method. These techniques can be used for finding the correct crystal symmetry in the case of structures of type 4.

Structures of other types produce diffraction patterns with enhanced symmetry even when Friedel's law does not hold. Furthermore, in the case of type 3, the diffraction enhancement also occurs in centrosymmetric structures. For example, if a centre of inversion is added to the structure with the symmetry $P4_2$ described above, the resultant structure will belong to the space group $P4_2/m$, and the diffraction symmetry will become $4/mmm$.

The phenomena of the occurrence of hypersymmetry in diffraction patterns (diffraction enhancement of symmetry) will be encountered actually, though seldom, in crystal-structure analysis, especially in the case of inorganic compounds. The space group must not be determined by a cursory glance at the apparent diffraction symmetry. It is, in general, dangerous to assign atomic parameters by a naive comparison of Z with the number of general positions required by such a space group. Disregard of the Laue symmetry will sometimes be necessary to attain the correct structure.

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The X-ray Structure Factors of Strontium Chloride Powder at 300° K and 80° K Analysed in Terms of Non-spherical Atoms

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The X-ray structure factors of $SrCl_2$ powder have been measured with Cu $K\alpha$ radiation at 300 and 80°K for 25 reflexions, including the faint ones, which in the fluorite structure obey the relation $h+k+l = 2(2n+1)$. The absolute scale was determined by comparing the intensities with those measured for a NaCl specimen. The overall agreement between the measured and calculated structure factors was good. The Debye–Waller coefficients were $B_{Sr} = 1\cdot30 \pm 0\cdot05$, $B_{Cl} = 1\cdot47 \pm 0\cdot05$ Å^2 at 300°K and $B_{Sr} = 0\cdot42 \pm 0\cdot05$, $B_{Cl} = 0\cdot50 \pm 0\cdot05$ Å^2 at 80°K. For the length of the unit-cell edge the values $6\cdot9783 \pm 0\cdot0004$ and $6\cdot9442 \pm 0\cdot0004$ Å were obtained at 300 and 80°K respectively. An analysis based on the spherical harmonic expansion shows the electron distribution around the cation and the anion to be almost spherically symmetric. Some traces of tetrahedral deformation in Cl$^-$ seem, however, to be present.

1. Introduction

The structure of strontium chloride has been found to be similar to the calcium fluoride structure (Mark & Tolksdorf, 1925). As the number of electrons in Sr^{2+} is twice as large as that in Cl$^-$, the reflexions $h+k+l = 2(2n-1)$, $n=1,2,3,\ldots$, are very weak, their intensity being less than 1% relative to the intensity of the strongest (220) reflexion (Swanson, Fuyat & Ugrinic, 1955). The edge of the unit cell has been measured to be 7·01 Å (Mark & Tolksdorf, 1925), 6·979 Å (20°C; Ott, 1926) and 6·9767 Å (26°C; Swanson, Fuyat & Ugrinic, 1955).

Thermal vibrations in fluorite structures have been studied with both neutron and X-ray diffraction. Some neutron-diffraction results have been analysed by Dawson, Hurley & Maslen (1967), who report anharmonic thermal vibrations in UO_2, ThO_2 and CaF_2 associated with the tetrahedral symmetry of the anionic sites. Cooper (1970) analysed single-crystal X-ray measurements for CaF_2 and found anharmonic components consistent with the neutron results. Calculations by Cooper & Panke (1970) based on X-ray diffraction measurements for Mg_2Si gave similar results. Non-spherical deformations of the ions in CaF_2 have been studied by Kurki-Suonio & Meisalo (1966)

and further with improved methods by Kurki-Suonio & Ruuskanen (1972). They found cubic deformations in the ions, but tetrahedral deformations in F⁻ are unlikely. Their calculations were based on X-ray powder results.

In order to obtain more information about possible non-spherical deformations in the fluorite structures we measured 25 reflexions of $SrCl_2$ using X-ray powder techniques. We have extended our measurements to liquid-air temperature to reveal new features of the effect of thermal vibrations.

