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THE CRYSTAL AND MOLECULAR STRUCTURE OF TETRAPHENYLARSONIUM CIS-DIOAQUOTETRACHLORO RUTHENATE MONOHYDRATE

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# THE CRYSTAL AND MOLECULAR STRUCTURE OF TETRAPHENYLARSONIUM CIS-DIAQUOTETRACHLORO RUTHENATE MONOHYDRATE

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# The Crystal and Molecular Structure of Tetraphenylarsonium cis-Diaquotetrachloro Ruthenate Monohydrate [1]

BY TED E. HOPKINS, ALLAN ZALKIN, DAVID H. TEMPLETON, AND MARTYN G. ADAMSON

X-ray diffraction study of a single crystal of $(C_6H_5)_4As\ Ru\ Cl_4(H_2O)_2 \cdot H_2O$ showed that it is monoclinic with $\underline{a}$ = 15.059 Å, $\underline{b}$ = 16.711 Å, $\underline{c}$ = 10.996 Å, $\beta$ = 99.88°, $\underline{D}_{\underline{x}}$ = 1.619 g cm$^{-3}$. The space group is $\underline{P2_1/n}$ amd there are four formula units per unit cell. The ruthenium is surrounded by an octahedron composed of the four chlorine atoms and two water molecules. A cis-configuration was found for the waters in the octahedron. The average Ru - O and Ru - Cl distances are 2.12 Å and 2.34 Å. An unsymmetrical configuration was found for the tetraphenylarsonium ion, with an average As- C bond length of 1.91 Å.

## INTRODUCTION

In the course of a series of studies of aqueous ruthenium species by Professor Connick and others at this laboratory, a number of ruthenium salts have been prepared. We have determined the crystal structure of a cesium aquopentachlororuthenate, and of a hexachlororuthenate [2]. The diaquochloro complex is interesting because of the possibility for cis-trans isomers. When it was found that single crystals of the complex could be obtained using the tetraphenylarsonium cation, the structure determination was undertaken to determine the configuration of the ruthenium complex.

## EXPERIMENTAL

A solution of chlororuthenate species containing a high proportion of the complex ion $RuCl_4(H_2O)_2^-$ was prepared by shaking a solution of 0.1 M ruthenium (III) in 2.5 M hydrochloric acid with clean mercury and allowing the Ru (III) solution to stand over the mercury for several hours. After the solution was separated from the mercury, it was filtered and sufficient aqueous tetraphenylarsonium chloride solution (0.3M) was added, dropwise with stirring, to give equimolar amounts of $AsPh_4^+$ and Ru (III). On standing at $0^\circ$ for 48 hours, the solution yielded a number of fairly large ruby-red prisms which were collected on a filter pad, washed well with ice-cold water, and finally dried over "anhydrone" in an evacuated desiccator.

The nature of the anion in this salt was shown to be exclusively one isomer of the complex. This was done by carrying out ion exchange and spectral analysis on a freshly prepared solution of the salt in 1 M hydrochloric acid at $0^\circ$. Study of the aqueous complexes will be reported elsewhere [3,4].

The preliminary determination of the space group and cell dimensions was made using the Weissenberg technique and copper radiation. A single crystal roughly cubic in shape with dimensions 0.15 x 0.17 x 0.18 mm was used. The crystal was mounted for rotation around the b axis. The cell dimensions and intensities were measured with a General Electric XRD-5 diffractometer with a scintillation counter, pulse height discriminator and a quarter circle Eulerian cradle goniostat. A molybdenum tube was used, operated at 50 KV and 20 ma, with a Zr filter used at the receiving slit. The wavelength of Mo $K\alpha_1$ was taken as 0.70926 Å.

There are 2731 independent reflections permitted within the sphere of reflection for $\sin \theta/\lambda < 0.494$ ($2\theta < 41^\circ$). The intensities were measured by taking 10 second counts, with the crystal stationary. No correction was made for either absorption or extinction. The calculated linear absorption coefficient is $\mu = 22.4\ cm^{-1}$ for molybdenum radiation. For this crystal, then, $\mu R \sim 0.2$.

Calculations were made using a IBM 7044 computer, and in the last stages of the least squares refinement when it was desired to increase the number of parameters, a CDC 6600 computer was used. The programs used were the Fourier and distance programs written by Zalkin, and our version (unpublished) of the Gantzel-Sparks-Trueblood full-matrix least squares program which minimizes $\sum w(|F_o| - |F_c|)^2/\sum w|F_o|^2$. $F_o$ and $F_c$ are the observed and calculated structure factors, and the weights, $w$, were all taken as unity. The atomic scattering factors were chosen as follows: As neutral, Ru +3, values taken from Thomas and Umeda[5], Cl -1, and neutral O, C, H from the International Tables[6].

Corrections for the real part of the anomalous dispersion ($\Delta f'$) were made for arsenic, ruthenium and chlorine by adding +0.1, -1.3 and +0.1, respectively, to their atomic scattering functions[7].

## UNIT CELL AND SPACE GROUP

The primitive cell contains four formula units of $(C_6H_5)_4As\ RuCl_4(H_2O)\cdot H_2O$. It is monoclinic with dimensions

$$a = 15.059 \pm 0.005,\ b = 16.711 \pm 0.005\ \ c = 10.996 \pm 0.005\ \text{Å}$$

$$\beta = 99.88 \pm 0.01^{\circ}.$$

The calculated density is 1.619 g $cm^{-3}$, and a rough measurement gave 1.7 g $cm^{-3}$.

The Weissenberg photographs showed the following reflection restrictions: $h0\ell$: $h + \ell = 2n$. Measurements with the goniostat confirmed this observation and the restriction $0k0$: $k = 2n$ was observed. These conditions correspond to space group $P2_1/n$. The observed and calculated structure factor magnitudes are given in Table I.

## DETERMINATION OF THE STRUCTURE

A three dimensional Patterson function was calculated from which the Ru-Ru, Ru-Cl and Ru-As vectors were identified. After several series of least squares refinements and adjustments of the structure, the R factor was 27%. A three dimensional Fourier was then calculated from which all of the carbon atoms were located, as well as an additional molecule of water. All of the atoms are in general positions:

$$4(e):\ \pm(x, y, z;\ 1/2 - x, 1/2 + y, 1/2 - z).$$

The isotropic thermal paramaters had the form $\exp(-B\ \lambda^{-2}\sin^2\theta)$. The anisotropic thermal paramaters were introduced in the form

Table I. Observed and Calculated Structure Factors (X 1.0) for

$(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$.

H,K= 0, 0

| L | FOB | FCA |
|---|---|---|
| 2 | 336 | -344 |
| 4 | 69 | 88 |
| 6 | 140 | -147 |
| 8 | 76 | 79 |
| 10 | 45 | -48 |

H,K= 0, 1

| L | FOB | FCA |
|---|---|---|
| 1 | 37 | -35 |
| 2 | 20 | 16 |
| 3 | 106 | 111 |
| 4 | 68 | -81 |
| 5 | 92 | -85 |
| 6 | 21 | 14 |
| 7 | 37 | 40 |
| 8 | 27 | 27 |
| 9 | 76 | -82 |
| 10 | 31 | -28 |

H,K= 0, 2

| L | FOB | FCA |
|---|---|---|
| -0 | 309 | 304 |
| 1 | 180 | 180 |
| 2 | 286 | -285 |
| 3 | 42 | -50 |
| 4 | 130 | 128 |
| 5 | 41 | 37 |
| 6 | 118 | -120 |
| 7 | 66 | -62 |
| 8 | 70 | 68 |
| 9 | 32 | 30 |
| 10 | 53 | -52 |

H,K= 0, 3

| L | FOB | FCA |
|---|---|---|
| 1 | 6 | 13 |
| 2 | 0 | -1 |
| 3 | 48 | -45 |
| 4 | 8 | 9 |
| 5 | 48 | -46 |
| 6 | 10 | -14 |
| 7 | 29 | 29 |
| 8 | 55 | 54 |
| 9 | 21 | -21 |
| 10 | 45 | -46 |

H,K= 0, 4

| L | FOB | FCA |
|---|---|---|
| -0 | 69 | -75 |
| 1 | 216 | 211 |
| 2 | 38 | 35 |
| 3 | 99 | -97 |
| 4 | 115 | 117 |
| 5 | 85 | 85 |
| 6 | 114 | -118 |
| 7 | 77 | -76 |
| 8 | 23 | 24 |
| 9 | 54 | 50 |
| 10 | 13 | -14 |

H,K= 0, 5

| L | FOB | FCA |
|---|---|---|
| 1 | 125 | 131 |
| 2 | 109 | -115 |
| 3 | 47 | -50 |
| 4 | 57 | 57 |
| 5 | 13 | -14 |
| 6 | 35 | -39 |
| 7 | 14 | 6 |
| 8 | 31 | 27 |
| 9 | 10 | -3 |
| 10 | 8 | -6 |

H,K= 0, 6

| L | FOB | FCA |
|---|---|---|
| -0 | 41 | -33 |
| 1 | 0 | 8 |
| 2 | 32 | 26 |
| 3 | 76 | -84 |
| 4 | 0 | 3 |
| 5 | 46 | 48 |
| 6 | 61 | -60 |
| 7 | 34 | -28 |
| 8 | 12 | -16 |
| 9 | 43 | 39 |

H,K= 0, 7

| L | FOB | FCA |
|---|---|---|
| 1 | 51 | 54 |
| 2 | 44 | -52 |
| 3 | 48 | -45 |
| 4 | 16 | -13 |
| 5 | 26 | 21 |
| 6 | 11 | 8 |
| 7 | 12 | -14 |
| 8 | 7 | -5 |
| 9 | 17 | 17 |

