TABLE IV

DISTANCES AND ANGLES IN $(C_6H_5)_4AsRuCl_4(H_2O)_2 \cdot H_2O$

Atom 1–atom 2	Bond, A	Bond angles	Deg (±1)
Ru–O(1)	2.12 ± 0.01	Cl(1)–Ru–O(2)	177
Ru–O(2)	2.11 ± 0.01	Cl(2)–Ru–O(1)	178
Ru–O(3)	3.92 ± 0.01	Cl(2)–Ru–O(2)	90
Ru–Cl(1)	2.33 ± 0.01	Cl(2)–Ru–Cl(1)	93
Ru–Cl(2)	2.32 ± 0.01	Cl(2)–Ru–Cl(3)	94
Ru–Cl(3)	2.35 ± 0.01	Cl(2)–Ru–Cl(4)	90
Ru–Cl(4)	2.36 ± 0.01		
As–C(1)	1.91 ± 0.01 (av of 4)		
C–C	1.396 ± 0.03 (av of 24)		

Ru–Cl and Ru–O distances of 2.34 and 2.12 A are in agreement with the values we have found for the cesium salt[2a] 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 hundredths of an angstrom shorter than those for which the opposite atoms were both chlorines.

The possibilities for hydrogen bonding are shown in Figure 2. 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 and 3.16 A 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 A, 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.

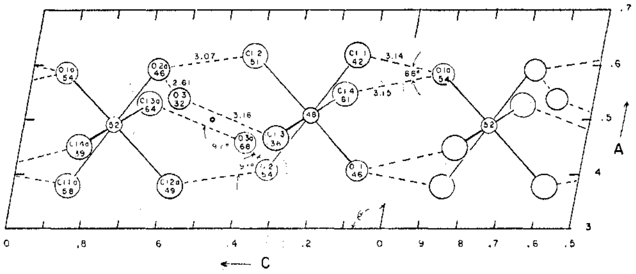

Figure 2.—Possibilities for hydrogen bonding in $(C_6H_5)_4AsRuCl_4$-$(H_2O)_2 \cdot H_2O$.

Water molecule O(3) appears to be vibrating quite anisotropically, with $B_{11} \sim 12$, $B_{22} \sim 4$, $B_{33} \sim 8$. This would indicate that most of the vibration is occurring in the *ac* 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.

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[12] T. S. Khodashova, *Zh. Strukt. Khim.*, **1**, 333 (1960).

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The Crystal Structure of Cesium Aquopentachlororuthenate[1]

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

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X-Ray diffraction study of a single crystal of $Cs_2RuCl_5H_2O$ showed that it is orthorhombic with $a = 7.986$ A, $b = 17.289$ A, and $c = 7.400$ A, $Z = 4$, $d_x = 3.65$ g cm^{-3}. The space group is Amam. The ruthenium is surrounded by an octahedron composed of the five chlorine atoms and one water molecule. The Ru–O and average Ru–Cl distances are 2.10 and 2.34 A.

Introduction

Aqueous ruthenium species have been studied extensively by Connick, *et al.*, with particular emphasis on ruthenium(III).[2] In the course of their work, a number of aquochlororuthenates with various cations have been prepared, and it seemed of interest to determine the crystal structures of some of them. Aquopentachlororuthenates with cations of potassium, rubidium, and cesium have been obtained. As far as we know, the crystal structure of only the potassium salt has been reported.[3] None of the salts in this series is isostructural with either of the others. This paper is a report on the cesium salt.

Experimental Section

Small well-shaped crystals of $Cs_2RuCl_5H_2O$ were obtained by adding sufficient 1 *M* cesium chloride solution to a ruthenium(III) solution in hydrochloric acid to give the following concentrations: $[Ru(III)] = 0.05$ *M*, $[Cs^+] = 0.25$ *M*, and $[Cl^-] \cong 2$ *M*. Under these conditions, the chloride ion concentration is low enough to assure that crystal growth is slow. After standing at 0° for 48 hr, crystals were separated from the mother liquor on a Buchner funnel, quickly washed twice with ice-cold water,

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[1] Work done under the auspices of the U. S. Atomic Energy Commission.