2. Experimental

Our raw material was strontium chloride hexahydrate ($SrCl_2.6H_2O$). It was 'Baker-analysed' reagent manufactured by Noury–Baker N.V., Holland, and the main impurities (0·05%) were reported to be Mg and alkalis (like SO_4). Crystalline water was removed by heating for several hours at 250°C. Two different techniques were used in preparing fine powder: (1) grinding in an agate mortar and (2) dissolving $SrCl_2$ in methanol and precipitating it by diethylether. The size of crystallites in the powders was about 1μ in both cases. Several specimens were prepared with different moulding pressures (600–2500 kp.cm⁻²) and with varying surface treatment. Comparisons between the intensities measured with 'soft' and 'hard' specimens indicated that the influence of porosity and surface roughness was small. Furthermore we did not notice any traces of specific orientation. Nine specimens were chosen for the final measurements. Because strontium chloride is not stable in normal atmosphere (it hydrates very easily) the specimens were stored and measured inside a vacuum chamber. Every specimen was checked for the presence of extra reflexions.

A detailed description of the measuring system, including the low-temperature equipment, and of the method of measurement has been given previously (Linkoaho, 1968). The measuring system has been tested in connexion with the Powder Intensity Project of the IUCr (Linkoaho, Rantavuori & Korhonen, 1971). We used Cu $K\alpha$ radiation monochromated by a diffracted-beam monochromator. The polarization factor of the monochromator was measured by the Miyake method (Linkoaho, Rantavuori & Korhonen, 1971). The result $k = 0·90 \pm 0·02$ is near the value $k = 0·89$ expected for a perfect crystal. The relative intensities of each reflexion were measured 12–16 times for the reflexions 111–531 and 6–8 times for the reflexions 442–660. The weak reflexion 200 was measured separately. The intensities of the other faint reflexions were obtained by a two-step procedure: first, the total intensity of the weak reflexion and the neighbouring strong reflexion (420 and 331, for instance) was measured just as in the case of a single reflexion. Then the line profile was drawn on a millimeter paper, the reflexions were separated and the total intensity was divided according to the ratio of their areas.

We determined the absolute scale of the structure factors by comparing the intensity of the 220 reflexion of $SrCl_2$ with the intensities of the 200 and 220 reflexions of NaCl. In this case we have

$$F = F_s \left[\frac{\mu V^2 p_s(\theta) j_s E}{\mu_s V_s^2 p(\theta) j E_s} \right]^{1/2} = F_s \left[\frac{\mu_e V M p_s(\theta) j_s E}{\mu_{es} V_s M_s p(\theta) j E_s} \right]^{1/2} \quad (1)$$

where F is the structure factor, μ the linear and μ_e the mass-absorption coefficient, M the mass and V the volume of the unit cell, $p(\theta)$ the Lorentz–polarization factor, j the multiplicity factor and E the measured integrated intensity. The subscript s refers to the values for NaCl, for which the absolute structure factors are accurately known (Linkoaho, 1968). The scale at 80°K was determined by a comparison of the integrated intensity of the 220 reflexion at 80°K with that at room temperature.

The TDS corrections at 300°K were determined according to Chipman & Paskin (1959) with the use of

$$I_{corr} = I_{meas}/(1 + \sigma) \quad (2)$$

$$\sigma = 0·05 \cos \theta \left(\frac{\sin \theta}{\lambda} \right)^2 \varDelta \quad (3)$$

where σ is the TDS correction, θ the Bragg angle, λ the wavelength, $\varDelta$ the scanning width in degrees (2θ); I_{corr} and I_{meas} are the corrected and measured integrated intensities respectively. At 80°K we used one fourth of those at room temperature for the values of σ. In applying the formula of Chipman & Paskin (1959) the value

$$\bar{B} = \tfrac{2}{3} \frac{m_{Sr} B_{Sr} + 2 m_{Cl} B_{Cl}}{m_{Sr} + 2 m_{Cl}} \quad (3a)$$

was used, where the weighting factor $\tfrac{2}{3}$ (instead of the usual $\tfrac{1}{2}$) is due to the dominant contribution of acoustic phonons to the Debye–Waller factor.