H,K= 0, 8

| L | FOB | FCA |
|---|---|---|
| -0 | 56 | 57 |
| 1 | 15 | -10 |
| 2 | 15 | 6 |
| 3 | 10 | -2 |
| 4 | 15 | -16 |
| 5 | 9 | 6 |
| 6 | 6 | -10 |
| 7 | 7 | 6 |
| 8 | 0 | 6 |
| 9 | 8 | 6 |

H,K= 0, 9

| L | FOB | FCA |
|---|---|---|
| 1 | 20 | -17 |
| 2 | 18 | 17 |
| 3 | 45 | 50 |
| 4 | 58 | -56 |
| 5 | 21 | -19 |
| 6 | 0 | 5 |
| 7 | 24 | -29 |
| 8 | 0 | 1 |

H,K= 0,10

| L | FOB | FCA |
|---|---|---|
| -0 | 82 | 83 |
| 1 | 14 | -10 |
| 2 | 42 | -42 |
| 3 | 6 | -4 |
| 4 | 16 | 20 |
| 5 | 15 | 18 |
| 6 | 55 | -56 |
| 7 | 19 | -19 |
| 8 | 30 | 31 |

H,K= 0,11

| L | FOB | FCA |
|---|---|---|
| 1 | 9 | -11 |
| 2 | 0 | 3 |
| 3 | 55 | 56 |
| 4 | 15 | -16 |
| 5 | 71 | -72 |
| 6 | 10 | -4 |
| 7 | 7 | -2 |

H,K= 0,12

| L | FOB | FCA |
|---|---|---|
| -0 | 52 | 49 |
| 1 | 0 | -1 |
| 2 | 57 | -57 |
| 3 | 48 | -47 |
| 4 | 82 | 83 |
| 5 | 66 | 68 |
| 6 | 34 | -41 |
| 7 | 36 | -37 |

H,K= 0,13

| L | FOB | FCA |
|---|---|---|
| 1 | 10 | 8 |
| 2 | 37 | -33 |
| 3 | 14 | 8 |
| 4 | 31 | 29 |
| 5 | 13 | -20 |
| 6 | 20 | -19 |

H,K= 0,14

| L | FOB | FCA |
|---|---|---|
| -0 | 48 | 49 |
| 1 | 66 | 71 |
| 2 | 34 | -41 |
| 3 | 90 | -90 |
| 4 | 25 | 28 |
| 5 | 42 | 47 |

H,K= 0,15

| L | FOB | FCA |
|---|---|---|
| 1 | 10 | 6 |
| 2 | 34 | -33 |
| 3 | 11 | -15 |
| 4 | 15 | 17 |

H,K= 0,16

| L | FOB | FCA |
|---|---|---|
| -0 | 11 | 3 |
| 1 | 97 | 100 |
| 2 | 13 | 9 |

H,K= 1, 0

| L | FOB | FCA |
|---|---|---|
| -9 | 23 | 30 |
| -7 | 0 | -9 |
| -5 | 0 | -10 |
| -3 | 33 | 24 |
| -1 | 101 | -107 |
| 1 | 129 | 128 |
| 3 | 135 | -116 |
| 5 | 99 | 95 |
| 7 | 111 | -114 |
| 9 | 39 | 40 |

H,K= 1, 1

| L | FOB | FCA |
|---|---|---|
| -10 | 13 | -14 |
| -9 | 20 | 15 |
| -8 | 21 | 17 |
| -7 | 22 | -21 |
| -6 | 28 | 25 |
| -5 | 9 | -9 |
| -4 | 164 | -164 |
| -3 | 45 | 38 |
| -2 | 6 | -9 |
| -1 | 37 | 37 |
| -0 | 136 | 126 |
| 1 | 34 | -25 |
| 2 | 52 | -60 |
| 3 | 44 | -40 |
| 4 | 76 | 80 |
| 5 | 11 | -12 |
| 6 | 40 | -47 |
| 7 | 49 | 51 |
| 8 | 0 | -2 |
| 9 | 0 | -1 |
| 10 | 50 | -49 |

H,K= 1, 2

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | 3 |
| -9 | 14 | -18 |
| -8 | 33 | -30 |
| -7 | 14 | 15 |
| -6 | 6 | 4 |
| -5 | 47 | -50 |
| -4 | 83 | 83 |
| -3 | 40 | 38 |
| -2 | 104 | -109 |
| -1 | 45 | -46 |
| -0 | 78 | -67 |
| 1 | 75 | 79 |
| 2 | 84 | -69 |
| 3 | 58 | 63 |
| 4 | 47 | -51 |
| 5 | 40 | 39 |
| 6 | 55 | 53 |
| 7 | 51 | -52 |
| 8 | 30 | -26 |
| 9 | 0 | 5 |
| 10 | 0 | 9 |

H,K= 1, 3

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -7 |
| -9 | 14 | 10 |
| -8 | 65 | 65 |
| -7 | 11 | -7 |
| -6 | 150 | -153 |
| -5 | 35 | 31 |
| -4 | 44 | 50 |
| -3 | 49 | -51 |
| -2 | 62 | -72 |
| -1 | 102 | 97 |
| -0 | 223 | 204 |
| 1 | 79 | -68 |
| 2 | 35 | -30 |
| 3 | 9 | 10 |
| 4 | 120 | 122 |
| 5 | 7 | -4 |
| 6 | 108 | -114 |
| 7 | 0 | 7 |
| 8 | 43 | 40 |
| 9 | 0 | -5 |
| 10 | 45 | -40 |

H,K= 1, 4

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -4 |
| -9 | 34 | -37 |
| -8 | 7 | 4 |
| -7 | 61 | 63 |
| -6 | 34 | -31 |
| -5 | 65 | -70 |
| -4 | 43 | -40 |
| -3 | 6 | 8 |
| -2 | 104 | 107 |
| -1 | 8 | 11 |
| -0 | 23 | 18 |
| 1 | 18 | -9 |
| 2 | 12 | 14 |
| 3 | 17 | 19 |
| 4 | 48 | -42 |
| 5 | 48 | -51 |
| 6 | 14 | 11 |
| 7 | 44 | 44 |
| 8 | 45 | -45 |
| 9 | 49 | -45 |
| 10 | 34 | 33 |

H,K= 1, 5

| L | FOB | FCA |
|---|---|---|
| -10 | 13 | -14 |
| -9 | 14 | -16 |
| -8 | 76 | 77 |
| -7 | 47 | 54 |
| -6 | 154 | -158 |
| -5 | 13 | -13 |
| -4 | 161 | 164 |
| -3 | 65 | -62 |
| -2 | 150 | -165 |
| -1 | 61 | 54 |
| -0 | 187 | 176 |
| 1 | 64 | 55 |
| 2 | 119 | -113 |
| 3 | 41 | 34 |
| 4 | 134 | 131 |
| 5 | 43 | 41 |
| 6 | 151 | -157 |
| 7 | 30 | -30 |
| 8 | 64 | 67 |
| 9 | 41 | 38 |
| 10 | 22 | -24 |

H,K= 1, 6

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -4 |
| -9 | 34 | -37 |
| -8 | 0 | -7 |
| -7 | 49 | 49 |
| -6 | 6 | 5 |
| -5 | 64 | -68 |
| -4 | 63 | -66 |
| -3 | 55 | -64 |
| -2 | 149 | 148 |
| -1 | 84 | 83 |
| -0 | 28 | -10 |
| 1 | 44 | 33 |
| 2 | 110 | -103 |
| 3 | 10 | -8 |
| 4 | 55 | 59 |
| 5 | 49 | -49 |
| 6 | 31 | -28 |
| 7 | 67 | 67 |
| 8 | 0 | -4 |
| 9 | 78 | -80 |

H,K= 1, 7

| L | FOB | FCA |
|---|---|---|
| -9 | 48 | -44 |
| -8 | 45 | 40 |
| -7 | 52 | 55 |
| -6 | 82 | -82 |
| -5 | 78 | -84 |
| -4 | 151 | 152 |
| -3 | 100 | 102 |
| -2 | 225 | -234 |
| -1 | 136 | -137 |
| -0 | 226 | 225 |
| 1 | 106 | 104 |
| 2 | 97 | -95 |
| 3 | 113 | -112 |
| 4 | 135 | 133 |
| 5 | 30 | 36 |
| 6 | 91 | -93 |
| 7 | 47 | -51 |
| 8 | 10 | 10 |
| 9 | 30 | 30 |

H,K= 1, 8

| L | FOB | FCA |
|---|---|---|
| -9 | 13 | -13 |
| -8 | 41 | -38 |
| -7 | 22 | 20 |
| -6 | 6 | 10 |
| -5 | 39 | -39 |
| -4 | 15 | -17 |
| -3 | 26 | -31 |
| -2 | 53 | 46 |
| -1 | 46 | 35 |
| -0 | 76 | 74 |
| 1 | 0 | -6 |
| 2 | 52 | -52 |
| 3 | 56 | 58 |
| 4 | 12 | 10 |
| 5 | 53 | -52 |
| 6 | 61 | -64 |
| 7 | 29 | 34 |
| 8 | 50 | 51 |
| 9 | 51 | -53 |

H,K= 1, 9

| L | FOB | FCA |
|---|---|---|
| -9 | 46 | -43 |
| -8 | 31 | 30 |
| -7 | 46 | 44 |
| -6 | 33 | -28 |
| -5 | 120 | -125 |
| -4 | 64 | 62 |
| -3 | 152 | 160 |
| -2 | 120 | -126 |
| -1 | 155 | -158 |
| -0 | 94 | 84 |
| 1 | 123 | 124 |
| 2 | 51 | -55 |
| 3 | 99 | -105 |
| 4 | 47 | 48 |
| 5 | 89 | 91 |
| 6 | 20 | -19 |
| 7 | 58 | -59 |
| 8 | 8 | 7 |

