in order to make an empirical assessment of the *relative* powers of the traditional and reinforced inequalities. It was then found that the reinforced criterion can give definite signs and several exclusions of sign combinations, even when the traditional inequalities gave no information.

If the known atoms are in positions having the same symmetry as the rest of the structure, no particular type of inequality is expected to be especially affected. In the case where the atoms with known positions define a higher symmetry than the rest, certain inequalities will be reinforced to a greater extent than others. However, since it would be natural to calculate

$$\sum_n' g f_{(n)} \cdot \exp\left[2\pi i \mathbf{h} \cdot \mathbf{r}_{(n)}\right]$$

for all **h**'s simultaneously, there is little point in discussing particular situations in detail. It is evident that a sum,

$$\sum_n' g f_{(n)} \cdot \exp\left[2\pi i \mathbf{h} \cdot \mathbf{r}_{(n)}\right],$$

that is large, whatever the cause might be, is particularly capable of increasing the power of an inequality.

It seems specially valuable to consider the reinforcement proposed here in the case in which some atomic positions are determined by symmetry, because

$$\sum_n' g f_{(n)} \cdot \exp\left[2\pi i \mathbf{h} \cdot \mathbf{r}_{(n)}\right]$$

is then exactly known, and V very easily found from U.

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Cell parameters and space groups of potassium, rubidium, and cesium acid chloromaleates.*

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The cell parameters and space groups of the potassium, rubidium, and cesium acid chloromaleates

(HOOC.CCl : CH.COOM, where M = K, Rb, or Cs)

grown from aqueous solution were determined. Preliminary values of the cell constants as well as symmetry information were found from photographs prepared with Mo $K\alpha$ radiation on the precession camera. Powder diffraction data taken with a Debye–Scherrer camera and Cr $K\alpha$ radiation were used in subsequent least-squares refinements of the cell dimensions. Densities were measured pycnometrically; the supporting liquid was *n*-decane.

Potassium acid chloromaleate was found to be orthorhombic. Precession camera pictures indexed as $h0l$, $h1l$, $h2l$, $0kl$, $1kl$, $2kl$, and $hk0$ display the following systematic absences: none among reflections hkl; $hk0$ reflections present only if $h+k=2n$; $h0l$, only if $l=2n$; and $0kl$, only if $k=2n$. These absences indicate the space group *Pbcn*. A previous report (Yardley, 1925) gave cell dimensions in good agreement with those of this study, but a different space group (*Pmcn*, referred to the present axis orientation). The disagreement rests on two weak reflections which are absent on our photographs.

The space group of the two isomorphous monoclinic salts rubidium and cesium acid chloromaleate was not uniquely determined. On the precession camera pictures $hk0$, $hk1$, $hk2$, $0kl$, $1kl$, and $2kl$, the only systematic absences noted were those for which $h+k+l=2n+1$. Of the three space groups *Im*, *I*2 and *I*2/*m*, which are consistent with these absences, the last is considered unlikely because it requires that two chloromaleate ions lie in mirror planes in the approximately five by eight Ångström face of the cell.

The findings of this study are summarized in Table 1. In the monoclinic cases, the more usual *C*-centered cell is included, but the body-centered cell with β close to 90° is retained for convenience. The observed interplanar spacings, corrected for error due to absorption in the specimen (Klug & Alexander, 1954), are compared with the calculated values in Tables 2, 3, and 4. Indexing of

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Table 1. *Crystallographic data for potassium, rubidium, and cesium acid chloromaleates*

		Rubidium		Cesium	
	Potassium	Body-centered indexing	*C*-centered indexing	Body-centered indexing	*C*-centered indexing
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
a	15·815 ± 0·015 Å	8·112 ± 0·003 Å	9·61 Å	8·352 ± 0·007 Å	9·87 Å
b	10·928 ± 0·006	16·638 ± 0·011	16·64	17·325 ± 0·014	17·33
c	7·707 ± 0·005	5·090 ± 0·003	5·09	5·152 ± 0·004	5·15
β	—	90° 28′ ± 4′	122° 26′	90° 45′ ± 5′	122° 12′
Space group	*Pbcn*	*Im* or *I*2	*Cm* or *C*2	*Im* or *I*2	*Cm* or *C*2
Molecules/cell	8	4		4	
Calculated density	1·881 g.cm.$^{-3}$	2·272 g.cm.$^{-3}$		2·516 g.cm.$^{-3}$	
Observed density	1·868	2·246		2·515	

The errors listed are least-squares standard deviations.

