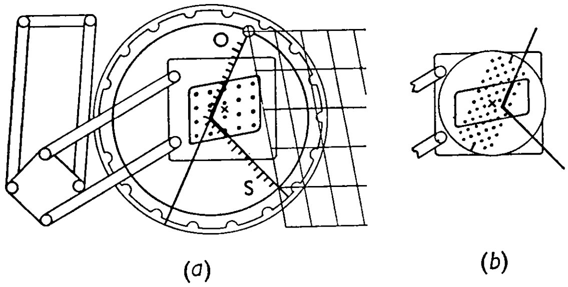
reasonably large scale (say, $1/\lambda = 5$ in.). This chart is also used for determining counter and crystal settings in a manner similar to that of Evans (1953). Two Bernal circles (Fig. 1(*a*)) have been cut from perspex. The bottom one rotates about the origin, O, of the reciprocal lattice and its diameter defines the direction of the incident beam. The top circle carries a scribed radius to define the direction of the reflected beam and rotates about a pin through the centre of the lower Bernal circle. To define the directions of the incident and reflected rays, both circles are rotated as a whole about the origin of the reciprocal lattice until the particular lattice point S lies on the Bernal circle. The upper circle is then rotated until the scribed radius also meets the lattice point S.



(*a*) (*b*)

Fig. 1. (*a*) The heavy lines indicate the distances l_1 and l_2 which give μx. The medium lines show the outline of the crystal model, and the incident and reflected directions and the Bernal circle. The pantograph device is not drawn to scale. (*b*) For cases (3) and (4) the distribution of scattering elements is determined by the direction of the incident beam and is displayed by another chart which rotates about the rotation centre of the crystal.

Along each of the direction-defining radii is pasted a replaceable strip of paper carrying a scale calibrated in terms of μx, where μ is the linear absorption coefficient of the crystal and x is proportional to length (the proportionality is determined by the magnification of the crystal model, see below).

A scale model of the crystal is drawn on another sheet of perspex and a suitable number (N) of points representing equal volume elements are marked in. This model is then attached to a pantograph device so that it can be moved to any required position over the Bernal circles whilst maintaining its correct angular orientation with respect to the reciprocal lattice net. (A T-square may be used in lieu of the pantograph but it would normally require both hands for operation, whereas the pantograph leaves one hand free for recording results.) For the nth volume element, $\mu x = l_1+l_2$. l_1 and l_2 are read from the scales, summed, and recorded. Then the absorption factor (A) is given by

$$A = N^{-1}\sum^{N}\exp\{-(l_1+l_2)\}\,,$$

where N remains constant (in contrast to previous methods). Should it be desired to measure the exponentials directly, then the use of a scale and dividers, as outlined by Rogers & Moffett (1956), is perfectly feasible.

The method as outlined here is applicable to prismatic crystals of constant cross-section (i) bathed completely in a uniform incident beam, and (ii) of length in the direction of the rotation axis extending beyond the incident beam. The method could be extended in the following ways:

(1) For crystals whose cross-sections vary in the direction of the rotation axis, a suitable number of different cross-sections can be drawn on the crystal model.

(2) For crystals falling in category (ii) above, it is possible to use this graphical aid for the computation of absorption factors in cases where either or both the incident and reflected beams are not normal to the rotation axis by modifying the μx scales by the relevant cosine factors.

(3) For crystals whose cross sections extend beyond the incident beam (Fig. 1(*b*)), the centres of equal volume elements may be represented on a fourth perspex sheet, which is attached to and rotated about the rotation centre of the crystal model. For each reflexion, the orientation of this sheet is defined by the direction of the incident beam. The number, N, which will now normally be variable, will also give an indication of the effective reflecting volume of the crystal.

(4) Where the incident-beam cross-section is not uniform, and is known, the distribution of reflecting points on the fourth perspex sheet of (3) may be approximately arranged to represent the intensity distribution of the incident beam, and once again N will give an indication of the effective reflecting volume of the crystal.

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Evans, H. T. (1953). *Rev. Sci. Instrum.* **24**, 156.
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A preliminary investigation of some heterocyclic compounds.

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A preliminary survey has been made of the crystallographic data for the compounds listed below. The unit-cell and space-group data (Table 1) were obtained from oscillation and Weissenberg photographs; the crystal densities were determined by flotation.

2-Hydroxypyrimidine

$\overline{\mathrm{N.C(OH).N.CH.CH.CH}}$

Source: Dr D. J. Brown, Australian National University.

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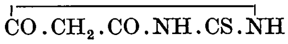
Table 1. *Unit-cell and space-group data*

Compound	System	*a* (Å)	*b* (Å)	*c* (Å)	β (°)	Space group	Mols. in cel
2-Hydroxypyrimidine	Tetragonal	8·54	—	12·35	90·0	$P4_12_1$	8
Thiobarbituric acid	Monoclinic	8·44	13·14	10·42	92·7	$P2_1/n$	8
Pseudothiohydantoin	Monoclinic	13·79	9·00	4·04	110·0	$P2_1/a$	4
6-Methyl 2-thiouracil	Monoclinic	13·05	14·49	4·44	132·5	$P2_1/a$	4

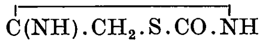
Crystallization: Slow cooling of a saturated solution in absolute alcohol.
Habit: Thin needles, extended along [001]; bounded by {110}.
Cleavage: (110).
Optical data: Small negative birefringence. $1{\cdot}60 < \varepsilon < 1{\cdot}62$, $1{\cdot}62 < \omega < 1{\cdot}64$.
Density: Observed 1·40 g.cm.$^{-3}$, calculated 1·412 g.cm.$^{-3}$.

