starting value of *a*, and the average slope of the high- and low-angle part of the curve through the tabulated data as starting values of *b* and *c*, respectively.

Starting from these, a least-squares refinement converged in about five cycles to the final values, except in the cases of the smallest values of μR, where the curve is essentially a straight line. Progress of the refinement of the constants was followed by inspection of the constants and the r.m.s. relative discrepancy between observed and calculated values of μR after every cycle. As a final safeguard $(A^*_{\text{obs}}-A^*_{\text{calc}})/A^*_{\text{obs}}$ was checked for all data in the Tables. In no case did this quantity exceed 1%, so that even in the most unfavourable cases (those with high μR) the structure factors computed with the use of our constants will not be in error by more than 0·5%, and usually by considerably less than that. It should be noted that the original data in the tables are in some places only accurate to within 0·5% owing to round-off.

Table 1. *Analytical constants for the absorption correction factor for spherical crystals*

μR	$A^*_{\theta=0}$	*a*	*b*	*c*	r.m.s. dev.
0·0	1·00	1·000	0·0000	0·0000	0·0%
0·1	1·16	1·160	0·0000	0·0000	0·0
0·2	1·35	1·426	0·0361	0·5831	0·3
0·3	1·56	1·625	0·0581	0·6316	0·1
0·4	1·80	1·820	0·0650	2·3688	0·3
0·5	2·08	2·115	0·1053	0·6462	0·5
0·6	2·39	2·427	0·1395	1·4448	0·2
0·7	2·75	2·812	0·1954	4·2075	0·4
0·8	3·15	3·157	0·2159	4·6021	0·1
0·9	3·61	3·595	0·2592	6·1161	0·1
1·0	4·12	4·058	0·2984	3·0039	0·1
1·1	4·70	4·508	0·3304	2·7231	0·1
1·2	5·35	5·021	0·3670	2·9234	0·1
1·3	6·08	5·671	0·4191	3·7131	0·1
1·4	6·90	6·253	0·4531	3·7853	0·1
1·5	7·80	6·872	0·4869	3·8224	0·1
1·6	8·81	7·620	0·5317	4·2486	0·1
1·7	9·92	8·314	0·5646	4·3171	0·1
1·8	11·2	9·219	0·6145	4·9735	0·2
1·9	12·5	9·839	0·6310	4·5913	0·2
2·0	14·0	10·80	0·6765	5·0185	0·2
2·1	15·6	11·73	0·7125	5·2362	0·2
2·2	17·4	12·69	0·7469	5·5129	0·1
2·3	19·4	13·81	0·7889	6·1126	0·2
2·4	21·5	14·85	0·8209	6·2846	0·2
2·5	23·8	15·96	0·8542	6·5276	0·3
2·6	26·3	17·26	0·8953	7·0784	0·3
2·7	29·0	18·37	0·9211	7·2568	0·4
2·8	31·9	19·68	0·9554	7·6692	0·4
2·9	35·0	20·94	0·9844	7·8883	0·5
3·0	38·4	22·27	1·0128	8·2616	0·5

Table 2. *Analytical constants for the absorption correction factor for cylindrical crystals*

μR	$A^*_{\theta=0}$	*a*	*b*	*c*	r.m.s. dev.
0·0	1·00	1·000	0·0000	0·0000	0·0%
0·1	1·18	1·180	0·0000	0·0000	0·0
0·2	1·40	1·503	0·0607	0·9750	0·4
0·3	1·65	1·615	0·0123	1·8912	0·5
0·4	1·95	1·979	0·0874	2·6509	0·1
0·5	2·29	2·320	0·1229	5·1682	0·1
0·6	2·69	2·721	0·1677	5·4849	0·1
0·7	3·16	3·177	0·2152	13·015	0·1
0·8	3·70	1·850	0·2731	0·2567	0·2
0·9	4·33	0·973	0·3312	0·3281	0·3
1·0	5·06	4·804	0·3538	2·6397	0·2
1·1	5·90	5·302	0·3823	2·1766	0·1
1·2	6·86	6·094	0·4393	2·7487	0·2
1·3	7·96	6·810	0·4792	3·0203	0·1
1·4	9·23	7·716	0·5327	3·5630	0·3
1·5	10·7	8·808	0·5971	4·3757	0·1
1·6	12·3	9·634	0·6276	4·3361	0·2
1·7	14·2	10·82	0·6845	4·9628	0·2
1·8	16·3	11·98	0·7310	5·3459	0·2
1·9	18·6	13·11	0·7701	5·5386	0·2
2·0	21·3	14·47	0·8184	6·0845	0·2
2·1	24·2	15·82	0·8600	6·4849	0·2
2·2	27·5	17·22	0·8997	6·8418	0·3
2·3	31·2	18·72	0·9405	7·3176	0·3
2·4	35·3	20·45	0·9887	7·8436	0·5