Spacings for K, Rb, Cs *acid chloromaleates*

Table 2. K H Cl Maleate

h	*k*	*l*	d_c, Å	d_o, Å	I_o	*h*	*k*	*l*	d_c, Å	d_o, Å	I_o
1	1	0	8.990	9.013	VW– *	2	2	3	2.230	2.230	W
2	0	0	7.907	7.923	W *	0	4	2	2.229		
1	1	1	5.851			7	1	0	2.212		
0	2	0	5.464			1	4	2	2.207		
2	1	1	4.927	4.915	W– *	4	3	2	2.200		
3	1	0	4.748	4.742	M *	6	0	2	2.176	2.170	M+
2	2	0	4.495			1	5	0	2.165		
0	2	1	4.457			4	4	1	2.158		
1	2	1	4.290	4.299	S *	2	4	2	2.145	2.146	W–
3	1	1	4.042			6	1	2	2.134	2.130	W–
4	0	0	3.954			3	2	3	2.127		
2	2	1	3.883	3.884	S– *	7	1	1	2.127		
0	0	2	3.854			4	1	3	2.114		
1	0	2	3.744	3.744	S– *	1	5	1	2.084	2.083	W+ *
1	3	0	3.550			1	3	3	2.081		
1	1	2	3.542	3.540	M+ *	6	3	1	2.058		
4	0	1	3.518			3	4	2	2.053		
2	0	2	3.464	3.469	W+ *	2	5	1	2.032		
3	2	1	3.404			5	3	2	2.030		
4	1	1	3.349			2	3	3	2.029		
2	1	2	3.302	3.297	M *	6	2	2	2.021	2.020	VW–
1	3	1	3.224	3.231	W b*	3	5	0	2.019		
4	2	0	3.203			7	2	1	2.015		
0	2	2	3.149	3.149	S *	4	2	3	2.004		
3	0	2	3.111			5	4	1	1.997		
1	2	2	3.088	3.091	M	8	0	0	1.977		
2	3	1	3.040			5	1	3	1.962		
5	1	0	3.038	3.036	M+	3	5	1	1.953		
3	3	0	2.997	2.994	M	3	3	3	1.950	1.949	VW–
3	1	2	2.992			7	0	2	1.949		
4	2	1	2.958	2.958	M+ *	4	4	2	1.941		
2	2	2	2.926			0	0	4	1.927		
5	1	1	2.827			7	3	0	1.920		
3	3	1	2.793	2.792	W *	7	1	2	1.919		
4	0	2	2.760	2.760	W+ *	1	0	4	1.913		
5	2	0	2.737			6	4	0	1.897		
0	4	0	2.732			1	5	2	1.888		
3	2	2	2.703	2.704	W– *	8	1	1	1.886		
4	1	2	2.676			1	1	4	1.884		
6	0	0	2.636	2.629	VW– b	5	2	3	1.873		
1	3	2	2.611			2	0	4	1.872		
2	4	0	2.582			0	4	3	1.872		
5	2	1	2.580			6	3	2	1.868		
0	4	1	2.575			7	3	1	1.863		
1	4	1	2.542			8	2	0	1.859	1.859	W–
4	3	1	2.530	2.525	VW– b	1	4	3	1.859		
2	3	2	2.510			4	5	1	1.856		
1	1	3	2.470	2.472	VW– b	4	3	3	1.854		
4	2	2	2.463			2	5	2	1.848		
2	4	1	2.448			2	1	4	1.845		
5	0	2	2.445			6	4	1	1.842		
6	1	1	2.431			7	2	2	1.836		
5	3	0	2.388			5	4	2	1.822		
5	1	2	2.386			0	6	0	1.821		
2	1	3	2.384			2	4	3	1.821		
6	2	0	2.374	2.371	W– b	0	2	4	1.817		
3	3	2	2.366			6	1	3	1.814		
0	2	3	2.325	2.326	M+	3	0	4	1.810		
3	4	1	2.314			8	2	1	1.807		
1	2	3	2.300			1	2	4	1.805		
5	3	1	2.281	2.279	W b	5	5	0	1.798		
6	2	1	2.269			3	5	2	1.788	1.788	W
3	1	3	2.259			3	1	4	1.785		
4	4	0	2.248			2	6	0	1.775		
5	2	2	2.232			0	6	1	1.773		

The observed spacings have been corrected for absorption error. Specimen radius = 0.075 mm.

b Indicates a broad line.

* Observations that were used in the least-squares refinement of the cell.

V = very, S = strong, M = medium, W = weak.

Table 3. Rb H Cl Maleate

(Indexing based on body-centered cell)