[2] H. H. Cady and R. E. Connick, *J. Am. Chem. Soc.*, **80**, 2646 (1958); R. E. Connick and D. A. Fine, *ibid.*, **83**, 3414 (1961).

[3] T. S. Khodashova, *Zh. Struckt. Khim.*, **1**, 333 (1960).

and partially dried by suction. Final traces of moisture were removed by heating at 105° for 30 min. Analyses for Ru, Cl, and H_2O confirmed the formula $Cs_2RuCl_5H_2O$.

The preliminary determination of the space group and cell dimensions was made using the Weissenberg technique and copper radiation. A single crystal in the form of a prism 0.14 × 0.021 × 0.02 mm was used. The sides parallel to the long axis comprised the form $\{120\}$. The measured dihedral angle was $\sim 85°$, while the calculated angle is 85° 28′. The crystal was mounted with the c axis as the axis of rotation in ϕ. The cell dimensions and intensities were measured with a General Electric XRD-5 goniostat equipped with a scintillation counter, using Mo Kα radiation (λ 0.70926 A for Kα_1).

There are 525 independent reflections permitted by the space group in the sphere of reflection with $\sin \theta/\lambda < 0.596$ ($2\theta < 50°$). These were measured with counting times of 10 sec each and 95 were recorded as zero intensity. No correction was made for either absorption or extinction. The calculated linear absorption coefficient is $\mu = 100.0$ cm^{-1} for molybdenum radiation. For the crystal used, μR was less than 0.7.

Calculations were made using an IBM 7044 computer and our version (unpublished) of the Gantzel–Sparks–Trueblood full-matrix least-squares program which minimizes $\Sigma w(F_o - |F_c|)^2/(\Sigma w F_o^2)$, where F_o and F_c are the observed and calculated structure factors, and the weights w were all taken as unity. The Fourier and distance programs were written by Zalkin. The atomic scattering factors were chosen as follows: Cs^+ and Ru^{3+} values from Thomas and Umeda,[4] Cl^- and O values from the International Tables.[5] Corrections for anomalous dispersion ($\Delta f'$) were made for cesium, ruthenium, and chlorine by adding −0.5, −1.3, and +0.1, respectively, to their atomic scattering functions.

Unit Cell and Space Group

The A-centered cell contains four formula units of $Cs_2RuCl_5H_2O$ and is orthorhombic with dimensions $a = 7.986 \pm 0.005$, $b = 17.289 \pm 0.008$, $c = 7.400 \pm 0.004$ A. The calculated density is 3.65 g cm^{-3}. The crystals sank in methylene iodide (density 3.3 g cm^{-3}).

The Weissenberg photographs showed the following reflection restrictions: hkl: $k + l = 2n$; $h0l$: $h = 2n$. Measurements with the goniostat confirmed these observations. The axes were chosen according to the $c < a < b$ convention. The extinctions correspond to the space groups A2am, Ama2, and Amam, for the particular choice of axes for the crystal. The success of the structure determination confirmed the choice of the centrosymmetric space group Amam. The observed and calculated structure factor magnitudes are given in Table I.

Determination of the Structure

A three-dimensional Patterson function was calculated from the observed intensities after correction for Lorentz and polarization effects. The cesium–ruthenium and ruthenium–chlorine vectors were identified and coordinates for the trial structure were chosen.

Except for one set of chlorines, all of the atoms are in special positions: 4(c): ($^1/_4$, y, 0; $^3/_4$, $-y$, 0) + (0, 0, 0; 0, $^1/_2$, $^1/_2$). A set of four chlorines are in the general positions: 16(h): $\pm$(x, y, z; $-x$, $-y$, z; $^1/_2 - x$, y, z; $^1/_2 + x$, $-y$, z) + (0, 0, 0; 0, $^1/_2$, $^1/_2$).

