quartz, thereby forming elementary silicon and scandium oxide.

The axial ratios of the unit cells of Sc_5Ga_3 and Y_5Ga_3 agree with the axial ratios of the six other known $D8_8$ phases containing Sc, Y or rare earth metals: Sc_5Si_3, Sc_5Ge_3, Y_5Si_3, Y_5Ge_3, La_5Ge_3 and Ce_5Ge_3. All these phases have very high axial ratios of about 0·75 while the axial ratios of the other known $D8_8$ phases are between 0·68 and 0·70. The characteristic high axial ratio of a $D8_8$ phase with a metal of the third group is nearly the same for gallide, silicide and germanide phase, but changes slightly with the transition metal component.

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The length of the I–Cl bond in tetramethylammonium dichloroiodide.

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The polyhalide ions in $KICl_4.H_2O$ (Mooney, 1937) and in $N(CH_3)_4ICl_2$ (Mooney, 1939) aroused our interest as the reported bond lengths are remarkably short in comparison with those in other polyhalide ions (Elema, de Boer & Vos, 1963). Refinement of the crystal structure of $KICl_4.H_2O$ (Elema *et al.*, 1963) showed that the I–Cl bonds in the ICl_4^- ion range from 2·42 to 2·60 Å and are thus considerably longer than the value determined by Mooney, 2·34 Å. It will appear from this paper that also in ICl_2^- the bonds are long.

$N(CH_3)_4ICl_2$ is tetragonal, space group $P\bar{4}2_1m$, with the two $N(CH_3)_4$ and ICl_2 groups in special positions (Mooney, 1939). Cell dimensions determined from a powder diffractogram with CaF_2 as a reference are $a=9{\cdot}35$, $c=5{\cdot}94$ Å with an e.s.d. of $2\,^0/_{00}$.

Fig. 3 in Mooney's paper shows that the I–Cl bond length in the ICl_2^- ion with symmetry 2 can be obtained both from the [001] and from the [1$\bar{1}$0] projection. Intensities of 56 *hk*0 reflexions were measured from a single crystal of dimensions $0{\cdot}17\times0{\cdot}25\times0{\cdot}28$ mm by counter techniques, 34 *hhl* reflexions were obtained from integrated zero-layer Weissenberg photographs about the [1$\bar{1}$0] axis of a crystal with dimensions $0{\cdot}18\times0{\cdot}10\times0{\cdot}20$ mm. Molybdenum radiation, with balanced Zr and Y filters and Zr-filtered Mo radiation respectively, was used. Corrections for the Lorentz and polarization effect and for absorption ($\mu=35{\cdot}6$ cm^{-1}) were applied.

The [001] projection was refined first. Isotropic refinement by successive Fourier syntheses failed to yield satisfactory agreement between the observed and calculated values of the individual structure factors. Good agreement ($R=0{\cdot}041$) was achieved by anisotropic least-squares refinement which was kindly carried out by Dr J. S. Rollett on the Mercury computer at Oxford.

The final coordinates listed in Table 1 and the thermal parameters U_{ij} (Cruickshank, 1956*a*) in Table 2 were obtained by anisotropic least-squares refinement of the 34 reflexions *hhl* and the 56 more accurately measured reflexions *hk*0; a weighting scheme corresponding to rough estimates of the experimental accuracy was applied. F_o-F_c syntheses of the two projections calculated after the refinement showed only small changes, less than 0·004 Å, in the I–Cl bond length. The calculated structure factors in Table 3 correspond to the parameters in Tables 1 and 2. $R=0{\cdot}045$.

Table 1. *Final coordinates*

Atom	*x*	e.s.d.	*y*	e.s.d.	*z*	e.s.d.
I	0		0·5		$0{\cdot}103_9$	0·001
Cl	$0{\cdot}193_1$	0·0015	$0{\cdot}693_1$	0·0015	$0{\cdot}105_5$	0·0025
N	0		0		0·5	
C	0·108	0·003	0·063	0·003	0·350	0·005

Table 2. *Thermal parameters* U_{ij} (Å^2) *relative to* [110] (1), [1$\bar{1}$0] (2) *and* z(3)

The e.s.d. for U_{ii}(I) and U_{ii}(Cl) are 0·002 and 0·004 Å^2 respectively

Atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
I	0·084	0·031	0·053	0	0	0
Cl	0·064	0·052	0·053	0	0	0*
N	0·042	0·042	0·058	0	0	0
C	0·058	0·091	0·097	0·004	0·023	0·000

* U_{13}(Cl) was assumed to be zero during the refinement in agreement with a rigid body description of the ICl_2^- ion; the remaining zeroes are due to symmetry.