H,K= 1,10

| L | FOB | FCA |
|---|---|---|
| -8 | 46 | -43 |
| -7 | 16 | -21 |
| -6 | 31 | 34 |
| -5 | 27 | -22 |
| -4 | 13 | 14 |
| -3 | 26 | 25 |
| -2 | 59 | -53 |
| -1 | 30 | -29 |
| -0 | 41 | 36 |
| 1 | 18 | 16 |
| 2 | 10 | 11 |
| 3 | 51 | 53 |
| 4 | 16 | 19 |
| 5 | 28 | -29 |
| 6 | 41 | -46 |
| 7 | 0 | -4 |
| 8 | 69 | 68 |

H,K= 1,11

| L | FOB | FCA |
|---|---|---|
| -8 | 19 | 23 |
| -7 | 59 | 56 |
| -6 | 28 | -28 |
| -5 | 116 | -114 |
| -4 | 40 | -42 |
| -3 | 135 | 138 |
| -2 | 39 | 33 |
| -1 | 75 | -78 |
| -0 | 0 | -0 |
| 1 | 52 | 54 |
| 2 | 31 | 31 |
| 3 | 87 | -89 |
| 4 | 16 | -17 |
| 5 | 73 | 74 |
| 6 | 0 | -3 |
| 7 | 65 | -60 |

H,K= 1,12

| L | FOB | FCA |
|---|---|---|
| -7 | 11 | -16 |
| -6 | 24 | 24 |
| -5 | 7 | 6 |
| -4 | 0 | -0 |
| -3 | 24 | 16 |
| -2 | 11 | 30 |
| -1 | 37 | -32 |
| -0 | 17 | 15 |
| 1 | 45 | 42 |
| 2 | 25 | -21 |
| 3 | 13 | 0 |
| 4 | 0 | -0 |
| 5 | 16 | 9 |
| 6 | 42 | -45 |
| 7 | 36 | -42 |

H,K= 1,13

| L | FOB | FCA |
|---|---|---|
| -6 | 8 | 5 |
| -5 | 35 | -38 |
| -4 | 32 | -32 |
| -3 | 53 | 53 |
| -2 | 49 | 49 |
| -1 | 32 | -32 |
| -0 | 34 | -35 |
| 1 | 43 | 35 |
| 2 | 14 | 12 |
| 3 | 35 | -37 |
| 4 | 16 | -21 |
| 5 | 39 | 37 |
| 6 | 0 | 1 |

H,K= 1,14

| L | FOB | FCA |
|---|---|---|
| -5 | 0 | 3 |
| -4 | 30 | -29 |
| -3 | 13 | -9 |
| -2 | 40 | 38 |
| -1 | 16 | -8 |
| -0 | 21 | -20 |
| 1 | 38 | 35 |
| 2 | 0 | 2 |
| 3 | 28 | -29 |
| 4 | 7 | -8 |
| 5 | 26 | 30 |

H,K= 1,15

| L | FOB | FCA |
|---|---|---|
| -4 | 0 | -4 |
| -3 | 8 | -12 |
| -2 | 7 | 7 |
| -1 | 20 | -22 |
| -0 | 13 | -12 |
| 1 | 56 | 54 |
| 2 | 7 | 5 |
| 3 | 24 | -23 |
| 4 | 8 | 11 |

H,K= 1,16

| L | FOB | FCA |
|---|---|---|
| -2 | 26 | 25 |
| -1 | 8 | 6 |
| -0 | 23 | -25 |
| 1 | 19 | 6 |
| 2 | 11 | 15 |

H,K= 2, 0

| L | FOB | FCA |
|---|---|---|
| -10 | 70 | -68 |
| -8 | 135 | 137 |
| -6 | 169 | -167 |
| -4 | 51 | 53 |
| -2 | 271 | -275 |
| -0 | 281 | 286 |
| 2 | 266 | -280 |
| 4 | 152 | 157 |
| 6 | 14 | 11 |
| 8 | 44 | -46 |
| 10 | 51 | -49 |

H,K= 2, 1

| L | FOB | FCA |
|---|---|---|
| -10 | 29 | 27 |
| -9 | 39 | -40 |
| -8 | 30 | -29 |
| -7 | 15 | 14 |
| -6 | 39 | -39 |
| -5 | 40 | 38 |
| -4 | 64 | 68 |
| -3 | 92 | -90 |
| -2 | 71 | 58 |
| -1 | 52 | 44 |
| -0 | 87 | 79 |
| 1 | 59 | -47 |
| 2 | 79 | 78 |
| 3 | 146 | 151 |
| 4 | 13 | -11 |
| 5 | 111 | -115 |
| 6 | 28 | -30 |
| 7 | 59 | 56 |
| 8 | 27 | 25 |
| 9 | 24 | -26 |
| 10 | 23 | -22 |

H,K= 2, 2

| L | FOB | FCA |
|---|---|---|
| -10 | 37 | -34 |
| -9 | 33 | -28 |
| -8 | 125 | 120 |
| -7 | 61 | 58 |
| -6 | 113 | -119 |
| -5 | 93 | -89 |
| -4 | 86 | 89 |
| -3 | 36 | 37 |
| -2 | 173 | -178 |
| -1 | 51 | -46 |
| -0 | 222 | 210 |
| 1 | 134 | 130 |
| 2 | 141 | -134 |
| 3 | 92 | -98 |
| 4 | 152 | 149 |
| 5 | 38 | 38 |
| 6 | 68 | -73 |
| 7 | 0 | -5 |
| 8 | 22 | 23 |
| 9 | 0 | 9 |
| 10 | 41 | -41 |

H,K= 2, 3

| L | FOB | FCA |
|---|---|---|
| -10 | 32 | 32 |
| -9 | 7 | -9 |
| -8 | 34 | -36 |
| -7 | 69 | 67 |
| -6 | 42 | -39 |
| -5 | 24 | -30 |
| -4 | 90 | 88 |
| -3 | 19 | 15 |
| -2 | 30 | -37 |
| -1 | 114 | -113 |
| -0 | 12 | -2 |
| 1 | 0 | 3 |
| 2 | 26 | -18 |
| 3 | 87 | 84 |
| 4 | 61 | 56 |
| 5 | 19 | 14 |
| 6 | 85 | -84 |
| 7 | 18 | 18 |
| 8 | 54 | 52 |
| 9 | 44 | -47 |
| 10 | 21 | -21 |

H,K= 2, 4

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -5 |
| -9 | 43 | -39 |
| -8 | 46 | 47 |
| -7 | 104 | 103 |
| -6 | 74 | -74 |
| -5 | 147 | -151 |
| -4 | 63 | 67 |
| -3 | 95 | 93 |
| -2 | 186 | -183 |
| -1 | 100 | -92 |
| -0 | 56 | 46 |
| 1 | 28 | 38 |
| 2 | 109 | 96 |
| 3 | 69 | -67 |
| 4 | 132 | 139 |
| 5 | 16 | 17 |
| 6 | 131 | -136 |
| 7 | 25 | -28 |
| 8 | 62 | 58 |
| 9 | 22 | 24 |
| 10 | 44 | -39 |

H,K= 2, 5

| L | FOB | FCA |
|---|---|---|
| -10 | 11 | 11 |
| -9 | 7 | -8 |
| -8 | 0 | 8 |
| -7 | 59 | 61 |
| -6 | 10 | -13 |
| -5 | 128 | -130 |
| -4 | 5 | -10 |
| -3 | 12 | 10 |
| -2 | 108 | 102 |
| -1 | 39 | 36 |
| -0 | 15 | -8 |
| 1 | 60 | 56 |
| 2 | 38 | -39 |
| 3 | 74 | -73 |
| 4 | 100 | 98 |
| 5 | 75 | 79 |
| 6 | 101 | -101 |
| 7 | 37 | -37 |
| 8 | 16 | 17 |
| 9 | 24 | -22 |

H,K= 2, 6

| L | FOB | FCA |
|---|---|---|
| -10 | 13 | 14 |
| -9 | 27 | -27 |
| -8 | 14 | -9 |
| -7 | 38 | 34 |
| -6 | 11 | 5 |
| -5 | 60 | -63 |
| -4 | 0 | 6 |
| -3 | 85 | 89 |
| -2 | 65 | -76 |
| -1 | 83 | -80 |
| -0 | 81 | 77 |
| 1 | 40 | 46 |
| 2 | 7 | 5 |
| 3 | 15 | -15 |
| 4 | 74 | 77 |
| 5 | 57 | 58 |
| 6 | 78 | -81 |
| 7 | 54 | -58 |
| 8 | 44 | 41 |
| 9 | 25 | 27 |

H,K= 2, 7

| L | FOB | FCA |
|---|---|---|
| -9 | 7 | -11 |
| -8 | 7 | -9 |
| -7 | 48 | 49 |
| -6 | 6 | -6 |
| -5 | 70 | -73 |
| -4 | 86 | -87 |
| -3 | 21 | 21 |
| -2 | 105 | 106 |
| -1 | 59 | -54 |
| -0 | 76 | -67 |
| 1 | 53 | 47 |
| 2 | 19 | 17 |
| 3 | 107 | -106 |
| 4 | 6 | -2 |
| 5 | 97 | 97 |
| 6 | 6 | -7 |
| 7 | 53 | -54 |
| 8 | 0 | -3 |
| 9 | 0 | -2 |

H,K= 2, 8

| L | FOB | FCA |
|---|---|---|
| -9 | 0 | 9 |
| -8 | 0 | 1 |
| -7 | 19 | -18 |
| -6 | 29 | 31 |
| -5 | 6 | 5 |
| -4 | 39 | -40 |
| -3 | 40 | 42 |
| -2 | 46 | -53 |
| -1 | 80 | -82 |
| -0 | 54 | 57 |
| 1 | 73 | 70 |
| 2 | 87 | -86 |
| 3 | 44 | -43 |
| 4 | 83 | 87 |
| 5 | 51 | 53 |
| 6 | 18 | -17 |
| 7 | 35 | -36 |
| 8 | 25 | 20 |

