# The Crystal and Molecular Structure Analysis of the Centrosymmetric Polynuclear Ferrocene Complex $(C_{10}H_9Fe)_3C(C_4OH_7)$

[a]F. HANIC, [b]J. ŠEVČÍK and [c]E. L. McGANDY

[a]*Institute of Inorganic Chemistry, Slovak Academy of Sciences, Bratislava 9*

[b]*Biological Institute, Slovak Academy of Sciences, Bratislava 9*

[c]*Crystallography Laboratory, University of Pittsburgh, Pittsburgh, Pa., USA*

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The crystal and molecular structure of the polynuclear ferrocene complex $(C_{10}H_9Fe)_3C(C_4OH_7)$ has been explained by X-ray structure analysis using direct methods. The space group symmetry is $P\bar{1}$. The asymmetric part of the unit cell contains two molecules $(C_{10}H_9Fe)_3C(C_4OH_7)$. The polynuclear molecules consist of three ferrocenyl groups bonded to the common carbon atom. The fourth group bonded to the same carbon atom is a tetrahydrofuran ring. The ring atoms of the cyclopentadiene rings do not deviate significantly from planarity. The angle of tilt between the least-squares planes is between 2.9° to 8.9°. The diffractometric intensities of 2292 independent reflections have been used. The final $R$ factor was 0.063.

The ferrocene molecule behaves as a typical covalent compound. The two $C_5H_5$ rings are parallel, with the metal atom lying symmetrically between them, and the rings in a staggered formation. The molecule possesses a centre of symmetry. There is no symmetry centre in the ferrocene groups of the complex

$$(C_{10}H_9Fe)_3C(C_4OH_7)$$

where each group is bonded through one $sp^2$ hybridized carbon atom of the cyclopentadienyl ring to the $sp^3$ hybridized central carbon atom. The effect of the symmetry distortion in the ferrocene group on the molecular geometry of $(C_{10}H_9Fe)_3C(C_4OH_7)$ was studied in details by the X-ray structure analysis.

This work gives an example of solving the crystal and molecular structure of the centrosymmetric polynuclear ferrocene complex $(C_{10}H_9Fe)_3C(C_4OH_7)$ directly from experimental data. Correct set of phases $\varphi_s$ were obtained by application of a fully automatic program written in ALGOL on a GIER computer [5].

## Experimental

The red brown crystals of $C_{35}H_{34}OFe_3$ have been synthesized by Drs. *Benkeser* and *Cunico* from Purdue University, Lafayette, Indiana, U.S.A. The formula given by the authors [13] differed only by 2.9% in content of carbon from the correct composition.

This difference could not influence the further correct solution of the crystal structure by X-ray methods.

The unit cell dimensions of $C_{35}H_{34}OFe_3$ were obtained from X-ray precession photographs and diffractometric measurements. The triclinic unit cell has the following parameters:

$a = 10.943 \pm 0.005$, $b = 14.434 \pm 0.008$, $c = 17.237 \pm 0.009$ Å,
$\alpha = 98.7 \pm 0.5°$, $\beta = 95.0 \pm 0.5°$, $\gamma = 96.3 \pm 0.5°$.

The space group is $P\bar{1}$. The symmetry centre was verified from X-ray statistics. The measured density, $D_m = 1.60 \pm 0.02$ g cm$^{-3}$, corresponds to four molecules of the molecular weight 642.1 in the unit cell. The calculated density $D_x$ corresponding to the formula $C_{35}H_{34}OFe_3$ ($M = 638.2$) is 1.59 g cm$^{-3}$.

For the structure analysis, the intensities of 2292 independent reflections were collected with a Picker automatic four-circle diffractometer using Mo$K$ radiation and balanced Zr, $Y_2O_3$ filters. All the intensities were corrected for background. The expression used to derive the integrated intesities $I$ is

$$I = (c_{T\beta} - c_{T\alpha}) - t\,[(c_{B1} + c_{B2})_\beta - (c_{B1} + c_{B2})_\alpha]. \qquad (1)$$

B1 and B2 are the extreme positions of the scan made across the reciprocal lattice point in experiment, $c_T$ is the total number of counts obtained by the continuous sampling technique and $t$ is the ratio of total measurement time to that used in the background measurement. $c_{i,\alpha,\beta}$ is the count obtained using a member of a balanced filter pair at the $i$-th point.

The integrated intensities $I$ were each reduced to structure factors $(F_o)_{rel}$ on the relative scale by use of the appropriate Lorentz and polarization factors. The absorption corrections were not applied as the maximum error due to absorption was as much as 5 per cent in this experiment.

The corrections of intensity data for vibrational effects and for a scale factor were computed by use of a statistical relationship between the mean intensity $\langle(F_o)^2_{rel}\rangle$ within a limited range of $\sin^2\Theta$ values and the sum of squared atomic scattering factors of all atoms in the unit cell

$$\sum_{j=1}^{N} f_j^2 = \sigma_2$$

at the average value of $\langle\sin^2\Theta\rangle$.

A plot of the logarithm of $\langle(F_o)^2_{rel}\rangle/\sigma_2$ *vs.* $\sin^2\Theta$ at average values of $\langle\sin^2\Theta\rangle$ within each selected group led to a straight line graph. The $B$ value was calculated from the slope of the straight line ($B = 3.17$) and the $-\log k$ value was given as intercept when $\sin^2\Theta = 0$.

The normalized structure factors $E_s$ were calculated by means of relation [1]:

$$E_s^2 = \frac{k(F_o)^2_{rel}\exp(B\sin^2\Theta/\lambda^2)}{\sigma_2}. \qquad (2)$$

Incorrect chemical formula caused an error of 2% in the $\sigma_2$ value.

The mean values $\langle E_s^2\rangle$, $\langle E_s^2 - 1\rangle$, $\langle E_s\rangle$ gave evidence for presence of the symmetry centre. Consequently, only an even number of molecules is allowed to be present in

the unit cell. Permissible molecular weights could have the following values: 1276.3, 638.2, 319.1, *etc.* taking into account the measured density value. This result confirmed the presence of 12 Fe atoms in the unit cell irrespective of the molecular weight.

### *Application of the probability relations*

Typical phase determining formulae for the space group $P\bar{1}$ are [1—4, 6]:

$$\sum_1: \; sg\, E_{2s} \sim sg(E_s^2 - 1), \tag{3}$$

$$\sum_2: \; sg\, E_s \sim sg \sum_p E_p E_{s-p}, \tag{4}$$

$$\sum_3: \; sg\, E_s \sim sg \sum_p E_p \left(E^2_{\frac{s+p}{2}} - 1\right) \tag{5}$$

where *sg* means „sign of", *s* represents integers $h_1$, $k_1$, $l_1$; *p* represents another three integers $h_2$, $k_2$, $l_2$.

The starting set for the phase determination procedure includes the sign of origin specifying linearly independent reflections and the assignments of signs to some other reflections with letters $a, b, c, \ldots$. Each letter represents + or − as the phase $\varphi_s$ in (2) can be either 0° or 180°, for the centrosymmetric structure. Table 1 gives the starting set for the phase determination of $C_{35}H_{34}OFe_3$.

*Table 1*

The starting set of reflections for the phase determination of $C_{35}H_{34}OFe_3$

| *s* | $E_s$ | *sg* |
|---|---|---|
| $\bar{1}\,2\,\bar{2}$ | 3.59 | + |
| $\bar{6}\,1\,\bar{2}$ | 4.54 | − |
| $\bar{2}\,0\,1$ | 3.02 | − |
| $\bar{4}\,7\,\bar{3}$ | 3.55 | *a* |
| $6\,1\,\bar{1}$ | 2.96 | *b* |
| $\bar{6}\,1\,2$ | 3.35 | *c* |
| $\bar{1}\,2\,2$ | 2.92 | *d* |

The starting set of reflections was selected with regard to the fact that they have many relationships applicable to the $\sum_2$ formula (4). In addition, the assignments are all associated with large values for $|E_s|$, giving high probabilities that the indications from $\sum_2$ formula are correct. A special program in ALGOL was written for this purpose [5]. This program puts $E_s$ values in a row of decreasing $E_s$ and it calculates the number of all triple-products of type $E_s E_p E_{s-p}$ for each $E_s$ value.

In the course of application of the starting set of 7 reflections (Table 1) for determination of new signs, an automatic program selects for each $E_s$ all contributors $E_p E_{s-p}$ to $\sum_2$, signs of which are known and it calculates the corresponding probability $P_+(E_s)$ in agreement with [1]. Only those signs are accepted where $P_+ \geqslant P_{\min}$ ($P_{\min} = 0.98$

in this calculation). All $E_s$ values with $E_s \geqslant E_{min}$ are included in procedure. With a value $E_{min} = 1.5$, 273 reflections were applied in the calculation of new signs using the $\sum_2$ formula.

The assignment of signs to four reflections with letters $a$, $b$, $c$, $d$ (Table 1) allows 16 possible combinations of signs in the basic set of reflections as each of letters may be + or −. Only one of these combinations represents a correct starting set of signs. Another combination of signs is a trivial one corresponding to the signs of Patterson coefficients with origin of the function in one of the symmetry centers. All possible combinations of signs are subsequently substituted for the symbols $a$, $b$, $c$, $d$ by the automatic program [5] with exception of the trivial one, as the presence of a heavy atom in the symmetry centre having influence upon all signs, can be refused. The development of new signs on a GIER computer is automatically interrupted for a given starting set of $E_s$, when any accepted sign of a normalized structure factor with $|E| \geqslant E_{tr}$ is either changed into opposite one or when the probability $P_+$ for such sign is reduced to a value $P_+ \geqslant P_+(\mathrm{tr})$ where $E_{tr}$ and $P_+(\mathrm{tr})$ are selected threshold values ($E_{tr} = 2.0$ and $P_+(\mathrm{tr}) = 0.85$ or $P_-(\mathrm{tr}) = 0.15$ in this calculation). After interruption, a new starting set of signs is applied. The calculation of signs is finished when all signs of $E_s$ with $E \geqslant E_{min}$ are established. Table 2 indicates fractions of signs calculated from the starting groups of reflections $II-XVI$ by application of $\sum_2$ till automatic interruption of computation. In two cases (combination $III$ and $VI$) there were more than 97% of all signs found until interruption. The correct starting set of signs is given in the last column. The 273 correct signs in combination $XVI$ (Table 2) were found in iteration cycles including six steps. The number of signs established in subsequent iteration cycles are given in Table 3.

Application of $\sum_3$ is limited to the same parity group of $E_s$. New signs can be developed when a part of phases are already known.

The crystal structure analysis of $C_{35}H_{34}OFe_3$ proceeded by calculation of Fourier synthesis $D(xyz)$ using the normalized structure factors $E_s$ with $|E| \geqslant 1.5$:

$$D(xyz) = \sum h \sum k \sum l\, E(hkl) \cos [2\pi(hx + ky + lz)]. \qquad (6)$$

*Table 2*

Possible combination of signs in the basic set of reflections. The correct set of signs is given in the last columm. The last row indicates fractions of signs calculated from the starting groups of reflections by application of $\sum_2$ till automatic interruption $E_{min} = 1.5$, $E_{tr} = 2.0$, $P_+(\mathrm{tr}) = 0.85$. Total number of $E_s$ used: 273

| | *I* | *II* | *III* | *IV* | *V* | *VI* | *VII* | *VIII* | *IX* | *X* | *XI* | *XII* | *XIII* | *XIV* | *XV* | *XVI* |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| *a* | + | + | + | + | + | + | + | − | − | − | − | − | − | − | − | + |
| *b* | + | + | + | + | − | − | − | + | + | + | + | − | − | − | − | − |
| *c* | − | + | + | − | + | − | − | + | + | − | − | + | + | − | − | + |
| *d* | + | + | − | − | + | + | − | + | − | + | − | + | − | + | − | − |
| % | Trivial combination | 12.2 | 98.9 | 12.2 | 12.2 | 97.8 | 12.2 | 12.2 | 46.1 | 46.1 | 12.2 | 12.2 | 78.6 | 44.3 | 12.2 | 100.0 |

*Table 3*

Establishment of 273 correct signs (starting set of signs $a = +$, $b = -$, $c = +$, $d = -$) during iteration cycles using the probability function $\sum_2$

| Iteration cycle | Number of developed signs | Fraction of signs (%) established in one cycle |
|---|---|---|
| 0 | 7 | 2.6 |
| 1 | 28 | 7.7 |
| 2 | 173 | 53.5 |
| 3 | 216 | 15.9 |
| 4 | 221 | 1.9 |
| 5 | 268 | 17.3 |
| 6 | 271 | 1.1 |

Three sets of signs were used to calculate the $D(xyz)$ functions. They were established from the sign combinations *III*, *VI*, *XVI* of Table 2. The Fourier syntheses were calculated with 268—273 coefficients. This is not enough to give complete information on positions of all 78 atoms in the asymmetric part of the unit cell, as it is only one reflection per one positional parameter available. However, positions of the Fe atoms should be concerned first because of the ability of the $D(xyz)$ function, calculated from the correct set of signs, to distinguish positions of the heavier Fe atoms. In fact, only set of signs developed from the combination *XVI* (Table 2) gave the $D(xyz)$ function with six well distinguished main maxima of the same height. The set of signs from the combination *III* gave a $D(xyz)$ function with seven main maxima. From the combination *VI* a $D(xyz)$ function resulted with six main maxima, one of them of double height. In this way, Fourier synthesis gave another evidence on the correctness of signs developed from the initial combination *XVI*. The positions of the Fe atoms are given in Table 4.

*Table 4*

Preliminary positions of the Fe atoms from the $D(xyz)$ synthesis

| Atom | $x/a$ | $y/b$ | $z/c$ |
|---|---|---|---|
| Fe(1) | 0.060 | 0.460 | 0.345 |
| Fe(2) | 0.067 | 0.166 | 0.626 |
| Fe(3) | 0.185 | 0.450 | 0.893 |
| Fe(4) | 0.250 | 0.190 | 0.130 |
| Fe(5) | 0.345 | 0.825 | 0.165 |
| Fe(6) | 0.462 | 0.130 | 0.410 |

Probable signs of all structure factors $F_s$ could be now inferred from the contribution $F_H$ of the heavy atoms Fe only whose positions were found (Table 4). *Sim* [7] calculated the actual number of structure factors $F_s$ of the centrosymmetric structure having tne same sign as $F_H$ in term of $[(\sigma_2)_H/(\sigma_2)_L]^{1/2}$. In the case of $C_{35}H_{34}OFe_3$, $[(\sigma_2)_H/(\sigma_2)_L]^{1/2}$ equals 1.14. According to probability relation of *Sim* [7], the expected theoretical fraction of correct signs found from the contribution of $F_H$, is 77%. This fraction is much higher than the fraction of $E_s$ used in symbolic addition procedure (11.9%).

*Table 5*

Final fractional atomic parameters, and their standard deviations

| Atom | $x$ ($\sigma$) | $y$ ($\sigma$) | $z$ ($\sigma$) |
|---|---|---|---|
| C(11) | 0.2015(14) | 0.4597(13) | 0.2735(11) |
| C(21) | 0.2115(15) | 0.3913(13) | 0.3294(11) |
| C(31) | 0.2151(13) | 0.4439(11) | 0.4085(9) |
| C(41) | 0.2123(15) | 0.5398(13) | 0.4020(10) |
| C(51) | 0.2009(15) | 0.5516(13) | 0.3216(11) |
| C(61) | −0.1098(12) | 0.5156(10) | 0.3256(9) |
| C(71) | −0.1069(13) | 0.4300(11) | 0.2726(9) |
| C(81) | −0.0921(14) | 0.3553(12) | 0.3207(10) |
| C(91) | −0.0800(13) | 0.3961(12) | 0.3999(9) |
| C(101) | −0.0928(13) | 0.4965(12) | 0.4066(9) |
| Fe(1) | 0.0556(2) | 0.4591(2) | 0.3439(1) |
| C(12) | 0.0393(15) | 0.0237(11) | 0.6377(10) |
| C(22) | 0.0873(14) | 0.0782(12) | 0.7147(10) |
| C(32) | 0.2033(15) | 0.1243(12) | 0.7001(9) |
| C(42) | 0.2289(14) | 0.0975(11) | 0.6212(10) |
| C(52) | 0.1247(16) | 0.0374(12) | 0.5835(10) |
| C(62) | −0.1014(15) | 0.1978(12) | 0.5963(10) |
| C(72) | −0.0467(15) | 0.2569(12) | 0.6650(10) |
| C(82) | 0.0774(16) | 0.2731(11) | 0.5614(10) |
| C(92) | 0.0664(13) | 0.3082(11) | 0.6444(9) |
| C(102) | −0.0264(15) | 0.2035(12) | 0.5313(10) |
| Fe(2) | 0.0692(2) | 0.1620(2) | 0.6259(1) |
| C(13) | 0.2111(15) | 0.3251(11) | 0.8265(9) |
| C(23) | 0.1541(14) | 0.3033(11) | 0.8936(9) |
| C(33) | 0.0408(15) | 0.3484(13) | 0.8939(10) |
| C(43) | 0.0320(14) | 0.3978(12) | 0.8255(9) |
| C(53) | 0.1331(13) | 0.3792(12) | 0.7816(9) |
| C(63) | 0.3608(16) | 0.5120(14) | 0.9383(10) |
| C(73) | 0.2985(15) | 0.4781(13) | 0.0020(10) |
| C(83) | 0.1852(16) | 0.5224(13) | 0.0044(10) |
| C(93) | 0.1824(16) | 0.5820(12) | 0.9431(10) |
| C(103) | 0.2913(15) | 0.5763(12) | 0.9043(9) |
| Fe(3) | 0.1898(2) | 0.4455(2) | 0.8970(1) |
| C(10) | 0.1482(13) | 0.3910(11) | 0.6938(9) |
| O(1) | 0.3039(9) | 0.3998(7) | 0.5985(6) |
| C(20) | 0.2883(13) | 0.3844(10) | 0.6774(9) |
| C(40) | 0.3969(16) | 0.4775(13) | 0.5952(10) |
| C(50) | 0.4721(18) | 0.4852(16) | 0.6734(12) |
| C(120) | 0.3810(14) | 0.4572(12) | 0.7298(9) |
| C(14) | 0.3909(15) | 0.2945(12) | 0.1454(10) |
| C(24) | 0.3951(13) | 0.2335(11) | 0.2051(10) |
| C(34) | 0.4039(14) | 0.1405(11) | 0.1701(9) |
| C(44) | 0.4058(14) | 0.1350(12) | 0.0827(10) |
| C(54) | 0.3963(15) | 0.2331(12) | 0.0713(10) |
| C(64) | 0.1022(17) | 0.0817(14) | 0.0868(13) |
| C(74) | 0.1019(16) | 0.1507(14) | 0.0374(11) |
| C(84) | 0.0893(15) | 0.2375(13) | 0.0822(11) |
| C(94) | 0.0842(15) | 0.2240(14) | 0.1619(11) |
| C(104) | 0.0911(15) | 0.1239(14) | 0.1650(10) |
| Fe(4) | 0.2460(2) | 0.1841(2) | 0.1236(1) |

*Table 5* (Continued)

| Atom | $x$ ($\sigma$) | $y$ ($\sigma$) | $z$ ($\sigma$) |
|---|---|---|---|
| C(15) | 0.4886(14) | 0.7945(12) | 0.2413(10) |
| C(25) | 0.5135(14) | 0.7712(11) | 0.1584(10) |
| C(35) | 0.3789(16) | 0.7375(13) | 0.2521(11) |
| C(45) | 0.3351(15) | 0.6797(11) | 0.1732(10) |
| C(55) | 0.4197(15) | 0.7079(13) | 0.1193(10) |
| C(65) | 0.3427(13) | 0.9650(11) | 0.1733(9) |
| C(75) | 0.3349(15) | 0.9199(12) | 0.0915(10) |
| C(85) | 0.2283(15) | 0.8484(13) | 0.0775(10) |
| C(95) | 0.1666(14) | 0.8544(12) | 0.1476(10) |
| C(105) | 0.2357(15) | 0.9250(12) | 0.2072(10) |
| Fe(5) | 0.3441(2) | 0.8219(2) | 0.1674(1) |
| C(16) | 0.4493(16) | 0.0158(12) | 0.3579(10) |
| C(26) | 0.4014(13) | 0.0683(12) | 0.2995(9) |
| C(36) | 0.3052(14) | 0.1165(12) | 0.3306(9) |
| C(46) | 0.2856(14) | 0.0916(12) | 0.4080(10) |
| C(56) | 0.3763(14) | 0.0276(12) | 0.4236(10) |
| C(66) | 0.4746(16) | 0.2590(13) | 0.5003(11) |
| C(76) | 0.4861(14) | 0.3012(12) | 0.4280(10) |
| C(86) | 0.6388(15) | 0.2042(14) | 0.4427(11) |
| C(96) | 0.5705(16) | 0.1991(12) | 0.5099(10) |
| C(106) | 0.5893(16) | 0.2664(12) | 0.3937(11) |
| Fe(6) | 0.4608(2) | 0.1556(2) | 0.4057(1) |
| C(60) | 0.4287(15) | 0.0546(12) | 0.2121(10) |
| O(2) | 0.4084(9) | 0.9942(9) | 0.8729(7) |
| C(80) | 0.3376(15) | 0.8791(13) | 0.7646(10) |
| C(90) | 0.2437(19) | 0.8842(18) | 0.8238(14) |
| C(100) | 0.4320(15) | 0.9651(13) | 0.7899(10) |
| C(110) | 0.2832(19) | 0.9639(17) | 0.8803(14) |

Next Fourier synthesis was calculated from all observed structure factors $F_o$ using weighted coefficients $sg\ (w|F_o|)$. $sg$ means the sign of the structure factor $F_H$ calculated from the known positions of the Fe atoms (Table 4) and the weight $w$ expresses the probability that the sign of $F_s$ is the same as that of $F_H$ [8]:

$$w = 2P_+ - 1 \tag{7}$$

where $P_+$ is

$$P_+ = \frac{1}{2} + \frac{1}{2} \tanh\ (|F_s|\ |F_H|/\Sigma f_L^2). \tag{8}$$

$f_L$ represents atomic scattering factor of a light atom with unknown position. Introduction of the weighting function $w$ improves resolution of the light atoms. The three-dimensional Fourier function $\varrho(xyz)$ calculated from the weighted coefficients $wF_s$ clearly resolved the positions of all 72 light atoms in the asymmetric unit.

