order of magnitude ought to be correct, however. The final R value obtained was 0·114. No attempt was made to refine anisotropic thermal parameters. A more detailed report also containing structure factors and powder data, will be given in *Acta Chem. Scand.*

The atomic positions in a c.c.p. layer and in an h.c.p. layer are represented in Fig. 1. Interatomic distances are summarized in Table 1. There are no Y–Y contacts in the structure.

Table 1. *Interatomic distances in* YAl₃

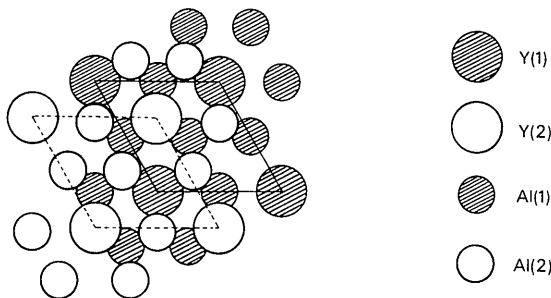| Atom	Neighbour	Number of neighbours	Distance
Y(1)	Al(1)	6	$3 \cdot 09_8$ Å
Y(1)	Al(2)	6	$3 \cdot 09_7$
Y(2)	Al(1)	3	$3 \cdot 02_3$
Y(2)	Al(2)	3	$3 \cdot 03_0$
Y(2)	Al(2)	6	$3 \cdot 10_7$
Al(1)	Al(1)	4	$3 \cdot 09_8$
Al(1)	Al(2)	4	$2 \cdot 88_9$
Al(1)	Y(1)	2	$3 \cdot 09_8$
Al(1)	Y(2)	2	$3 \cdot 02_3$
Al(2)	Al(1)	2	$2 \cdot 88_9$
Al(2)	Al(2)	2	$3 \cdot 49_8$
Al(2)	Al(2)	2	$2 \cdot 69_7$
Al(2)	Al(2)	2	$2 \cdot 81_8$
Al(2)	Y(1)	1	$3 \cdot 09_7$
Al(2)	Y(2)	1	$3 \cdot 03_0$
Al(2)	Y(2)	2	$3 \cdot 10_7$

Fig. 1. Two superposed YAl₃ layers.
Open circles: h.c.p. layer $z_{Al}=0 \cdot 111$ $z_Y=0 \cdot 115$.
Filled circles: c.c.p. layer $z_{Al}=z_Y=0$.
The Al(2) positions deviate from ideal h.c.p. positions which are at the centres of the broken lines.

The c.c.p. layers at $z=0$, $z=\frac{1}{3}$ and $z=\frac{2}{3}$ are exactly planar, subject to space group requirements. The arrangement of Al(1) around Y(1) in these layers is perfectly hexagonal, resulting in a rather long Al(1)–Al(1) distance, equal to the Y(1)–Al(1) distance.

The aluminum structure of the h.c.p. layers is planar. These layers occur at $z=\frac{1}{9}$, $z=\frac{2}{9}$, $z=\frac{4}{9}$ etc. within the accuracy of the refinement. An yttrium atom in such a layer is displaced toward the neighboring h.c.p. layer where the contacting aluminum triangle is expanded, the Al(2)–Al(2) distance being 3·50 Å. Remaining Al(2)–Al(2) distances within the h.c.p. layer are short, 2·70 Å, in comparison with the contact distance, 2·86 Å, in the pure element.

The coordination of Al around Y(1) is quite regular, all twelve Y–Al distances being equal to 3·10 Å.

Around Y(2) there are six long, 3·11 Å, Y(2)–Al(2) contacts within the h.c.p. layer. The remaining six Y(2)–Al distances, of which three are Y(2)–Al(1) and three Y(2)–Al(2) are short and approximately equal, ~3·03 Å. The mean Y(2)–Al distance is 3·07 Å.

A recent article, (Runnalls & Boucher, 1965) reports a partial refinement of the structure of PuAl₃, which is isostructural with YAl₃. In that work, $z_{Pu}=0 \cdot 2185$ is given, which indicates that the deviation from ideal close packing of equal spheres is of the same type in the two phases. In PuAl₃, however, the h.c.p. Al layers have been assumed to be displaced from the ideal z (1/9, 2/9 etc.) so as to produce equal distortions of the coordination around Pu(1) and Pu(2).

The same structure type has been observed (Giessen & Grant, 1965) for Ta(Pd₀·₈₈Ru₀·₁₂)₃ and Ta(Pd₀·₇₂Rh₀·₂₈)₃. No refinement of these structures has apparently been reported.

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Über trigonale Doppelselenate. Von W. FRANKE, *Freie Universität Berlin, Mineralogisches Institut, Berlin - Lichterfelde - West, Holbeinstrasse 45, Deutschland*

Die Anhydrate der Alaune kristallisieren meist trigonal, wahrscheinliche Raumgruppe $P321$ (D_3^2), Zahl der Formeleinheiten in der Elementarzelle = 1 (Vegard & Maurstad, 1928; Franke & Henning, 1965.) Entsprechende Doppelselenate wurden bisher noch nicht untersucht. Die allgemeine Formel lautet: $A^+B^{3+}(SeO_4)_2$ (mit A : Cs, Rb, Tl, NH₄, K und B: Al, Ga, Cr, Fe, In.)

