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The crystal structure of $GdCl_3$*

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The structure of $GdCl_3$ is determined with a space group $P6_3/m$ and atom parameters, Gd in (*c*) at $(\frac{1}{3},\frac{2}{3},\frac{1}{4})$ and Cl in (*h*) at $(x,y,\frac{1}{4})$, $x=0{\cdot}3900\pm0{\cdot}0011$, $y=0{\cdot}3027\pm0{\cdot}0011$.

The chlorine nuclear resonance of ferromagnetic $GdCl_3$ (Wolf, Leask, Mangum & Wyatt, 1961) is being studied in this laboratory (Carlson, 1966) and the Cl positions are needed for analysis. $GdCl_3$ is of the UCl_3 structure type (Bommer & Hohmann, 1941; Zachariasen, 1948). Clear hygroscopic crystals were grown from the melt (Anderson & Hutchinson, 1955) by the Stockbarger method.

An irregular X-ray sample of about 0.1 mm × 0.2 mm × 0.3 mm was chipped from a larger crystal and sealed in glass in a dry atmosphere. Data were collected at room temperature on a General Electric XRD-5 diffractometer using a single-crystal orienter with filtered Mo $K\alpha$ radiation. The ($h\bar{k}0$), ($\bar{h}k0$) reciprocal lattice was covered. 98 % of the reflections were observable. The space group was checked as well as the lattice constants; both agreed with previous measurements (Templeton & Dauben, 1954). Reflections were corrected for Lorentz-polarization and a $\chi=90°$, φ rotation absorption correction was applied. A theoretical absorption correction was attempted but the exact shape of the crystal could not be ascertained.

The positions of the Gd and Cl ions were easily determined from a sharpened Patterson function. Final positions were determined by averaging the equivalent reflections and from the individual isotropic temperature factors in *OR FLS*, (Busing, Martin & Levy, 1962), a least-squares computer program which was modified for the CDC 3600. It converged after 4 cycles.

Each gadolinium ion is surrounded by six chloride ions at distances of Gd–Cl = 2.820 ± 0.005 Å and three chloride ions at distances of 2.911 ± 0.007 Å. The large value of $R=0.137$ is due to uncorrected absorption in the irregular chip. The absorption coefficient for this crystal is $\mu=196$.

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Table 1. *Unit-cell dimensions for* $GdCl_3$ *and* UCl_3

For $GdCl_3$ from Templeton & Dauben (1954) and for UCl_3 from Zachariasen (1948) (changed from kX units).
Space group $P6_3/m$ (no. 176)

	$GdCl_3$	UCl_3
a_0	7·363 ± 0·004 Å	7·443 ± 0·003 Å
c_0	4·105 ± 0·004	4·320 ± 0·003

Table 2. *Atomic positions in* $GdCl_3$ *and* UCl_3, *and the isotropic temperature factors*
The results for UCl_3 are from Zachariasen (1954).

		x	*y*	*z*	*B*
$GdCl_3$	Cl	0·3900 ± 0·0011	0·3027 ± 0·0011	$\frac{1}{4}$	0·96 ± 0·10 Å²
	Gd	0·3333	0·6667	$\frac{1}{4}$	0·73 ± 0·04
UCl_3	Cl	0·375 ± 0·014	0·292 ± 0·014	$\frac{1}{4}$	
	U	$\frac{1}{3}$	$\frac{2}{3}$	$\frac{1}{4}$	

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Table 3. *Observed and calculated structure factors*

Within each group, the columns, reading from left to right, contain the values of *h*, $|F_o|$, and F_c. Unobserved reflections were omitted. A zero for $|F_o|$ indicates negligible intensity above background.