The positions of all atoms together with their anisotropic temperature factors were refined by least squares using a block diagonal approximation and the *Cruickshank*'s weighting scheme [9]. First three cycles of refinement were calculated with an assump-

*Table 6*

Final thermal parameters and calculated standard deviations ($\times 10^4$), according to the expression for the temperature factor: $\exp[-2\pi^2(h^2a^{*2}U_{11} + 2hka^*b^*U_{12} + \ldots)]$

| Atom | $U_{11}$ ($\sigma$) | $U_{22}$ ($\sigma$) | $U_{33}$ ($\sigma$) | $U_{12}$ ($\sigma$) | $U_{13}$ ($\sigma$) | $U_{23}$ ($\sigma$) |
|---|---|---|---|---|---|---|
| C(11) | 129(17) | 857(14) | 649(9) | 461(27) | 177(21) | 589(19) |
| C(21) | 263(18) | 604(14) | 886(10) | 780(27) | 341(23) | 465(20) |
| C(31) | 208(17) | 520(13) | 258(8) | −143(24) | −40(19) | −37(16) |
| C(41) | 364(19) | 580(13) | 473(9) | 139(26) | 155(22) | −156(17) |
| C(51) | 225(17) | 605(14) | 699(10) | 350(26) | 594(22) | 270(19) |
| C(61) | 106(15) | 256(11) | 371(7) | 46(21) | −11(17) | 250(14) |
| C(71) | 159(15) | 403(12) | 402(8) | 238(22) | 58(18) | 6(15) |
| C(81) | 284(18) | 555(13) | 550(9) | −6(26) | 5(22) | 282(18) |
| C(91) | 199(16) | 520(12) | 326(8) | 69(24) | 124(19) | 284(16) |
| C(101) | 224(17) | 419(12) | 410(8) | 296(24) | 121(20) | 178(16) |
| Fe(1) | 226(2) | 325(2) | 313(1) | 233(3) | 173(3) | 159(2) |
| C(12) | 388(18) | 304(11) | 677(9) | 87(25) | 253(22) | 371(17) |
| C(22) | 348(17) | 507(12) | 464(8) | 473(25) | 201(21) | 645(17) |
| C(32) | 399(18) | 378(12) | 309(8) | 69(25) | 36(21) | 77(16) |
| C(42) | 290(17) | 192(11) | 629(9) | 271(24) | 12(21) | 129(16) |
| C(52) | 746(19) | 291(12) | 468(9) | 590(27) | 181(23) | −75(17) |
| C(62) | 507(19) | 330(12) | 516(9) | 307(26) | −273(22) | 268(17) |
| C(72) | 344(18) | 265(12) | 569(9) | 155(24) | −105(21) | −69(16) |
| C(82) | 691(21) | 244(11) | 592(9) | 393(26) | −202(23) | 671(17) |
| C(92) | 365(16) | 323(11) | 245(8) | 164(23) | −14(18) | −10(15) |
| C(102) | 400(19) | 503(12) | 493(8) | 186(26) | −113(21) | 554(17) |
| Fe(2) | 236(3) | 291(2) | 308(1) | 97(4) | 47(3)$_5$ | 126(2) |
| C(13) | 521(19) | 256(12) | 221(8) | 75(25) | −116(20) | −108(15) |
| C(23) | 431(17) | 300(11) | 330(8) | 80(23) | 293(20) | −34(15) |
| C(33) | 299(18) | 542(13) | 448(9) | −264(26) | −88(21) | 364(17) |
| C(43) | 323(17) | 489(12) | 126(7) | 174(24) | 314(19) | −7(15) |
| C(53) | 226(17) | 459(12) | 290(8) | 155(23) | 41(19) | 114(15) |
| C(63) | 384(21) | 857(15) | 554(10) | 83(30) | 2(24) | 138(19) |
| C(73) | 352(18) | 582(13) | 566(9) | −81(26) | −311(22) | −17(17) |
| C(83) | 558(20) | 599(14) | 331(8) | 164(28) | −145(22) | −443(17) |
| C(93) | 729(22) | 449(13) | 385(9) | 218(29) | 109(23) | −96(17) |
| C(103) | 552(19) | 494(12) | 314(8) | 71(26) | −149(21) | −24(16) |
| Fe(3) | 312(3) | 416(2) | 252(1) | 165(4) | 71(3) | 66(2) |
| C(10) | 294(15) | 399(11) | 192(7) | 144(22) | 346(18) | 12(14) |
| O(1) | 114(11) | 181(7) | 304(5) | −158(15) | 181(13) | −115(10) |
| C(20) | 150(15) | 223(11) | 401(8) | 28(21) | 212(18) | −177(14) |
| C(40) | 488(21) | 660(14) | 452(9) | 103(29) | −167(23) | 114(18) |
| C(50) | 540(22) | 1295(19) | 658(11) | −323(35) | −10(26) | 339(23) |
| C(120) | 307(18) | 663(13) | 438(9) | −464(26) | −54(21) | 24(17) |
| C(14) | 435(19) | 641(13) | 398(8) | 36(27) | 351(21) | 223(17) |
| C(24) | 142(16) | 182(11) | 694(9) | 195(23) | 110(20) | 46(16) |
| C(34) | 298(17) | 369(11) | 413(8) | −154(24) | −43(20) | 616(16) |
| C(44) | 173(17) | 706(13) | 492(8) | 229(25) | 107(20) | 358(17) |
| C(54) | 354(18) | 555(12) | 570(9) | 190(26) | 469(21) | 791(17) |
| C(64) | 346(20) | 668(15) | 1210(13) | −106(29) | −321(28) | 652(24) |
| C(74) | 456(20) | 743(15) | 712(10) | 109(30) | −115(24) | 493(20) |
| C(84) | 397(18) | 754(15) | 723(10) | 417(28) | −377(22) | 231(19) |
| C(94) | 338(18) | 996(16) | 532(10) | 328(29) | 129(23) | −608(20) |
| C(104) | 358(19) | 1141(16) | 417(8) | −230(29) | 136(22) | 804(21) |
| Fe(4) | 319(3) | 462(2) | 412(1) | 223(4) | 106(3) | 306(3) |

*Table 6* (Continued)

| Atom | $U_{11}$ (σ) | $U_{22}$ (σ) | $U_{33}$ (σ) | $U_{12}$ (σ) | $U_{13}$ (σ) | $U_{23}$ (σ) |
|---|---|---|---|---|---|---|
| C(15) | 353(17) | 361(12) | 714(9) | 388(25) | 61(21) | 292(17) |
| C(25) | 355(18) | 350(11) | 683(9) | 455(25) | 154(21) | 129(17) |
| C(35) | 478(20) | 511(13) | 688(9) | 315(27) | −5(23) | 483(18) |
| C(45) | 601(20) | 378(11) | 556(9) | 390(26) | 246(22) | 367(16) |
| C(55) | 358(18) | 509(14) | 637(9) | 255(26) | 211(22) | 117(18) |
| C(65) | 310(16) | 232(11) | 215(7) | −112(22) | 122(18) | −98(14) |
| C(75) | 535(19) | 384(12) | 318(8) | 330(25) | −179(21) | 143(16) |
| C(85) | 297(18) | 780(14) | 456(9) | 254(27) | −302(21) | 480(18) |
| C(95) | 298(18) | 435(13) | 693(9) | 21(26) | −93(22) | 48(18) |
| C(105) | 358(18) | 268(12) | 673(9) | 253(25) | 171(22) | 243(17) |
| Fe(5) | 294(3) | 344(2) | 400(1) | 144(4) | 101(3) | 93(2) |
| C(16) | 553(20) | 378(13) | 427(9) | 310(26) | 121(22) | 203(17) |
| C(26) | 348(17) | 401(11) | 228(8) | 265(24) | 101(19) | −4(15) |
| C(36) | 266(16) | 526(12) | 307(8) | 181(24) | 177(19) | 289(16) |
| C(46) | 219(17) | 631(14) | 489(9) | 108(26) | 445(21) | 286(18) |
| C(56) | 316(18) | 466(12) | 612(9) | −456(25) | 176(22) | 462(17) |
| C(66) | 594(21) | 492(15) | 610(10) | 24(30) | −128(25) | −282(19) |
| C(76) | 424(17) | 326(12) | 560(9) | −149(24) | 244(21) | −343(16) |
| C(86) | 307(19) | 621(15) | 718(10) | 219(28) | −535(23) | −88(19) |
| C(96) | 644(22) | 520(13) | 426(9) | 350(29) | −181(24) | −104(18) |
| C(106) | 551(21) | 345(13) | 625(9) | −382(28) | 171(24) | −25(18) |
| Fe(6) | 284(3) | 313(2) | 358(1) | 155(4) | 25(3) | 57(2) |
| C(60) | 480(19) | 283(12) | 498(9) | 189(25) | 19(21) | 201(17) |
| O(2) | 346(11) | 185(9) | 61(5) | −125(16) | 103(13) | −227(11) |
| C(80) | 402(19) | 631(14) | 520(9) | −211(27) | 471(23) | 20(18) |
| C(90) | 613(24) | 1131(22) | 1332(14) | −818(38) | 1217(34) | −734(28) |
| C(100) | 248(17) | 469(13) | 599(9) | 82(25) | −129(21) | −79(17) |
| C(110) | 756(25) | 1170(21) | 754(13) | −115(39) | 386(30) | −439(26) |

tion that all light atoms are the carbon atoms. The negative temperature coefficients $B_{11}$, $B_{22}$, $B_{33}$ of two light atoms and the higher electron density at their positions proved the presence of the oxygen atoms. During another three cycles of refinement the reliability index $R = \sum ||F_o| - |F_c|| / \sum |F_o|$ decreased to 0.063. The standard deviations σ for the positional parameters are 0.0002 considering the Fe atoms and 0.0009 to 0.0016 as regards the light atoms. The final positional parameters together with their standard deviations are given in Table 5. The final thermal parameters are listed in Table 6. The atoms in Tables 5 and 6 are labelled according to Fig. 1. The observed $F_o$ and calculated $F_c$ structure factors are given in Table 7.

## Discussion of the structure

The asymmetric part of the unit cell contains two molecules $(C_{10}H_9Fe)_3C(C_4OH_7)$. The polynuclear molecules consist of three ferrocene groups bonded to the common carbon atom (Fig. 1). The fourth group bonded to the same carbon atom is a tetrahydrofuran ring.

The least-squares planes through each of the cyclopentadienyl rings are given in Table 8. The ring atoms do not deviate significantly from planarity. The angle

*Table 7*

Observed and calculated structure factors

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| | H 0 0 | |
| 1 | 10.57 | 16.50 |
| 2 | 11.57 | 14.21 |
| 3 | 6.89 | 6.56 |
| 4 | 44.53 | 41.55 |
| 6 | 88.31 | 78.76 |
| 7 | 112.87 | 113.53 |
| 8 | 68.81 | 60.58 |
| | H 1 0 | |
| 1 | 235.89 | 249.30 |
| 2 | 63.83 | 70.07 |
| 3 | 5.32 | 5.53 |
| 4 | 18.34 | 18.52 |
| 5 | 161.28 | 160.25 |
| 6 | 34.23 | 32.23 |
| 7 | 37.30 | 37.95 |
| 8 | 32.60 | 33.91 |
| $\bar{1}$ | 52.85 | 53.97 |
| $\bar{2}$ | 175.40 | 165.43 |
| $\bar{3}$ | 119.55 | 120.21 |
| $\bar{4}$ | 33.76 | 33.26 |
| $\bar{5}$ | 105.16 | 95.13 |
| $\bar{6}$ | 67.79 | 58.43 |
| $\bar{7}$ | 18.48 | 17.27 |
| $\bar{8}$ | 41.94 | 43.08 |
| | H 2 0 | |
| 0 | 33.14 | 36.21 |
| 1 | 90.36 | 90.24 |
| 2 | 98.61 | 100.69 |
| 3 | 103.39 | 97.95 |
| 5 | 57.22 | 55.14 |
| 6 | 62.06 | 62.88 |
| 7 | 67.65 | 66.84 |
| 8 | 16.64 | 20.78 |
| $\bar{1}$ | 43.31 | 51.42 |
| $\bar{2}$ | 57.63 | 69.64 |
| $\bar{3}$ | 50.19 | 50.50 |
| $\bar{5}$ | 155.97 | 146.21 |
| $\bar{6}$ | 45.62 | 46.90 |
| $\bar{7}$ | 47.94 | 51.25 |
| $\bar{8}$ | 74.27 | 74.07 |
| | H 3 0 | |
| 0 | 224.09 | 265.02 |
| 1 | 78.49 | 89.61 |
| 2 | 12.96 | 10.68 |
| 3 | 42.49 | 46.10 |
| 4 | 22.16 | 21.91 |
| $\bar{1}$ | 41.87 | 43.55 |
| $\bar{2}$ | 64.31 | 61.12 |
| $\bar{3}$ | 35.46 | 36.13 |
| $\bar{4}$ | 75.02 | 76.75 |
| $\bar{5}$ | 31.10 | 31.46 |
| $\bar{6}$ | 36.76 | 32.14 |
| $\bar{7}$ | 56.47 | 61.43 |
| $\bar{8}$ | 138.58 | 142.82 |
| | 46.71 | 47.55 |
| | H 4 0 | |
| $\bar{1}$ | 98.75 | 96.82 |
| $\bar{2}$ | 61.92 | 46.10 |
| $\bar{3}$ | 24.07 | 22.63 |
| $\bar{4}$ | 24.41 | 19.68 |
| $\bar{5}$ | 63.97 | 61.85 |
| $\bar{6}$ | 35.60 | 34.49 |
| $\bar{7}$ | 23.19 | 25.71 |
| 2 | 101.95 | 97.36 |
| 3 | 6.41 | 3.16 |
| 4 | 49.31 | 43.45 |
| 5 | 134.62 | 133.92 |
| 6 | 13.91 | 18.03 |
| 7 | 6.34 | 4.92 |
| | H 5 0 | |
| 0 | 45.76 | 55.19 |
| 1 | 20.73 | 21.02 |
| 2 | 15.62 | 17.69 |
| 4 | 9.00 | 5.48 |
| 5 | 44.87 | 49.82 |
| 6 | 40.71 | 41.72 |
| $\bar{7}$ | 13.57 | 8.96 |
| $\bar{1}$ | 10.91 | 11.30 |
| $\bar{2}$ | 11.80 | 12.43 |
| $\bar{3}$ | 29.12 | 26.88 |
| $\bar{4}$ | 29.53 | 31.66 |
| $\bar{5}$ | 68.54 | 68.06 |
| $\bar{6}$ | 60.56 | 59.95 |
| $\bar{7}$ | 13.57 | 8.96 |
| 7 | 12.14 | 14.04 |
| | H 6 0 | |
| 0 | 78.36 | 79.90 |
| 1 | 14.80 | 13.92 |
| 2 | 58.99 | 59.31 |
| 3 | 71.40 | 76.61 |
| 4 | 8.52 | 13.81 |
| 5 | 9.07 | 8.12 |
| $\bar{6}$ | 8.32 | 10.64 |
| $\bar{1}$ | 71.81 | 64.17 |
| $\bar{2}$ | 23.66 | 25.58 |
| $\bar{3}$ | 47.40 | 47.14 |
| $\bar{5}$ | 50.81 | 46.47 |
| $\bar{6}$ | 52.99 | 52.97 |
| $\bar{7}$ | 81.36 | 85.71 |
| | H 7 0 | |
| 1 | 20.60 | 20.86 |
| 2 | 55.58 | 53.31 |
| 3 | 65.40 | 64.60 |
| 4 | 15.14 | 14.25 |
| 5 | 63.76 | 56.47 |
| $\bar{1}$ | 16.23 | 17.13 |
| $\bar{2}$ | 96.02 | 94.13 |
| $\bar{5}$ | 129.23 | 130.09 |
| $\bar{6}$ | 39.35 | 43.08 |
| $\bar{7}$ | 9.68 | 5.51 |
| | H 8 0 | |
| 2 | 36.62 | 36.51 |
| 3 | 16.30 | 17.10 |
| $\bar{5}$ | 41.39 | 40.24 |
| $\bar{1}$ | 27.96 | 30.04 |
| $\bar{2}$ | 49.72 | 53.72 |
| $\bar{3}$ | 24.41 | 22.08 |
| $\bar{4}$ | 36.01 | 33.55 |
| $\bar{5}$ | 9.00 | 12.08 |
| $\bar{6}$ | 45.62 | 48.99 |
| | H 9 0 | |
| 0 | 37.10 | 40.01 |
| 1 | 6.07 | 8.15 |
| 2 | 7.30 | 10.81 |
| 3 | 84.70 | 85.38 |
| 4 | 8.80 | 5.32 |
| $\bar{1}$ | 44.67 | 40.57 |
| $\bar{2}$ | 46.31 | 40.57 |
| $\bar{3}$ | 58.17 | 52.50 |
| $\bar{4}$ | 32.67 | 38.45 |
| $\bar{5}$ | 55.31 | 55.42 |
| | H 10 0 | |
| 1 | 10.71 | 10.96 |
| 2 | 6.68 | 7.50 |
| $\bar{1}$ | 25.03 | 29.19 |
| $\bar{2}$ | 79.24 | 77.72 |
| $\bar{3}$ | 18.55 | 20.78 |
| $\bar{4}$ | 22.10 | 22.98 |
| | H 11 0 | |
| $\bar{1}$ | 31.57 | 33.95 |
| | H 0 1 | |
| 1 | 81.09 | 85.18 |
| 2 | 58.44 | 42.44 |
| 3 | 12.48 | 12.64 |
| 4 | 19.98 | 17.16 |
| 5 | 45.42 | 44.77 |
| 6 | 8.25 | 9.97 |
| 7 | 15.82 | 14.66 |
| 8 | 63.56 | 58.53 |
| $\bar{1}$ | 9.82 | 14.67 |
| $\bar{2}$ | 337.64 | 338.42 |
| $\bar{4}$ | 55.99 | 49.36 |
| $\bar{5}$ | 105.91 | 98.30 |
| $\bar{6}$ | 71.74 | 65.08 |
| $\bar{7}$ | 26.67 | 27.21 |
| $\bar{8}$ | 8.59 | 7.14 |
| | H 1 1 | |
| 0 | 54.22 | 54.45 |
| 1 | 19.44 | 20.77 |
| 2 | 13.50 | 18.31 |
| 3 | 20.05 | 28.98 |
| 4 | 15.00 | 14.73 |
| 5 | 27.21 | 25.96 |
| 6 | 37.78 | 39.72 |
| 7 | 20.73 | 20.74 |
| 8 | 18.07 | 16.68 |
| $\bar{1}$ | 171.99 | 163.85 |
| $\bar{2}$ | 18.75 | 19.28 |
| $\bar{3}$ | 88.86 | 81.83 |
| $\bar{4}$ | 84.29 | 91.33 |
| $\bar{5}$ | 103.39 | 96.34 |
| $\bar{7}$ | 127.19 | 120.07 |
| $\bar{8}$ | 16.41 | 18.21 |
| | H 2 1 | |
| 0 | 57.49 | 62.37 |
| 1 | 151.60 | 159.31 |
| 2 | 5.93 | 4.20 |
| 3 | 33.08 | 34.89 |
| 4 | 48.56 | 44.84 |
| 5 | 50.33 | 49.54 |
| 6 | 22.57 | 22.42 |
| 7 | 22.64 | 25.73 |
| 8 | 78.22 | 77.31 |
| $\bar{1}$ | 62.95 | 57.82 |
| $\bar{2}$ | 106.59 | 91.87 |
| $\bar{3}$ | 41.19 | 36.00 |
| $\bar{4}$ | 22.03 | 21.97 |
| $\bar{5}$ | 5.46 | 3.86 |
| $\bar{6}$ | 54.56 | 58.53 |
| $\bar{7}$ | 87.50 | 82.60 |
| | H 3 1 | |
| 0 | 11.05 | 16.93 |
| 1 | 164.08 | 182.76 |
| 2 | 15.96 | 14.63 |
| 3 | 26.05 | 28.48 |
| 4 | 44.40 | 40.59 |
| 5 | 73.66 | 70.13 |
| 6 | 16.09 | 12.89 |
| 7 | 9.69 | 12.52 |
| $\bar{1}$ | 143.28 | 128.21 |
| $\bar{2}$ | 70.38 | 69.24 |
| $\bar{3}$ | 27.35 | 33.73 |
| $\bar{4}$ | 33.42 | 36.21 |
| $\bar{5}$ | 43.85 | 45.63 |
| $\bar{6}$ | 6.27 | 6.73 |
| $\bar{8}$ | 29.53 | 33.48 |
| | H 4 1 | |
| 0 | 3.89 | 6.83 |
| 1 | 31.64 | 36.86 |
| 2 | 90.97 | 77.82 |
| 3 | 65.25 | 72.91 |
| 4 | 26.87 | 23.97 |
| 5 | 40.03 | 41.69 |
| 6 | 56.13 | 60.27 |
| 7 | 23.39 | 22.41 |
| $\bar{2}$ | 20.32 | 22.62 |
| $\bar{3}$ | 56.06 | 54.75 |
| $\bar{4}$ | 170.22 | 145.85 |
| $\bar{6}$ | 18.62 | 20.99 |
| $\bar{7}$ | 47.19 | 48.05 |
| $\bar{8}$ | 7.43 | 8.37 |
| | H 5 1 | |
| 0 | 25.44 | 23.10 |
| 1 | 86.13 | 88.88 |
| 2 | 35.87 | 35.72 |
| 3 | 28.71 | 30.74 |
| 4 | 101.27 | 103.85 |
| 5 | 23.39 | 21.38 |
| $\bar{1}$ | 18.62 | 16.32 |
| $\bar{2}$ | 68.33 | 63.84 |
| $\bar{3}$ | 95.82 | 87.51 |
| $\bar{4}$ | 15.96 | 14.88 |
| $\bar{5}$ | 7.71 | 6.45 |
| $\bar{6}$ | 19.78 | 17.19 |
| $\bar{7}$ | 27.82 | 26.44 |
| | H 6 1 | |
| 1 | 37.24 | 40.16 |
| 2 | 9.48 | 6.59 |
| 3 | 78.29 | 81.23 |
| 5 | 59.94 | 62.17 |
| 6 | 42.35 | 44.22 |
| $\bar{1}$ | 22.78 | 28.0 |
| $\bar{2}$ | 59.06 | 58.29 |
| $\bar{3}$ | 79.38 | 80.46 |
| $\bar{4}$ | 20.25 | 19.49 |
| $\bar{5}$ | 7.71 | 6.54 |
| $\bar{6}$ | 10.03 | 9.34 |
| $\bar{7}$ | 25.71 | 29.04 |
| | H 7 1 | |
| 1 | 24.07 | 10.40 |
| 2 | 61.04 | 60.24 |
| 3 | 98.07 | 96.81 |
| 4 | 25.23 | 26.54 |
| 5 | 33.28 | 35.69 |
| $\bar{2}$ | 74.88 | 71.86 |
| $\bar{3}$ | 82.38 | 77.24 |
| $\bar{4}$ | 148.87 | 146.60 |
| $\bar{5}$ | 25.64 | 30.44 |
| $\bar{6}$ | 13.09 | 11.26 |
| $\bar{7}$ | 14.59 | 17.03 |
| | H 8 1 | |
| 0 | 13.71 | 16.14 |
| 1 | 147.85 | 152.54 |
| 2 | 26.67 | 23.50 |
| 3 | 81.29 | 80.21 |
| 4 | 19.03 | 18.21 |
| $\bar{2}$ | 93.36 | 96.79 |
| $\bar{3}$ | 49.85 | 49.02 |
| $\bar{4}$ | 56.33 | 58.45 |
| $\bar{5}$ | 56.60 | 51.97 |
| $\bar{6}$ | 8.66 | 9.22 |
| | H 9 1 | |
| 0 | 8.32 | 9.04 |
| 1 | 51.35 | 51.90 |
| 2 | 18.62 | 20.46 |
| 3 | 58.99 | 54.41 |
| $\bar{1}$ | 14.12 | 17.15 |
| $\bar{2}$ | 34.58 | 33.46 |
| $\bar{3}$ | 40.64 | 35.44 |
| $\bar{4}$ | 77.06 | 74.30 |
| $\bar{5}$ | 16.16 | 17.37 |
| | H 10 1 | |
| 0 | 7.91 | 9.00 |
| 2 | 22.78 | 20.56 |
| $\bar{2}$ | 39.62 | 34.55 |
| $\bar{4}$ | 62.81 | 63.49 |
| | H 1 $\bar{1}$ | |
| 0 | 30.82 | 41.85 |
| 1 | 40.03 | 43.43 |
| 2 | 79.93 | 82.47 |
| 3 | 33.21 | 37.86 |
| 4 | 7.84 | 6.08 |
| 5 | 52.10 | 55.58 |
| 6 | 180.93 | 183.31 |
| 7 | 64.31 | 68.54 |
| $\bar{1}$ | 162.10 | 144.09 |
| $\bar{2}$ | 100.32 | 92.42 |
| $\bar{4}$ | 13.03 | 17.92 |
| $\bar{5}$ | 29.80 | 24.64 |
| $\bar{6}$ | 37.64 | 32.18 |
| $\bar{7}$ | 25.16 | 25.08 |
| $\bar{8}$ | 90.77 | 84.95 |
| | H 2 $\bar{1}$ | |
| 0 | 40.85 | 43.30 |
| 1 | 155.63 | 141.68 |
| 2 | 54.42 | 56.48 |
| 3 | 56.26 | 54.18 |
| 4 | 37.92 | 40.56 |
| 5 | 52.10 | 58.28 |
| 6 | 51.35 | 52.14 |
| 7 | 140.42 | 144.75 |
| $\bar{8}$ | 33.83 | 35.85 |
| $\bar{1}$ | 55.92 | 57.76 |
| $\bar{2}$ | 86.88 | 70.95 |
| $\bar{3}$ | 17.80 | 29.47 |
| $\bar{4}$ | 25.03 | 21.60 |
| $\bar{5}$ | 6.00 | 6.46 |
| $\bar{8}$ | 10.37 | 7.56 |
| | H 3 $\bar{1}$ | |
| 0 | 25.37 | 28.98 |
| 2 | 97.18 | 116.43 |
| 3 | 33.28 | 30.37 |
| 4 | 19.09 | 19.00 |
| 5 | 55.65 | 57.43 |

