3 | 204 | 200 |
| 1 | -4 | 4 | 90 | -78 |
| 1 | -4 | 5 | 136 | 140 |
| 1 | -4 | 6 | 23 | -30 |
| 1 | -4 | 7 | 42 | 53 |
| 1 | -4 | 8 | 75 | -79 |
| 1 | -4 | 9 | 39 | 55 |
| 1 | -4 | 10 | 16 | -15 |
| 1 | -4 | 11 | 28 | 37 |
| 1 | -5 | 0 | 147 | 126 |
| 1 | -5 | 1 | 62 | 46 |
| 1 | -5 | 2 | 194 | 173 |
| 1 | -5 | 3 | 18 | 13 |
| 1 | -5 | 4 | 208 | 197 |
| 1 | -5 | 5 | 28 | 14 |
| 1 | -5 | 6 | 76 | 69 |
| 1 | -5 | 8 | 39 | 38 |
| 1 | -5 | 9 | 12 | -16 |
| 1 | -5 | 10 | 36 | 38 |
| 1 | -6 | 1 | 126 | 107 |
| 1 | -6 | 3 | 125 | 107 |
| 1 | -6 | 4 | 14 | 19 |
| 1 | -6 | 5 | 76 | 71 |
| 1 | -6 | 6 | 19 | 14 |
| 1 | -6 | 7 | 22 | 19 |
| 1 | -6 | 9 | 51 | 60 |
| 1 | -7 | 0 | 75 | 71 |
| 1 | -7 | 1 | 20 | -24 |
| 1 | -7 | 2 | 55 | 45 |
| 1 | -7 | 3 | 14 | 15 |
| 1 | -7 | 4 | 37 | 37 |
| 1 | -7 | 5 | 22 | 25 |
| 1 | -7 | 6 | 11 | 8 |
| 1 | -7 | 8 | 41 | 39 |
| 1 | -8 | 1 | 69 | 59 |
| 1 | -8 | 2 | 23 | -27 |
| 1 | -8 | 3 | 50 | 45 |
| 1 | -8 | 4 | 10 | 7 |
| 1 | -8 | 5 | 26 | 29 |
| 1 | -8 | 6 | 24 | -27 |
| 1 | -9 | 0 | 31 | 27 |
| 1 | -9 | 1 | 21 | -22 |
| 1 | -9 | 2 | 37 | 36 |
| 1 | 1 | 2 | 96 | 115 |
| 1 | 1 | 3 | 69 | -69 |
| 1 | 1 | 4 | 61 | 71 |
| 1 | 1 | 5 | 25 | -34 |
| 1 | 1 | 6 | 119 | 135 |
| 1 | 1 | 8 | 82 | 93 |
| 1 | 1 | 9 | 34 | -32 |
| 1 | 1 | 10 | 59 | 80 |
| 1 | 1 | 11 | 12 | -20 |
| 1 | 1 | 12 | 48 | 73 |
| 1 | 2 | 3 | 114 | 122 |
| 1 | 2 | 4 | 176 | 185 |
| 1 | 2 | 5 | 129 | 128 |
| 1 | 2 | 7 | 98 | 114 |
| 1 | 2 | 9 | 66 | 79 |
| 1 | 2 | 11 | 50 | 73 |
| 1 | 2 | 12 | 25 | 30 |
| 1 | 3 | 3 | 142 | 130 |
| 1 | 3 | 4 | 98 | 97 |
| 1 | 3 | 5 | 63 | 56 |
| 1 | 3 | 6 | 115 | 113 |
| 1 | 3 | 7 | 43 | -47 |
| 1 | 3 | 8 | 58 | 69 |
| 1 | 3 | 10 | 63 | 76 |
| 1 | 3 | 11 | 14 | 13 |
| 1 | 3 | 12 | 20 | 28 |
| 1 | 4 | 3 | 121 | 118 |
| 1 | 4 | 4 | 43 | 53 |
| 1 | 4 | 5 | 156 | 134 |
| 1 | 4 | 6 | 69 | -66 |
| 1 | 4 | 7 | 67 | 67 |
| 1 | 4 | 8 | 39 | -46 |
| 1 | 4 | 9 | 54 | 54 |
| 1 | 4 | 10 | 11 | -16 |
| 1 | 4 | 11 | 32 | 35 |
| 1 | 5 | 4 | 118 | 116 |
| 1 | 5 | 5 | 42 | 34 |
| 1 | 5 | 6 | 90 | 97 |
| 1 | 5 | 7 | 19 | -24 |
| 1 | 5 | 8 | 28 | 31 |
| 1 | 5 | 10 | 34 | 41 |
| 1 | 6 | 2 | 40 | -41 |
| 1 | 6 | 3 | 70 | 61 |
| 1 | 6 | 4 | 34 | 28 |
| 1 | 6 | 5 | 115 | 115 |
| 1 | 6 | 6 | 13 | 14 |
| 1 | 6 | 7 | 32 | 39 |
| 1 | 6 | 8 | 10 | -15 |
| 1 | 6 | 9 | 21 | 24 |
| 1 | 7 | 2 | 71 | 67 |
| 1 | 7 | 4 | 100 | 86 |
| 1 | 7 | 5 | 37 | 41 |
| 1 | 7 | 6 | 55 | 57 |
| 1 | 7 | 8 | 19 | 25 |
| 1 | 8 | 1 | 58 | 58 |
| 1 | 8 | 2 | 22 | -21 |
| 1 | 8 | 3 | 49 | 43 |
| 1 | 8 | 4 | 9 | -13 |
| 1 | 8 | 5 | 27 | 26 |
| 1 | 8 | 6 | 7 | 12 |
| 1 | 9 | 0 | 41 | 47 |
| 1 | 9 | 1 | 10 | -8 |
| 2 | 0 | 2 | 52 | -17 |
| 2 | 0 | 3 | 68 | -53 |
| 2 | 0 | 4 | 208 | 210 |
| 2 | 0 | 5 | 102 | -101 |
| 2 | 0 | 6 | 118 | 127 |
| 2 | 0 | 7 | 33 | 29 |
| 2 | 0 | 8 | 47 | 62 |
| 2 | 0 | 10 | 66 | 88 |
| 2 | 0 | 12 | 27 | 43 |
| 2 | -1 | 2 | 150 | 101 |
| 2 | -1 | 3 | 315 | 340 |
| 2 | -1 | 4 | 112 | -106 |
| 2 | -1 | 5 | 289 | 328 |
| 2 | -1 | 6 | 61 | -62 |
| 2 | -1 | 7 | 73 | 72 |
| 2 | -1 | 9 | 47 | 49 |
| 2 | -1 | 11 | 19 | 21 |
| 2 | -1 | 12 | 8 | -7 |
| 2 | -2 | 0 | 96 | 111 |
| 2 | -2 | 1 | 22 | 31 |
| 2 | -2 | 2 | 222 | 217 |
| 2 | -2 | 3 | 83 | 57 |
| 2 | -2 | 4 | 333 | 317 |
| 2 | -2 | 5 | 56 | -62 |
| 2 | -2 | 6 | 145 | 136 |
| 2 | -2 | 7 | 12 | -8 |
| 2 | -2 | 8 | 56 | 59 |
| 2 | -2 | 9 | 22 | 21 |
| 2 | -2 | 10 | 36 | 36 |
| 2 | -2 | 11 | 20 | -19 |
| 2 | -2 | 12 | 13 | 17 |
| 2 | -3 | 1 | 174 | 141 |
| 2 | -3 | 2 | 104 | 89 |
| 2 | -3 | 3 | 242 | 204 |
| 2 | -3 | 4 | 145 | 119 |
| 2 | -3 | 5 | 134 | 105 |
| 2 | -3 | 6 | 17 | -11 |
| 2 | -3 | 7 | 87 | 83 |
| 2 | -3 | 8 | 74 | 69 |
| 2 | -3 | 9 | 82 | 85 |
| 2 | -3 | 10 | 28 | 28 |
| 2 | -3 | 11 | 29 | 32 |
| 2 | -4 | 0 | 130 | 108 |
| 2 | -4 | 1 | 28 | -23 |
| 2 | -4 | 2 | 176 | 159 |
| 2 | -4 | 3 | 95 | 80 |
| 2 | -4 | 4 | 60 | 56 |
| 2 | -4 | 5 | 65 | -50 |
| 2 | -4 | 6 | 33 | 38 |
| 2 | -4 | 7 | 68 | -67 |
| 2 | -4 | 8 | 100 | 109 |
| 2 | -4 | 9 | 20 | 20 |
| 2 | -4 | 10 | 51 | 65 |
| 2 | -4 | 11 | 11 | -13 |
| 2 | -5 | 1 | 155 | 126 |
| 2 | -5 | 2 | 20 | 14 |
| 2 | -5 | 3 | 122 | 111 |
| 2 | -5 | 4 | 37 | 34 |
| 2 | -5 | 5 | 13 | 5 |
| 2 | -5 | 6 | 91 | -86 |
| 2 | -5 | 7 | 70 | 78 |
| 2 | -5 | 8 | 12 | -11 |
| 2 | -5 | 9 | 56 | 67 |
| 2 | -5 | 10 | 11 | 12 |
| 2 | -6 | 0 | 160 | 129 |
| 2 | -6 | 1 | 18 | -16 |
| 2 | -6 | 2 | 183 | 165 |
| 2 | -6 | 3 | 34 | 23 |
| 2 | -6 | 4 | 92 | 79 |
| 2 | -6 | 5 | 13 | -12 |
| 2 | -6 | 6 | 65 | 58 |
| 2 | -6 | 7 | 16 | -24 |
| 2 | -6 | 8 | 61 | 58 |
| 2 | -6 | 9 | 19 | 21 |
| 2 | -7 | 3 | 70 | 64 |
| 2 | -7 | 5 | 34 | 35 |
| 2 | -7 | 7 | 55 | 54 |
| 2 | -7 | 8 | 21 | 24 |
| 2 | -8 | 0 | 40 | 36 |
| 2 | -8 | 1 | 11 | -5 |
| 2 | -8 | 2 | 45 | 39 |
| 2 | -8 | 3 | 14 | -17 |
| 2 | -8 | 4 | 28 | 26 |
| 2 | -8 | 5 | 8 | 9 |
| 2 | -8 | 6 | 42 | 41 |
| 2 | -9 | 1 | 38 | 35 |
| 2 | -9 | 2 | 9 | -6 |
| 2 | -9 | 3 | 15 | 16 |
| 2 | 1 | 2 | 141 | 120 |
| 2 | 1 | 3 | 131 | 132 |
| 2 | 1 | 4 | 154 | -139 |
| 2 | 1 | 5 | 175 | 176 |
| 2 | 1 | 6 | 86 | 90 |
| 2 | 1 | 7 | 67 | 73 |
| 2 | 1 | 8 | 40 | 45 |
| 2 | 1 | 9 | 90 | 100 |
| 2 | 1 | 11 | 53 | 66 |
| 2 | 1 | 12 | 8 | -6 |
| 2 | 2 | 3 | 87 | -75 |
| 2 | 2 | 4 | 130 | 138 |
| 2 | 2 | 5 | 18 | 26 |
| 2 | 2 | 6 | 104 | 103 |
| 2 | 2 | 7 | 125 | 130 |
| 2 | 2 | 8 | 68 | 69 |
| 2 | 2 | 9 | 25 | 19 |
| 2 | 2 | 10 | 67 | 84 |
| 2 | 2 | 11 | 10 | 5 |
| 2 | 2 | 12 | 21 | 28 |
| 2 | 3 | 4 | 156 | -143 |
| 2 | 3 | 5 | 115 | 118 |
| 2 | 3 | 6 | 12 | 5 |
| 2 | 3 | 7 | 79 | 74 |
| 2 | 3 | 8 | 13 | -20 |
| 2 | 3 | 9 | 49 | 54 |
| 2 | 3 | 10 | 19 | -22 |
| 2 | 3 | 11 | 42 | 57 |
| 2 | 4 | 4 | 99 | 100 |
| 2 | 4 | 5 | 25 | -27 |
| 2 | 4 | 6 | 89 | 88 |
| 2 | 4 | 7 | 13 | -17 |
| 2 | 4 | 8 | 45 | 46 |
| 2 | 4 | 9 | 11 | -9 |
| 2 | 4 | 10 | 38 | 49 |
| 2 | 4 | 11 | 8 | 9 |
| 2 | 5 | 3 | 94 | 76 |
| 2 | 5 | 4 | 41 | 34 |
| 2 | 5 | 5 | 53 | 56 |
| 2 | 5 | 6 | 22 | -29 |
| 2 | 5 | 7 | 53 | 56 |
| 2 | 5 | 8 | 16 | -18 |
| 2 | 5 | 9 | 26 | 33 |
| 2 | 5 | 10 | 14 | 19 |
| 2 | 6 | 3 | 60 | 59 |
| 2 | 6 | 4 | 96 | 87 |
| 2 | 6 | 5 | 12 | 11 |
| 2 | 6 | 6 | 56 | 55 |
| 2 | 6 | 7 | 25 | -24 |
| 2 | 6 | 8 | 30 | 32 |
| 2 | 6 | 9 | 11 | 16 |
| 2 | 7 | 2 | 12 | -15 |
| 2 | 7 | 3 | 78 | 81 |
| 2 | 7 | 4 | 22 | 25 |
| 2 | 7 | 5 | 50 | 47 |
| 2 | 7 | 6 | 15 | -18 |
| 2 | 7 | 7 | 24 | 29 |
| 2 | 8 | 0 | 9 | 7 |
| 2 | 8 | 1 | 37 | -39 |
| 2 | 8 | 2 | 43 | 41 |
| 2 | 8 | 3 | 14 | -15 |
| 2 | 8 | 4 | 58 | 56 |
| 2 | 8 | 5 | 7 | -9 |
| 3 | 0 | 3 | 183 | 207 |
| 3 | 0 | 4 | 38 | 13 |
| 3 | 0 | 5 | 46 | 50 |
| 3 | 0 | 6 | 11 | 3 |
| 3 | 0 | 7 | 152 | 158 |
| 3 | 0 | 8 | 23 | 22 |
| 3 | 0 | 9 | 58 | 65 |
| 3 | 0 | 10 | 12 | -11 |
| 3 | 0 | 11 | 17 | 21 |
| 3 | -1 | 2 | 212 | 219 |
| 3 | -1 | 3 | 71 | 66 |
| 3 | -1 | 4 | 49 | 56 |
| 3 | -1 | 5 | 21 | -12 |
| 3 | -1 | 6 | 67 | 78 |
| 3 | -1 | 7 | 38 | -44 |
| 3 | -1 | 8 | 127 | 149 |
| 3 | -1 | 9 | 13 | -13 |
| 3 | -1 | 10 | 24 | 30 |
| 3 | -1 | 11 | 20 | 17 |
| 3 | -2 | 1 | 272 | 252 |
| 3 | -2 | 2 | 97 | 63 |
| 3 | -2 | 3 | 265 | 271 |
| 3 | -2 | 5 | 53 | 56 |
| 3 | -2 | 6 | 74 | -79 |
| 3 | -2 | 7 | 136 | 146 |
| 3 | -2 | 8 | 80 | -91 |
| 3 | -2 | 9 | 50 | 61 |
| 3 | -2 | 11 | 9 | 9 |
| 3 | -3 | 0 | 198 | 167 |
| 3 | -3 | 1 | 46 | 40 |
| 3 | -3 | 2 | 239 | 218 |
| 3 | -3 | 3 | 48 | 33 |
| 3 | -3 | 4 | 95 | 96 |
| 3 | -3 | 5 | 56 | 49 |
| 3 | -3 | 6 | 89 | 84 |
| 3 | -3 | 7 | 19 | -18 |
| 3 | -3 | 8 | 93 | 98 |
| 3 | -3 | 9 | 12 | -9 |
| 3 | -3 | 10 | 15 | 221 |
| 3 | -4 | 1 | 189 | 179 |
| 3 | -4 | 2 | 29 | -27 |
| 3 | -4 | 3 | 109 | 103 |
| 3 | -4 | 4 | 41 | 31 |
| 3 | -4 | 5 | 84 | 71 |
| 3 | -4 | 6 | 78 | 76 |
| 3 | -4 | 7 | 97 | 89 |
| 3 | -4 | 9 | 54 | 58 |
| 3 | -4 | 10 | 21 | 19 |
| 3 | -5 | 0 | 160 | 143 |
| 3 | -5 | 1 | 60 | -53 |
| 3 | -5 | 2 | 48 | 40 |
| 3 | -5 | 3 | 94 | -78 |
| 3 | -5 | 4 | 13 | 21 |
| 3 | -5 | 5 | 19 | 23 |
| 3 | -5 | 6 | 59 | 59 |
| 3 | -5 | 7 | 13 | 7 |
| 3 | -5 | 8 | 55 | 64 |
| 3 | -5 | 9 | 10 | -17 |
| 3 | -6 | 1 | 132 | 131 |
| 3 | -6 | 2 | 63 | -59 |
| 3 | -6 | 3 | 29 | 26 |
| 3 | -6 | 5 | 66 | 72 |
| 3 | -6 | 6 | 21 | 19 |
| 3 | -6 | 7 | 49 | 46 |
| 3 | -7 | 0 | 137 | 131 |
| 3 | -7 | 1 | 26 | -23 |
| 3 | -7 | 2 | 63 | 51 |
| 3 | -7 | 4 | 75 | 67 |
| 3 | -7 | 5 | 16 | 9 |
| 3 | -7 | 6 | 63 | 67 |
| 3 | -8 | 1 | 32 | 32 |
| 3 | -8 | 3 | 22 | 19 |
| 3 | 1 | 2 | 257 | 282 |
| 3 | 1 | 3 | 19 | 17 |
| 3 | 1 | 4 | 189 | 210 |
| 3 | 1 | 5 | 41 | 33 |
| 3 | 1 | 6 | 145 | 150 |
| 3 | 1 | 7 | 82 | 88 |
| 3 | 1 | 8 | 100 | 95 |
| 3 | 1 | 9 | 36 | 39 |
| 3 | 1 | 11 | 14 | -17 |
| 3 | 2 | 3 | 169 | 166 |
| 3 | 2 | 4 | 47 | -56 |
| 3 | 2 | 5 | 143 | 153 |
| 3 | 2 | 6 | 17 | -28 |
| 3 | 2 | 7 | 99 | 107 |
| 3 | 2 | 8 | 32 | 31 |
| 3 | 2 | 9 | 25 | 30 |
| 3 | 2 | 10 | 22 | -31 |
| 3 | 3 | 4 | 106 | 98 |
| 3 | 3 | 5 | 62 | -66 |
| 3 | 3 | 6 | 113 | 112 |
| 3 | 3 | 8 | 60 | 65 |
| 3 | 3 | 10 | 28 | 38 |
| 3 | 4 | 4 | 13 | 5 |
| 3 | 4 | 5 | 57 | 57 |
| 3 | 4 | 6 | 12 | 6 |
| 3 | 4 | 7 | 59 | 59 |
| 3 | 4 | 8 | 29 | 33 |
| 3 | 4 | 9 | 52 | 71 |
| 3 | 5 | 4 | 37 | 32 |
| 3 | 5 | 6 | 67 | 64 |
| 3 | 5 | 7 | 16 | 15 |
| 3 | 5 | 8 | 41 | 46 |
| 3 | 6 | 3 | 38 | 30 |
| 3 | 6 | 4 | 12 | -8 |
| 3 | 6 | 5 | 62 | 71 |
| 3 | 6 | 6 | 11 | 5 |
| 3 | 6 | 7 | 40 | 38 |
| 3 | 7 | 1 | 23 | 20 |
| 3 | 7 | 2 | 25 | 20 |
| 3 | 7 | 4 | 36 | 38 |
| 4 | 0 | 1 | 44 | 38 |
| 4 | 0 | 2 | 197 | 198 |
| 4 | 0 | 3 | 51 | 45 |
| 4 | 0 | 4 | 228 | 233 |
| 4 | 0 | 5 | 73 | 58 |
| 4 | 0 | 6 | 102 | 95 |
| 4 | 0 | 8 | 46 | 49 |
| 4 | 0 | 9 | 11 | -14 |
| 4 | 0 | 10 | 37 | 40 |
| 4 | 0 | 11 | 20 | 29 |
| 4 | -1 | 1 | 65 | 73 |
| 4 | -1 | 2 | 39 | -33 |
| 4 | -1 | 3 | 92 | 82 |
| 4 | -1 | 4 | 75 | 63 |
| 4 | -1 | 5 | 97 | 95 |
| 4 | -1 | 6 | 31 | 23 |
| 4 | -1 | 7 | 31 | 36 |
| 4 | -1 | 9 | 65 | 90 |
| 4 | -1 | 10 | 14 | 8 |
| 4 | -1 | 11 | 38 | 53 |