TABLE I

OBSERVED AND CALCULATED STRUCTURE FACTORS FOR $Cs_2RuCl_5H_2O$

H,K=	L	FOB	FCA
0, 0	2	186	190
	4	237	255
	6	110	111
	8	85	83
0, 1	1	3	-8
	3	44	-50
	5	22	20
	7	28	-25
0, 2	0	10	7
	2	30	-30
	4	0	-1
	6	12	-10
	8	12	-5
0, 3	1	125	-128
	3	68	-74
	5	78	-83
	7	25	-28
0, 4	0	32	27
	2	199	200
	4	32	33
	6	62	62
	8	17	18
0, 5	1	111	-110
	3	42	-43
	5	82	-89
	7	15	-12
0, 6	0	135	-132
	2	37	-37
	4	76	-75
	6	33	-32
	8	24	-26
0, 7	1	0	-4
	3	6	-8
	5	7	1
	7	12	-5
0, 8	0	220	222
	2	93	98
	4	136	139
	6	57	62
	8	53	51
0, 9	1	86	65
	3	35	37
	5	72	75
	7	8	4
0,10	0	8	-10
	2	96	-89
	4	9	-15
	6	34	-34
0,11	1	13	7
	3	6	-2
	5	7	7
	7	0	-4
0,12	0	22	-15
	2	33	31
	4	10	-9
	6	6	10
0,13	1	0	-1
	3	21	20
	5	15	-20
0,14	0	148	-148
	2	70	-70
	4	101	-103
	6	47	-50
0,15	1	14	10
	3	20	20
	5	0	-2
0,16	0	41	41
	2	26	27
	4	28	33
0,17	1	70	70
	3	48	50
0,18	0	22	-8
	2	54	-54
	4	9	-9
0,19	1	20	21
	3	0	7
0,20	0	16	10
	2	9	3
1, 1	1	15	-3
	3	9	5
	5	9	-4
	7	0	2
1, 2	0	75	-67
	2	14	-9
	4	43	-40
	6	17	-15
	8	16	-15
1, 3	1	178	-173
	3	131	-130
	5	103	-103
	7	57	-56
1, 4	0	31	29
	2	41	39
	4	20	18
	6	15	14
	8	8	5
1, 5	1	33	28
	3	26	23
	5	20	22
	7	8	12
1, 6	0	163	164
	2	108	113
	4	105	106
	6	55	60
	8	47	43
1, 7	1	55	-60
	3	53	-56
	5	30	-26
	7	22	-22
1, 8	0	99	98
	2	68	69
	4	67	65
	6	36	37
	8	27	25
1, 9	1	21	-26
	3	19	-22
	5	16	-15
	7	8	-10
1,10	0	18	19
	2	33	33
	4	9	11
	6	11	12
1,11	1	127	-130
	3	104	-105
	5	89	-85
	7	51	-49
1,12	0	9	-10
	2	9	8
	4	8	-9
	6	0	-1
1,13	1	3	1
	3	3	3
	5	2	-1
1,14	0	61	63
	2	53	52
	4	45	47
	6	32	30
1,15	1	0	-2
	3	0	-4
	5	0	4
1,16	0	31	33
	2	17	17
	4	28	25
1,17	1	30	24
	3	23	19
1,18	0	0	-4
	2	0	-4
	4	9	-4
1,19	1	31	-30
	3	24	-25
1,20	0	42	-40
2, 0	0	209	-199
	2	332	-338
	4	146	-149
	6	142	-137
	8	73	-72
2, 1	1	34	35
	3	14	-11
	5	39	34
	7	15	-16
2, 2	0	30	27
	2	14	-4
	4	14	13
	6	9	4
	8	10	4
2, 3	1	98	98
	3	103	102
	5	43	46
