$$\begin{split} \sigma^2 & (\tan \alpha) = \left(\frac{1}{F_A}\right)^2 \sigma^2(F_B) + \left(\frac{F_B}{F_A^2}\right)^2 \sigma^2(F_A) \\ &= \left\{\frac{1}{F_A^2} \frac{1}{8(\Delta B)^2} + \frac{F_B^2}{F_A^4} \left[\frac{1}{2} + \frac{(I_1 - I_2)^2}{32(\Delta B)^4}\right] \frac{1}{4F_A^2}\right\} \sigma^2(I) \\ \text{or} \\ \sigma & (\tan \alpha) = \frac{1}{2\pi} \int \frac{1}{F_B^2} \left[\frac{1}{4} + \frac{F_B^2}{F_B^2}\right]^{\frac{1}{2}} \sigma(I) \end{split}$$

$$\sigma (\tan \alpha) = \frac{1}{F \cos \alpha} \left\{ \frac{1}{8(\Delta B)^2} + \frac{F_B^2}{4F_A^4} \left[\frac{1}{2} + \frac{F_B^2}{2(\Delta B)^2} \right] \right\}^{\frac{1}{2}} \sigma(I)$$

$$= \frac{1}{F \cos \alpha} \left\{ \frac{1}{8(\Delta B)^2} + \frac{\tan^2 \alpha}{8F^2 \cos^2 \alpha} + \frac{\tan^4 \alpha}{8(\Delta B)^2} \right\}^{\frac{1}{2}} \sigma(I).$$

Now

$$\begin{split} &\sigma(\alpha) = \frac{1}{\sec^2 \alpha} \, \sigma \, (\tan \, \alpha) \\ &\sigma(\alpha) = \frac{\cos \alpha}{F} \left\{ \frac{1}{8(\Delta B)^2} + \frac{\tan^2 \alpha}{8F^2 \cos \alpha} + \frac{\tan^4 \alpha}{8(\Delta B)^2} \right\}^{\frac{1}{2}} \! \sigma(I) \; . \end{split}$$

If $\varepsilon = \sigma(F)/F$ is the fractional error in F then

$$\sigma(\alpha) = \cos \alpha \left\{ \left(\frac{F}{\Delta B} \right)^2 (1 + \tan^4 \alpha) + \frac{\tan^2 \alpha}{\cos^2 \alpha} \right\}^{\frac{1}{2}} \varepsilon.$$

The variation of $\sigma(\alpha)$ with α is shown in Fig. 1; the error in α is reasonably constant up to a phase angle of about 55°, but increases rapidly as α approaches 90°. The value of $\sigma(\alpha)$ for the 'constant' portion will depend on ε and the ratio $F/\Delta B$; Table 2 shows the value of $\sigma(\alpha)$ for this portion for values of ε and the ratio $F/\Delta B$.

Table 2. $\sigma(\alpha)$ for values of ε and $F/\Delta B$

$F/\Delta B$	ε				
	0.01	0.02	0.03	0.04	0.05
2	1.1°	2·3°	3·4°	4.6°	5·7°
5	2.9	5.7	8.6	11.5	14.3
10	5.7	11.5	17.2	$22 \cdot 9$	27.6
20	11.5	$22 \cdot 9$	$34 \cdot 4$	45.8	$57 \cdot 3$

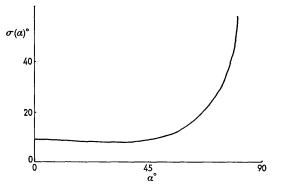


Fig. 1. A graph of $\sigma(\alpha)$ against α for $F/\Delta B = 5$ and $\varepsilon = 0.03$.

Reference

RAMACHANDRAN, G. N. & RAMAN, S. (1956). Curr. Sci. 25, 348.

Acta Cryst. (1963). 16, 852

Unit cell and space group of 4-aminopyridine.* By George M. Brown† and Harold J. Zabsky,‡
Department of Chemistry, University of Maryland, College Park, Maryland, U.S.A.

(Received 11 February 1963)

A sample of 4-aminopyridine was kindly furnished by Dr K. G. Stone of Michigan State University. The melting point was 159–161 °C; the melting point reported by Heilbron (1953) is 158 °C. Small irregular crystals of 4-aminopyridine were grown by evaporation of an aqueous solution at room temperature.

Weissenberg and precession photographs (Cu $K\alpha$ radiation) were taken of a single crystal mounted along the c axis of the orthorhombic system found to describe the crystal. Since the only systematic absences noted were the h00 reflections for odd h, the 0k0 reflections for odd k,

and the 00l reflections for odd l, the space group appears uniquely determined as $P2_12_12_1$.

The cell dimensions derived from measurements of the film are: $a=5\cdot57$, $b=7\cdot32$, $c=12\cdot1$ Å, all $\pm1\%$. The density calculated for Z=4 is $1\cdot27$ g.cm⁻³; the density observed, by the flotation method, is $1\cdot25$ g.cm⁻³.

No crystal specimens were obtained which yielded films suitable for intensity estimation. Diffraction spots were characteristically elongated and drawn out into streaks, evidencing some disorder in growth of the crystals. The structure analysis originally planned was not undertaken.

Reference

HEILBRON, I. & BUNBURY, H. M. (1953). Dictionary of Organic Compounds. Vol. I, p. 133. New York: Oxford University Press.

^{*} This research was supported by the U.S. National Science Foundation.

[†] Present address: Chemistry Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee.

[†] Present address: Chemistry Division, St. Louis University, S. Louis, Missouri.