TABLE 5 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 4 | -2 | 0 | 240 | 231 |
| 4 | -2 | 1 | 126 | -105 |
| 4 | -2 | 2 | 113 | 114 |
| 4 | -2 | 3 | 21 | -10 |
| 4 | -2 | 4 | 98 | 93 |
| 4 | -2 | 5 | 33 | 28 |
| 4 | -2 | 6 | 53 | 46 |
| 4 | -2 | 7 | 21 | -28 |
| 4 | -2 | 8 | 68 | 69 |
| 4 | -2 | 9 | 10 | -0 |
| 4 | -2 | 10 | 70 | 92 |
| 4 | -3 | 1 | 236 | 212 |
| 4 | -3 | 2 | 123 | -112 |
| 4 | -3 | 3 | 112 | 102 |
| 4 | -3 | 4 | 31 | 25 |
| 4 | -3 | 5 | 89 | 83 |
| 4 | -3 | 6 | 56 | -57 |
| 4 | -3 | 7 | 32 | 38 |
| 4 | -3 | 8 | 23 | -26 |
| 4 | -3 | 9 | 62 | 76 |
| 4 | -3 | 11 | 26 | 48 |
| 4 | -4 | 0 | 190 | 158 |
| 4 | -4 | 1 | 91 | -76 |
| 4 | -4 | 2 | 140 | 121 |
| 4 | -4 | 3 | 45 | 38 |
| 4 | -4 | 4 | 132 | 115 |
| 4 | -4 | 5 | 53 | 47 |
| 4 | -4 | 6 | 71 | 71 |
| 4 | -4 | 8 | 39 | 31 |
| 4 | -4 | 9 | 30 | 32 |
| 4 | -4 | 10 | 37 | 47 |
| 4 | -5 | 1 | 64 | 54 |
| 4 | -5 | 2 | 53 | -47 |
| 4 | -5 | 3 | 122 | 99 |
| 4 | -5 | 4 | 46 | 38 |
| 4 | -5 | 5 | 108 | 104 |
| 4 | -5 | 6 | 6 | 3 |
| 4 | -5 | 7 | 45 | 42 |
| 4 | -5 | 8 | 21 | 20 |
| 4 | -5 | 9 | 19 | 15 |
| 4 | -6 | 0 | 29 | -22 |
| 4 | -6 | 1 | 46 | -35 |
| 4 | -6 | 2 | 38 | 34 |
| 4 | -6 | 3 | 17 | -17 |
| 4 | -6 | 4 | 73 | 73 |
| 4 | -6 | 6 | 51 | 57 |
| 4 | -6 | 8 | 13 | 14 |
| 4 | -7 | 1 | 55 | 49 |
| 4 | -7 | 2 | 11 | -13 |
| 4 | -7 | 3 | 83 | 81 |
| 4 | -7 | 5 | 53 | 56 |
| 4 | -7 | 7 | 25 | 32 |
| 4 | -8 | 0 | 39 | 33 |
| 4 | -8 | 1 | 17 | 20 |
| 4 | -8 | 2 | 57 | 55 |
| 4 | -8 | 3 | 8 | 4 |
| 4 | -8 | 4 | 41 | 41 |
| 4 | 1 | 2 | 48 | 64 |
| 4 | 1 | 3 | 219 | 219 |
| 4 | 1 | 4 | 13 | -5 |
| 4 | 1 | 5 | 153 | 141 |
| 4 | 1 | 6 | 23 | 13 |
| 4 | 1 | 7 | 58 | 60 |
| 4 | 1 | 8 | 50 | -55 |
| 4 | 1 | 9 | 35 | 45 |
| 4 | 1 | 11 | 20 | 18 |
| 4 | 2 | 3 | 59 | -66 |
| 4 | 2 | 4 | 138 | 135 |
| 4 | 2 | 5 | 30 | -31 |
| 4 | 2 | 6 | 67 | 68 |
| 4 | 2 | 7 | 27 | -30 |
| 4 | 2 | 8 | 59 | 69 |
| 4 | 2 | 9 | 49 | -60 |
| 4 | 2 | 10 | 32 | 34 |
| 4 | 3 | 3 | 133 | 121 |
| 4 | 3 | 4 | 30 | -31 |
| 4 | 3 | 5 | 53 | 46 |
| 4 | 3 | 6 | 78 | 81 |
| 4 | 3 | 7 | 73 | 73 |
| 4 | 3 | 8 | 19 | 11 |
| 4 | 3 | 9 | 45 | 50 |
| 4 | 4 | 3 | 55 | -58 |
| 4 | 4 | 4 | 82 | 66 |
| 4 | 4 | 5 | 29 | 31 |
| 4 | 4 | 6 | 54 | 51 |
| 4 | 4 | 7 | 61 | 63 |
| 4 | 4 | 8 | 50 | 54 |
| 4 | 4 | 9 | 8 | -11 |
| 4 | 5 | 3 | 114 | 108 |
| 4 | 5 | 4 | 23 | -17 |
| 4 | 5 | 5 | 62 | 55 |
| 4 | 5 | 6 | 31 | 34 |
| 4 | 5 | 7 | 54 | 56 |
| 4 | 5 | 8 | 10 | 10 |
| 4 | 6 | 2 | 54 | 51 |
| 4 | 6 | 4 | 31 | 26 |
| 4 | 6 | 6 | 35 | 36 |
| 4 | 7 | 1 | 51 | 50 |
| 4 | 7 | 3 | 17 | 14 |
| 4 | 7 | 4 | 11 | 13 |
| 4 | 7 | 5 | 12 | 16 |
| 5 | 0 | 1 | 178 | 196 |
| 5 | 0 | 2 | 27 | 23 |
| 5 | 0 | 3 | 162 | 160 |
| 5 | 0 | 4 | 73 | 66 |
| 5 | 0 | 5 | 46 | 38 |
| 5 | 0 | 6 | 63 | -62 |
| 5 | 0 | 7 | 76 | 70 |
| 5 | 0 | 8 | 12 | 4 |
| 5 | 0 | 9 | 51 | 58 |
| 5 | 0 | 10 | 22 | 23 |
| 5 | -1 | 1 | 11 | -13 |
| 5 | -1 | 2 | 172 | 174 |
| 5 | -1 | 3 | 77 | 53 |
| 5 | -1 | 4 | 99 | 80 |
| 5 | -1 | 6 | 75 | 62 |
| 5 | -1 | 7 | 22 | -25 |
| 5 | -1 | 8 | 67 | 65 |
| 5 | -1 | 9 | 27 | 32 |
| 5 | -1 | 10 | 25 | 34 |
| 5 | -2 | 1 | 65 | 53 |
| 5 | -2 | 2 | 18 | -9 |
| 5 | -2 | 3 | 96 | 79 |
| 5 | -2 | 4 | 16 | 17 |
| 5 | -2 | 5 | 59 | 53 |
| 5 | -2 | 6 | 13 | 13 |
| 5 | -2 | 7 | 78 | 74 |
| 5 | -2 | 8 | 37 | 35 |
| 5 | -2 | 9 | 26 | 34 |
| 5 | -2 | 10 | 17 | 22 |
| 5 | -3 | 0 | 116 | 90 |
| 5 | -3 | 1 | 20 | -16 |
| 5 | -3 | 2 | 119 | 100 |
| 5 | -3 | 3 | 75 | -71 |
| 5 | -3 | 4 | 86 | 83 |
| 5 | -3 | 5 | 25 | -28 |
| 5 | -3 | 6 | 90 | 86 |
| 5 | -3 | 7 | 22 | 11 |
| 5 | -3 | 8 | 45 | 42 |
| 5 | -3 | 9 | 10 | 3 |
| 5 | -3 | 10 | 14 | 25 |
| 5 | -4 | 1 | 120 | 100 |
| 5 | -4 | 3 | 73 | 68 |
| 5 | -4 | 4 | 67 | -61 |
| 5 | -4 | 5 | 85 | 81 |
| 5 | -4 | 7 | 55 | 56 |
| 5 | -4 | 9 | 15 | 21 |
| 5 | -5 | 0 | 145 | 127 |
| 5 | -5 | 1 | 75 | 59 |
| 5 | -5 | 2 | 94 | 77 |
| 5 | -5 | 3 | 22 | 14 |
| 5 | -5 | 4 | 87 | 79 |
| 5 | -5 | 6 | 86 | 73 |
| 5 | -5 | 7 | 21 | 22 |
| 5 | -5 | 8 | 26 | 25 |
| 5 | -6 | 1 | 49 | 42 |
| 5 | -6 | 2 | 65 | 65 |
| 5 | -6 | 3 | 30 | 23 |
| 5 | -6 | 4 | 12 | -13 |
| 5 | -6 | 5 | 70 | 67 |
| 5 | -6 | 6 | 10 | -10 |
| 5 | -6 | 7 | 28 | 32 |
| 5 | -7 | 0 | 44 | 40 |
| 5 | -7 | 1 | 40 | 40 |
| 5 | -7 | 2 | 15 | 11 |
| 5 | -7 | 3 | 15 | 18 |
| 5 | -7 | 4 | 41 | 40 |
| 5 | -7 | 5 | 14 | -20 |
| 5 | -7 | 6 | 29 | 41 |
| 5 | -8 | 1 | 51 | 51 |
| 5 | -8 | 2 | 12 | 12 |
| 5 | -8 | 3 | 18 | 27 |
| 5 | 1 | 2 | 133 | 118 |
| 5 | 1 | 3 | 54 | 35 |
| 5 | 1 | 4 | 69 | 61 |
| 5 | 1 | 5 | 46 | -49 |
| 5 | 1 | 6 | 26 | 30 |
| 5 | 1 | 7 | 61 | -70 |
| 5 | 1 | 8 | 62 | 70 |
| 5 | 1 | 9 | 15 | 8 |
| 5 | 1 | 10 | 38 | 54 |
| 5 | 2 | 3 | 132 | 116 |
| 5 | 2 | 4 | 46 | 39 |
| 5 | 2 | 5 | 77 | 75 |
| 5 | 2 | 6 | 32 | -35 |
| 5 | 2 | 7 | 43 | 42 |
| 5 | 2 | 8 | 23 | 18 |
| 5 | 2 | 9 | 46 | 50 |
| 5 | 2 | 10 | 11 | 7 |
| 5 | 3 | 3 | 52 | 43 |
| 5 | 3 | 4 | 126 | 124 |
| 5 | 3 | 5 | 18 | 10 |
| 5 | 3 | 6 | 52 | 53 |
| 5 | 3 | 7 | 16 | 13 |
| 5 | 3 | 8 | 25 | 22 |
| 5 | 3 | 9 | 24 | 28 |
| 5 | 4 | 3 | 123 | 118 |
| 5 | 4 | 5 | 106 | 105 |
| 5 | 4 | 6 | 16 | -17 |
| 5 | 4 | 7 | 27 | 19 |
| 5 | 5 | 2 | 60 | 48 |
| 5 | 5 | 4 | 70 | 73 |
| 5 | 5 | 5 | 15 | -19 |
| 5 | 5 | 6 | 31 | 30 |
| 5 | 5 | 7 | 7 | 3 |
| 5 | 6 | 1 | 33 | 29 |
| 5 | 6 | 3 | 28 | 27 |
| 5 | 6 | 4 | 31 | -34 |
| 5 | 6 | 5 | 21 | 24 |
| 5 | 7 | 0 | 39 | 38 |
| 5 | 7 | 1 | 10 | 13 |

oxygen orbitals. Using the terminology of Martin and Waterman,[23] the hydrogen-bonds are in both the *syn*- and *anti*-positions, and the copper–oxygen bond in the chelate ring is *anti* (see Figure 15). When the non-chelating carboxy-oxygen makes a short contact to the copper atom (glycollate and lactate), this contact is neither *syn* nor *anti*. The oxygen forms a strong hydrogen-bond in the *syn*-positions, suggesting that there is $sp^2$ hybridisation of the oxygen orbitals. However, the weak copper oxygen interaction is directed out of the plane of the carboxy-group and above the oxygen lone-pair rather than in the direction of the lone-pair. The interactions may be purely electrostatic and non-directional with respect to the oxygen, or perhaps utilise the oxygen π-electrons. The latter alternative seems less likely, since the interaction becomes weaker as its direction moves nearer to the perpendicular to the carboxy-group of the oxygen (lactate). Strong copper interactions in the *anti,anti*-configuration at a carboxy-group, as in the formate tetrahydrate,[24] lead to super-exchange effects. However, these effects are no longer observed as the direction of interaction moves out of the plane and interaction becomes weaker.

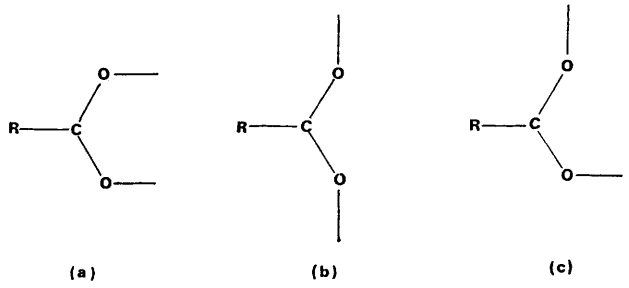


FIGURE 15 Carboxylate configurations (a) *syn,syn*, (b) *anti,anti*, (c) *syn,anti*

The methoxy- and phenoxy-acetate crystal structures differ from those of the 2-hydroxycarboxylates. No hydrogen-bond can be formed between O(2) and O(3), and the molecules are now linked into three-dimensional networks by hydrogen-bonds between the water molecules and the carboxylate groups. In the methoxy-acetate, there are two hydrogen-bonds, one *syn* and one *anti*, to aquo-ligands of two neighbouring complexes. In the phenoxyacetate, hydrogen-bonding is to the chelating as well as to the non-chelating carboxy-oxygens, and bifurcated hydrogen bonds may be formed [Figure 1(b)].

## EXPERIMENTAL

*Preparations.*—Crystals were obtained by slow growth from aqueous solutions of pH < 5 in order to repress hydrolysis. All solutions were prepared in one of two ways.

(A) Basic copper carbonate was dissolved in carboxylic acid and any excess of carbonate filtered off.

(B) Carboxylic acid–sodium carboxylate buffers were added to dilute solutions of copper perchlorate containing a small amount of perchloric acid. These solutions, which had been prepared in connection with our related thermodynamic studies,[2,20] were all made up in a 3M-sodium perchlorate ionic medium. Crystals were analysed for copper

[23] R. L. Martin and H. Waterman, *J. Chem. Soc.*, 1959, 1359.
[24] R. Kiriyama, H. Ibamoto, and K. Matsuo, *Acta Cryst.*, 1954, **7**, 482.

