

BENCE-ALBEE AFTER 20 YEARS: REVIEW OF THE ACCURACY OF α -FACTOR
 CORRECTION PROCEDURES FOR OXIDE AND SILICATE MINERALS

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Twenty years ago, Arden Albee and Ted Bence wrote a paper in the *Journal of Geology* proposing the use of empirical α -factors to correct electron microprobe analyses of oxide and silicate minerals,¹ similar to procedures proposed by Ziebold and Ogilvie for binary metal alloys² and by Lachance and Traill for x-ray fluorescence analyses.³ This paper has become one of, if not *the* most cited paper in the geological sciences, which is a tribute both to the success and popularity of the analytical technique and to the important role microbeam analysis plays in geology. In the intervening years, although the original papers emphasized that new empirical α -factors should be developed,^{1,4} and other studies indicated that the original α -factors produced some systematic errors in processing geological data, most investigators have continued to use the corrections as originally formulated. In the present study, the Bence-Albee correction is evaluated in comparison with the current generation of ZAF, $\phi(\rho z)$, and Monte Carlo corrections. We show that with some modifications the α -factor corrections can be as accurate as any other correction procedure currently available and much easier and quicker to process.

Basics of the α -factor Procedures

The Bence-Albee correction is based on two assumptions.^{1,4}

1. In binary oxide systems AB, there is a hyperbolic relation between concentration and intensity such that

$$(1 - K_{AB}^A)/K_{AB}^A = \alpha_{AB}^A (1 - C_{AB}^A)/C_{AB}^A \quad (1)$$

or

$$C_{AB}^A/K_{AB}^A = \alpha_{AB}^A + (1 - \alpha_{AB}^A)C_{AB}^A \quad (2)$$

where C_{AB}^A is the concentration of A in the binary relative to the end member oxide (i.e., the oxide weight fraction), K_{AB}^A is the ratio of the background-subtracted x-ray intensity of A in the binary relative to that in the end member oxide, and α_{AB}^A , the α -factor, is a con-

stant for the binary. If this assumption is correct, the plot of C/K vs C is a straight line, the y-intercept of which is equal to the α -factor, as is 1 minus the slope.

2. In multicomponent oxide systems, C/K is equal to the concentration-weighted sum of the α -factors for each of the binaries:

$$C_{ABC\dots n}^A/K_{ABC\dots n}^A = \sum_1^i (C_{ABC\dots n}^i \alpha_{Ai}^A) / \sum_1^i C_{ABC\dots n}^i \quad (3)$$

One can determine the α -factors either experimentally by performing a multiple least-squares fit of C/K vs composition for a series of analyzed standards,^{1,5} or theoretically by calculating C/K from a ZAF correction procedure for various compositions in binary oxide systems, and then performing least squares fits of C/K vs C.⁴

Bence and Albee noted in their initial paper that in binary systems where there was either a large fluorescence or a large absorption correction, the linear relationship between C/K and C did not hold. Other investigators have proposed that more accurate results could be obtained if the constant α -factor term was replaced with a polynomial function of concentration,^{6,7} although this conclusion has been disputed.⁵ In none of these papers were the magnitudes of the deviations from linearity of the Bence-Albee equation evaluated for any considerable range of binary oxides. In a recent series of papers,⁸⁻¹⁰ Armstrong has demonstrated that the α -factor approach can be successfully applied to the quantitative analysis of particles and thin films, in addition to conventional thick polished specimens, but that the accuracy of the procedure can be significantly improved if α -factors are calculated from newer ZAF and $\phi(\rho z)$ algorithms. However, these papers did not evaluate the magnitude of the nonlinearity in C/K vs C relations, either.

α -factor Calculations

Series of α -factors were calculated for a 102×102 oxide matrix spanning the periodic table. ZAF and $\phi(\rho z)$ correction procedures employed were those tabulated in a companion paper (see Table 1 in Ref. 11). Correction factors were calculated for the 1:0, 3:1, 1:1, 1:3, and 0:1 oxide combinations for each binary (e.g., CaO, Ca₃SiO₅, CaSiO₃, CaSi₃O₇, and SiO₂ for the binary CaO--SiO₂). From these values a least-squares fit was made of C/K vs C, and the α -factor was calculated. The maximum deviations of C/K from the least-squares-fit lines were stored along with the α -factors. In cases where the deviation exceeded a threshold value (typically 0.05%),

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the nominal α -factor for each composition was calculated from the relation:

$$\alpha = [(C/K) - C]/(1 - C) \quad (4)$$

and a second-order polynomial fit was performed to determine the variation of the α -factors with concentration.

