Formfaktorwerte für die *K*-Schale. Dadurch wird bei der Differenzenbildung nur die vom Bindungszustand recht unabhängige Elektronendichte der *K*-Schale abgezogen und die gesamte Elektronendichte der 4 Valenzelektronen bleibt zurück, ohne dass man dabei irgendwelche Modelle für die Verteilung der Bindungselektronen in die Rechnung hineinstecken muss. Obwohl man dadurch 4 von 6 Elektronen pro Kohlenstoff belässt, ist doch der Einfluss des Abbrucheffektes selbst bei Verwendung der relativ langwelligen Cu *Kα*-Strahlung weitgehend eliminiert (vergl. Tabelle 1).

Tabelle 2. *Einfluss von Temperaturfaktor und Abbruchseffekt auf die Höhe der maximalen Gesamt-Elektronendichte* $\varrho(0)$ *in* e.Å^{-3}

$(\sin\theta/\lambda)_{\max}$	Temperaturfaktor B in Å^2				
in a.u.$^{-1}$	0·0	1·0	2·5	5·0	8·0
∞	841·2	(47·5)	(17·6)	(7·9)	(4·6)
3·0	523·1	47·5	17·6	7·9	4·6
0·75	101·7	41·7	17·5	7·9	4·6
0·35	18·1	14·4	10·6	6·8	4·4

In Tabelle 2 sind die maximalen Gesamt-Elektronendichten des Kohlenstoffs für die durchgerechneten Fälle in e.Å^{-3} angegeben. Daraus folgt z.B., dass man bei Atomen mit einem Temperaturfaktor von $B \leq 1$ Å^2 bei Verwendung von Mo *Kα*-Daten (gesamte Ausbreitungskugel) einen 3–5-mal höheren Wert für das Elektronendichtemaximum erhält als bei Verwendung von Cu *Kα*-Daten. Bei grösseren Temperaturfaktorwerten fällt der Abbruchseffekt weniger stark ins Gewicht.

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On the relation between the monoclinic and the orthorhombic form of yttrium hydroxychloride, $[YCl(OH)_2]_n$.

By K. DORNBERGER-SCHIFF, *Institut für Strukturforschung der Deutschen Akademie der Wissenschaften zu Berlin, Berlin-Adlershof, German Democratic Republic, and* R. F. KLEVTSOVA, *Institute of Inorganic Chemistry, Siberian Department, Academy of Sciences of the USSR, Novosibirsk, USSR*

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The two known modifications of yttrium hydroxychloride are the two structures of maximum degree of order belonging to one and the same family of OD-structures built of two kinds of layer of composition $[Y(OH)_2]_n$ and Cl_n respectively. The Cl_n layer possesses higher symmetry than the $Y(OH)_n$ layer and this explains the OD-character and the polymorphism. The energies of interaction of these layers are discussed qualitatively.

The monoclinic and the orthorhombic form of $YCl(OH)_2$ have recently been investigated (Klevtsova & Klevtsov, 1965, 1966). They are closely related. They both consist of layers of composition $[YCl(OH)_2]_n$ which are very similar, with the translational vectors of the single layer, *i.e.* the *a* and *b* axis, of the monoclinic form corresponding to those of the orthorhombic form, and the distances between consecutive layers are also very similar (Table 1). Thus, not only the atomic distances and coordination numbers but also the bond angles and the way the coordination polyhedra around the Y ion are joined together are practically the same. This can most easily be seen if the coordinates of one of these layers, *e.g.* the layer around $z=0$ of the monoclinic form, are referred to orthogonal axes, taking $c_{\text{orthog}} = 2c_{\text{mon}} \times \sin\beta$. This leads to the transformed coordinates given in Table 2, in which the coordinates of the orthorhombic form are also given for comparison.

Table 1. *Cell parameters of the two forms of yttrium hydroxychloride*

	Orthorhombic*	Monoclinic	
a	6·21 Å	6·14 Å	
b	3·62	3·62	$\beta=107°$
c	12·56	6·60	
	$c/2=6·28$	$c \sin\beta=6·31$	

* For convenience of comparison the *b* and *c* axes of the orthorhombic form have been interchanged as compared with the notation used earlier (Klevtsov & Klevtsova, 1965). Thus the space group *Pcmn* results.

The question arises, how it is to be explained that these two modes of stacking the layers, which lead to different pairs of adjacent layers, occur within the same charge of crystallization in greater or lesser proportion. The answer to this question may be obtained, if we consider either of these structures as consisting of two different kinds of layer, one kind to consist of $[Y(OH)_2]_n$ groups and the other of Cl atoms. The symmetry of the yttrium hydroxide layers is $P12_1/m(1)$, where the brackets around the symbol 1 indicate that the **c** direction is the direction of missing periodicity of the layer. The symmetry of the Cl layers is $P2_1/m\,2_1/m\,(2/n)$ (Figs. 1 and 2).

The fact that the symmetry of the Cl layers is higher than the symmetry of the yttrium hydroxide layers explains the polymorphism as a kind of polytypism. In the monoclinic form successive yttrium hydroxide layers L_{2n} and L_{2n+2} are connected by the symmetry centre and the screw axis parallel to **b** which convert the Cl layer L_{2n+1} lying between

Table 2. *Atomic coordinates of the monoclinic form (referred to monoclinic and orthogonal axes) and the orthorhombic form of* $YCl(OH)_2$

The orthogonal coordinates were obtained through the following transformation:
$x_{\rm orthog} = x - (z\,c\,.\,\cos\beta)/a = x - 0{\cdot}316z$ $\quad y_{\rm orthog} = y$; $\quad z_{\rm orthog} = z/2$.

