five-membered rings indicate a rotation of only a few degrees (which is however apparent on the *a*-axis electron-density projection) from the *cis* configuration.

Accurate molecular dimensions are not available from this two-dimensional study, and since the object was the determination of the molecular configuration, no three-dimensional analysis was carried out. The acetocyclopentadienyl residues are approximately planar and parallel, and the mean molecular dimensions are Ru–C = 2·18 Å (omitting one very short distance from the averaging), $C_{ar}-C_{ar}$ = 1·41 Å, other C–C = 1·48 Å, C=O = 1·23 Å, ∠ C–C–C (in five membered rings) = 108°.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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On the most probable differences occurring in the Lipson-Hesse difference method for indexing powder photographs.

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During our work we have found that the method described by Hesse (1948) and Lipson (1949) is one of the most powerful for indexing powder photographs with orthorhombic, hexagonal or tetragonal unit cells. But we have learned also that it is very important to know exactly what kind of differences may occur at all.

If we form the differences of the values

$$Q_{hkl} = 4\sin^2\theta_{hkl} = h^2a^{*2} + k^2b^{*2} + l^2c^{*2} + 2hka^*b^*\cos\gamma^* + 2klb^*c^*\cos\alpha^* + 2hla^*c^*\cos\beta^*,$$

we get in the monoclinic system (1st setting)

$$Q_{hkl} - Q_{hkl'} = N_3c^{*2}, \qquad \text{(I)}$$

in the orthorhombic system

$$Q_{hkl} - Q_{h'kl} = N_1a^{*2}, \text{ etc.} \qquad \text{(II)}$$

in the hexagonal system

$$Q_{hkl} - Q_{h'k'l} = Na^{*2}, \qquad \text{(III}a\text{)}$$

$$Q_{hkl} - Q_{hkl'} = N_3c^{*2}, \qquad \text{(III}b\text{)}$$

in the tetragonal system

$$Q_{hkl} - Q_{h'k'l} = Na^{*2}, \qquad \text{(IV}a\text{)}$$

$$Q_{hkl} - Q_{hkl'} = N_3c^{*2}, \qquad \text{(IV}b\text{)}$$

in the cubic system

$$Q_{hkl} - Q_{h'k'l'} = Na^{*2}, \qquad \text{(V)}$$

where N, N_1, N_2, N_3 are integers, the possible values of which (see Table 1) are determined by the Bravais lattice properties. (From these numbers all those which, in the form N_1a^{*2}, can also represent possible values of Q_{hkl} are printed in italics.) It is obvious that there are some forbidden values even for primitive unit cells; $N_3 = l^2 - l'^2$ cannot be equal to 2, 6, 10, 14, ... For

Table 1. *Possible values of* N, N_1, N_2, N_3

		Monoclinic
P		N_3 = *1*, –, 3, *4*, 5, –, 7, 8, *9*, –, 11, 12, 13, –, ...
B		N_3 = *4*, 8, 12, *16*, 20, 24, ...
		Orthorhombic
P	N_1, N_2, N_3	= *1*, –, 3, *4*, 5, –, 7, 8, *9*, –, 11, 12, 13, –, ...
C	N_1, N_2	= *4*, 8, 12, *16*, 20, 24, ...
	N_3	= *1*, –, 3, *4*, 5, –, 7, 8, *9*, –, 11, 12, 13, –, ...
F, *I*	N_1, N_2, N_3	= *4*, 8, 12, *16*, 20, 24, ...
		Hexagonal
H	N	= *1*, 2, *3*, *4*, 5, 6, *7*, 8, *9*, 10, ...
	N_3	= *1*, –, 3, *4*, 5, –, 7, 8, *9*, –, 11, 12, 13, –, ...
R	$\frac{1}{3}$N	= *1*, 2, *3*, *4*, 5, 6, *7*, 8, *9*, 10, ...
	$\frac{1}{3}N_3$	= 1, –, *3*, 4, 5, –, 7, 8, 9, –, 11, *12*, 13, –, ...
		Tetragonal
P	N	= *1*, *2*, 3, *4*, *5*, 6, 7, *8*, *9*, *10*, ...
	N_3	= *1*, –, 3, *4*, 5, –, 7, 8, *9*, –, 11, 12, 13, –, ...
I	N	= *2*, *4*, 6, *8*, *10*, 12, 14, *16*, *18*, ...
	N_3	= *4*, 8, 12, *16*, 20, 24, 28, 32, ...
		Cubic
P	N	= *1*, *2*, *3*, *4*, *5*, *6*, 7, *8*, *9*, *10*, ...
I	N	= *2*, *4*, *6*, *8*, *10*, *12*, *14*, *16*, ...
F	N	= *1*, –, *3*, *4*, *5*, –, 7, *8*, 9, –, *11*, ...