*Table 7* (Continued)

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| 6 | 32.19 | 30.69 |
| 7 | 25.98 | 27.10 |
| $\bar{1}$ | 19.37 | 12.16 |
| $\bar{2}$ | 233.98 | 236.85 |
| $\bar{3}$ | 29.80 | 25.74 |
| $\bar{4}$ | 18.21 | 17.09 |
| $\bar{5}$ | 49.03 | 41.74 |
| $\bar{6}$ | 44.80 | 40.79 |
| $\bar{7}$ | 17.59 | 14.77 |
| $\bar{8}$ | 70.79 | 67.65 |
| | H 4 $\bar{1}$ | |
| 1 | 23.05 | 26.40 |
| 2 | 30.28 | 32.86 |
| 3 | 44.60 | 42.99 |
| 4 | 12.34 | 17.58 |
| 6 | 78.84 | 84.47 |
| 7 | 18.07 | 18.62 |
| $\bar{1}$ | 167.42 | 167.41 |
| $\bar{2}$ | 70.31 | 70.07 |
| $\bar{3}$ | 17.25 | 20.12 |
| $\bar{4}$ | 60.90 | 56.15 |
| $\bar{6}$ | 12.48 | 11.66 |
| $\bar{7}$ | 36.28 | 41.64 |
| $\bar{8}$ | 56.33 | 53.54 |
| | H 5 $\bar{1}$ | |
| 0 | 29.46 | 32.74 |
| 1 | 38.26 | 45.42 |
| 2 | 10.09 | 12.76 |
| 3 | 14.05 | 12.32 |
| 4 | 17.59 | 14.05 |
| 5 | 16.09 | 18.24 |
| 6 | 10.84 | 8.16 |
| 7 | 63.22 | 66.45 |
| $\bar{1}$ | 31.10 | 38.55 |
| $\bar{2}$ | 15.41 | 15.63 |
| $\bar{3}$ | 85.45 | 84.55 |
| $\bar{4}$ | 28.37 | 25.92 |
| $\bar{5}$ | 14.32 | 14.38 |
| $\bar{6}$ | 52.65 | 53.95 |
| $\bar{7}$ | 20.46 | 23.69 |
| | H 6 $\bar{1}$ | |
| 0 | 23.80 | 25.10 |
| 1 | 7.43 | 6.18 |
| 2 | 157.12 | 168.42 |
| 3 | 81.09 | 79.81 |
| 4 | 39.15 | 41.93 |
| 5 | 13.37 | 13.14 |
| 6 | 33.42 | 37.83 |
| $\bar{1}$ | 53.47 | 52.26 |
| $\bar{2}$ | 83.13 | 80.09 |
| $\bar{3}$ | 81.56 | 77.02 |
| $\bar{4}$ | 66.22 | 63.40 |
| $\bar{5}$ | 170.29 | 168.00 |
| $\bar{6}$ | 6.96 | 7.83 |
| $\bar{7}$ | 17.12 | 20.15 |
| | H 7 $\bar{1}$ | |
| 0 | 40.58 | 36.08 |
| 1 | 14.73 | 13.77 |
| 2 | 48.08 | 50.63 |
| 3 | 88.18 | 82.97 |
| 4 | 53.74 | 53.72 |
| 5 | 39.21 | 38.80 |
| 6 | 21.35 | 20.64 |
| $\bar{1}$ | 55.44 | 49.56 |
| $\bar{3}$ | 162.17 | 154.95 |
| $\bar{5}$ | 26.60 | 29.18 |
| $\bar{6}$ | 18.69 | 18.91 |
| $\bar{7}$ | 25.78 | 26.01 |
| | H 8 $\bar{1}$ | |
| 0 | 50.06 | 54.56 |
| 1 | 60.90 | 61.01 |
| 2 | 70.92 | 69.49 |
| 4 | 11.53 | 11.47 |
| 5 | 25.10 | 25.87 |
| $\bar{1}$ | 59.88 | 57.74 |
| $\bar{2}$ | 17.66 | 14.54 |
| $\bar{3}$ | 91.86 | 93.16 |
| $\bar{4}$ | 50.74 | 51.53 |
| $\bar{5}$ | 6.75 | 6.19 |
| $\bar{6}$ | 10.37 | 8.96 |
| | H 9 $\bar{1}$ | |
| 0 | 54.83 | 63.72 |
| 1 | 21.62 | 21.02 |
| 2 | 118.25 | 115.93 |
| 3 | 32.33 | 33.16 |
| 4 | 21.21 | 21.82 |
| $\bar{2}$ | 5.93 | 6.41 |
| $\bar{3}$ | 80.88 | 82.15 |
| $\bar{4}$ | 65.20 | 67.88 |
| $\bar{5}$ | 77.88 | 76.97 |
| | H 10 $\bar{1}$ | |
| 0 | 33.62 | 37.99 |
| 1 | 25.64 | 29.12 |
| $\bar{2}$ | 34.98 | 31.66 |
| $\bar{2}$ | 30.82 | 30.43 |
| $\bar{3}$ | 96.23 | 98.81 |
| $\bar{4}$ | 20.46 | 23.07 |
| | H 11 $\bar{1}$ | |
| 0 | 9.41 | 7.84 |
| $\bar{1}$ | 12.07 | 15.86 |
| $\bar{2}$ | 47.33 | 49.53 |
| | H 0 2 | |
| 0 | 77.40 | 81.64 |
| 1 | 93.77 | 87.99 |
| 2 | 25.78 | 27.15 |
| 3 | 117.37 | 111.18 |
| 4 | 114.57 | 93.87 |
| 5 | 32.39 | 28.47 |
| 6 | 6.75 | 3.18 |
| 7 | 136.73 | 130.89 |
| 8 | 32.05 | 29.16 |
| $\bar{1}$ | 85.38 | 76.59 |
| $\bar{2}$ | 17.87 | 19.53 |
| $\bar{3}$ | 54.56 | 50.32 |
| $\bar{4}$ | 172.88 | 161.51 |
| $\bar{5}$ | 39.35 | 37.39 |
| $\bar{6}$ | 7.98 | 6.27 |
| $\bar{7}$ | 90.16 | 87.90 |
| $\bar{8}$ | 36.08 | 37.17 |
| | H 1 2 | |
| 0 | 25.37 | 20.89 |
| 1 | 202.07 | 201.94 |
| 2 | 45.15 | 43.41 |
| 3 | 16.98 | 17.69 |
| 4 | 42.21 | 41.38 |
| 5 | 7.30 | 5.36 |
| 7 | 39.15 | 41.55 |
| 8 | 45.76 | 46.58 |
| $\bar{1}$ | 59.47 | 62.15 |
| $\bar{2}$ | 192.86 | 167.19 |
| $\bar{3}$ | 62.40 | 66.04 |
| $\bar{4}$ | 24.21 | 22.93 |
| $\bar{6}$ | 200.36 | 207.52 |
| $\bar{7}$ | 57.97 | 55.63 |
| $\bar{8}$ | 50.67 | 50.84 |
| | H 2 2 | |
| 0 | 126.16 | 136.81 |
| 1 | 75.02 | 81.08 |
| 2 | 106.32 | 105.82 |
| 3 | 65.74 | 61.33 |
| 4 | 18.48 | 17.34 |
| 5 | 11.32 | 11.60 |
| 6 | 190.54 | 200.84 |
| 7 | 17.94 | 19.82 |
| $\bar{1}$ | 320.46 | 297.34 |
| $\bar{2}$ | 75.70 | 72.19 |
| $\bar{3}$ | 50.60 | 49.36 |
| $\bar{4}$ | 37.17 | 32.31 |
| $\bar{5}$ | 87.22 | 68.27 |
| $\bar{6}$ | 38.94 | 39.16 |
| $\bar{7}$ | 57.76 | 59.41 |
| | H 3 2 | |
| 0 | 18.07 | 25.23 |
| 1 | 146.35 | 160.14 |
| 2 | 18.82 | 16.15 |
| 3 | 50.81 | 47.47 |
| 4 | 38.94 | 45.96 |
| 5 | 7.09 | 5.92 |
| 6 | 38.76 | 39.08 |
| 7 | 95.61 | 101.03 |
| $\bar{2}$ | 23.60 | 19.52 |
| $\bar{3}$ | 7.16 | 3.20 |
| $\bar{4}$ | 31.71 | 32.30 |
| $\bar{5}$ | 9.21 | 8.24 |
| $\bar{6}$ | 40.99 | 38.50 |
| $\bar{7}$ | 6.21 | 6.01 |
| $\bar{8}$ | 20.66 | 20.82 |
| | H 4 2 | |
| 0 | 31.37 | 32.83 |
| 1 | 42.96 | 47.56 |
| 2 | 66.08 | 59.24 |
| 3 | 13.71 | 15.74 |
| 4 | 20.12 | 17.81 |
| 5 | 24.55 | 30.85 |
| 6 | 21.69 | 21.65 |
| $\bar{7}$ | 28.37 | 26.24 |
| $\bar{1}$ | 17.53 | 17.48 |
| $\bar{2}$ | 102.70 | 103.24 |
| $\bar{3}$ | 30.14 | 32.70 |
| $\bar{4}$ | 27.69 | 20.71 |
| $\bar{5}$ | 13.91 | 12.99 |
| $\bar{6}$ | 74.27 | 73.11 |
| $\bar{7}$ | 19.78 | 20.60 |
| $\bar{8}$ | 54.97 | 55.87 |
| | H 5 2 | |
| 0 | 17.73 | 17.95 |
| 1 | 45.49 | 46.71 |
| 2 | 50.67 | 41.66 |
| 3 | 87.70 | 81.12 |
| 4 | 31.17 | 31.74 |
| 5 | 40.51 | 41.67 |
| 6 | 57.15 | 56.06 |
| $\bar{1}$ | 130.66 | 120.50 |
| $\bar{3}$ | 73.45 | 71.79 |
| $\bar{4}$ | 76.18 | 72.02 |
| $\bar{5}$ | 34.10 | 31.08 |
| 6 | 52.58 | 56.67 |
| $\bar{7}$ | 49.37 | 53.15 |
| | H 6 2 | |
| 0 | 41.80 | 46.68 |
| 1 | 73.99 | 80.75 |
| 3 | 54.69 | 51.03 |
| 4 | 92.95 | 92.75 |
| 6 | 68.95 | 69.89 |
| $\bar{1}$ | 20.39 | 19.58 |
| $\bar{2}$ | 81.97 | 68.93 |
| $\bar{3}$ | 13.16 | 8.03 |
| $\bar{4}$ | 36.28 | 40.40 |
| $\bar{5}$ | 6.68 | 4.70 |
| $\bar{6}$ | 60.76 | 61.96 |
| $\bar{7}$ | 8.93 | 11.77 |
| | H 7 2 | |
| 0 | 60.83 | 64.31 |
| 1 | 16.50 | 19.15 |
| 2 | 15.96 | 17.03 |
| 3 | 37.24 | 36.58 |
| 4 | 42.76 | 41.93 |
| 5 | 31.71 | 31.48 |
| $\bar{1}$ | 69.08 | 61.27 |
| $\bar{3}$ | 19.23 | 20.94 |
| $\bar{4}$ | 33.08 | 31.20 |
| $\bar{5}$ | 36.08 | 35.62 |
| $\bar{6}$ | 55.79 | 54.79 |
| | H 8 2 | |
| 0 | 19.37 | 21.45 |
| 1 | 99.70 | 103.71 |
| 2 | 31.92 | 31.66 |
| 3 | 53.53 | 52.65 |
| 4 | 13.50 | 14.83 |
| $\bar{1}$ | 80.34 | 75.29 |
| $\bar{2}$ | 63.56 | 59.47 |
| $\bar{3}$ | 34.17 | 31.40 |
| $\bar{4}$ | 46.51 | 45.25 |
| $\bar{5}$ | 6.48 | 9.37 |
| $\bar{6}$ | 29.39 | 26.76 |
| | H 9 2 | |
| 0 | 8.87 | 6.44 |
| 1 | 93.84 | 92.13 |
| 2 | 24.69 | 23.62 |
| 3 | 13.09 | 15.33 |
| $\bar{1}$ | 65.33 | 70.16 |
| $\bar{2}$ | 60.35 | 58.64 |
| $\bar{4}$ | 18.34 | 15.23 |
| | H 10 2 | |
| $\bar{1}$ | 61.24 | 60.94 |
| $\bar{3}$ | 8.73 | 5.40 |
| 2 | 24.69 | 25.36 |
| | H 1 $\bar{2}$ | |
| 0 | 9.96 | 8.92 |
| 1 | 300.47 | 293.04 |
| 2 | 200.16 | 194.58 |
| 3 | 26.39 | 26.49 |
| 4 | 7.16 | 2.64 |
| 5 | 15.28 | 8.42 |
| 6 | 15.14 | 13.83 |
| 7 | 18.75 | 20.60 |
| 8 | 38.60 | 39.47 |
| $\bar{1}$ | 70.72 | 58.58 |
| $\bar{2}$ | 152.22 | 130.22 |
| $\bar{3}$ | 61.24 | 57.45 |
| $\bar{4}$ | 7.50 | 6.67 |
| $\bar{5}$ | 70.45 | 61.55 |
| $\bar{6}$ | 273.13 | 260.20 |
| $\bar{7}$ | 21.48 | 20.90 |
| $\bar{8}$ | 16.98 | 19.36 |
| | H 2 $\bar{2}$ | |
| 0 | 73.17 | 72.64 |
| 1 | 58.17 | 14.29 |
| 2 | 8.52 | 11.44 |
| 3 | 14.53 | 18.76 |
| 4 | 8.18 | 10.03 |
| 5 | 5.86 | 5.52 |
| 6 | 139.26 | 140.62 |
| 7 | 66.36 | 63.84 |
| $\bar{8}$ | 8.46 | 6.56 |
| $\bar{1}$ | 400.31 | 366.42 |
| $\bar{2}$ | 68.40 | 71.73 |
| $\bar{3}$ | 8.32 | 9.57 |
| $\bar{5}$ | 60.69 | 58.66 |
| $\bar{6}$ | 19.03 | 18.01 |
| $\bar{7}$ | 43.85 | 44.74 |
| $\bar{8}$ | 13.37 | 11.78 |
| | H 3 $\bar{2}$ | |
| 0 | 78.15 | 95.54 |
| 1 | 136.87 | 125.43 |
| 2 | 14.59 | 13.98 |
| 3 | 42.21 | 39.56 |
| 4 | 46.17 | 42.28 |
| 5 | 34.85 | 26.02 |
| 6 | 13.09 | 10.27 |
| 7 | 74.47 | 78.26 |
| $\bar{1}$ | 30.55 | 27.73 |
| $\bar{2}$ | 40.78 | 37.59 |
| $\bar{3}$ | 25.16 | 17.70 |
| $\bar{5}$ | 53.40 | 53.37 |
| $\bar{6}$ | 52.03 | 51.05 |
| $\bar{7}$ | 65.20 | 68.52 |
| $\bar{8}$ | 24.14 | 22.91 |
| | H 4 $\bar{2}$ | |
| 0 | 37.17 | 42.95 |
| 1 | 24.82 | 23.97 |
| 2 | 50.81 | 56.21 |
| 3 | 27.01 | 29.04 |
| 4 | 73.79 | 73.85 |
| 5 | 5.86 | 2.84 |
| 6 | 12.82 | 14.90 |
| 7 | 11.53 | 13.79 |
| $\bar{1}$ | 92.27 | 90.69 |
| $\bar{2}$ | 58.65 | 63.91 |
| $\bar{3}$ | 18.96 | 13.75 |
| $\bar{4}$ | 10.84 | 13.05 |
| $\bar{5}$ | 40.71 | 43.82 |
| $\bar{6}$ | 135.44 | 136.70 |
| $\bar{7}$ | 31.17 | 32.03 |
| $\bar{8}$ | 14.05 | 13.88 |
| | H 5 $\bar{2}$ | |
| 1 | 29.46 | 26.36 |
| 2 | 12.75 | 10.82 |
| 3 | 14.39 | 10.79 |
| $\bar{4}$ | 69.83 | 70.65 |
| $\bar{1}$ | 82.93 | 93.65 |
| $\bar{2}$ | 42.90 | 45.39 |
| $\bar{3}$ | 28.16 | 20.62 |
| | H 0 3 | |
| 1 | 167.22 | 157.06 |

*Table 7* (Continued)

