

symptoms of distress (respiration 95 per min., pulse 120 per min.) and was slightly blown; the heifers, although full in the flank, were neither blown nor showing signs of discomfort. Blood samples taken at this stage were analysed for hydrocyanic acid content; the bullock's blood contained 0.1 mgm. hydrocyanic acid per 100 ml. blood, while the heifers' had 0.04 mgm. per 100 ml. blood.

The possible role of hydrocyanic acid in the etiology of acute bloat in sheep has been considered before by Clark and Quin⁷, but they prefer the 'saponin foam theory' of its pathogenesis (see also Clark⁸).

It seems probable to us that in a complex syndrome like bloat several factors may operate; a satisfactory theory of the cause must not only account for the sequence of symptoms in the animal, but must also explain observations of agriculturists on predisposing environmental conditions. We believe that our findings are significant in this connexion.

We wish to acknowledge our grateful thanks to the Welsh Plant Breeding Station for providing facilities in the field.

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DETERMINATION OF ABSOLUTE INTENSITIES OF X-RAY REFLEXIONS FROM RELATIVE INTENSITY DATA

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RECENTLY, owing to the advent of various methods¹ of direct determination of phase angles of Bragg reflexions from a crystal, a convenient method of determination of absolute intensities of Bragg reflexions seems urgently needed². In 1942 I proposed a simple method of determination of absolute from relative intensities³, which has since been made rigorous and so should be reliable in general cases if used properly. Accordingly, I present here the final result of the method, which is applicable to practical cases immediately.

Suppose we have a crystal containing t atoms in the unit cell, the number of shell electrons of the i th atom being Z_i . Let the relative intensities of reflexions for the crystal at room temperature be denoted by $I'(hkl)$ for hkl and $I'(000)$ for 000. We have

$$|F(hkl)|^2 = \frac{F^2(000)}{I'(000)} I'(hkl). \quad (1)$$

We see that if we can determine $I'(000)$ we can deduce $|F(hkl)|^2$ from $I'(hkl)$, for we have the known $F(000) = \sum_{i=1}^t Z_i$. Let us introduce

$$\bar{f}(hkl) = \frac{\sum_{i=1}^t f_i(hkl)}{\sum_{i=1}^t Z_i}, \quad (2)$$

where $f_i(hkl)$ is the atomic structure factor at room temperature of the i th atom in the cell. If only $f_i(hkl)$ for atoms at rest are available, such as those obtained from James and Brindley's table, suitable temperature correction must be made in order to obtain the room temperature value of $f_i(hkl)$. We further form the sum $\sum_{i=1}^t Z_i^2$. Then from the theory of a new X-ray synthesis developed by me, it can be shown that:

$$I'(000) = F^2(000) \frac{\sum' U_{n,h} U_{n,k} U_{n,l} I'(hkl) / \bar{f}^2(hkl)}{\sum_{i=1}^t Z_i^2 - U_{n,0} U_{n,0} U_{n,0} \cdot F^2(000)} \quad (3)$$

where Σ' denotes the sum $\sum_{h=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} \sum_{l=-\infty}^{\infty}$, excluding the term of $h = k = l = 0$. U_{nh} are known functions of n and h , the numerical values of which are negligibly small for $h > n/2$; $U_{nh} = U_{n\bar{h}}$ when $\bar{h} = -h$. Thus, if the maximum h, k, l of our available set of $I'(hkl)$ are h_M, k_M, l_M , we may choose $n_1 \doteq 2h_M, n_2 \doteq 2k_M, n_3 \doteq 2l_M$. The values of U_{nh} for some values of n and h are given below:

n	$U_{nh} \times 10^4$									
	48	44	40	36	32	28	24	20	16	12
0	334	364	400	443	498	568	660	790	981	1297
1	325	354	388	430	481	547	633	751	920	1187
2	315	341	371	409	455	511	584	679	809	989
3	303	328	357	391	433	484	547	626	729	848
4	294	316	342	372	407	449	499	557	617	646
5	282	303	327	354	386	421	462	505	540	528
6	272	291	311	334	360	387	414	433	422	176
7	256	278	296	316	338	359	377	385	360	
8	251	265	280	296	312	324	328	308	131	
9	239	253	266	278	290	297	294	272		
10	230	240	250	258	263	261	240	104		
11	218	227	235	240	242	235	216			
12	209	215	219	220	215	196	87			
13	198	202	204	203	196	181				
14	187	189	189	181	164	73				
15	177	177	174	167	155					
16	166	164	157	142	64					
17	156	152	145	135						
18	144	138	124	57						
19	135	128	120							
20	122	110	51							
21	115	108								
22	99	46								
23	98									
24	42									
ΣU_{nh}	0.9998	1.0010	1.0016	1.0022	1.0037					

The last row gives the sum $\sum_{-h_M/2}^{h_M/2} U_{nh}$ for $n = 48, 40, 32, 24, 16$. Apparently all the sums differ from the theoretical limit $\sum_{h=-\infty}^{\infty} U_{nh} = 1$ only by fractions of 1 per cent, indicating the rapidity of convergence of the infinite series.

The accuracy of $I'(000)$ deduced from (3) depends essentially upon the following four factors:

- (1) The accuracy of the observed $I'(hkl)$.
- (2) The order of approximation of the equation

$$f_i(hkl) = Z_i \cdot \bar{f}(hkl), \quad (4)$$

which forms the basis of equation (2). The error introduced by the failure of equation (4) is usually not very serious.

(3) The proper correction of the temperature effect in $f_i(hkl)$. If we actually do a suitable experiment to correct this effect, the error introduced is, of course, limited. Otherwise we have to correct the effect with reference to similar crystals of known structures, and

the error resulting in $I'(000)$ may be very large. This uncertain correction of the temperature effect constitutes the chief source of errors in the value deduced for $I'(000)$.

(4) The correct choice of n_1, n_2, n_3 . The strict condition is

$$d_m \geq \frac{1.2a}{n_1}, \frac{1.2b}{n_2}, \frac{1.2c}{n_3},$$

where d_m denotes the shortest interatomic distance between any two atoms in contact in the crystal. Because this condition is rather too strict to be satisfied easily, let us introduce a much more approximate condition,

$$d_a \geq 1.2 \left\{ \left(\frac{a}{n_1} \right)^2 + \left(\frac{b}{n_2} \right)^2 + \frac{2ab}{n_1 n_2} |\cos \gamma| \right\}^{1/2},$$

$$1.2 \left\{ \left(\frac{b}{n_2} \right)^2 + \left(\frac{c}{n_3} \right)^2 + \frac{2bc}{n_2 n_3} |\cos \alpha| \right\}^{1/2},$$

$$1.2 \left\{ \left(\frac{a}{n_1} \right)^2 + \left(\frac{c}{n_3} \right)^2 + \frac{2ac}{n_1 n_3} |\cos \beta| \right\}^{1/2},$$

where d_a denotes the average interatomic distance between any two contact atoms in the crystal: d_a can be roughly estimated from the nature of the atoms contained. In case the structure contains a number of very heavy small atoms, their effect on $I'(000)$ can be estimated.

When all of the foregoing four points have been provided for, it is believed that the error in $I'(000)$ would fall in the range of 5–20 per cent in the usual cases.

To illustrate the use of (3), let us first take a crystal consisting of only one atom at the origin in the unit cell, the number of electrons in the shell of the atom being Z and the atomic structure factor, $f(hkl)$. Then $F(hkl) = f(hkl) = Zf(hkl)$. $F^2(000) = Z^2$. If we assume $I'(hkl) = F^2(hkl)$, we have $I'(hkl)/F^2(hkl) = Z^2$. Substituting these values in (3) we obtain

$$I'(000) = \frac{Z^2 \left(\sum_{h=-\infty}^{\infty} U_{n_1 h} \right) \left(\sum_{k=-\infty}^{\infty} U_{n_2 k} \right) \left(\sum_{l=-\infty}^{\infty} U_{n_3 l} \right) - U_{n_1 0} U_{n_2 0} U_{n_3 0}}{1 - U_{n_1 0} U_{n_2 0} U_{n_3 0}}.$$

Using U_{nh} given in the table, with $n_1 = 48, n_2 = 32, n_3 = 16$, we obtain $I'(000) = 1.0051Z^2$, which differs from the assumed $I'(000) = F^2(000) = Z^2$ only by 0.51 per cent. The choice of U_{nh} of any other n_1, n_2, n_3 will give similar results.