Thiobarbituric acid


$CO.CH_2.CO.NH.CS.NH$

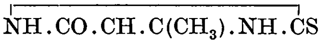
Source: Messrs Genatosan, Limited.
Crystallization: Sublimation at 182° C. Recrystallization from organic solvents yielded feathery clusters of very small crystals.
Habit: Small prisms, (010) well developed.
Cleavage: None.
Optical data: Negative birefringence. $\alpha = 1{\cdot}55$, $\beta = 1{\cdot}67$, $\gamma = 1{\cdot}75$. α is parallel to *b*, β lies at 40° to *c* in the obtuse angle of the cell.
Density: Observed 1·661 g.cm.$^{-3}$, calculated 1·666 g.cm.$^{-3}$.

Pseudothiohydantoin (2-imino 4-thiazolidine)†


$C(NH).CH_2.S.CO.NH$

Source: Messrs Genatosan, Limited.
Crystallization: Slow cooling of a saturated aqueous solution.
Habit: Pale yellow needles extended along [001]; bounded by {110} and {001}.
Cleavage: (001).
Optical data: Negative birefringence. $\alpha = 1{\cdot}54$, $\beta = 1{\cdot}74$, $2V = 70°$, $\gamma = 1{\cdot}91$ (extrapolated value). β is parallel to *b*, γ approximately parallel to *a*.
Density: Observed 1·637 g.cm.$^{-3}$, calculated 1·635 g.cm.$^{-3}$.

6-methyl 2-thiouracil†


$NH.CO.CH.C(CH_3).NH.CS$

Source: Messrs Genatosan, Limited.
Crystallization: Slow cooling of a saturated solution in 1:1 glacial acetic acid: water.
Habit: Pale yellow needles, extended along [001]; bounded by {110} and to a lesser extent {010}. Crystals twin frequently on (100).
Optical data: Strong negative birefringence. $\alpha = 1{\cdot}613$, $\beta, \gamma > 1{\cdot}86$. β is parallel to *b*, γ approximately parallel to *a*.
Cleavage: (001).
Density: Observed 1·519 g.cm.$^{-3}$, calculated 1·498 g.cm.$^{-3}$.

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† The crystal structure of these compounds has been obtained and will be reported in subsequent papers.

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Die K_2NiF_4-Struktur beim La_2NiO_4.

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(*Eingegangen am* 4. *Dezember* 1957)

Einleitung

Balz & Plieth (1955) haben in ihrer Arbeit über die K_2NiF_4-Struktur bereits auf den Zusammenhang mit dem Perowskittyp hingewiesen. So ist der von Goldschmidt für den Perowskittyp ABO_3 abgeleitete Toleranzfaktor

$$t = (r_A+r_O)/(r_B+r_O)\sqrt{2}$$

auch ein Mass für die Bildung der K_2NiF_4-Struktur. Weitere Untersuchungen (Randall, Katz & Ward, 1957; Ruddlesden & Popper, 1957) schienen zu zeigen, dass der Toleranzfaktor im Falle der A_2BO_4-Verbindungen in den engen Grenzen von $0{,}90 < t < 1{,}00$* liegt.

Demgegenüber konnten wir feststellen, dass diese Struktur auch beim La_2NiO_4 ($t = 0{,}855$) auftritt. Die Verbindung bildet sich leicht beim Tempern von Lanthanoxyd mit der entsprechenden Menge Nickelkarbonat bei 1200°–1400° C. an der Luft.† Die Ursache für dieses Verhalten ist darin zu suchen, dass — wie Bestimmungen des Oxydationswertes zeigen — ein kleiner Teil des Nickels in höherwertigem Zustand vorliegt. Ersetzt man das Nickel durch das etwa gleichgrosse Magnesium, das nicht zu einem Wertigkeitswechsel fähig ist, wird die Verbindung nicht gebildet (Rabenau, 1956). Dagegen kann auch La_2CoO_4 ($t = 0{,}84$) erhalten werden, wenn die Bildung des Perowskits $LaCoO_3$ durch Arbeiten in geeigneter CO_2/H_2-Atmosphäre unterdrückt wird.

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* Goldschmidtradien, 6er Koordination.

† Die Struktur wird auch noch bei Nd_2NiO_4 gebildet ($t = 0{,}83_2$; orthorhombisch deformiert) nicht mehr bei Sm_2NiO_4 ($t = 0{,}82_5$). Dagegen existiert $LaSmNiO_4$ ($t = 0{,}84$). Die von Wold, Post & Banks (1957) angegebenen *d*-Werte für die aus La_2O_3, Sm_2O_3 und NiO gebildete Phase lässt sich vollständig, die aus Nd_2O_3 und NiO mit einer Ausnahme entsprechend der K_2NiF_4-Struktur indizieren.