H,K= 2, 9

| L | FOB | FCA |
|---|---|---|
| -9 | 0 | 2 |
| -8 | 32 | -33 |
| -7 | 12 | 15 |
| -6 | 38 | 36 |
| -5 | 35 | -38 |
| -4 | 60 | -66 |
| -3 | 39 | 39 |
| -2 | 50 | 49 |
| -1 | 66 | -66 |
| -0 | 15 | -5 |
| 1 | 61 | 55 |
| 2 | 79 | 80 |
| 3 | 17 | 21 |
| 4 | 105 | -103 |
| 5 | 15 | 15 |
| 6 | 34 | 32 |
| 7 | 10 | -11 |
| 8 | 15 | -17 |

H,K= 2,10

| L | FOB | FCA |
|---|---|---|
| -8 | 49 | 45 |
| -7 | 0 | -7 |
| -6 | 36 | -35 |
| -5 | 9 | -7 |
| -4 | 34 | 39 |
| -3 | 32 | 34 |
| -2 | 39 | -39 |
| -1 | 35 | -31 |
| -0 | 62 | 58 |
| 1 | 62 | 63 |
| 2 | 52 | -50 |
| 3 | 32 | -36 |
| 4 | 50 | 48 |
| 5 | 41 | 37 |
| 6 | 21 | -22 |
| 7 | 57 | -57 |
| 8 | 11 | 14 |

H,K= 2,11

| L | FOB | FCA |
|---|---|---|
| -8 | 41 | -40 |
| -7 | 0 | 5 |
| -6 | 21 | 24 |
| -5 | 7 | -6 |
| -4 | 59 | -60 |
| -3 | 11 | 10 |
| -2 | 47 | 46 |
| -1 | 21 | -23 |
| -0 | 19 | -8 |
| 1 | 14 | -5 |
| 2 | 58 | 56 |
| 3 | 77 | 80 |
| 4 | 78 | -78 |
| 5 | 63 | -62 |
| 6 | 10 | 15 |
| 7 | 22 | 21 |

H,K= 2,12

| L | FOB | FCA |
|---|---|---|
| -7 | 19 | 18 |
| -6 | 73 | -73 |
| -5 | 53 | -55 |
| -4 | 57 | 55 |
| -3 | 34 | 38 |
| -2 | 55 | -54 |
| -1 | 13 | -12 |
| -0 | 41 | 39 |
| 1 | 11 | 16 |
| 2 | 39 | -35 |
| 3 | 38 | -39 |
| 4 | 12 | 16 |
| 5 | 48 | 50 |
| 6 | 29 | -30 |

H,K= 2,13

| L | FOB | FCA |
|---|---|---|
| -6 | 15 | 18 |
| -5 | 7 | 13 |
| -4 | 12 | -11 |
| -3 | 47 | -53 |
| -2 | 32 | 27 |
| -1 | 17 | 18 |
| -0 | 15 | -10 |
| 1 | 15 | -16 |
| 2 | 7 | -1 |
| 3 | 53 | 52 |
| 4 | 13 | 11 |
| 5 | 20 | -23 |
| 6 | 0 | -11 |

H,K= 2,14

| L | FOB | FCA |
|---|---|---|
| -5 | 54 | -55 |
| -4 | 30 | 31 |
| -3 | 51 | 52 |
| -2 | 39 | -41 |
| -1 | 41 | -41 |
| -0 | 12 | 9 |
| 1 | 62 | 63 |
| 2 | 7 | -6 |
| 3 | 53 | -55 |
| 4 | 23 | 25 |
| 5 | 30 | 32 |

H,K= 2,15

| L | FOB | FCA |
|---|---|---|
| -4 | 0 | 3 |
| -3 | 29 | -31 |
| -2 | 7 | -7 |
| -1 | 28 | 29 |
| -0 | 26 | 28 |
| 1 | 0 | 0 |
| 2 | 23 | -21 |
| 3 | 11 | -3 |

H,K= 2,16

| L | FOB | FCA |
|---|---|---|
| -2 | 11 | 11 |
| -1 | 69 | -67 |
| -0 | 0 | -3 |
| 1 | 88 | 87 |

H,K= 3, 0

| L | FOB | FCA |
|---|---|---|
| -9 | 87 | -85 |
| -7 | 121 | 123 |
| -5 | 83 | -85 |
| -3 | 62 | 61 |
| -1 | 244 | -255 |
| 1 | 172 | 172 |
| 3 | 115 | -101 |
| 5 | 69 | 66 |
| 7 | 40 | -36 |
| 9 | 7 | 8 |

H,K= 3, 1

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -0 |
| -9 | 20 | 21 |
| -8 | 55 | 54 |
| -7 | 9 | -6 |
| -6 | 10 | -11 |
| -5 | 40 | 41 |
| -4 | 42 | -36 |
| -3 | 7 | -2 |
| -2 | 75 | -85 |
| -1 | 96 | -90 |
| -0 | 264 | 252 |
| 1 | 75 | -66 |
| 2 | 228 | -234 |
| 3 | 22 | -22 |
| 4 | 242 | 243 |
| 5 | 36 | 35 |
| 6 | 77 | -85 |
| 7 | 22 | -22 |
| 8 | 50 | 48 |
| 9 | 0 | -1 |
| 10 | 63 | -63 |

H,K= 3, 2

| L | FOB | FCA |
|---|---|---|
| -10 | 37 | 36 |
| -9 | 52 | -51 |
| -8 | 78 | -77 |
| -7 | 93 | 94 |
| -6 | 64 | 63 |
| -5 | 82 | -78 |
| -4 | 11 | 16 |
| -3 | 66 | 65 |
| -2 | 15 | -9 |
| -1 | 120 | -131 |
| -0 | 38 | -36 |
| 1 | 82 | 83 |
| 2 | 157 | 152 |
| 3 | 56 | -47 |
| 4 | 143 | -142 |
| 5 | 56 | 53 |
| 6 | 56 | 59 |
| 7 | 0 | -6 |
| 8 | 0 | -9 |
| 9 | 0 | 1 |

H,K= 3, 3

| L | FOB | FCA |
|---|---|---|
| -10 | 21 | -18 |
| -9 | 48 | 48 |
| -8 | 82 | 79 |
| -7 | 18 | -15 |
| -6 | 56 | -60 |
| -5 | 0 | -10 |
| -4 | 122 | 120 |
| -3 | 0 | 7 |
| -2 | 202 | -209 |
| -1 | 5 | 8 |
| -0 | 29 | -38 |
| 1 | 95 | 87 |
| 2 | 57 | -57 |
| 3 | 25 | -30 |
| 4 | 178 | 179 |
| 5 | 77 | 78 |
| 6 | 68 | -73 |
| 7 | 55 | -54 |
| 8 | 48 | 48 |
| 9 | 17 | 17 |

H,K= 3, 4

| L | FOB | FCA |
|---|---|---|
| -10 | 34 | 31 |
| -9 | 0 | -5 |
| -8 | 55 | -54 |
| -7 | 58 | 57 |
| -6 | 35 | 36 |
| -5 | 51 | -58 |
| -4 | 107 | -102 |
| -3 | 27 | 29 |
| -2 | 59 | 60 |
| -1 | 9 | -14 |
| -0 | 104 | -99 |
| 1 | 84 | -74 |
| 2 | 233 | 216 |
| 3 | 24 | 24 |
| 4 | 41 | -43 |
| 5 | 6 | -5 |
| 6 | 9 | -8 |
| 7 | 25 | 26 |
| 8 | 26 | -26 |
| 9 | 40 | -37 |

H,K= 3, 5

| L | FOB | FCA |
|---|---|---|
| -10 | 33 | -29 |
| -9 | 10 | 5 |
| -8 | 73 | 71 |
| -7 | 21 | 23 |
| -6 | 90 | -91 |
| -5 | 70 | -69 |
| -4 | 125 | 121 |
| -3 | 5 | 3 |
| -2 | 192 | -193 |
| -1 | 34 | -32 |
| -0 | 52 | 51 |
| 1 | 17 | 18 |
| 2 | 45 | -47 |
| 3 | 88 | -84 |
| 4 | 75 | 80 |
| 5 | 30 | 32 |
| 6 | 53 | -53 |
| 7 | 35 | -35 |
| 8 | 45 | 43 |
| 9 | 41 | 42 |

H,K= 3, 6

| L | FOB | FCA |
|---|---|---|
| -10 | 13 | 15 |
| -9 | 7 | 9 |
| -8 | 0 | 1 |
| -7 | 23 | 23 |
| -6 | 16 | -17 |
| -5 | 0 | 2 |
| -4 | 37 | -35 |
| -3 | 34 | -34 |
| -2 | 90 | 91 |
| -1 | 92 | 84 |
| -0 | 69 | -70 |
| 1 | 103 | -97 |
| 2 | 7 | -3 |
| 3 | 106 | 100 |
| 4 | 10 | 12 |
| 5 | 16 | 15 |
| 6 | 29 | -33 |
| 7 | 45 | 44 |
| 8 | 0 | -3 |
| 9 | 39 | -42 |

H,K= 3, 7

| L | FOB | FCA |
|---|---|---|
| -9 | 36 | -37 |
| -8 | 62 | 61 |
| -7 | 47 | 50 |
| -6 | 28 | -29 |
| -5 | 21 | -25 |
| -4 | 51 | 48 |
| -3 | 84 | 84 |
| -2 | 168 | -166 |
| -1 | 63 | -67 |
| -0 | 108 | 105 |
| 1 | 67 | 67 |
| 2 | 39 | -41 |
| 3 | 40 | -40 |
| 4 | 46 | 46 |
| 5 | 18 | 16 |
| 6 | 9 | -10 |
| 7 | 0 | 1 |
| 8 | 13 | 8 |
| 9 | 27 | 25 |

