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The Crystal Structure of Mercury(II) Chromate Hemihydrate $HgCrO_4.\frac{1}{2}H_2O$

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The crystal structure of $HgCrO_4.\frac{1}{2}H_2O$, space group $C2/c$, has been determined from single crystal X-ray photographic intensity data (1702 independent reflections). The unit cell contains eight formula units and has the dimensions $a = 11.832(1)$, $b = 5.2616(6)$, $c = 14.637(2)$ Å, $\beta = 121.01(1)°$, and $V = 911.2(1)$ Å^3.

Every mercury atom is only bonded to two oxygen atoms, each belonging to a chromate tetrahedron, at the distances 2.05(2) and 2.06(2) Å. The angle O–Hg–O is 176.2(9)°. As each mercury atom is bonded to two chromate groups and each chromate group bonded to two mercury atoms, the structure is built up of endless chains of the composition $(HgCrO_4)_n$. There are four crystallographically equivalent chains running through the unit cell parallel to the diagonals of the *ab*-plane. The chromate tetrahedra are slightly distorted. The distances Cr–O for such oxygen atoms that are bonded to mercury are elongated. The water molecules of the unit cell are situated in cavities between the chains. Possible hydrogen bonds are discussed.

Studies on the crystal chemistry of mercury(II) have revealed that the fundamental building elements of the oxides and some oxide halides are infinite chains $-O-Hg-O-$.[1] Only a few accurately determined crystal structures of mercury(II) salts containing tetrahedral anions are hitherto known[2] and in none of them infinite chains are reported. In order to find out whether chains $-O-Hg-O-$ are compatible with the presence of tetrahedral anions, the crystal structure of the compound $HgCrO_4.\frac{1}{2}H_2O$ has now been determined.

STRUCTURE DETERMINATION

The present author has previously reported the existence of the compound $HgCrO_4.\frac{1}{2}H_2O$.[3] The preparation and the analysis, the cell dimensions and space group of the compound were given in the earlier report. The cell parameters of the monoclinic unit cell have now been refined by the method of least-squares and are as follows: $a = 11.832 \pm 0.001$ Å, $b = 5.2616 \pm 0.0006$ Å,

$c = 14.637 \pm 0.002$ Å, and $\beta = 121.01° \pm 0.01°$. The observed density was 5.51 and the calculated value 5.52 g cm^{-3}, assuming a cell content of eight formula units. The systematically absent spectra were hkl with $h+k=2n+1$ and $h0l$ with $l=2n+1$ which is characteristic of the space groups Cc (No. 9) and $C2/c$ (No. 15) as numbered by the International Tables.[4]

SINGLE CRYSTAL WORK AND DATA REDUCTION

Zr-filtered MoK radiation was used for the single crystal work. The reflections $h0l - h9l$ were registered with the aid of an integrating Weissenberg camera. The multiple film technique was used, with three films interleaved by steel foils of thickness 0.005 cm. The integrated spots of the films were visually compared with a calibrated scale. As the linear absorption coefficient for the compound is 428 cm^{-1} for the radiation used,[5] it was necessary to correct for the absorption. A suitable single crystal was ground to a sphere using an apparatus described by Buerger.[6] From the grinding a slightly ellipsoidal specimen resulted with the axes 0.023 and 0.025 cm. A mean value of 0.024 cm was used as the diameter of the "sphere" and a μR value of 5.2 was obtained. The absorption correction factors were obtained from graphical interpolation between the values given for $\mu R = 5.2$ in the International Tables.[7] The corrections for Lorentz and polarization effects were performed in the usual way.

POSITIONS OF THE ATOMS

A three-dimensional Patterson function (program *DRF*) was used to find preliminary positions of the mercury and chromium atoms. Approximate layer line scale factors for this calculation were obtained from the exposure times of the photographs. The Patterson sections were interpreted assuming the space group to be $C2/c$, with the mercury and the chromium atoms occupying general point positions 8(f). The solution of the problem was somewhat complicated by the fact that the parameters of the mercury atoms were $x \sim 0$, $y \sim 0$, and $z \sim \frac{1}{8}$. The parameters of the chromium atoms were found to be $x = 0.20$, $y = 0.43$, and $z = 0.10$. A least-squares refinement (program *LALS*) was then carried out, based on the approximate positions of the mercury and the chromium atoms and on all the 1702 observed independent reflections. The resulting R-factor was 13.7 %. Isotropic temperature factors were used at this stage. Following this, three-dimensional Fourier-sections were calculated, with the contributions of the mercury and of the chromium atoms subtracted. Apart from maxima in the vicinity of the subtracted mercury atoms all remaining large peaks could be interpreted as resulting from oxygen atoms. The positions of the light atoms thus arrived at yielded reasonable oxygen – oxygen as well as oxygen – metal distances. The angles O – Cr – O were nearly tetrahedral. As the peaks in the sections were distinct and as the interatomic distances and angles were reasonable it was assumed that the space group $C2/c$ was the correct one or that the deviations from $C2/c$ to Cc must be very small.

The intensities of the strongest and of the weakest reflections were considered rather uncertain due to the photographic method. Therefore, 23 out of 1702 reflections were omitted in the following calculations. The parameters of all atoms were refined using isotropic temperature factors, giving a final R-value of 11.0 %. The isotropic temperature factors obtained, 0.7 and 0.5 for the mercury and chromium atoms, and 1.1 – 1.4 for the oxygen atoms, respectively, do not contradict the assumption of the space group $C2/c$.

A least-squares refinement was then performed using anisotropic temperature factors for the mercury atoms and isotropic ones for the chromium and oxygen atoms. The resulting R-factor was reduced from 11.0 to 10.1 %. The anisotropic thermal movement of the mercury atoms is significant at

Table 1. Final positional and thermal parameters for $HgCrO_4 \cdot \frac{1}{2}H_2O$. The anisotropic thermal parameters for the mercury and chromium atoms are based on the expression $\exp -(h^2\beta_{11}+k^2\beta_{22}+l^2\beta_{33}+hk\beta_{12}+hl\beta_{13}+kl\beta_{23})$. The root-mean-square components R_i (Å) of thermal vibration along principal axes of the ellipsoids of vibration of the mercury atoms. Standard deviations are given within brackets.

	x	y	z	B (Å^2)
Hg	−0.00126(10)	0.02676(12)	0.12468(8)	–
Cr	0.19990(31)	0.43854(42)	0.09891(24)	–
O(1)	0.3687(17)	0.3925(27)	0.1646(14)	1.11(16)
O(2)	0.1610(20)	0.6187(31)	0.1660(16)	1.44(21)
O(3)	0.1195(17)	0.1562(28)	0.0728(14)	1.10(17)
O(4)	0.1494(20)	0.5757(35)	−0.0161(16)	1.53(22)
O(5)	0	0.3989(44)	1/4	1.38(28)

	β_{11}	β_{22}	β_{33}	β_{12}	β_{13}	β_{23}
Hg	0.00244(4)	0.00775(15)	0.00128(3)	−0.00215(21)	0.00200(5)	−0.00029(15)
Cr	0.00166(17)	0.00334(49)	0.00087(11)	−0.00070(40)	0.00124(23)	0.00010(30)

Atom	R_1	R_2	R_3
Hg	0.125(3)	0.092(3)	0.101(2)

Table 2. The weighting scheme used in the last cycle of the least-squares refinement. The averages $w(|F_o|-|F_c|)^2 = w\Delta^2$ are normalized. $w = (52.00 + |F_o| + 0.0040|F_o|^2 + 0.00010|F_o|^3)^{-1}$. $R = 10.1$ % (1679 independent reflections).

$\lvert F_o\rvert$ interval	$\overline{w\Delta^2}$	No. of reflections	$\sin\theta$ interval	$\overline{w\Delta^2}$	No. of reflections
0.0 – 67.9	1.10	163	0.00 – 0.39	1.32	348
67.9 – 80.2	1.06	168	0.39 – 0.50	0.68	319
80.2 – 88.8	1.02	167	0.50 – 0.57	0.60	297
88.8 – 98.8	1.10	172	0.57 – 0.63	0.67	263
98.8 – 109.5	1.10	166	0.63 – 0.67	0.55	189
109.5 – 123.5	0.98	169	0.67 – 0.72	0.80	152
123.5 – 145.8	0.81	168	0.72 – 0.75	0.86	69
145.8 – 172.2	1.05	169	0.75 – 0.79	1.46	27
172.2 – 223.8	0.92	168	0.79 – 0.82	2.50	11
223.8 – 495.9	0.86	169	0.82 – 0.85	0.55	4

Table 3.