TABLE 6

Observed structure amplitudes and calculated structure factors for bis(glycollato)copper(II)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 0 | 0 | 2 | 20 | 16 |
| 0 | 0 | 4 | 24 | 50 |
| 0 | 0 | 6 | 195 | 185 |
| 0 | 0 | 8 | 115 | 110 |
| 0 | 0 | 10 | 55 | 61 |
| 0 | 1 | 2 | 191 | 173 |
| 0 | 1 | 3 | 101 | -84 |
| 0 | 1 | 4 | 198 | 197 |
| 0 | 1 | 5 | 10 | 9 |
| 0 | 1 | 6 | 103 | 104 |
| 0 | 1 | 7 | 22 | 24 |
| 0 | 1 | 8 | 94 | 90 |
| 0 | 1 | 9 | 10 | 11 |
| 0 | 1 | 10 | 70 | 77 |
| 0 | 2 | 0 | 71 | -29 |
| 0 | 2 | 1 | 229 | -184 |
| 0 | 2 | 2 | 309 | 248 |
| 0 | 2 | 3 | 79 | -59 |
| 0 | 2 | 4 | 267 | 265 |
| 0 | 2 | 5 | 67 | 56 |
| 0 | 2 | 6 | 66 | 61 |
| 0 | 2 | 7 | 16 | 18 |
| 0 | 2 | 8 | 74 | 75 |
| 0 | 2 | 9 | 13 | -10 |
| 0 | 2 | 10 | 60 | 60 |
| 0 | 3 | 0 | 122 | 103 |
| 0 | 3 | 1 | 90 | -63 |
| 0 | 3 | 2 | 154 | 131 |
| 0 | 3 | 3 | 56 | 47 |
| 0 | 3 | 4 | 171 | 152 |
| 0 | 3 | 5 | 38 | -29 |
| 0 | 3 | 6 | 115 | 109 |
| 0 | 3 | 7 | 13 | 11 |
| 0 | 3 | 8 | 68 | 66 |
| 0 | 3 | 9 | 5 | 9 |
| 0 | 4 | 0 | 163 | 138 |
| 0 | 4 | 1 | 70 | 52 |
| 0 | 4 | 2 | 89 | 68 |
| 0 | 4 | 3 | 85 | 73 |
| 0 | 4 | 4 | 108 | 95 |
| 0 | 4 | 5 | 85 | -73 |
| 0 | 4 | 6 | 108 | 90 |
| 0 | 4 | 8 | 40 | 35 |
| 0 | 5 | 0 | 96 | 80 |
| 0 | 5 | 1 | 10 | 7 |
| 0 | 5 | 2 | 89 | 73 |
| 0 | 5 | 3 | 20 | 18 |
| 0 | 5 | 4 | 66 | 49 |
| 0 | 5 | 6 | 57 | 47 |
| 0 | 6 | 0 | 54 | 47 |
| 0 | 6 | 1 | 34 | -33 |
| 0 | 6 | 2 | 59 | 70 |
| 1 | -6 | 1 | 78 | 65 |
| 1 | -6 | 2 | 46 | 41 |
| 1 | -6 | 3 | 23 | 16 |
| 1 | -5 | 1 | 110 | 88 |
| 1 | -5 | 2 | 12 | -8 |
| 1 | -5 | 3 | 100 | 72 |
| 1 | -5 | 4 | 29 | 19 |
| 1 | -5 | 5 | 58 | 36 |
| 1 | -4 | 2 | 116 | -98 |
| 1 | -4 | 3 | 148 | 118 |
| 1 | -4 | 4 | 64 | 44 |
| 1 | -4 | 5 | 28 | 12 |
| 1 | -4 | 6 | 20 | 18 |
| 1 | -3 | 1 | 164 | 141 |
| 1 | -3 | 2 | 25 | -22 |
| 1 | -3 | 3 | 208 | 185 |
| 1 | -3 | 4 | 29 | -22 |
| 1 | -3 | 5 | 85 | 71 |
| 1 | -3 | 6 | 22 | -28 |
| 1 | -3 | 7 | 105 | 99 |
| 1 | -3 | 8 | 71 | 69 |
| 1 | -2 | 1 | 91 | 81 |
| 1 | -2 | 2 | 97 | 71 |
| 1 | -2 | 3 | 258 | 280 |
| 1 | -2 | 4 | 92 | -83 |
| 1 | -2 | 5 | 176 | 198 |
| 1 | -2 | 7 | 79 | 65 |
| 1 | -2 | 8 | 60 | 49 |
| 1 | -2 | 9 | 61 | 49 |
| 1 | -1 | 1 | 202 | 218 |
| 1 | -1 | 2 | 48 | 35 |
| 1 | -1 | 3 | 152 | 168 |
| 1 | -1 | 4 | 24 | -18 |
| 1 | -1 | 5 | 195 | 215 |
| 1 | -1 | 6 | 71 | 64 |
| 1 | -1 | 7 | 171 | 166 |
| 1 | -1 | 8 | 78 | -72 |
| 1 | -1 | 9 | 16 | 9 |
| 1 | -1 | 10 | 15 | 14 |
| 1 | -1 | 11 | 35 | 47 |
| 1 | 0 | 2 | 127 | 113 |
| 1 | 0 | 3 | 123 | 131 |
| 1 | 0 | 4 | 41 | 41 |
| 1 | 0 | 5 | 99 | 108 |
| 1 | 0 | 6 | 7 | -8 |
| 1 | 0 | 7 | 196 | 215 |
| 1 | 0 | 8 | 75 | -73 |
| 1 | 0 | 9 | 30 | 21 |
| 1 | 0 | 10 | 37 | 37 |
| 1 | 0 | 11 | 39 | 45 |
| 1 | 1 | 1 | 235 | 220 |
| 1 | 1 | 2 | 28 | 46 |
| 11 | 1 | 3 | 308 | 306 |
| 1 | 1 | 4 | 58 | 39 |
| 1 | 1 | 5 | 74 | 73 |
| 1 | 1 | 6 | 34 | -35 |
| 1 | 1 | 7 | 79 | 65 |
| 1 | 1 | 8 | 20 | -19 |
| 1 | 1 | 9 | 111 | 108 |
| 1 | 1 | 10 | 20 | 24 |
| 1 | 2 | 1 | 231 | 195 |
| 1 | 2 | 2 | 86 | -70 |
| 1 | 2 | 3 | 215 | 200 |
| 1 | 2 | 4 | 26 | -23 |
| 1 | 2 | 5 | 118 | 110 |
| 1 | 2 | 6 | 64 | 54 |
| 1 | 2 | 7 | 30 | 18 |
| 1 | 2 | 8 | 10 | -13 |
| 1 | 2 | 9 | 109 | 121 |
| 1 | 3 | 1 | 228 | 183 |
| 1 | 3 | 2 | 21 | 14 |
| 1 | 3 | 3 | 68 | 50 |
| 1 | 3 | 4 | 102 | -89 |
| 1 | 3 | 5 | 139 | 122 |
| 1 | 3 | 6 | 62 | 56 |
| 1 | 3 | 7 | 84 | 79 |
| 1 | 3 | 8 | 11 | 10 |
| 1 | 3 | 9 | 52 | 51 |
| 1 | 4 | 1 | 111 | 83 |
| 1 | 4 | 2 | 44 | 32 |
| 1 | 4 | 3 | 94 | 73 |
| 1 | 4 | 4 | 51 | -39 |
| 1 | 4 | 5 | 117 | 101 |
| 1 | 4 | 6 | 11 | 6 |
| 1 | 4 | 7 | 79 | 63 |
| 1 | 4 | 8 | 9 | 13 |
| 1 | 5 | 1 | 58 | 41 |
| 1 | 5 | 2 | 35 | -28 |
| 1 | 5 | 3 | 94 | 70 |
| 1 | 5 | 4 | 46 | 40 |
| 1 | 5 | 5 | 86 | 74 |
| 2 | -6 | -1 | 28 | -19 |
| 2 | -6 | 0 | 48 | 45 |
| 2 | -6 | 2 | 48 | 40 |
| 2 | -5 | -5 | 39 | -29 |
| 2 | -5 | -4 | 127 | 112 |
| 2 | -5 | -3 | 32 | -27 |
| 2 | -5 | -2 | 74 | 65 |
| 2 | -5 | -1 | 50 | 42 |
| 2 | -5 | 0 | 69 | 55 |
| 2 | -5 | 6 | 50 | 34 |
| 2 | -4 | -6 | 64 | 42 |
| 2 | -4 | -5 | 14 | -12 |
| 2 | -4 | -4 | 123 | 105 |
| 2 | -4 | -3 | 44 | -33 |
| 2 | -4 | -2 | 90 | 77 |
| 2 | -4 | -1 | 11 | 15 |
| 2 | -4 | 0 | 204 | 197 |
| 2 | -3 | -6 | 62 | 57 |
| 2 | -3 | -5 | 77 | 85 |
| 2 | -3 | -4 | 106 | 104 |
| 2 | -3 | -3 | 27 | -19 |
| 2 | -3 | -2 | 147 | 140 |
| 2 | -3 | -1 | 131 | -118 |
| 2 | -3 | 0 | 258 | 275 |
| 2 | -2 | -6 | 94 | 102 |
| 2 | -2 | -5 | 26 | 35 |
| 2 | -2 | -4 | 127 | 148 |
| 2 | -2 | -3 | 34 | 35 |
| 2 | -2 | -2 | 202 | 225 |
| 2 | -2 | -1 | 63 | 52 |
| 2 | -2 | 0 | 197 | 199 |
| 2 | -1 | -3 | 37 | 20 |
| 2 | -1 | 0 | 280 | 287 |
| 2 | -1 | 1 | 366 | -377 |
| 2 | -1 | 2 | 178 | 180 |
| 2 | -1 | 4 | 130 | 141 |
| 2 | -1 | 5 | 83 | 72 |
| 2 | -1 | 6 | 165 | 205 |
| 2 | 0 | 0 | 192 | 195 |
| 2 | 0 | 1 | 153 | -128 |
| 2 | 0 | 2 | 150 | 164 |
| 2 | 0 | 3 | 105 | 87 |
| 2 | 0 | 4 | 183 | 228 |
| 2 | 0 | 5 | 30 | -15 |
| 2 | 0 | 6 | 147 | 178 |
| 2 | 1 | 0 | 81 | -52 |
| 2 | 1 | 1 | 156 | 119 |
| 2 | 1 | 2 | 284 | 270 |
| 2 | 1 | 3 | 99 | 78 |
| 2 | 1 | 4 | 257 | 269 |
| 2 | 1 | 5 | 57 | -43 |
| 2 | 1 | 6 | 71 | 64 |
| 2 | 2 | 0 | 103 | 111 |
| 2 | 2 | 1 | 56 | 49 |
| 2 | 2 | 2 | 271 | 242 |
| 2 | 2 | 3 | 26 | 24 |
| 2 | 2 | 4 | 80 | 75 |
| 2 | 2 | 6 | 99 | 85 |
| 2 | 3 | 0 | 239 | 214 |
| 2 | 3 | 2 | 162 | 140 |
| 2 | 3 | 3 | 17 | 14 |
| 2 | 3 | 4 | 17 | -15 |
| 2 | 3 | 5 | 24 | -24 |
| 2 | 3 | 6 | 130 | 110 |
| 2 | 4 | 0 | 125 | 97 |
| 2 | 4 | 1 | 20 | -18 |
| 2 | 4 | 2 | 103 | 82 |
| 2 | 4 | 3 | 24 | -19 |
| 2 | 4 | 4 | 78 | 57 |
| 2 | 4 | 6 | 71 | 57 |
| 2 | 5 | 0 | 26 | 18 |
| 2 | 5 | 1 | 18 | -12 |
| 2 | 5 | 2 | 80 | 57 |
| 2 | 5 | 3 | 59 | -44 |
| 2 | 5 | 4 | 90 | 71 |
| 3 | -6 | 1 | 50 | 47 |
| 3 | -6 | 2 | 17 | -22 |
| 3 | -6 | 3 | 58 | 57 |
| 3 | -5 | -5 | 81 | 71 |
| 3 | -5 | -2 | 24 | 29 |
| 3 | -5 | -1 | 37 | 32 |
| 3 | -5 | 3 | 145 | 128 |
| 3 | -5 | 5 | 83 | 71 |
| 3 | -5 | 6 | 63 | 49 |
| 3 | -4 | -6 | 20 | -15 |
| 3 | -4 | -5 | 78 | 74 |
| 3 | -4 | -4 | 33 | 34 |
| 3 | -4 | -3 | 139 | 125 |
| 3 | -4 | -2 | 68 | -63 |
| 3 | -4 | -1 | 100 | 91 |
| 3 | -3 | -6 | 43 | 55 |
| 3 | -3 | -5 | 108 | 105 |
| 3 | -3 | -4 | 34 | 31 |
| 3 | -3 | -3 | 115 | 114 |
| 3 | -3 | -2 | 160 | -162 |
| 3 | -3 | -1 | 175 | 177 |
| 3 | -2 | 1 | 277 | 273 |
| 3 | -2 | 2 | 17 | -28 |
| 3 | -2 | 3 | 104 | 94 |
| 3 | -2 | 4 | 44 | 38 |
| 3 | -2 | 5 | 138 | 146 |
| 3 | -2 | 6 | 22 | 13 |
| 3 | -1 | 1 | 320 | 340 |
| 3 | -1 | 2 | 184 | -170 |
| 3 | -1 | 3 | 61 | 66 |
| 3 | -1 | 4 | 22 | 13 |
| 3 | -1 | 5 | 141 | 134 |
| 3 | -1 | 6 | 101 | 94 |
| 3 | 0 | 1 | 178 | 168 |
| 3 | 0 | 3 | 231 | 234 |
| 3 | 0 | 4 | 85 | -81 |
| 3 | 0 | 5 | 125 | 128 |
| 3 | 0 | 6 | 34 | 26 |
| 3 | 1 | 1 | 56 | 54 |
| 3 | 1 | 2 | 13 | 16 |
| 3 | 1 | 3 | 253 | 269 |
| 3 | 1 | 4 | 24 | -21 |
| 3 | 1 | 5 | 162 | 170 |
| 3 | 1 | 6 | 30 | -29 |
| 3 | 2 | 1 | 168 | 150 |
| 3 | 2 | 3 | 70 | 60 |
| 3 | 2 | 4 | 48 | 44 |
| 3 | 2 | 5 | 181 | 170 |
| 3 | 2 | 6 | 33 | -29 |
| 3 | 3 | 1 | 187 | 151 |
| 3 | 3 | 2 | 43 | 38 |
| 3 | 3 | 3 | 18 | 15 |
| 3 | 3 | 4 | 23 | 21 |
| 3 | 3 | 5 | 113 | 97 |
| 3 | 3 | 6 | 30 | -29 |
| 3 | 4 | 1 | 95 | 68 |
| 3 | 4 | 3 | 121 | 90 |
| 3 | 4 | 4 | 23 | 16 |
| 3 | 4 | 6 | 8 | -11 |
| 3 | 5 | 1 | 52 | 40 |
| 3 | 5 | 2 | 41 | -39 |
| 4 | -6 | 0 | 25 | 26 |
| 4 | -6 | 1 | 17 | -15 |
| 4 | -6 | 2 | 78 | 81 |
| 4 | -6 | 3 | 14 | 9 |
| 4 | -6 | 4 | 40 | 47 |
| 4 | -5 | 0 | 38 | 41 |
| 4 | -5 | 1 | 68 | -66 |
| 4 | -5 | 2 | 95 | 108 |
| 4 | -5 | 3 | 5 | -2 |
| 4 | -5 | 4 | 61 | 65 |
| 4 | -5 | 6 | 40 | 29 |
| 4 | -4 | 0 | 123 | 147 |
| 4 | -4 | 2 | 73 | 81 |
| 4 | -4 | 3 | 10 | 6 |
| 4 | -4 | 4 | 67 | 69 |
| 4 | -4 | 5 | 42 | -42 |
| 4 | -4 | 6 | 115 | 114 |
| 4 | -3 | -2 | 121 | 119 |
| 4 | -3 | 0 | 77 | 106 |
| 4 | -3 | 1 | 63 | 59 |
| 4 | -3 | 3 | 16 | 15 |
| 4 | -3 | 4 | 119 | 132 |
| 4 | -3 | 5 | 27 | -33 |
| 4 | -3 | 6 | 127 | 138 |
| 4 | -2 | 1 | 45 | -33 |
| 4 | -2 | 2 | 218 | 233 |
| 4 | -2 | 3 | 16 | 9 |
| 4 | -2 | 4 | 136 | 137 |
| 4 | -2 | 5 | 87 | 78 |
| 4 | -2 | 6 | 131 | 109 |
| 4 | -1 | 0 | 144 | 161 |
| 4 | -1 | 1 | 27 | -30 |
| 4 | -1 | 2 | 259 | 266 |
| 4 | -1 | 3 | 47 | 40 |
| 4 | -1 | 4 | 42 | 59 |
| 4 | -1 | 5 | 52 | 37 |
| 4 | -1 | 6 | 104 | 91 |
| 4 | 0 | 0 | 192 | 206 |
| 4 | 0 | 1 | 127 | 105 |
| 4 | 0 | 2 | 238 | 205 |
| 4 | 0 | 3 | 22 | 13 |
| 4 | 0 | 4 | 98 | 109 |
| 4 | 0 | 5 | 73 | -71 |
| 4 | 0 | 6 | 63 | 55 |
| 4 | 1 | 0 | 160 | 166 |
| 4 | 1 | 1 | 61 | 54 |
| 4 | 1 | 2 | 137 | 132 |
| 4 | 1 | 3 | 88 | -89 |
| 4 | 1 | 4 | 145 | 135 |
| 4 | 1 | 5 | 19 | 6 |
| 4 | 1 | 6 | 85 | 76 |
| 4 | 2 | 0 | 144 | 151 |
| 4 | 2 | 1 | 8 | -7 |
| 4 | 2 | 2 | 92 | 87 |
| 4 | 2 | 3 | 97 | -79 |
| 4 | 2 | 4 | 81 | 69 |
| 4 | 2 | 5 | 69 | 55 |
| 4 | 2 | 6 | 129 | 122 |
| 4 | 3 | 0 | 79 | 65 |
| 4 | 3 | 1 | 8 | 6 |
| 4 | 3 | 2 | 88 | 72 |
| 4 | 3 | 3 | 10 | 4 |
| 4 | 3 | 4 | 88 | 79 |
| 4 | 3 | 6 | 96 | 73 |
| 4 | 4 | 0 | 37 | 31 |
| 4 | 4 | 1 | 9 | 5 |
| 4 | 4 | 2 | 65 | 47 |
| 4 | 4 | 3 | 33 | 22 |
| 4 | 4 | 4 | 116 | 97 |
| 5 | -6 | 1 | 38 | 38 |
| 5 | -6 | 2 | 22 | 27 |
| 5 | -6 | 3 | 50 | 67 |
| 5 | -5 | 1 | 98 | 108 |
| 5 | -5 | 2 | 16 | 16 |
| 5 | -5 | 3 | 27 | 31 |
| 5 | -5 | 4 | 14 | -17 |
| 5 | -5 | 5 | 59 | 61 |
| 5 | -5 | 6 | 31 | 20 |
| 5 | -4 | 1 | 146 | 166 |
| 5 | -4 | 3 | 20 | 16 |
| 5 | -4 | 4 | 23 | -35 |
| 5 | -4 | 5 | 56 | 63 |
| 5 | -4 | 6 | 19 | 11 |
| 5 | -3 | 1 | 97 | 108 |
| 5 | -3 | 2 | 64 | -71 |
| 5 | -3 | 3 | 104 | 130 |
| 5 | -3 | 4 | 33 | 21 |
| 5 | -3 | 5 | 92 | 104 |
| 5 | -2 | 1 | 70 | 75 |
| 5 | -2 | 2 | 116 | -133 |
| 5 | -2 | 3 | 156 | 180 |
| 5 | -2 | 4 | 83 | 81 |
| 5 | -2 | 5 | 158 | 158 |
| 5 | -1 | 1 | 126 | 134 |
| 5 | -1 | 2 | 73 | 62 |
| 5 | -1 | 3 | 125 | 125 |
| 5 | -1 | 5 | 141 | 144 |
| 5 | -1 | 6 | 38 | -31 |
| 5 | 0 | 1 | 151 | 141 |
| 5 | 0 | 2 | 146 | 153 |
| 5 | 0 | 3 | 143 | 144 |
| 5 | 0 | 4 | 27 | -37 |
| 5 | 0 | 5 | 78 | 75 |
| 5 | 0 | 6 | 49 | -52 |
| 5 | 1 | 1 | 171 | 148 |
| 5 | 1 | 2 | 29 | -29 |
| 5 | 1 | 3 | 116 | 108 |
| 5 | 1 | 4 | 52 | 40 |
| 5 | 1 | 5 | 44 | 33 |
| 5 | 2 | 1 | 154 | 136 |
| 5 | 2 | 2 | 89 | -83 |
| 5 | 2 | 3 | 53 | 44 |
| 5 | 2 | 4 | 48 | 42 |
| 5 | 2 | 5 | 55 | 40 |
| 5 | 3 | 1 | 65 | 54 |
| 5 | 3 | 3 | 107 | 78 |
| 5 | 3 | 4 | 18 | -18 |
| 5 | 3 | 5 | 65 | 50 |
| 5 | 3 | 6 | 6 | 8 |
| 5 | 4 | 1 | 14 | 8 |
| 5 | 4 | 2 | 12 | 13 |
| 6 | -6 | 0 | 15 | -22 |
| 6 | -6 | 1 | 25 | 34 |
| 6 | -6 | 2 | 50 | 73 |
| 6 | -5 | 0 | 51 | 68 |
| 6 | -5 | 1 | 13 | 13 |
| 6 | -5 | 2 | 56 | 77 |
| 6 | -5 | 3 | 8 | 11 |
| 6 | -5 | 4 | 18 | 22 |
| 6 | -5 | 5 | 10 | 9 |
| 6 | -5 | 6 | 74 | 77 |
| 6 | -4 | 1 | 24 | 20 |
| 6 | -4 | 2 | 52 | 73 |
| 6 | -4 | 3 | 14 | 22 |
| 6 | -4 | 4 | 22 | 28 |
| 6 | -4 | 5 | 6 | -0 |
| 6 | -4 | 6 | 73 | 75 |
| 6 | -3 | 0 | 94 | 118 |
| 6 | -3 | 1 | 23 | 13 |
| 6 | -3 | 2 | 89 | 110 |
| 6 | -3 | 3 | 30 | -40 |
| 6 | -3 | 4 | 93 | 110 |
| 6 | -3 | 5 | 42 | 34 |
| 6 | -3 | 6 | 20 | 18 |
| 6 | -2 | 0 | 83 | 93 |
| 6 | -2 | 2 | 117 | 136 |
| 6 | -2 | 3 | 83 | -91 |
| 6 | -2 | 4 | 98 | 115 |
| 6 | -2 | 5 | 56 | 50 |
| 6 | -2 | 6 | 38 | 39 |
| 6 | -1 | 0 | 112 | 130 |
| 6 | -1 | 1 | 56 | 44 |
| 6 | -1 | 2 | 90 | 101 |
| 6 | -1 | 3 | 24 | -24 |
| 6 | -1 | 4 | 92 | 97 |
| 6 | -1 | 5 | 34 | -36 |
| 6 | -1 | 6 | 97 | 102 |
| 6 | 0 | 0 | 103 | 122 |
| 6 | 0 | 1 | 31 | 25 |
| 6 | 0 | 2 | 49 | 55 |
| 6 | 0 | 3 | 33 | 35 |
| 6 | 0 | 4 | 125 | 142 |
| 6 | 0 | 5 | 34 | -38 |
| 6 | 0 | 6 | 88 | 91 |
| 6 | 1 | 0 | 134 | 142 |
| 6 | 1 | 1 | 29 | -30 |
| 6 | 1 | 2 | 30 | 40 |
| 6 | 1 | 3 | 17 | 15 |
| 6 | 1 | 4 | 100 | 111 |
| 6 | 1 | 5 | 43 | 40 |
| 6 | 1 | 6 | 70 | 61 |
| 6 | 2 | 0 | 114 | 119 |
| 6 | 2 | 2 | 68 | 62 |
| 6 | 2 | 3 | 9 | 9 |
| 6 | 2 | 4 | 45 | 44 |
| 6 | 2 | 5 | 19 | 15 |
| 6 | 2 | 6 | 44 | 35 |
| 6 | 3 | 0 | 40 | 40 |
| 6 | 3 | 2 | 82 | 72 |
| 6 | 3 | 3 | 22 | 17 |
| 6 | 3 | 4 | 39 | 41 |
| 7 | -6 | 1 | 27 | 40 |
| 7 | -5 | 1 | 49 | 69 |
| 7 | -5 | 2 | 19 | -31 |
| 7 | -5 | 3 | 19 | 17 |
| 7 | -5 | 4 | 11 | 17 |
| 7 | -5 | 5 | 57 | 77 |
| 7 | -4 | 1 | 38 | 58 |
| 7 | -4 | 2 | 17 | 24 |
| 7 | -4 | 3 | 61 | 86 |
| 7 | -4 | 4 | 14 | 11 |
| 7 | -4 | 5 | 39 | 54 |
| 7 | -4 | 6 | 14 | -17 |
| 7 | -3 | 1 | 38 | 48 |
| 7 | -3 | 2 | 18 | 17 |
| 7 | -3 | 3 | 131 | 165 |
| 7 | -3 | 4 | 36 | 29 |
| 7 | -3 | 5 | 18 | 19 |
| 7 | -3 | 6 | 24 | -27 |
| 7 | -2 | 1 | 121 | 126 |
| 7 | -2 | 3 | 63 | 84 |
| 7 | -2 | 4 | 16 | 15 |
| 7 | -2 | 5 | 27 | 27 |
| 7 | -1 | 1 | 131 | 151 |
| 7 | -1 | 2 | 18 | 25 |
| 7 | -1 | 3 | 35 | 26 |
| 7 | -1 | 4 | 37 | -46 |
| 7 | -1 | 5 | 46 | 60 |
| 7 | -1 | 6 | 18 | 7 |
| 7 | 0 | 1 | 66 | 71 |
| 7 | 0 | 2 | 17 | -16 |
| 7 | 0 | 3 | 93 | 94 |
| 7 | 0 | 4 | 27 | -35 |
| 7 | 0 | 5 | 62 | 67 |
| 7 | 0 | 6 | 47 | 42 |
| 7 | 1 | 1 | 35 | 37 |
| 7 | 1 | 2 | 36 | -48 |
| 7 | 1 | 3 | 96 | 104 |
| 7 | 1 | 4 | 14 | 15 |
| 7 | 1 | 6 | 53 | 51 |
| 7 | 2 | 1 | 49 | 46 |
| 7 | 2 | 2 | 21 | 21 |
| 7 | 2 | 3 | 58 | 57 |
| 8 | -5 | 3 | 13 | -23 |
| 8 | -4 | 0 | 30 | 42 |
| 8 | -4 | 1 | 12 | -19 |
| 8 | -4 | 2 | 29 | 47 |
| 8 | -4 | 3 | 8 | 8 |
| 8 | -4 | 4 | 64 | 96 |
| 8 | -4 | 5 | 12 | -16 |
| 8 | -3 | 0 | 35 | 43 |
| 8 | -3 | 3 | 16 | 14 |