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| 2 | 110.75 | 106.25 |
| 3 | 26.32 | 28.46 |
| 4 | 48.28 | 41.46 |
| 5 | 96.98 | 94.97 |
| 7 | 8.05 | 5.89 |
| 8 | 24.35 | 24.23 |
| $\bar{1}$ | 168.79 | 159.86 |
| $\bar{2}$ | 25.98 | 29.45 |
| $\bar{3}$ | 19.57 | 23.75 |
| $\bar{4}$ | 17.19 | 14.01 |
| $\bar{5}$ | 8.05 | 6.16 |
| $\bar{6}$ | 103.86 | 110.50 |
| $\bar{7}$ | 43.58 | 47.32 |
| $\bar{8}$ | 91.79 | 91.15 |
| | H 1 3 | |
| 0 | 191.84 | 202.09 |
| 1 | 15.28 | 17.63 |
| 2 | 71.95 | 75.68 |
| 3 | 10.71 | 12.37 |
| 4 | 39.83 | 35.87 |
| 5 | 44.87 | 47.88 |
| 6 | 16.91 | 19.18 |
| 7 | 62.13 | 61.62 |
| $\bar{1}$ | 275.58 | 241.10 |
| $\bar{2}$ | 40.92 | 38.46 |
| $\bar{3}$ | 16.91 | 16.39 |
| $\bar{4}$ | 12.55 | 7.37 |
| $\bar{5}$ | 14.19 | 15.69 |
| $\bar{6}$ | 28.44 | 30.08 |
| $\bar{7}$ | 89.88 | 88.70 |
| $\bar{8}$ | 77.74 | 75.01 |
| | H 2 3 | |
| 0 | 110.82 | 120.64 |
| 1 | 15.57 | 18.53 |
| 2 | 20.46 | 21.83 |
| 3 | 15.28 | 8.84 |
| 4 | 88.38 | 81.06 |
| 5 | 26.73 | 24.94 |
| 6 | 22.91 | 25.05 |
| 7 | 63.90 | 65.13 |
| $\bar{1}$ | 45.76 | 43.17 |
| $\bar{2}$ | 17.87 | 16.18 |
| $\bar{3}$ | 138.71 | 129.18 |
| $\bar{4}$ | 25.44 | 25.45 |
| $\bar{5}$ | 69.29 | 62.82 |
| $\bar{6}$ | 35.60 | 26.89 |
| $\bar{7}$ | 21.48 | 24.51 |
| $\bar{8}$ | 22.78 | 25.19 |
| | H 3 3 | |
| 1 | 85.38 | 93.45 |
| 2 | 89.47 | 93.92 |
| 3 | 11.93 | 11.31 |
| 4 | 49.17 | 45.80 |
| 5 | 44.40 | 49.19 |
| 6 | 11.12 | 9.60 |
| 7 | 10.16 | 7.29 |
| $\bar{1}$ | 56.74 | 55.9 |
| $\bar{2}$ | 75.97 | 71.05 |
| $\bar{3}$ | 27.55 | 23.37 |
| $\bar{4}$ | 65.74 | 59.59 |
| $\bar{5}$ | 50.87 | 50.38 |
| $\bar{6}$ | 88.38 | 85.85 |
| $\bar{8}$ | 45.56 | 48.28 |
| | H 4 3 | |
| 0 | 17.88 | 20.89 |
| 1 | 26.67 | 21.76 |
| 3 | 123.30 | 118.85 |
| 4 | 39.96 | 41.12 |
| 5 | 9.41 | 9.55 |
| 6 | 7.71 | 7.69 |
| 7 | 48.35 | 46.51 |
| $\bar{1}$ | 56.74 | 55.97 |
| $\bar{2}$ | 75.97 | 71.05 |
| $\bar{3}$ | 27.55 | 23.37 |
| $\bar{4}$ | 65.74 | 59.59 |
| $\bar{5}$ | 50.87 | 50.38 |
| $\bar{6}$ | 88.38 | 85.85 |
| | H 5 3 | |
| 0 | 36.14 | 35.72 |
| 2 | 20.87 | 19.53 |
| 3 | 105.16 | 98.65 |
| 4 | 28.78 | 28.31 |
| 5 | 22.78 | 20.43 |
| 6 | 13.03 | 13.68 |
| $\bar{1}$ | 59.06 | 51.27 |
| $\bar{2}$ | 16.03 | 14.49 |
| $\bar{3}$ | 139.26 | 126.31 |
| $\bar{4}$ | 17.53 | 18.54 |
| $\bar{5}$ | 86.27 | 86.15 |
| $\bar{6}$ | 30.35 | 25.89 |
| $\bar{7}$ | 10.57 | 13.28 |
| | H 6 3 | |
| 0 | 47.40 | 43.02 |
| 1 | 29.87 | 28.51 |
| 2 | 180.79 | 190.68 |
| 3 | 40.99 | 39.58 |
| 4 | 110.21 | 109.45 |
| 5 | 19.37 | 19.53 |
| $\bar{1}$ | 46.65 | 38.71 |
| $\bar{2}$ | 52.51 | 51.90 |
| $\bar{3}$ | 69.42 | 72.44 |
| $\bar{4}$ | 115.18 | 117.34 |
| $\bar{5}$ | 81.70 | 77.46 |
| $\bar{6}$ | 51.83 | 49.01 |
| $\bar{7}$ | 35.19 | 39.99 |
| | H 7 3 | |
| 0 | 35.05 | 34.81 |
| 1 | 83.88 | 83.02 |
| 2 | 91.79 | 90.32 |
| 3 | 119.41 | 123.68 |
| 4 | 49.17 | 51.50 |
| 5 | 18.82 | 17.28 |
| $\bar{1}$ | 75.43 | 68.45 |
| $\bar{2}$ | 36.96 | 37.68 |
| $\bar{3}$ | 121.19 | 120.08 |
| $\bar{4}$ | 37.78 | 35.10 |
| $\bar{5}$ | 40.58 | 37.50 |
| $\bar{6}$ | 10.78 | 11.88 |
| | H 8 3 | |
| 0 | 28.44 | 31.51 |
| 2 | 63.97 | 63.09 |
| 3 | 32.12 | 36.35 |
| 4 | 11.32 | 13.19 |
| $\bar{1}$ | 47.40 | 44.54 |
| $\bar{2}$ | 34.58 | 37.89 |
| $\bar{3}$ | 38.46 | 43.09 |
| $\bar{4}$ | 54.49 | 52.65 |
| $\bar{5}$ | 69.08 | 68.08 |
| | H 9 3 | |
| 1 | 12.75 | 9.37 |
| $\bar{2}$ | 65.67 | 61.17 |
| $\bar{1}$ | 8.25 | 8.27 |
| $\bar{3}$ | 57.28 | 53.35 |
| $\bar{4}$ | 100.86 | 95.73 |
| $\bar{5}$ | 39.55 | 38.56 |
| | H 10 3 | |
| 0 | 14.87 | 16.42 |
| 1 | 14.73 | 12.91 |
| $\bar{1}$ | 27.07 | 31.22 |
| $\bar{2}$ | 13.03 | 15.37 |
| $\bar{3}$ | 85.04 | 81.06 |
| | H 1 $\bar{3}$ | |
| 0 | 98.68 | 93.44 |
| 1 | 65.47 | 61.17 |
| 2 | 67.31 | 64.69 |
| 3 | 73.04 | 91.97 |
| 4 | 44.46 | 52.83 |
| 5 | 17.87 | 20.94 |
| 7 | 18.89 | 18.73 |
| 8 | 38.67 | 38.91 |
| $\bar{1}$ | 161.83 | 145.38 |
| $\bar{3}$ | 15.41 | 10.97 |
| $\bar{4}$ | 160.26 | 133.22 |
| $\bar{5}$ | 26.05 | 25.12 |
| $\bar{6}$ | 17.25 | 17.49 |
| $\bar{7}$ | 40.64 | 40.71 |
| $\bar{8}$ | 44.05 | 42.84 |
| | H 2 $\bar{3}$ | |
| 0 | 220.62 | 229.71 |
| 1 | 205.41 | 189.00 |
| 2 | 19.71 | 25.14 |
| 3 | 36.35 | 34.17 |
| 4 | 106.32 | 93.63 |
| 5 | 5.25 | 7.38 |
| 7 | 52.78 | 48.64 |
| 8 | 40.78 | 41.17 |
| $\bar{1}$ | 75.36 | 70.69 |
| $\bar{2}$ | 16.84 | 16.42 |
| $\bar{3}$ | 38.74 | 41.97 |
| $\bar{5}$ | 7.43 | 6.33 |
| $\bar{6}$ | 17.59 | 18.22 |
| $\bar{7}$ | 20.19 | 13.70 |
| $\bar{8}$ | 27.69 | 23.79 |
| | H 3 $\bar{3}$ | |
| 0 | 51.83 | 65.28 |
| 1 | 119.62 | 116.44 |
| 2 | 5.39 | 9.96 |
| 3 | 41.12 | 35.14 |
| 4 | 11.80 | 10.06 |
| 5 | 117.57 | 119.44 |
| 6 | 16.62 | 39.58 |
| 7 | 26.19 | 28.34 |
| $\bar{1}$ | 118.39 | 105.50 |
| $\bar{2}$ | 30.01 | 31.93 |
| $\bar{3}$ | 16.91 | 24.04 |
| $\bar{4}$ | 16.98 | 14.11 |
| $\bar{5}$ | 88.31 | 82.71 |
| $\bar{6}$ | 25.37 | 21.03 |
| $\bar{7}$ | 19.30 | 18.32 |
| $\bar{8}$ | 43.24 | 44.99 |
| | H 4 $\bar{3}$ | |
| 1 | 44.67 | 42.86 |
| 3 | 77.47 | 80.95 |
| 4 | 93.57 | 85.47 |
| 5 | 28.78 | 26.21 |
| 6 | 56.19 | 57.18 |
| 7 | 6.48 | 8.63 |
| $\bar{1}$ | 142.33 | 143.95 |
| $\bar{2}$ | 36.35 | 35.43 |
| $\bar{3}$ | 55.03 | 51.87 |
| $\bar{4}$ | 157.12 | 137.08 |
| $\bar{5}$ | 22.16 | 20.01 |
| $\bar{6}$ | 9.96 | 11.74 |
| $\bar{7}$ | 57.49 | 61.92 |
| | H 5 $\bar{3}$ | |
| 1 | 94.86 | 85.87 |
| 2 | 29.26 | 27.73 |
| 3 | 37.78 | 33.13 |
| 4 | 66.42 | 69.93 |
| 5 | 50.53 | 49.29 |
| 6 | 28.03 | 30.24 |
| 7 | 8.80 | 8.44 |
| $\bar{1}$ | 27.48 | 29.34 |
| $\bar{3}$ | 51.69 | 49.96 |
| $\bar{4}$ | 19.50 | 15.25 |
| $\bar{6}$ | 20.39 | 24.22 |
| | H 6 $\bar{3}$ | |
| 0 | 19.64 | 17.33 |
| 1 | 110.34 | 101.37 |
| 2 | 18.89 | 16.90 |
| 3 | 93.57 | 84.96 |
| 4 | 15.62 | 17.58 |
| 5 | 62.67 | 60.55 |
| 6 | 24.07 | 26.14 |
| $\bar{1}$ | 45.08 | 35.82 |
| $\bar{2}$ | 5.18 | 0.64 |
| $\bar{3}$ | 43.24 | 37.65 |
| $\bar{4}$ | 49.72 | 48.94 |
| $\bar{5}$ | 98.41 | 99.35 |
| $\bar{7}$ | 38.05 | 37.46 |
| | H 7 $\bar{3}$ | |
| 1 | 70.99 | 70.40 |
| 2 | 24.75 | 23.04 |
| 3 | 66.97 | 69.16 |
| 4 | 44.53 | 45.16 |
| 5 | 19.91 | 19.42 |
| $\bar{6}$ | 47.19 | 40.40 |
| $\bar{1}$ | 10.30 | 10.10 |
| $\bar{2}$ | 54.15 | 54.32 |
| $\bar{3}$ | 149.96 | 138.97 |
| $\bar{4}$ | 204.86 | 203.49 |
| $\bar{5}$ | 36.76 | 39.20 |
| $\bar{6}$ | 35.05 | 38.84 |
| | H 8 $\bar{3}$ | |
| 0 | 68.20 | 74.69 |
| 1 | 96.63 | 90.20 |
| 2 | 37.99 | 39.76 |
| 3 | 22.03 | 20.46 |
| $\bar{5}$ | 24.28 | 22.44 |
| $\bar{1}$ | 70.92 | 73.78 |
| $\bar{2}$ | 85.72 | 86.02 |
| $\bar{3}$ | 9.75 | 9.26 |
| $\bar{4}$ | 50.26 | 49.74 |
| $\bar{5}$ | 39.96 | 43.30 |
| $\bar{6}$ | 26.46 | 31.32 |
| | H 9 $\bar{3}$ | |
| 1 | 50.12 | 47.38 |
| 3 | 67.38 | 63.24 |
| $\bar{4}$ | 31.44 | 27.90 |
| $\bar{1}$ | 18.62 | 14.10 |
| $\bar{2}$ | 41.67 | 40.13 |
| $\bar{4}$ | 85.11 | 81.75 |
| $\bar{5}$ | 41.46 | 41.23 |
| | H 10 $\bar{3}$ | |
| 0 | 47.33 | 47.89 |
| $\bar{1}$ | 54.56 | 56.22 |
| $\bar{2}$ | 51.62 | 50.54 |
| $\bar{3}$ | 27.89 | 31.82 |
| $\bar{4}$ | 49.03 | 48.26 |
| | H 11 $\bar{3}$ | |
| $\bar{1}$ | 56.67 | 50.71 |
| $\bar{2}$ | 29.19 | 28.66 |
| | H 0 4 | |
| 0 | 296.18 | 333.82 |
| 1 | 12.55 | 10.79 |
| 2 | 41.26 | 42.49 |
| 3 | 18.28 | 13.54 |
| 4 | 76.52 | 67.02 |
| 5 | 33.14 | 33.78 |
| 6 | 36.01 | 36.49 |
| 7 | 88.31 | 87.68 |
| $\bar{1}$ | 132.57 | 137.22 |
| $\bar{2}$ | 48.69 | 52.63 |
| $\bar{3}$ | 13.37 | 11.21 |
| $\bar{4}$ | 6.00 | 6.08 |
| $\bar{5}$ | 67.38 | 61.42 |
| $\bar{6}$ | 92.61 | 93.33 |
| $\bar{7}$ | 30.42 | 28.66 |
| $\bar{8}$ | 96.23 | 94.21 |
| | H 1 4 | |
| 0 | 18.75 | 37.56 |
| 1 | 75.08 | 76.51 |
| 2 | 62.95 | 67.74 |
| 4 | 81.84 | 79.50 |
| 5 | 161.01 | 162.73 |
| 6 | 31.98 | 34.32 |
| 7 | 24.48 | 21.12 |
| $\bar{1}$ | 51.76 | 53.03 |
| $\bar{3}$ | 118.80 | 116.72 |
| $\bar{4}$ | 17.80 | 13.79 |
| $\bar{5}$ | 86.34 | 86.23 |
| $\bar{6}$ | 43.71 | 44.58 |
| $\bar{7}$ | 27.82 | 29.32 |
| $\bar{8}$ | 16.09 | 17.55 |
| | H 2 4 | |
| 0 | 29.12 | 32.56 |
| 1 | 25.71 | 23.65 |
| 3 | 29.19 | 25.40 |
| 5 | 34.23 | 30.52 |
| 6 | 71.06 | 72.43 |
| 7 | 38.94 | 40.95 |
| $\bar{1}$ | 25.03 | 28.45 |
| $\bar{2}$ | 16.71 | 19.12 |
| $\bar{3}$ | 16.09 | 14.00 |
| $\bar{4}$ | 60.22 | 59.20 |
| $\bar{5}$ | 86.61 | 86.20 |
| $\bar{6}$ | 32.05 | 27.16 |
| $\bar{7}$ | 44.80 | 47.25 |
| $\bar{8}$ | 23.12 | 25.35 |
| | H 3 4 | |
| 0 | 77.61 | 99.39 |
| 1 | 17.19 | 11.55 |
| 2 | 20.66 | 20.99 |
| 3 | 59.13 | 49.22 |
| 4 | 58.58 | 63.20 |
| 5 | 12.96 | 11.04 |
| 6 | 8.32 | 8.64 |
| 7 | 41.74 | 42.09 |
| $\bar{1}$ | 9.00 | 10.83 |
| $\bar{2}$ | 67.99 | 71.59 |
| $\bar{3}$ | 61.10 | 53.09 |
| $\bar{5}$ | 50.19 | 52.90 |

*Table 7* (Continued)

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| $\bar{6}$ | 69.08 | 68.22 |
| $\bar{7}$ | 66.70 | 71.44 |
| $\bar{8}$ | 52.72 | 55.19 |
| **H 4 4** | | |
| 0 | 68.13 | 63.84 |
| 1 | 75.29 | 73.07 |
| 3 | 5.86 | 6.99 |
| 4 | 27.28 | 25.49 |
| 5 | 121.12 | 128.54 |
| $\bar{1}$ | 47.74 | 53.72 |
| $\bar{2}$ | 82.25 | 75.67 |
| $\bar{3}$ | 149.01 | 130.33 |
| $\bar{4}$ | 8.46 | 1.92 |
| $\bar{5}$ | 78.49 | 76.61 |
| $\bar{6}$ | 13.23 | 13.60 |
| $\bar{7}$ | 12.48 | 16.21 |
| **H 5 4** | | |
| 0 | 55.85 | 54.28 |
| 1 | 28.23 | 24.92 |
| 2 | 25.57 | 24.06 |
| 3 | 21.41 | 22.72 |
| 4 | 43.58 | 45.89 |
| 5 | 26.67 | 27.39 |
| $\bar{6}$ | 62.95 | 60.38 |
| $\bar{1}$ | 33.69 | 34.66 |
| $\bar{2}$ | 50.40 | 36.10 |
| $\bar{4}$ | 72.42 | 67.74 |
| $\bar{5}$ | 109.32 | 108.35 |
| $\bar{7}$ | 10.16 | 9.35 |
| **H 6 4** | | |
| 0 | 127.80 | 129.02 |
| 1 | 21.89 | 20.20 |
| 2 | 94.59 | 92.48 |
| 3 | 40.58 | 37.19 |
| $\bar{5}$ | 13.03 | 13.53 |
| $\bar{1}$ | 27.55 | 30.37 |
| $\bar{2}$ | 55.85 | 49.33 |
| $\bar{3}$ | 30.35 | 29.87 |
| $\bar{4}$ | 19.85 | 20.88 |
| $\bar{6}$ | 41.19 | 42.37 |
| $\bar{7}$ | 35.87 | 34.95 |
| **H 7 4** | | |
| 0 | 99.16 | 106.71 |
| 1 | 36.69 | 38.84 |
| 2 | 36.96 | 42.74 |
| $\bar{4}$ | 27.01 | 28.06 |
| $\bar{1}$ | 51.28 | 52.77 |
| $\bar{2}$ | 69.49 | 70.04 |
| $\bar{3}$ | 73.24 | 72.05 |
| $\bar{4}$ | 69.22 | 70.85 |
| $\bar{5}$ | 77.54 | 72.00 |
| $\bar{6}$ | 19.57 | 16.81 |
| **H 8 4** | | |
| 0 | 66.70 | 72.11 |
| 1 | 24.69 | 25.21 |
| $\bar{2}$ | 6.55 | 0.32 |
| $\bar{1}$ | 43.85 | 43.60 |
| $\bar{3}$ | 40.78 | 40.43 |
| $\bar{4}$ | 47.40 | 40.59 |
| $\bar{5}$ | 27.14 | 22.38 |
| **H 9 4** | | |
| 0 | 39.69 | 39.38 |
| 1 | 50.47 | 51.41 |

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| $\bar{2}$ | 30.69 | 34.02 |
| $\bar{1}$ | 15.68 | 15.11 |
| $\bar{2}$ | 16.50 | 19.22 |
| $\bar{3}$ | 14.39 | 13.26 |
| **H 10 4** | | |
| 0 | 40.30 | 39.07 |
| $\bar{1}$ | 37.07 | 38.20 |
| $\bar{2}$ | 24.35 | 23.71 |
| **H 1 $\bar{4}$** | | |
| 1 | 178.54 | 174.84 |
| 2 | 32.19 | 32.27 |
| 3 | 22.10 | 20.42 |
| 4 | 64.04 | 64.00 |
| 5 | 65.40 | 66.99 |
| 6 | 20.73 | 22.25 |
| 7 | 52.31 | 55.16 |
| 8 | 26.60 | 29.64 |
| $\bar{1}$ | 12.00 | 13.67 |
| $\bar{2}$ | 62.33 | 58.34 |
| $\bar{3}$ | 54.15 | 42.63 |
| $\bar{4}$ | 8.18 | 6.03 |
| $\bar{5}$ | 43.92 | 42.49 |
| $\bar{6}$ | 38.67 | 37.62 |
| $\bar{7}$ | 13.16 | 11.21 |
| **H 2 $\bar{4}$** | | |
| 0 | 29.19 | 25.68 |
| 1 | 5.66 | 4.95 |
| 2 | 58.24 | 66.66 |
| 3 | 89.06 | 83.59 |
| 5 | 74.27 | 77.67 |
| 6 | 30.76 | 26.26 |
| 7 | 7.02 | 6.70 |
| 8 | 13.57 | 12.07 |
| $\bar{1}$ | 17.39 | 20.64 |
| $\bar{2}$ | 13.37 | 15.84 |
| $\bar{3}$ | 51.22 | 47.74 |
| $\bar{4}$ | 81.84 | 73.21 |
| $\bar{5}$ | 114.57 | 112.02 |
| $\bar{6}$ | 41.74 | 36.88 |
| $\bar{7}$ | 11.18 | 8.87 |
| **H 3 $\bar{4}$** | | |
| 0 | 71.81 | 95.17 |
| 1 | 116.89 | 116.86 |
| 2 | 12.96 | 11.67 |
| 3 | 35.67 | 32.32 |
| 4 | 30.42 | 24.34 |
| 5 | 27.21 | 27.57 |
| 6 | 49.24 | 52.89 |
| 7 | 14.12 | 9.31 |
| $\bar{1}$ | 3.61 | 4.16 |
| $\bar{2}$ | 7.09 | 4.59 |
| $\bar{3}$ | 22.30 | 21.15 |
| $\bar{4}$ | 85.65 | 77.35 |
| $\bar{5}$ | 27.96 | 23.72 |
| $\bar{6}$ | 53.60 | 52.01 |
| $\bar{7}$ | 111.37 | 108.00 |
| **H 4 $\bar{4}$** | | |
| 1 | 79.65 | 81.76 |
| 2 | 69.22 | 63.15 |
| 3 | 42.69 | 44.59 |
| 4 | 51.42 | 52.45 |
| 5 | 58.72 | 57.26 |
| 6 | 28.30 | 30.50 |
| 7 | 7.09 | 5.89 |
| $\bar{1}$ | 14.32 | 17.45 |

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| $\bar{2}$ | 25.03 | 25.53 |
| $\bar{3}$ | 87.43 | 85.35 |
| $\bar{4}$ | 25.85 | 27.33 |
| $\bar{5}$ | 65.06 | 63.39 |
| $\bar{6}$ | 27.55 | 24.09 |
| $\bar{7}$ | 7.37 | 1.83 |
| **H 5 $\bar{4}$** | | |
| 0 | 28.98 | 33.57 |
| 1 | 14.73 | 14.72 |
| 2 | 161.28 | 150.88 |
| 3 | 56.60 | 51.93 |
| 4 | 20.25 | 23.22 |
| 5 | 54.63 | 55.41 |
| 7 | 25.23 | 21.32 |
| $\bar{1}$ | 32.19 | 31.59 |
| $\bar{2}$ | 32.60 | 33.61 |
| $\bar{4}$ | 41.67 | 45.06 |
| $\bar{5}$ | 30.96 | 29.06 |
| $\bar{6}$ | 36.08 | 38.07 |
| $\bar{7}$ | 18.89 | 17.78 |
| **H 6 $\bar{4}$** | | |
| 0 | 59.33 | 56.65 |
| 1 | 58.31 | 63.68 |
| 2 | 44.46 | 44.65 |
| 3 | 143.35 | 139.80 |
| 4 | 31.64 | 30.74 |
| 5 | 40.64 | 42.48 |
| 6 | 47.26 | 42.60 |
| $\bar{1}$ | 32.94 | 33.90 |
| $\bar{2}$ | 97.86 | 82.58 |
| $\bar{3}$ | 61.92 | 57.34 |
| $\bar{4}$ | 55.24 | 54.15 |
| $\bar{6}$ | 82.18 | 87.24 |
| $\bar{7}$ | 74.47 | 74.52 |
| **H 7 $\bar{4}$** | | |
| 0 | 54.97 | 62.41 |
| 1 | 55.03 | 52.23 |
| 2 | 41.60 | 38.81 |
| 3 | 113.00 | 109.14 |
| 5 | 52.31 | 48.89 |
| $\bar{1}$ | 8.46 | 9.45 |
| $\bar{2}$ | 131.69 | 130.42 |
| $\bar{3}$ | 39.15 | 43.61 |
| $\bar{4}$ | 69.56 | 68.34 |
| $\bar{5}$ | 133.19 | 137.58 |
| $\bar{6}$ | 15.41 | 17.71 |
| **H 8 $\bar{4}$** | | |
| 0 | 34.58 | 37.18 |
| 1 | 68.54 | 69.72 |
| 2 | 118.80 | 116.22 |
| 3 | 32.80 | 30.58 |
| $\bar{2}$ | 90.22 | 83.10 |
| $\bar{3}$ | 8.87 | 9.19 |
| $\bar{4}$ | 24.69 | 23.07 |
| $\bar{6}$ | 44.53 | 49.13 |
| **H 9 $\bar{4}$** | | |
| 2 | 15.34 | 15.83 |
| 3 | 90.09 | 81.66 |
| 4 | 18.69 | 18.11 |
| $\bar{1}$ | 21.41 | 21.67 |
| $\bar{2}$ | 74.40 | 73.54 |
| $\bar{3}$ | 50.67 | 53.12 |
| $\bar{4}$ | 39.96 | 40.47 |
| $\bar{5}$ | 48.83 | 48.09 |

