Tabelle 1. *Gitterkonstanten und Achsenverhältnisse*

Formel	a_0	c_0	c/a
$CsFe(SeO_4)_2$	$5{\cdot}04_3$ Å	$9{\cdot}02_8$ Å	$1{\cdot}79_0$
$RbFe(SeO_4)_2$	$4{\cdot}99_7$	$8{\cdot}53_1$	$1{\cdot}70_7$
$TlFe(SeO_4)_2$	$5{\cdot}01_2$	$8{\cdot}48_6$	$1{\cdot}69_3$
$NH_4Fe(SeO_4)_2$	$5{\cdot}00_4$	$8{\cdot}46_5$	$1{\cdot}69_1$
$RbGa(SeO_4)_2$	$4{\cdot}90_7$	$8{\cdot}59_2$	$1{\cdot}75_0$
$TlGa(SeO_4)_2$	$4{\cdot}93_1$	$8{\cdot}55_2$	$1{\cdot}73_4$
$NH_4Ga(SeO_4)_2$	$4{\cdot}91_9$	$8{\cdot}51_8$	$1{\cdot}73_1$
$RbAl(SeO_4)_2$	$4{\cdot}89_7$	$8{\cdot}54_9$	$1{\cdot}74_6$
$TlAl(SeO_4)_2$	$4{\cdot}88_4$	$8{\cdot}49_5$	$1{\cdot}73_9$
$NH_4Al(SeO_4)_2$	$4{\cdot}89_2$	$8{\cdot}47_0$	$1{\cdot}73_1$

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} cm^3 pro Formeleinheit; den gleichen Wert fand auch Haussühl (1961) für die Alaune.

Der Deutschen Forschungsgemeinschaft danke ich für ihre finanzielle Unterstützung.

Literatur

FRANKE, W. & HENNING, G. (1965). *Acta Cryst.* **19**, 870.
HAUSSÜHL, (1961). *Z. Kristallogr.* **116**, 371.
VEGARD, L. & MAURSTAD, A. (1928). *Z. Kristallogr.* **69**, 519.

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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.*

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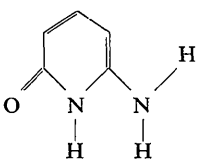
As a part of our interest in bases closely related to those found in nucleic acids we have examined crystals of 2-amino-6-hydroxypyridine, $C_5H_6N_2O$, by the methods of X-ray diffraction. Acicular crystals, elongated along **a**, were obtained by recrystallization from ethanol. Crystal data, as determined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

Triclinic

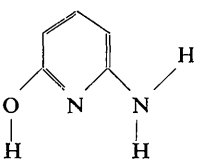
$a=4{\cdot}85\pm2$ Å	$\alpha=98°$
$b=9{\cdot}30\pm3$	$\beta=91$
$c=13{\cdot}57\pm5$	$\gamma=92$

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)

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Note on reliability indices*.

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

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

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

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 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

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