Our Tables 1 and 2 contain the following information in the consecutive columns: the value of μR for which the constants were computed; the value of $A^*_{\theta=0}$, *a*, *b*, *c*, and the r.m.s. value of $(A^*_{\text{obs}}-A^*_{\text{calc}})/A^*_{\text{obs}}$ over the 19 entries for the particular value of μR.

We are planning to extend this work to a five-constant formula (Moore, 1963) after a forthcoming change of computer.

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Estimation of error in the measured structure factor.

By S. C. ABRAHAMS, *Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey, U.S.A.*

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In a recent paper on automatic diffractometer programs (Cetlin & Abrahams, 1963), two formulae were given for computing the variance in the mean structure amplitude. In the notation of that paper, $\sigma^2(\bar{F}^2)$ gave the variance due to a Poisson distribution in the counting statistics and $V(\bar{F}^2)$ gave the variance due to those effects that are unequal with respect to reflections constrained by symmetry to be equivalent. It was also suggested that the variance ratio $V(\bar{F}^2)/\sigma^2(\bar{F}^2)$ be used as an indicator of systematic error. In practice, the *F*-distribution could not be interpreted satisfactorily. Table 1 (column 4) illustrates part of the very wide range found in a typical

Table 1. *Structure factors and error measures in ludlamite*

hkl	$\sigma^2(\bar{F}^2)$	$V(\bar{F}^2)$	$V(\bar{F}^2)/\sigma^2(\bar{F}^2)$	$\bar{F}$	$\sqrt{V(\bar{F})}$	$\sigma(\bar{F})$
$20\bar{1}$	$0{\cdot}832\times10^7$	$2{\cdot}104\times10^8$	25·296	970	7·5	1·5
$60\bar{3}$	$0{\cdot}644\times10^8$	$5{\cdot}922\times10^7$	0·919	1551	2·5	2·6
6,0,13	$0{\cdot}488\times10^7$	$2{\cdot}714\times10^4$	0·006	184	0·4	5·9

study (on ludlamite, using a relative scale). It may be noted that the large individual values of the structure amplitude variances in columns 2 and 3 are equivalent to the fairly small 'standard deviations' in columns 6 and 7. The largest 'standard deviation' in column 6 is 0·8% of $|\bar{F}(20\bar{1})|$ and in column 7 is 3·2% of $|\bar{F}(6, 0, 13)|$.

A more realistic measure of the error in the mean structure factor includes three distinct sources of error. Source 1 is random; source 2 is systematic and anisotropic; source 3 is systematic and isotropic. Source 1 includes (*a*) the Poisson distribution in each N_j, which is given by $\sigma^2(\bar{F}^2)$; (*b*) short-term variations in the X-ray supply; and (*c*) short-term variations in the stability of the electronic recording system. For PEXRAD, an adequate measure of the variance in 1(*b*) + 1(*c*) is obtained from the reproducibility which is typically about $0{\cdot}005F$ (Abrahams, 1964), *i.e.* the variance in the structure amplitude due to short-term instability is $V(S)=10^{-4}\bar{F}^4$. Source 2 contains (*a*) variations in the *effective*† radii (r) from the mean radius ($\bar{r}$) for an imperfect sphere, or in the *actual* linear dimensions of a polyhedron from the measured values. Such variations make the absorption correction systematically in error for each reflection for which $r \neq \bar{r}$; (*b*) variations in extinction, anomalous dispersion and multiple scattering with crystal direction; and (*c*) variations in the spectral distribution. All the anisotropic systematic errors are given by $V(\bar{F}^2)$, except for the triclinic case as pointed out by Jeffery (1964).