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| **H 10 $\bar{4}$** | | |
| $\bar{1}$ | 16.50 | 14.87 |
| $\bar{1}$ | 23.26 | 21.41 |
| $\bar{2}$ | 66.76 | 73.33 |
| $\bar{3}$ | 41.74 | 39.07 |
| $\bar{4}$ | 66.22 | 66.24 |
| **H 11 $\bar{4}$** | | |
| 0 | 32.67 | 32.75 |
| **H 0 5** | | |
| 1 | 7.84 | 5.82 |
| 2 | 43.99 | 39.20 |
| 3 | 39.08 | 34.96 |
| 4 | 30.35 | 23.44 |
| 5 | 103.80 | 92.58 |
| $\bar{6}$ | 21.21 | 22.93 |
| $\bar{1}$ | 108.84 | 118.00 |
| $\bar{2}$ | 110.89 | 119.61 |
| $\bar{3}$ | 43.44 | 43.58 |
| $\bar{4}$ | 70.04 | 60.93 |
| $\bar{5}$ | 19.44 | 23.21 |
| $\bar{6}$ | 29.87 | 32.11 |
| $\bar{7}$ | 30.42 | 29.23 |
| $\bar{8}$ | 8.73 | 8.52 |
| **H 1 5** | | |
| 0 | 27.35 | 29.15 |
| 1 | 37.78 | 43.46 |
| 2 | 18.41 | 24.48 |
| 3 | 173.08 | 160.32 |
| 4 | 5.59 | 5.09 |
| 5 | 58.79 | 61.38 |
| 6 | 20.73 | 21.60 |
| 7 | 12.00 | 10.99 |
| $\bar{1}$ | 16.23 | 20.38 |
| $\bar{2}$ | 19.23 | 25.04 |
| $\bar{3}$ | 48.83 | 44.33 |
| $\bar{4}$ | 70.11 | 68.10 |
| $\bar{5}$ | 127.87 | 118.62 |
| $\bar{6}$ | 12.62 | 12.39 |
| $\bar{7}$ | 36.01 | 28.33 |
| $\bar{8}$ | 14.53 | 18.04 |
| **H 2 5** | | |
| 0 | 37.30 | 48.68 |
| 1 | 12.34 | 16.67 |
| 2 | 56.81 | 52.53 |
| 3 | 17.32 | 20.54 |
| 4 | 125.21 | 124.74 |
| 5 | 12.27 | 12.86 |
| 6 | 21.48 | 21.62 |
| 7 | 28.51 | 25.69 |
| $\bar{1}$ | 13.98 | 12.27 |
| $\bar{2}$ | 65.47 | 66.92 |
| $\bar{3}$ | 35.80 | 33.19 |
| $\bar{4}$ | 37.44 | 33.73 |
| $\bar{5}$ | 16.03 | 16.76 |
| $\bar{6}$ | 54.49 | 54.05 |
| $\bar{7}$ | 93.84 | 95.33 |
| $\bar{8}$ | 39.96 | 46.02 |
| **H 3 5** | | |
| 0 | 32.33 | 31.41 |
| 1 | 34.37 | 28.63 |
| 2 | 48.62 | 37.27 |
| 3 | 19.37 | 18.37 |
| 4 | 40.99 | 43.49 |
| $\bar{5}$ | 40.30 | 39.67 |
| $\bar{1}$ | 64.24 | 64.76 |

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| $\bar{2}$ | 132.92 | 108.24 |
| $\bar{3}$ | 19.37 | 18.37 |
| $\bar{4}$ | 40.99 | 43.49 |
| $\bar{4}$ | 111.30 | 104.82 |
| $\bar{5}$ | 18.96 | 20.92 |
| $\bar{6}$ | 13.71 | 12.71 |
| **H 4 5** | | |
| 0 | 21.41 | 22.56 |
| 1 | 58.99 | 55.43 |
| 2 | 33.76 | 35.45 |
| 3 | 82.99 | 91.14 |
| 4 | 15.68 | 15.58 |
| 5 | 67.58 | 71.42 |
| 6 | 7.84 | 7.69 |
| $\bar{1}$ | 45.35 | 32.76 |
| $\bar{2}$ | 66.70 | 63.22 |
| $\bar{3}$ | 75.36 | 80.78 |
| $\bar{4}$ | 141.92 | 135.74 |
| $\bar{5}$ | 72.77 | 67.30 |
| $\bar{6}$ | 58.04 | 59.79 |
| $\bar{7}$ | 8.80 | 10.28 |
| **H 5 5** | | |
| 0 | 52.72 | 53.94 |
| 1 | 77.68 | 79.73 |
| 2 | 130.87 | 125.92 |
| 3 | 52.85 | 53.24 |
| 4 | 108.36 | 113.90 |
| 5 | 17.66 | 20.21 |
| $\bar{1}$ | 16.64 | 19.76 |
| $\bar{2}$ | 54.49 | 55.24 |
| $\bar{3}$ | 57.49 | 60.63 |
| $\bar{4}$ | 15.28 | 1.85 |
| $\bar{5}$ | 70.31 | 71.16 |
| $\bar{6}$ | 19.09 | 18.74 |
| $\bar{7}$ | 70.51 | 68.00 |
| **H 6 5** | | |
| 0 | 52.03 | 59.43 |
| 2 | 64.72 | 62.99 |
| 3 | 85.72 | 92.26 |
| $\bar{5}$ | 29.67 | 33.34 |
| $\bar{1}$ | 13.50 | 14.20 |
| $\bar{2}$ | 109.93 | 105.81 |
| $\bar{3}$ | 39.28 | 39.21 |
| $\bar{4}$ | 23.80 | 23.34 |
| $\bar{5}$ | 17.53 | 17.19 |
| $\bar{6}$ | 48.35 | 44.59 |
| **H 7 5** | | |
| 1 | 46.10 | 39.13 |
| 2 | 54.76 | 55.76 |
| 3 | 29.12 | 31.74 |
| $\bar{4}$ | 34.23 | 36.78 |
| $\bar{1}$ | 26.26 | 27.38 |
| $\bar{2}$ | 70.65 | 68.03 |
| $\bar{3}$ | 49.51 | 51.00 |
| $\bar{4}$ | 54.69 | 56.18 |
| $\bar{6}$ | 66.63 | 65.67 |
| **H 8 5** | | |
| 0 | 27.07 | 26.58 |
| 1 | 68.06 | 69.63 |
| 2 | 62.26 | 58.16 |
| 3 | 63.90 | 60.53 |
| $\bar{1}$ | 28.64 | 29.55 |
| $\bar{2}$ | 57.22 | 57.19 |
| $\bar{3}$ | 13.84 | 15.05 |
| $\bar{4}$ | 26.67 | 24.06 |

*Table 7* (Continued)

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| 5 | 80.06 | 77.64 |
| | H 9 5 | |
| 0 | 45.28 | 47.50 |
| 1 | 25.44 | 21.05 |
| 1̄ | 19.50 | 19.96 |
| 2̄ | 43.85 | 42.40 |
| | H 1 5̄ | |
| 0 | 123.44 | 141.60 |
| 1 | 46.78 | 41.54 |
| 2 | 81.63 | 73.53 |
| 3 | 33.76 | 30.96 |
| 4 | 28.37 | 17.06 |
| 6 | 132.98 | 135.03 |
| 7 | 68.27 | 69.05 |
| 8 | 33.28 | 27.63 |
| 1̄ | 61.04 | 63.21 |
| 2̄ | 16.03 | 10.90 |
| 3̄ | 26.80 | 19.11 |
| 4̄ | 62.74 | 65.59 |
| 7̄ | 24.89 | 20.98 |
| | H 2 5̄ | |
| 1 | 25.51 | 22.72 |
| 2 | 40.44 | 43.30 |
| 3 | 58.04 | 55.01 |
| 4 | 18.62 | 15.17 |
| 5 | 66.76 | 70.08 |
| 6 | 23.32 | 23.72 |
| 7 | 77.06 | 74.33 |
| 1̄ | 12.07 | 11.57 |
| 2̄ | 101.82 | 99.94 |
| 3̄ | 182.63 | 159.05 |
| 4̄ | 43.51 | 43.21 |
| 5̄ | 56.81 | 57.97 |
| 6̄ | 9.62 | 10.46 |
| 7̄ | 66.29 | 60.76 |
| | H 3 5̄ | |
| 0 | 22.85 | 27.80 |
| 1 | 65.47 | 72.20 |
| 2 | 92.61 | 88.29 |
| 3 | 41.80 | 45.75 |
| 4 | 40.37 | 35.58 |
| 5 | 41.60 | 40.36 |
| 6 | 83.81 | 86.24 |
| 7 | 31.57 | 29.57 |
| 1̄ | 56.33 | 54.35 |
| 2̄ | 108.02 | 104.88 |
| 3̄ | 28.78 | 25.40 |
| 4̄ | 34.10 | 31.70 |
| 5̄ | 86.47 | 80.97 |
| 6̄ | 79.86 | 77.09 |
| | H 4 5̄ | |
| 0 | 36.42 | 35.31 |
| 1 | 21.28 | 16.84 |
| 2 | 82.59 | 76.32 |
| 3 | 48.42 | 49.41 |
| 4 | 25.30 | 22.28 |
| 5 | 17.59 | 18.25 |
| 6 | 49.99 | 74.50 |
| 7 | 12.82 | 15.16 |
| 1̄ | 79.04 | 75.78 |
| 2̄ | 26.05 | 24.65 |
| 3̄ | 31.98 | 26.88 |
| 4̄ | 70.72 | 65.41 |
| 5̄ | 47.06 | 47.84 |
| 6̄ | 22.10 | 18.72 |
| 7̄ | 20.87 | 18.30 |
| | H 5 5̄ | |
| 0 | 40.37 | 44.36 |
| 1 | 50.33 | 41.97 |
| 2 | 69.42 | 66.16 |
| 3 | 82.18 | 80.75 |
| 4 | 50.53 | 50.16 |
| 5 | 47.46 | 52.19 |
| 6 | 38.94 | 35.50 |
| 1̄ | 18.89 | 20.13 |
| 2̄ | 48.90 | 45.09 |
| 3̄ | 135.03 | 131.01 |
| 5̄ | 55.85 | 58.34 |
| 6̄ | 22.91 | 22.78 |
| 7̄ | 28.71 | 25.08 |
| | H 6 5̄ | |
| 0 | 77.47 | 87.74 |
| 1 | 37.85 | 36.96 |
| 2 | 122.00 | 115.30 |
| 3 | 91.45 | 88.68 |
| 4 | 21.41 | 21.83 |
| 5 | 42.96 | 43.46 |
| 1̄ | 26.94 | 22.64 |
| 2̄ | 27.14 | 25.97 |
| 4̄ | 103.93 | 100.38 |
| 5̄ | 92.82 | 96.84 |
| 6̄ | 51.62 | 49.48 |
| | H 7 5̄ | |
| 0 | 28.44 | 32.07 |
| 1 | 5.93 | 4.92 |
| 2 | 56.33 | 56.66 |
| 3 | 24.89 | 24.05 |
| 4 | 20.94 | 23.32 |
| 5 | 63.08 | 59.69 |
| 1̄ | 67.11 | 63.22 |
| 2̄ | 54.08 | 52.44 |
| 3̄ | 90.16 | 88.44 |
| 4̄ | 59.33 | 57.48 |
| 5̄ | 26.12 | 24.42 |
| 6̄ | 17.73 | 21.26 |
| | H 8 5̄ | |
| 0 | 73.58 | 81.72 |
| 1 | 72.42 | 68.71 |
| 2 | 37.37 | 37.11 |
| 3 | 33.76 | 33.85 |
| 4 | 17.66 | 15.97 |
| 5 | 39.42 | 39.33 |
| 1̄ | 54.97 | 53.71 |
| 2̄ | 83.68 | 82.18 |
| 3̄ | 56.40 | 55.59 |
| 4̄ | 9.82 | 11.05 |
| 5̄ | 36.35 | 43.20 |
| | H 9 5̄ | |
| 0 | 77.33 | 83.40 |
| 1 | 24.14 | 23.27 |
| 2 | 75.02 | 68.27 |
| 3 | 52.51 | 49.03 |
| 4̄ | 6.62 | 1.16 |
| 1̄ | 5.93 | 6.83 |
| 3̄ | 43.99 | 43.70 |
| 4̄ | 69.15 | 70.52 |
| | H 10 5̄ | |
| 1 | 9.21 | 10.18 |
| 2 | 12.00 | 14.30 |
| 1̄ | 75.56 | 77.33 |
| 2̄ | 58.38 | 50.04 |
| 3̄ | 33.55 | 32.87 |
| | H 0 6 | |
| 1 | 52.78 | 55.66 |
| 2 | 20.25 | 21.50 |
| 3 | 59.54 | 65.39 |
| 4 | 43.24 | 42.31 |
| 5 | 16.23 | 16.06 |
| 6 | 35.60 | 29.08 |
| 7 | 50.26 | 43.58 |
| 1̄ | 48.01 | 45.56 |
| 2̄ | 21.28 | 23.36 |
| 3̄ | 110.27 | 96.55 |
| 4̄ | 30.28 | 38.17 |
| 5̄ | 54.49 | 59.67 |
| 6̄ | 19.37 | 17.44 |
| | H 1 6 | |
| 0 | 9.96 | 6.96 |
| 1 | 64.65 | 66.76 |
| 2 | 67.17 | 69.54 |
| 3 | 28.92 | 29.83 |
| 4 | 8.32 | 0.03 |
| 6 | 7.84 | 4.63 |
| 1̄ | 35.53 | 40.03 |
| 2̄ | 120.78 | 111.33 |
| 3̄ | 17.46 | 15.92 |
| 6̄ | 7.84 | 4.63 |
| 6̄ | 43.03 | 41.83 |
| 7̄ | 79.93 | 79.48 |
| | H 2 6 | |
| 0 | 26.46 | 33.09 |
| 1 | 34.78 | 32.70 |
| 2 | 24.96 | 25.62 |
| 3 | 36.08 | 42.84 |
| 4 | 51.76 | 51.36 |
| 5 | 23.12 | 22.71 |
| 6 | 80.74 | 80.62 |
| 1̄ | 92.95 | 87.89 |
| 2̄ | 81.43 | 84.57 |
| 3̄ | 49.99 | 47.00 |
| 4̄ | 39.01 | 38.63 |
| 5̄ | 11.12 | 10.95 |
| 6̄ | 33.28 | 32.28 |
| 7̄ | 46.44 | 43.85 |
| | H 3 6 | |
| 0 | 24.55 | 29.55 |
| 1 | 67.51 | 66.70 |
| 2 | 12.14 | 11.46 |
| 3 | 28.98 | 30.46 |
| 4 | 70.65 | 75.45 |
| 5 | 30.35 | 30.93 |
| 6 | 35.80 | 32.31 |
| 1̄ | 33.01 | 28.76 |
| 2̄ | 40.71 | 37.54 |
| 3̄ | 15.00 | 19.74 |
| 4̄ | 146.69 | 134.25 |
| 5̄ | 72.83 | 70.29 |
| | H 4 6 | |
| 1 | 75.15 | 75.80 |
| 2 | 82.93 | 88.90 |
| 3 | 16.03 | 17.26 |
| 4 | 67.86 | 70.06 |
| 5 | 26.19 | 24.55 |
| 1̄ | 37.17 | 32.45 |
| 2̄ | 8.52 | 6.99 |
| 3̄ | 46.44 | 43.87 |
| 4̄ | 21.89 | 21.54 |
| 5̄ | 23.73 | 19.70 |
| 6̄ | 75.63 | 76.26 |
| 7̄ | 28.92 | 28.15 |
| | H 5 6 | |
| 0 | 61.85 | 56.78 |
| 1 | 39.15 | 40.66 |
| 2 | 72.56 | 72.66 |
| 3 | 43.65 | 43.62 |
| 4 | 21.48 | 20.34 |
| 1̄ | 82.59 | 80.23 |
| 2̄ | 89.75 | 88.43 |
| 3̄ | 113.48 | 113.87 |
| 5̄ | 6.68 | 5.10 |
| 6̄ | 16.37 | 17.40 |
| | H 6 6 | |
| 0 | 85.11 | 86.87 |
| 1 | 57.42 | 56.49 |
| 2 | 54.35 | 57.96 |
| 3 | 45.01 | 47.58 |
| 4 | 43.10 | 46.50 |
| 1̄ | 10.30 | 9.20 |
| 2̄ | 105.91 | 107.10 |
| 4̄ | 144.03 | 134.19 |
| 5̄ | 18.62 | 18.38 |
| 6̄ | 15.48 | 14.78 |
| | H 7 6 | |
| 1 | 64.24 | 65.27 |
| 2 | 50.60 | 49.17 |
| 3̄ | 55.65 | 60.93 |
| 2̄ | 30.89 | 29.17 |
| 3̄ | 44.74 | 42.80 |
| 5̄ | 28.16 | 26.27 |
| | H 8 6 | |
| 0 | 28.92 | 33.47 |
| 1 | 54.49 | 53.87 |
| 2̄ | 6.55 | 6.24 |
| 1̄ | 41.19 | 41.90 |
| 3̄ | 59.81 | 55.87 |
| | H 9 6 | |
| 0̄ | 27.69 | 30.88 |
| 1̄ | 54.22 | 53.95 |
| 2̄ | 58.79 | 53.71 |
| | H 1 6̄ | |
| 0 | 19.64 | 25.82 |
| 1 | 50.47 | 57.22 |
| 2 | 99.63 | 106.95 |
| 3 | 19.85 | 18.35 |
| 4 | 104.89 | 94.34 |
| 5 | 31.57 | 31.96 |
| 6 | 14.46 | 16.90 |
| 7̄ | 48.97 | 44.98 |
| 1̄ | 48.28 | 45.94 |
| 2̄ | 68.33 | 57.19 |
| 3̄ | 52.03 | 44.90 |
| 4̄ | 11.39 | 17.02 |
| 5̄ | 102.29 | 95.63 |
| 6̄ | 124.80 | 108.52 |
| | H 2 6̄ | |
| 0 | 72.36 | 75.24 |
| 1 | 37.78 | 40.04 |
| 2 | 107.34 | 92.83 |
| 3 | 16.78 | 14.93 |
| 4 | 24.01 | 21.87 |
| 5 | 44.87 | 44.27 |
| 6 | 11.73 | 14.39 |
| 7 | 56.33 | 53.53 |
| 1̄ | 116.82 | 118.34 |
| 2̄ | 102.70 | 93.35 |
| 3̄ | 47.60 | 45.55 |
| 5̄ | 119.82 | 108.39 |
| 6̄ | 7.71 | 7.99 |
| 7̄ | 32.67 | 33.94 |
| | H 3 6̄ | |
| 0 | 31.57 | 30.71 |
| 1 | 14.32 | 14.95 |
| 2 | 14.87 | 9.86 |
| 3 | 129.98 | 128.58 |
| 4 | 5.11 | 7.64 |
| 5 | 43.92 | 43.86 |
| 7 | 42.08 | 43.92 |
| 1̄ | 61.85 | 58.63 |
| 2̄ | 31.17 | 26.06 |
| 3̄ | 44.19 | 40.19 |
| 4̄ | 77.13 | 73.07 |
| 5̄ | 19.85 | 18.85 |
| 6̄ | 10.23 | 9.79 |
| 7̄ | 23.73 | 19.54 |
| | H 4 6̄ | |
| 0 | 18.14 | 21.39 |
| 1 | 6.00 | 5.95 |
| 2 | 132.37 | 123.50 |
| 3 | 49.72 | 45.34 |
| 4 | 144.78 | 142.33 |
| 5 | 23.32 | 22.18 |
| 6 | 32.46 | 37.59 |
| 7 | 28.51 | 25.56 |
| 1̄ | 5.80 | 4.67 |
| 2̄ | 49.17 | 46.39 |
| 3̄ | 34.03 | 31.52 |
| 4̄ | 35.53 | 37.56 |
| 5̄ | 107.75 | 103.12 |
| 6̄ | 51.35 | 48.75 |
| 7̄ | 43.58 | 39.26 |
| | H 5 6̄ | |
| 0 | 75.02 | 74.13 |
| 1 | 9.07 | 7.21 |
| 2 | 8.32 | 8.72 |
| 3 | 14.12 | 0.29 |
| 4 | 89.13 | 85.57 |
| 5 | 51.56 | 52.94 |
| 6 | 10.43 | 10.35 |
| 1̄ | 30.21 | 27.47 |
| 2̄ | 11.59 | 10.95 |
| 3̄ | 64.10 | 59.75 |
| 4̄ | 47.06 | 46.14 |
| 5̄ | 90.97 | 88.98 |
| 6̄ | 35.60 | 39.51 |
| | H 6 6̄ | |
| 0 | 8.05 | 9.27 |
| 1 | 28.51 | 33.59 |
| 2 | 82.11 | 78.46 |
| 3 | 98.61 | 99.12 |
| 4 | 10.23 | 12.60 |
| 5 | 40.44 | 39.45 |
| 1̄ | 30.28 | 31.58 |
| 2̄ | 37.71 | 42.09 |
| 3̄ | 10.43 | 12.91 |
| 4̄ | 100.93 | 100.75 |
| 5̄ | 13.91 | 13.06 |
| 6̄ | 34.64 | 33.18 |
| | H 7 6̄ | |

*Table 7* (Continued)

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| 0 | 57.97 | 62.83 |
| 1 | 68.40 | 71.41 |
| 2 | 27.96 | 29.51 |
| 4 | 96.77 | 90.20 |
| 5 | 50.87 | 50.17 |
| $\bar{1}$ | 47.26 | 50.86 |
| $\bar{2}$ | 84.63 | 86.30 |
| $\bar{3}$ | 57.28 | 56.57 |
| $\bar{4}$ | 43.31 | 45.67 |
| $\bar{5}$ | 64.17 | 62.07 |
| $\bar{6}$ | 37.51 | 36.51 |

H 8 $\bar{6}$

| | | |
|---|---|---|
| 0 | 20.32 | 21.35 |
| 1 | 13.98 | 12.97 |
| 2 | 56.33 | 53.79 |
| 3 | 71.06 | 70.61 |
| 4 | 52.65 | 47.97 |
| $\bar{1}$ | 47.46 | 45.91 |
| $\bar{3}$ | 120.44 | 122.28 |
| $\bar{5}$ | 35.74 | 36.56 |

H 9 $\bar{6}$

| | | |
|---|---|---|
| 0 | 34.58 | 41.46 |
| 1 | 20.66 | 18.09 |
| 2 | 55.51 | 50.05 |
| $\bar{3}$ | 10.91 | 13.47 |
| $\bar{1}$ | 54.28 | 50.78 |
| $\bar{3}$ | 34.78 | 36.09 |
| $\bar{4}$ | 58.24 | 56.50 |

H 10 $\bar{6}$

| | | |
|---|---|---|
| 0 | 46.99 | 45.48 |
| 1 | 59.06 | 56.44 |
| 2 | 16.64 | 17.53 |
| $\bar{1}$ | 10.43 | 11.60 |
| $\bar{2}$ | 52.51 | 52.94 |
| $\bar{3}$ | 54.15 | 54.61 |