In calculating the I–Cl bond length no correction for thermal motion (Cruickshank, 1956*b*) could be applied as may be seen from the parameters U_{ij} in Table 2 (Cl–I–Cl along [110]). The difference $U_{22}(\mathrm{Cl})-U_{22}(\mathrm{I})$, which might be ascribed to libration, is approximately

Table 3. *Observed and calculated structure factors*

In order to obtain F_o and F_c on the absolute scale, the values in the Table must be divided by 10

hk0	$\|F_o\|$	F_c	hk0	$\|F_o\|$	F_c	hhl	$\|F_o\|$	$\|F_o\|$	$\alpha/2\pi$
200	838	787	730	331	346-	001	868	896	0.000
400	697	716	830	105	103	002	321	331	0.000
600	568	551	930	156	166-	003	276	278	0.500
800	162	158	440	586	557	004	577	603	0.500
10,0,0	216	234	540	120	117-	005	454	468	0.500
12,0,0	48	66	640	418	412	006	219	178	0.500
110	595	637-	840	246	253	111	1100	1079	0.286
210	415	372	940	144	152-	112	508	470	0.436
310	667	573-	10,4,0	150	158	113	373	365	0.112
410	270	260-	12,4,0	81	70	114	385	391	0.034
510	682	681-	550	472	469-	115	303	286	0.757
610	234	245	650	108	98	221	796	775	0.811
710	303	311-	750	144	138-	222	310	283	0.783
910	171	178-	850	81	91	223	358	330	0.580
11,1,0	99	111-	950	129	134-	224	409	404	0.527
220	1280	1253	10,5,0	75	70	225	355	360	0.265
320	123	104	11,5,0	111	108-	331	733	741	0.506
420	598	591	660	352	351	332	267	261	0.416
520	63	49	760	153	158-	333	201	188	0.060
620	373	355	860	141	152	334	427	418	0.004
720	102	108-	10,6,0	123	133	335	294	293	0.009
820	361	381	11,6,0	72	75-	441	406	417	0.845
10,2,0	114	114	770	207	201-	442	295	285	0.907
11,2,0	54	61-	870	90	80	443	255	264	0.642
12,2,0	99	94	970	111	116-	444	249	232	0.569
330	967	905-	880	156	172	551	439	461	0.280
430	261	255	980	66	82-	554	258	250	0.021
530	246	246-	990	99	94-	661	234	218	0.818

equal to the difference $|U_{11}(\mathrm{Cl}) - U_{11}(\mathrm{I})|$, which should be zero for the ion to be a rigid body.

As the z coordinates of iodine and chlorine show no significant difference, the ICl_2^- ion is linear within experimental error. The I–Cl bond length, 2·55 e.s.d. 0·02 Å, is much larger than the value reported by Mooney, 2·34 Å. It is also much larger than the sum of the covalent radii, 2·32 Å. This is compatible with a bonding scheme in which delocalized molecular orbitals are formed by a linear combination of *p*-orbitals of the halogen atoms (Havinga & Wiebenga, 1959).

It is remarkable that the N–C distance obtained from the least-squares refinement, 1·47 e.s.d. 0·03 Å, is close to the usually accepted value, 1·48 Å, although the carbon atoms look rather blurred in the Fourier syntheses.

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Diffraction symbols.

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In reporting the results of a crystallographic investigation a problem of symbolism arises: how to represent, in as compact a form as possible, all the information that has been obtained by X-ray diffraction concerning the symmetry of a crystalline species.

Two solutions have been proposed: one by Donnay & Harker (1940), the other by Buerger (1942). Both are presented in *International Tables for X-ray Crystallography* (1952). The former has been reprinted as an Appendix to *Crystal Data* (1954, 1963).

Donnay & Harker have introduced the concept of *aspect* (either as 'morphological aspect' or as 'diffraction aspect'). An *aspect* is a statement of a set of criteria that govern the systematic absences in one or several space groups, in any given crystal system. Examples: In the orthorhombic system $P{*}{*}{*}$ stands for $Pmmm$, $P222$, $Pmm2$, $P2mm$, $Pm2m$. In the tetragonal system $I4_1{*}{*}$ stands for $I4_1$ and $I4_122$.

Buerger's *diffraction symbol* is more informative. It gives the Laue class symbol, followed by the aspect symbol. The above examples become: $mmmP{-}{-}{-}$, which stands for the same space groups as $P{*}{*}{*}$; $4/mI4_1{-}{-}$ and $4/mmmI4_1{-}{-}$, which stand respectively for $I4_1$ and $I4_122$.

Both notations are based on the fact that only those elements of symmetry that involve a translation component (glide planes and screw axes) can be symbolized. Other elements of symmetry (mirrors, rotation axes, inversion axes) are replaced by asterisks (in the aspect symbol) or by hyphens (in the diffraction symbol).† The asterisk, in some cases, stands for the absence of symmetry element, as in the tetragonal aspect $Pn{*}{*}$, which stands for $P4/nmm$ and $P4/n$.

Neither solution is completely satisfactory. The aspect symbolism has the following drawbacks:

(1) Any aspect that corresponds to a single space group is unnecessary; the space-group symbol itself should be used. Example: $P222_1$ instead of $P{*}{*}2_1$.

(2) Some aspect symbols are identical with space-group symbols. Example: Two space groups, $C2/c$ and Cc, are represented by the aspect symbol Cc, which gives no indication of its being an aspect rather than a space-group symbol.

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† Asterisks and hyphens have been changed to dots in *International Tables*.