H,K= 3, 8

| L | FOB | FCA |
|---|---|---|
| -9 | 0 | 4 |
| -8 | 13 | 14 |
| -7 | 0 | 2 |
| -6 | 28 | -28 |
| -5 | 27 | 30 |
| -4 | 10 | 12 |
| -3 | 32 | -29 |
| -2 | 5 | -12 |
| -1 | 12 | -2 |
| -0 | 74 | 69 |
| 1 | 72 | -66 |
| 2 | 26 | -26 |
| 3 | 81 | 76 |
| 4 | 41 | 41 |
| 5 | 13 | -11 |
| 6 | 34 | -33 |
| 7 | 0 | 7 |
| 8 | 0 | 1 |

H,K= 3, 9

| L | FOB | FCA |
|---|---|---|
| -9 | 42 | -43 |
| -8 | 40 | 40 |
| -7 | 32 | 33 |
| -6 | 20 | -22 |
| -5 | 52 | -52 |
| -4 | 21 | 19 |
| -3 | 58 | 59 |
| -2 | 45 | -50 |
| -1 | 120 | -123 |
| -0 | 72 | 68 |
| 1 | 102 | 100 |
| 2 | 44 | -46 |
| 3 | 9 | -7 |
| 4 | 17 | 16 |
| 5 | 15 | 15 |
| 6 | 21 | -20 |
| 7 | 31 | -31 |
| 8 | 0 | 7 |

H,K= 3,10

| L | FOB | FCA |
|---|---|---|
| -8 | 0 | 1 |
| -7 | 0 | 3 |
| -6 | 23 | -26 |
| -5 | 21 | -20 |
| -4 | 0 | -2 |
| -3 | 41 | 36 |
| -2 | 51 | -51 |
| -1 | 103 | -96 |
| -0 | 97 | 93 |
| 1 | 54 | 50 |
| 2 | 37 | -39 |
| 3 | 14 | 14 |
| 4 | 0 | 3 |
| 5 | 7 | -11 |
| 6 | 31 | -30 |
| 7 | 8 | 4 |

H,K= 3,11

| L | FOB | FCA |
|---|---|---|
| -8 | 0 | 7 |
| -7 | 50 | 51 |
| -6 | 12 | -14 |
| -5 | 71 | -74 |
| -4 | 19 | 19 |
| -3 | 82 | 81 |
| -2 | 11 | 4 |
| -1 | 78 | -77 |
| -0 | 34 | -26 |
| 1 | 32 | 28 |
| 2 | 19 | -17 |
| 3 | 7 | 7 |
| 4 | 58 | 53 |
| 5 | 40 | 37 |
| 6 | 7 | -15 |
| 7 | 45 | -45 |

H,K= 3,12

| L | FOB | FCA |
|---|---|---|
| -7 | 27 | 24 |
| -6 | 7 | 9 |
| -5 | 34 | -34 |
| -4 | 24 | -27 |
| -3 | 25 | 23 |
| -2 | 0 | -1 |
| -1 | 77 | -72 |
| -0 | 26 | 26 |
| 1 | 79 | 77 |
| 2 | 7 | -8 |
| 3 | 59 | -55 |
| 4 | 22 | 22 |
| 5 | 27 | 26 |
| 6 | 28 | -28 |

H,K= 3,13

| L | FOB | FCA |
|---|---|---|
| -6 | 0 | 8 |
| -5 | 73 | -75 |
| -4 | 16 | 18 |
| -3 | 59 | 57 |
| -2 | 10 | 5 |
| -1 | 31 | -28 |
| -0 | 17 | -14 |
| 1 | 35 | 33 |
| 2 | 10 | -10 |
| 3 | 49 | -45 |
| 4 | 31 | 35 |
| 5 | 36 | 37 |

H,K= 3,14

| L | FOB | FCA |
|---|---|---|
| -5 | 11 | -11 |
| -4 | 45 | -44 |
| -3 | 19 | -13 |
| -2 | 39 | 40 |
| -1 | 19 | -22 |
| -0 | 40 | -38 |
| 1 | 39 | 37 |
| 2 | 38 | 36 |
| 3 | 33 | -34 |
| 4 | 0 | 6 |

H,K= 3,15

| L | FOB | FCA |
|---|---|---|
| -4 | 0 | -4 |
| -3 | 8 | 8 |
| -2 | 17 | -15 |
| -1 | 26 | -24 |
| -0 | 18 | 16 |
| 1 | 79 | 74 |
| 2 | 15 | -11 |
| 3 | 65 | -64 |

H,K= 3,16

| L | FOB | FCA |
|---|---|---|
| -1 | 0 | 0 |
| -0 | 44 | -44 |

H,K= 4, 0

| L | FOB | FCA |
|---|---|---|
| -10 | 62 | -60 |
| -8 | 79 | 78 |
| -6 | 45 | -47 |
| -4 | 82 | 89 |
| -2 | 27 | -31 |
| -0 | 23 | 8 |
| 2 | 194 | -200 |
| 4 | 164 | 166 |
| 6 | 21 | 21 |
| 8 | 0 | -7 |

H,K= 4, 1

| L | FOB | FCA |
|---|---|---|
| -10 | 7 | -10 |
| -9 | 19 | -21 |
| -8 | 11 | -11 |
| -7 | 42 | 42 |
| -6 | 16 | 16 |
| -5 | 30 | 31 |
| -4 | 50 | 42 |
| -3 | 17 | -24 |
| -2 | 194 | -198 |
| -1 | 43 | 34 |
| -0 | 27 | 34 |
| 1 | 68 | -69 |
| 2 | 22 | 17 |
| 3 | 38 | 31 |
| 4 | 12 | 12 |
| 5 | 20 | -19 |
| 6 | 6 | -2 |
| 7 | 25 | 27 |
| 8 | 7 | -4 |
| 9 | 0 | -0 |

H,K= 4, 2

| L | FOB | FCA |
|---|---|---|
| -10 | 37 | -34 |
| -9 | 12 | 12 |
| -8 | 82 | 82 |
| -7 | 6 | -3 |
| -6 | 58 | -58 |
| -5 | 57 | -55 |
| -4 | 80 | 81 |
| -3 | 74 | 82 |
| -2 | 157 | -155 |
| -1 | 70 | 68 |
| -0 | 22 | -20 |
| 1 | 82 | -72 |
| 2 | 82 | -79 |
| 3 | 39 | -39 |
| 4 | 140 | 144 |
| 5 | 21 | 20 |
| 6 | 37 | -38 |
| 7 | 38 | 41 |
| 8 | 17 | 15 |
| 9 | 30 | -31 |

H,K= 4, 3

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -9 |
| -9 | 17 | -18 |
| -8 | 7 | 2 |
| -7 | 54 | 53 |
| -6 | 16 | -13 |
| -5 | 48 | -50 |
| -4 | 81 | 80 |
| -3 | 50 | 52 |
| -2 | 187 | -192 |
| -1 | 87 | -88 |
| -0 | 92 | 94 |
| 1 | 16 | -15 |
| 2 | 17 | -10 |
| 3 | 0 | 2 |
| 4 | 19 | -17 |
| 5 | 10 | 14 |
| 6 | 33 | -33 |
| 7 | 24 | 23 |
| 8 | 17 | 18 |
| 9 | 0 | -1 |

H,K= 4, 4

| L | FOB | FCA |
|---|---|---|
| -10 | 20 | -18 |
| -9 | 0 | -3 |
| -8 | 53 | 49 |
| -7 | 61 | 59 |
| -6 | 44 | -46 |
| -5 | 59 | -62 |
| -4 | 97 | 104 |
| -3 | 57 | 57 |
| -2 | 125 | -133 |
| -1 | 0 | 3 |
| -0 | 16 | 18 |
| 1 | 41 | -41 |
| 2 | 37 | -38 |
| 3 | 39 | 32 |
| 4 | 86 | 85 |
| 5 | 13 | 12 |
| 6 | 70 | -71 |
| 7 | 7 | 10 |
| 8 | 105 | 104 |
| 9 | 0 | -11 |

H,K= 4, 5

| L | FOB | FCA |
|---|---|---|
| -10 | 0 | -2 |
| -9 | 51 | -46 |
| -8 | 17 | 14 |
| -7 | 73 | 70 |
| -6 | 35 | -35 |
| -5 | 67 | -69 |
| -4 | 14 | -15 |
| -3 | 135 | 133 |
| -2 | 14 | -2 |
| -1 | 101 | -103 |
| -0 | 17 | 12 |
| 1 | 11 | 7 |
| 2 | 25 | 21 |
| 3 | 76 | -76 |
| 4 | 58 | 58 |
| 5 | 71 | 72 |
| 6 | 60 | -60 |
| 7 | 7 | -11 |
| 8 | 15 | 11 |
| 9 | 0 | 3 |

H,K= 4, 6

| L | FOB | FCA |
|---|---|---|
| -10 | 16 | -16 |
| -9 | 30 | -26 |
| -8 | 27 | 27 |
| -7 | 46 | 47 |
| -6 | 16 | 14 |
| -5 | 41 | -42 |
| -4 | 73 | 71 |
| -3 | 47 | 51 |
| -2 | 101 | -104 |
| -1 | 91 | -88 |
| -0 | 122 | 119 |
| 1 | 75 | 76 |
| 2 | 134 | -139 |
| 3 | 0 | -6 |
| 4 | 81 | 83 |
| 5 | 35 | 36 |
| 6 | 79 | -80 |
| 7 | 30 | -28 |
| 8 | 85 | 82 |
| 9 | 8 | 12 |