H 0 7

| | | |
|---|---|---|
| 0 | 18.14 | 15.82 |
| 1 | 127.39 | 122.65 |
| 2 | 86.95 | 80.22 |
| 3 | 74.06 | 75.40 |
| 4 | 77.27 | 75.06 |
| 5 | 41.74 | 40.96 |
| $\bar{6}$ | 42.08 | 37.66 |
| $\bar{2}$ | 64.72 | 47.56 |
| $\bar{3}$ | 42.76 | 39.26 |
| $\bar{4}$ | 72.77 | 71.75 |
| $\bar{5}$ | 48.49 | 51.13 |
| $\bar{6}$ | 96.98 | 94.22 |
| $\bar{7}$ | 50.33 | 53.72 |

H 1 7

| | | |
|---|---|---|
| 0 | 40.03 | 45.80 |
| 1 | 25.44 | 27.88 |
| 2 | 34.58 | 25.54 |
| 3 | 50.06 | 54.52 |
| 4 | 40.10 | 41.04 |
| $\bar{6}$ | 52.58 | 49.90 |
| $\bar{1}$ | 64.04 | 59.43 |
| $\bar{2}$ | 67.11 | 53.72 |
| $\bar{3}$ | 6.55 | 7.85 |
| $\bar{4}$ | 19.30 | 22.91 |
| $\bar{5}$ | 10.03 | 10.50 |
| $\bar{6}$ | 7.91 | 7.70 |
| $\bar{7}$ | 34.44 | 33.40 |

H 2 7

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| 0 | 18.14 | 22.36 |
| 1 | 89.54 | 90.46 |
| 2 | 48.90 | 49.70 |
| 4 | 48.49 | 44.12 |
| 5 | 29.32 | 27.33 |
| 6 | 30.14 | 27.29 |
| $\bar{1}$ | 13.44 | 12.54 |
| $\bar{2}$ | 7.02 | 4.05 |
| $\bar{3}$ | 43.65 | 41.60 |
| $\bar{4}$ | 78.02 | 68.55 |
| $\bar{5}$ | 103.11 | 103.18 |
| $\bar{6}$ | 28.37 | 22.74 |

H 3 7

| | | |
|---|---|---|
| 0 | 62.20 | 53.71 |
| 1 | 22.37 | 19.55 |
| 2 | 113.00 | 111.81 |
| 3 | 70.45 | 69.04 |
| 4 | 31.10 | 33.12 |
| 5 | 36.89 | 32.87 |
| $\bar{1}$ | 15.89 | 13.77 |
| $\bar{2}$ | 5.86 | 9.62 |
| $\bar{3}$ | 21.48 | 21.75 |
| $\bar{4}$ | 116.14 | 110.59 |
| $\bar{5}$ | 30.08 | 28.02 |
| $\bar{6}$ | 88.04 | 82.83 |
| $\bar{7}$ | 18.69 | 18.32 |

H 4 7

| | | |
|---|---|---|
| 0 | 21.41 | 15.35 |
| 1 | 44.87 | 42.05 |
| 2 | 47.81 | 48.50 |
| 3 | 54.56 | 54.39 |
| 4 | 40.44 | 39.42 |
| $\bar{5}$ | 11.18 | 10.34 |
| $\bar{1}$ | 84.97 | 85.56 |
| $\bar{3}$ | 55.92 | 51.59 |
| $\bar{4}$ | 9.07 | 6.58 |
| $\bar{5}$ | 15.68 | 15.05 |
| $\bar{6}$ | 23.66 | 21.87 |

H 5 7

| | | |
|---|---|---|
| 0 | 38.19 | 41.99 |
| 1 | 25.78 | 28.88 |
| 2 | 15.89 | 17.56 |
| 3 | 23.94 | 25.35 |
| 4 | 42.08 | 44.72 |
| $\bar{1}$ | 58.65 | 52.15 |
| $\bar{2}$ | 23.12 | 21.12 |
| $\bar{3}$ | 65.06 | 59.31 |
| $\bar{4}$ | 38.74 | 37.11 |
| $\bar{5}$ | 112.39 | 105.60 |
| $\bar{6}$ | 20.05 | 17.42 |

H 6 7

| | | |
|---|---|---|
| 0 | 77.61 | 80.73 |
| 1 | 18.14 | 20.72 |
| 2 | 73.58 | 78.75 |
| 3 | 30.21 | 28.36 |
| 4 | 45.21 | 45.78 |
| $\bar{1}$ | 22.16 | 19.22 |
| $\bar{2}$ | 26.26 | 26.35 |
| $\bar{3}$ | 47.19 | 45.00 |
| $\bar{4}$ | 96.70 | 89.01 |
| $\bar{5}$ | 32.19 | 32.35 |

H 7 7

| | | |
|---|---|---|
| 1 | 103.93 | 111.22 |
| 2 | 24.69 | 26.47 |
| $\bar{3}$ | 31.98 | 25.84 |
| $\bar{1}$ | 70.38 | 70.41 |
| $\bar{2}$ | 40.85 | 41.22 |
| $\bar{3}$ | 36.01 | 32.28 |
| $\bar{4}$ | 30.14 | 28.86 |

H 8 7

| | | |
|---|---|---|
| 0 | 26.60 | 31.16 |
| 1 | 12.82 | 15.95 |
| $\bar{1}$ | 16.64 | 12.64 |
| $\bar{2}$ | 24.01 | 22.16 |
| $\bar{3}$ | 14.19 | 13.21 |

H 1 $\bar{7}$

| | | |
|---|---|---|
| 0 | 18.48 | 13.95 |
| 1 | 45.76 | 44.04 |
| 2 | 17.46 | 16.75 |
| 3 | 63.70 | 60.97 |
| 4 | 40.30 | 39.05 |
| 5 | 57.15 | 57.19 |
| 6 | 7.43 | 7.07 |
| 7 | 32.46 | 31.88 |
| $\bar{1}$ | 99.50 | 96.88 |
| $\bar{2}$ | 35.26 | 33.90 |
| $\bar{3}$ | 84.15 | 71.43 |
| $\bar{4}$ | 126.16 | 112.02 |
| $\bar{5}$ | 53.60 | 48.56 |
| $\bar{6}$ | 28.51 | 25.99 |

H 2 $\bar{7}$

| | | |
|---|---|---|
| 0 | 78.09 | 77.55 |
| 1 | 85.79 | 82.59 |
| 3 | 9.75 | 2.27 |
| 4 | 58.65 | 63.65 |
| 5 | 24.28 | 26.11 |
| 6 | 18.21 | 22.55 |
| 7 | 23.19 | 22.44 |
| $\bar{1}$ | 21.82 | 28.32 |
| $\bar{2}$ | 11.05 | 12.43 |
| $\bar{3}$ | 9.55 | 10.87 |
| $\bar{4}$ | 41.87 | 39.11 |
| $\bar{5}$ | 13.64 | 13.70 |
| $\bar{6}$ | 58.72 | 59.03 |

H 3 $\bar{7}$

| | | |
|---|---|---|
| 0 | 30.14 | 33.07 |
| 1 | 24.01 | 24.37 |
| 2 | 40.24 | 45.54 |
| 3 | 6.14 | 9.04 |
| 4 | 64.86 | 59.98 |
| 5 | 93.50 | 90.01 |
| 6 | 60.49 | 66.68 |
| 7 | 42.96 | 42.25 |
| $\bar{1}$ | 95.88 | 94.79 |
| $\bar{2}$ | 5.52 | 5.47 |
| $\bar{3}$ | 60.56 | 60.71 |
| $\bar{4}$ | 33.14 | 29.00 |
| $\bar{5}$ | 36.49 | 51.76 |
| $\bar{6}$ | 26.05 | 20.90 |

H 4 $\bar{7}$

| | | |
|---|---|---|
| 1 | 28.23 | 32.44 |
| 2 | 5.32 | 8.80 |
| 3 | 82.45 | 83.38 |
| 4 | 87.77 | 83.80 |
| 5 | 30.76 | 28.43 |
| 6 | 42.21 | 37.48 |
| $\bar{2}$ | 65.33 | 68.05 |
| $\bar{3}$ | 39.15 | 43.65 |
| $\bar{4}$ | 90.43 | 92.65 |
| $\bar{5}$ | 57.42 | 51.76 |
| $\bar{6}$ | 39.35 | 35.37 |

H 5 $\bar{7}$

| | | |
|---|---|---|
| 0 | 62.40 | 62.92 |
| 1 | 47.87 | 48.51 |
| 2 | 70.86 | 64.76 |
| 3 | 18.28 | 19.26 |
| 5 | 46.65 | 44.17 |
| 6 | 36.76 | 37.25 |
| $\bar{1}$ | 65.33 | 57.30 |
| $\bar{2}$ | 39.21 | 37.51 |
| $\bar{3}$ | 12.68 | 12.26 |
| $\bar{4}$ | 32.12 | 27.31 |
| $\bar{5}$ | 16.84 | 17.43 |
| $\bar{6}$ | 32.33 | 30.84 |

H 6 $\bar{7}$

| | | |
|---|---|---|
| 0 | 22.44 | 27.13 |
| 1 | 90.22 | 90.08 |
| 2 | 55.51 | 53.56 |
| 3 | 9.00 | 8.30 |
| 4 | 55.72 | 52.22 |
| $\bar{5}$ | 68.40 | 61.51 |
| $\bar{1}$ | 61.17 | 63.69 |
| $\bar{2}$ | 34.37 | 33.41 |
| $\bar{3}$ | 64.65 | 66.17 |
| $\bar{4}$ | 38.80 | 39.89 |
| $\bar{5}$ | 67.86 | 66.91 |
| $\bar{6}$ | 8.66 | 7.55 |

H 7 $\bar{7}$

| | | |
|---|---|---|
| 1 | 70.86 | 71.80 |
| 2 | 126.91 | 120.61 |
| 4 | 60.01 | 53.30 |
| $\bar{5}$ | 13.03 | 13.15 |
| $\bar{1}$ | 15.55 | 13.35 |
| $\bar{2}$ | 7.84 | 11.04 |
| $\bar{3}$ | 80.74 | 77.17 |
| $\bar{4}$ | 109.46 | 111.05 |
| $\bar{5}$ | 24.41 | 27.20 |

H 8 $\bar{7}$

| | | |
|---|---|---|
| 0 | 52.78 | 59.08 |
| 1 | 28.64 | 26.67 |
| 2 | 7.77 | 5.18 |
| $\bar{3}$ | 33.96 | 32.19 |
| $\bar{1}$ | 73.38 | 76.68 |
| $\bar{2}$ | 16.98 | 18.22 |
| $\bar{3}$ | 13.30 | 13.88 |
| $\bar{4}$ | 16.16 | 15.96 |

H 9 $\bar{7}$

| | | |
|---|---|---|
| 1 | 73.65 | 71.74 |
| 2 | 14.59 | 11.98 |
| $\bar{3}$ | 9.55 | 10.66 |
| $\bar{2}$ | 34.30 | 37.26 |
| $\bar{3}$ | 32.05 | 32.29 |

H 10 $\bar{7}$

| | | |
|---|---|---|
| 0 | 48.28 | 50.36 |
| 1 | 8.59 | 6.71 |
| $\bar{1}$ | 25.78 | 27.11 |
| $\bar{2}$ | 37.85 | 39.64 |

H 0 8

| | | |
|---|---|---|
| 1 | 21.82 | 18.57 |
| 2 | 26.39 | 25.41 |
| 4 | 99.57 | 93.28 |
| 5 | 48.56 | 44.28 |
| $\bar{6}$ | 16.03 | 15.89 |
| $\bar{1}$ | 64.45 | 71.98 |
| $\bar{2}$ | 20.25 | 24.54 |
| $\bar{3}$ | 37.37 | 41.76 |
| $\bar{5}$ | 46.71 | 48.13 |
| $\bar{6}$ | 68.67 | 70.56 |
| $\bar{7}$ | 35.80 | 35.51 |

H 1 8

| | | |
|---|---|---|
| 1 | 9.75 | 13.00 |
| 4 | 91.45 | 92.19 |
| 5 | 63.42 | 65.77 |
| 6 | 28.51 | 26.87 |
| $\bar{1}$ | 43.71 | 43.85 |
| $\bar{2}$ | 28.57 | 26.07 |
| $\bar{3}$ | 100.18 | 97.69 |
| $\bar{4}$ | 105.16 | 102.18 |
| $\bar{5}$ | 24.21 | 29.03 |
| $\bar{6}$ | 20.73 | 23.40 |
| $\bar{7}$ | 8.87 | 6.17 |

H 2 8

| | | |
|---|---|---|
| 0 | 15.21 | 11.72 |
| 2 | 61.31 | 66.22 |
| 3 | 67.79 | 66.81 |
| 4 | 27.89 | 27.65 |
| $\bar{5}$ | 7.09 | 3.27 |
| $\bar{1}$ | 42.69 | 42.51 |
| $\bar{2}$ | 42.35 | 40.14 |
| $\bar{3}$ | 79.52 | 76.42 |
| $\bar{4}$ | 92.07 | 86.98 |
| $\bar{5}$ | 56.40 | 56.64 |
| $\bar{6}$ | 71.68 | 74.12 |

H 3 8

| | | |
|---|---|---|
| 0 | 43.78 | 44.18 |
| 2 | 28.64 | 31.05 |
| 3 | 43.51 | 47.39 |
| 4 | 47.26 | 49.96 |
| $\bar{5}$ | 18.21 | 15.76 |
| $\bar{1}$ | 54.28 | 54.34 |
| $\bar{2}$ | 79.58 | 75.88 |
| $\bar{3}$ | 81.77 | 78.35 |
| $\bar{5}$ | 29.53 | 24.34 |
| $\bar{6}$ | 55.65 | 55.60 |

H 4 8

| | | |
|---|---|---|
| 0 | 9.96 | 11.18 |
| 1 | 27.82 | 32.60 |
| 2 | 27.35 | 31.60 |
| 3 | 48.56 | 51.08 |
| 4 | 40.44 | 38.47 |
| $\bar{1}$ | 85.65 | 86.32 |
| $\bar{2}$ | 16.57 | 17.00 |
| $\bar{3}$ | 148.81 | 138.18 |
| $\bar{4}$ | 13.37 | 13.49 |

H 5 8

| | | |
|---|---|---|
| 0 | 34.58 | 35.72 |
| 2 | 82.18 | 89.65 |
| 3 | 14.19 | 14.07 |
| 4 | 61.31 | 62.90 |
| $\bar{2}$ | 62.81 | 63.02 |
| $\bar{3}$ | 45.69 | 39.64 |
| $\bar{4}$ | 23.39 | 23.58 |
| $\bar{5}$ | 81.70 | 81.39 |

H 6 8

| | | |
|---|---|---|
| 0 | 66.70 | 67.77 |
| 1 | 16.50 | 18.25 |
| 2 | 17.39 | 24.34 |
| $\bar{3}$ | 65.40 | 63.17 |
| $\bar{1}$ | 35.67 | 31.16 |

*Table 7* (Continued)

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| $\bar{2}$ | 44.46 | 49.09 |
| $\bar{3}$ | 7.84 | 7.74 |
| $\bar{4}$ | 40.58 | 37.85 |
| $\bar{5}$ | 16.44 | 17.25 |
| | H 7 8 | |
| 0 | 44.87 | 45.84 |
| $\bar{1}$ | 53.19 | 52.39 |
| $\bar{1}$ | 87.22 | 92.75 |
| $\bar{2}$ | 20.94 | 18.03 |
| $\bar{3}$ | 68.95 | 66.30 |
| $\bar{4}$ | 56.19 | 55.96 |
| | H 1 $\bar{8}$ | |
| 0 | 35.67 | 28.44 |
| 1 | 24.48 | 23.23 |
| 2 | 6.55 | 6.05 |
| 3 | 44.67 | 46.40 |
| 4 | 86.40 | 83.53 |
| 5 | 12.48 | 14.74 |
| 6 | 58.51 | 62.03 |
| 7 | 21.28 | 23.30 |
| $\bar{1}$ | 74.06 | 78.92 |
| $\bar{2}$ | 119.21 | 108.94 |
| $\bar{3}$ | 151.94 | 144.34 |
| $\bar{4}$ | 32.87 | 29.66 |
| $\bar{5}$ | 11.39 | 10.06 |
| $\bar{6}$ | 14.59 | 12.97 |
| | H 2 $\bar{8}$ | |
| 0 | 23.39 | 25.11 |
| 1 | 56.13 | 54.43 |
| 2 | 14.12 | 15.86 |
| 3 | 28.10 | 34.43 |
| 4 | 57.69 | 61.90 |
| 5 | 62.95 | 64.92 |
| $\bar{6}$ | 6.75 | 0.57 |
| $\bar{1}$ | 18.62 | 14.77 |
| $\bar{2}$ | 42.76 | 45.35 |
| $\bar{3}$ | 71.47 | 69.43 |
| $\bar{4}$ | 135.30 | 119.78 |
| $\bar{5}$ | 39.69 | 40.01 |
| $\bar{6}$ | 9.48 | 6.93 |
| | H 3 $\bar{8}$ | |
| 0 | 46.37 | 44.72 |
| 1 | 91.59 | 92.05 |
| 3 | 15.55 | 14.90 |
| 4 | 32.26 | 33.12 |
| 5 | 44.87 | 46.26 |
| $\bar{6}$ | 61.65 | 54.25 |
| $\bar{1}$ | 31.71 | 27.23 |
| $\bar{2}$ | 26.12 | 34.50 |
| $\bar{3}$ | 31.64 | 23.12 |
| $\bar{4}$ | 117.64 | 105.59 |
| $\bar{5}$ | 12.21 | 12.12 |
| $\bar{6}$ | 35.39 | 31.58 |
| | H 4 $\bar{8}$ | |
| 0 | 35.67 | 27.21 |
| 1 | 46.51 | 42.29 |
| 2 | 7.57 | 5.97 |
| 4 | 11.18 | 11.29 |
| 6 | 41.26 | 43.89 |
| $\bar{1}$ | 86.00 | 85.16 |
| $\bar{2}$ | 33.96 | 33.93 |
| $\bar{3}$ | 161.01 | 152.92 |
| $\bar{4}$ | 10.50 | 13.16 |
| $\bar{5}$ | 12.75 | 12.54 |
| $\bar{6}$ | 35.33 | 31.19 |

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| | H 5 $\bar{8}$ | |
| 0 | 7.77 | C.37 |
| 1 | 47.60 | 51.56 |
| 2 | 85.25 | 89.76 |
| 3 | 30.96 | 25.38 |
| 4 | 84.97 | 79.70 |
| 5 | 41.80 | 40.34 |
| 6 | 17.05 | 18.18 |
| $\bar{1}$ | 23.53 | 23.76 |
| $\bar{2}$ | 80.40 | 79.78 |
| $\bar{3}$ | 69.36 | 64.90 |
| $\bar{4}$ | 45.35 | 43.36 |
| $\bar{5}$ | 12.14 | 9.45 |
| | H 6 $\bar{8}$ | |
| 0 | 10.57 | 9.49 |
| 1 | 107.27 | 110.36 |
| 2 | 30.28 | 27.14 |
| 3 | 102.64 | 100.94 |
| 4 | 34.58 | 37.02 |
| $\bar{5}$ | 13.84 | 10.63 |
| $\bar{1}$ | 42.62 | 45.60 |
| $\bar{2}$ | 38.46 | 41.75 |
| $\bar{3}$ | 12.62 | 14.01 |
| $\bar{4}$ | 29.60 | 26.02 |
| | H 7 $\bar{8}$ | |
| 0 | 20.87 | 22.66 |
| 1 | 41.12 | 44.16 |
| 2 | 6.62 | 5.99 |
| 3 | 46.17 | 40.06 |
| 4 | 67.51 | 66.48 |
| $\bar{1}$ | 34.03 | 31.82 |
| $\bar{2}$ | 11.59 | 14.04 |
| $\bar{3}$ | 44.26 | 50.42 |
| $\bar{4}$ | 49.17 | 58.68 |
| $\bar{5}$ | 21.96 | 22.54 |
| | H 8 $\bar{8}$ | |
| 1 | 66.22 | 64.02 |
| 2 | 82.25 | 76.90 |
| $\bar{1}$ | 11.18 | 11.70 |
| $\bar{2}$ | 64.10 | 64.49 |
| $\bar{3}$ | 11.73 | 10.75 |
| $\bar{4}$ | 12.82 | 13.19 |
| | H 9 $\bar{8}$ | |
| $\bar{1}$ | 57.01 | 62.05 |
| $\bar{2}$ | 34.10 | 30.99 |
| $\bar{3}$ | 49.78 | 48.54 |
| 2 | 8.59 | 5.69 |
| | H 0 9 | |
| 0 | 10.43 | 6.12 |
| 1 | 24.89 | 25.37 |
| 2 | 71.74 | 75.82 |
| 3 | 7.43 | 6.33 |
| 4 | 47.19 | 41.30 |
| 5 | 37.78 | 34.58 |
| $\bar{1}$ | 62.40 | 64.75 |
| $\bar{2}$ | 9.14 | 8.64 |
| $\bar{3}$ | 62.26 | 61.61 |
| $\bar{4}$ | 52.65 | 48.86 |
| $\bar{5}$ | 15.75 | 15.77 |
| | H 1 9 | |
| 0 | 46.17 | 39.88 |
| 1 | 53.13 | 54.82 |
| 2 | 52.03 | 54.07 |

