Short Communications

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Diamagnetic anisotropies of some organic molecules. Corrigenda. By M. A. Lasheen, *Physics Department, Faculty of Science, Alexandria University, Alexandria, U. A. R.*

Attention is drawn to a printing error as a result of which some data for potassium acid phthalate were attributed to 10,10′-dianthronyl in *Acta Cryst.* (1969) A25, 581.

In the paper (Lasheen, 1969) under the above title two parts of the text were accidentally transposed just before the final printing. The paper reads as originally intended if the part beginning at the heading '10,10′-dianthronyl, $(C_{14}H_9O)_2$' and ending with the words 'towards the second half' (half way down the second column of page 582) is transferred to the beginning of the text. The figures for direction cosines and for molecular susceptibilities and anisotropy in the remaining part of the second column of page 582 refer to potassium acid phthalate. To clear up any possible confusion the final part of the original text, consisting of the section on potassium acid phthalate and the concluding paragraph, is reprinted below in full.

Potassium acid phthalate $C_6H_4(COOH)(COOK)$

Lasheen (1964a) measured the crystal magnetic anisotropies and Lasheen & Heddewi (1967) measured the mean molecular susceptibility. These are:

$\chi_b - \chi_a = 35\cdot6$, $\chi_c - \chi_a = 41\cdot7$, $\chi_c - \chi_b = 6\cdot0$, $\bar{\chi}_M = -99\cdot25$ Hence, $\chi_a = -125\cdot02 \pm 0\cdot12$, $\chi_b = -89\cdot42 \pm 0\cdot19$, $\chi_c = -83\cdot32 \pm 0\cdot20$ (10^{-6} e.m.u. g^{-1}).
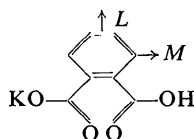
The molecular susceptibilities of this molecule were pre-viously calculated (Lasheen, 1964a) by the use of the direction cosines of ammonium acid phthalate, whose crystal structure had been determined by Okaya & Pepinsky (1957).

The crystal structure of potassium acid phthalate was later determined by Okaya (1965) who found:

$a = 6\cdot46_6$, $b = 9\cdot60_9$, $c = 13\cdot85_7$ Å, $Z = 4$, $P2_1ab$.

The angles between the plane of the benzene ring and those of the two carboxyl groups are 31·7 and 75·4° respectively.

The direction cosines of the molecular axes L, M and N are:

	a	b	c
L	0·1609	0·4349	0.8858
M	0·5148	−0·8029	0·3006
N	−0·8399	−0·4111	0·3543

Thus the molecular susceptibilities and anisotropy are:

$K_L = -73\cdot92 \pm 0\cdot10$
$K_M = -79\cdot12 \pm 0\cdot13$ $\qquad \Delta K = 68\cdot27 \pm 0\cdot12$
$K_N = -144\cdot79 \pm 0\cdot08$

The variances in the crystal magnetic susceptibilities and the resulting probable errors in the molecular susceptibilities and anisotropies were calculated by the method given for orthorhombic crystals by Lasheen & Tadros (1968) and for monoclinic crystals by Walley (1967).

Reference

Lasheen, M. A. (1969). *Acta Cryst.* A25, 581.

The multiple-film technique: the effect of angle of incidence on the absorption of Co *K*α radiation by X-ray film. By J. E. Derry and T. A. Hamor, *Department of Chemistry, The University, Birmingham* 15, *England*

Film absorption factors of Ilford Industrial G X-ray film for Co *K*α radiation have been determined over a range of angles of incidence.

Experimental data for the variation of the film absorption factor, *R*, with angle of incidence for Cu *K*α radiation have been given by Bullen (1953) and Grenville-Wells (1955). These authors assumed that this variation could be ex-

pressed by

$$R_v = (I_0/I)_v = \exp(\mu t \sec v),\qquad(1)$$

where I_0 and I are the intensities of the incident and transmitted beams, μt is the sum of the separate products of the linear absorption coefficients with the thickness of emulsion, film base and any interleaving paper, and v is the angle the incident X-rays make with the normal to the film. Rossmann (1956) improved the agreement between the experimental and calculated values of R using the relationship

$$R_v = [1/(1-C)] \exp(\mu t \sec v),\qquad(2)$$

where C is a factor to allow for the absorption of energy by the photochemical effect (Cox & Shaw, 1930).