H,K= 4, 7

| L | FOB | FCA |
|---|---|---|
| -9 | 53 | -49 |
| -8 | 7 | -9 |
| -7 | 70 | 70 |
| -6 | 0 | -0 |
| -5 | 66 | -69 |
| -4 | 66 | -65 |
| -3 | 95 | 95 |
| -2 | 99 | 102 |
| -1 | 93 | -97 |
| -0 | 52 | -54 |
| 1 | 44 | 40 |
| 2 | 40 | 38 |
| 3 | 38 | -41 |
| 4 | 26 | 22 |
| 5 | 70 | 67 |
| 6 | 13 | -19 |
| 7 | 21 | -22 |
| 8 | 11 | -10 |

H,K= 4, 8

| L | FOB | FCA |
|---|---|---|
| -9 | 27 | -22 |
| -8 | 25 | 25 |
| -7 | 15 | 16 |
| -6 | 11 | 14 |
| -5 | 0 | -5 |
| -4 | 18 | 18 |
| -3 | 26 | 29 |
| -2 | 102 | -105 |
| -1 | 143 | -144 |
| -0 | 102 | 104 |
| 1 | 120 | 118 |
| 2 | 130 | -129 |
| 3 | 100 | -101 |
| 4 | 121 | 116 |
| 5 | 53 | 49 |
| 6 | 27 | -23 |
| 7 | 54 | -55 |
| 8 | 40 | 40 |

H,K= 4, 9

| L | FOB | FCA |
|---|---|---|
| -8 | 41 | -43 |
| -7 | 27 | 26 |
| -6 | 51 | 52 |
| -5 | 9 | -10 |
| -4 | 86 | -87 |
| -3 | 21 | 20 |
| -2 | 61 | 62 |
| -1 | 105 | -106 |
| -0 | 49 | -44 |
| 1 | 25 | 30 |
| 2 | 67 | 66 |
| 3 | 12 | 12 |
| 4 | 43 | -41 |
| 5 | 14 | 13 |
| 6 | 36 | 34 |
| 7 | 13 | 16 |

H,K= 4,10

| L | FOB | FCA |
|---|---|---|
| -8 | 26 | 30 |
| -7 | 13 | 14 |
| -6 | 36 | -36 |
| -5 | 45 | -47 |
| -4 | 40 | 38 |
| -3 | 72 | 73 |
| -2 | 29 | -32 |
| -1 | 102 | -106 |
| -0 | 24 | 20 |
| 1 | 113 | 114 |
| 2 | 44 | -44 |
| 3 | 88 | -89 |
| 4 | 13 | 13 |
| 5 | 70 | 70 |
| 6 | 0 | -5 |
| 7 | 59 | -59 |

H,K= 4,11

| L | FOB | FCA |
|---|---|---|
| -7 | 0 | 2 |
| -6 | 74 | 75 |
| -5 | 37 | 33 |
| -4 | 83 | -79 |
| -3 | 16 | -19 |
| -2 | 41 | 42 |
| -1 | 9 | 6 |
| -0 | 46 | -42 |
| 1 | 17 | -10 |
| 2 | 64 | 67 |
| 3 | 18 | 14 |
| 4 | 14 | -11 |
| 5 | 31 | -35 |
| 6 | 17 | 17 |

H,K= 4,12

| L | FOB | FCA |
|---|---|---|
| -7 | 33 | 33 |
| -6 | 36 | -37 |
| -5 | 63 | -58 |
| -4 | 48 | 47 |
| -3 | 69 | 70 |
| -2 | 20 | -20 |
| -1 | 83 | -80 |
| -0 | 19 | -14 |
| 1 | 54 | 51 |
| 2 | 30 | 29 |
| 3 | 36 | -37 |
| 4 | 7 | -13 |
| 5 | 66 | 64 |
| 6 | 11 | 10 |

H,K= 4,13

| L | FOB | FCA |
|---|---|---|
| -6 | 17 | 18 |
| -5 | 25 | 26 |
| -4 | 39 | -38 |
| -3 | 61 | -61 |
| -2 | 32 | 32 |
| -1 | 48 | 46 |
| -0 | 36 | -31 |
| 1 | 38 | -35 |
| 2 | 19 | 19 |
| 3 | 10 | 13 |
| 4 | 0 | -5 |
| 5 | 0 | 0 |

H,K= 4,14

| L | FOB | FCA |
|---|---|---|
| -5 | 30 | -30 |
| -4 | 19 | 17 |
| -3 | 21 | 19 |
| -2 | 7 | -5 |
| -1 | 34 | -37 |
| -0 | 19 | -21 |
| 1 | 40 | 39 |
| 2 | 0 | 2 |
| 3 | 15 | -15 |
| 4 | 0 | -6 |

H,K= 4,15

| L | FOB | FCA |
|---|---|---|
| -3 | 15 | -22 |
| -2 | 26 | -27 |
| -1 | 15 | 21 |
| -0 | 8 | 9 |
| 1 | 11 | -15 |
| 2 | 0 | 0 |

H,K= 5, 0

| L | FOB | FCA |
|---|---|---|
| -9 | 87 | -78 |
| -7 | 104 | 99 |
| -5 | 98 | -104 |
| -3 | 165 | 162 |
| -1 | 10 | 6 |
| 1 | 35 | 33 |
| 3 | 114 | -118 |
| 5 | 13 | 17 |
| 7 | 57 | 53 |
| 9 | 0 | 1 |

H,K= 5, 1

| L | FOB | FCA |
|---|---|---|
| -10 | 50 | -48 |
| -9 | 0 | 1 |
| -8 | 61 | 64 |
| -7 | 0 | 4 |
| -6 | 38 | -41 |
| -5 | 23 | -25 |
| -4 | 123 | 119 |
| -3 | 65 | 64 |
| -2 | 164 | -166 |
| -1 | 93 | -86 |
| -0 | 62 | 70 |
| 1 | 19 | 17 |
| 2 | 246 | -241 |
| 3 | 60 | -56 |
| 4 | 197 | 198 |
| 5 | 41 | 45 |
| 6 | 110 | -110 |
| 7 | 25 | -23 |
| 8 | 84 | 82 |
| 9 | 13 | 17 |

H,K= 5, 2

| L | FOB | FCA |
|---|---|---|
| -10 | 34 | 32 |
| -9 | 70 | -67 |
| -8 | 80 | -76 |
| -7 | 87 | 85 |
| -6 | 107 | 109 |
| -5 | 73 | -73 |
| -4 | 39 | -38 |
| -3 | 111 | 109 |
| -2 | 84 | -87 |
| -1 | 102 | -106 |
| -0 | 71 | 72 |
| 1 | 24 | 20 |
| 2 | 37 | 36 |
| 3 | 49 | -47 |
| 4 | 52 | -54 |
| 5 | 0 | 3 |
| 6 | 14 | 12 |
| 7 | 30 | 28 |
| 8 | 18 | 19 |
| 9 | 0 | -0 |

H,K= 5, 3

| L | FOB | FCA |
|---|---|---|
| -10 | 30 | -30 |
| -9 | 0 | -2 |
| -8 | 35 | 36 |
| -7 | 13 | 15 |
| -6 | 66 | -70 |
| -5 | 86 | -87 |
| -4 | 190 | 192 |
| -3 | 143 | 144 |
| -2 | 98 | -105 |
| -1 | 151 | -145 |
| -0 | 42 | 41 |
| 1 | 74 | 70 |
| 2 | 107 | -105 |
| 3 | 78 | -75 |
| 4 | 76 | 79 |
| 5 | 86 | 89 |
| 6 | 59 | -57 |
| 7 | 68 | -66 |
| 8 | 90 | 87 |
| 9 | 35 | 34 |

H,K= 5, 4

| L | FOB | FCA |
|---|---|---|
| -10 | 34 | 34 |
| -9 | 23 | -24 |
| -8 | 47 | -48 |
| -7 | 36 | 41 |
| -6 | 89 | 86 |
| -5 | 25 | -23 |
| -4 | 76 | -77 |
| -3 | 86 | 93 |
| -2 | 33 | 30 |
| -1 | 43 | -44 |
| -0 | 8 | 1 |
| 1 | 5 | -4 |
| 2 | 87 | 82 |
| 3 | 27 | 25 |
| 4 | 20 | -23 |
| 5 | 9 | 6 |
| 6 | 17 | -18 |
| 7 | 0 | -0 |
| 8 | 25 | 25 |
| 9 | 0 | -1 |

H,K= 5, 5

| L | FOB | FCA |
|---|---|---|
| -10 | 22 | -20 |
| -9 | 0 | -4 |
| -8 | 32 | 31 |
| -7 | 28 | 25 |
| -6 | 26 | -31 |
| -5 | 64 | -66 |
| -4 | 78 | 82 |
| -3 | 110 | 115 |
| -2 | 69 | -74 |
| -1 | 67 | -83 |
| -0 | 37 | 34 |
| 1 | 40 | 54 |
| 2 | 24 | -27 |
| 3 | 74 | -74 |
| 4 | 26 | 21 |
| 5 | 74 | 70 |
| 6 | 7 | 2 |
| 7 | 58 | -57 |
| 8 | 39 | 38 |

H,K= 5, 6

| L | FOB | FCA |
|---|---|---|
| -9 | 18 | -19 |
| -8 | 0 | 6 |
| -7 | 9 | -8 |
| -6 | 11 | 14 |
| -5 | 8 | 2 |
| -4 | 53 | -52 |
| -3 | 8 | 4 |
| -2 | 59 | 57 |
| -1 | 28 | -28 |
| -0 | 122 | -123 |
| 1 | 65 | -69 |
| 2 | 71 | 67 |
| 3 | 26 | -23 |
| 4 | 22 | 22 |
| 5 | 18 | 15 |
| 6 | 19 | -16 |
| 7 | 16 | -16 |
| 8 | 0 | 0 |