	7	52	51
2, 4	0	207	-199
	2	39	-37
	4	108	-102
	6	30	-27
	8	24	-22
2, 5	1	72	73
	3	99	100
	5	23	24
	7	61	57
2, 6	0	39	37
	2	94	95
	4	37	36
	6	43	41
	8	23	24
2, 7	1	5	6
	3	0	1
	5	0	6
	7	0	-3
2, 8	0	101	-101
	2	173	-171
	4	77	-79
	6	84	-81
2, 9	1	55	-60
	3	81	-81
	5	17	-19
	7	51	-49
2,10	0	88	87
	2	16	14
	4	51	53
	6	16	15
2,11	1	0	-3
	3	7	-8
	5	0	3
	7	0	-4
2,12	0	29	-28
	2	9	11
	4	16	-16
	6	8	5
2,13	1	11	-10
	3	12	13
	5	11	-15
2,14	0	72	72
	2	121	123
	4	61	61
	6	64	62
2,15	1	16	-17
	3	0	-3
	5	20	-16
2,16	0	28	-28
	2	34	-35
	4	23	-22
2,18	0	56	53
	2	8	10
2,19	1	14	-14
2,20	0	0	-2
3, 1	1	9	-4
	3	15	13
	5	9	-11
	7	13	13
3, 2	0	29	-28
	2	80	78
	4	0	-4
	6	35	35
	8	8	9
3, 3	1	136	132
	3	131	131
	5	65	67
	7	69	68
3, 4	0	46	-48
	2	13	-11
	4	29	-28
	6	0	-7
	8	0	-7
3, 5	1	22	-20
	3	26	-25
	5	10	-11
	7	19	-17
3, 6	0	83	-79
	2	143	-144
	4	62	-61
	6	74	-70
3, 7	1	53	55
	3	26	26
	5	41	42
	7	0	-1
3, 8	0	50	-49
	2	89	-89
	4	40	-39
	6	45	-43
3, 9	1	20	25
	3	19	19
	5	16	15
	7	8	9
3,10	0	46	-45
	2	0	-1
	4	30	-28
	6	0	2
3,11	1	107	106
	3	105	105
	5	59	58
3,12	0	25	-24
	2	23	22
	4	13	-12
	6	12	11
3,13	1	0	-2
	3	0	4
	5	0	-5
3,14	0	45	-43
	2	58	-56
	4	33	-33
3,15	1	0	3
	3	0	-7
	5	0	5
3,16	0	0	-4
	2	40	-39
	4	12	-7
3,17	1	19	-18
	3	25	-22
3,18	0	8	4
	2	0	5
3,19	1	27	25
4, 0	0	256	255
	2	160	163
	4	167	163
	6	98	96
4, 1	1	10	-8
	3	25	-26
	5	0	9
	7	11	-13
4, 2	0	7	6
	2	8	-6
	4	0	1
	6	0	-3
4, 3	1	88	-86
	3	62	-60
	5	59	-60
	7	26	-26
4, 4	0	43	45
	2	98	96
	4	38	36
	6	32	33
4, 5	1	77	-76
	3	43	-43
	5	63	-62
	7	12	-18
4, 6	0	69	-69
	2	38	-39
	4	43	-46
	6	24	-27
4, 7	1	0	-2
	3	0	-5
	5	0	1
	7	0	-2
4, 8	0	135	134
	2	84	86
	4	96	92
	6	56	55
4, 9	1	64	62
	3	36	34
	5	53	52
4,10	0	16	-18
	2	49	-49
	4	18	-17
	6	18	-18
4,11	1	0	5
	3	0	0
	5	0	5
4,12	0	10	-7
	2	11	10
	4	8	-5
	6	0	1
4,13	1	0	-2
	3	11	9
	5	12	-13
4,14	0	101	-100
	2	66	-65
	4	73	-71