Using powder mixtures we measured the positions of the $K\alpha$ and $K\beta$ reflexions of $SrCl_2$ at 300 and 80°K relative to the positions of the reflexions of NaCl. This way we obtained the values $6·9783 \pm 0·0004$ and $6·9442 \pm 0·0004$ Å for the length of the unit-cell edge at 300 and 80°K respectively. The room-temperature value differs from the value reported by Swanson et al. (1955) but is very near the much older value of Ott (1926). Our results give the mean value of $2·23 \pm 0·05 . 10^{-5}/°C$ for the coefficient of thermal expansion of $SrCl_2$ between 80 and 300°K.

3. Results

For comparison, the integrated intensities of the strong reflexions for $SrCl_2$ measured by us are shown in Table 1 together with the NBS results (Swanson, Fuyat & Ugrinic, 1955) obtained with photographic techniques.

Table 1. *The relative integrated intensities of* $SrCl_2$ *powder for strong reflexions measured at* 300°K *with* Cu Kα *radiation together with the values given by the National Bureau of Standards* (NBS; *Swanson, Fuyat & Ugrinic*, 1955)

hkl	NBS	This work
111	59	74·0
220	100	100
311	44	36·4
400	20	14·8
331	17	13·8
422	28	27·1
511	12	9·4
440	10	7·9
531	11	8·8
620	12	10·7
533	4	2·9
444	4	2·6
711	7	4·9
642	14	13·8
731	7	6·7
800	3	2·1
733	2	2·2
822	10	11·1

The measured structure factors at 300 and 80°K are shown in Table 2 (without dispersion corrections). The error estimates are for the relative values, and they are in each case obtained from the scatter of the measured relative intensity values. The inaccuracies in the TDS corrections, the geometrical aberrations and the porosity affect the accuracy relatively little in comparison with the influence of the statistical fluctuations and the differences between the specimens (*cf.* Korhonen, Rantavuori & Linkoaho, 1971). Thus the accuracy of the relative measurements seems to be about 0·5% for the strong reflexions and about 10% for the weak ones.

The accuracy of the absolute scale depends almost entirely on the accuracy of the absorption factors used in equation (1). As the absorption factor of strontium chloride for Cu Kα radiation is relatively high ($\mu \simeq 350$ cm⁻¹) it is difficult to measure it directly. There are at least three different sets of theoretical absorption factors available, namely those of *International Tables for X-ray Crystallography* (1962), of Guttmann & Wagenfeld (1967) and of Cromer & Liberman (1970). The values of *International Tables for X-ray Crystallography* are based on an empirical relation, the values of Guttmann & Wagenfeld have been calculated using multipole expansion of matrix elements with hydrogen-like eigenfunctions for K, L, M and N electrons and, finally, the values of Cromer & Liberman are based on calculations of photoelectric cross-sections with relativistic Dirac–Slater wave functions. In Fig. 1 we have compared these theoretical absorption factors with some experimental ones. We see that the values of *International Tables for X-ray Crystallography* are too low in the vicinity of $Z = 11$ (Na) and $Z = 17$ (Cl) but too high in the vicinity of $Z = 38$ (Sr). Since we need the ratio of the absorption coefficients for $SrCl_2$ and NaCl

in equation (1), we prefer to use the values of Cromer & Liberman, although the values of Guttmann & Wagenfeld seem to be almost equally suitable. According to Fig. 1 we estimate the accuracy of the ratio of the absorption coefficients in this case to be about ±4% which means about ±2% in the scale factor.