TABLE 6 (*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 | $\|F_o\|$ | $F_c$ | h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| 8 | -3 | 5 | 10 | -12 | 8 | -1 | 2 | 61 | 78 | 8 | 0 | 4 | 45 | 54 | 9 | -4 | 2 | 15 | 26 | 9 | -2 | 5 | 48 | 70 |
| 8 | -3 | 6 | 30 | 29 | 8 | -1 | 3 | 38 | 40 | 8 | 0 | 5 | 9 | 5 | 9 | -4 | 3 | 43 | 71 | 9 | -1 | 1 | 36 | 57 |
| 8 | -2 | 0 | 96 | 126 | 8 | -1 | 4 | 14 | 16 | 8 | 0 | 6 | 19 | 19 | 9 | -3 | 1 | 26 | 41 | 9 | -1 | 2 | 18 | 21 |
| 8 | -2 | 1 | 18 | 25 | 8 | -1 | 5 | 15 | -26 | 8 | 1 | 0 | 40 | 49 | 9 | -3 | 3 | 48 | 74 | 9 | -1 | 3 | 23 | 33 |
| 8 | -2 | 2 | 34 | 49 | 8 | -1 | 6 | 50 | 62 | 8 | 1 | 1 | 43 | -52 | 9 | -3 | 4 | 20 | -30 | 9 | 0 | 1 | 31 | 40 |
| 8 | -2 | 3 | 19 | 20 | 8 | 0 | 0 | 43 | 56 | 8 | 1 | 2 | 48 | 57 | 9 | -3 | 5 | 21 | 39 | 9 | 0 | 2 | 10 | 11 |
| 8 | -2 | 4 | 36 | 51 | 8 | 0 | 1 | 62 | -66 | 8 | 1 | 3 | 9 | -13 | 9 | -2 | 1 | 50 | 69 | 9 | 0 | 3 | 43 | 65 |
| 8 | -2 | 6 | 58 | 72 | 8 | 0 | 2 | 66 | 85 | 8 | 1 | 4 | 47 | 51 | 9 | -2 | 3 | 13 | 20 | 10 | -1 | 0 | 16 | -20 |
| 8 | -1 | 0 | 86 | 121 | 8 | 0 | 3 | 23 | 19 | 9 | -4 | 1 | 27 | 45 | | | | | | | | | | |

by complexometric titration using EDTA with murexide as indicator.[25]

*Bis(glycollato)copper*(II). Method B (Found: C, 22·4; H, 2·75; Cu, 29·3. $C_4H_6CuO_6$ requires C, 22·5; H, 2·85; Cu, 29·7%.)

*Aquobis*-(DL-*lactato*)*copper*(II) *hemihydrate*. Method A, the blue surfaces of these crystals became coated with a white sheen on standing, owing to efflorescence. Analyses of various batches indicated a variable loss of water. An anhydrous sample was obtained by dehydration in a vacuum-desiccator over phosphorus pentoxide (Found: C, 29·9; H, 4·15; Cu, 26·3. $C_6H_{10}CuO_6$ requires C, 29·8; H, 4·15; Cu, 26·3%).

*Diaquobis*-(2-*hydroxy*-2-*methylpropionato*)*copper*(II). Method A (Found: C, 31·3; H, 6·2; Cu, 20·6. $C_8H_{18}CuO_8$ requires C, 31·4; H, 5·95; Cu, 20·8%).

*Diaquobis*(*methoxyacetato*)*copper*(II). Method B (Found: C, 25·8; H, 5·1; Cu, 23·0. $C_6H_{14}CuO_8$ requires C, 25·9; H, 5·05; Cu, 22·9%).

*Diaquobis*(*phenoxyacetato*)*copper*(II). Method B (Found: C, 47·9; H, 4·5; Cu, 15·6. $C_{16}H_{18}CuO_8$ requires C, 47·8; H, 4·5; Cu, 15·8%). In the absence of sodium perchlorate, clusters of green needle-shaped anhydrous bis(phenoxyacetato)copper(II) crystals were obtained. These are the subject of a continuing investigation.

X-*Ray Photography*.—Crystals of all five complexes were monoclinic needles. The unit cell dimensions were obtained from calibrated zero-layer Weissenberg photographs taken about the needle axis and a second principal axis of the crystal so that one photograph was taken about the unique axis of the crystal. The *X*-ray intensities were estimated visually from sets of multiple-film Weissenberg photographs about the needle axis of the crystals. The results from individual layers were placed on a common scale either by using the exposure time to *X*-rays from a stabilised source and standardised development conditions [diaquobis(phenoxyacetato)copper(II), diaquobis-(2-hydroxy-2-methylpropionato)copper(II), and aquobis-(lactato)copper(II) hemihydrate] or by using intensities collected about a second axis [bis(glycollato)copper(II) and diaquobis(methoxyacetato)copper(II)] with layer scale factor calculated by the method of Hamilton, Rollett, and Sparks.[26] All intensities were corrected for Lorentz and polarisation factors but not for extinction or absorption.

*Calculations*.—Structure factors, cycles of least-squares refinement, Fourier syntheses, and interatomic distances were computed on an English Electric KDF9 computer using J. S. Rollett's 'Novtape' programme [27] as modified and extended by J. Hodder. Atomic scattering factors for carbon, oxygen, hydrogen, and copper were taken from International Tables.[28] An anomalous-dispersion correction was applied to the scattering curve for copper.

[25] G. Schwarzenbach, 'Complexometric Titrations,' Methuen, London, 1957.

[26] W. C. Hamilton, J. S. Rollett, and R. A. Sparks, *Acta Cryst.*, 1965, **18**, 129.

Details of individual structure analyses follow. In each case, the authors mainly responsible for the experimental work are given in parentheses.

*Diaquobis*(*phenoxyacetato*)*copper*(II) (R. A. Armstrong).—$C_{16}H_{18}CuO_8$, $M$ 401·85, Monoclinic prismatic, $a = 16·26 \pm 0·04$, $b = 7·28 \pm 0·03$, $c = 23·99 \pm 0·06$ Å, $\gamma = 110·4 \pm 0·3°$. $U = 2653$ Å$^3$, $D_m = 1·531 \pm 0·01$ (by flotation), $Z = 6$, $D_c = 1·510$. Space group $P2_1/n$ ($C_{2h}^5$, No. 14), general positions $\pm (x, y, z; \frac{1}{2} + x, \frac{1}{2} + y, \frac{1}{2} - z)$. Cu-$K_\alpha$ radiation, $\mu = 15·35$ cm.$^{-1}$, crystal size 0·12 × 0·15 × 1·0 mm. Optically biaxial.

To have six bis(phenoxyacetato)copper(II) molecules in a unit cell in space group $P2_1/n$ it is necessary that they should be of at least two crystallographically dissimilar types. If two molecules lie with their copper atoms at the inversion centres at 0,0,0 and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$, then the other four may have copper atoms in general positions and the molecules need not be centrosymmetric. The oscillation photographs about the *a*-axis shows layers 0, 3, 6, and 9 much more intense than the rest, suggesting molecules in similar orientations separated from each other by *a*/3.

A three-dimensional Patterson function sharpened to 'point atoms at rest' was computed from 2383 independent reflections. The most prominent vectors could be explained if two copper atoms were at the special positions 0,0,0 and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$, and a further four at the general positions 0·33, 0·08, 0, and symmetry-related positions. A three-dimensional electron-density distribution was computed from the phases given by the proposed copper positions. Prominent independent maxima in this distribution correspond to three phenoxyacetate residues and three water molecules. The trial parameters were refined by two least-squares cycles assuming isotropic thermal motion for all atoms and unit weights for all observations. The weighting scheme

$$w = \{1 + [(|F_o| - a)/b]^2\}^{-1} \qquad (2)$$

was then adopted with $a = b = 100$ [on the scale of Table 4]. After two further refinement cycles $R = 0·131$. At this stage it was possible to locate hydrogen atoms from a three-dimensional difference synthesis calculated so that the two-dimensional sections were parallel to the plane of the phenoxyacetate molecules of the complexes. The hydrogen atoms were placed within the maxima on the difference synthesis at accepted bonded distances from the atoms to which they were attached. Three very strong reflections showing very considerable extinction effects were removed, and after two further least-squares cycles convergence was reached with $R = 0·113$. In all least-squares refinement cycles, a block diagonal approximation to the normal matrix was reduced to three blocks 39 × 39, 36 × 36, and 75 × 75, such that interactions of the temperature and overall scale parameters, and the space parameters, and of

[27] J. S. Rollett, unpublished work.

[28] 'International Tables for *X*-ray Crystallography,' vol. 3 Kynoch Press, Birmingham, 1962, p. 220.

TABLE 7

Observed structure amplitudes and calculated structure factors for aquobis-(DL-lactato)copper(II) hemihydrate