4,15	1	0	9
	3	14	15
4,16	0	30	28
	2	23	23
	4	24	23
4,17	1	60	55
	3	46	42
4,18	0	8	-12
	2	30	-31
5, 1	1	8	-10
	3	0	3
	5	18	-20
	7	8	7
5, 2	0	77	-77
	2	23	21
	4	53	-53
	6	8	-2
5, 3	1	107	-107
	3	71	-68
	5	85	-83
	7	24	-26
5, 4	0	0	5
	2	33	33
	4	0	5
	6	11	13
5, 5	1	15	17
	3	0	8
	5	21	19
	7	0	1
5, 6	0	132	129
	2	47	48
	4	93	89
	6	36	34
5, 7	1	27	-26
	3	43	-43
	5	0	3
5, 8	0	79	83
	2	32	30
	4	57	56
	6	20	22
5, 9	1	22	-21
	3	19	-19
	5	14	-13
5,10	0	28	-8
	2	35	34
	4	0	-6
	6	15	12
5,11	1	89	-89
	3	61	-60
	5	75	-71
5,12	0	25	-27
	2	21	22
	4	16	-19
5,13	1	0	-4
	3	0	3
	5	9	-7
5,14	0	53	50
	2	32	30
	4	40	38
5,15	1	8	6
	3	0	-4
5,16	0	41	41
	2	0	0
5,17	1	0	17
6, 0	0	137	-138
	2	133	-133
	4	108	-106
	6	69	-67
6, 1	1	9	12
	3	0	2
	5	0	8
6, 2	0	6	-4
	2	0	-5
	4	0	-3
	6	0	0
6, 3	1	57	57
	3	58	53
	5	36	35
6, 4	0	50	-49
	2	41	-40
	4	28	-28
	6	23	-23
6, 5	1	49	49
	3	46	51
	5	25	29
6, 6	0	30	31
	2	31	33
	4	26	27
	6	17	17
6, 7	1	0	2
	3	0	-0
	5	0	1
6, 8	0	72	-76
	2	72	-73
	4	62	-60
6, 9	1	37	-39
	3	43	-42
	5	20	-23
6,10	0	21	24
	2	19	18
	4	11	14
6,11	1	0	-3
	3	0	-4
6,12	0	12	2
	2	0	3
	4	8	4
6,13	1	0	0
	3	0	5
6,14	0	58	59
	2	55	59
6,15	1	12	-10
7, 1	1	0	4
	3	18	13
	5	8	-5
7, 2	0	14	-15
	2	50	50
	4	0	-4
7, 3	1	60	60
	3	72	71
	5	31	27
7, 4	0	27	-26
	2	0	-2
	4	16	-16
7, 5	1	0	-6
	3	0	-12
	5	0	-1
7, 6	0	39	-34
	2	75	-82
	4	32	-31
7, 7	1	21	23
	3	0	-1
	5	27	25
7, 8	0	0	-21
	2	55	-54
	4	20	-20
7, 9	1	16	18
	3	12	15
7,10	0	25	-25
	2	0	8
	4	17	-14
7,11	1	51	54
	3	62	62
7,12	0	18	-19
	0	16	-19
7,13	1	8	2
8, 0	0	82	77
	2	98	95
	4	54	55
8, 1	1	0	-4
	3	8	-2
8, 2	0	0	5
	2	0	8
	4	0	3
8, 3	1	40	-39
	3	34	-34
8, 4	0	33	34
	2	11	10
	4	21	25
8, 5	1	37	-35
	3	29	-32
8, 6	0	0	-14
	2	20	-23
8, 7	1	0	0
	3	0	1
8, 8	0	42	42
	2	50	54
8, 9	1	29	29
8,10	0	17	-16
	2	0	-3
9, 1	1	0	-12
9, 2	0	31	-33
	2	0	1
9, 3	1	44	-43
9, 4	0	0	2
	2	12	12
9, 5	1	0	5
9, 6	0	55	54