Group 3 includes (*a*) incorrect values of μ (*i.e.* experimental or extrapolation errors in *International Tables*) and/or breakdown of the additivity relation $\mu = D_m\Sigma p(\mu/\varrho)$; (*b*) incorrect value of measured $\bar{r}$ as compared with the mean of all the effective radii; (*c*) scattering received by the counter of wavelengths different from the given λ; (*d*) thermal diffuse scattering (this could also have an anisotropic component); (*e*) incorrect extinction parameters; and (*f*) long-term drift in the stability both of the X-ray supply and of the electronic recording system. The published values of μ/ϱ are probably in error by about 2–5% (*cf. International Tables for X-ray Crystallography*, 1962). For an error of 2%, the resulting systematic error in A^* for $\mu\bar{r}=1$ is 1%; for an error of 5% in μ/ϱ, the corresponding error in A^* is 2·5%. For absolute measurements, and for larger μr‡, the error in A^* is larger. Let us assume μ/ϱ is in error by 3%. Then the resulting variance in $\bar{F}^2$ is $V(\mu) = 9\times10^{-4}\bar{F}^4$. The error in $\bar{r}$ can be directly estimated by averaging many microscopic measurements, and is comparable to the above error in μ/ϱ. In favorable cases, it can be reduced to 1–2%. In the writer's experience, for $\bar{r} < 0{\cdot}2$ mm, this is usually a lower limit. For an error in $\bar{r}$ of 3%, the resulting variance in $\bar{F}^2$ is $V(\bar{r}) = 9\times10^{-4}\bar{F}^4$, in the case $\mu r = 1$. Spectral contamination in (*c*) is experimentally reduced to a small value in PEXRAD and is probably less than about 1%, corresponding to a variance of $V(\lambda) = 4\times10^{-4}\bar{F}^4$. The errors due to (*d*) and (*e*) are difficult to estimate, but could be taken at a nominal 1% with $V(T,E) = 4\times10^{-4}\bar{F}^4$. The error in (*f*) is small in PEXRAD, and generally is less than the short-term variations in X-ray supply and electronic stability.

Assuming no correlations among these different variances, the total variance in the value of $\bar{F}_{\text{meas}}$ is given by

$$V(\bar{F}^2_{\text{meas}}) = \sigma^2(\bar{F}^2) + V(S) + V(\bar{F}^2) + V(\mu) + V(\bar{r}) + V(\lambda) + V(T, E)$$

and substituting the estimated numerical values above,

$$V(\bar{F}^2_{\text{meas}}) = \sigma^2(\bar{F}^2) + V(\bar{F}^2) + 27\times10^{-4}\bar{F}^4\,.$$

Defining the best estimated error in $\bar{F}_{\text{meas}}$ as

$$\delta(\bar{F}_{\text{meas}}) = \sqrt{[V(\bar{F}^2_{\text{meas}})]}/2\bar{F}\,,$$

the resulting errors in the $\bar{F}_{\text{meas}}$ given in Table 1 become $\delta(\bar{F}(20\bar{1})) = 26$ or 2·7% $|\bar{F}(20\bar{1})|$; $\delta(\bar{F}(60\bar{3})) = 40$ or 2·6% $|\bar{F}(60\bar{3})|$ and $\delta(\bar{F}(6, 0, 13)) = 8$ or 4·4% $|\bar{F}(6, 0, 13)|$.

The importance of absorption as a primary source of error has been recently emphasized by MacGillavry (1963), Burbank (1964), and Jeffery & Rose (1964).

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† The effective radius here is that length which gives the correct transmission factor

$$A = (1/V)\iiint \exp\left[-\mu(p+q)\right]dx\,dy\,dz\,,$$

where μ is the correct linear absorption coefficient, for a particular reflection.

‡ In this case, the percentage error is a function of θ.