Monte Carlo calculations of electron trajectories were performed by use of both multiple-scattering and single-scattering models to calculate $\phi(\rho z)$ distributions for similar ranges of compositions in selected binary oxide systems. These $\phi(\rho z)$ distributions were then used to calculate absorption and atomic number corrections and combined with a conventional characteristic fluorescence correction¹¹ to calculate C/K vs C. The calculations were performed with modified versions of the Monte Carlo programs written by David Joy.^{12,13} The multiple-scattering program uses a screened Rutherford cross section based on the models of Curgenvin and Duncumb¹⁴ and constants of Bishop¹⁵ and Myklebust et al.¹⁶ The single-scattering model is similar to that developed by Newbury et al.¹⁶⁻¹⁸ The programs were modified to work with multi-element samples by generating a random number at each electron step and determining which element in the sample is involved in the scattering by application of the random number to the relative values of the atom-concentration-weighted ionization cross sections for the given electron energy. The number and energy distribution of electrons passing through each ρz increment were stored and then multiplied by a series of ionization cross section expressions to calculate the $\phi(\rho z)$ distributions. The ionization cross section expressions tested were those of Green and Cosslett, Worthington and Tomlin, Hutchins, Gryzinski, and Fabre (see Powell¹⁹ for equations and references).

All the ZAF, $\phi(\rho z)$, and Monte Carlo corrections agree closely in the shapes of the C/K vs C curves or lines for all the systems tested, although the magnitude of the intercepts and slopes varies from expression to expression. Table 1 lists selected α -factors calculated for an accelerating potential of 15 keV and a take-off angle of 40° with the $\phi(\rho z)$ absorption correction of Armstrong and atomic-number correction of Love and Scott (Arms-LS).¹¹ Figure 1 shows typical C/K vs C values determined from Monte Carlo calculations.

Table 2 lists the maximum percentage deviations of C/K from the best-fit α -factor lines for the binary systems given in Table 1. As can be seen, many of the binary systems show significant deviations from the constant α -factor assumption. In many cases, the deviations exceed 1% (including geologically important binaries such as Na₂O:Al₂O₃, MgO:Al₂O₃, Al₂O₃:SiO₂, MgO:FeO, and Na₂O:CaO) and in extreme cases are greater than 30%.

All the correction procedures tested give similar results regarding the frequency and nature of the deviations from linear fits of

C/K vs C. An element in a binary system that has small absorption and fluorescence corrections closely fits the straight-line C/K vs C relation (i.e., it has a composition-independent, constant α -factor). In binary systems where the two elements are similar in atomic number, but one is heavily absorbed (the fluorescing element), that element exhibits significant deviations from a straight-line C/K vs C relation. However, the calculated α -factors in those cases are found to vary linearly with concentration. In binary systems where the two elements are dissimilar in atomic number and one is heavily absorbed (particularly when it is also heavily absorbed by oxygen), a plot of calculated α -factor vs oxide concentration precisely fits a second-order polynomial function. In binary systems where one of the elements is significantly fluoresced by other, a plot of α -factor vs oxide concentration for the fluoresced element approximately fits a second-order polynomial. Figure 2 shows typical α -factor vs concentration plots for these cases.

Table 3 gives the results of second-order polynomial fits of α -factors vs concentration for selected of the binary systems presented in Table 1 (using the same Armstrong--Love/Scott correction) and Table 4 lists the maximum percentage deviations of C/K from the second-order polynomial α -factor fits for all the cases shown in Table 2. As can be seen, the deviations drop dramatically when the polynomial expression is used. The maximum relative deviation is 1% and deviations greater than 0.1% are rare. This has been found to be true for all of the binaries spanning the periodic table and all the major ZAF, $\phi(\rho z)$, and Monte Carlo calculations examined. In other words, replacing the constant α -factor approximation with a simple second-order polynomial function of concentration results in the α -factor procedure *exactly* duplicating the results or the correction procedure on which it is based. The only modifications to the conventional Bence-Albee procedure required to use this polynomial approach are (1) to replace the constant α -factor in Eq. (3) with the polynomial equation:

$$\alpha_{AB}^A = c + d[C_A/(C_A + C_B)] + e[C_A/(C_A + C_B)]^2 \quad (5)$$

where C_A and C_B are the oxide weight fractions of the elements in each calculated binary, and (2) to store three matrices of c , d , and e coefficients instead of the single α -factor matrix. Under these circumstances, there is no reason not to replace the ZAF, $\phi(\rho z)$, or Monte Carlo correction by the much simpler and faster polynomial-modified Bence-Albee correction when one is analyzing silicates or oxides.

