It is clear that this simple formulation cannot be successful unless the relationships are linear in phase angles and the weights are assumed to be independent of phase angles. Otherwise, variable symbols would enter the sums.

Two rationales for this matrix formulation can be offered. The first is that the phases of those reflections to which the phase set is most sensitive should be determined first (or fixed at the beginning). The second is that those important reflections with phase angles which are most easily varied must have their phases fixed early. Consider the meaning of the matrix which contributes to the sum. If the weight for a contributing matrix is large, then the corresponding equation is an important one in the set of all equations. In the latter case, each of the contributions to the sum is correspondingly large. If the element, kl, of the sum matrix is large, then there are many equations with large weight which involve the kth and lth phase angles. In this case assigning the phase angles of the kth and lth reflections will aid in the phasing of many other reflections. Correspondingly, if these phase angles are not assigned, then these reflections which enter many strong relationships will be phased by other (probably weaker) reflections through a weaker chain of phase relationships.

Several routes to a starting set are possible once the matrix sum is formed from all available relationships. The simplest is to compute the magnitude (norm) of each row (or column) and to choose some number of reflections whose rows have large magnitudes to be the starting set. Space-group symmetry restrictions on origin fixing must, of course, be taken into account. A second procedure might be to choose some number of reflections from the row with the largest magnitude. Still another method might be to choose reflections corresponding to large elements from the eigenvector associated with the smallest eigenvalue. By successive choice of smaller elements at each stage (in any method), a tree for phase determination may be set up. Clearly some thought toward connecting the series of reflections is required.

The first method above has been tried in preliminary tests. In the first test, two previously solved structures for which poor origins were determined by the CM were used. All reflections with $|E| > 1{\cdot}5$ were used. For both, fewer reflections had α (Germain, Main & Woolfson, 1970) equal to zero at elimination if a starting set was chosen by the first method described above than by CM. The second test involved oxytocin data. All reflections (141) for which $|E|$ exceeded 1·8 were included. The CM chose poor origins, chiefly with reflections that connected badly with the bulk of the reflections. The present method immediately indicated a group of reflections most of which had been found to be important by laborious tracing of many alternative starting sets (Andrews & Koenig, 1978). The other indicated reflections were also useful.

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X-ray linear absorption coefficients for silicon and germanium in the energy range 5 to 50 keV.

By G. Hildebrandt, *Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg* 4–6, *D*-1000 *Berlin* 33 (*Dahlem*), *Federal Republic of Germany*

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Abstract

Experimental absorption data from different authors are commented on and, critically evaluated, presented in a table.

In a paper published two years ago, Lawrence (1977) contributed two experimental absorption coefficients for Si measured at the wavelengths of Cu $K\alpha$ and Mo $K\alpha$ [data (*a*) in Table 1] and made the statement that 'no recent experimental determination of the absorption coefficient of silicon appears to have been carried out'. One year later, Suorrti (1978) tried to explain the apparent deviation of the measured values from the data given in *International Tables for X-ray Crystallography* [1974; marked (*f*) in Table 1].

Evidently, both authors were not aware of extended measurements of X-ray absorption coefficients in the range 5 to 25 keV which have been published from 1973 to 1976, mainly in *Z. Naturforsch.*, and of a recent extension of the measurements to 50 keV, so important for experiments with synchrotron radiation, presented in the same journal in 1977.

Table 1. *Comparison of attenuation coefficients*, μ_0(cm^{-1}), *for* Si *and* Ge *at* Cu $K\alpha$ *and* Mo $K\alpha$ *wavelengths*

Line	E (keV)			Si		
Cu $K\alpha$	8·041	132·4^{a}	144^{b}	144·9^{c}	143·9^{e}	152·0^{f}
Mo $K\alpha$	17·44	14·18^{a}	14·6^{b}	14·4^{d}	14·58^{e}	15·21^{f}
				Ge		
Cu $K\alpha$	8·041		354^{b}	352^{g}	353·9^{e}	361·6^{f}
Mo $K\alpha$	17·44		320^{b}	318^{g}	320·2^{e}	321·9^{f}

References: (*a*) Lawrence (1977); (*b*) Hildebrandt, Stephenson & Wagenfeld (1973); (*c*) Gerward & Thuesen (1977); (*d*) Pike (1941); (*e*) interpolated from Table 2; (*f*) *International Tables for X-ray Crystallography* (1974); (*g*) Persson & Efimov (1970).

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It seems, therefore, necessary to review the main content of these papers very briefly, to mention important theoretical approaches and, what might be most useful, to present a table of absorption coefficients in the energy range 5 to 50 keV as the result of a critical evaluation of existing experimental data.