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
0	0	0	540.9	449.5	10	0	-10	87.5	58.0	1	1	3	100.9	78.9	3	1	-12	367.5	291.9
4	0	0	374.0	445.1	12	0	-10	83.0	77.1	5	1	3	93.4	73.3	5	1	-12	510.0	432.9
8	0	0	451.1	552.1	2	0	-12	417.0	364.6	1	1	4	518.2	518.4 *	7	1	-12	426.1	347.1
1	0	0	285.9	349.1	4	0	-12	516.5	473.1 *	3	1	4	685.4	583.2 *	9	1	-12	249.2	267.5
10	0	0	335.4	355.3	6	0	-12	253.1	226.8	5	1	4	312.5	270.7	11	1	-12	356.9	391.0
12	0	0	214.2	194.7	8	0	-12	376.7	401.2	7	1	4	387.1	360.4	13	1	-12	220.9	235.6
14	0	0	232.1	217.8	10	0	-12	294.1	316.4	9	1	4	350.8	308.7	15	1	-12	196.0	218.1
16	0	0	186.0	169.2	12	0	-12	234.9	267.8	11	1	4	172.9	169.1	17	1	-12	171.2	190.8
18	0	0	107.9	95.0	14	0	-12	236.2	279.8	13	1	4	200.3	208.2	19	1	-12	115.4	139.4
20	0	0	106.0	113.1	16	0	-12	161.2	152.6	15	1	4	104.8	113.2	21	1	-12	126.4	146.6
22	0	0	70.9	67.9	18	0	-12	210.8	196.8	17	1	4	97.7	110.3	23	1	-12	61.8	66.2
2	0	2	202.5	168.0	22	0	-12	114.7	101.3	19	1	4	76.7	86.1	25	1	-12	67.8	79.8
4	0	2	149.9	118.1	24	0	-12	99.2	91.2	3	1	5	83.1	73.2	1	1	-13	79.2	64.1
6	0	2	91.6	73.4	2	0	-14	61.3	49.9	5	1	6	66.1	62.9	7	1	-13	64.3	49.1
14	0	2	64.1	55.3	4	0	-14	113.3	78.2	7	1	6	102.6	84.9	5	1	-14	72.8	63.2
0	0	4	502.8	612.4 *	6	0	-14	61.0	38.3	1	1	7	174.7	126.7	7	1	-14	59.3	50.7
2	0	4	427.0	476.5	10	0	-14	61.3	51.8	5	1	7	52.6	59.4	9	1	-14	94.5	73.1
4	0	4	480.4	598.6	12	0	-14	85.7	74.1	1	1	8	374.6	296.3	3	1	-15	81.3	64.3
6	0	4	418.1	349.2	2	0	-16	312.0	298.8	3	1	8	503.9	429.7 *	1	1	-16	326.7	299.4
8	0	4	241.0	212.9	4	0	-16	308.6	320.8	5	1	8	367.2	276.4	3	1	-16	252.1	216.1
10	0	4	310.4	313.7	6	0	-16	268.6	227.5	7	1	8	228.7	212.7	5	1	-16	348.7	303.5
12	0	4	190.3	161.2	8	0	-16	345.4	339.3	9	1	8	245.0	239.4	7	1	-16	295.1	253.1
14	0	4	133.6	120.3	10	0	-16	256.9	201.7	11	1	8	131.4	132.4	9	1	-16	313.2	273.7
16	0	4	153.2	149.2	12	0	-16	285.9	290.7	13	1	8	133.2	152.3	11	1	-16	308.9	293.8
18	0	4	67.6	72.4	14	0	-16	248.4	212.7	15	1	8	73.5	86.9	13	1	-16	197.5	177.5
20	0	4	85.4	78.1	16	0	-16	183.5	194.5	17	1	8	63.6	67.4	15	1	-16	221.9	238.6
2	0	6	94.0	66.0	18	0	-16	223.8	226.4	19	1	8	55.4	73.8	17	1	-16	154.5	160.5
4	0	6	194.2	140.1	20	0	-16	119.5	107.2	3	1	10	101.9	78.6	19	1	-16	168.3	143.9
10	0	6	118.1	90.2	22	0	-16	116.1	114.6	1	1	11	79.5	69.3	21	1	-16	124.3	138.9
0	0	8	478.7	448.4	24	0	-16	124.7	95.4	11	1	11	48.3	32.6	25	1	-16	75.3	93.7
2	0	8	485.9	453.9	26	0	-16	71.3	57.4	1	1	12	301.8	257.5	1	1	-17	47.9	44.5
4	0	8	315.1	297.6	28	0	-16	65.1	67.6	3	1	12	311.1	278.2	7	1	-17	96.2	82.4
6	0	8	353.1	335.7	6	0	-18	86.1	52.9	5	1	12	259.2	248.6	1	1	-20	190.0	189.4
8	0	8	214.9	186.1	2	0	-20	243.1	230.1	7	1	12	151.6	154.5	3	1	-20	167.6	168.5
10	0	8	222.4	215.0	4	0	-20	199.4	170.4	9	1	12	177.9	182.6	5	1	-20	247.5	246.6
12	0	8	170.0	169.9	6	0	-20	237.6	203.2	11	1	12	89.5	98.9	7	1	-20	197.1	179.1
14	0	8	77.5	57.5	8	0	-20	275.5	269.3	13	1	12	79.2	106.3	9	1	-20	249.3	250.0
16	0	8	111.5	116.2	10	0	-20	212.9	175.6	1	1	14	47.2	50.0	11	1	-20	221.6	225.5
0	0	10	170.1	73.2 *	12	0	-20	267.0	235.5	3	1	14	55.4	57.1	13	1	-20	170.1	161.1
3	0	12	298.3	243.0	14	0	-20	192.2	165.9	1	1	15	47.6	42.5	15	1	-20	206.7	222.5
2	0	12	387.4	329.1	16	0	-20	201.1	177.6	1	1	16	219.5	190.6	17	1	-20	136.0	138.4
4	0	12	241.1	217.6	18	0	-20	179.1	171.2	3	1	16	160.9	160.8	19	1	-20	141.0	151.6
6	0	12	234.2	211.8	22	0	-20	161.2	127.7	5	1	16	191.0	202.9	21	1	-20	101.6	115.9
8	0	12	167.0	145.6	24	0	-20	63.0	61.7	7	1	16	87.7	98.9	23	1	-20	82.0	78.2
10	0	12	141.2	124.7	26	0	-20	99.2	84.2	9	1	16	104.0	110.2	25	1	-20	86.3	101.0
12	0	12	133.4	137.7	28	0	-20	74.0	61.4	1	1	20	175.1	171.1	1	1	-24	97.7	109.6
14	0	12	81.3	76.8	8	0	-22	63.7	55.2	3	1	20	87.4	104.0	3	1	-24	110.4	127.5
0	0	14	89.9	56.8	2	0	-24	165.3	161.3	5	1	20	108.7	139.0	5	1	-24	159.1	166.7
1	0	14	77.5	65.3	4	0	-24	134.6	113.4	1	1	24	103.3	129.9	7	1	-24	120.4	129.1
0	0	16	197.7	139.3	6	0	-24	210.1	177.2	1	1	28	72.4	90.9	9	1	-24	189.6	198.6
2	0	16	234.9	212.8	8	0	-24	197.3	176.4	3	1	-1	99.1	91.2	11	1	-24	138.5	133.8
4	0	16	167.0	147.1	10	0	-24	155.7	137.0	5	1	-1	99.1	92.8	13	1	-24	150.2	148.2
6	0	16	170.9	161.0	12	0	-24	232.0	203.8	9	1	-1	88.4	90.1	15	1	-24	168.3	181.4
8	0	16	148.6	143.0	14	0	-24	169.4	128.9	7	1	-2	78.1	71.6	17	1	-24	105.1	101.3
12	0	16	77.9	96.0	16	0	-24	183.5	166.1	11	1	-2	71.0	60.9	19	1	-24	119.0	134.8
0	0	20	156.3	139.5	18	0	-24	165.3	138.0	1	1	-3	146.7	128.0	21	1	-24	88.8	94.1
2	0	20	168.4	146.9	20	0	-24	100.6	77.5	9	1	-3	60.4	56.6	23	1	-24	70.3	85.8
4	0	20	102.6	109.4	22	0	-24	154.3	125.1	1	1	-4	628.9	566.6 *	25	1	-24	70.0	82.2
6	0	20	90.6	106.2	24	0	-24	54.9	69.7	3	1	-4	525.6	513.2 *	3	1	-28	70.0	106.0
8	0	24	102.6	101.5	26	0	-24	80.6	72.0	5	1	-4	440.3	460.1	5	1	-28	92.3	111.4
2	0	24	99.9	108.7	2	0	-28	86.1	103.6	7	1	-4	511.4	540.3 *	7	1	-28	81.0	92.2
4	0	24	74.0	92.6	4	0	-28	57.5	69.2	9	1	-4	261.4	230.1	9	1	-28	105.8	104.8
0	0	28	53.7	75.5	6	0	-28	147.4	142.6	11	1	-4	293.3	316.1	11	1	-28	83.1	96.8
4	0	-2	189.4	206.8	8	0	-28	118.1	104.1	13	1	-4	260.6	274.8	13	1	-28	112.6	133.4
6	0	-2	120.5	89.5	10	0	-28	119.4	105.5	15	1	-4	158.0	173.6	15	1	-28	100.5	121.9
8	0	-2	118.1	98.8	12	0	-28	174.2	145.1	17	1	-4	181.8	191.0	17	1	-28	86.3	91.2
14	0	-2	74.0	59.0	14	0	-28	108.5	101.0	19	1	-4	83.5	94.1	19	1	-28	99.4	118.7
18	0	-2	63.7	48.7	16	0	-28	142.6	133.4	21	1	-4	88.1	104.1	21	1	-28	57.2	59.9
2	0	-4	304.8	356.6	18	0	-28	97.5	83.9	23	1	-4	73.2	78.7	23	1	-28	64.3	99.2
4	0	-4	405.7	588.8	20	0	-28	90.6	96.2	1	1	-5	107.2	90.9					
6	0	-4	329.2	466.8	22	0	-28	125.7	101.7	3	1	-5	157.3	139.6	2	2	0	307.9	402.4
8	0	-4	309.9	408.7	24	0	-28	57.9	47.1	5	1	-5	100.1	103.5	4	2	0	371.3	440.8
10	0	-4	282.4	365.6	26	0	-28	75.9	72.1	1	1	-6	151.6	108.9	6	2	0	384.9	425.1
12	0	-4	221.8	193.7	6	0	-32	69.9	94.7	11	1	-6	80.3	77.1	8	2	0	250.8	276.2
14	0	-4	258.3	286.9	10	0	-32	99.3	98.8	15	1	-6	70.7	74.9	10	2	0	269.5	305.5
16	0	-4	166.3	169.5	12	0	-32	101.2	93.1	1	1	-7	58.2	51.5	12	2	0	195.5	191.5
18	0	-4	117.1	118.5	14	0	-32	76.4	74.1	5	1	-7	143.9	127.7	14	2	0	179.2	189.3
20	0	-4	124.7	128.1	16	0	-32	111.6	108.5	9	1	-7	51.5	53.3	16	2	0	130.1	143.4
22	0	-4	58.5	61.4	18	0	-32	68.9	60.2	1	1	-8	576.7	470.2 *	20	2	0	92.0	100.7
24	0	-4	62.7	77.7	20	0	-32	80.6	90.3	3	1	-8	480.1	410.6	2	2	1	156.7	134.4
8	0	-6	135.7	99.0	22	0	-32	61.5	71.3	5	1	-8	512.9	448.5 *	4	2	1	113.1	134.5
10	0	-6	90.2	89.8						7	1	-8	443.9	453.4	8	2	1	124.8	115.8
12	0	-6	69.6	64.1	3	1	0	564.6	662.4 *	9	1	-8	262.1	203.2	2	2	2	88.6	61.0
2	0	-8	363.7	345.8	5	1	0	306.8	297.3	11	1	-8	345.0	374.0	0	2	3	82.4	72.6
4	0	-8	533.8	638.7 *	7	1	0	424.0	498.7	13	1	-8	216.9	246.6	2	2	3	209.4	186.7
6	0	-8	382.6	420.9	9	1	0	331.7	328.7	15	1	-8	175.8	200.6	4	2	3	83.1	71.2
8	0	-8	353.0	430.7	11	1	0	229.0	233.6	17	1	-8	176.1	200.5	6	2	3	106.3	105.2
10	0	-8	273.1	339.3	13	1	0	253.5	228.2	19	1	-8	97.3	101.6	8	2	3	141.0	119.7
12	0	-8	251.4	272.0	15	1	0	130.7	137.0	21	1	-8	117.5	132.4	12	2	3	104.9	86.0
14	0	-8	284.4	334.9	17	1	0	154.5	161.3	23	1	-8	65.3	76.3	0	2	4	495.9	516.2
16	0	-8	171.1	147.6	19	1	0	82.7	83.3	3	1	-9	166.5	127.9	2	2	4	410.1	387.5
18	0	-8	207.7	165.4	21	1	0	64.3	65.0	9	1	-9	73.9	72.3	4	2	4	367.9	357.6
20	0	-8	168.1	149.6	23	1	0	59.7	71.8	3	1	-10	131.7	99.2	6	2	4	386.9	366.0
22	0	-8	140.2	80.7	3	1	1	90.9	77.9	5	1	-10	154.1	116.7	8	2	4	214.6	214.0
24	0	-8	104.0	89.7	5	1	1	92.3	79.3	7	1	-10	93.7	74.0	10	2	4	226.2	249.9
26	0	-8	76.8	59.6 *	11	1	1	74.2	67.3	11	1	-10	99.7	90.3	12	2	4	156.7	165.9
2	0	-10	199.0	135.1	1	1	2	223.0	160.2	15	1	-10	61.8	59.7	14	2	4	150.6	127.9
4	0	-10	133.3	60.6 *	7	1	2	101.2	91.1	5	1	-11	72.4	63.9	16	2	4	128.1	129.0
8	0	-10	156.7	129.9	11	1	2	77.4	68.0	1	1	-12	432.9	338.7	18	2	4	104.9	83.6