Die den angegebenen Kationenkombinationen entsprechenden Verbindungen wurden durch thermischen Abbau der Alaune dargestellt. Wasserfreie Doppelselenate, deren zugehörige Alaune nicht existieren, wurden durch Eindunsten einer Lösung der jeweiligen Zusammensetzung bei 5°C und Tempern des Rückstandes bei 150°C gewonnen.

Alle Chromverbindungen waren röntgenamorph, bei Erhöhung der Abbautemperatur zersetzten sie sich.

Die Pulverdiagramme (Zählrohrdiffraktometer, Cu $K\alpha$-, bzw. Fe $K\alpha$-Strahlung) der in Tabelle 1 aufgeführten Substanzen liessen sich einwandfrei trigonal indizieren. Ein Vergleich der Intensitätsverhältnisse und Gitterdaten zeigt, dass Doppelsulfate und Doppelselenate isotyp sind.

Tabelle 1. *Gitterkonstanten und Achsenverhältnisse*

Formel	a_0	c_0	c/a
$CsFe(SeO_4)_2$	5.04_3 Å	9.02_8 Å	1.79_0
$RbFe(SeO_4)_2$	4.99_7	8.53_1	1.70_7
$TlFe(SeO_4)_2$	5.01_2	8.48_6	1.69_3
$NH_4Fe(SeO_4)_2$	5.00_4	8.46_5	1.69_1
$RbGa(SeO_4)_2$	4.90_7	8.59_2	1.75_0
$TlGa(SeO_4)_2$	4.93_1	8.55_2	1.73_4
$NH_4Ga(SeO_4)_2$	4.91_9	8.51_8	1.73_1
$RbAl(SeO_4)_2$	4.89_7	8.54_9	1.74_6
$TlAl(SeO_4)_2$	4.88_4	8.49_5	1.73_9
$NH_4Al(SeO_4)_2$	4.89_2	8.47_0	1.73_1

Die *d*-Werte werden im *X-Ray Powder Data File* veröffentlicht.
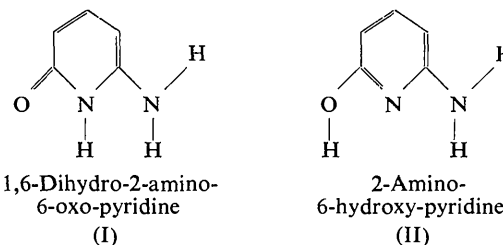
Die Volumeninkremente sind von gleicher Grössenordnung wie bei den Doppelsulfaten und lassen sich analog erklären. Die Inkremente für den Übergang SeO_4–SO_4 schwanken geringfügig um den Werte $15,4 . 10^{-24}$ cm³ pro Formeleinheit; den gleichen Wert fand auch Haussühl (1961) für die Alaune.

Der Deutschen Forschungsgemeinschaft danke ich für ihre finanzielle Unterstützung.

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Crystal data for 2-amino-6-hydroxypyridine.

By BRAHAMA D. SHARMA, *Department of Chemistry, Oregon State University, Corvallis, Oregon* 97331, *U.S.A.*

As a part of our interest in bases closely related to those found in nucleic acids we have examined crystals of 2-amino-6-hydroxypyridine, $C_5H_6N_2O$, by the methods of X-ray diffraction. Acicular crystals, elongated along **a**, were obtained by recrystallization from ethanol. Crystal data, as determined from the analysis of rotation and Weissenberg (zero and upper level) photographs about *a* and *b* axes, are:

Triclinic

$a = 4.85 \pm 2$ Å $\alpha = 98°$
$b = 9.30 \pm 3$ $\beta = 91$
$c = 13.57 \pm 5$ $\gamma = 92$

The density measured in methylchloroform and benzene mixture by the flotation method is 1.298 g.cm⁻³. Calculated density for four ($C_5H_6N_2O . \frac{1}{2}H_2O$) formula units per unit cell is 1.306 g.cm⁻³. Presence of water of crystallization was also confirmed by elementary analyses (Found: C, 51.23; H, 6.22; N, 22.71%. Required: C, 50.42; H, 5.88; N, 23.53%), and drying of the recrystallized material.

Heavily exposed (72 hours, unfiltered radiation) Weissenberg photographs show a marked fall-off of intensity beyond a *d* value of 1 Å. No further crystallographic work on this compound, which is likely to have either of the tautomeric structures (I) and (II), is contemplated.

| 1,6-Dihydro-2-amino-6-oxo-pyridine (I) | 2-Amino-6-hydroxy-pyridine (II) |

Note on reliability indices*.

By GEORGE M. BROWN, *Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee, U.S.A.*

Continued use by crystallographers of the discrepancy indices (or residuals) R_k given by the equation

$$R_k \equiv \frac{\Sigma ||F|_o^k - |F|_c^k|}{\Sigma |F|_o^k} \quad (k = 1 \text{ or } 2) \quad (1)$$

justifies some remarks on R_k values from experience in this laboratory in neutron-diffraction analysis. We have found that for a set of $|F|_o^2$ and $|F|_c^2$ values at convergence

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in least-squares refinement the index R_1 may be as large as R_2, or even somewhat larger (Table 1). This finding has caused reactions among various crystallographic colleagues varying from mild surprise to incredulity, apparently because the usual result in X-ray analyses based on data recorded photographically is that R_1 is about one-half of R_2.

It is helpful in considering the relation between R_1 and R_2 to define the fractional discrepancy f_k of an individual observation by the equation