In Table 2 we have compared our measured values of the structure factors with the semi-theoretical ones based on the relativistic Hartree–Fock atomic factors of Doyle & Turner (1968). Calculating the semi-theoretical values we need also the Debye–Waller coefficients and the dispersion corrections. We find the appropriate values for the Debye–Waller coefficients applying the Fourier-difference method (Kurki-Suonio & Fontell, 1964). The results are $B_{Sr} = 1.30 \pm 0.05$, $B_{Cl} = 1.47 \pm 0.05$ Å² and $B_{Sr} = 0.42 \pm 0.05$, $B_{Cl} = 0.50 \pm 0.05$ Å² at 300 and 80°K respectively. The scale obtained by this method agrees within 1% with the experimental one at both room and liquid-air temperatures. In Table 2 we show also the total dispersion corrections obtained by using the relativistic values of Cromer & Liberman (1970).

4. Non-spherical analysis of charge density

At first, we tried to define the atomic region for each atom independently of the other atoms by seeking the most natural way to separate it from its surroundings. It has been pointed out by Kurki-Suonio & Salmo (1971) that a sphere is the most natural shape to use for any structure. The problem is to find the radius of best separation. Consequently we have calculated the spherical electron density $4\pi r^2 \varrho_0(r)$ around both atoms, ϱ_0 being

$$\varrho_0(r) = \frac{1}{V} \sum_j F_j \frac{\sin 2\pi b_j r}{2\pi b_j r}. \tag{4}$$

Here the F_j's are the measured structure factors, V is the volume of the unit cell and the b_j's are the reciprocal lattice vectors. We define the radius of best separation to be the value of r which gives a minimum in $4\pi r^2 \varrho_0(r)$ (Kurki-Suonio & Salmo, 1971). These values appeared to be 1·5 and 1·8 Å for Sr^{2+} and Cl^- respectively. The residual term due to the early breaking off of the measured structure factors has been calculated by the use of a Gaussian representation of the theoretical atomic factors (Kurki-Suonio & Salmo, 1971). However, some inconvenient oscillations were still present in the electron density curves rendering the determination of the ionic radii difficult. The electron density reached a lower value around the cation, which means better separability from the surroundings.

Secondly, we calculated the electron count $Z(R)$ inside spheres around both kinds of atoms according to

$$Z(R) = \frac{1}{V} \sum_j F_j \frac{j_1(2\pi b_j R)}{2\pi b_j R} \tag{5}$$

where R is the radius obtained by the use of equation (4) and j_1 is the spherical Bessel function (Kurki-Suonio & Salmo, 1971). The absolute and relative electron counts obtained inside the Sr and Cl spheres are given in Table 3 together with the radii of these spheres. Table 3 shows that our definition of the ionic spheres leaves about 3·5 electrons per unit cell hidden. However, if we use 0·1 Å larger radii for both spheres, we get about four more electrons, and only a minute fraction of this is due to overlapping of the spheres. Calculations of the electron density show the big holes around the points $\frac{1}{2}00$, $0\frac{1}{2}0$, $00\frac{1}{2}$, and $\frac{1}{2}\frac{1}{2}\frac{1}{2}$ to be completely empty. The hidden electron distribution seems to accumulate inside the cubes with Sr ions in the centre and Cl ions in the corners.

Preliminary calculations of the cubic harmonic expansions (Kurki-Suonio, 1968) indicated that the large differences between the experimental and theoretical structure factors of the reflexions 800–660, 822 were not consistent with the other data. We, therefore, omitted these reflexions in our final calculations. The results of these calculations are shown schematically in Table 4. We see that the aspherical components are generally small, but we want to make the following remarks:

– There seem to be some difficulties in the use of cubic harmonic expansions for electron distribution analysis in crystals with heavy atoms (cf. also Linkoaho, 1969). The reasons may be that (a) the theoretical values do not give the residual term accurately enough and that (b) the binding effects are probably

similar on an absolute scale and, therefore, are relatively smaller in heavy ions. Thus it is difficult to find significant deformations in this case.
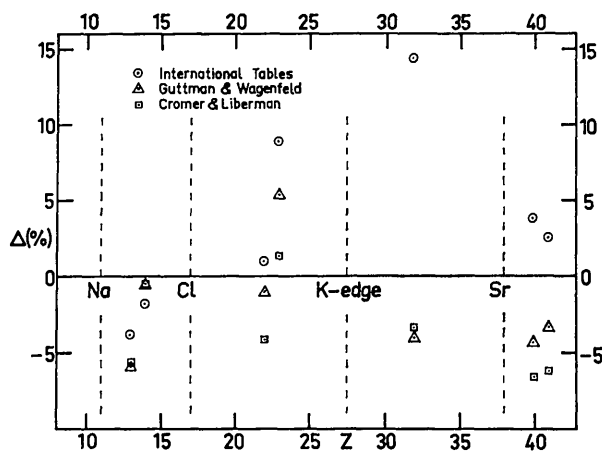

Fig. 1. The percentage differences between some theoretical and measured absorption factors for Cu $K\alpha$ radiation as a function of atomic number. The theoretical values are taken from the *International Tables for X-ray Crystallography* (circles, 1962), from the work of Guttmann & Wagenfeld (triangles, 1967) and from Cromer & Liberman (squares, 1970). The experimental values have been measured by Hughes, Woodhouse & Bucklow (1968) for Al, Ti, Zr and Nb, by Cooper (1965) for Al and V and by Hildebrandt (cf. Jennings, 1969) for Si and Ge. The position of the K edge for Cu $K\alpha$ radiation is shown as well as the positions of the atoms in NaCl and SrCl₂.

Table 2. *The measured structure factors of* SrCl₂ *at* 300 *and* 80°K *together with the dispersion corrections, the error estimates, the semi-theoretical values and the differences between the measured and semi-theoretical values*

In calculations the values $B_{Sr}=1·30$ Å², $B_{Cl}=1·47$ and $B_{Sr}=0·42$, $B_{Cl}=0·50$ Å² have been used at 300 and 80°K respectively.

	300°K, $a=6·9783$ Å					80°K, $a=6·9442$ Å				
hkl	F_{meas}	$-\Delta f$	Error	F_{calc}	$F_m - F_c$	$\sin\theta/\lambda$	F_{meas}	$-\Delta f$	Error	F_{calc}	$F_m - F_c$
111	31·08	0·41	±0·15	32·26	−1·18	0·1247	32·05	0·41	±0·32	32·68	−0·63
200	3·79	1·11	0·28	3·43	0·36	0·1440	3·29	1·13	0·40	3·46	−0·17
220	50·16	−0·31	0·25	51·13	−0·97	0·2037	52·99	−0·32	0·26	52·98	0·01
311	25·66	0·38	0·13	26·03	−0·37	0·2388	27·25	0·40	0·14	27·31	−0·06
222	5·59	1·05	0·25	5·35	0·24	0·2494	5·91	1·11	0·60	5·53	0·38
400	40·78	−0·30	0·83	41·34	−0·56	0·2880	45·04	−0·33	0·23	44·46	0·58
331	21·84	0·35	0·11	22·02	−0·18	0·3139	24·14	0·38	0·12	23·93	0·21
420	5·50	0·99	0·27	5·19	0·31	0·3220	6·05	1·09	0·60	5·51	0·54
422	35·23	−0·29	0·71	35·33	−0·10	0·3527	39·82	−0·33	0·20	39·44	0·38
333, 511	19·26	0·33	0·38	19·16	0·10	0·3741	21·77	0·37	0·11	21·58	0·19
440	31·41	−0·28	0·95	31·06	0·35	0·4073	36·58	−0·33	1·10	36·00	0·58
531	17·27	0·31	0·09	16·97	0·30	0·4260	19·70	0·36	0·39	19·81	−0·11
442, 600	4·42	0·88	0·22	4·15	0·27	0·4320	4·92	1·05	0·50	4·62	0·30
620	28·29	−0·27	0·56	27·73	0·56	0·4554	33·27	−0·33	1·33	33·37	−0·10
533	15·05	0·29	0·30	15·19	−0·14	0·4722	17·94	0·35	0·54	18·38	−0·44
622	3·85	0·83	0·34	3·69	0·16	0·4776	4·55	1·02	0·46	4·20	0·35
444	24·72	−0·25	0·74	24·97	−0·25	0·4988	30·70	−0·33	2·15	31·20	−0·50
551, 711	13·84	0·27	0·42	13·69	0·15	0·5142	17·24	0·34	0·52	17·17	0·07
640	3·84	0·78	0·36	3·30	0·54	0·5192	4·79	1·00	0·48	3·83	0·96
642	22·58	−0·24	0·45	22·60	−0·02	0·5388	29·18	−0·33	0·87	29·32	−0·14
553, 731	12·49	0·25	0·62	12·40	0·09	0·5531	16·16	0·33	0·65	16·11	0·05
800	22·41	−0·23	1·13	20·52	1·89	0·5760	31·10	−0·32	0·78	27·63	3·47
733	11·12	0·24	0·56	11·26	−0·14	0·5894	14·93	0·32	0·89	15·17	−0·24
820, 644	2·24	0·69	0·24	2·69	−0·45	0·5937	3·01	0·96	0·30	3·27	−0·26
660, 822	17·95	−0·22	0·18	18·67	−0·72	0·6110	25·82	−0·32	1·29	26·09	−0·27