	h 0 0		5	27.9	-25.4	16	12.3	-13.7	20	14.2	16.7
			6	63.2	69.0	17	10.6	-8.3			
1	84.6	-67.7	7	48.9	-52.3	18	18.6	20.4		h -11 0	
2	73.4	-60.2	8	44.8	-45.5	19	8.9	-10.0			
3	125.8	131.6	9	67.5	69.5				12	27.8	-25.0
4	84.0	-70.4	10	19.1	-20.0		h -7 0		13	40.0	37.5
5	74.5	-56.2	11	32.2	-32.0				14	0.0	-6.7
6	69.5	55.7	12	50.6	48.3	8	79.3	91.8	15	14.2	-16.6
7	44.2	-33.3	14	17.8	-18.6	9	32.7	-30.4	16	29.6	29.2
8	43.2	-32.5	15	33.8	31.2	10	22.1	-22.7	17	8.3	-7.4
9	49.7	39.3	16	4.4	-8.8	11	48.3	56.7	18	13.0	-12.3
10	2.5	-1.2	17	14.6	-12.3	12	26.4	-29.1	19	14.4	15.2
11	20.5	-16.4	18	14.5	14.3	13	20.2	-22.6	20	8.1	-8.3
12	38.4	30.3				14	20.8	25.3			
13	0.0	-2.0		h -4 0		15	13.7	-15.3		h -12 0	
14	18.9	-14.1				16	12.6	-14.4			
15	22.8	17.3	5	97.3	107.9	17	11.9	17.3	13	23.6	-18.8
16	11.6	-8.7	6	6.1	-5.3	19	1.7	-7.5	14	17.0	-16.3
17	10.9	-9.1	7	46.8	-49.5	20	12.2	10.3	15	21.5	18.6
			8	72.4	83.3				16	12.7	-11.4
	h -1 0		9	19.4	-20.0		h -8 0		17	0.8	-6.7
			10	36.5	-39.0				18	15.3	14.6
2	72.2	80.6	11	38.0	40.8	9	34.7	-30.8	19	2.1	-4.5
3	10.0	6.5	12	26.0	-26.2	10	38.2	36.7	20	2.7	-2.9
4	37.3	-34.9	13	12.7	-19.5	11	0.0	-3.6			
5	76.8	77.5	14	20.9	22.0	12	16.8	-16.6		h -13 0	
6	2.8	-1.0	15	7.9	-11.9	13	28.8	32.5			
7	47.2	-39.0	16	4.2	-4.4	14	2.3	-0.7	14	13.3	20.1
8	57.6	47.6	17	17.7	15.7	15	13.4	-15.4	15	11.3	-9.5
9	35.6	-27.0	18	1.7	-4.2	16	19.8	20.7	16	10.2	-9.6
10	40.7	-31.2	19	5.3	-3.3	17	5.8	-9.7	17	13.9	14.6
11	40.5	33.0				18	12.3	-11.9	18	10.5	-10.5
12	31.3	-25.5		h -5 0		19	12.0	13.4	19	9.8	-9.4
13	15.5	-9.0				20	8.7	-9.0	20	12.9	13.8
14	36.1	27.0	6	49.5	-44.4						
15	17.7	-13.1	7	57.6	52.1		h -9 0			h -14 0	
17	20.6	16.3	8	32.7	-33.4						
18	10.0	-7.8	9	6.4	-5.9	10	25.5	-20.7	15	15.3	-10.9
			10	37.3	42.0	11	30.7	-29.0	16	27.1	27.5
	h -2 0		11	7.1	-11.5	12	31.4	31.0	17	12.2	-9.9
			12	4.4	-3.2	13	24.2	-25.5	18	7.4	-6.8
3	70.8	-79.3	13	23.9	26.5	14	9.8	-11.4	19	16.0	17.3
4	75.5	82.4	14	8.7	-13.0	15	26.4	28.8			
5	64.8	-70.9	15	7.2	-13.6	16	14.5	-15.2		h -15 0	
6	26.3	-25.7	16	14.2	17.7	17	1.3	-1.6			
7	79.5	81.8	17	11.6	-12.7	18	19.2	19.8	16	7.1	-10.8
8	44.7	-41.7	18	11.1	-10.4	19	8.2	-9.4	17	11.7	-10.0
9	9.3	0.4	19	14.5	15.7	20	4.8	-4.1	18	14.3	12.6
10	61.3	56.6							19	5.9	-3.3
11	30.8	-27.9		h -6 0			h -10 0				
12	12.6	-10.3								h -16 0	
13	27.8	26.1	7	38.3	-32.0	11	54.7	46.8			
14	21.4	-18.4	8	32.9	-30.7	12	24.8	-24.0	17	17.3	13.8
15	19.2	-15.5	9	39.1	41.7	13	8.6	-7.8	18	7.4	-6.0
16	1.1	18.0	10	31.4	-35.1	14	23.7	26.0			
17	6.5	-7.6	11	27.8	-31.7	15	16.8	-18.3		h -17 0	
18	10.6	-9.4	12	40.1	46.3	16	15.9	-15.1			
	h -3 0		13	18.4	-21.9	17	17.0	18.1	18	5.6	-2.3
			14	12.9	-14.1	18	8.2	-8.6			
4	67.0	-71.5	15	34.5	39.3	19	7.8	-10.7			