| h | k | l | $\|F_o\|$ | $F_o$ | α |
|---|---|---|---|---|---|
| 0 | 2 | 4 | 145 | 213 | 171 |
| 0 | 3 | 3 | 194 | 246 | 175 |
| 0 | 4 | 0 | 75 | 49 | 180 |
| 0 | 4 | 2 | 275 | 194 | 129 |
| 0 | 4 | 4 | 94 | 102 | -50 |
| 0 | 5 | 1 | 297 | 310 | 24 |
| 0 | 5 | 3 | 298 | 302 | -21 |
| 0 | 6 | 0 | 137 | 137 | 0 |
| 0 | 6 | 2 | 300 | 232 | -115 |
| 0 | 6 | 4 | 77 | 90 | 145 |
| 0 | 7 | 1 | 239 | 245 | 173 |
| 0 | 7 | 3 | 322 | 320 | 157 |
| 0 | 8 | 0 | 343 | 270 | 180 |
| 0 | 8 | 2 | 105 | 79 | 124 |
| 0 | 8 | 4 | 71 | 75 | -128 |
| 0 | 9 | 1 | 273 | 295 | -17 |
| 0 | 9 | 3 | 300 | 283 | -6 |
| 0 | 10 | 0 | 102 | 78 | 0 |
| 0 | 10 | 2 | 87 | 95 | 32 |
| 0 | 10 | 4 | 67 | 82 | 22 |
| 0 | 11 | 1 | 292 | 214 | 157 |
| 0 | 11 | 3 | 172 | 170 | -170 |
| 0 | 12 | 2 | 144 | 132 | -151 |
| 0 | 12 | 4 | 47 | 55 | 176 |
| 0 | 13 | 1 | 72 | 70 | -56 |
| 0 | 13 | 3 | 46 | 40 | 73 |
| 0 | 14 | 0 | 195 | 163 | 0 |
| 0 | 14 | 2 | 238 | 218 | 7 |
| 0 | 14 | 4 | 66 | 74 | -5 |
| 0 | 15 | 3 | 52 | 50 | -40 |
| 0 | 16 | 0 | 195 | 183 | 180 |
| 0 | 16 | 2 | 217 | 190 | 177 |
| 0 | 16 | 4 | 44 | 50 | -176 |
| 0 | 17 | 3 | 32 | 39 | 168 |
| 0 | 18 | 2 | 125 | 129 | -6 |
| 0 | 18 | 4 | 21 | 33 | 34 |
| 0 | 19 | 1 | 94 | 91 | -8 |
| 0 | 19 | 3 | 71 | 65 | 7 |
| 0 | 24 | 2 | 52 | 55 | 174 |
| 0 | 21 | 1 | 78 | 78 | 164 |
| 0 | 21 | 3 | 43 | 52 | -176 |
| 0 | 22 | 0 | 48 | 64 | -180 |
| 1 | -23 | -1 | 26 | 31 | -42 |
| 1 | -22 | -2 | 79 | 79 | -166 |
| 1 | -22 | 0 | 62 | 73 | -180 |
| 1 | -21 | -3 | 27 | 33 | -81 |
| 1 | -21 | -1 | 42 | 52 | 158 |
| 1 | -20 | -4 | 29 | 43 | -7 |
| 1 | -20 | -2 | 90 | 103 | -1 |
| 1 | -20 | 0 | 62 | 54 | 0 |
| 1 | -19 | -3 | 32 | 34 | 4 |
| 1 | -19 | -1 | 113 | 125 | -10 |
| 1 | -18 | -4 | 14 | 24 | 151 |
| 1 | -18 | -2 | 81 | 70 | 161 |
| 1 | -17 | -3 | 96 | 110 | 161 |
| 1 | -17 | -1 | 217 | 221 | 172 |
| 1 | -16 | -4 | 25 | 32 | -138 |
| 1 | -16 | -2 | 33 | 34 | -153 |
| 1 | -16 | 0 | 70 | 58 | -180 |
| 1 | -15 | -3 | 70 | 74 | -12 |
| 1 | -15 | -1 | 144 | 144 | -13 |
| 1 | -14 | -4 | 78 | 82 | 15 |
| 1 | -14 | -2 | 153 | 147 | -12 |
| 1 | -14 | 0 | 75 | 52 | 0 |
| 1 | -13 | -3 | 94 | 90 | -180 |
| 1 | -13 | -1 | 162 | 171 | 152 |
| 1 | -12 | -4 | 118 | 132 | -178 |
| 1 | -12 | -2 | 301 | 225 | 167 |
| 1 | -12 | 0 | 54 | 46 | -180 |
| 1 | -11 | -3 | 159 | 154 | 15 |
| 1 | -11 | -1 | 309 | 252 | -26 |
| 1 | -10 | -4 | 191 | 208 | -9 |
| 1 | -10 | -2 | 340 | 316 | 3 |
| 1 | -10 | 0 | 321 | 266 | 0 |
| 1 | -9 | -3 | 157 | 157 | -56 |
| 1 | -9 | -1 | 148 | 163 | 23 |
| 1 | -8 | -4 | 187 | 212 | 167 |
| 1 | -8 | -2 | 305 | 346 | -151 |
| 1 | -8 | 0 | 520 | 532 | 180 |
| 1 | -7 | -3 | 237 | 237 | 149 |
| 1 | -7 | -1 | 350 | 277 | -177 |
| 1 | -6 | -4 | 143 | 131 | -5 |
| 1 | -6 | -2 | 304 | 297 | 70 |
| 1 | -6 | 0 | 503 | 484 | 0 |
| 1 | -5 | -3 | 173 | 168 | -11 |
| 1 | -5 | -1 | 92 | 139 | -1 |
| 1 | -4 | -4 | 58 | 69 | 173 |
| 1 | -4 | -2 | 124 | 95 | -108 |
| 1 | -3 | -3 | 364 | 365 | -178 |
| 1 | 0 | 4 | 97 | 102 | 43 |
| 1 | 1 | 1 | 392 | 398 | 163 |
| 1 | 1 | 3 | 254 | 209 | -160 |
| 1 | 2 | 0 | 140 | 132 | 180 |
| 1 | 2 | 2 | 347 | 306 | 143 |
| 1 | 2 | 4 | 156 | 204 | 150 |
| 1 | 3 | 1 | 220 | 226 | -26 |
| 1 | 3 | 3 | 237 | 237 | 43 |
| 1 | 4 | 0 | 53 | 38 | 0 |
| 1 | 4 | 2 | 353 | 372 | -5 |
| 1 | 4 | 4 | 210 | 222 | 12 |
| 1 | 5 | 1 | 149 | 120 | 52 |
| 1 | 5 | 3 | 115 | 113 | -94 |
| 1 | 6 | 0 | 45 | 114 | -180 |
| 1 | 6 | 2 | 444 | 420 | -173 |
| 1 | 6 | 4 | 169 | 201 | -180 |
| 1 | 7 | 1 | 153 | 147 | -135 |
| 1 | 7 | 3 | 42 | 50 | 158 |
| 1 | 8 | 0 | 490 | 387 | 0 |
| 1 | 8 | 2 | 473 | 434 | 1 |
| 1 | 8 | 4 | 190 | 207 | -5 |
| 1 | 9 | 1 | 297 | 275 | 28 |
| 1 | 9 | 3 | 150 | 150 | 35 |
| 1 | 10 | 0 | 314 | 268 | 180 |
| 1 | 10 | 2 | 212 | 192 | 167 |
| 1 | 10 | 4 | 97 | 105 | 168 |
| 1 | 11 | 1 | 383 | 330 | -162 |
| 1 | 11 | 3 | 156 | 159 | -153 |
| 1 | 12 | 0 | 68 | 58 | 180 |
| 1 | 12 | 2 | 171 | 121 | -163 |
| 1 | 12 | 4 | 47 | 54 | -163 |
| 1 | 13 | 1 | 203 | 195 | 11 |
| 1 | 13 | 3 | 67 | 59 | -31 |
| 1 | 14 | 0 | 107 | 100 | 0 |
| 1 | 14 | 2 | 108 | 113 | -7 |
| 1 | 14 | 4 | 50 | 59 | -3 |
| 1 | 15 | 1 | 154 | 146 | -175 |
| 1 | 15 | 3 | 62 | 73 | 114 |
| 1 | 16 | 0 | 38 | 52 | 180 |
| 1 | 16 | 2 | 49 | 53 | 127 |
| 1 | 16 | 4 | 24 | 37 | 157 |
| 1 | 17 | 1 | 94 | 102 | 9 |
| 1 | 17 | 3 | 40 | 51 | -47 |
| 1 | 18 | 0 | 87 | 70 | 0 |
| 1 | 18 | 2 | 54 | 47 | -28 |
| 1 | 18 | 4 | 57 | 50 | -5 |
| 1 | 19 | 1 | 28 | 30 | -133 |
| 1 | 19 | 3 | 16 | 14 | 175 |
| 1 | 20 | 0 | 35 | 48 | 180 |
| 1 | 20 | 2 | 48 | 40 | -173 |
| 1 | 22 | 0 | 28 | 34 | 0 |
| 2 | -24 | 0 | 46 | 56 | 0 |
| 2 | -23 | -1 | 49 | 53 | -179 |
| 2 | -22 | -2 | 78 | 74 | 179 |
| 2 | -22 | 0 | 27 | 49 | 180 |
| 2 | -21 | -3 | 46 | 52 | 28 |
| 2 | -21 | -1 | 50 | 57 | -23 |
| 2 | -20 | -4 | 31 | 42 | -2 |
| 2 | -20 | -2 | 110 | 122 | -16 |
| 2 | -20 | 0 | 72 | 68 | 0 |
| 2 | -19 | -3 | 24 | 32 | -102 |
| 2 | -19 | -1 | 46 | 57 | 90 |
| 2 | -18 | -4 | 45 | 59 | -179 |
| 2 | -18 | -2 | 105 | 102 | 157 |
| 2 | -18 | 0 | 71 | 52 | -180 |
| 2 | -17 | -3 | 64 | 73 | 164 |
| 2 | -17 | -1 | 98 | 108 | -134 |
| 2 | -16 | -4 | 42 | 58 | -2 |
| 2 | -16 | -2 | 33 | 45 | 7 |
| 2 | -16 | 0 | 86 | 90 | 0 |
| 2 | -15 | -3 | 119 | 127 | 13 |
| 2 | -15 | -1 | 119 | 99 | 42 |
| 2 | -14 | -4 | 93 | 105 | 164 |
| 2 | -14 | -2 | 151 | 146 | -150 |
| 2 | -14 | 0 | 332 | 307 | 180 |
| 2 | -13 | -3 | 201 | 205 | -165 |
| 2 | -13 | -1 | 147 | 126 | 180 |
| 2 | -12 | -4 | 91 | 97 | -41 |
| 2 | -12 | -2 | 207 | 189 | 33 |
| 2 | -12 | 0 | 405 | 318 | 0 |
| 2 | -11 | -3 | 231 | 261 | 5 |
| 2 | -11 | -1 | 284 | 281 | -18 |
| 2 | -10 | -4 | 80 | 83 | 48 |
| 2 | -10 | -2 | 76 | 66 | -108 |
| 2 | -10 | 0 | 223 | 191 | 0 |
| 2 | -9 | -3 | 273 | 272 | -177 |
| 2 | -8 | -4 | 185 | 189 | -180 |
| 2 | -8 | -2 | 219 | 198 | 172 |
| 2 | -7 | -3 | 194 | 193 | 4 |
| 2 | -7 | -1 | 354 | 345 | 8 |
| 2 | -6 | -4 | 281 | 241 | -6 |
| 2 | -6 | -2 | 233 | 257 | -5 |
| 2 | -5 | -3 | 27 | 30 | 53 |
| 2 | -5 | -1 | 204 | 201 | -69 |
| 2 | -4 | -4 | 244 | 188 | -175 |
| 2 | -4 | -2 | 132 | 131 | 143 |
| 2 | -3 | -3 | 143 | 134 | -110 |
| 2 | -3 | -1 | 231 | 216 | 115 |
| 2 | -2 | -4 | 232 | 191 | 12 |
| 2 | -2 | -2 | 303 | 285 | -44 |
| 2 | -2 | 0 | 263 | 234 | 0 |
| 2 | -1 | -3 | 266 | 230 | 57 |
| 2 | -1 | -1 | 70 | 113 | -50 |
| 2 | 0 | 2 | 362 | 320 | -153 |
| 2 | 0 | 4 | 193 | 182 | 153 |
| 2 | 1 | 1 | 582 | 520 | -177 |
| 2 | 1 | 3 | 421 | 434 | 167 |
| 2 | 2 | 0 | 64 | 75 | -180 |
| 2 | 2 | 2 | 109 | 121 | -12 |
| 2 | 2 | 4 | 122 | 106 | -63 |
| 2 | 3 | 1 | 258 | 283 | -3 |
| 2 | 3 | 3 | 340 | 320 | -2 |
| 2 | 4 | 0 | 89 | 80 | 180 |
| 2 | 4 | 2 | 100 | 81 | 113 |
| 2 | 5 | 1 | 115 | 135 | 156 |
| 2 | 5 | 3 | 125 | 146 | -179 |
| 2 | 6 | 2 | 149 | 148 | -159 |
| 2 | 6 | 4 | 48 | 67 | 149 |
| 2 | 7 | 1 | 393 | 375 | -7 |
| 2 | 7 | 3 | 158 | 168 | 12 |
| 2 | 8 | 0 | 296 | 256 | 0 |
| 2 | 8 | 2 | 266 | 272 | 4 |
| 2 | 8 | 4 | 91 | 92 | -7 |
| 2 | 9 | 1 | 188 | 203 | 173 |
| 2 | 9 | 3 | 23 | 28 | -139 |
| 2 | 10 | 0 | 296 | 267 | 180 |
| 2 | 10 | 2 | 296 | 262 | 179 |
| 2 | 10 | 4 | 59 | 77 | -162 |
| 2 | 11 | 1 | 43 | 35 | 170 |
| 2 | 11 | 3 | 86 | 84 | -177 |
| 2 | 12 | 0 | 237 | 192 | 0 |
| 2 | 12 | 2 | 259 | 225 | -1 |
| 2 | 12 | 4 | 57 | 68 | 30 |
| 2 | 13 | 1 | 86 | 85 | -39 |
| 2 | 13 | 3 | 54 | 55 | -11 |
| 2 | 14 | 0 | 29 | 38 | 180 |
| 2 | 14 | 2 | 155 | 129 | 177 |
| 2 | 14 | 4 | 24 | 29 | -160 |
| 2 | 15 | 1 | 97 | 118 | 144 |
| 2 | 15 | 3 | 66 | 62 | -180 |
| 2 | 16 | 0 | 23 | 28 | 180 |
| 2 | 16 | 2 | 55 | 63 | -5 |
| 2 | 17 | 1 | 88 | 100 | -31 |
| 2 | 17 | 3 | 85 | 75 | 19 |
| 2 | 18 | 2 | 31 | 28 | 165 |
| 2 | 19 | 1 | 60 | 59 | 154 |
| 2 | 20 | 2 | 44 | 50 | -157 |
| 3 | -25 | -1 | 38 | 54 | 1 |
| 3 | -24 | -2 | 53 | 61 | 173 |
| 3 | -24 | 0 | 15 | 17 | -180 |
| 3 | -23 | -1 | 35 | 63 | -178 |
| 3 | -22 | -2 | 21 | 32 | 7 |
| 3 | -21 | -3 | 61 | 69 | -21 |
| 3 | -21 | -1 | 90 | 95 | -13 |
| 3 | -20 | -4 | 17 | 21 | 64 |
| 3 | -20 | 0 | 33 | 52 | -180 |
| 3 | -19 | -3 | 88 | 102 | 169 |
| 3 | -19 | -1 | 138 | 127 | 155 |
| 3 | -18 | -4 | 44 | 64 | -168 |
| 3 | -18 | -2 | 87 | 90 | 167 |
| 3 | -17 | -3 | 81 | 98 | 20 |
| 3 | -17 | -1 | 97 | 111 | -25 |
| 3 | -16 | -4 | 123 | 152 | -4 |
| 3 | -16 | -2 | 226 | 213 | 6 |
| 3 | -16 | 0 | 293 | 271 | 0 |
| 3 | -15 | -3 | 85 | 101 | -116 |
| 3 | -15 | -1 | 68 | 67 | -180 |
| 3 | -14 | -4 | 115 | 132 | 173 |
| 3 | -14 | -2 | 187 | 170 | -145 |
| 3 | -14 | 0 | 338 | 319 | -180 |
| 3 | -13 | -3 | 72 | 80 | 93 |
| 3 | -13 | -1 | 54 | 53 | 45 |
| 3 | -12 | -4 | 91 | 90 | -9 |
| 3 | -12 | -2 | 101 | 111 | 70 |
| 3 | -12 | 0 | 233 | 240 | 0 |
| 3 | -11 | -3 | 103 | 105 | -10 |
| 3 | -11 | -1 | 161 | 142 | -10 |
| 3 | -10 | -4 | 120 | 148 | 170 |
| 3 | -10 | -2 | 210 | 201 | 168 |
| 3 | -10 | 0 | 391 | 365 | -180 |
| 3 | -9 | -3 | 249 | 240 | -168 |
| 3 | -9 | -1 | 416 | 409 | -173 |
| 3 | -8 | -4 | 77 | 77 | 43 |
| 3 | -8 | -2 | 202 | 185 | -65 |
| 3 | -8 | 0 | 101 | 73 | 0 |
| 3 | -7 | -3 | 282 | 282 | 8 |
| 3 | -7 | -1 | 500 | 465 | 13 |
| 3 | -6 | -4 | 132 | 121 | -86 |
| 3 | -6 | -2 | 211 | 201 | 87 |
| 3 | -6 | 0 | 74 | 27 | 180 |
| 3 | -5 | -3 | 368 | 303 | 163 |
| 3 | -5 | -1 | 370 | 373 | -171 |
| 3 | -4 | -4 | 96 | 75 | 61 |
| 3 | -4 | -2 | 260 | 234 | -55 |
| 3 | -3 | -3 | 396 | 313 | -35 |
| 3 | -3 | -1 | 248 | 240 | -3 |
| 3 | -2 | -4 | 257 | 179 | -12 |
| 3 | -2 | -2 | 436 | 407 | 8 |
| 3 | -2 | 0 | 35 | 8 | 0 |
| 3 | -1 | -3 | 249 | 210 | 146 |
| 3 | -1 | -1 | 174 | 172 | -174 |
| 3 | 0 | 0 | 540 | 511 | -180 |
| 3 | 0 | 4 | 377 | 325 | -176 |
| 3 | 1 | 1 | 218 | 178 | -61 |
| 3 | 1 | 3 | 73 | 81 | -50 |
| 3 | 2 | 0 | 472 | 427 | 0 |
| 3 | 2 | 2 | 458 | 466 | -3 |
| 3 | 2 | 4 | 241 | 221 | -4 |
| 3 | 3 | 1 | 353 | 333 | 45 |
| 3 | 3 | 3 | 200 | 208 | 53 |
| 3 | 4 | 0 | 244 | 249 | -180 |
| 3 | 4 | 2 | 204 | 207 | 168 |
| 3 | 4 | 4 | 95 | 109 | 176 |
| 3 | 5 | 1 | 338 | 325 | -155 |
| 3 | 5 | 3 | 124 | 124 | -157 |
| 3 | 6 | 0 | 13 | 17 | 0 |
| 3 | 6 | 2 | 24 | 21 | -56 |
| 3 | 7 | 1 | 220 | 219 | 4 |
| 3 | 7 | 3 | 81 | 88 | -72 |
| 3 | 8 | 0 | 64 | 41 | 0 |
| 3 | 8 | 2 | 24 | 26 | -87 |
| 3 | 8 | 4 | 47 | 37 | -10 |
| 3 | 9 | 1 | 303 | 306 | 177 |
| 3 | 9 | 3 | 117 | 127 | 142 |
| 3 | 10 | 2 | 59 | 59 | 47 |
| 3 | 10 | 4 | 17 | 27 | 155 |
| 3 | 11 | 1 | 215 | 214 | 1 |
| 3 | 11 | 3 | 119 | 115 | -12 |
| 3 | 12 | 0 | 79 | 67 | 0 |
| 3 | 12 | 2 | 33 | 37 | -23 |
| 3 | 12 | 4 | 48 | 54 | -11 |
| 3 | 13 | 1 | 33 | 40 | -136 |
| 3 | 13 | 3 | 44 | 43 | -165 |
| 3 | 14 | 0 | 77 | 83 | -180 |
| 3 | 14 | 2 | 92 | 76 | -174 |
| 3 | 14 | 4 | 79 | 68 | 160 |
| 3 | 15 | 3 | 35 | 38 | 25 |
| 3 | 16 | 0 | 109 | 92 | 0 |
| 3 | 16 | 2 | 86 | 84 | 12 |
| 3 | 17 | 3 | 16 | 15 | 138 |
| 3 | 18 | 0 | 139 | 104 | -180 |
| 3 | 18 | 2 | 90 | 69 | -167 |
| 3 | 19 | 1 | 53 | 51 | -173 |
| 4 | -25 | -1 | 30 | 44 | 104 |
| 4 | -24 | -2 | 15 | 32 | 159 |
| 4 | -24 | 0 | 27 | 29 | -180 |
| 4 | -23 | -1 | 31 | 47 | -80 |
| 4 | -22 | -2 | 35 | 49 | 11 |
| 4 | -22 | 0 | 90 | 110 | 0 |
| 4 | -21 | -3 | 15 | 21 | 33 |
| 4 | -21 | -1 | 43 | 54 | 152 |
| 4 | -20 | -4 | 78 | 89 | 163 |
| 4 | -20 | -2 | 73 | 97 | -161 |
| 4 | -20 | 0 | 186 | 200 | -180 |
| 4 | -19 | -3 | 96 | 121 | -173 |
| 4 | -19 | -1 | 73 | 80 | 167 |
| 4 | -18 | -4 | 48 | 72 | -34 |
| 4 | -18 | -2 | 103 | 108 | 20 |
| 4 | -18 | 0 | 142 | 155 | 0 |
| 4 | -17 | -3 | 151 | 183 | 6 |
| 4 | -17 | -1 | 203 | 210 | -8 |
| 4 | -16 | -2 | 61 | 58 | -148 |
| 4 | -16 | 0 | 78 | 81 | 0 |
| 4 | -15 | -3 | 119 | 123 | -164 |
| 4 | -15 | -1 | 170 | 177 | -175 |
| 4 | -14 | -4 | 59 | 63 | 163 |
| 4 | -14 | -2 | 33 | 21 | 104 |
| 4 | -14 | 0 | 353 | 343 | -180 |
| 4 | -13 | -3 | 162 | 159 | -7 |
| 4 | -13 | -1 | 288 | 264 | 12 |
| 4 | -12 | -4 | 91 | 87 | -12 |
| 4 | -12 | -2 | 28 | 42 | -20 |
| 4 | -12 | 0 | 480 | 438 | 0 |
| 4 | -11 | -3 | 176 | 180 | 148 |
| 4 | -11 | -1 | 231 | 204 | -158 |
| 4 | -10 | -4 | 122 | 125 | -180 |
| 4 | -10 | -2 | 158 | 168 | 161 |
| 4 | -10 | 0 | 366 | 420 | -180 |
| 4 | -9 | -3 | 129 | 131 | -75 |
| 4 | -9 | -1 | 84 | 90 | 118 |
| 4 | -8 | -4 | 199 | 206 | 11 |
| 4 | -8 | -2 | 332 | 368 | -13 |
| 4 | -8 | 0 | 432 | 400 | 0 |
| 4 | -7 | -3 | 143 | 110 | 67 |
| 4 | -7 | -1 | 109 | 92 | -64 |
| 4 | -6 | -4 | 212 | 211 | -157 |
| 4 | -6 | -2 | 340 | 341 | 178 |
| 4 | -6 | 0 | 130 | 191 | -180 |
| 4 | -5 | -3 | 237 | 193 | -171 |
| 4 | -5 | -1 | 182 | 157 | 137 |
| 4 | -4 | -4 | 146 | 100 | 23 |
| 4 | -4 | -2 | 170 | 155 | 14 |
| 4 | -4 | 0 | 41 | 37 | 180 |
| 4 | -3 | -3 | 272 | 244 | 7 |
| 4 | -3 | -1 | 149 | 182 | -22 |
| 4 | -2 | -4 | 67 | 79 | 145 |
| 4 | -2 | -2 | 156 | 149 | -166 |
| 4 | -2 | 0 | 94 | 104 | -180 |
| 4 | -1 | -3 | 221 | 231 | -170 |
| 4 | 0 | 0 | 58 | 37 | 0 |
| 4 | 0 | 2 | 71 | 61 | -60 |
| 4 | 0 | 4 | 46 | 39 | 79 |
| 4 | 1 | 1 | 562 | 568 | -5 |
| 4 | 1 | 3 | 208 | 209 | -2 |
| 4 | 2 | 0 | 281 | 254 | 0 |
| 4 | 2 | 2 | 184 | 219 | 14 |
| 4 | 2 | 4 | 85 | 94 | 12 |
| 4 | 3 | 1 | 286 | 308 | 173 |
| 4 | 3 | 3 | 43 | 37 | -173 |
| 4 | 4 | 0 | 177 | 205 | -180 |
| 4 | 4 | 2 | 223 | 222 | -175 |
| 4 | 4 | 4 | 52 | 66 | -146 |
| 4 | 5 | 1 | 85 | 93 | 32 |
| 4 | 5 | 3 | 51 | 49 | 127 |
| 4 | 6 | 0 | 175 | 152 | 0 |
| 4 | 6 | 2 | 244 | 237 | -2 |
| 4 | 6 | 4 | 40 | 41 | 18 |
| 4 | 7 | 1 | 126 | 127 | -94 |