Table 3. Continued.

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
0	2	5	134.9	114.9
4	2	5	208.5	196.1
2	2	6	111.0	97.6
4	2	6	117.2	94.9
2	2	7	127.6	110.6
4	2	7	97.4	83.6
8	2	7	115.0	95.1
0	2	8	449.6	410.5
2	2	8	396.5	368.2
4	2	8	252.1	240.8
6	2	8	297.1	295.4
8	2	8	194.5	187.7
10	2	8	179.9	177.6
12	2	8	134.9	142.2
0	2	9	115.0	85.4
4	2	9	146.5	123.8
0	2	10	96.7	86.2
2	2	11	118.5	99.5
4	2	11	102.9	102.2
8	2	11	99.5	84.6
0	2	12	303.2	283.2
2	2	12	327.7	292.6
4	2	12	175.3	185.7
6	2	12	213.9	208.8
8	2	12	150.6	144.4
10	2	12	105.6	117.3
12	2	12	102.2	117.3
0	2	13	143.7	125.5
0	2	15	81.7	63.0
0	2	16	170.3	178.4
2	2	16	214.6	227.1
4	2	16	132.2	140.8
6	2	16	135.6	137.4
8	2	16	109.7	119.6
0	2	17	98.8	76.2
0	2	19	83.8	66.9
0	2	20	124.7	123.3
2	2	20	139.7	146.5
4	2	20	103.5	109.1
6	2	-1	185.3	202.7
12	2	-1	145.8	120.0
4	2	-2	83.8	93.3
6	2	-2	87.2	86.9
8	2	-2	87.9	74.0
2	2	-3	201.6	239.3
6	2	-3	158.0	171.6
2	2	-4	367.9	394.2
4	2	-4	459.8	532.9
6	2	-4	310.6	360.5
8	2	-4	285.4	331.3
10	2	-4	310.0	350.7
12	2	-4	197.6	202.6
14	2	-4	218.0	228.6
16	2	-4	154.0	153.5
18	2	-4	130.1	119.5
20	2	-4	121.3	115.1
2	2	-5	209.8	199.2
6	2	-5	196.2	219.2
8	2	-5	68.1	65.9
12	2	-5	129.4	118.7
8	2	-6	87.2	87.6
2	2	-7	207.1	189.8
6	2	-7	89.2	71.4
8	2	-7	140.3	156.8
2	2	-8	351.5	332.2
4	2	-8	506.2	475.0 *
6	2	-8	306.6	337.4
8	2	-8	331.8	374.6
10	2	-8	287.5	321.6
12	2	-8	218.7	233.2
14	2	-8	222.8	259.6
16	2	-8	144.6	151.4
18	2	-8	167.6	156.8
20	2	-8	123.3	123.2
24	2	-8	92.0	81.4
2	2	-9	133.5	125.8
4	2	-9	96.1	69.7
6	2	-9	130.8	113.3
10	2	-9	139.0	132.6
12	2	-9	87.9	75.5
16	2	-9	91.3	77.3
8	2	-10	83.1	70.1
2	2	-11	136.9	127.9
4	2	-11	74.9	62.3
6	2	-11	148.5	124.9
8	2	-11	68.8	59.4
12	2	-11	102.2	91.4
2	2	-12	302.5	301.3
4	2	-12	355.6	364.3
6	2	-12	285.4	259.1
8	2	-12	352.2	363.9
10	2	-12	250.7	268.0
12	2	-12	224.1	233.2
14	2	-12	231.6	249.7
16	2	-12	153.3	157.2
18	2	-12	163.5	172.6
20	2	-12	118.5	112.1
22	2	-12	88.6	92.3
24	2	-12	95.4	87.9
2	2	-13	100.1	78.4
4	2	-13	78.3	64.8
6	2	-13	110.1	88.0
8	2	-13	78.3	72.5
10	2	-13	147.1	140.8
16	2	-13	98.4	82.7
2	2	-15	80.4	66.3
6	2	-15	145.1	115.6
10	2	-15	62.0	47.9
12	2	-15	89.2	76.9
2	2	-16	243.9	245.7
4	2	-16	274.5	268.3
6	2	-16	233.5	231.5
8	2	-16	322.2	292.9
10	2	-16	222.1	210.0
12	2	-16	235.8	248.3
14	2	-16	216.4	210.9
16	2	-16	154.9	152.5
18	2	-16	155.3	179.2
20	2	-16	98.4	104.2
22	2	-16	95.4	107.3
24	2	-16	67.4	85.1
4	2	-17	82.4	75.9
10	2	-17	121.9	107.5
6	2	-19	98.1	83.1
10	2	-19	90.6	80.2
12	2	-19	74.3	47.6
2	2	-20	194.8	200.4
4	2	-20	154.0	170.3
6	2	-20	166.9	136.2
8	2	-20	223.4	225.0
10	2	-20	148.5	162.7
12	2	-20	205.1	215.3
14	2	-20	149.1	163.4
16	2	-20	140.3	149.9
18	2	-20	144.4	153.3
22	2	-20	100.1	114.7
10	2	-21	74.9	55.8
14	2	-21	92.0	87.2
2	2	-24	109.0	144.2
4	2	-24	98.1	111.9
6	2	-24	134.2	152.7
8	2	-24	134.9	142.7
10	2	-24	133.5	135.7
12	2	-24	158.7	176.4
14	2	-24	111.7	115.9
16	2	-24	138.1	162.2
18	2	-24	131.5	125.6
20	2	-24	94.0	88.2
22	2	-24	101.5	105.0
6	2	-28	103.5	118.3
10	2	-28	100.8	105.0
12	2	-28	100.8	124.1
14	2	-28	93.3	88.9
16	2	-28	104.9	121.2
18	2	-28	83.8	86.2
22	2	-28	81.7	86.2
1	3	0	272.9	365.4
3	3	0	321.9	433.1
5	3	0	318.1	332.9
7	3	0	303.5	312.7
9	3	0	239.9	224.3
11	3	0	221.5	210.8
13	3	0	195.5	197.2
15	3	0	124.2	113.4
17	3	0	116.5	111.6
19	3	0	104.2	83.4
1	3	1	176.3	226.2
3	3	1	73.6	85.2
5	3	1	168.6	195.5
7	3	1	93.5	71.3
11	3	1	143.3	129.0
1	3	3	128.8	128.7
5	3	3	220.0	212.3
7	3	3	75.1	63.1
9	3	3	118.0	113.1
11	3	3	80.5	77.7
1	3	4	282.8	288.0
3	3	4	331.9	343.1
5	3	4	306.6	293.3
7	3	4	273.6	262.4
9	3	4	195.5	199.3
11	3	4	157.1	151.0
13	3	4	154.8	158.6
15	3	4	113.4	99.2
1	3	5	213.1	195.1
3	3	5	97.3	98.0
5	3	5	89.7	78.0
7	3	5	109.6	94.4
1	3	7	236.1	211.5
3	3	7	179.4	159.2
7	3	7	97.3	81.7
9	3	7	99.6	84.8
11	3	7	92.0	86.0
1	3	8	293.6	259.4
3	3	8	289.7	277.6
5	3	8	224.6	232.1
7	3	8	212.3	195.8
9	3	8	178.6	182.2
11	3	8	108.8	114.2
1	3	9	158.7	144.0
3	3	9	101.2	83.2
7	3	9	120.3	118.4
1	3	11	184.7	168.5
5	3	11	99.6	106.9
7	3	11	100.4	81.5
1	3	12	234.5	224.4
3	3	12	229.9	211.7
5	3	12	167.9	171.8
7	3	12	116.5	111.7
9	3	12	117.3	143.5
11	3	12	90.4	86.9
3	3	13	90.4	66.7
1	3	15	134.9	120.3
1	3	16	169.4	176.6
3	3	16	154.9	153.3
5	3	16	117.3	117.3
1	3	20	124.2	129.6
1	3	-1	90.4	104.2
5	3	-1	168.6	201.9
5	3	-1	181.7	196.3
9	3	-1	199.3	194.2
13	3	-1	99.6	89.6
1	3	-3	190.1	229.1
5	3	-3	170.9	178.8
9	3	-3	105.2	102.6
11	3	-3	102.7	98.3
1	3	-4	341.8	426.5
3	3	-4	309.7	413.1
5	3	-4	259.8	296.7
7	3	-4	304.3	338.1
9	3	-4	207.7	254.1
11	3	-4	226.1	250.5
13	3	-4	174.8	223.2
15	3	-4	141.4	132.8
17	3	-4	131.1	148.9
19	3	-4	108.1	97.0
3	3	-5	228.1	284.1
5	3	-5	156.9	164.2
9	3	-5	150.2	138.6
13	3	-5	119.6	113.1
1	3	-6	42.0	36.2
3	3	-6	73.6	69.6
1	3	-7	136.0	135.4
3	3	-7	83.5	74.5
5	3	-7	220.0	227.0
9	3	-7	136.4	139.3
1	3	-8	379.4	391.2
3	3	-8	334.2	332.8
5	3	-8	290.5	277.5
7	3	-8	331.1	340.9
9	3	-8	265.2	282.0
11	3	-8	231.5	261.0
13	3	-8	169.4	148.3
15	3	-8	158.7	171.5
17	3	-8	149.5	162.1
19	3	-8	117.3	109.6
1	3	-9	78.9	68.6
3	3	-9	234.5	220.3
5	3	-9	85.1	79.4
7	3	-9	142.6	135.3
9	3	-9	173.2	173.0
13	3	-9	137.2	144.6
1	3	-11	98.1	91.4
3	3	-11	89.7	75.9
5	3	-11	141.8	128.9
9	3	-11	151.0	133.2
13	3	-11	89.7	77.7
1	3	-12	291.3	281.4
3	3	-12	254.5	233.3
5	3	-12	301.2	276.6
7	3	-12	295.9	290.3
9	3	-12	229.2	244.5
11	3	-12	231.5	239.4
13	3	-12	160.2	176.7
15	3	-12	167.9	193.6
17	3	-12	149.5	156.0
19	3	-12	92.0	99.7
21	3	-12	92.9	105.9
3	3	-13	175.5	152.2
7	3	-13	158.7	138.4
9	3	-13	121.9	104.3
11	3	-13	88.1	79.5
13	3	-13	138.7	122.0
17	3	-13	109.6	106.0
19	3	-13	92.7	54.0
3	3	-15	153.3	131.2
5	3	-15	96.6	86.5
9	3	-15	141.0	129.5
13	3	-15	90.4	97.9
1	3	-16	213.1	197.8
3	3	-16	192.4	184.3
5	3	-16	261.4	252.5
7	3	-16	221.5	218.8
9	3	-16	203.1	204.3
11	3	-16	224.6	216.0
13	3	-16	172.5	172.2
15	3	-16	174.8	189.3
17	3	-16	131.1	135.1
19	3	-16	109.6	108.1
21	3	-16	106.5	112.5
1	3	-17	100.4	87.0
3	3	-17	90.4	82.0
7	3	-17	154.1	163.1
11	3	-17	90.4	82.8
13	3	-17	129.5	117.4
17	3	-17	92.7	98.7
3	3	-19	108.8	103.4
13	3	-19	101.2	96.6
1	3	-20	138.0	135.5
3	3	-20	149.5	148.2
5	3	-20	197.7	194.1
7	3	-20	147.9	149.0
9	3	-20	164.8	167.1
11	3	-20	184.7	179.9
13	3	-20	149.5	152.2
15	3	-20	154.8	153.3
17	3	-20	117.3	111.8
19	3	-20	122.6	117.9
21	3	-20	105.0	100.3
7	3	-21	117.3	104.1
11	3	-21	101.2	86.4
13	3	-21	72.0	63.7
17	3	-21	92.0	81.4
5	3	-24	100.4	130.4
7	3	-24	116.5	109.9
9	3	-24	130.3	142.9
11	3	-24	130.3	132.5
13	3	-24	124.2	125.9
15	3	-24	115.7	122.4
17	3	-24	107.3	97.2
19	3	-24	105.0	114.4
21	3	-24	93.5	80.4
11	3	-25	100.4	97.0
9	3	-28	102.7	109.4
11	3	-28	87.4	86.5
13	3	-28	95.0	97.7
15	3	-28	101.2	93.4
2	4	0	190.0	297.9
4	4	0	233.0	315.2
6	4	0	214.3	285.3
8	4	0	194.5	191.0
10	4	0	194.5	192.1
12	4	0	172.2	194.8
14	4	0	146.9	119.7
16	4	0	119.4	96.7
0	4	1	79.5	92.4
2	4	1	140.4	161.4
4	4	1	181.5	185.7
6	4	1	163.8	160.2
14	4	1	98.3	73.4
0	4	3	71.1	62.2
2	4	3	210.5	255.9
4	4	3	138.5	128.5
6	4	3	152.5	143.5
8	4	3	179.7	166.0
0	4	4	214.3	279.3
2	4	4	234.9	268.6
4	4	4	232.1	250.5
6	4	4	242.4	232.4
8	4	4	190.0	189.3
10	4	4	158.1	143.8
12	4	4	159.4	128.7
14	4	4	130.1	111.1
16	4	4	95.4	78.8
0	4	5	180.6	175.5
2	4	5	86.1	66.7
4	4	5	179.7	190.3
8	4	5	131.9	109.0
0	4	7	101.1	81.8
2	4	7	170.3	152.1
4	4	7	151.6	127.1
6	4	7	112.3	96.3
8	4	7	149.7	146.0
0	4	8	248.0	256.6
2	4	8	220.9	210.9
4	4	8	190.0	178.1
6	4	8	187.1	163.3
8	4	8	167.5	152.0
10	4	8	119.8	104.0
12	4	8	109.5	98.5
0	4	9	172.2	167.1
4	4	9	164.7	144.5
0	4	11	108.5	94.4
2	4	11	131.0	118.6
4	4	11	142.2	132.4
0	4	12	219.0	224.5
2	4	12	175.0	183.5
4	4	12	151.6	140.4
6	4	12	138.5	138.1
8	4	12	120.7	119.3
0	4	13	173.1	162.3
4	4	13	108.5	93.5
0	4	15	126.3	107.8
4	4	15	110.4	109.1