Recently we used Co $K\alpha$ radiation and the multiple-film technique (Robertson, 1943) to record intensity data on equi-inclination Weissenberg photographs, but were unable to find the relevant film-factor data in the literature. Owing to the much stronger absorption of Co radiation and the limited range of linearity of response of X-ray film, it was not possible to determine the film factors with sufficient accuracy by comparing reflexion intensities on successive films of the multiple-film pack, and the following procedure was therefore adopted.

For each equi-inclination angle, v, a 60° Weissenberg exposure was recorded twice, on different portions of a twin-pack of Ilford Industrial G film (each film wrapped in its black paper folder as supplied by the manufacturers). The exposure times, t_1 and t_2, were chosen so that t_2/t_1 was approximately equal to the film factor at the equi-inclination angle under consideration. Then, if the intensity of a reflexion of the shorter (time t_1) exposure on the first (nearer to crystal) film is S_1, and that of the same reflexion of the longer (time t_2) exposure on the second film is S_2, the film absorption factor is given by

$$R = t_2 S_1/t_1 S_2.$$

S_1 and S_2 are approximately equal and errors due to non-linearity are avoided.

The film factors, R (exp), derived in this way are listed in Table 1, together with those calculated according to equation (1), the value of $\mu t(=1\cdot951)$ being determined by least squares. Application of equation (2) gives virtually identical results ($\mu t = 1\cdot950$, $C = 0\cdot001$).

Table 1. *Experimental and calculated R values*

v	$\sec v$	R (exp)	R (calc) $\mu t = 1\cdot951$
0·0°	1·000	7·02	7·04
4·7	1·003	7·21	7·08
9·5	1·014	7·26	7·23
15·9	1·040	7·40	7·60
22·6	1·083	8·47	8·27
29·6	1·150	8·99	9·43
33·2	1·195	10·62	10·29

The average discrepancy between experimental and calculated values is 2·35 % and the root-mean-square deviation is 0·24. The standard deviation in μt is 0·010 and the standard deviations in the calculated film factors range from 0·07 at $v = 0$ to 0·12 at $v = 33\cdot2°$.

References

BULLEN, G. J. (1953). *Acta Cryst.* **6**, 825.
Cox, E. G. & SHAW, W. F. B. (1930). *Proc. Roy. Soc.* **A127**, 71.
GRENVILLE-WELLS, H. J. (1955). *Acta Cryst.* **8**, 512.
ROBERTSON, J. M. (1943). *J. Sci. Instrum.* **20**, 175.
ROSSMANN, M. G. (1956). *Acta Cryst.* **9**, 819.

Absorption corrections for neutron diffraction.

By K. D. ROUSE and M. J. COOPER, *Materials Physics Division, A.E.R.E., Harwell, Berkshire, England,* and E. J. YORK and A. CHAKERA, *Computer Analysts and Programmers Ltd., Reading, Berkshire, England*

Absorption corrections for cylindrical and spherical crystals have been evaluated by numerical integration for values of μR in the range 0 to 1·0, where μ is the mean linear absorption coefficient and R is the radius of the crystal. For this range of μR, which is that normally required for neutron diffraction data, interpolation from existing tables is unsatisfactory. The transmission factor A_{hkl} is tabulated as a function of μR and $\sin^2 \theta$, accurate to four decimal places. The intervals chosen for the tabulation are such that linear interpolation may be used for intermediate values. Analytical expressions, which may be used for calculating the transmission factor when a lower accuracy is acceptable, are also given.

In passing through a crystal a neutron or X-ray beam is attenuated by normal absorption processes, resulting in a reduction in the observed intensity of a given Bragg reflexion. The exact reduction depends on the paths through the crystal and the magnitude of the mean absorption coefficient of the crystal, the transmission factor being

$$A_{hkl} = \frac{1}{V} \int \exp\{-\mu(p+q)\}dV \qquad(1)$$

(*International Tables for X-ray Crystallography*, 1959), where μ is the mean linear absorption coefficient, p and q are the lengths of the paths of the incident and reflected beams in the crystal for radiation reflected in an element of volume dV, and V is the volume of the crystal.

This integral can be evaluated rigorously only for certain crystal shapes, two of the most convenient of which are a cylinder and a sphere. For these the integral over all path lengths can be computed to give an absorption factor A^*