TABLE 7 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ | α |
|---|---|---|---|---|---|
| 4 | 7 | 3 | 25 | 39 | -80 |
| 4 | 8 | 0 | 232 | 211 | -180 |
| 4 | 8 | 2 | 320 | 310 | 178 |
| 4 | 8 | 4 | 103 | 107 | 178 |
| 4 | 9 | 1 | 149 | 156 | 129 |
| 4 | 9 | 3 | 83 | 70 | -150 |
| 4 | 10 | 0 | 115 | 105 | 0 |
| 4 | 10 | 2 | 198 | 182 | -2 |
| 4 | 10 | 4 | 91 | 91 | -1 |
| 4 | 11 | 1 | 139 | 131 | -36 |
| 4 | 11 | 3 | 125 | 120 | 38 |
| 4 | 12 | 0 | 47 | 23 | 0 |
| 4 | 12 | 2 | 23 | 21 | 83 |
| 4 | 12 | 4 | 28 | 35 | -173 |
| 4 | 13 | 1 | 94 | 85 | 157 |
| 4 | 13 | 3 | 107 | 109 | -155 |
| 4 | 14 | 0 | 21 | 29 | 180 |
| 4 | 14 | 2 | 63 | 70 | -158 |
| 4 | 14 | 4 | 20 | 20 | 63 |
| 4 | 15 | 1 | 72 | 58 | -2 |
| 4 | 15 | 3 | 98 | 77 | -0 |
| 4 | 16 | 0 | 25 | 12 | 0 |
| 4 | 16 | 2 | 73 | 56 | 20 |
| 4 | 17 | 1 | 39 | 41 | -165 |
| 4 | 18 | 0 | 21 | 17 | 180 |
| 5 | -25 | -1 | 47 | 54 | 155 |
| 5 | -24 | -2 | 15 | 27 | 171 |
| 5 | -23 | -3 | 58 | 71 | 20 |
| 5 | -23 | -1 | 59 | 75 | -6 |
| 5 | -22 | -2 | 36 | 48 | 17 |
| 5 | -22 | 0 | 61 | 86 | 0 |
| 5 | -21 | -3 | 42 | 74 | -143 |
| 5 | -21 | -1 | 82 | 92 | -157 |
| 5 | -21 | -4 | 62 | 71 | 166 |
| 5 | -21 | -2 | 66 | 67 | -153 |
| 5 | -21 | 0 | 122 | 150 | -180 |
| 5 | -19 | -3 | 30 | 46 | 43 |
| 5 | -19 | -1 | 56 | 64 | 31 |
| 5 | -18 | -4 | 45 | 58 | -14 |
| 5 | -18 | -2 | 77 | 54 | 23 |
| 5 | -18 | 0 | 134 | 151 | 0 |
| 5 | -17 | -3 | 19 | 14 | 37 |
| 5 | -17 | -1 | 31 | 46 | -8 |
| 5 | -16 | -4 | 52 | 68 | -165 |
| 5 | -16 | -2 | 92 | 90 | 167 |
| 5 | -16 | 0 | 150 | 173 | -180 |
| 5 | -15 | -3 | 105 | 97 | -154 |
| 5 | -15 | -1 | 177 | 177 | -168 |
| 5 | -14 | -4 | 93 | 112 | 36 |
| 5 | -14 | -2 | 144 | 148 | -28 |
| 5 | -14 | 0 | 166 | 212 | 0 |
| 5 | -13 | -3 | 115 | 113 | 7 |
| 5 | -13 | -1 | 157 | 170 | 12 |
| 5 | -12 | -4 | 127 | 133 | -154 |
| 5 | -12 | -2 | 213 | 218 | 142 |
| 5 | -12 | 0 | 316 | 338 | -180 |
| 5 | -11 | -3 | 201 | 179 | 158 |
| 5 | -10 | -4 | 75 | 73 | 21 |
| 5 | -10 | -2 | 131 | 151 | -67 |
| 5 | -10 | 0 | 343 | 319 | 0 |
| 5 | -9 | -3 | 334 | 328 | -19 |
| 5 | -9 | -1 | 373 | 384 | -11 |
| 5 | -8 | -4 | 138 | 130 | -18 |
| 5 | -8 | -2 | 337 | 327 | 7 |
| 5 | -8 | 0 | 111 | 126 | 0 |
| 5 | -7 | -3 | 215 | 210 | 178 |
| 5 | -7 | -1 | 305 | 300 | -178 |
| 5 | -6 | -4 | 225 | 218 | 171 |
| 5 | -6 | -2 | 436 | 446 | 178 |
| 5 | -6 | 0 | 321 | 336 | -180 |
| 5 | -5 | -3 | 127 | 129 | 88 |
| 5 | -5 | -1 | 181 | 165 | 80 |
| 5 | -4 | -4 | 204 | 168 | -5 |
| 5 | -4 | -2 | 277 | 304 | -0 |
| 5 | -4 | 0 | 230 | 258 | 0 |
| 5 | -3 | -3 | 129 | 104 | -110 |
| 5 | -3 | -1 | 197 | 199 | -109 |
| 5 | -2 | -4 | 117 | 107 | 175 |
| 5 | -2 | -2 | 231 | 236 | -177 |
| 5 | -2 | 0 | 183 | 237 | 180 |
| 5 | -1 | -3 | 21 | 19 | -91 |
| 5 | -1 | -1 | 138 | 139 | 144 |
| 5 | 0 | 0 | 158 | 145 | 0 |
| 5 | 0 | 2 | 217 | 180 | -7 |
| 5 | 0 | 4 | 45 | 40 | -18 |
| 5 | 1 | 1 | 373 | 356 | -3 |
| 5 | 1 | 3 | 118 | 112 | -30 |
| 5 | 2 | 0 | 140 | 145 | 180 |
| 5 | 2 | 2 | 201 | 195 | -177 |
| 5 | 2 | 4 | 22 | 32 | 160 |
| 5 | 3 | 1 | 262 | 272 | 167 |
| 5 | 3 | 3 | 92 | 94 | 153 |
| 5 | 4 | 0 | 101 | 59 | 0 |
| 5 | 4 | 2 | 122 | 115 | 19 |
| 5 | 4 | 4 | 31 | 16 | 57 |
| 5 | 5 | 1 | 196 | 183 | -8 |
| 5 | 5 | 3 | 125 | 121 | -2 |
| 5 | 6 | 0 | 67 | 64 | 0 |
| 5 | 6 | 2 | 37 | 41 | -36 |
| 5 | 6 | 4 | 53 | 57 | -46 |
| 5 | 7 | 1 | 153 | 148 | -169 |
| 5 | 7 | 3 | 158 | 153 | -171 |
| 5 | 8 | 0 | 66 | 61 | -180 |
| 5 | 8 | 2 | 74 | 56 | -176 |
| 5 | 8 | 4 | 71 | 73 | 132 |
| 5 | 9 | 1 | 65 | 72 | 30 |
| 5 | 9 | 3 | 103 | 103 | 0 |
| 5 | 10 | 0 | 176 | 142 | 0 |
| 5 | 10 | 2 | 119 | 110 | 20 |
| 5 | 10 | 4 | 89 | 93 | -13 |
| 5 | 11 | 3 | 53 | 45 | 146 |
| 5 | 12 | 0 | 217 | 177 | -180 |
| 5 | 12 | 2 | 136 | 100 | -161 |
| 5 | 12 | 4 | 106 | 96 | -176 |
| 5 | 13 | 1 | 48 | 41 | -153 |
| 5 | 13 | 3 | 33 | 27 | -127 |
| 5 | 14 | 0 | 111 | 92 | 0 |
| 5 | 14 | 2 | 19 | 10 | 2 |
| 5 | 15 | 1 | 64 | 47 | 34 |
| 5 | 16 | 0 | 82 | 66 | -180 |
| 6 | -26 | 0 | 67 | 94 | -180 |
| 6 | -25 | -1 | 28 | 28 | 157 |
| 6 | -24 | -2 | 45 | 56 | 19 |
| 6 | -24 | 0 | 48 | 67 | 0 |
| 6 | -23 | -3 | 41 | 60 | 24 |
| 6 | -23 | -1 | 38 | 62 | -1 |
| 6 | -22 | -2 | 39 | 60 | -160 |
| 6 | -21 | -3 | 38 | 58 | -175 |
| 6 | -21 | -1 | 75 | 94 | -169 |
| 6 | -20 | -4 | 15 | 33 | 16 |
| 6 | -20 | -2 | 85 | 96 | 3 |
| 6 | -19 | -3 | 71 | 103 | -26 |
| 6 | -19 | -1 | 131 | 137 | 10 |
| 6 | -18 | -2 | 38 | 6 | -0 |
| 6 | -18 | 0 | 106 | 134 | 0 |
| 6 | -17 | -3 | 110 | 129 | 148 |
| 6 | -17 | -1 | 122 | 114 | -168 |
| 6 | -16 | -4 | 73 | 92 | 180 |
| 6 | -16 | -2 | 160 | 179 | 176 |
| 6 | -16 | 0 | 261 | 273 | -180 |
| 6 | -15 | -3 | 122 | 114 | -28 |
| 6 | -15 | -1 | 98 | 97 | 21 |
| 6 | -14 | -4 | 92 | 98 | 19 |
| 6 | -14 | -2 | 155 | 160 | 0 |
| 6 | -13 | -3 | 56 | 59 | 158 |
| 6 | -13 | -1 | 121 | 120 | -146 |
| 6 | -12 | -4 | 128 | 131 | -172 |
| 6 | -12 | -2 | 188 | 191 | -179 |
| 6 | -12 | 0 | 73 | 78 | -180 |
| 6 | -11 | -3 | 56 | 60 | -163 |
| 6 | -11 | -1 | 107 | 98 | 73 |
| 6 | -10 | -4 | 151 | 147 | -13 |
| 6 | -10 | -2 | 232 | 249 | -1 |
| 6 | -10 | 0 | 128 | 132 | 0 |
| 6 | -9 | -3 | 147 | 141 | 24 |
| 6 | -9 | -1 | 95 | 110 | -34 |
| 6 | -8 | -4 | 46 | 52 | 150 |
| 6 | -8 | -2 | 148 | 148 | -160 |
| 6 | -7 | -3 | 201 | 194 | -162 |
| 6 | -7 | -1 | 309 | 345 | -179 |
| 6 | -6 | -4 | 25 | 25 | 8 |
| 6 | -6 | -2 | 151 | 164 | 30 |
| 6 | -6 | 0 | 67 | 76 | 0 |
| 6 | -5 | -3 | 157 | 149 | 5 |
| 6 | -5 | -1 | 401 | 448 | 7 |
| 6 | -4 | -4 | 46 | 38 | -161 |
| 6 | -4 | -2 | 119 | 106 | -153 |
| 6 | -4 | 0 | 91 | 93 | -180 |
| 6 | -3 | -3 | 71 | 50 | 113 |
| 6 | -2 | -2 | 148 | 139 | 177 |
| 6 | -2 | 0 | 88 | 116 | 180 |
| 6 | -1 | -3 | 120 | 116 | -49 |
| 6 | 0 | 0 | 253 | 250 | 0 |
| 6 | 0 | 4 | 76 | 67 | -12 |
| 6 | 1 | 1 | 236 | 217 | -135 |
| 6 | 1 | 3 | 85 | 91 | -173 |
| 6 | 2 | 0 | 306 | 282 | -180 |
| 6 | 2 | 2 | 344 | 354 | 179 |
| 6 | 2 | 4 | 144 | 137 | 174 |
| 6 | 3 | 1 | 165 | 164 | 125 |
| 6 | 3 | 3 | 119 | 116 | -119 |
| 6 | 4 | 0 | 168 | 140 | 0 |
| 6 | 4 | 2 | 200 | 182 | -1 |
| 6 | 4 | 4 | 145 | 131 | -2 |
| 6 | 5 | 1 | 120 | 115 | -52 |
| 6 | 5 | 3 | 138 | 121 | 51 |
| 6 | 6 | 2 | 27 | 26 | 56 |
| 6 | 6 | 4 | 78 | 75 | -175 |
| 6 | 7 | 1 | 47 | 50 | 132 |
| 6 | 7 | 3 | 80 | 79 | -159 |
| 6 | 8 | 0 | 48 | 45 | 0 |
| 6 | 8 | 2 | 52 | 46 | -145 |
| 6 | 8 | 4 | 61 | 52 | 26 |
| 6 | 9 | 1 | 122 | 110 | 3 |
| 6 | 9 | 3 | 134 | 120 | -8 |
| 6 | 10 | 0 | 45 | 56 | -180 |
| 6 | 10 | 2 | 29 | 26 | 65 |
| 6 | 11 | 1 | 116 | 100 | -170 |
| 6 | 11 | 3 | 106 | 87 | 163 |
| 6 | 12 | 0 | 13 | 1 | 0 |
| 6 | 12 | 2 | 17 | 13 | -105 |
| 6 | 13 | 1 | 70 | 60 | 11 |
| 6 | 14 | 0 | 74 | 49 | 0 |
| 7 | -26 | 0 | 20 | 40 | 180 |
| 7 | -24 | -2 | 24 | 20 | 31 |
| 7 | -24 | 0 | 28 | 54 | 0 |
| 7 | -23 | -3 | 13 | 29 | 164 |
| 7 | -22 | -2 | 35 | 50 | 175 |
| 7 | -22 | 0 | 64 | 96 | -180 |
| 7 | -21 | -3 | 17 | 35 | -30 |
| 7 | -21 | -1 | 30 | 26 | -51 |
| 7 | -20 | -4 | 62 | 80 | 19 |
| 7 | -20 | -2 | 84 | 99 | -25 |
| 7 | -20 | 0 | 116 | 159 | 0 |
| 7 | -19 | -3 | 40 | 49 | -7 |
| 7 | -19 | -1 | 56 | 65 | -1 |
| 7 | -18 | -4 | 83 | 107 | -173 |
| 7 | -18 | -2 | 112 | 139 | 144 |
| 7 | -18 | 0 | 209 | 223 | -180 |
| 7 | -17 | -3 | 103 | 116 | 169 |
| 7 | -17 | -1 | 122 | 127 | 161 |
| 7 | -16 | -4 | 50 | 64 | 19 |
| 7 | -16 | -2 | 57 | 74 | -59 |
| 7 | -16 | 0 | 148 | 159 | 0 |
| 7 | -15 | -3 | 140 | 149 | -2 |
| 7 | -15 | -1 | 183 | 186 | -15 |
| 7 | -14 | -4 | 52 | 68 | -37 |
| 7 | -14 | -2 | 108 | 109 | 4 |
| 7 | -14 | 0 | 23 | 20 | 0 |
| 7 | -13 | -3 | 133 | 134 | -163 |
| 7 | -13 | -1 | 203 | 201 | -179 |
| 7 | -12 | -4 | 99 | 86 | 160 |
| 7 | -12 | -2 | 98 | 105 | 170 |
| 7 | -12 | 0 | 30 | 39 | -180 |
| 7 | -11 | -3 | 83 | 85 | 44 |
| 7 | -11 | -1 | 147 | 158 | 30 |
| 7 | -10 | -4 | 72 | 69 | -11 |
| 7 | -10 | -2 | 113 | 117 | -7 |
| 7 | -10 | 0 | 102 | 91 | 0 |
| 7 | -9 | -3 | 63 | 72 | -165 |
| 7 | -9 | -1 | 134 | 148 | -145 |
| 7 | -8 | -4 | 100 | 104 | -176 |
| 7 | -8 | -2 | 263 | 275 | -178 |
| 7 | -8 | 0 | 260 | 294 | -180 |
| 7 | -7 | -3 | 40 | 41 | -3 |
| 7 | -7 | -1 | 28 | 34 | 121 |
| 7 | -6 | -4 | 86 | 70 | 31 |
| 7 | -6 | -2 | 245 | 253 | 6 |
| 7 | -6 | 0 | 210 | 231 | 0 |
| 7 | -5 | -3 | 31 | 11 | -23 |
| 7 | -4 | -4 | 40 | 31 | -151 |
| 7 | -4 | -2 | 169 | 163 | 177 |
| 7 | -4 | 0 | 103 | 106 | 180 |
| 7 | -3 | -3 | 27 | 34 | -169 |
| 7 | -3 | -1 | 146 | 147 | -144 |
| 7 | -2 | -2 | 151 | 166 | -19 |
| 7 | -2 | 0 | 110 | 132 | 0 |
| 7 | -1 | -1 | 179 | 188 | 15 |
| 7 | 0 | 0 | 45 | 49 | 180 |
| 7 | 0 | 2 | 57 | 58 | -144 |
| 7 | 0 | 4 | 61 | 72 | -111 |
| 7 | 1 | 1 | 227 | 200 | -177 |
| 7 | 1 | 3 | 233 | 206 | -179 |
| 7 | 2 | 0 | 61 | 59 | -180 |
| 7 | 2 | 2 | 66 | 58 | -151 |
| 7 | 2 | 4 | 61 | 65 | 142 |
| 7 | 3 | 1 | 117 | 110 | 11 |
| 7 | 3 | 3 | 156 | 156 | -6 |
| 7 | 4 | 0 | 116 | 98 | 0 |
| 7 | 4 | 2 | 76 | 75 | 54 |
| 7 | 4 | 4 | 76 | 74 | -4 |
| 7 | 5 | 1 | 47 | 37 | 175 |
| 7 | 5 | 3 | 96 | 78 | 172 |
| 7 | 6 | 0 | 187 | 149 | -180 |
| 7 | 6 | 2 | 71 | 57 | -144 |
| 7 | 6 | 4 | 87 | 78 | -177 |
| 7 | 7 | 1 | 31 | 34 | -103 |
| 7 | 7 | 3 | 18 | 12 | 28 |
| 7 | 8 | 0 | 220 | 177 | 0 |
| 7 | 8 | 2 | 86 | 66 | -1 |
| 7 | 8 | 4 | 89 | 63 | 1 |
| 7 | 9 | 1 | 28 | 41 | 82 |
| 7 | 9 | 3 | 11 | 15 | -63 |
| 7 | 10 | 0 | 171 | 138 | -180 |
| 7 | 10 | 2 | 86 | 69 | 173 |
| 7 | 11 | 1 | 44 | 35 | -140 |
| 7 | 12 | 0 | 92 | 52 | 0 |
| 7 | 12 | 2 | 44 | 38 | 2 |
| 8 | -25 | -1 | 49 | 58 | 6 |
| 8 | -24 | 0 | 17 | 37 | 0 |
| 8 | -23 | -3 | 54 | 70 | 158 |
| 8 | -23 | -1 | 50 | 65 | -175 |
| 8 | -22 | -2 | 30 | 54 | -173 |
| 8 | -22 | 0 | 46 | 69 | -180 |
| 8 | -21 | -3 | 60 | 69 | -10 |
| 8 | -21 | -1 | 59 | 73 | 12 |
| 8 | -20 | -4 | 40 | 46 | -1 |
| 8 | -20 | -2 | 52 | 63 | 2 |
| 8 | -20 | 0 | 32 | 32 | 0 |
| 8 | -19 | -3 | 54 | 74 | 173 |
| 8 | -19 | -1 | 95 | 121 | -162 |
| 8 | -18 | -4 | 69 | 73 | 165 |
| 8 | -18 | -2 | 79 | 97 | 177 |
| 8 | -18 | 0 | 38 | 26 | 180 |
| 8 | -17 | -3 | 23 | 24 | -87 |
| 8 | -17 | -1 | 69 | 75 | 44 |
| 8 | -16 | -4 | 41 | 65 | -17 |
| 8 | -16 | -2 | 113 | 131 | 7 |
| 8 | -16 | 0 | 29 | 32 | 0 |
| 8 | -15 | -3 | 85 | 87 | 28 |
| 8 | -15 | -1 | 65 | 80 | -26 |
| 8 | -14 | -4 | 27 | 36 | -173 |
| 8 | -14 | -2 | 138 | 153 | -150 |
| 8 | -14 | 0 | 46 | 51 | 180 |
| 8 | -13 | -3 | 52 | 48 | -136 |
| 8 | -13 | -1 | 85 | 96 | -171 |
| 8 | -12 | -4 | 54 | 64 | 0 |
| 8 | -12 | -2 | 201 | 224 | 13 |
| 8 | -12 | 0 | 125 | 163 | 0 |
| 8 | -11 | -3 | 42 | 37 | -30 |
| 8 | -11 | -1 | 163 | 180 | 14 |
| 8 | -10 | -4 | 68 | 72 | 170 |
| 8 | -10 | -2 | 133 | 136 | -174 |
| 8 | -10 | 0 | 122 | 124 | -180 |
| 8 | -9 | -3 | 139 | 127 | 142 |
| 8 | -8 | -4 | 35 | 35 | -30 |
| 8 | -8 | -2 | 72 | 74 | -174 |
| 8 | -8 | 0 | 45 | 53 | -180 |
| 8 | -7 | -3 | 120 | 110 | -27 |
| 8 | -6 | -4 | 53 | 46 | 22 |
| 8 | -6 | -2 | 235 | 224 | 1 |
| 8 | -6 | 0 | 172 | 174 | 0 |
| 8 | -5 | -3 | 107 | 86 | -147 |
| 8 | -5 | -1 | 165 | 156 | 133 |
| 8 | -4 | -2 | 232 | 240 | 177 |
| 8 | -4 | 0 | 166 | 199 | -180 |
| 8 | -3 | -1 | 138 | 130 | -70 |
| 8 | -2 | 0 | 73 | 76 | 0 |
| 8 | -1 | -1 | 86 | 81 | 92 |
| 8 | 0 | 0 | 108 | 89 | 180 |
| 8 | 0 | 2 | 27 | 21 | 117 |
| 8 | 0 | 4 | 115 | 106 | -178 |
| 8 | 1 | 1 | 47 | 42 | 157 |
| 8 | 1 | 3 | 83 | 69 | -169 |
| 8 | 2 | 0 | 223 | 184 | 0 |
| 8 | 2 | 2 | 73 | 63 | -26 |
| 8 | 2 | 4 | 105 | 101 | 7 |
| 8 | 3 | 1 | 102 | 85 | 15 |
| 8 | 3 | 3 | 112 | 98 | -10 |
| 8 | 4 | 0 | 120 | 92 | -180 |
| 8 | 4 | 2 | 42 | 31 | 114 |
| 8 | 4 | 4 | 41 | 26 | 166 |
| 8 | 5 | 1 | 129 | 107 | -167 |
| 8 | 5 | 3 | 118 | 85 | 170 |
| 8 | 7 | 1 | 121 | 98 | 5 |
| 8 | 7 | 3 | 63 | 51 | 4 |
| 8 | 8 | 2 | 34 | 27 | -115 |
| 8 | 9 | 1 | 117 | 71 | 178 |
| 8 | 10 | 0 | 114 | 77 | -180 |
| 9 | -26 | 0 | 38 | 90 | 0 |
| 9 | -24 | -2 | 34 | 45 | 132 |
| 9 | -24 | 0 | 71 | 81 | -180 |
| 9 | -23 | -3 | 25 | 44 | -164 |
| 9 | -23 | -1 | 33 | 48 | 143 |
| 9 | -22 | -2 | 24 | 36 | -30 |
| 9 | -22 | 0 | 51 | 79 | 0 |
| 9 | -21 | -3 | 40 | 59 | 18 |
| 9 | -21 | -1 | 48 | 73 | -26 |
| 9 | -20 | -4 | 21 | 28 | -128 |
| 9 | -20 | -2 | 40 | 57 | -180 |
| 9 | -20 | 0 | 62 | 93 | -180 |
| 9 | -19 | -3 | 33 | 48 | -160 |
| 9 | -19 | -1 | 53 | 79 | 175 |
| 9 | -18 | -4 | 17 | 29 | 144 |
| 9 | -17 | -3 | 42 | 45 | 10 |
| 9 | -17 | -1 | 107 | 107 | 16 |
| 9 | -16 | -4 | 22 | 37 | 3 |
| 9 | -16 | -2 | 70 | 80 | -6 |
| 9 | -16 | 0 | 79 | 91 | 0 |
| 9 | -15 | -3 | 67 | 74 | -173 |
| 9 | -15 | -1 | 135 | 135 | -164 |
| 9 | -14 | -4 | 34 | 40 | -130 |
| 9 | -14 | -2 | 107 | 125 | -174 |
| 9 | -14 | 0 | 128 | 126 | -180 |
| 9 | -13 | -3 | 63 | 61 | 30 |
| 9 | -13 | -1 | 33 | 47 | 9 |
| 9 | -12 | -4 | 42 | 46 | 34 |
| 9 | -12 | -2 | 155 | 155 | 2 |
| 9 | -12 | 0 | 113 | 141 | 0 |
| 9 | -11 | -3 | 58 | 57 | -157 |
| 9 | -11 | -1 | 46 | 54 | 104 |
| 9 | -10 | -4 | 65 | 55 | 168 |
| 9 | -10 | -2 | 135 | 133 | 167 |
| 9 | -10 | 0 | 100 | 112 | 180 |
| 9 | -8 | -4 | 83 | 79 | -32 |
| 9 | -8 | -2 | 103 | 108 | -23 |
| 9 | -8 | 0 | 91 | 104 | 0 |
| 9 | -7 | -3 | 139 | 141 | 2 |
| 9 | -7 | -1 | 178 | 175 | 15 |
| 9 | -6 | -2 | 72 | 82 | 174 |
| 9 | -6 | 0 | 91 | 108 | -180 |
| 9 | -5 | -1 | 173 | 142 | -178 |
| 9 | -4 | 0 | 53 | 56 | 0 |
| 9 | -3 | -1 | 52 | 40 | -9 |
| 9 | -1 | -1 | 113 | 97 | -172 |
| 9 | 0 | 0 | 177 | 129 | 180 |
| 9 | 0 | 2 | 56 | 41 | -150 |
| 9 | 0 | 4 | 85 | 56 | 178 |