Table 3. Continued.

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
0	4	16	153.5	150.9
2	4	16	130.1	132.4
4	4	16	98.3	112.5
6	4	17	119.8	103.2
0	4	19	98.3	90.9
2	4	20	120.7	102.4
2	4	20	96.4	98.6
2	4	-1	148.8	248.1
4	4	-1	102.0	105.5
0	4	-1	194.6	202.8
6	4	-1	134.7	115.0
10	4	-1	101.1	93.5
12	4	-1	177.8	166.7
2	4	-3	173.1	223.7
4	4	-3	132.9	177.7
6	4	-3	106.7	87.1
8	4	-3	154.4	163.9
12	4	-3	132.9	116.5
2	4	-4	219.9	313.0
4	4	-4	226.4	319.2
0	4	-4	203.1	244.2
6	4	-4	193.7	220.3
10	4	-4	203.1	235.1
12	4	-4	174.0	181.2
14	4	-4	136.6	131.5
16	4	-4	120.7	120.1
18	4	-4	119.8	99.7
2	4	-5	215.2	246.2
4	4	-5	81.4	68.6
6	4	-5	174.0	228.9
8	4	-5	123.5	123.6
10	4	-5	152.5	145.1
12	4	-5	146.9	145.8
14	4	-5	130.1	123.1
2	4	-7	224.6	250.9
4	4	-7	81.4	67.7
6	4	-7	121.6	115.1
8	4	-7	149.7	165.8
12	4	-7	121.6	123.2
2	4	-8	240.5	257.9
4	4	-8	225.5	244.5
6	4	-8	201.2	229.9
8	4	-8	201.2	231.4
10	4	-8	196.5	225.0
12	4	-8	166.6	169.5
14	4	-8	143.2	138.1
16	4	-8	138.5	135.8
12	4	-8	110.4	110.2
2	4	-9	150.7	129.7
4	4	-9	118.8	103.1
6	4	-9	194.6	207.2
8	4	-9	94.5	76.0
10	4	-9	166.6	171.7
12	4	-9	113.2	118.6
14	4	-9	87.4	71.3
16	4	-9	138.5	134.6
2	4	-11	203.1	196.3
4	4	-11	85.2	80.5
8	4	-11	165.6	158.2
10	4	-11	123.5	119.5
10	4	-11	100.1	77.6
12	4	-11	131.9	125.6
14	4	-11	97.3	88.4
2	4	-12	199.3	201.2
4	4	-12	195.6	202.0
6	4	-12	234.0	241.8
8	4	-12	213.3	227.7
10	4	-12	182.5	187.6
12	4	-12	175.0	173.8
14	4	-12	173.1	163.6
16	4	-12	134.5	147.2
18	4	-12	120.7	117.0
20	4	-12	108.5	87.0
2	4	-13	83.6	71.1
4	4	-13	134.7	117.6
6	4	-13	179.7	170.4
8	4	-13	98.8	82.0
10	4	-13	172.2	158.0
12	4	-13	95.0	77.5
14	4	-13	127.3	126.0
16	4	-13	129.1	134.9
20	4	-13	108.5	95.7
2	4	-15	132.9	132.5
6	4	-15	168.4	166.9
10	4	-15	94.5	74.9
12	4	-15	125.0	86.0
16	4	-15	96.3	90.9
20	4	-15	68.1	58.1 *
4	4	-17	151.0	131.9
6	4	-17	105.7	80.1
8	4	-17	87.4	72.2
10	4	-17	159.1	149.4
14	4	-17	129.1	119.9
16	4	-17	98.3	81.2
0	4	-19	138.5	123.2
10	4	-19	119.1	103.5
16	4	-19	98.3	93.0
2	4	-20	120.7	123.0
4	4	-20	147.9	139.2
6	4	-20	153.1	148.9
8	4	-20	146.9	140.5
10	4	-20	139.4	134.0
12	4	-20	147.3	141.7
14	4	-20	147.3	135.2
16	4	-20	111.4	99.0
18	4	-20	97.3	97.4
20	4	-20	106.7	93.3
4	4	-21	120.7	117.8
10	4	-21	109.6	100.4
14	4	-21	120.7	116.5
10	4	-23	85.2	81.1
4	4	-24	96.4	97.7
6	4	-24	97.3	93.8
8	4	-24	108.5	103.0
10	4	-24	119.8	110.0
12	4	-24	108.5	107.5
14	4	-24	97.3	97.7
16	4	-24	95.4	89.4
14	4	-25	83.3	87.4
1	5	0	205.0	236.1
3	5	0	196.9	181.9
5	5	0	218.6	230.5
7	5	0	152.0	162.6
9	5	0	150.3	149.1
11	5	0	141.8	138.3
13	5	0	108.5	105.0
15	5	0	99.4	92.6
19	5	0	74.6	63.9
1	5	1	208.4	221.7
3	5	1	69.5	66.5
5	5	1	175.1	187.6
7	5	1	136.7	127.2
9	5	1	61.0	49.6
11	5	1	115.2	111.3
15	5	1	70.0	63.8
19	5	1	44.6	10.0 *
1	5	2	38.4	39.4
1	5	3	126.0	148.1
3	5	3	126.5	125.2
5	5	3	215.8	229.7
7	5	3	94.3	80.9
9	5	3	139.5	134.9
11	5	3	119.2	112.5
15	5	3	85.3	95.6
1	5	4	175.1	192.4
3	5	4	157.6	158.9
5	5	4	198.3	202.2
7	5	4	150.3	129.1
9	5	4	119.8	109.7
11	5	4	123.1	123.8
13	5	4	75.7	74.4
15	5	4	68.9	71.5
1	5	5	194.9	220.4
3	5	5	101.1	86.0
5	5	5	129.4	106.2
7	5	5	154.2	135.2
11	5	5	106.8	89.1
13	5	5	63.8	52.2 *
1	5	7	173.4	174.7
3	5	7	97.7	91.0
5	5	7	182.5	178.0
7	5	7	111.8	89.9
9	5	7	81.9	98.7
11	5	7	90.9	101.8
1	5	8	200.0	194.5
3	5	8	155.9	140.4
5	5	8	171.2	154.4
7	5	8	152.0	131.9
9	5	8	85.3	89.7
11	5	8	90.8	94.9
1	5	9	175.7	161.8
3	5	9	113.0	106.2
7	5	9	128.3	112.6
11	5	9	75.1	65.0
1	5	11	189.2	175.2
3	5	11	66.7	55.7
5	5	11	134.4	120.0
7	5	11	119.7	97.9
11	5	11	73.4	57.2
1	5	12	138.2	140.0
3	5	12	132.7	116.9
5	5	12	113.5	101.7
7	5	12	119.7	101.9
1	5	13	94.9	91.6
3	5	13	134.4	124.2
7	5	13	75.7	75.5
1	5	15	138.4	138.9
3	5	15	83.9	73.8
7	5	15	74.0	64.3
1	5	16	124.7	121.6
3	5	16	80.4	63.3
5	5	16	57.1	43.0
7	5	16	67.1	51.0
3	5	17	80.9	95.9
1	5	19	94.9	91.0
3	5	19	68.9	58.5
1	5	20	74.5	75.4
3	5	20	61.0	75.0
1	5	-1	110.9	105.0
3	5	-1	140.1	141.3
5	5	-1	172.3	197.2
7	5	-1	94.3	91.6
9	5	-1	107.2	109.3
11	5	-1	108.5	100.7
13	5	-1	102.2	102.7
15	5	-1	94.9	102.2
1	5	-2	42.9	49.6
1	5	-3	162.1	213.2
3	5	-3	89.0	100.6
5	5	-3	166.6	205.6
7	5	-3	98.3	92.1
9	5	-3	105.6	102.4
11	5	-3	113.5	111.1
15	5	-3	82.5	89.6
17	5	-3	49.1	16.2 *
1	5	-4	161.0	204.0
3	5	-4	187.8	209.7
5	5	-4	158.7	146.6
7	5	-4	132.7	148.8
9	5	-4	104.4	105.1
11	5	-4	120.7	131.6
13	5	-4	163.4	110.4
15	5	-4	60.8	105.0
17	5	-4	63.0	70.4
1	5	-5	111.3	107.6
3	5	-5	186.4	202.7
5	5	-5	136.1	157.5
7	5	-5	115.3	105.6
9	5	-5	187.6	202.6
11	5	-5	83.0	90.0
13	5	-5	120.7	136.4
15	5	-5	75.1	62.4
1	5	-7	172.3	146.6
3	5	-7	131.0	133.8
5	5	-7	179.6	198.5
9	5	-7	145.7	150.6
11	5	-7	97.7	105.2
15	5	-7	93.8	90.1
17	5	-7	63.8	18.4 *
1	5	-8	211.3	182.6
3	5	-8	219.2	206.4
5	5	-8	174.0	184.5
7	5	-8	162.7	172.2
9	5	-8	161.6	196.6
11	5	-8	117.5	128.2
13	5	-8	120.9	137.3
15	5	-8	101.7	115.7
17	5	-8	75.7	83.3
1	5	-9	111.8	95.0
3	5	-9	192.6	189.7
5	5	-9	111.8	101.6
7	5	-9	166.6	174.8
9	5	-9	169.5	177.6
11	5	-9	69.5	69.4
13	5	-9	137.3	161.6
15	5	-9	89.2	89.4
1	5	-11	120.3	103.8
3	5	-11	146.3	133.0
5	5	-11	150.8	145.6
7	5	-11	89.8	69.4
9	5	-11	170.6	169.5
11	5	-11	65.5	62.6
15	5	-11	80.2	87.5
1	5	-12	158.2	135.6
3	5	-12	189.8	179.5
5	5	-12	153.1	134.6
7	5	-12	168.3	153.3
9	5	-12	180.8	177.7
11	5	-12	116.9	110.5
13	5	-12	131.6	128.1
15	5	-12	105.6	111.3
1	5	-13	106.2	72.6
3	5	-13	184.1	172.1
5	5	-13	100.0	85.8
7	5	-13	174.0	163.0
9	5	-13	132.2	123.7
11	5	-13	93.8	95.5
13	5	-13	140.1	154.2
1	5	-15	66.1	55.0
3	5	-15	146.3	134.4
5	5	-15	107.3	105.2
7	5	-15	75.7	78.3
9	5	-15	153.6	141.7
11	5	-15	55.4	44.3
13	5	-15	85.3	93.3
15	5	-15	70.0	64.8
1	5	-16	116.4	102.9
3	5	-16	164.9	141.3
5	5	-16	155.3	128.9
7	5	-16	162.7	145.4
9	5	-16	126.5	132.9
11	5	-16	115.2	119.3
15	5	-16	148.8	132.0
1	5	-17	122.0	119.2
5	5	-17	78.5	69.5
7	5	-17	134.8	143.5
9	5	-17	78.5	74.3
11	5	-17	105.1	114.4
13	5	-17	136.1	127.3
15	5	-17	97.1	99.0
3	5	-19	127.7	112.0
5	5	-19	75.7	66.3
7	5	-19	106.2	93.7
9	5	-19	106.2	90.2
11	5	-19	57.1	58.2
13	5	-19	114.7	109.0
1	5	-20	70.0	81.1
1	5	-20	70.0	61.1
3	5	-20	107.3	98.1
5	5	-20	102.8	92.1
7	5	-20	121.4	119.6
11	5	-20	114.1	100.7
13	5	-20	124.3	112.6
15	5	-20	80.8	77.4
1	5	-21	80.2	82.9
3	5	-21	80.8	71.9
5	5	-21	64.4	58.0
7	5	-21	107.3	115.2
9	5	-21	97.1	95.8
11	5	-21	121.4	119.0
13	5	-21	75.7	76.0
15	5	-21	57.6	60.8
3	5	-23	88.1	90.2
7	5	-23	94.3	94.0
13	5	-23	85.3	86.7
5	5	-24	78.5	75.3
7	5	-24	84.7	90.0
9	5	-24	74.3	66.9
11	5	-24	97.7	85.5
13	5	-24	92.6	95.1
15	5	-24	67.1	65.1
7	5	-25	67.9	74.3
11	5	-25	103.9	96.8
15	5	-25	72.9	66.0
2	6	0	169.3	177.9
4	6	0	123.9	121.6
6	6	0	110.1	97.4
8	6	0	142.0	135.0
10	6	0	91.1	73.0
12	6	0	158.9	157.7
0	6	1	120.7	132.3
2	6	1	117.7	146.3
4	6	1	151.1	149.1
6	6	1	97.2	85.4
8	6	1	141.2	142.0
10	6	1	69.9	67.6
12	6	1	88.1	91.8
0	6	3	94.1	105.5
2	6	3	194.9	215.3
4	6	3	114.6	118.9
6	6	3	120.7	126.5
8	6	3	146.5	151.3
10	6	3	79.7	78.9
12	6	3	109.3	113.1
0	6	4	114.6	113.8
2	6	4	158.7	154.1
4	6	4	132.9	131.6
6	6	4	91.1	81.8
8	6	4	123.8	129.8
12	6	4	97.2	79.1
0	6	5	142.0	150.7
2	6	5	126.8	111.7
4	6	5	151.8	147.9
6	6	5	80.5	63.2
8	6	5	110.8	111.3
0	6	7	110.8	109.7
2	6	7	177.7	163.7
4	6	7	148.8	132.7
6	6	7	120.0	102.5
8	6	7	134.4	132.7
12	6	7	81.2	90.4
0	6	8	113.1	99.3
2	6	8	116.9	93.8
4	6	8	145.8	136.6
6	6	8	69.9	60.4
8	6	8	96.4	88.8
0	6	9	168.6	156.2
2	6	9	107.8	95.7
4	6	9	136.7	124.1
6	6	9	71.4	59.6
8	6	9	72.9	73.5
0	6	11	119.2	102.8
2	6	11	113.9	105.5
4	6	11	128.3	126.7
8	6	11	89.6	99.0
0	6	12	144.3	118.4
2	6	12	78.2	66.0
4	6	12	120.0	106.0
0	6	13	159.4	133.4
2	6	13	79.7	64.8
4	6	13	96.4	87.6

Table 3. Continued.