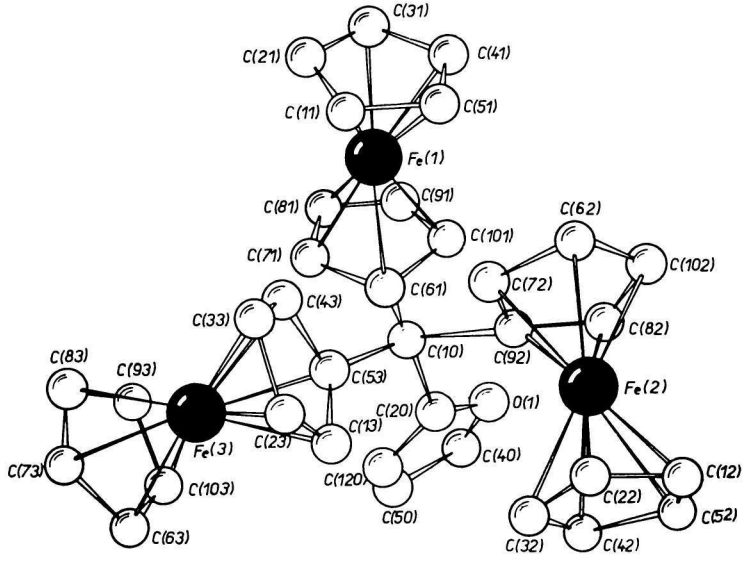
| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| 3 | 85.25 | 89.44 |
| 4 | 9.75 | 11.12 |
| 5 | 42.69 | 43.54 |
| $\bar{1}$ | 76.11 | 77.86 |
| $\bar{2}$ | 55.38 | 49.26 |
| $\bar{3}$ | 77.13 | 74.87 |
| $\bar{4}$ | 27.82 | 27.10 |
| $\bar{5}$ | 54.28 | 55.01 |
| $\bar{6}$ | 20.12 | 19.00 |
| | H 2 9 | |
| 0 | 121.46 | 117.07 |
| 2 | 80.40 | 83.39 |
| 4 | 24.69 | 26.25 |
| 5 | 13.23 | 10.99 |
| $\bar{1}$ | 24.82 | 20.93 |
| $\bar{2}$ | 37.17 | 39.41 |
| $\bar{3}$ | 31.10 | 28.56 |
| $\bar{4}$ | 7.91 | 8.16 |
| $\bar{5}$ | 22.91 | 18.21 |
| | H 3 9 | |
| 0 | 5.89 | 8.99 |
| 1 | 45.49 | 42.66 |
| 2 | 10.57 | 10.63 |
| 3 | 22.23 | 24.45 |
| 4 | 20.94 | 20.85 |
| $\bar{1}$ | 42.01 | 43.72 |
| $\bar{2}$ | 70.99 | 68.42 |
| $\bar{3}$ | 55.03 | 59.19 |
| $\bar{4}$ | 57.63 | 53.27 |
| $\bar{5}$ | 9.96 | 9.33 |
| $\bar{6}$ | 28.23 | 34.97 |
| | H 4 9 | |
| 0 | 61.58 | 62.06 |
| 1 | 79.24 | 85.03 |
| 2 | 11.18 | 7.94 |
| 3 | 55.03 | 55.17 |
| 4 | 11.12 | 8.09 |
| $\bar{1}$ | 13.16 | 12.03 |
| $\bar{2}$ | 23.80 | 26.41 |
| $\bar{3}$ | 58.58 | 54.64 |
| $\bar{5}$ | 55.38 | 46.41 |
| | H 5 9 | |
| 0 | 55.03 | 59.34 |
| 1 | 49.58 | 50.72 |
| 2 | 87.36 | 89.51 |
| 3 | 10.30 | 8.07 |
| $\bar{2}$ | 22.23 | 26.94 |
| $\bar{3}$ | 8.93 | 9.52 |
| $\bar{4}$ | 16.44 | 15.62 |
| $\bar{5}$ | 85.25 | 78.28 |
| | H 6 9 | |
| 0 | 21.41 | 20.74 |
| 1 | 19.03 | 20.01 |
| 2 | 34.98 | 35.88 |
| $\bar{1}$ | 17.94 | 21.55 |
| $\bar{2}$ | 35.39 | 33.67 |
| $\bar{3}$ | 53.33 | 49.86 |
| $\bar{4}$ | 7.30 | 9.35 |
| | H 7 9 | |
| $\bar{1}$ | 33.35 | 34.97 |
| | H 1 $\bar{9}$ | |
| 0 | 101.89 | 99.65 |

| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| 1 | 73.79 | 71.23 |
| 2 | 87.50 | 81.56 |
| 3 | 18.96 | 13.91 |
| 4 | 24.89 | 23.75 |
| 5 | 34.30 | 37.48 |
| 6 | 21.21 | 21.90 |
| $\bar{1}$ | 73.79 | 71.23 |
| $\bar{2}$ | 103.18 | 101.11 |
| $\bar{3}$ | 37.71 | 31.05 |
| $\bar{4}$ | 40.03 | 37.21 |
| $\bar{5}$ | 11.80 | 10.32 |
| | H 2 $\bar{9}$ | |
| 0 | 12.34 | 8.30 |
| 1 | 12.07 | 11.10 |
| 2 | 73.86 | 70.82 |
| 3 | 101.82 | 104.74 |
| $\bar{5}$ | 41.80 | 42.66 |
| $\bar{1}$ | 17.87 | 17.34 |
| $\bar{2}$ | 120.03 | 125.18 |
| $\bar{3}$ | 100.02 | 92.44 |
| $\bar{4}$ | 10.71 | 13.85 |
| $\bar{5}$ | 42.01 | 46.47 |
| | H 3 $\bar{9}$ | |
| 0 | 79.86 | 81.61 |
| 1 | 22.71 | 22.11 |
| 2 | 7.23 | 4.73 |
| 3 | 31.23 | 31.37 |
| 4 | 53.47 | 51.64 |
| 5 | 6.21 | 6.51 |
| 6 | 25.30 | 26.71 |
| $\bar{2}$ | 101.20 | 96.02 |
| $\bar{3}$ | 17.94 | 17.91 |
| $\bar{4}$ | 45.62 | 47.80 |
| $\bar{5}$ | 21.21 | 22.22 |
| | H 4 $\bar{9}$ | |
| 0 | 44.46 | 46.08 |
| 1 | 66.08 | 72.62 |
| 2 | 68.95 | 69.18 |
| $\bar{1}$ | 73.45 | 71.64 |
| $\bar{2}$ | 57.35 | 58.15 |
| $\bar{5}$ | 44.12 | 46.56 |
| | H 5 $\bar{9}$ | |
| 0 | 15.55 | 18.03 |
| 1 | 24.96 | 24.43 |
| 2 | 53.13 | 50.73 |
| 3 | 139.67 | 132.88 |
| 4 | 38.19 | 38.34 |
| $\bar{5}$ | 11.12 | 11.91 |
| $\bar{2}$ | 56.53 | 58.87 |
| $\bar{3}$ | 42.83 | 47.21 |
| $\bar{4}$ | 19.57 | 20.42 |
| $\bar{5}$ | 38.67 | 38.55 |
| | H 6 $\bar{9}$ | |
| 0 | 41.67 | 43.63 |
| 1 | 12.00 | 10.28 |
| 2 | 14.32 | 13.72 |
| 3 | 48.42 | 48.18 |
| 4 | 38.19 | 36.52 |
| $\bar{1}$ | 5.18 | 8.17 |
| $\bar{2}$ | 52.24 | 55.96 |
| $\bar{4}$ | 20.66 | 20.73 |
| | H 7 $\bar{9}$ | |
| 1 | 33.08 | 33.19 |
| 2 | 45.76 | 42.92 |

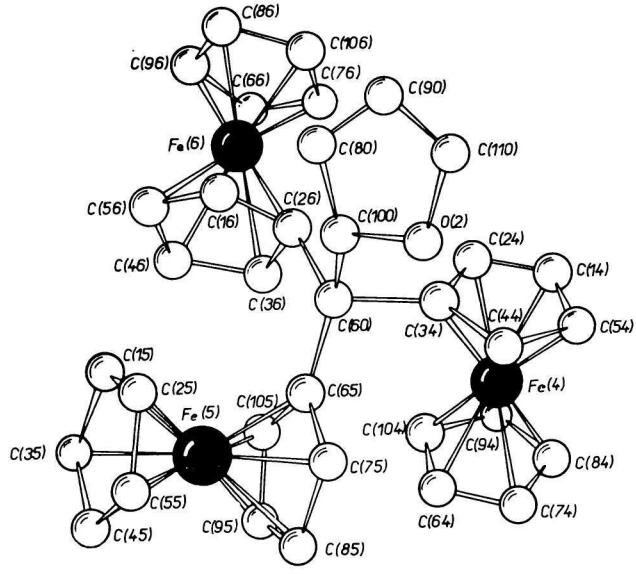
| H | $\|F_o\|$ | $\|F_c\|$ |
|---|---|---|
| 3 | 14.25 | 18.15 |
| 4 | 34.58 | 34.37 |
| $\bar{1}$ | 50.47 | 61.08 |
| $\bar{2}$ | 39.49 | 51.28 |
| $\bar{4}$ | 28.57 | 32.03 |
| | H 8 $\bar{9}$ | |
| 0 | 47.74 | 46.44 |
| 1 | 27.07 | 28.31 |
| 3 | 93.22 | 80.93 |
| $\bar{1}$ | 6.21 | 7.10 |
| $\bar{2}$ | 44.46 | 47.70 |
| $\bar{3}$ | 18.21 | 19.98 |
| | H 9 $\bar{9}$ | |
| 0 | 34.92 | 33.31 |
| 1 | 37.78 | 32.35 |
| $\bar{1}$ | 14.66 | 13.86 |
| | H 0 10 | |
| 0 | 63.63 | 63.60 |
| 1 | 36.76 | 39.96 |
| 2 | 84.56 | 82.95 |
| 3 | 57.76 | 54.31 |
| $\bar{4}$ | 13.64 | 11.74 |
| $\bar{1}$ | 24.96 | 23.54 |
| $\bar{3}$ | 91.45 | 88.96 |
| $\bar{4}$ | 20.19 | 22.25 |
| $\bar{5}$ | 107.55 | 114.80 |
| $\bar{6}$ | 21.55 | 25.97 |
| | H 1 10 | |
| 0 | 83.54 | 85.78 |
| 1 | 36.96 | 36.41 |
| 2 | 52.51 | 52.30 |
| 3 | 8.66 | 10.36 |
| $\bar{4}$ | 16.09 | 15.18 |
| $\bar{1}$ | 24.07 | 21.71 |
| $\bar{2}$ | 73.72 | 77.09 |
| $\bar{3}$ | 30.08 | 33.79 |
| $\bar{4}$ | 44.94 | 45.04 |
| | H 2 10 | |
| 0 | 40.10 | 44.93 |
| 1 | 6.62 | 6.84 |
| 2 | 12.96 | 11.00 |
| 3 | 58.17 | 56.18 |
| $\bar{4}$ | 40.99 | 37.71 |
| $\bar{1}$ | 6.41 | 10.26 |
| $\bar{2}$ | 64.45 | 65.45 |
| $\bar{3}$ | 21.62 | 18.79 |
| $\bar{4}$ | 19.85 | 20.06 |
| $\bar{5}$ | 41.46 | 40.38 |
| | H 3 10 | |
| 1 | 17.46 | 15.24 |
| 2 | 8.59 | 7.33 |
| 3 | 40.17 | 40.14 |
| $\bar{1}$ | 26.05 | 22.44 |
| $\bar{2}$ | 43.78 | 45.59 |
| $\bar{3}$ | 8.59 | 5.65 |
| $\bar{4}$ | 86.95 | 84.34 |
| $\bar{5}$ | 95.07 | 88.85 |
| | H 4 10 | |
| 0 | 11.12 | 12.31 |
| 1 | 49.44 | 52.02 |
| 2 | 23.94 | 22.65 |

*Table 7* (Continued)

| H | $\lvert F_o \rvert$ | $\lvert F_c \rvert$ |
|---|---|---|
| 2 | 14.87 | 15.45 |
| 3 | 35.26 | 33.16 |
| 4 | 41.12 | 39.38 |
| $\bar{1}$ | 22.98 | 26.31 |
| $\bar{3}$ | 11.46 | 6.66 |
| H 5 10 | | |
| 0 | 50.53 | 52.82 |
| 1 | 32.19 | 34.23 |
| $\bar{2}$ | 36.01 | 35.34 |
| $\bar{1}$ | 17.46 | 18.13 |
| $\bar{2}$ | 46.44 | 43.25 |
| $\bar{3}$ | 52.38 | 45.45 |
| H 6 10 | | |
| 0 | 31.78 | 32.35 |
| 2 | 75.70 | 71.07 |
| H 1 $\bar{10}$ | | |
| 0 | 68.27 | 69.77 |
| 1 | 49.24 | 47.19 |
| 2 | 95.13 | 93.53 |
| 3 | 40.44 | 46.79 |
| 4 | 66.01 | 65.43 |
| 6 | 47.40 | 50.27 |
| $\bar{1}$ | 11.66 | 14.43 |
| $\bar{2}$ | 13.44 | 12.40 |
| $\bar{3}$ | 60.01 | 52.36 |
| $\bar{5}$ | 65.74 | 55.44 |
| H 2 $\bar{10}$ | | |
| 0 | 117.43 | 122.29 |
| 1 | 14.32 | 12.61 |
| 2 | 62.06 | 64.14 |
| 3 | 21.00 | 18.33 |
| $\bar{5}$ | 70.17 | 70.43 |
| $\bar{1}$ | 7.84 | 6.46 |
| $\bar{2}$ | 87.09 | 86.55 |
| $\bar{3}$ | 25.30 | 27.97 |
| $\bar{4}$ | 17.32 | 18.95 |
| $\bar{5}$ | 48.97 | 48.58 |
| H 3 $\bar{10}$ | | |
| 1 | 19.16 | 16.90 |
| 2 | 10.37 | 9.34 |
| 3 | 85.25 | 86.69 |
| $\bar{5}$ | 60.49 | 55.54 |
| $\bar{1}$ | 85.25 | 84.85 |
| $\bar{2}$ | 80.54 | 79.43 |
| $\bar{3}$ | 53.67 | 59.43 |
| $\bar{4}$ | 47.81 | 49.57 |
| $\bar{5}$ | 15.68 | 13.88 |
| H 4 $\bar{10}$ | | |
| 0 | 83.20 | 83.64 |
| 1 | 5.86 | 4.51 |
| 2 | 85.18 | 84.55 |
| 3 | 69.42 | 65.00 |
| 4 | 78.63 | 78.75 |
| 5 | 20.66 | 22.18 |
| $\bar{1}$ | 41.12 | 40.32 |
| $\bar{2}$ | 7.91 | 6.82 |
| $\bar{4}$ | 12.41 | 11.47 |
| H 5 $\bar{10}$ | | |
| 0 | 53.87 | 62.81 |
| 1 | 10.98 | 9.05 |
| 2 | 40.64 | 38.95 |
| 3 | 32.94 | 34.99 |
| $\bar{4}$ | 15.82 | 14.73 |
| $\bar{3}$ | 6.14 | 3.13 |
| $\bar{4}$ | 27.89 | 29.41 |
| H 6 $\bar{10}$ | | |
| 1 | 13.03 | 12.08 |
| 2 | 41.26 | 45.67 |
| 3 | 46.37 | 46.27 |
| $\bar{4}$ | 32.80 | 30.20 |
| $\bar{1}$ | 28.16 | 28.11 |
| $\bar{2}$ | 20.32 | 19.00 |
| $\bar{3}$ | 12.89 | 12.77 |
| $\bar{4}$ | 70.38 | 62.27 |
| H 7 $\bar{10}$ | | |
| 0 | 75.02 | 79.64 |
| 1 | 21.62 | 22.83 |
| 2 | 33.21 | 31.25 |
| $\bar{3}$ | 56.88 | 49.79 |
| $\bar{1}$ | 21.00 | 22.61 |
| $\bar{2}$ | 48.90 | 48.73 |
| $\bar{3}$ | 52.51 | 49.43 |
| H 8 $\bar{10}$ | | |
| 0 | 24.41 | 22.69 |
| 1 | 29.19 | 26.75 |
| $\bar{1}$ | 30.21 | 34.40 |
| $\bar{2}$ | 50.19 | 52.73 |
| H 0 11 | | |
| 1 | 102.29 | 104.61 |
| 2 | 21.14 | 19.03 |
| 3 | 91.86 | 87.25 |
| $\bar{4}$ | 14.39 | 10.66 |
| $\bar{2}$ | 29.80 | 25.99 |
| $\bar{3}$ | 18.14 | 14.38 |
| $\bar{4}$ | 64.45 | 65.38 |
| $\bar{5}$ | 34.44 | 28.22 |
| H 1 11 | | |
| 1 | 55.17 | 57.02 |
| 2 | 44.46 | 49.30 |
| $\bar{3}$ | 17.87 | 16.69 |
| $\bar{1}$ | 39.90 | 41.32 |
| $\bar{2}$ | 102.98 | 112.98 |
| $\bar{3}$ | 36.35 | 35.46 |
| $\bar{4}$ | 25.51 | 24.06 |
| H 2 11 | | |
| 0 | 24.55 | 23.47 |
| 1 | 39.55 | 40.14 |
| 2 | 18.48 | 19.07 |
| $\bar{3}$ | 28.57 | 25.81 |
| $\bar{1}$ | 34.37 | 33.53 |
| $\bar{2}$ | 8.66 | 10.35 |
| 4 | 53.60 | 66.87 |
| H 3 11 | | |
| 0 | 44.74 | 45.22 |
| 1 | 9.48 | 11.02 |
| 2 | 35.60 | 39.58 |
| $\bar{2}$ | 32.80 | 29.86 |
| $\bar{4}$ | 67.86 | 67.52 |
| H 4 11 | | |
| $\bar{1}$ | 56.13 | 58.00 |
| $\bar{1}$ | 39.83 | 40.13 |
| $\bar{2}$ | 53.47 | 51.39 |
| $\bar{3}$ | 25.51 | 26.47 |
| H 1 $\bar{11}$ | | |
| 1 | 19.85 | 0.60 |
| 2 | 29.46 | 35.80 |
| 4 | 22.23 | 24.90 |
| $\bar{1}$ | 54.42 | 54.36 |
| $\bar{3}$ | 72.70 | 68.71 |
| $\bar{4}$ | 17.19 | 13.83 |
| H 2 $\bar{11}$ | | |
| 0 | 50.06 | 48.82 |
| 1 | 20.66 | 21.29 |
| 2 | 60.90 | 63.15 |
| 3 | 41.46 | 44.87 |
| 4 | 9.34 | 9.06 |
| $\bar{1}$ | 36.28 | 36.73 |
| $\bar{2}$ | 9.68 | 12.07 |
| $\bar{3}$ | 28.98 | 26.22 |
| $\bar{4}$ | 58.24 | 52.70 |
| H 3 $\bar{11}$ | | |
| 0 | 60.15 | 59.39 |
| 1 | 45.62 | 45.86 |
| 2 | 30.48 | 33.76 |
| 3 | 8.93 | 8.04 |
| 4 | 82.31 | 79.78 |
| $\bar{1}$ | 60.42 | 66.17 |
| $\bar{2}$ | 16.23 | 15.94 |
| $\bar{3}$ | 62.47 | 53.23 |
| $\bar{4}$ | 19.23 | 18.92 |
| H 4 $\bar{11}$ | | |
| 0 | 27.76 | 30.06 |
| 1 | 48.90 | 46.76 |
| 2 | 55.31 | 51.23 |
| $\bar{4}$ | 10.71 | 8.66 |
| $\bar{1}$ | 27.07 | 33.47 |
| $\bar{2}$ | 10.30 | 14.00 |
| $\bar{3}$ | 24.21 | 28.14 |
| $\bar{4}$ | 9.75 | 10.39 |
| H 5 $\bar{11}$ | | |
| 0 | 39.08 | 43.18 |
| 1 | 39.28 | 40.84 |
| 2 | 74.47 | 72.42 |
| 3 | 24.01 | 29.13 |
| $\bar{4}$ | 8.05 | 2.91 |
| $\bar{1}$ | 15.68 | 11.90 |
| $\bar{2}$ | 23.80 | 27.44 |
| $\bar{3}$ | 29.53 | 26.36 |
| H 6 $\bar{11}$ | | |
| 0 | 55.65 | 56.57 |
| 1 | 60.97 | 63.95 |
| 2 | 8.80 | 8.74 |
| 3 | 6.55 | 6.62 |
| $\bar{1}$ | 20.12 | 20.12 |
| $\bar{2}$ | 33.14 | 36.28 |
| $\bar{3}$ | 79.04 | 75.52 |
| H 7 $\bar{11}$ | | |
| 0 | 19.98 | 21.35 |
| 1 | 48.21 | 48.99 |
| 2 | 88.86 | 84.52 |
| $\bar{1}$ | 23.12 | 26.10 |
| $\bar{2}$ | 19.64 | 26.10 |
| H 0 12 | | |
| 0 | 48.08 | 58.81 |
| 1 | 14.39 | 15.19 |
| 2 | 22.98 | 22.91 |
| $\bar{1}$ | 49.31 | 49.88 |
| $\bar{3}$ | 28.30 | 29.14 |
| $\bar{4}$ | 33.89 | 33.72 |
| H 1 12 | | |
| 0 | 20.39 | 22.64 |
| $\bar{1}$ | 66.36 | 70.59 |
| $\bar{3}$ | 33.76 | 32.91 |
| H 2 12 | | |
| 1 | 58.65 | 57.43 |
| $\bar{1}$ | 15.55 | 18.76 |
| $\bar{3}$ | 61.85 | 63.36 |
| H 3 12 | | |
| 0 | 14.59 | 26.04 |
| $\bar{1}$ | 61.24 | 60.04 |
| $\bar{2}$ | 45.15 | 42.34 |
| H 1 $\bar{12}$ | | |
| 0 | 68.06 | 70.45 |
| 2 | 10.78 | 12.30 |
| 3 | 37.58 | 39.46 |
| 4 | 21.48 | 19.23 |
| $\bar{1}$ | 78.97 | 75.69 |
| $\bar{2}$ | 23.46 | 24.37 |
| $\bar{3}$ | 42.83 | 43.50 |
| H 2 $\bar{12}$ | | |
| 0 | 12.55 | 17.43 |
| 1 | 116.21 | 115.43 |
| 2 | 19.37 | 23.52 |
| 3 | 27.82 | 24.72 |
| 4 | 73.86 | 75.35 |
| $\bar{1}$ | 25.64 | 25.75 |
| $\bar{2}$ | 47.94 | 41.90 |
| $\bar{3}$ | 39.76 | 38.09 |
| H 3 $\bar{12}$ | | |
| 0 | 30.89 | 34.15 |
| 1 | 45.62 | 44.74 |
| 2 | 20.66 | 25.63 |
| $\bar{3}$ | 10.16 | 11.84 |
| $\bar{1}$ | 65.88 | 59.28 |
| $\bar{2}$ | 11.46 | 13.50 |
| $\bar{3}$ | 23.39 | 20.30 |
| H 4 $\bar{12}$ | | |
| $\bar{1}$ | 20.25 | 19.24 |
| $\bar{1}$ | 60.83 | 61.54 |
| H 5 $\bar{12}$ | | |
| 0 | 12.34 | 16.22 |
| $\bar{1}$ | 52.51 | 50.81 |
| $\bar{1}$ | 9.82 | 9.74 |
| $\bar{2}$ | 78.77 | 77.01 |
| H 6 $\bar{12}$ | | |
| 0 | 14.53 | 15.01 |
| $\bar{1}$ | 30.55 | 29.38 |
| $\bar{1}$ | 83.81 | 87.22 |
| H 0 $\bar{13}$ | | |
| 0 | 13.71 | 20.85 |
| 2 | 24.55 | 20.72 |
| H 1 $\bar{13}$ | | |
| 1 | 106.05 | 105.34 |
| 2 | 52.58 | 50.56 |
| H 2 $\bar{13}$ | | |
| 1 | 19.37 | 22.48 |
| 2 | 39.69 | 42.68 |
| H 3 $\bar{13}$ | | |
| 2 | 24.69 | 19.99 |




*a*




*b*

*Fig. 1.* Atomic arrangement in the trisferrocenyl complex $(C_{10}H_9Fe)_3C(C_4OH_7)$. Two independent molecules of the unit cell are represented with the central carbon atom C(10) (*a*) and C(60) (*b*), respectively.