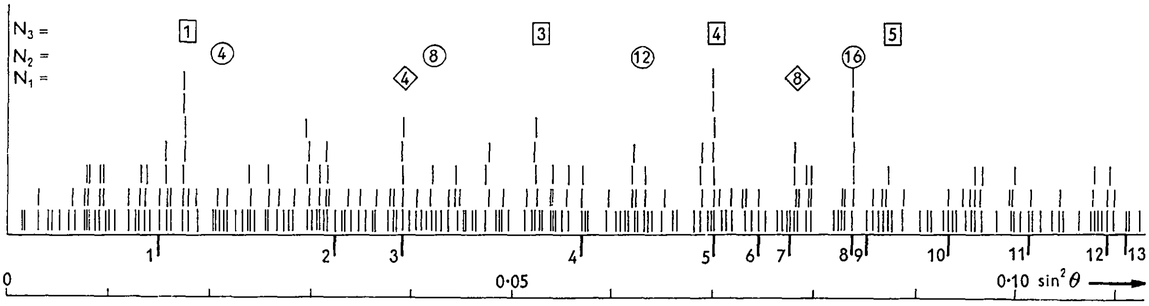

Fig. 1. The first part of the difference diagram of the powder photograph of α-$Cu(NH_3)_2Cl_2$. The unit cell is orthorhombic C centered with $a = 7{\cdot}78$, $b = 10{\cdot}65$, $c = 5{\cdot}82$ Å. Instead of Q we have used directly $\sin^2\theta$. The thick numbered lines below the horizontal axis mark the first $\sin^2\theta$ values measured, and each line above the axis represents a difference between a pair of measured $\sin^2\theta$. The whole number of the measured lines was 34.

centered cells, further values become forbidden. For example with a B centered monoclinic cell, for a given hk, l is either always even or odd. Therefore the difference of the squares is divisible by four.

For a trigonal unit cell (with hexagonal indices), the situation is more complicated. Here for a given h, k

$$l = l_0 + 3n, \quad (n = 0, \pm 1, \pm 2, \ldots) \tag{1}$$

where $l_0 = -1, 0, +1$, depending on h and k. So for example

$$\tfrac{1}{3}N_3 = \tfrac{1}{3}(l^2 - l'^2) = (n - n')\,[3(n + n') + 2l_0]\,. \tag{2}$$

Both factors on the right-hand side have the same parity (and are odd only when n is even and n' is odd or conversely). Using the abbreviations

$$A = n - n'; \quad B = 3(n + n') + 2l_0\,, \tag{3}$$

$$\begin{aligned}\tfrac{1}{3}N_3 &= A\,.\,B \\ &= [(A+B)/2 + (A-B)/2]\,.\,[(A+B)/2 - (A-B)/2]\,. \end{aligned} \tag{4}$$

But $A + B$ is always even, therefore $\tfrac{1}{2}(A \pm B)$ is integral; that is

$$\tfrac{1}{3}N_3 = (m + m')\,.\,(m - m') = m^2 - m'^2, \tag{5}$$

where m and m' are integers. It can be shown in a similar way that we can find an appropriate n and n' to each m and m'.

Now if we prepare in the usual way (see Fig. 1), the difference diagram from the data measured, we find quite a few maxima. We have to group these into two sets (tetragonal and hexagonal system) or three sets (orthorhombic system). Knowing the forbidden values mentioned above, this process is considerably facilitated. Of course there are always some accidentally appearing fortuitous maxima, and on the other hand, it can happen that no maxima belong to some permissible value.

Our experience shows, that—at least in the orthorhombic and tetragonal systems—the highest maxima belong usually to N (or N_1, N_2, N_3) = 4, 8, 16, ... and here are to be found most of the differences for the strongest lines.

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The crystallography of the hydrates of sodium carbonate and of sodium sulphite.

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Though the goniometric data are recorded by Groth (Vol. II, 1908), the unit-cell dimensions of common 'washing soda', $Na_2CO_3.10H_2O$, are not given in any of the standard compilations and appear not to have been measured. Whilst remedying this omission, we were led to a study of the heptahydrate, $Na_2CO_3.7H_2O$, and of the similarly hydrated sulphite, $Na_2SO_3.7H_2O$.

Crystals of all three hydrates can be grown from aqueous solution. $Na_2CO_3.7H_2O$, in contact with aqueous solution, is thermodynamically stable only between 35 and 32 °C; but it was sometimes obtained at lower temperatures—presumably an example of the operation of Ostwald's law of successive reactions. Suitable fragments of $Na_2SO_3.7H_2O$ could alternatively be cut from the interior of the large crystals commercially available. All three substances effloresce rapidly when exposed to normal atmospheric conditions, and the small crystals suitable for X-ray study had immediately to be sealed into thin-walled glass tubes. Copper $K\alpha$-radiation was used. Internal calibration was procured by superposing on the same Weissenberg diagram the powder lines from a fine copper or aluminium wire, for which a at 20° was taken as 3·6149 and 4·04907 Å respectively. The new crystal data are collected in Table 1. The standard deviations shown are based, in each case, on a least-squares treatment of about 20 high-order reflexions