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
0	6	15	125.3	104.4
4	6	15	110.1	109.6
0	6	16	109.3	105.1
4	6	16	72.9	73.5
0	6	17	103.3	100.0
4	6	17	72.1	57.9
0	6	19	89.6	88.0
0	6	20	88.1	81.6
2	6	-1	198.2	226.2
4	6	-1	96.4	118.3
6	6	-1	156.4	167.5
8	6	-1	140.5	151.4
10	6	-1	112.4	111.4
12	6	-1	113.1	132.7
2	6	-3	120.0	159.7
4	6	-3	127.6	156.4
6	6	-3	97.2	112.6
8	6	-3	117.7	134.3
12	6	-3	97.9	112.8
2	6	-4	136.7	175.2
4	6	-4	99.5	101.1
6	6	-4	146.5	156.4
8	6	-4	124.5	131.2
10	6	-4	66.1	77.0
12	6	-4	110.4	121.9
2	6	-5	156.4	179.6
4	6	-5	85.8	109.3
6	6	-5	154.9	148.3
8	6	-5	112.4	126.0
10	6	-5	118.8	135.1
12	6	-5	110.1	128.4
2	6	-7	184.5	183.7
4	6	-7	115.4	121.0
6	6	-7	137.4	141.0
8	6	-7	110.1	121.3
12	6	-7	114.6	129.8
2	6	-8	160.2	158.5
4	6	-8	95.7	90.5
6	6	-8	149.6	148.4
8	6	-8	87.3	98.9
10	6	-8	103.3	99.7
12	6	-8	117.7	112.3
2	6	-9	144.5	121.4
4	6	-9	133.6	129.1
6	6	-9	179.9	195.1
8	6	-9	108.6	100.0
10	6	-9	132.1	155.5
12	6	-9	110.1	125.5
2	6	-11	177.7	163.3
4	6	-11	104.6	84.0
6	6	-11	141.2	140.9
8	6	-11	91.1	106.1
10	6	-11	88.8	79.7
12	6	-11	104.4	120.4
2	6	-12	152.1	115.2
4	6	-12	101.7	89.4
6	6	-12	161.7	150.7
8	6	-12	73.6	74.3
10	6	-12	113.1	116.0
12	6	-12	109.3	107.6
2	6	-13	82.6	77.4
4	6	-13	137.4	125.2
6	6	-13	169.3	155.6
8	6	-13	82.0	82.3
10	6	-13	129.1	145.5
12	6	-13	106.3	104.6
2	6	-15	127.6	128.3
4	6	-15	75.9	69.2
6	6	-15	100.2	134.5
8	6	-15	78.2	68.1
10	6	-15	93.4	93.1
12	6	-15	107.8	95.0
2	6	-16	88.1	77.7
4	6	-16	87.3	74.5
6	6	-16	117.7	107.1
8	6	-16	76.7	69.5
10	6	-16	113.1	113.5
12	6	-16	72.9	64.3
2	6	-17	72.9	62.9
4	6	-17	130.6	120.7
6	6	-17	107.8	101.9
10	6	-17	125.3	133.9
12	6	-17	89.6	83.5
2	6	-19	89.6	80.2
4	6	-19	73.6	66.8
6	6	-19	103.3	103.3
10	6	-19	103.3	96.3
4	6	-20	89.6	81.1
6	6	-20	82.0	80.8
8	6	-20	72.9	59.2
10	6	-20	103.3	98.7
4	6	-21	96.4	93.3
6	6	-21	73.6	55.9
10	6	-21	101.7	99.3
6	6	-23	80.5	76.1
10	6	-23	80.5	87.2
10	6	-24	71.4	66.1
10	6	-25	69.9	66.7
1	7	0	103.1	108.9
3	7	0	34.2	36.0
5	7	0	124.0	117.3
7	7	0	63.6	43.2
9	7	0	91.4	80.5
11	7	0	62.5	60.8
15	7	0	79.6	67.7
1	7	1	157.6	172.6
3	7	1	82.8	95.3
5	7	1	118.1	120.0
7	7	1	121.3	112.1
9	7	1	78.6	73.5
11	7	1	86.0	81.0
15	7	1	63.1	51.1
1	7	2	40.1	35.2
1	7	3	138.9	152.6
3	7	3	125.6	131.0
5	7	3	166.2	147.7
7	7	3	106.9	100.3
9	7	3	140.0	124.8
11	7	3	104.7	100.1
1	7	4	118.1	120.6
3	7	4	51.3	39.7
5	7	4	109.0	97.5
9	7	4	57.7	48.1
11	7	4	87.6	75.2
1	7	5	154.4	160.2
3	7	5	109.5	104.3
5	7	5	116.5	104.1
7	7	5	111.1	104.0
9	7	5	79.6	58.8
11	7	5	72.7	74.7
1	7	7	112.2	135.9
3	7	7	120.2	113.6
5	7	7	136.3	126.5
7	7	7	85.5	80.2
9	7	7	83.9	88.2
11	7	7	90.3	89.7
1	7	8	133.6	121.2
5	7	8	79.6	66.6
7	7	8	76.4	65.4
11	7	8	75.9	63.0
1	7	9	127.2	116.0
3	7	9	114.4	100.9
5	7	9	84.8	72.5
7	7	9	86.6	79.7
3	7	10	46.0	37.2
1	7	11	135.7	121.9
3	7	11	102.6	98.0
5	7	11	93.0	104.3
7	7	11	83.4	78.7
1	7	12	80.2	78.3
7	7	12	67.9	64.2
1	7	13	81.8	85.0
3	7	13	87.1	93.5
7	7	13	70.0	62.9
1	7	15	90.3	95.9
3	7	15	87.1	66.4
3	7	17	63.1	71.9
1	7	-1	107.0	134.1
3	7	-1	98.9	127.3
7	7	-1	118.6	118.2
9	7	-1	140.5	134.9
11	7	-1	87.6	92.7
13	7	-1	83.9	96.1
15	7	-1	90.3	87.3
1	7	-2	59.3	59.5
3	7	-2	49.4	42.3
11	7	-2	57.2	54.8
1	7	-3	122.4	159.7
3	7	-3	88.2	108.5
5	7	-3	122.9	148.9
7	7	-3	107.9	115.6
9	7	-3	106.9	97.1
11	7	-3	86.0	89.5
13	7	-3	63.6	59.4
15	7	-3	76.4	71.1
1	7	-4	57.2	56.2
3	7	-4	72.7	69.3
5	7	-4	102.6	117.5
9	7	-4	113.0	104.9
11	7	-4	56.1	44.6
15	7	-4	83.9	71.2
1	7	-5	106.3	124.1
3	7	-5	123.4	144.7
5	7	-5	123.4	146.6
7	7	-5	135.7	140.4
9	7	-5	145.9	141.6
11	7	-5	87.6	92.0
15	7	-5	126.6	118.7
15	7	-5	90.3	95.3
1	7	-6	47.0	43.0
3	7	-6	48.6	44.1
5	7	-6	42.2	43.7
1	7	-7	114.6	118.4
3	7	-7	112.2	117.3