*Table 8*

The least-squares planes through the rings and deviations of the ring atoms from the plane

| The least-square plane | Atom | Deviation (Å) |
|---|---|---|
| | C(11) | 0.001 |
| $B = 0.03882$ | C(21) | 0.008 |
| $C = 0.02681$ | C(31) | 0.014 |
| $D = 2.12512$ | C(41) | 0.015 |
| | C(51) | 0.010 |
| | Fe(1) | 1.660 |
| | C(61) | 0.006 |
| $B = 0.09335$ | C(71) | 0.014 |
| $C = -0.01082$ | C(81) | 0.017 |
| $D = 1.12476$ | C(91) | 0.014 |
| | C(101) | 0.004 |
| | Fe(1) | 1.658 |
| | C(12) | 0.001 |
| $B = -2.27579$ | C(22) | 0.010 |
| $C = 0.57907$ | C(32) | 0.016 |
| $D = -8.97878$ | C(42) | 0.017 |
| | C(52) | 0.010 |
| | Fe(2) | 1.648 |
| | C(62) | 0.017 |
| $B = -1.80507$ | C(72) | 0.016 |
| $C = 0.53057$ | C(82) | 0.001 |
| $D = -0.98985$ | C(92) | 0.009 |
| | C(102) | 0.010 |
| | Fe(2) | 1.655 |
| | C(13) | 0.024 |
| $B = 1.54127$ | C(23) | 0.007 |
| $C = 1.10639$ | C(33) | 0.012 |
| $D = -20.09418$ | C(43) | 0.023 |
| | C(53) | 0.029 |
| | Fe(3) | 1.607 |
| | C(63) | 0.010 |
| $B = 1.50117$ | C(73) | 0.006 |
| $C = 1.50776$ | C(83) | 0.001 |
| $D = -33.39765$ | C(93) | 0.008 |
| | C(103) | 0.011 |
| | Fe(3) | 1.616 |
| | C(14) | 0.004 |
| $B = 0.06832$ | C(24) | 0.002 |
| $C = 0.10458$ | C(34) | 0.001 |
| $D = -4.52267$ | C(44) | 0.004 |
| | C(54) | 0.005 |
| | Fe(4) | 1.658 |
| | C(64) | 0.001 |
| $B = 0.06255$ | C(74) | 0.006 |
| $C = 0.15616$ | C(84) | 0.008 |
| $D = -1.26793$ | C(94) | 0.007 |
| | C(104) | 0.003 |
| | Fe(4) | 1.659 |

*Table 8* (Continued)

| The least-square plane | Atom | Deviation (Å) |
|---|---|---|
| | C(15) | 0.013 |
| $B = -1.69208$ | C(25) | 0.026 |
| $C = 0.39783$ | C(35) | 0.002 |
| $D = 10.18701$ | C(45) | 0.015 |
| | C(55) | 0.026 |
| | Fe(5) | 1.653 |
| | C(65) | 0.018 |
| $B = -1.65044$ | C(75) | 0.023 |
| $C = 0.57011$ | C(85) | 0.021 |
| $D = 15.87818$ | C(95) | 0.012 |
| | C(105) | 0.005 |
| | Fe(5) | 1.654 |
| | C(16) | 0.018 |
| $B = 1.08022$ | C(26) | 0.018 |
| $C = 0.65766$ | C(36) | 0.012 |
| $D = -6.95702$ | C(46) | 0.002 |
| | C(56) | 0.010 |
| | Fe(6) | 1.619 |
| | C(66) | 0.002 |
| $B = 1.16013$ | C(76) | 0.001 |
| $C = 0.90171$ | C(86) | 0.006 |
| $D = -14.18905$ | C(96) | 0.005 |
| | C(106) | 0.005 |
| | Fe(6) | 1.654 |
| | O(1) | 0.013 |
| $B = -1.35176$ | C(20) | 0.030 |
| $C = -0.20962$ | C(40) | 0.144 |
| $D = 4.77750$ | C(50) | 0.262 |
| | C(120) | 0.161 |
| | O(2) | 0.193 |
| $B = -1.73487$ | C(80) | 0.067 |
| $C = 0.98482$ | C(90) | 0.017 |
| $D = 1.96443$ | C(100) | 0.091 |
| | C(110) | 0.152 |

The values of $B$, $C$, $D$ are the coefficients of the best plane $x + By + Cz + D = 0$ with respect to the orthogonal axes $a_0$, $b_0$ and $c_0$. The transformation matrix: the triclinic axes → the orthogonal axes has a form

$$\begin{pmatrix} a \sin\beta & b\cos\psi & 0 \\ 0 & b\cos\varrho & 0 \\ a\cos\beta & b\cos\alpha & c \end{pmatrix}$$

where $\cos\psi = \dfrac{\cos\gamma - \cos\beta\cos\alpha}{\sin\beta}$; $\cos\varrho = (1 - \cos^2\alpha - \cos^2\psi)^{1/2}$.

The Fe atoms were not included in the calculation of the plane.

*Table 9*

Interatomic distances ($\sigma$) and angles showing the ring tilting in the ferrocene groups. $\omega$ is the angle of tilt *i.e.* the angle between the ring normals; $T(a) - T(b)$ is the inter-ring distance between the points of gravities

| | |
|---|---|
| Fe(1)—C(11): 2.09(1) Å | Fe(1)—C(61)*: 2.09(1) Å |
| Fe(1)—C(21): 2.07(1) Å | Fe(1)—C(71): 2.04(1) Å |
| Fe(1)—C(31): 2.04(1) Å | Fe(1)—C(81): 2.05(1) Å |
| Fe(1)—C(41): 2.05(1) Å | Fe(1)—C(91): 2.04(1) Å |
| Fe(1)—C(51): 2.06(1) Å | Fe(1)—C(101): 2.05(1) Å |
| Mean Fe—C: 2.06 Å | Mean Fe—C: 2.05 Å |
| | |
| C(11) ... C(71): 3.35(2) Å | |
| C(21) ... C(81): 3.29(2) Å | $T(a)-T(b)$: 3.34 Å |
| C(31) ... C(91): 3.21(2) Å | $\omega$: 176.2° |
| C(41) ... C(101): 3.34(2) Å | $180-\omega$: 3.8° |
| C(51) ... C(61)*: 3.39(2) Å | |
| | |
| Fe(2)—C(12): 2.03(1) Å | Fe(2)—C(62): 2.04(1) Å |
| Fe(2)—C(22): 2.10(1) Å | Fe(2)—C(72): 2.05(1) Å |
| Fe(2)—C(32): 2.04(1) Å | Fe(2)—C(82): 2.08(1) Å |
| Fe(2)—C(42): 2.07(1) Å | Fe(2)—C(92)*: 2.09(1) Å |
| Fe(2)—C(52): 2.02(2) Å | Fe(2)—C(102): 2.06(1) Å |
| Mean Fe—C: 2.05 Å | Mean Fe—C: 2.06 Å |
| | |
| C(12) ... C(62): 3.23(2) Å | |
| C(22) ... C(72): 3.29(2) Å | $T(a)-T(b)$: 3.31 Å |
| C(32) ... C(92)*: 3.41(2) Å | $\omega$: 174.7° |
| C(42) ... C(82): 3.42(2) Å | $180-\omega$: 5.3° |
| C(52) ... C(102): 3.25(2) Å | |
| | |
| Fe(3)—C(13): 2.01(1) Å | Fe(3)—C(63): 2.02(1) Å |
| Fe(3)—C(23): 2.04(1) Å | Fe(3)—C(73): 2.04(1) Å |
| Fe(3)—C(33): 2.02(1) Å | Fe(3)—C(83): 2.02(1) Å |
| Fe(3)—C(43): 2.02(1) Å | Fe(3)—C(93): 2.02(1) Å |
| Fe(3)—C(53)*: 2.08(1) Å | Fe(3)—C(103): 2.06(1) Å |
| Mean Fe—C: 2.03 Å | Mean Fe—C: 2.03 Å |
| | |
| C(13) ... C(63): 3.25(2) Å | |
| C(23) ... C(73): 3.09(2) Å | $T(a)-T(b)$: 3.22 Å |
| C(33) ... C(83): 3.10(2) Å | $\omega$: 171.1° |
| C(43) ... C(93): 3.27(2) Å | $180-\omega$: 8,9° |
| C(53)*...C(103): 3.46(2) Å | |
| | |
| Fe(4)—C(14): 2.09(1) Å | Fe(4)—C(64): 2.02(1) Å |
| Fe(4)—C(24): 2.04(1) Å | Fe(4)—C(74): 2.03(1) Å |
| Fe(4)—C(34)*: 2.04(1) Å | Fe(4)—C(84): 2.07(1) Å |
| Fe(4)—C(44): 2.10(1) Å | Fe(4)—C(94): 2.05(1) Å |
| Fe(4)—C(54): 2.05(1) Å | Fe(4)—C(104): 2.05(1) Å |
| Mean Fe—C: 2.06 Å | Mean Fe—C: 2.05 Å |
| | |
| C(14) ... C(84): 3.35(2) Å | |
| C(24) ... C(94): 3.40(2) Å | $T(a)-T(b)$: 3.32 Å |
| C(34)*...C(104): 3.40(2) Å | $\omega$: 177.1° |
| C(44) ... C(64): 3.40(2) Å | $180-\omega$: 2.9° |
| C(54) ... C(74): 3.28(2) Å | |

*Table 9* (Continued)

| | |
|---|---|
| Fe(5)—C(15): 2.05(1) Å | Fe(5)—C(65)*: 2.05(1) Å |
| Fe(5)—C(25): 2.08(1) Å | Fe(5)—C(75): 2.07(1) Å |
| Fe(5)—C(35): 2.08(1) Å | Fe(5)—C(85): 2.02(1) Å |
| Fe(5)—C(45): 2.06(1) Å | Fe(5)—C(95): 2.06(1) Å |
| Fe(5)—C(55): 2.02(1) Å | Fe(5)—C(105): 2.08(1) Å |
| Mean Fe—C: 2.06 Å | Mean Fe—C: 2.06 Å |
| C(15) ... C(65)*: 3.38(2) Å | |
| C(25) ... C(75): 3.32(2) Å | $T(a)-T(b)$: 3.31 Å |
| C(35) ... C(105): 3.43(2) Å | $\omega$: 174.9° |
| C(45) ... C(95): 3.34(2) Å | $180-\omega$: 5.1° |
| C(55) ... C(85): 3.19(2) Å | |
| Fe(6)—C(16): 2.05(1) Å | Fe(6)—C(66): 2.02(1) Å |
| Fe(6)—C(26)*: 2.07(1) Å | Fe(6)—C(76): 2.06(1) Å |
| Fe(6)—C(36): 2.02(1) Å | Fe(6)—C(86): 2.01(1) Å |
| Fe(6)—C(46): 2.04(1) Å | Fe(6)—C(96): 2.04(1) Å |
| Fe(6)—C(56): 2.05(1) Å | Fe(6)—C(106): 2.06(1) Å |
| Mean Fe—C: 2.04 Å | Mean Fe—C: 2.04 Å |
| C(16) ... C(86): 3.29(2) Å | |
| C(26)*...C(106): 3.42(2) Å | $T(a)-T(b)$: 3.27 Å |
| C(36) ... C(76): 3.28(2) Å | $\omega$: 173.3° |
| C(46) ... C(66): 3.13(2) Å | $180-\omega$: 6.7° |
| C(56) ... C(96): 3.16(2) Å | |

The carbon atoms indicated by an asterisk (*) are bonded to the central carbon atom C(10) or C(60).

of tilt, *i.e.* the angle between the least-squares planes of the two cyclopentadiene rings is between 2.9 and 8.9°. *Ballhausen* and *Dahl* [10] predicted that the cyclopentadienyl rings in metallocenes could be tilted by as much as 45° without affecting the energy of the metal-ring bonding. The angle of tilt in the $(C_{10}H_9Fe)_3C(C_4OH_7)$ complex is well within this limit. Similar deviation from coplanarity of the two cyclopentadienyl rings has been observed in the crystal structures of α-keto-1,1--trimethyleneferrocene $C_{13}H_{12}OFe$ (8.8°) [11] and 1,1-tetramethyleneferrocene $C_{16}H_{20}Fe$ (23.2°) [12]. α-Keto-1,1-trimethyleneferrocene is a derivative of ferrocene with a two-carbon bridge between the cyclopentadienyl rings, α-keto-1,1-trimethyleneferrocene is a bridged „sandwich" compound with a three-carbon bridge. The shortness of these bridges causes tilting of the two cyclopentadienyl rings so they are no longer parallel as in the parent compound, ferrocene. No such influence would be expected in the complex $(C_{10}H_9Fe)_3C(C_4OH_7)$ where only one cyclopentadienyl ring of the ferrocene group is bonded to the central carbon atom. Table 9 summarizes data on the interatomic distances and angles which show the ring tilting. The steepest decrease of the inter-ring distances is in the direction of C—C bond connecting the ring atom with the central carbon atom. This splaying is indicated by the pairs of C...C distances between the rings (Table 9) (the angle of rotation of one ring with respect to the other about the straight line between the points of gravities of the two cyclopentadienyl rings is rather close to the eclipsed orientation). The largest distances exist between the pairs of those ring atoms where

one atom is attached to the central carbon atom. These distances are: 3.39, 3.41, 3.46, 3.40, 3.38 and 3.42 Å, average distance being 3.41 Å. Average inter-ring distances are shown in Fig. 2.

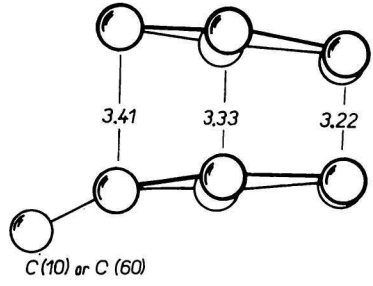



*Fig. 2.* Side view of the ferrocenyl group showing average distances of the ring atoms.

The significant lengthenings of distances between the ring atoms attached to the central atom and their closest neighbours in the opposite rings are probably caused by their mutual repulsion. This repulsion can be explained by the increase of the effective negative charge on the aromatic carbon atoms bonded to the central carbon atoms. The $sp^3$ hybridized central carbon atom cannot withdraw electrons

*Table 10*

Bond lengths (Å) and bond angles around the $sp^3$ hybridized carbon atoms. Deviation $\varepsilon$ of the $\sigma$ bond from the ring plane

| Atoms | Distances ($\sigma$) | Atoms | Angle ($\sigma$) |
|---|---|---|---|
| C(10)—C(61): | 1.53(2) | C(61)—C(10)—C(20): | 110(1)° |
| C(10)—C(92): | 1.51(2) | C(92)—C(10)—C(20): | 109(1)° |
| C(10)—C(53): | 1.57(2) | C(53)—C(10)—C(20): | 109(1)° |
| C(10)—C(20): | 1.59(2) | C(61)—C(10)—C(92): | 111(1)° |
| | | C(53)—C(10)—C(92): | 105(1)° |
| C(60)—C(34): | 1.57(2) | C(61)—C(10)—C(53): | 112(2)° |
| C(60)—C(65): | 1.54(2) | | |
| C(60)—C(26): | 1.55(2) | C(34)—C(60)—C(100): | 111(1)° |
| C(60)—C(100): | 1.58(2) | C(65)—C(60)—C(100): | 109(1)° |
| | | C(26)—C(60)—C(100): | 108(1)° |
| | | C(34)—C(60)—C(65): | 111(1)° |
| | | C(26)—C(60)—C(65): | 104(2)° |
| | | C(34)—C(60)—C(26): | 113(1)° |
| $\varepsilon$(C(10)—C(61)): | 8.3° | | |
| $\varepsilon$(C(10)—C(92)): | 0.2° | | |
| $\varepsilon$(C(10)—C(53)): | 1.2° | | |
| $\varepsilon$(C(60)—C(34)): | 7.1° | | |
| $\varepsilon$(C(60)—C(65)): | 14.7° | | |
| $\varepsilon$(C(60)—C(26)): | 12.9° | | |

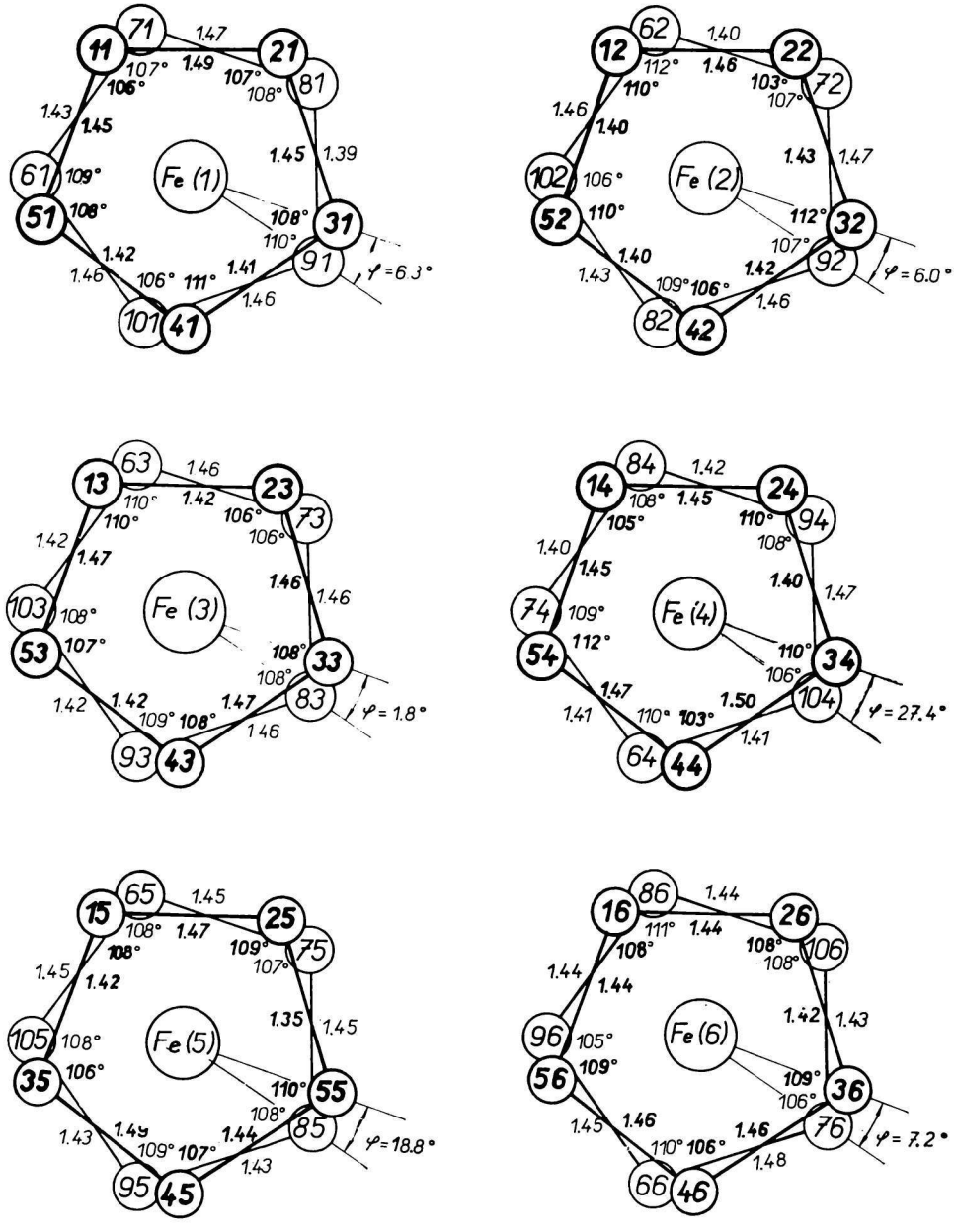



*Fig. 3.* Bond distances and angles in the ferrocenyl groups.
The groups are viewed along the normals to the planes of the rings. Darker numbers refer to the nearer ring. $\varphi$ is the angle of rotation of one ring with respect to the other about the straight line between the points of gravities.

from the aromatic rings since it would lead to the increase of the effective negative charge on the central atom causing instability of the molecular arrangement. The opposite shift of electrons is more probable. In fact, the electron density distribution shows lower peak electron density at the positions of the $sp^3$ hybridized central carbon atoms (about 30%) than the average value of the peak electron density of the ring carbon atoms.

The $\sigma$ bonds between the $sp^2$ ring atoms and $sp^3$ hybridized central carbon atoms show a lengthening from the expected 1.54 Å to 1.56 Å (Table 10). This is only on the border of significance, although it is certainly suggestive. The internal bond angles of the bonds are not significantly different from the tetrahedral angle 109.5° (Table 10). In an unstrained system, the $\sigma$ bonds between the $sp^2$ hybridized ring

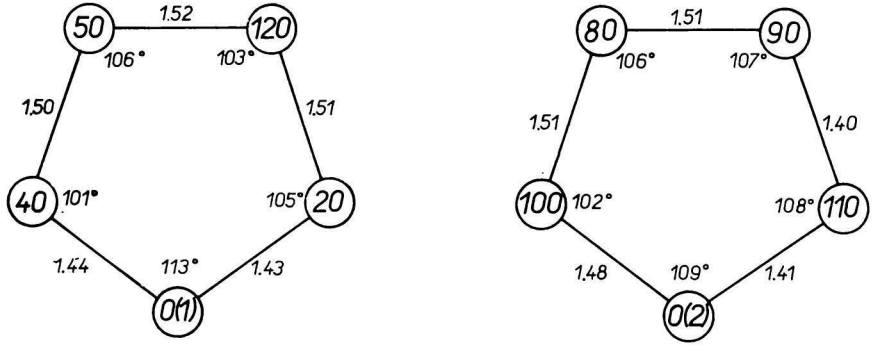



*Fig. 4.* Bond distances and angles in the tetrahydrofuran groups. C atoms are labelled according to Fig. 1.

atoms and $sp^3$ hybridized central carbon atoms, would be coplanar with the rings. There are, however, distortions of the coplanarity between the rings and $\sigma$ bonds probably caused by steric effects of the molecular packing of bulky molecules. Deviations $\varepsilon$ of the $\sigma$ bonds from the ring planes are between 0.2 and 14.7° (Table 10).

The geometry of the rings seems to agree well with the bond lengths and bond angles in 1,1-tetramethylethyleneferrocene [12] and α-keto-1,1-trimethyleneferrocene [11]. The average ring C—C bond length in 1,1-tetramethylferrocene is 1.44 Å and the average Fe—C bond is 2.04 Å; for the α-keto-1,1-trimethyleneferrocene these bonds are 1.43 and 2.04 Å. These values are comparable to the values observed in $(C_{10}H_9Fe)_3C(C_4OH_7)$: 1.44 and 2.05 Å, respectively. The distortions of some bond angles in the rings from 108° are not considered to be significant. The data on the ring geometry are summarized in Fig. 3. Average bond angle is 108°. Fig. 4 represents tetrahydrofuran groups. The assumed positions of the hydrogene atoms are not included in the calculated distances and angles.

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