Let us next illustrate the method by studying a real crystal, say, *paradinitrobenzene*, the structure of which was determined carefully by James, King and Horrocks⁴, who made the determination on the basis of reflexions $hkl, h0l$ and $0kl$. Strictly speaking, we should determine $I'(000)$ from equation (3), based on the relative intensities of the whole set of reflexions hkl . But in the case of the present structure, as we know already from James, King and Horrocks' paper that there is no overlapping of atoms directly upon each other in the projection of the structure in direction b to the ac plane (see ref. 4, Fig. 3), a study of the relative intensities of reflexions $h0l$ is sufficient for our purpose of illustration. Then let us take their observed $F^2(h0l)$ directly as our $I'(h0l)$ and take Robertson's f -values⁵ directly as our $\bar{f}(h0l)$. Since no further temperature correction has been made, the values of $\bar{f}(h0l)$ so obtained are under-corrected for the temperature effect as revealed

from my studies of the same structure. But we may deliberately use such rough values of $\bar{f}(hkl)$ in order to see if $I'(000)$ so deduced still proves reliable. The structure has

$$F^2(000) = 164^2, \sum_{i=1}^t Z_i^2 = 1140$$

when the contribution of the hydrogen atoms is neglected. $h_M = 13$ such as in $h0l = 13 0 1$, and $l_M = 7$ such as in $h0l = 1 0 7$. Accordingly, we take $n_1 = 24, n_2 = 12$. The two-dimensional equation for $I'(000)$ is given by

$$I'(000) = F^2(000) \frac{\sum' U_{n_1 h} U_{n_2} I'(h0l) / \bar{f}^2(h^0l)}{\sum_{i=1}^t Z_i^2 - U_{n_1 0} U_{n_2 0} F^2(000)}, \quad (3a)$$

where Σ' denotes $\sum_{h=-\infty}^{\infty} \sum_{l=-\infty}^{\infty}$,

excluding the term with $h = l = 0$. Substituting in (3a) the appropriate U_{nh} from the table and the other quantities mentioned above, we obtain $I'(000) = 0.85F^2(000)$, differing from the assumed $I'(000) = F^2(000)$ by 15 per cent; an acceptable error obtained by deliberately choosing rather rough values of $\bar{f}(hkl)$.

Details of this work, including the method of correcting for the effect of small heavy atoms, will be presented elsewhere.

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FRACTURE OF SOLIDS

A CONFERENCE on "The Fracture of Solids" was held by the British Rheologists' Club on October 29. Prof. N. F. Mott, recently elected president of the Club, opened the conference by pointing out that, quite apart from its practical importance, fracture was the most interesting property of solids to the theoreticians because it is the least understood property, no progress having been made beyond the Griffith crack-theory of 1924. It is not known how cracks exist nor what causes them; experimental work has made clear what happens during fracture, but not how it occurs.

Dr. C. F. Tipper then presented a paper describing some beautiful experimental work on the subject of fracture in mild steel. She divided fracture into three types: the first corresponds to a parting along a shear plane; the second along two intersecting planes, giving a wedge-shaped fracture; and the third along a plane quite different from the shear plane, often at right angles to the principal tensile stress. Iron and mild steel show all three types of fracture, and it is possible to have all in the same test-piece, even in adjacent crystals. The amount of energy absorbed in fracture depends on how much of each type goes to make up the total fracture. The third type, which is generally brittle, can always be