TABLE 7 (*Continued*)

| h | k | l | $\|F_o\|$ | $F_c$ | α |
|---|---|---|---|---|---|
| 9 | 1 | 1 | 94 | 85 | -33 |
| 9 | 1 | 3 | 86 | 68 | 21 |
| 9 | 2 | 0 | 260 | 205 | 0 |
| 9 | 2 | 2 | 129 | 106 | -0 |
| 9 | 2 | 4 | 105 | 64 | 3 |
| 9 | 3 | 1 | 46 | 54 | 93 |
| 9 | 4 | 0 | 200 | 149 | -180 |
| 9 | 4 | 2 | 117 | 97 | 176 |
| 9 | 5 | 1 | 26 | 24 | -110 |
| 9 | 5 | 3 | 14 | 8 | -158 |
| 9 | 6 | 0 | 86 | 44 | 0 |
| 9 | 6 | 2 | 47 | 39 | 2 |
| 9 | 7 | 1 | 48 | 33 | -18 |
| 10 | -23 | -1 | 30 | 54 | 31 |
| 10 | -22 | -2 | 59 | 66 | 19 |
| 10 | -21 | -3 | 14 | 18 | 107 |
| 10 | -20 | -2 | 84 | 103 | -163 |
| 10 | -20 | 0 | 25 | 25 | 180 |
| 10 | -18 | -4 | 50 | 63 | -14 |
| 10 | -18 | -2 | 140 | 162 | 5 |
| 10 | -18 | 0 | 107 | 124 | 0 |
| 10 | -17 | -3 | 28 | 34 | -69 |
| 10 | -17 | -1 | 75 | 97 | 21 |
| 10 | -16 | -4 | 69 | 67 | 165 |
| 10 | -16 | -2 | 76 | 88 | -179 |
| 10 | -16 | 0 | 89 | 87 | 180 |
| 10 | -15 | -3 | 67 | 72 | 143 |
| 10 | -15 | -1 | 158 | 170 | -176 |
| 10 | -14 | -4 | 32 | 24 | -21 |
| 10 | -14 | -2 | 40 | 47 | 177 |
| 10 | -13 | -3 | 68 | 64 | -4 |
| 10 | -12 | -2 | 67 | 56 | -6 |
| 10 | -11 | -3 | 89 | 79 | -153 |
| 10 | -10 | -4 | 72 | 48 | -173 |
| 10 | -10 | -2 | 56 | 59 | 168 |
| 10 | -10 | 0 | 34 | 39 | -180 |
| 10 | -9 | -3 | 88 | 82 | 28 |
| 10 | -9 | -1 | 130 | 111 | -50 |
| 10 | -8 | -2 | 59 | 65 | -2 |
| 10 | -8 | 0 | 100 | 110 | 0 |
| 10 | -7 | -1 | 72 | 61 | 140 |
| 10 | -6 | 0 | 125 | 133 | -180 |
| 10 | -3 | -1 | 31 | 45 | -47 |
| 10 | -1 | -1 | **98** | 82 | 165 |
| 10 | 0 | 0 | **81** | 63 | 0 |
| 10 | 0 | 2 | 34 | 35 | 28 |
| 10 | 1 | 1 | 145 | 111 | 2 |
| 10 | 1 | 3 | 70 | 49 | -4 |
| 10 | 2 | 2 | 30 | 24 | -102 |
| 10 | 3 | 1 | 145 | 105 | -180 |
| 10 | 4 | 0 | 60 | 35 | -180 |
| 10 | 4 | 2 | 46 | 32 | 153 |
| 10 | 5 | 1 | 54 | 31 | 8 |
| 11 | -23 | -1 | 47 | 50 | 18 |
| 11 | -22 | -2 | 14 | 21 | -10 |
| 11 | -22 | 0 | 15 | 28 | 0 |
| 11 | -21 | -1 | 72 | 69 | -165 |
| 11 | -20 | -2 | 38 | 45 | 180 |
| 11 | -20 | 0 | 31 | 44 | -180 |
| 11 | -19 | -3 | 60 | 72 | 18 |
| 11 | -19 | -1 | 62 | 82 | -6 |
| 11 | -18 | -2 | 60 | 56 | -12 |
| 11 | -18 | 0 | 44 | 54 | 0 |
| 11 | -17 | -3 | 58 | 51 | -166 |
| 11 | -16 | -2 | 41 | 50 | 156 |
| 11 | -16 | 0 | 56 | 55 | 180 |
| 11 | -14 | -2 | 56 | 68 | -12 |
| 11 | -14 | 0 | 66 | 90 | 0 |
| 11 | -13 | -3 | 75 | 50 | 20 |
| 11 | -13 | -1 | 116 | 39 | 46 |
| 11 | -12 | -2 | 83 | 81 | -176 |
| 11 | -12 | 0 | 86 | 105 | -180 |
| 11 | -11 | -3 | 103 | 87 | -175 |
| 11 | -11 | -1 | 30 | 29 | -174 |
| 11 | -10 | -2 | 90 | 88 | 15 |
| 11 | -10 | 0 | 97 | 89 | 0 |
| 11 | -9 | -1 | 67 | 57 | -0 |
| 11 | -8 | 0 | 44 | 43 | 180 |
| 11 | -7 | -1 | 129 | 96 | -164 |
| 11 | -5 | -1 | 110 | 92 | 34 |
| 11 | -3 | -1 | 70 | 56 | -131 |
| 11 | 0 | 0 | 82 | 46 | 0 |
| 11 | 0 | 2 | 53 | 43 | -2 |
| 11 | 2 | 0 | 92 | 46 | 180 |
| 12 | -22 | 0 | 33 | 49 | -180 |
| 12 | -21 | -1 | 46 | 65 | -170 |
| 12 | -20 | 0 | 40 | 48 | 0 |
| 12 | -19 | -1 | 21 | 36 | -34 |
| 12 | -18 | 0 | 26 | 30 | -180 |
| 12 | -17 | -1 | 89 | 70 | 138 |
| 12 | -15 | -1 | 89 | 76 | -31 |
| 12 | -14 | -2 | 30 | 22 | 10 |
| 12 | -14 | 0 | 56 | 62 | 0 |
| 12 | -13 | -1 | 44 | 38 | 180 |
| 12 | -12 | 0 | 88 | 87 | -180 |
| 12 | -11 | -1 | 68 | 70 | 21 |
| 12 | -9 | -1 | 26 | 33 | -128 |
| 12 | -7 | -1 | 104 | 80 | 170 |
| 12 | -5 | -1 | 129 | 84 | -3 |
| 12 | -3 | -1 | 97 | 62 | 170 |
| 13 | -15 | -1 | 75 | 40 | 12 |
| 13 | -13 | -1 | 115 | 67 | -155 |
| 13 | -11 | -1 | 100 | 58 | 37 |
| 13 | -9 | -1 | 59 | 37 | -153 |
| 13 | -7 | -1 | 42 | 38 | -10 |

the space parameters of the centrosymmetric molecule and the space parameters of the molecule in the general position, were ignored. Table 4 gives the observed structure amplitudes and the structures factors calculated from the atomic parameters in Table 3(a).

*Diaquobis(methoxyacetato)copper*(II) (J. G. Forrest).—$C_6H_{14}CuO_8$, $M = 277{\cdot}6$, Monoclinic prismatic, $a = 6{\cdot}92 \pm 0{\cdot}02$, $b = 7{\cdot}26 \pm 0{\cdot}02$, $c = 10{\cdot}10 \pm 0{\cdot}03$ Å, $\gamma = 96{\cdot}7 \pm 0{\cdot}3°$, $U = 505{\cdot}2$ Å$^3$, $D_m = 1{\cdot}820 \pm 0{\cdot}005$ (by flotation), $Z = 2$, $D_c = 1{\cdot}819$. Space group $P2_1/n$ ($C_{2h}^5$, No. 14), general position $\pm (x, y, z; \frac{1}{2} + x, \frac{1}{2} + y, \frac{1}{2} - z)$. Cu-$K_\alpha$ radiation, $\mu = 33{\cdot}8$ cm.$^{-1}$. Crystal size $0{\cdot}4 \times 0{\cdot}15 \times 0{\cdot}08$ mm. Optically biaxial.

A trial structure was deduced from a Patterson function sharpened to 'point atoms at rest' computed from 722 independent reflections. The trial was refined by $F_o$ synthesis and six cycles of full matrix least-squares refinement, assuming isotropic temperature factors and giving each observation unit weight. The refinement converged with $R = 0{\cdot}115$. Some adjustment at the layer scale factors was made after the third refinement cycle. At no stage was it possible to locate hydrogen atoms from a difference synthesis. Table 5 gives observed structure amplitude and structure factors calculated from the atomic parameters in Table 3(b).

*Bis(glycollato)copper*(II) (J. G. Forrest).—$C_4H_6CuO_6$, $M = 213{\cdot}6$, Monoclinic prismatic, $a = 7{\cdot}93 \pm 0{\cdot}02$, $b = 5{\cdot}08 \pm 0{\cdot}02$, $c = 8{\cdot}68 \pm 0{\cdot}02$ Å, $\gamma = 111{\cdot}1 \pm 0{\cdot}3°$, $U = 326{\cdot}3$ Å, $D_m = 2{\cdot}164 \pm 0{\cdot}01$ (by flotation), $Z = 2$, $D_c = 2{\cdot}165$. Space group $P2_1/a$ ($C_{2h}^5$, No. 14), general positions $\pm (x, y, z; \frac{1}{2} - x, \bar{y}, \frac{1}{2} + z)$. Cu-$K_\alpha$ radiation, $\mu = 46{\cdot}0$ cm.$^{-1}$. Crystal size $0{\cdot}4 \times 0{\cdot}2 \times 0{\cdot}15$ mm. Optically biaxial.

A trial structure was deduced from a three-dimensional Patterson function sharpened to 'point atoms at rest' computed from 602 independent reflections. The trial structure was improved firstly by $F_o$ synthesis and then by four cycles of full matrix least-squares refinement assuming isotropic temperature factors and giving each observation unit weight. The refinement converged with $R = 0{\cdot}136$. Attempts to locate the hydrogen atoms by difference synthesis failed. Table 6 gives the observed structure amplitudes and structure factors calculated from the atomic parameters in Table 3(c).

*Aquobis-*(DL-*lactato*)*copper*(II) *Hemihydrate* (J. R. Carruthers and R. A. Armstrong).—$C_6H_{10}CuO_6, 1\frac{1}{2}H_2O$, $M = 268{\cdot}7$, Monoclinic, $a = 10{\cdot}53 \pm 0{\cdot}03$, $b = 20{\cdot}55 \pm 0{\cdot}05$, $c = 5{\cdot}66 \pm 0{\cdot}02$, $\gamma = 119{\cdot}3° \pm 0{\cdot}30$, $U = 1{\cdot}067{\cdot}9$ Å$^3$, $D_m = 1{\cdot}71 \pm 0{\cdot}03$ (by flotation), $Z = 4$, $D_c = 1{\cdot}671$. Space group $A2$($C_2^3$, No. 5); a piezoelectric test shows no inversion centre. Cu-$K_\alpha$ radiation, $\mu = 32{\cdot}3$ cm.$^{-1}$.

From the three-dimensional Patterson function sharpened to 'point atoms at rest' computed from 981 independent reflections, it was clear that the copper atom was in a general position in space group $A2$. The $F_o$ synthesis computed from the phases given by the tentative copper atom position and the three-dimensional minimum function constructed by superposing the copper–copper vectors had similar sets of maxima. Surprisingly, after careful study of both maps, it was only possible to assign maxima to four atoms [O(1), O(13), O(3), and O(11)] of the copper co-ordination polyhedron and no others. However, the $F_o$ synthesis phased on the five proposed atom positions showed the location of both lactate groups and a water molecule. This trial structure was improved by six cycles of full matrix least-squares refinement, assuming isotropic thermal motion, unit weights for the observations, and applying 0·5 shifts. After the third cycle the layer scale factors were adjusted manually, and the residual was 0·15. A difference map computed at this residual had a maximum of about four electrons at the site O(5). The agreement between observed and calculated densities assuming a monohydrate was not good nor were the analytical results. It was therefore decided to introduce one 'half water molecule' at this position, and to refine its positional and temperature parameters and occupation number along with all other atomic parameters for the structure at $R = 0{\cdot}15$ by the full matrix least-squares method with the weighting scheme (2) with $a = b = 1000$. The refinement converged after three cycles at $R = 0{\cdot}121$. At no stage in the refinement was it possible to locate hydrogen atoms from difference syntheses with any certainty. Table 7 lists observed structure amplitudes and calculated structure factors based on the final atomic parameters in Table 3(d).

*Diaquobis-*(2-*hydroxy*-2-*methylpropionato*)*copper*(II) (R. A. Armstrong).—When a pale blue needle crystal of this complex was first subjected to $X$-ray photography it showed a diffraction pattern expected for a triclinic twinned crystal with a needle axis spacing of 5·80 Å. As $X$-ray photography progressed the diffraction pattern changed during an exposure time of several days. One of several new

TABLE 8

Observed structure amplitudes and calculated stucture factors for diaquobis-(2-hydroxy-2-methylpropionato)copper(II)