5	7	-7	133.1	145.3
7	7	-7	82.1	82.0
9	7	-7	105.4	107.4
11	7	-7	81.3	84.4
13	7	-7	71.1	65.4
15	7	-7	80.2	76.4
3	7	-8	95.6	87.6
5	7	-8	104.7	101.4
7	7	-8	52.4	41.8
9	7	-8	104.2	97.0
13	7	-8	85.5	76.7
1	7	-9	99.9	96.5
3	7	-9	145.3	144.4
5	7	-9	115.4	118.4
7	7	-9	125.6	129.5
9	7	-9	123.4	127.6
11	7	-9	81.8	93.0
13	7	-9	123.4	126.0
15	7	-9	83.9	84.0
17	7	-9	75.9	68.8
5	7	-10	67.3	57.4
1	7	-11	89.8	94.5
3	7	-11	133.6	131.7
5	7	-11	130.9	134.0
7	7	-11	88.2	78.7
9	7	-11	113.3	118.4
11	7	-11	82.8	89.3
13	7	-11	79.1	75.2
15	7	-11	68.4	72.5
3	7	-12	117.6	105.9
7	7	-12	65.7	53.0
9	7	-12	100.5	92.5
13	7	-12	82.8	84.1
1	7	-13	92.4	89.9
3	7	-13	129.3	133.5
5	7	-13	96.7	97.2
7	7	-13	126.1	123.9
9	7	-13	122.9	117.3
11	7	-13	87.6	102.2
13	7	-13	122.4	119.9
15	7	-13	68.4	78.0
17	7	-13	95.6	84.8
9	7	-14	56.6	46.6
1	7	-15	86.0	76.4
3	7	-15	118.1	111.2
5	7	-15	96.2	93.8
7	7	-15	77.5	73.2
9	7	-15	110.1	106.2
11	7	-15	71.6	73.0
13	7	-15	72.7	74.1
15	7	-15	64.1	57.2
3	7	-16	95.6	88.1
7	7	-16	81.8	70.8
13	7	-16	72.7	81.4
17	7	-16	63.6	54.4
1	7	-17	68.4	73.5
3	7	-17	99.4	97.7
5	7	-17	79.6	74.3
7	7	-17	95.6	102.2
9	7	-17	89.8	90.4
11	7	-17	86.6	97.9
13	7	-17	80.2	92.7
15	7	-17	63.6	67.9
17	7	-17	89.2	90.5
1	7	-19	63.1	56.0
3	7	-19	30.2	19.3
5	7	-19	69.1	66.2
7	7	-19	63.4	58.2
9	7	-19	83.4	90.2
11	7	-19	64.1	58.0
13	7	-19	68.4	74.5
17	7	-19	57.7	55.3
7	7	-20	76.4	76.9
17	7	-20	57.2	59.0
5	7	-21	63.6	65.3
7	7	-21	67.9	7.2
9	7	-21	76.4	67.6
11	7	-21	83.4	90.4
13	7	-21	75.9	75.0
15	7	-21	71.1	66.1
17	7	-21	82.8	84.7
7	7	-23	70.5	74.4
9	7	-23	63.1	58.9
2	8	0	61.9	77.5
4	8	0	39.0	21.1
6	8	0	43.0	25.8
8	8	0	60.7	67.1
12	8	0	58.4	52.0
0	8	1	158.1	130.6
2	8	1	90.5	119.7
4	8	1	108.3	110.7
6	8	1	91.1	95.6
8	8	1	98.6	89.7
10	8	1	80.8	77.1
12	8	1	63.6	58.4
0	8	3	95.7	124.9
2	8	3	110.0	125.4
4	8	3	107.7	105.7
6	8	3	103.7	99.7
8	8	3	114.0	103.3
10	8	3	82.6	84.1
12	8	3	67.6	70.6
14	8	3	72.9	68.4
2	8	4	48.1	47.6
4	8	4	56.7	44.6
0	8	5	100.8	109.2
2	8	5	111.7	112.9
4	8	5	112.3	97.7
6	8	5	69.4	74.9
8	8	5	77.9	72.1
10	8	5	67.6	63.5
0	8	6	43.0	43.9
2	8	6	47.6	41.2
0	8	7	100.9	108.9
2	8	7	126.1	123.2
4	8	7	119.0	106.9
6	8	7	90.0	83.9
8	8	7	85.9	94.1
10	8	7	75.1	77.2
4	8	8	84.9	70.4
6	8	8	56.7	45.0
0	8	9	98.0	101.9
2	8	9	96.3	91.5
4	8	9	86.5	85.5
6	8	9	84.2	72.4
0	8	10	53.3	49.5
0	8	11	74.5	88.7
2	8	11	86.5	87.6
4	8	11	94.5	90.5
6	8	11	79.6	74.3
4	8	12	63.0	59.3
0	8	13	81.4	80.6
2	8	13	67.6	69.8
4	8	13	63.6	63.2
6	8	15	79.6	76.0
2	8	15	63.6	67.2
4	8	15	66.5	72.1
0	8	16	58.4	48.8
0	8	17	67.6	69.9
2	8	17	57.3	55.3
0	8	19	69.4	64.8
2	8	-1	118.0	131.0
4	8	-1	95.1	113.2
6	8	-1	118.6	120.1
8	8	-1	139.2	123.7
10	8	-1	99.7	94.1
12	8	-1	88.8	80.5
14	8	-1	79.1	77.3
16	8	-1	79.1	66.8
4	8	-2	82.4	49.0
6	8	-2	59.0	50.5
2	8	-3	85.9	112.9
4	8	-3	83.7	104.9
6	8	-3	97.4	103.6
8	8	-3	99.1	99.8
10	8	-3	90.0	75.4
12	8	-3	74.5	62.1
14	8	-3	67.6	59.5
2	8	-4	69.3	81.4
6	8	-4	67.6	59.7
8	8	-4	57.9	49.5
12	8	-4	70.5	64.0
2	8	-5	96.3	109.9
4	8	-5	107.1	120.6
6	8	-5	113.5	125.3
8	8	-5	99.7	107.7
10	8	-5	94.5	94.4
12	8	-5	94.0	95.4
14	8	-5	89.4	82.2
16	8	-5	82.5	69.8
8	8	-6	57.9	55.7
2	8	-7	101.4	106.3
4	8	-7	106.6	118.4
6	8	-7	107.1	114.2
8	8	-7	103.1	95.3
10	8	-7	79.6	79.9
12	8	-7	87.1	80.3
14	8	-7	67.6	66.4
16	8	-7	57.9	48.7
2	8	-8	82.5	75.5
6	8	-8	72.8	69.4
12	8	-8	61.9	55.2
2	8	-9	107.1	108.7
4	8	-9	112.9	115.6
6	8	-9	115.7	110.2
8	8	-9	99.5	104.5
10	8	-9	92.3	101.3
12	8	-9	111.7	104.9
14	8	-9	85.9	86.4
16	8	-9	79.1	73.2
2	8	-10	46.4	40.4
2	8	-11	103.7	100.7
4	8	-11	99.7	101.3
6	8	-11	102.0	97.8
8	8	-11	90.5	86.1
10	8	-11	79.6	75.3
12	8	-11	77.9	81.4
14	8	-11	63.9	64.3
16	8	-11	45.9	46.5
6	8	-12	70.9	69.7