H,K= 5, 7

| L | FOB | FCA |
|---|---|---|
| -9 | 21 | -22 |
| -8 | 74 | 24 |
| -7 | 26 | 28 |
| -6 | 18 | 17 |
| -5 | 6 | 9 |
| -4 | 20 | -18 |
| -3 | 0 | 6 |
| -2 | 16 | 15 |
| -1 | 65 | -70 |
| -0 | 41 | 34 |
| 1 | 46 | 49 |
| 2 | 93 | -88 |
| 3 | 51 | -46 |
| 4 | 6 | 4 |
| 5 | 37 | 37 |
| 6 | 23 | 25 |
| 7 | 0 | 1 |
| 8 | 13 | 11 |

H,K= 5, 8

| L | FOB | FCA |
|---|---|---|
| -9 | 15 | -13 |
| -8 | 0 | 2 |
| -7 | 0 | 2 |
| -6 | 21 | -22 |
| -5 | 48 | 47 |
| -4 | 0 | -1 |
| -3 | 18 | 14 |
| -2 | 18 | -17 |
| -1 | 13 | -12 |
| -0 | 37 | -37 |
| 1 | 16 | -16 |
| 2 | 24 | 25 |
| 3 | 15 | -17 |
| 4 | 18 | 19 |
| 5 | 10 | 10 |
| 6 | 26 | 24 |
| 7 | 0 | -2 |

H,K= 5, 9

| L | FOB | FCA |
|---|---|---|
| -8 | 36 | 36 |
| -7 | 22 | 22 |
| -6 | 0 | 1 |
| -5 | 30 | 32 |
| -4 | 20 | 19 |
| -3 | 31 | -29 |
| -2 | 24 | -24 |
| -1 | 36 | -34 |
| -0 | 32 | 32 |
| 1 | 62 | 61 |
| 2 | 44 | -44 |
| 3 | 9 | -12 |
| 4 | 33 | 31 |
| 5 | 7 | -8 |
| 6 | 0 | 1 |
| 7 | 13 | 12 |

H,K= 5,10

| L | FOB | FCA |
|---|---|---|
| -8 | 0 | 2 |
| -7 | 13 | 11 |
| -6 | 10 | -13 |
| -5 | 7 | -3 |
| -4 | 0 | -1 |
| -3 | 33 | 32 |
| -2 | 28 | -25 |
| -1 | 50 | -50 |
| -0 | 27 | 18 |
| 1 | 15 | 14 |
| 2 | 13 | 16 |
| 3 | 7 | -8 |
| 4 | 21 | -20 |

Table I. Observed and Calculated Structure Factors (X 1.0) for

$(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$.

| | | |

$\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}\ell^2 - 2\beta_{12}hk - 2\beta_{13}h\ell - 2\beta_{23}k\ell)$, with $4\beta_{ij} = a_i^* a_j^* \beta_{ij}$, where $a_i^*$ is the length of the $i$ th reciprocal axis. The carbon atoms were assigned isotropic temperature factors while the Ru, As, Cl and O atoms were given anisotropic temperature factors. With a full matrix treatment of all 178 parameters, the R factor was reduced to 0.067. The final values of the parameters are listed in Table II. The unit cell is shown in Figure 1.

Discussion of the Structure.-- Several structures involving tetraphenylarsonium and tetrphenylphosphonium cations have been reported: $(C_6H_5)_4AsI$ [8], $(C_6H_5)_4AsI_3$ [9], $(C_6H_5)_4AsFeCl_4$ [10], and $(C_6H_5)_4PI$ [11]. In the first two examples, the point symmetry at the arsenic is $\bar{4}2m$, with the planes of the phenyl rings perpendicular to the mirror planes. In the second two examples, the point symmetry is only $\bar{4}2$. The phenyl rings in $(C_6H_5)_4As\ Fe\ Cl_4$ point to the corners of a regular tetrahedron, but the planes of the rings are rotated 28°, destroying the mirror planes. In $(C_6H_5)_4PI$, the phenyl rings point to the corners of a distorted tetrahedron, forming angles about the phosphorus of 103° and 113°, and the planes are rotated 52° in this case. No simple description is possible for the configuration of the phenyl rings in the present example of the ruthenium salt. In this case, the arsenic is situated at a point of symmetry 1, and the phenyl groups have taken correspondingly free positions around the arsenic. The details of the configuration are given in Table III, where I, II, III, IV refer to the four phenyl rings.

Since the carbon atoms in the phenyl rings were not restrained in the least squares refinement, the individual rings departed slightly from 6/mm symmetry. The average of the 24 C - C bond lengths is 1.396 Å, with a spread

Table II. Positional and thermal parameters in $(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$ [a].

| Atom | x | y | z | $B_{11}$ | $B_{22}$ | $B_{33}$ | $B_{12}$ | $B_{13}$ | $B_{23}$ |
|---|---|---|---|---|---|---|---|---|---|
| Ru | 0.4872 | 0.5164 | 0.7585 | 3.28 | 3.72 | 3.32 | 0.11 | 0.41 | 0.00 |
| As | 0.4169 | 0.0785 | 0.7332 | 2.56 | 2.75 | 3.38 | 0.23 | 0.12 | -0.01 |
| Cl(1) | 0.3829 | 0.5818 | 0.8566 | 3.96 | 5.36 | 4.29 | 0.66 | 0.84 | -0.43 |
| Cl(2) | 0.3813 | 0.4884 | 0.5838 | 3.52 | 6.15 | 3.51 | -0.26 | 0.09 | -0.45 |
| Cl(3) | 0.5308 | 0.6382 | 0.6796 | 4.75 | 3.46 | 5.04 | 0.14 | 0.89 | 0.39 |
| Cl(4) | 0.4614 | 0.3895 | 0.8391 | 5.75 | 4.02 | 4.39 | -0.55 | 1.05 | 0.61 |
| O(1) | 0.5865 | 0.5358 | 0.9173 | 3.89 | 5.89 | 3.41 | -0.20 | 0.40 | 0.04 |
| O(2) | 0.5884 | 0.4623 | 0.6748 | 3.24 | 4.46 | 3.74 | 0.72 | 0.40 | -0.02 |
| O(3) | 0.0442 | 0.1822 | 0.0983 | 12.4 | 4.47 | 7.63 | -0.66 | 0.01 | 0.17 |
| C(I1) | 0.3493 | 0.1309 | 0.5926 | 3.0 [b] | | | | | |
| C(I2) | 0.3189 | 0.0852 | 0.4865 | 4.9 | | | | | |
| C(I3) | 0.2656 | 0.1249 | 0.3866 | 5.9 | | | | | |
| C(I4) | 0.2489 | 0.2063 | 0.3914 | 6.3 | | | | | |
| C(I5) | 0.2840 | 0.2497 | 0.4922 | 7.3 | | | | | |
| C(I6) | 0.3338 | 0.2124 | 0.5995 | 5.6 | | | | | |
| C(II1) | 0.3914 | 0.1309 | 0.8793 | 3.6 | | | | | |
| C(II2) | 0.3130 | 0.1121 | 0.9194 | 5.3 | | | | | |
| C(II3) | 0.2920 | 0.1577 | 1.0226 | 6.2 | | | | | |
| C(II4) | 0.3530 | 0.2161 | 1.0785 | 5.2 | | | | | |
| C(II5) | 0.4301 | 0.2313 | 1.0359 | 5.1 | | | | | |
| C(II6) | 0.4502 | 0.1898 | 0.9339 | 4.6 | | | | | |

(Table II. Continued)

| | | | | |
|---|---|---|---|---|
| C(III1) | 0.5421 | 0.0904 | 0.7312 | 3.6 |
| C(III2) | 0.6046 | 0.0611 | 0.8340 | 5.0 |
| C(III3) | 0.6969 | 0.0656 | 0.8253 | 5.4 |
| C(III4) | 0.7249 | 0.0968 | 0.7267 | 6.0 |
| C(III5) | 0.6651 | 0.1247 | 0.6252 | 5.4 |
| C(III6) | 0.5707 | 0.1204 | 0.6283 | 4.3 |
| C(IV1) | 0.3893 | 0.9670 | 0.7260 | 3.3 |
| C(IV2) | 0.3014 | -0.0579 | 0.7264 | 5.0 |
| C(IV3) | 0.2828 | -0.1419 | 0.7187 | 6.2 |
| C(IV4) | 0.3528 | -0.1957 | 0.7106 | 6.1 |
| C(IV5) | 0.4380 | -0.1698 | 0.7054 | 5.8 |
| C(IV6) | 0.4599 | -0.0871 | 0.7150 | 5.0 |

[a] Standard deviations of the positional parameters of Ru and As are 0.0001 or less, Cl 0.0003 or less, and O and C 0.001 or less.

Standard deviations of the thermal parameters are 0.05 or less for Ru and As, 0.2 or less for Cl, 0.4 or less for O and C, except for O(3) which was 0.8 or less.

[b] Only isotropic temperature factors were used for the carbon atoms..

Table III. Configuration of tetraphenylarsonium ion in $(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$.

| Bond angles around arsenic | | Dihedral angles between planes of phenyl rings | |
|---|---|---|---|
| C(I1)-As-C(II1) | $109^\circ \pm 1^\circ$ | I-II | $70^\circ \pm 3^\circ$ |
| C(II1)-As-C(III1) | $108^\circ$ | I-III | $89^\circ$ |
| C(I1)-As-C(IV1) | $110^\circ$ | I-IV | $70^\circ$ |
| C(III1)-As-C(IIII1) | $107^\circ$ | II-III | $36^\circ$ |
| C(III1)-As-C(IV1) | $114^\circ$ | II-IV | $70^\circ$ |

in bond lengths of 1.35 Å to 1.45 Å, and a standard deviation of about 0.03 Å. This bond length does not differ significantly from the benzene C - C bond of 1.397 Å. The C(1) - C(4) diameters of all four rings, pointing to the central arsenic, are shorter by about 0.02 Å compared to the average diameter of 2.79 Å. This apparent shortening may be the result of torsional thermal motion.