h	*k*	*l*	d_c, Å	d_o, Å	I_o	*h*	*k*	*l*	d_c, Å	d_o, Å	I_o
0	2	0	8.319	8.293	W *	3	0	1	2.380	2.383	W
1	1	0	7.291	7.281	W– *	1	6	–1	2.335		
0	1	1	4.867	4.861	tr *	1	6	1	2.330		
1	3	0	4.578	4.582	W+ *	3	2	–1	2.302	2.302	M+
1	0	–1	4.327	4.312	W+	2	5	–1	2.301		
1	0	1	4.296			2	5	1	2.291		
0	4	0	4.159			2	6	0	2.289		
2	0	0	4.056	4.056	tr *b	3	2	1	2.288		
1	2	–1	3.839	3.829	M+ b	1	7	0	2.281	2.280	M
1	2	1	3.817			1	3	–2	2.229	2.230	W– *b†
0	3	1	3.750			1	3	2	2.220		
2	2	0	3.646	3.645	M *	0	4	2	2.171		
2	1	–1	3.128			2	0	–2	2.164		
2	1	1	3.104	3.109	S– *†	0	7	1	2.154	2.151	W– b
1	5	0	3.079	3.080	W+ *	2	0	2	2.148		
1	4	–1	2.999	2.995	M– b	3	5	0	2.098	2.099	W *
1	4	1	2.988			2	2	–2	2.094		
2	4	0	2.904	2.910	W *	0	8	0	2.080	2.081	tr
0	5	–1	2.785			2	2	2	2.080		
0	5	1	2.785			3	4	–1	2.076		
0	6	0	2.773	2.767	W+	3	4	1	2.066	2.063	tr
2	3	–1	2.762			4	0	0	2.028	2.026	VW– *
2	3	1	2.745	2.748	W	4	2	0	1.970	1.970	W– *
3	1	0	2.669			1	5	–2	1.965		
0	0	2	2.545	2.544	VW– *	1	5	2	1.959	1.958	W– *†
0	2	2	2.434	2.434	W	2	4	–2	1.920	1.919	W– *†
3	3	0	2.430			2	4	2	1.908		
1	1	–2	2.408			2	7	–1	1.905		
1	1	2	2.397	2.397	W	2	7	1	1.899	1.898	W– *†
3	0	–1	2.396			4	1	–1	1.877		

†The choice between indices *hkl* and *hkl̄* was made in these cases by comparing the intensities with those on the single crystal patterns.

The observed spacings have been corrected for absorption error. Specimen radius = 0.15 mm.

Table 4. Cs H Cl Maleate

(Indexing based on body-centered cell)

h	*k*	*l*	d_c, Å	d_o, Å	I_o	*h*	*k*	*l*	d_c, Å	d_o, Å	I_o
0	2	0	8.663	8.676	W+ *	1	3	2	2.257		
1	1	0	7.523	7.508	W– *	0	7	1	2.231	2.231	W *
0	1	1	4.938	4.932	VW– *	0	4	2	2.214		
1	3	0	4.750	4.758	W+ *	2	0	–2	2.205		
1	0	–1	4.411	4.414	W *	2	0	2	2.179		
1	0	1	4.359	4.364	W	3	5	0	2.170	2.170	W
0	4	0	4.331			0	8	0	2.166		
2	0	0	4.176	4.183	W– *	3	4	–1	2.141	2.139	W– b
1	2	–1	3.930	3.925	M *	2	2	–2	2.137		
1	2	1	3.894	3.894	M *	3	4	1	2.123		
0	3	1	3.844	3.839	W– *	2	2	2	2.114	2.113	W– b
2	2	0	3.761	3.763	M *	4	0	0	2.088		
2	1	–1	3.209	3.205	M	4	2	0	2.030	2.029	W
1	5	0	3.201			1	5	–2	2.012		
2	1	1	3.169	3.171	M+ *	1	5	2	2.002	2.001	W– b
1	4	–1	3.090	3.089	M b	2	7	–1	1.972		
1	4	1	3.072			2	4	–2	1.965	1.964	W+
2	4	0	3.006	3.004	W+ *	2	7	1	1.963		
0	6	0	2.888	2.888	W b	2	4	2	1.947		
0	5	1	2.875			1	8	–1	1.944		
2	3	–1	2.842	2.842	W *	1	8	1	1.939		
2	3	1	2.814	2.814	W– *	4	1	–1	1.932		
3	1	0	2.748			2	8	0	1.922		
0	0	2	2.576	2.574	VW– *	0	6	2	1.922		
3	3	0	2.508	2.505	tr *	4	1	1	1.914		
0	2	2	2.469	2.466	W b	3	1	–2	1.892		
3	0	–1	2.463			4	4	0	1.881	1.878	W–
1	1	–2	2.446			1	9	0	1.876		
3	0	1	2.436	2.436	W	3	6	–1	1.874		
1	1	2	2.428			3	1	2	1.867		
1	6	–1	2.416			3	6	1	1.862		
1	6	1	2.407	2.403	tr	3	7	0	1.850		
2	5	–1	2.376			4	3	–1	1.842		
2	6	0	2.375	2.374	M b	4	3	1	1.827		
1	7	0	2.373			3	3	–2	1.808		
3	2	–1	2.369			0	9	1	1.803	1.803	W–
2	5	1	2.360			3	3	2	1.786		
3	2	1	2.345	2.345	W	2	6	–2	1.753		
1	3	–2	2.271	2.274	W– *	1	7	–2	1.749		

The observed spacings have been corrected for absorption error. Specimen radius = 0.33 mm.

the monoclinic patterns is on the basis of the body-centered cell.

An investigation of the structure of potassium acid chloromaleate is in progress, but no further work is planned on the rubidium and cesium salts.

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