Table 3. Continued.

h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$	h	k	l	$\lvert F_o \rvert$	$\lvert F_c \rvert$
10	8	-12	56.7	46.3	12	8	-19	63.0	59.4	5	9	9	76.3	68.6	9	9	-7	65.5	65.2
12	8	-12	57.9	58.1	10	8	-19	64.7	53.2	1	9	11	80.2	66.2	11	9	-7	80.2	67.5
10	8	-12	58.4	50.3	0	8	-21	57.3	62.2	3	9	11	95.6	86.5	13	9	-7	64.8	64.5
2	8	-13	97.4	89.0	8	8	-21	66.5	57.0	5	9	11	77.1	62.4	9	9	-8	60.1	36.0
4	8	-13	102.0	97.3	10	8	-21	57.9	70.2	1	9	13	76.3	68.6	1	9	-9	87.9	91.6
6	8	-13	98.0	95.0	12	8	-21	61.0	61.3	1	9	-1	99.5	106.0	3	9	-9	91.7	86.5
8	8	-13	84.9	89.0	14	8	-21	63.0	65.1	3	9	-1	74.8	96.8	5	9	-9	89.4	104.7
10	8	-13	80.5	100.9						5	9	-1	84.0	91.8	7	9	-9	77.1	81.6
12	8	-13	91.7	94.4	5	9	0	54.7	42.6	7	9	-1	106.4	103.7	9	9	-9	85.6	79.1
14	8	-13	67.6	73.6	1	9	1	82.5	59.4	9	9	-1	64.8	71.9	11	9	-9	69.4	98.5
16	8	-13	79.1	73.5	3	9	1	91.3	108.6	11	9	-1	81.7	80.6	13	9	-9	77.1	89.9
12	8	-14	67.0	54.6	5	9	1	73.7	72.2	1	9	-2	30.1	32.5	1	9	-11	94.1	87.4
2	8	-15	97.4	94.7	7	9	1	83.3	76.6	3	9	-2	40.1	28.1	3	9	-11	79.4	85.4
4	8	-15	91.1	86.7	9	9	1	84.0	76.6	5	9	-2	51.7	38.0	5	9	-11	79.4	82.5
6	8	-15	90.5	79.6	1	9	3	85.6	107.5	11	9	-2	70.2	51.9	7	9	-11	84.9	98.3
8	8	-15	80.8	71.2	3	9	3	100.2	106.7	1	9	-3	66.3	89.6	9	9	-11	67.8	61.4
10	8	-15	81.3	83.4	5	9	3	79.4	73.6	3	9	-3	80.9	107.3	11	9	-11	85.6	90.5
12	8	-15	80.8	76.6	7	9	3	109.5	97.3	7	9	-3	87.9	93.2	13	9	-11	64.8	59.4
14	8	-15	57.9	54.1	9	9	3	91.0	73.8	9	9	-3	80.9	72.6	1	9	-13	89.0	81.2
10	8	-16	64.9	62.5	1	9	4	55.5	42.7	11	9	-3	70.2	63.2	3	9	-13	79.4	66.5
2	8	-17	80.5	71.7	1	9	5	80.9	80.5	5	9	-4	50.9	42.1	5	9	-13	80.2	92.0
4	8	-17	82.5	76.0	3	9	5	94.1	95.3	1	9	-5	96.4	110.4	7	9	-13	79.4	74.4
6	8	-17	85.9	84.9	5	9	5	80.2	78.6	3	9	-5	77.1	90.9	9	9	-13	94.1	82.9
8	8	-17	82.5	84.9	7	9	5	79.4	61.1	5	9	-5	97.9	101.0	11	9	-13	81.7	81.5
10	8	-17	85.9	98.1	9	9	5	81.7	66.2	7	9	-5	90.2	103.2	13	9	-13	70.9	65.3
12	8	-17	83.1	90.8	1	9	7	87.9	84.9	9	9	-5	84.0	78.7	1	9	-15	96.4	80.1
14	8	-17	67.6	74.4	3	9	7	108.7	96.3	11	9	-5	84.8	89.0	3	9	-15	70.2	63.0
16	8	-17	70.5	73.3	5	9	7	84.0	68.6	13	9	-5	82.5	65.6	5	9	-15	70.2	71.8
2	8	-19	86.5	88.9	7	9	7	95.6	77.2	1	9	-7	91.0	94.0	7	9	-15	75.6	74.4
6	8	-19	63.3	66.7	1	9	8	63.2	47.9	3	9	-7	83.3	93.8	11	9	-15	81.7	73.2
8	8	-19	79.4	71.2	1	9	9	84.0	72.7	5	9	-7	68.6	78.8	13	9	-15	64.0	52.9
10	8	-19	63.0	67.7	3	9	9	92.5	74.7	7	9	-7	92.5	100.8					

the 0.005 confidence level (Hamilton's test [8]). Converting the isotropic temperature factors to anisotropic ones also for the chromium atoms in a further least-squares refinement resulted in nearly the same *R*-factor. The contributions of the mercury and the chromium atoms were also corrected for anomalous dispersion in a least-squares refinement, giving no significant decrease in the *R*-factor or in the standard deviations compared to the calculations based on the uncorrected values. The atomic scattering factors given by Cromer and Waber [9] for neutral mercury and by Hanson *et al.*[10] for neutral chromium and oxygen were used. No correction was applied for extinction as nothing in the intensity data indicates the presence of such effects.

Finally, three-dimensional Fourier-sections were calculated, the contributions of all atoms subtracted from the observed structure factors. The cuts showed only negligible rest peaks.

Positional and thermal parameters with estimated standard deviations are given in Table 1 together with the r.m.s. components of the thermal vibrations along principal axes of the ellipsoids of vibration of the mercury atoms. The weighting scheme used in the last cycle of the least-squares refinement is given in Table 2, and the observed and calculated structure factors in Table 3.

DESCRIPTION AND DISCUSSION OF THE STRUCTURE

The distances mercury to oxygen in the structure of mercury(II) chromate hemihydrate fall into three ranges (Table 4). It is seen that mercury is only bonded to two oxygen atoms (O(1), O(3)) at the distances of 2.05 and 2.06 Å, respectively. The dominant feature of the structure is thus the two-covalency of mercury(II). The two oxygen atoms in range I belong to the chromate tetrahedra. Each mercury atom is bonded to two chromate groups and each chromate group is bonded to two mercury atoms. In this way, endless chains of the

Table 4. Interatomic distances (Å) and angles (°) in the structure of $HgCrO_4.\frac{1}{2}H_2O$. Standard deviations are given within brackets.