The octahedral environment of the ruthenium is detailed in Table IV. The most interesting aspect of the configuration is the cis-arrangement of the two water molecules in the octahedron. The average Ru - Cl and Ru - O distances of 2.34 Å and 2.12 Å are in agreement with the values we have found for the cesium salt [2], and those reported by Khodashova for the potassium salt [12]. The Ru - Cl bonds opposite the oxygens in the octahedron were again found to be several hundreths of an Ångstrom shorter than those for which the opposite atoms were both chlorines.

The possibilities for hydrogen bonding are shown in Figure 2.

Table IV. Distances and angles in $(C_6H_5)_4AsRuCl_4(H_2O)_2 \cdot H_2O$.

| Atom 1-Atom 2 | Bond (Å) | Bond angles (degrees) | |
|---|---|---|---|
| Ru - O(1) | 2.12 ± 0.01 | Cl(1) - Ru - O(2) | 177° ± 1° |
| - O(2) | 2.11 ± 0.01 | Cl(2) - Ru - O(1) | 178° ± 1° |
| - O(3) | 3.92 ± 0.01 | Cl(2) - Ru - O(2) | 90° ± 1° |
| - Cl(1) | 2.33 ± 0.01 | Cl(2) - Ru - Cl(1) | 93° ± 1° |
| - Cl(2) | 2.32 ± 0.01 | Cl(2) - Ru - Cl(3) | 94° ± 1° |
| - Cl(3) | 2.35 ± 0.01 | Cl(2) - Ru - Cl(4) | 90° ± 1° |
| - Cl(4) | 2.36 ± 0.01 | | |
| As - C(1) | 1.91 ± 0.01 | (average of four) | |
| C - C | 1.396 ± 0.03 | (average of twenty four) | |

The water of crystallization, designated O(3) in the figure, is probably involved in two hydrogen bonds: to water molecule O(2), and to chlorine Cl(3). The distances of 2.61 Å and 3.16 Å, and the angle of 97° are acceptable evidence for bonding. In the case of the two water molecules in the octahedron surrounding the ruthenium, reasonable hydrogen bonds can only be postulated for one of the molecules, O(2). In addition to the bond to O(3), it appears to be bonded to chlorine, Cl(2) at a distance of 3.07 Å, giving an angle of about 91° between the bonds. The other water molecule in the octahedron, O(1), is not too distant from chlorines Cl(1) and Cl(4) of the neighboring octahedron, but the acute 66° angle is too small to indicate a pair of hydrogen bonds.

Water molecule O(3) appears to be vibrating quite anisotropically, with $\underline{B}_{11} \sim 12$, $\underline{B}_{22} \sim 4$, and $\underline{B}_{33} \sim 8$. This would indicate that most of the vibration is occurring in the <u>ac</u> plane, or alternatively, some disorder concerning the location of the oxygen atom.

It is interesting to note that the structure of this complex salt can be visualized as a series of alternating layers of ruthenium octahedra and tetraphenylarsonium ions. This is shown in figure 1, where the alternating planes run roughly parallel to the (110) planes.

References

(1) Work done under the auspices of the U. S. Atomic Energy Commission.

(2) To be published.

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Figure Captions

Figure 1. Unit cell of $(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$. Numbers are coordinates along the c axis.

Figure 2. Possibilities for hydrogen bonding in $(C_6H_5)_4As\ Rucl_4(H_2O)_2 \cdot H_2O$.

Figure 1. Unit cell of $(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$.

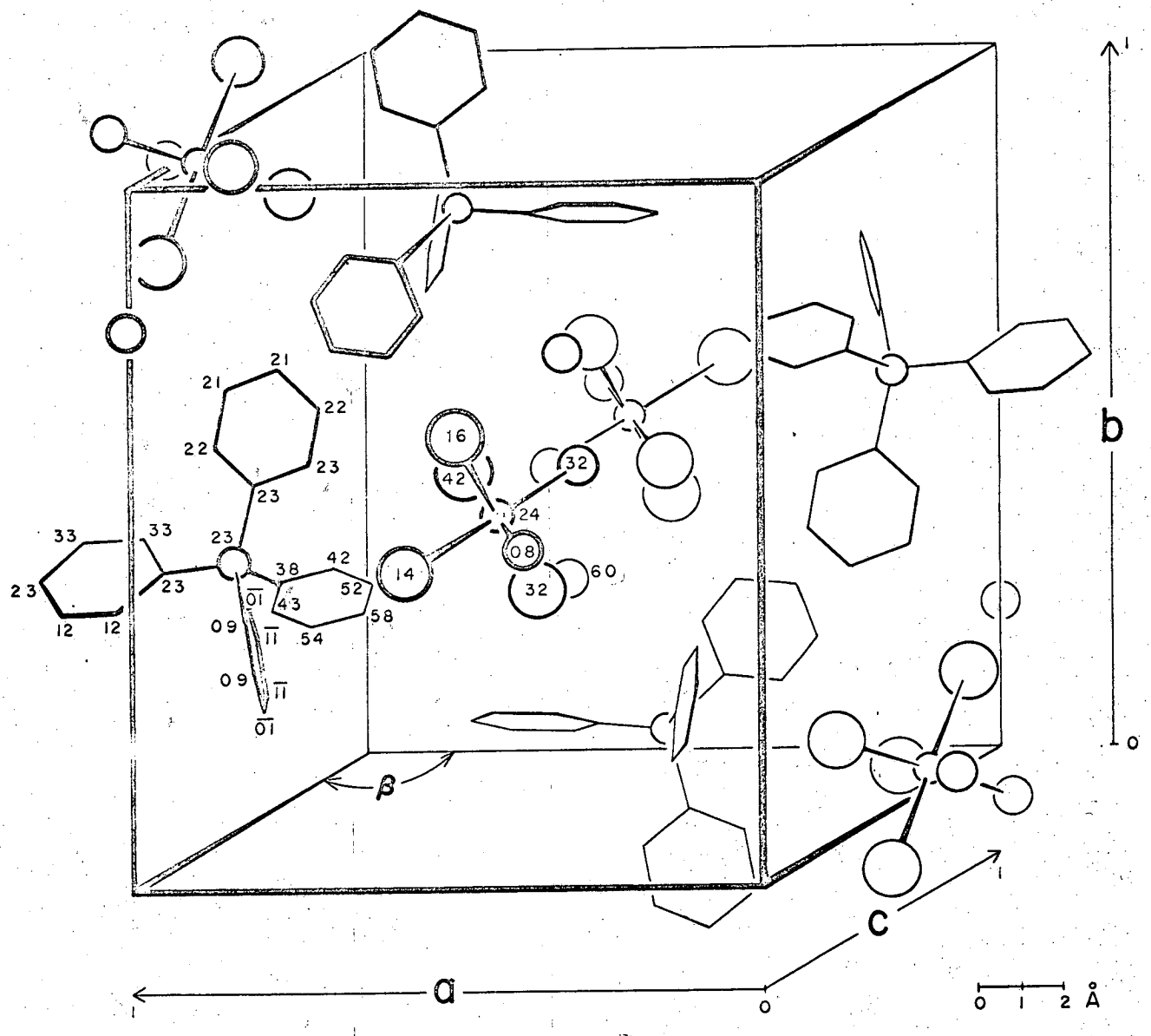


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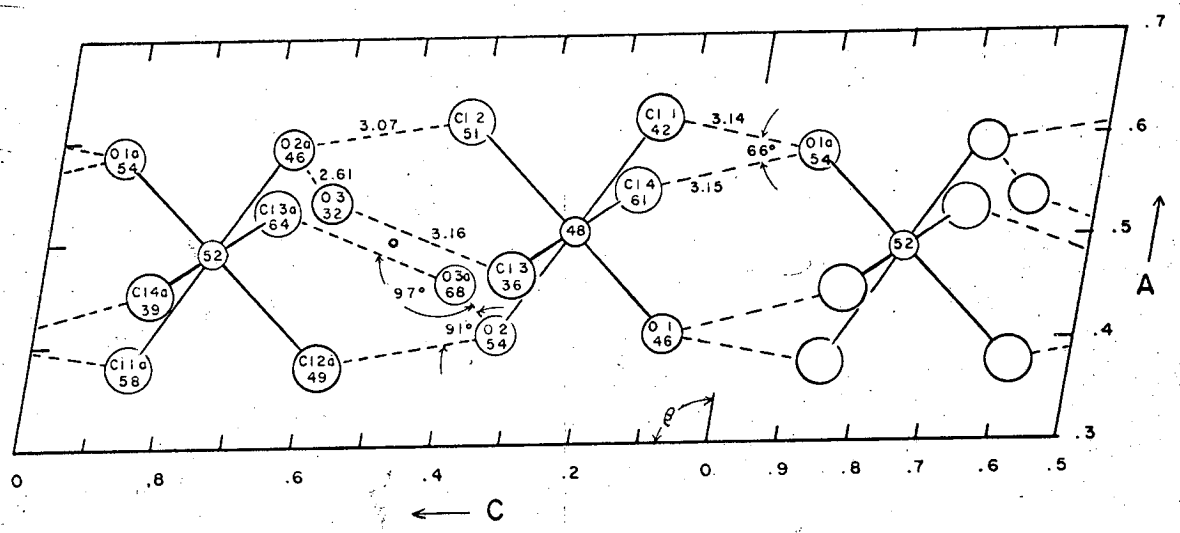
Figure 2. Possibilities for hydrogen bonding in $(C_6H_5)_4As\ RuCl_4(H_2O)_2 \cdot H_2O$.

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