Three cycles of least-squares refinement resulted in an R value of 0.09 with anisotropic temperature factors for cesium and ruthenium and isotropic temperature factors for the chlorines and oxygen. A three-dimensional Fourier was run on the basis of the refined structure. This did not show any unexpected features. Some reflections were then remeasured and all of the atoms were allowed anisotropic temperature factors. Several more cycles of least squares were run, and the final value for R was 0.069.

The anisotropic parameters were introduced in the form $\exp(-\beta_{11}h^2 - \beta_{22}k^2 - \beta_{33}l^2 - 2\beta_{12}hk - 2\beta_{13}hl - 2\beta_{23}kl)$, with $4\beta_{ij} = a^*_i a^*_j B_{ij}$, where a^*_i is the length of the ith reciprocal axis. With this notation, the anisotropic thermal parameters B_{ij} are in units of A^2 which are used for isotropic thermal parameters B in the temperature factor of the form $\exp(-B\lambda^{-2} \sin^2 \theta)$. The atoms in special positions lie on perpendicular mirror planes, thus requiring that the axes of the ellipsoids of thermal vibration be parallel to the reciprocal axes. Therefore, for these atoms, $B_{12} = B_{13} = B_{23} = 0$.

The atomic coordinates are listed in Table II, and the anisotropic temperature factors in Table III. An electron density difference function was calculated following the last cycle of least-squares refinement. The largest peak corresponded to 0.79 electron/A^3.

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[4] L. H. Thomas and K. Umeda, *J. Chem. Phys.*, **26**, 293 (1957).

[5] "International Tables for X-ray Crystallography," Vol. III, The Kynoch Press, Birmingham, England, 1962.

TABLE II

ATOMIC COORDINATES FROM LEAST-SQUARES REFINEMENT[a]

Atom	x	y	z
Cs(1)	(0.2500)[b]	0.4715	(0.0)
Cs(2)	(0.2500)	0.7534	(0.0)
Ru	(0.2500)	0.1153	(0.0)
Cl(1)	(0.2500)	0.2490	(0.0)
Cl(2)	0.4605	0.1112	0.2222
O	(0.2500)	0.9936	(0.0)

[a] Standard deviations are $\sigma(y) = 0.0001$ for Cs and Ru, 0.0004 for Cl, and 0.002 for O. For Cl(2), $\sigma(x) = \sigma(z) = 0.0006$. [b] Parentheses indicate parameters which were subject to constraints.

TABLE III

ANISOTROPIC THERMAL PARAMETERS FOR $Cs_2RuCl_5H_2O$

Atom	B_{11}	B_{22}	B_{33}	B_{12}	B_{13}	B_{23}
Cs(1)	2.69	3.36	3.21	(0)[a]	(0)	(0)
Cs(2)	4.05	2.63	2.86	(0)	(0)	(0)
Ru	1.60	1.63	1.66	(0)	(0)	(0)
Cl(1)	3.54	1.26	2.90	(0)	(0)	(0)
Cl(2)	2.73	2.95	3.03	−0.13	−1.07	0.37
O	1.79	4.44	3.70	(0)	(0)	(0)

[a] Parentheses indicate parameters which were subject to constraints.

Description of the Structure

Figure 1 is a drawing of the unit cell in a clinographic projection. The octahedral environment of the ruthenium is shown in Figure 2. A list of the distances and angles including the estimated standard deviation is given in Tables IV and V.

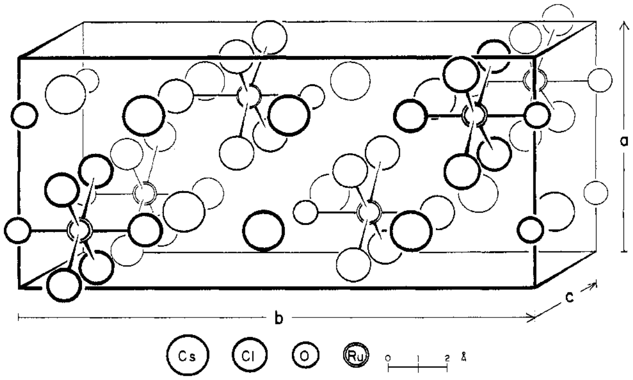

Figure 1.—Unit cell of $Cs_2RuCl_5H_2O$.

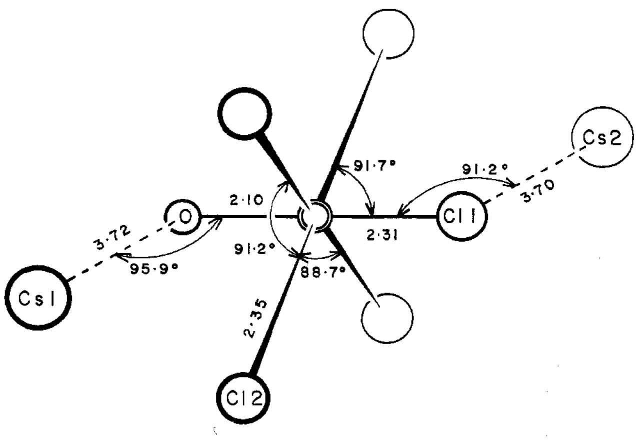

Figure 2.—Ruthenium environment in $Cs_2RuCl_5H_2O$.