		Monoclinic					
		Monoclinic axes		Orthogonal axes		Orthorhombic	
	y	x	z	$x_{\rm orthog}$	$z_{\rm orthog}$	$x_{\rm orthorh}$	$z_{\rm orthorh}$
Y	0·25	0·286	0·112	0·251	0·056	0·250	0·055
Cl	0·75	0·234	0·427	0·100	0·2135	0·108	0·215
O_I	0·75	0·104	−0·090	0·132	−0·045	0·125	−0·050
O_{II}	0·75	0·550	0·162	0·499	0·081	0·508	0·083

them into itself. Thus the pair (L_{2n}; L_{2n+1}) is converted by these operations into the pair (L_{2n+2}; L_{2n+1}). In the orthorhombic form the layers L_{2n} and L_{2n+2} are connected by the *n*-glide plane and the screw axis parallel to **a**, which convert L_{2n+1} into itself. Thus the pair (L_{2n}; L_{2n+1}) is converted by these operations into the pair (L_{2n+2}; L_{2n+1}). Thus not only the layers but also the pairs of adjacent layers are the same in both cases; *i.e.* the structures have to be looked upon as belonging to one and the same family of OD-structures consisting of two kinds of layer (Dornberger-Schiff, 1964).

The relation between successive Cl layers L_{2n-1} and L_{2n+1} is the same in both cases: they are related by the symmetry centre and the screw axis parallel to **b** converting the yttrium layer L_{2n} into itself.

The total energy of interaction may be thought of as consisting of the following parts:

(1) Energy of interaction between atoms of layers L_{2n} and L_{2n}
(2) L_{2n+1} L_{2n+1}
(3) L_q L_{q+1}
(4) L_{2n-1} L_{2n+1}
(5) L_{2n} L_{2n+2}
(6) L_q L_{q+r} $r \geq 3$

From the above it follows that the energies of interaction in the monoclinic and orthorhombic form differ only in terms (5) and (6), whereas terms (1) to (4) are the same in both cases. As regards term (5) we shall expect its influence to be mainly indirect: the Cl atoms will be polarized by the Y atoms to which they are attached. In the orthorhombic form this polarization will not tend to change the difference in x coordinates of the two Cl atoms belonging to one particular layer, whereas in the monoclinic form the polarization of the Cl atoms would tend to decrease the distance between Cl atoms joined by a vector roughly perpendicular to the respective Cl–Y bonds.

The coordinates as found experimentally, referred to orthogonal axes, are given in Table 2. The differences in coordinates of the Y atoms and OH groups are probably within the limits of error. The difference in coordinates of the Cl atoms may conceivably be just outside these limits, as the R index calculated for the data of the orthorhombic form with the coordinates of the monoclinic form rises from 16·1 to 17·3, and for the monoclinic data with orthorhombic coordinates from 10·4 to 13·0. For mean values of the coordinates the R values rise to 16·3 and 11·9 respectively. As, however, data for the orthorhombic form were taken from a fairly large crystal and were not corrected for absorption, the significance of these differences cannot be taken for granted. The differences in coordinates of the Cl atoms agree as regards their signs with the effect of polarization to be expected.

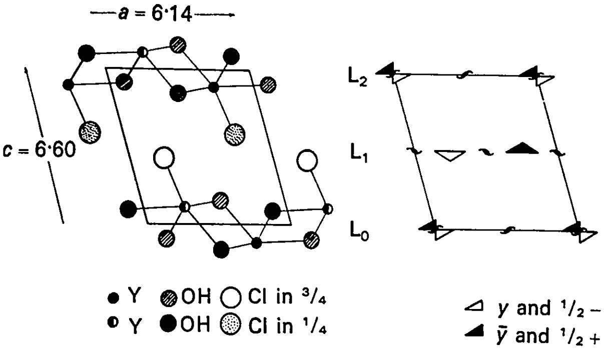

Fig. 1. Monoclinic form of yttrium hydroxide. Left: projection of structure. Right: schematic representation of the symmetry of the layers.

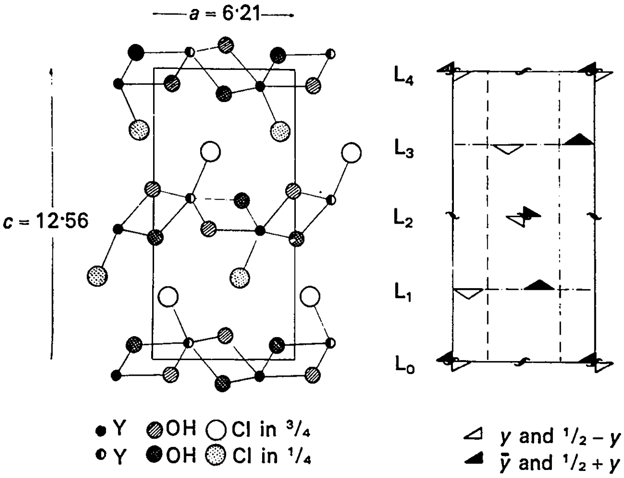

Fig. 2. Orthorhombic form of yttrium hydroxide. Left and right hand parts correspond to Fig. 1.

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