Distances mercury to oxygen

	Range I	Range II	Range III
Hg – O(1)	2.046(18)	2.75(2)	
Hg – O(2)		2.82(2)	3.63(2), 3.68(2)
Hg – O(3)	2.061(18)	2.68(2)	
Hg – O(4)		2.75(2)	3.56(2), 3.72(2)
Hg – O(5)		2.75(2)	3.92(2)

Angle O – Hg – O

∠O(1) – Hg – O(3)	176.2(9)

Distances and angles within the CrO_4 tetrahedron

Cr – O(1)	1.735(18)	O(1) – O(2)	2.77(3)	O(2) – O(3)	2.82(2)
Cr – O(2)	1.622(19)	O(1) – O(3)	2.85(3)	O(2) – O(4)	2.61(3)
Cr – O(3)	1.764(17)	O(1) – O(4)	2.78(3)	O(3) – O(4)	2.77(3)
Cr – O(4)	1.652(21)				
		∠O(1) – Cr – O(2)	111.0(9)	∠O(2) – Cr – O(3)	112.6(9)
		∠O(1) – Cr – O(3)	109.3(8)	∠O(2) – Cr – O(4)	105.6(10)
		∠O(1) – Cr – O(4)	110.1(9)	∠O(3) – Cr – O(4)	108.2(9)

Shortest distances Hg – Hg and Hg – Cr

Hg – Hg 3.654(2), 3.677(2); between the chains
Hg – Cr 3.394(4), 3.451(3); within the chains
Hg – Cr 3.809(4), 3.866(3); between the chains

Distances O – O ≤ 3.00 Å outside the tetrahedra

O(1) – O(1)	2.82(4),	O(4) – O(4)	2.91(4); between the chains
O(5) – 2 O(4)	2.94(2)		
O(5) – 2 O(2)	3.00(2)		

composition $(HgCrO_4)_n$ are formed. The chains are parallel to the diagonals of the *ab*-plane (Fig. 1). Four crystallographically equivalent chains run through the unit cell (Fig. 2).

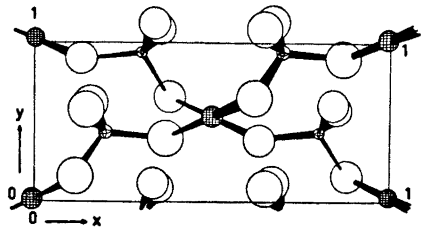

Fig. 1. Projection of the structure of $HgCrO_4.\frac{1}{2}H_2O$ along [001], showing the infinite chains $(HgCrO_4)_n$. The chains overlap each other two and two in the drawing. Large circles show the oxygen atoms, small the chromium atoms, and chequered ones the mercury atoms, which overlap each other four and four in the projection.

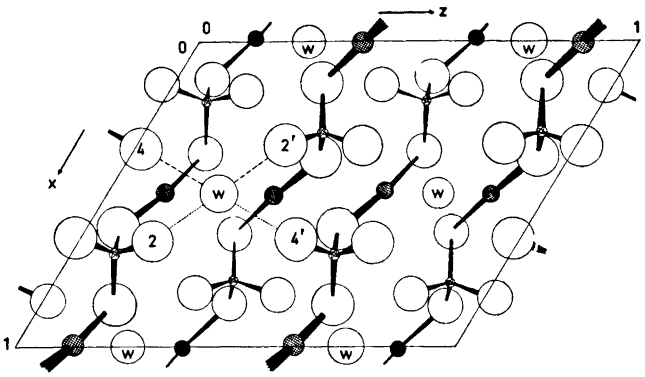

Fig. 2. Projection of the structure of $HgCrO_4 \cdot \frac{1}{2}H_2O$ along [010], showing the infinite chains $(HgCrO_4)_n$ and the water oxygen atoms. Possible hydrogen bonds between the water oxygen atom (denoted *w*) and oxygen atoms of the chromate tetrahedra are shown by dashed and dashed-dotted lines for one water oxygen atom. Designations as in Fig. 1.

The short distances mercury to oxygen and the angle O – Hg – O are close to the values found for orthorhombic mercury(II) oxide:[11]

Compound	Distances Hg – O (Å)	Angle O – Hg – O (°)
HgO	2.04(3) 2.07(3)	179.5(1.1)
$HgCrO_4 \cdot \frac{1}{2}H_2O$	2.05(2) 2.06(2)	176.2(9)

In orthorhombic mercury(II) oxide there are four additional oxygen atoms at distances varying from 2.81 to 2.85 Å. If these non-bonded oxygen atoms are also included in a coordination polyhedron, the result is a deformed octahedron. For the present structure the five oxygen atoms of range II (2.68 to 2.82 Å) lie approximately in a plane, forming a pentagon. From geometrical point of view the polyhedron around the mercury atom of $HgCrO_4 \cdot \frac{1}{2}H_2O$ is a deformed pentagonal bipyramid.

Each chromate group has two oxygen atoms (O(2), O(4)) which are not bonded to mercury; there are 16 such oxygen atoms in the unit cell, which also contains 8 hydrogen atoms.

For the two non-mercury oxygen atoms of a chromate group there are then the following three possibilities:

(*a*) They are not involved in any hydrogen bonding.
(*b*) One of them is bonded by a hydrogen bond to a water molecule.
(*c*) By means of a statistical distribution of the hydrogen atoms in the structure, each has on the average one half hydrogen bond.

The only conclusions that can be drawn from the available X-ray intensity data are the following. The water oxygen atom O(5) (denoted *w* in Fig. 2) is situated on a twofold axis at the distance 2.94(2) Å from the chromate oxygen atoms O(4), O(4′) and at 3.00(2) Å from the chromate oxygen atoms O(2), O(2′) (Fig. 2). In an ordered structure including the

hydrogen atoms, with space group $C2/c$, the hydrogen bonding angles O(2) – O(5) – O(2′) and O(4) – O(5) – O(4′) would be 132° and 175°, respectively; values very unlikely for a hydrogen bond (case *b* above). With space group *Cc* there is also another possibility; hydrogen bonding could occur either as O(2) – O(5) – O(4′) or as O(4) – O(5) – O(2′) (*cf.* Fig. 2, dashed and dashed-dotted lines, respectively), the hydrogen bonding angles being 109°. Thus case *b* could be fulfilled with space group *Cc* though it must be admitted that the hydrogen bonds would be quite long (2.94 and 3.00 Å).

Assuming space group $C2/c$, the present author prefers the interpretation that either no hydrogen bonding at all occurs (case *a*) or possibly that the hydrogen atoms are statistically distributed to give bonds O(4) – O(5) – O(2′) and O(2) – O(5) – O(4′) in equal amounts (case *c*).

Since in the present compound the mercury atoms are combined with tetrahedral anions as in $HgSO_4$ and $HgSO_4.H_2O$ and since the water content is intermediate between their contents, it seems appropriate to make a comparison between its structure and the known structures of the last-mentioned compounds. Though many authors [12,13] have worked on the structure of $HgSO_4$, its details do not seem to have been made clear. However, all authors report that mercury is coordinated to four oxygen atoms of sulphate groups in the form of a deformed tetrahedron and that the three-dimensional structure is built up of HgO_4 and SO_4 tetrahedra, which share corners only. The Hg – O distances given for the HgO_4 tetrahedron fall in the range 2.08 – 2.43 Å. No standard deviations in the distances are reported. At present, nothing definite can thus be said about the detailed coordination of mercury in $HgSO_4$.

In the structure of $HgSO_4.H_2O$ [2,14] mercury has two close oxygen atoms, *viz.* one sulphate oxygen atom and one water oxygen atom at the distances 2.17(1) and 2.24(1) Å, respectively.[2] The angle O – Hg – O is 169°. Four more sulphate oxygen atoms at distances 2.50, 2.51 Å complete a deformed octahedron around mercury. Of the four oxygen atoms of a sulphate group, three are in contact with mercury at distances 2.17, 2.50, and 2.51 Å. The fourth oxygen atom is suggested to form a hydrogen bond with the water molecule.

In $HgSO_4$ all sulphate oxygen atoms are believed to be in contact with mercury.

If a statistical distribution of the hydrogen atoms in the structure of $HgCrO_4.\frac{1}{2}H_2O$ is assumed (case *c*, above), two of the chromate oxygen atoms are bonded to mercury and two have on the average one half hydrogen bond each.

The two-covalency of mercury(II) seems to be more pronounced in $HgCrO_4.\frac{1}{2}H_2O$ than in $HgSO_4$ and $HgSO_4.H_2O$. This point is further stressed by the fact that the distances Cr – O for such oxygen atoms that are bonded to mercury are longer (1.75 Å) than the rest of the Cr – O distances (1.64 Å), the differences between the bonds being highly significant.

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REFERENCES

1. Aurivillius, K. *Arkiv Kemi* **24** (1965) 151.
2. Templeton, L. K., Templeton, D. H. and Zalkin, A. *Acta Cryst.* **17** (1964) 933.
3. Aurivillius, K. and Malmros, B. *Acta Chem. Scand.* **15** (1961) 1932.
4. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. I, p. 101.
5. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham 1962, Vol. III, p. 162 ff.
6. Buerger, M. J. *Crystal Structure Analysis*, Wiley, New York 1960, p. 75.
7. *International Tables for X-Ray Crystallography*, Kynoch Press, Birmingham 1959, Vol. II, p. 304.
8. Hamilton, W. C. *Acta Cryst.* **18** (1965) 502.
9. Cromer, D. T. and Waber, J. T. *Acta Cryst.* **18** (1965) 104.
10. Hanson, H. P., Herman, F., Lea, J. D. and Skillman, S. *Acta Cryst.* **17** (1964) 1040.
11. Aurivillius, K. *Acta Chem. Scand.* **18** (1964) 1305.
12. Bonefačić, A. *Croat. Chem. Acta* **35** (1963) 195.
13. Kokkoros, P. A. and Rentzeperis, P. J. *Z. Krist.* **119** (1963) 234.
14. Bonefačić, A. *Acta Cryst.* **14** (1961) 116.

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