– The Δf_3 component in Cl seems to be significant both at 300 and 80°K. We are not, however, able to decide whether it is due to aspherical thermal vibrations or to static deformation.

– The Δf_6 component in Sr, although not fully significant, may have a real physical meaning. Its existence indicates an electron concentration in the [111] direction, which is natural in BC symmetry.

– The Δf_4 components do not seem to have physical significance, because they have a different sign compared to fluorite (Kurki-Suonio & Ruuskanen, 1972), where this deformation is clearly significant.

Table 3. *The results of the calculations of the spherical electron density $4\pi r^2 \varrho_0(r)$ and the electron count $Z(R)$ performed to separate the ions of* SrCl$_2$ *from their surroundings*

The absolute charges inside the spheres are shown together with the radii of these spheres. The total charge includes two chlorine ions. The error estimates give the conceptual inaccuracies. The relative charges give the differences between the electron count on the neutral atom and the absolute charge. The total relative charge $+4\cdot1\pm0\cdot8$ appears to be near the ideal value $+4\cdot0$ corresponding to the completely ionized states.

Ion	Radius (Å)	Absolute charge ($-e$)	Relative charge (e)
Sr^{2+}	$1\cdot5\pm0\cdot1$	$35\cdot5\pm0\cdot2$	$+2\cdot5\pm0\cdot2$
Cl$^-$	$1\cdot8\pm0\cdot1$	$17\cdot8\pm0\cdot4$	$-0\cdot8\pm0\cdot4$
Total		$71\cdot1\pm0\cdot8$	$+4\cdot1\pm0\cdot8$

Table 4. *The results of the calculation of the spherical harmonic expansion in* SrCl$_2$

The plus sign indicates the presence of a deformation larger than the estimated experimental inaccuracy and the parentheses indicate deformations comparable to the experimental inaccuracy. The Δf_0 component is spherically symmetric and relates to radial changes in electron density.

Ion	Temperature	Δf_0	Δf_3	Δf_4	Δf_6	Δf_7	Δf_8
Sr^{2+}	300°K	+		(+)	(+)		−
	80	+		(+)	(+)		−
Cl$^-$	300	+	+	(+)	−	−	−
	80	+	+	(+)	−	−	−

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