| h | k | l | $\|F_o\|$ | $F_c$ |
|---|---|---|---|---|
| 0 | 0 | 13 | 25 | 41 |
| 0 | 0 | 12 | 60 | 61 |
| 0 | 0 | 11 | 106 | 102 |
| 0 | 0 | 10 | 79 | 74 |
| 0 | 0 | 9 | 45 | 60 |
| 0 | 0 | 8 | 80 | 90 |
| 0 | 0 | 7 | 93 | 92 |
| 0 | 0 | 6 | 103 | 122 |
| 0 | 0 | 5 | 116 | 114 |
| 0 | 0 | 4 | 130 | 143 |
| 0 | 0 | 3 | 225 | 218 |
| 0 | 0 | 2 | 14 | 13 |
| 2 | 0 | 13 | 27 | 38 |
| 2 | 0 | 12 | 49 | 50 |
| 2 | 0 | 11 | 101 | 78 |
| 2 | 0 | 10 | 74 | 66 |
| 2 | 0 | 9 | 18 | 66 |
| 2 | 0 | 8 | 52 | 44 |
| 2 | 0 | 7 | 78 | 73 |
| 2 | 0 | 6 | 38 | 36 |
| 2 | 0 | 5 | 48 | 30 |
| 2 | 0 | 4 | 102 | 93 |
| 2 | 0 | 3 | 18 | 22 |
| 2 | 0 | 2 | 114 | -86 |
| 2 | 0 | 1 | 117 | 142 |
| 4 | 0 | 12 | 33 | 45 |
| 4 | 0 | 11 | 67 | 64 |
| 4 | 0 | 10 | 70 | 74 |
| 4 | 0 | 8 | 32 | 44 |
| 4 | 0 | 7 | 98 | 106 |
| 4 | 0 | 6 | 39 | 45 |
| 4 | 0 | 5 | 63 | 66 |
| 4 | 0 | 4 | 159 | 165 |
| 4 | 0 | 3 | 45 | 44 |
| 4 | 0 | 2 | 37 | 41 |
| 4 | 0 | 1 | 224 | 231 |
| 4 | 0 | 0 | 229 | 292 |
| 6 | 0 | 12 | 20 | 27 |
| 6 | 0 | 11 | 41 | 46 |
| 6 | 0 | 10 | 40 | 37 |
| 6 | 0 | 8 | 23 | 19 |
| 6 | 0 | 7 | 37 | 37 |
| 6 | 0 | 6 | 26 | 15 |
| 6 | 0 | 4 | 56 | 47 |
| 6 | 0 | 5 | 12 | 14 |
| 6 | 0 | 3 | 22 | 9 |
| 6 | 0 | 2 | 65 | -32 |
| 6 | 0 | 1 | 66 | 71 |
| 6 | 0 | 0 | 131 | 64 |
| 8 | 0 | 10 | 18 | 21 |
| 8 | 0 | 9 | 11 | 12 |
| 8 | 0 | 8 | 17 | 22 |
| 8 | 0 | 7 | 18 | 20 |
| 8 | 0 | 6 | 32 | 28 |
| 8 | 0 | 5 | 35 | 24 |
| 8 | 0 | 4 | 37 | 31 |
| 8 | 0 | 3 | 45 | 41 |
| 8 | 0 | 1 | 50 | 53 |
| 8 | 0 | 0 | 127 | 144 |
| 10 | 0 | 2 | 26 | -18 |
| 10 | 0 | 0 | 45 | 59 |
| 12 | 0 | 4 | 18 | 16 |
| 12 | 0 | 1 | 16 | 22 |
| 12 | 0 | 0 | 28 | 33 |
| 1 | 1 | -4 | 41 | 49 |
| 1 | 1 | -5 | 26 | 13 |
| 1 | 1 | -6 | 152 | 128 |
| 1 | 1 | -7 | 160 | 126 |
| 1 | 1 | -8 | 130 | 110 |
| 1 | 1 | -9 | 133 | 105 |
| 1 | 1 | -10 | 71 | 54 |
| 1 | 1 | -11 | 44 | 46 |
| 1 | 1 | -12 | 54 | 58 |
| 1 | 1 | -13 | 52 | 49 |
| 3 | 1 | -1 | 70 | 58 |
| 3 | 1 | -2 | 155 | 119 |
| 3 | 1 | -3 | 54 | 44 |
| 3 | 1 | -4 | 27 | 30 |
| 3 | 1 | -5 | 80 | 64 |
| 3 | 1 | -6 | 88 | 65 |
| 3 | 1 | -7 | 126 | 116 |
| 3 | 1 | -8 | 137 | 113 |
| 3 | 1 | -9 | 79 | 67 |
| 3 | 1 | -10 | 65 | 56 |
| 3 | 1 | -11 | 43 | 43 |
| 3 | 1 | -12 | 37 | 40 |
| 3 | 1 | -13 | 47 | 49 |
| 5 | 1 | 0 | 101 | 80 |
| 5 | 1 | -1 | 51 | 36 |
| 5 | 1 | -2 | 84 | 76 |
| 5 | 1 | -3 | 21 | 23 |
| 5 | 1 | -4 | 37 | 14 |
| 5 | 1 | -5 | 52 | 40 |
| 5 | 1 | -6 | 41 | 40 |
| 5 | 1 | -7 | 106 | 82 |
| 5 | 1 | -8 | 100 | 83 |
| 5 | 1 | -9 | 47 | 46 |
| 5 | 1 | -10 | 43 | 39 |
| 5 | 1 | -11 | 21 | 30 |
| 5 | 1 | -12 | 21 | 28 |
| 7 | 1 | 0 | 84 | 64 |
| 7 | 1 | -1 | 56 | 44 |
| 7 | 1 | -2 | 13 | 12 |
| 7 | 1 | -3 | 52 | 36 |
| 7 | 1 | -4 | 35 | 15 |
| 7 | 1 | -6 | 45 | 42 |
| 7 | 1 | -7 | 53 | 50 |
| 7 | 1 | -8 | 46 | 47 |
| 7 | 1 | -9 | 42 | 43 |
| 9 | 1 | 5 | 41 | 40 |
| 9 | 1 | 4 | 28 | 30 |
| 9 | 1 | 3 | 18 | 19 |
| 9 | 1 | 2 | 24 | 21 |
| 9 | 1 | 1 | 18 | 15 |
| 9 | 1 | 0 | 45 | 33 |
| 9 | 1 | -1 | 24 | 21 |
| 9 | 1 | -2 | 14 | -4 |
| 9 | 1 | -3 | 28 | 15 |
| 9 | 1 | -4 | 14 | 5 |
| 9 | 1 | -6 | 27 | 20 |
| 9 | 1 | -7 | 20 | 27 |
| 9 | 1 | -8 | 29 | 28 |
| 9 | 1 | -9 | 25 | 25 |
| 11 | 1 | 4 | 20 | 25 |
| 11 | 1 | 1 | 16 | 18 |
| 11 | 1 | 0 | 16 | 15 |
| 1 | 1 | 2 | 167 | 149 |
| 1 | 1 | 3 | 123 | 109 |
| 1 | 1 | 4 | 177 | 154 |
| 1 | 1 | 5 | 201 | 188 |
| 1 | 1 | 6 | 80 | 70 |
| 1 | 1 | 7 | 16 | 29 |
| 1 | 1 | 8 | 50 | 48 |
| 1 | 1 | 9 | 35 | 41 |
| 1 | 1 | 10 | 74 | 67 |
| 1 | 1 | 11 | 83 | 70 |
| 1 | 1 | 12 | 39 | 39 |
| 3 | 1 | 1 | 226 | 191 |
| 3 | 1 | 2 | 53 | 54 |
| 3 | 1 | 3 | 113 | 98 |
| 3 | 1 | 4 | 182 | 174 |
| 3 | 1 | 5 | 126 | 114 |
| 3 | 1 | 6 | 67 | 76 |
| 3 | 1 | 7 | 35 | 37 |
| 3 | 1 | 9 | 38 | 48 |
| 3 | 1 | 10 | 68 | 59 |
| 3 | 1 | 11 | 60 | 52 |
| 5 | 1 | 3 | 85 | 64 |
| 5 | 1 | 4 | 123 | 120 |
| 5 | 1 | 5 | 82 | 77 |
| 5 | 1 | 6 | 71 | 52 |
| 5 | 1 | 7 | 20 | 23 |
| 5 | 1 | 9 | 33 | 32 |
| 7 | 1 | 1 | 55 | 42 |
| 7 | 1 | 2 | 45 | 46 |
| 7 | 1 | 3 | 44 | 40 |
| 7 | 1 | 4 | 42 | 58 |
| 7 | 1 | 10 | 19 | 29 |
| 0 | 2 | 11 | 23 | 34 |
| 0 | 2 | 10 | 77 | 73 |
| 0 | 2 | 9 | 53 | 58 |
| 0 | 2 | 8 | 51 | 56 |
| 0 | 2 | 7 | 103 | 98 |
| 0 | 2 | 6 | 113 | 110 |
| 0 | 2 | 5 | 131 | 125 |
| 0 | 2 | 4 | 116 | 112 |
| 0 | 2 | 3 | 154 | 158 |
| 0 | 2 | 2 | 234 | 262 |
| 0 | 2 | 1 | 43 | 47 |
| 0 | 2 | 0 | 74 | -54 |
| 0 | 2 | -2 | 128 | 162 |
| 0 | 2 | -3 | 129 | 128 |
| 0 | 2 | -4 | 233 | 248 |
| 0 | 2 | -5 | 141 | 139 |
| 0 | 2 | -6 | 60 | 82 |
| 0 | 2 | -7 | 125 | 127 |
| 0 | 2 | -8 | 140 | 138 |
| 0 | 2 | -9 | 119 | 117 |
| 0 | 2 | -10 | 19 | 43 |
| 0 | 2 | -11 | 23 | 23 |
| 0 | 2 | -12 | 62 | 64 |
| 0 | 2 | -13 | 45 | 50 |
| 2 | 2 | 11 | 17 | 28 |
| 2 | 2 | 10 | 63 | 53 |
| 2 | 2 | 9 | 59 | 52 |
| 2 | 2 | 8 | 32 | 34 |
| 2 | 2 | 7 | 78 | 59 |
| 2 | 2 | 6 | 104 | 95 |
| 2 | 2 | 5 | 74 | 65 |
| 2 | 2 | 4 | 61 | 44 |
| 2 | 2 | 3 | 111 | 123 |
| 2 | 2 | 2 | 124 | 129 |
| 2 | 2 | 1 | 57 | -37 |
| 2 | 2 | 0 | 119 | -91 |
| 2 | 2 | -1 | 22 | 40 |
| 2 | 2 | -2 | 87 | 82 |
| 2 | 2 | -3 | 76 | 59 |
| 2 | 2 | -4 | 111 | 106 |
| 2 | 2 | -5 | 104 | 96 |
| 2 | 2 | -6 | 32 | 28 |
| 2 | 2 | -7 | 67 | 57 |
| 2 | 2 | -8 | 129 | 120 |
| 2 | 2 | -9 | 107 | 82 |
| 2 | 2 | -12 | 58 | 46 |
| 2 | 2 | -13 | 41 | 39 |
| 4 | 2 | 10 | 37 | 42 |
| 4 | 2 | 9 | 62 | 58 |
| 4 | 2 | 8 | 28 | 35 |
| 4 | 2 | 7 | 54 | 51 |
| 4 | 2 | 5 | 70 | 65 |
| 4 | 2 | 4 | 60 | 59 |
| 4 | 2 | 3 | 163 | 167 |
| 4 | 2 | 2 | 121 | 120 |
| 4 | 2 | 1 | 49 | 30 |
| 4 | 2 | 0 | 46 | 27 |
| 4 | 2 | -1 | 65 | 52 |
| 4 | 2 | -2 | 149 | 143 |
| 4 | 2 | -3 | 127 | 122 |
| 4 | 2 | -4 | 96 | 97 |
| 4 | 2 | -5 | 126 | 139 |
| 4 | 2 | -6 | 55 | 58 |
| 4 | 2 | -7 | 39 | 53 |
| 4 | 2 | -8 | 130 | 135 |
| 4 | 2 | -9 | 83 | 77 |
| 4 | 2 | -10 | 16 | 14 |
| 4 | 2 | -12 | 27 | 37 |
| 4 | 2 | -13 | 26 | 34 |
| 6 | 2 | 10 | 27 | 30 |
| 6 | 2 | 9 | 26 | 28 |
| 6 | 2 | 8 | 21 | 14 |
| 6 | 2 | 7 | 27 | 31 |
| 6 | 2 | 6 | 54 | 53 |
| 6 | 2 | 5 | 32 | 31 |
| 6 | 2 | 3 | 62 | 67 |
| 6 | 2 | 2 | 68 | 64 |
| 6 | 2 | 1 | 34 | -20 |
| 6 | 2 | 0 | 55 | -44 |
| 6 | 2 | -2 | 38 | 42 |
| 6 | 2 | -3 | 37 | 32 |
| 6 | 2 | -4 | 59 | 53 |
| 6 | 2 | -5 | 52 | 49 |
| 6 | 2 | -7 | 28 | 27 |
| 6 | 2 | -8 | 80 | 70 |
| 6 | 2 | -9 | 48 | 45 |
| 6 | 2 | -12 | 21 | 24 |
| 8 | 2 | 7 | 27 | 30 |
| 8 | 2 | 6 | 26 | 32 |
| 8 | 2 | 5 | 32 | 32 |
| 8 | 2 | 4 | 28 | 26 |
| 8 | 2 | 3 | 43 | 42 |
| 8 | 2 | 2 | 63 | 67 |
| 8 | 2 | 1 | 16 | 1 |
| 8 | 2 | 0 | 16 | -25 |
| 8 | 2 | -1 | 51 | 44 |
| 8 | 2 | -2 | 43 | 35 |
| 8 | 2 | -3 | 36 | 28 |
| 8 | 2 | -4 | 61 | 64 |
| 8 | 2 | -5 | 36 | 32 |
| 8 | 2 | -7 | 32 | 35 |
| 8 | 2 | -8 | 39 | 45 |
| 8 | 2 | -9 | 31 | 37 |
| 10 | 2 | 2 | 18 | 23 |
| 10 | 2 | 0 | 24 | -23 |
| 10 | 2 | -8 | 21 | 28 |
| 10 | 2 | -9 | 16 | 16 |
| 1 | 3 | -13 | 30 | 41 |
| 1 | 3 | -12 | 44 | 51 |
| 1 | 3 | -11 | 44 | 54 |
| 1 | 3 | -10 | 35 | 53 |
| 1 | 3 | -9 | 24 | 37 |
| 1 | 3 | -8 | 68 | 62 |
| 1 | 3 | -7 | 52 | 65 |
| 1 | 3 | -5 | 109 | 117 |
| 1 | 3 | -4 | 151 | 178 |
| 1 | 3 | -3 | 91 | 107 |
| 1 | 3 | -2 | 79 | 116 |
| 1 | 3 | -1 | 71 | 90 |
| 1 | 3 | 0 | 18 | 32 |
| 1 | 3 | 1 | 45 | 73 |
| 1 | 3 | 2 | 71 | 91 |
| 1 | 3 | 3 | 73 | 82 |
| 1 | 3 | 4 | 30 | 43 |
| 1 | 3 | 6 | 62 | 73 |
| 3 | 3 | -12 | 38 | 49 |
| 3 | 3 | -11 | 38 | 52 |
| 3 | 3 | -9 | 40 | 46 |
| 3 | 3 | -8 | 43 | 52 |
| 3 | 3 | -7 | 25 | 31 |
| 3 | 3 | -6 | 32 | 55 |
| 3 | 3 | -5 | 69 | 85 |
| 3 | 3 | -4 | 116 | 130 |
| 3 | 3 | -3 | 102 | 137 |
| 3 | 3 | -2 | 54 | 64 |
| 3 | 3 | -1 | 57 | 70 |
| 3 | 3 | 0 | 57 | 66 |
| 3 | 3 | 2 | 65 | 89 |
| 3 | 3 | 3 | 82 | 89 |
| 3 | 3 | 6 | 56 | 67 |
| 3 | 3 | 7 | 59 | 71 |
| 3 | 3 | 8 | 42 | 60 |
| 5 | 3 | -12 | 25 | 37 |
| 5 | 3 | -11 | 30 | 38 |
| 5 | 3 | -9 | 20 | 32 |
| 5 | 3 | -8 | 35 | 35 |
| 5 | 3 | -6 | 18 | 37 |
| 5 | 3 | -5 | 47 | 58 |
| 5 | 3 | -4 | 72 | 89 |
| 5 | 3 | -3 | 70 | 96 |
| 5 | 3 | -2 | 36 | 41 |
| 5 | 3 | -1 | 46 | 45 |
| 5 | 3 | 0 | 33 | 42 |
| 5 | 3 | 2 | 51 | 63 |
| 5 | 3 | 3 | 50 | 62 |
| 5 | 3 | 6 | 34 | 49 |
| 5 | 3 | 7 | 37 | 53 |
| 5 | 3 | 8 | 29 | 45 |
| 7 | 3 | -11 | 14 | 21 |
| 7 | 3 | -8 | 20 | 22 |
| 7 | 3 | -5 | 30 | 46 |
| 7 | 3 | -4 | 39 | 69 |
| 7 | 3 | -3 | 24 | 40 |
| 7 | 3 | -2 | 33 | 44 |
| 7 | 3 | -1 | 28 | 31 |
| 7 | 3 | 2 | 29 | 37 |
| 7 | 3 | 3 | 24 | 31 |
| 7 | 3 | 6 | 21 | 31 |
| 7 | 3 | 7 | 29 | 45 |
| 0 | 4 | -13 | 49 | 50 |
| 0 | 4 | -12 | 60 | 48 |
| 0 | 4 | -11 | 95 | 71 |
| 0 | 4 | -10 | 83 | 76 |
| 0 | 4 | -9 | 27 | 39 |
| 0 | 4 | -8 | 31 | 34 |
| 0 | 4 | -7 | 57 | 50 |
| 0 | 4 | -6 | 132 | 96 |
| 0 | 4 | -5 | 131 | 102 |
| 0 | 4 | -4 | 37 | 27 |
| 0 | 4 | -3 | 94 | 78 |
| 0 | 4 | -1 | 93 | 78 |
| 0 | 4 | 0 | 149 | 113 |
| 0 | 4 | 1 | 186 | 136 |
| 0 | 4 | 2 | 83 | 62 |
| 2 | 4 | -13 | 34 | 39 |
| 2 | 4 | -12 | 45 | 46 |
| 2 | 4 | -11 | 58 | 53 |
| 2 | 4 | -10 | 66 | 59 |
| 2 | 4 | -9 | 27 | 32 |
| 2 | 4 | -8 | 12 | 0 |
| 2 | 4 | -7 | 40 | 30 |
| 2 | 4 | -6 | 85 | 75 |
| 2 | 4 | -5 | 51 | 46 |
| 2 | 4 | -4 | 11 | 8 |
| 2 | 4 | -3 | 47 | 44 |
| 2 | 4 | -2 | 83 | 75 |
| 2 | 4 | -1 | 65 | 61 |
| 2 | 4 | 0 | 80 | 69 |
| 2 | 4 | 1 | 101 | 86 |
| 2 | 4 | 2 | 58 | 52 |
| 2 | 4 | 3 | 18 | 17 |
| 2 | 4 | 4 | 15 | 24 |
| 2 | 4 | 5 | 25 | 37 |
| 4 | 4 | -13 | 16 | 33 |
| 4 | 4 | -12 | 45 | 48 |
| 4 | 4 | -11 | 40 | 44 |
| 4 | 4 | -10 | 51 | 55 |
| 4 | 4 | -9 | 41 | 44 |
| 4 | 4 | -8 | 18 | -3 |
| 4 | 4 | -7 | 46 | 42 |
| 4 | 4 | -6 | 87 | 87 |
| 4 | 4 | -5 | 39 | 39 |
| 4 | 4 | -4 | 49 | 38 |
| 4 | 4 | -3 | 86 | 60 |
| 4 | 4 | -2 | 85 | 66 |
| 4 | 4 | -1 | 108 | 89 |
| 4 | 4 | 0 | 90 | 72 |
| 4 | 4 | 1 | 68 | 76 |
| 4 | 4 | 2 | 89 | 74 |
| 4 | 4 | 3 | 30 | 18 |
| 4 | 4 | 4 | 23 | 25 |
| 4 | 4 | 5 | 50 | 47 |
| 6 | 4 | -12 | 16 | 27 |
| 6 | 4 | -11 | 33 | 30 |
| 6 | 4 | -10 | 34 | 34 |
| 6 | 4 | -9 | 23 | 15 |
| 6 | 4 | -8 | 12 | -8 |
| 6 | 4 | -7 | 12 | 12 |
| 6 | 4 | -6 | 48 | 43 |
| 6 | 4 | -5 | 24 | 23 |
| 6 | 4 | -3 | 24 | 20 |
| 6 | 4 | -2 | 43 | 41 |
| 6 | 4 | -1 | 40 | 34 |
| 6 | 4 | 0 | 32 | 35 |
| 6 | 4 | 1 | 35 | 46 |
| 6 | 4 | 2 | 35 | 29 |
| 8 | 4 | -10 | 16 | 26 |
| 8 | 4 | -6 | 28 | 30 |
| 8 | 4 | -5 | 35 | 31 |
| 8 | 4 | -3 | 17 | 16 |
| 8 | 4 | -2 | 47 | 44 |
| 8 | 4 | -1 | 29 | 21 |
| 8 | 4 | 0 | 29 | 31 |
| 8 | 4 | 1 | 45 | 43 |
| 8 | 4 | 2 | 26 | 16 |
| 8 | 4 | 3 | 21 | 9 |
| 8 | 4 | 4 | 13 | 9 |

monoclinic forms of the crystal resulted; one with unit cell dimensions $a = 10{\cdot}8 \pm 0{\cdot}05$, $b = 5{\cdot}80 \pm 0{\cdot}03$, $c = 39{\cdot}98 \pm 0{\cdot}1$ Å, $\alpha = 110 \pm 1°$ and space group $P2_1/c$; and another with the crystal data quoted below and whose structure has been determined. Investigation of the first form is in progress. Although crystals have been prepared and stored in a variety of ways, only the triclinic twin has been found at the beginning of *X*-ray photography of a particular crystal.

Diaquobis-(2-hydroxy-2-methylpropionato)copper(II), $C_8H_{18}CuO_8$, $M = 305{\cdot}8$, Monoclinic prismatic (after exposure to Cu-$K_\alpha$ radiation), $a = 10{\cdot}25 \pm 0{\cdot}05$, $b = 5{\cdot}80 \pm 0{\cdot}03$, $c = 11{\cdot}24 \pm 0{\cdot}05$, $\alpha = 105{\cdot}9° \pm 0{\cdot}5$, $U = 642{\cdot}5$ Å$^3$, $D_m = 1{\cdot}647 \pm 0{\cdot}01$, $Z = 2$, $D_c = 1{\cdot}581$. Space group $C2/m$ ($C_{2h}^3$, No. 12), general positions $(0,0,0;\ \frac{1}{2},\frac{1}{2},0) \pm (x,y,z;\ \bar{x},y,z)$. Cu-$K_\alpha$ radiation, $\mu = 17{\cdot}3$ cm.$^{-1}$. Crystal size $0{\cdot}15 \times 0{\cdot}18 \times 0{\cdot}32$ mm.

Space group $C2$ or $C2/m$ are possible, from absent reflections. With two molecules to the unit cell the copper atoms lie on the two-fold axis, and if space group $C2/m$ is used, then the chelate rings and the copper atom must lie in the mirror plane. A three-dimensional unsharpened Patterson function calculated from 406 independent reflections could be interpreted assuming that the space group was $C2/m$ with the copper atoms at 0,0,0 and $\frac{1}{2},\frac{1}{2},0$. After a preliminary $F_o$ synthesis, the trial was refined to convergence assuming isotropic thermal motion, and $R$ was 0·214. Examination of the difference synthesis and the *X*-ray photographs suggested that the copper atom was executing anisotropic vibrations with the maximum displacement along $a$ perpendicular to the plane of the chelate ring. There was no compelling evidence in the difference synthesis to suggest using anisotropic temperature factors for the light atoms. Refinement continued using an anisotropic temperature factor for the copper atom. After five more refinement cycles, $R$ dropped to 0·16, but a difference synthesis still indicated residual electron-density near the copper atom along $a$. After a re-examination of the difference synthesis at $R = 0{\cdot}214$, the copper atoms were replaced by an arrangement whereby one half copper atom was placed at 0,0,0 and $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ and two one quarter copper atoms were placed along $a$ at each side of the half copper atom, related by the mirror planes and about $\frac{1}{2}$ Å distant. Then, starting with the atomic parameters for $R = 0{\cdot}214$, the space and isotropic temperature factors of the light atoms and the occupation numbers only for the copper atoms were refined by least-squares using the full normal matrix. The refinement converged after five cycles with $R = 0{\cdot}129$. The difference synthesis was much cleaner in the region of the copper than after the anisotropic refinement. The thermal parameters of the light atoms were very similar after both refinements, but the bonded distances at $R = 0{\cdot}129$ were markedly better than at $R = 0{\cdot}160$, and the e.s.d.'s for the refined parameters calculated from the normal matrices were uniformly smaller at $R = 0{\cdot}129$ than at $R = 0{\cdot}160$. It was concluded that the last refinement came nearest to the true model. Table 8 gives observed structure amplitudes and structure factors calculated from the parameters in Table 3(e), which gave $R = 0{\cdot}129$.

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