Theoretically, the calculation of absorption cross sections has been treated rigorously with relativistic wave functions, mainly by Cromer & Liberman (1970) and Storm & Israel (1970). Proceeding from hydrogen-like eigenfunctions, Wagenfeld (1966), on the other hand, arrived at simple formulae, allowing fast calculations not only of normal but also of anomalous absorption cross sections important for the absorption of wave fields (Borrmann effect). Such calculations have been reported by Hildebrandt, Stephenson & Wagenfeld (1973, 1975*a*,*b*), Hildebrandt & Stephenson (1975), Stephenson (1976) and most recently by Gerward & Thuesen (1977) who also considered in detail contributions from thermal diffuse and Compton scattering.

Measurements of linear absorption coefficients of Ge and Si at 8 to 12 characteristic wavelengths in the energy range 5 to 25 keV have been reported by Hildebrandt, Stephenson & Wagenfeld (1973), together with comparisons with other experimental data and theory. The same paper presents the most extensive collection of measured and calculated anomalous absorption data; some supplements appeared later (1975*b*). Stephenson (1975) considered elements $Z = 6$ to 54, Persson & Efimov (1970) concentrated their measurements on the surroundings of the Ge–K absorption edge, and Gerward & Thuesen (1977) finally expanded the measurements and comparisons with theory to the whole energy range from 5 to 50 keV. For other experimental values see Table 2.

The further discussion will be restricted to Si and Ge; crystals from these elements are important for experiments with wavefields, as materials for monochromators and interferometers *etc*., and many new absorption data are available. The older measurements (1973) in the lower energy range (5 to 25 keV) are precisely confirmed by some newer ones (Gerward & Thuesen, 1977) and agree satisfactorily with theoretical data (hydrogen-like calculation); the data of *International Tables for X-ray Crystallography* (1974) coincide now for Ge, but are still a little too high for Si. In the upper energy range (25 to 50 keV), the Storm–Israel calculations turn out to be superior. There exist no data from *International Tables for X-ray Crystallography*. For a discussion of other contributions *cf*. the original paper (Gerward & Thuesen, 1977).

From the relation $\ln\mu = a_0 + a_1 \ln E$, mean values for the constants a_0 and a_1 have been calculated from the available experimental data separately, in four ranges (I) 5 to 15, (II) 11 to 27, (III) 23 to 39, (IV) 35 to 50 keV. The values mainly considered in (I) and (II) were those from Hildebrandt, Stephenson & Wagenfeld (1973) and, especially for Ge, those from Persson & Efimov (1970), and in the ranges (III) and (IV) those from Gerward & Thuesen (1977). In the case of Si, only small corrections were necessary in the three overlapping regions, and some corrections in (IV) to take into account the stronger influence of the Compton effect. For Ge, somewhat larger corrections between actually measured and extrapolated values were necessary only in the overlap (II)/(III). The same holds for values near the Ge–K edge.

Table 2 presents linear absorption coefficients for Si and Ge between 5 and 50 keV in steps of 1 keV. The accuracy, even of interpolated values, should be about 1%, at least in the ranges closely covered by characteristic wavelengths (6 to 9 and 17 to 25 keV). As an example four values interpolated from Table 2 are included in Table 1, marked (*e*).

I am grateful to Dr Gerward for valuable comments.

Table 2. *Attenuation coefficients*, μ_0(cm^{-1}), *for* Si *and* Ge *in the energy range* 5 *to* 50 keV, *based on experimental data*

Numbers underlined are more uncertain.

E (keV)	Si	Ge	*E* (keV)	Si	Ge
5	$\underline{555}$	$\underline{1347}$	28	3·77	89·8
6	331	806	29	3·43	81·5
7	213	523	30	3·13	74·1
8	146	359	31	2·86	67·3
9	104	258	32	2·62	61·3
10	76·3	193	33	2·41	56·0
11	57·4	$\underline{148}$	34	2·22	51·3
12	44·0	$\underline{910}$	35	2·05	47·2
13	34·4	$\underline{725}$	36	1·90	43·5
14	27·4	588	37	1·77	40·1
15	22·5	484	38	1·66	37·1
16	18·7	405	39	1·56	34·4
17	15·7	343	40	1·47	32·0
18	13·3	294	41	1·39	29·8
19	11·3	254	42	1·32	27·8
20	9·75	221	43	1·25	26·0
21	8·44	193	44	1·19	24·3
22	7·36	171	45	1·13	22·8
23	6·48	151	46	1·08	21·4
24	5·75	135	47	1·03	20·1
25	5·13	121	48	0·99	18·9
26	4·61	109	49	0·95	17·8
27	4·16	99·0	50	0·92	16·8

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