TABLE IV

DISTANCES IN $Cs_2RuCl_5H_2O$

Atom 1 to atom 2	Distance, A	Atom 1 to atom 2	Distance, A
Ru–O	2.104 ± 0.028	Cs(2)–4Cl(2)	3.619 ± 0.004
Ru–Cl(1)	2.311 ± 0.008	Cs(2)–2Cl(1)	3.701 ± 0.002
Ru–4Cl(2)	2.353 ± 0.004	Cs(2)–O	4.153 ± 0.028
Ru–Cs(2)	4.404 ± 0.002	Cl(1)–4Cl(2)	3.347 ± 0.007
Ru–Cs(1)	4.458 ± 0.003	Cl(1)–O	4.415 ± 0.028
Cs(1)–4Cl(2)	3.408 ± 0.004	Cl(2)–O	3.109 ± 0.018
Cs(1)–4Cl(2)	3.590 ± 0.004	Cl(2)–Cl(2)	3.289 ± 0.008
Cs(1)–2O	3.720 ± 0.003	Cl(2)–Cl(2)	3.363 ± 0.008
Cs(1)–Cl(1)	3.848 ± 0.008	O–2O	3.999 ± 0.004
Cs(1)–Cs(1)	4.113 ± 0.003		

TABLE V

BOND ANGLES IN $Cs_2RuCl_5H_2O$

Atom 1–atom 2–atom 3	Angle, deg
Cl(2)–Ru–O	88.3 ± 0.1
Cl(2)–Ru–Cl(2)	91.2 ± 0.2
Cl(2)–Ru–Cl(2)	88.7 ± 0.2
Cl(2)–Ru–Cl(1)	91.7 ± 0.1
Cs(1)–O–Cs(2)	84.1 ± 0.4
Cs(1)–O–Ru	95.9 ± 0.4

The ruthenium atom lies out of the plane of the four Cl(2) atoms a distance of 0.07 A, and the resulting Cl(1)–Ru–Cl(2) angles differ from 90° by several times the estimated standard deviation. In addition, the Cl(2) atoms lie on the corners of a rectangle instead of a square. Thus, the point group at the ruthenium is 2mm instead of the more symmetrical group 4mm. In the potassium salt,[3] the point group at the ruthenium is 1. The four chlorines do not lie in a plane, and the ruthenium lies on a line through two of the chlorines, rather than on the chlorine–oxygen line. The space group of the potassium salt is Pnma with $Z = 4$.

A review of Ru–Cl and Ru–O distances is given in the paper by Khodashova on the potassium salt. We may note here, however, that in the cesium salt the average Ru–Cl and Ru–O distances are the same as those found for the potassium salt, within the limits of the reported experimental errors: 2.10 ± 0.03 A compared with 2.12 ± 0.05 A, and 2.34 ± 0.005 A compared with 2.35 ± 0.02 A. In both cases, the Ru–Cl bond opposite the Ru–O bond was found to be shorter by about 0.05 A compared to the remaining Ru–Cl bonds.

The hydrogen atoms were not included in the calculation. A plausible location for hydrogen is at (0.34, 0.96, 0.00), a position in which each hydrogen is near two Cl(2) atoms of an adjacent molecule. This position coincides with a positive region of the electron density difference function, but we do not claim that this function is good enough to establish the hydrogen location. This structure for the hydrogen atoms would provide an explanation for the rectangular shape of the four Cl(2) atoms in the molecule, since it places the hydrogen atoms adjacent to the smaller Cl–Ru–Cl angles. Another explanation in terms of a Jahn–Teller distortion was suggested by a referee, but we see no necessity for it in this case.