Best-fit α -factors

To determine the accuracy of the newly calculated α -factors, a set of standards minerals and glasses in the system MgO-Al₂O₃-SiO₂-CaO previously described by Shaw and Albee⁵ were

TABLE 1.--Calculated oxide α -factors from Armstrong/Love-Scott correction.

EO = 15 KEV, PSI = 40 DEGREES

Emitting																								
Line:	O	K	C	K	F	K	Na	K	Mg	K	Al	K	Si	K	P	K	S	K	Cl	K	K	K	Ca	K
O	1.000	1.169	6.460	1.846	1.372	1.213	1.114	1.085	1.052	1.152	1.102	1.070												
CO2	2.003	1.000	5.546	1.625	1.258	1.145	1.074	1.061	1.038	1.144	1.102	1.072												
F	1.064	1.685	1.000	2.171	1.519	1.277	1.131	1.075	1.024	1.108	1.046	1.012												
Na2O	1.486	3.109	2.310	1.000	2.037	1.589	1.326	1.205	1.114	1.180	1.086	1.042												
MgO	1.693	3.598	3.183	1.154	1.000	1.722	1.414	1.271	1.158	1.226	1.120	1.073												
Al2O3	1.868	3.927	3.727	1.261	1.027	1.000	1.474	1.305	1.183	1.235	1.118	1.068												
SiO2	2.100	4.316	4.264	1.372	1.099	1.016	1.000	1.361	1.225	1.273	1.145	1.091												
P2O5	2.292	4.533	4.607	1.440	1.136	1.042	0.971	1.000	1.254	1.290	1.146	1.088												
SO3	2.545	4.854	5.036	1.522	1.187	1.082	1.007	0.975	1.000	1.325	1.169	1.108												
Cl	6.281	11.36	3.649	1.206	0.987	0.925	0.869	0.831	0.763	1.000	1.271	1.152												
K2O	7.025	1.098	5.078	1.571	1.199	1.074	0.988	0.951	0.898	0.943	1.000	1.203												
CaO	6.951	1.167	5.869	1.757	1.309	1.153	1.051	1.010	0.959	1.018	0.861	1.000												
TiO2	5.889	1.297	6.665	2.071	1.463	1.235	1.093	1.034	0.977	1.044	0.933	0.858												
V2O3	7.348	1.400	7.122	2.295	1.575	1.294	1.122	1.046	0.980	1.042	0.933	0.865												
Cr2O3	1.237	1.616	7.131	2.530	1.704	1.376	1.177	1.086	1.011	1.072	0.965	0.902												
MnO	1.326	1.797	7.653	2.913	1.900	1.484	1.235	1.116	1.024	1.075	0.961	0.901												
FeO	1.452	2.065	2.098	3.226	2.072	1.592	1.305	1.167	1.062	1.110	0.991	0.932												
NiO	1.755	2.684	2.247	4.002	2.490	1.846	1.464	1.275	1.139	1.172	1.034	0.975												
ZnO	2.103	3.472	2.382	3.081	3.017	2.145	1.633	1.371	1.191	1.202	1.038	0.971												
SrO	4.466	5.978	3.726	1.538	1.151	1.005	0.937	1.848	1.615	1.491	1.138	1.027												
ZrO2	4.740	4.694	4.529	1.727	1.266	1.089	0.967	0.951	1.536	1.549	1.181	1.066												
BaO	1.501	1.126	1.709	2.694	2.389	1.991	1.521	1.269	1.087	1.077	0.885	0.804												
HfO2	2.971	2.596	3.117	1.518	1.172	1.038	1.863	1.491	1.329	1.482	1.095	0.973												
ThO2	3.323	0.410	3.549	2.315	1.657	1.361	1.150	1.035	0.936	0.966	0.842	1.023												

Emitting																								
Line:	Ti	K	V	K	Cr	K	Mn	K	Fe	K	Ni	K	Zn	K	Sr	L	Zr	L	Ba	L	Hf	L	Th	M
O	1.114	1.149	1.142	1.184	1.175	1.177	1.240	1.169	1.129	1.340	1.548	1.255												
CO2	1.119	1.155	1.149	1.191	1.183	1.186	1.250	1.139	1.110	1.346	1.560	1.253												
F	1.050	1.080	1.072	1.110	1.101	1.102	1.160	1.208	1.135	1.262	1.447	1.204												
Na2O	1.070	1.098	1.088	1.124	1.113	1.112	1.169	1.389	1.263	1.287	1.459	1.258												
MgO	1.098	1.126	1.115	1.152	1.140	1.138	1.196	1.462	1.320	1.320	1.494	1.298												
Al2O3	1.089	1.115	1.103	1.139	1.127	1.124	1.181	1.518	1.354	1.309	1.475	1.299												
SiO2	1.110	1.137	1.123	1.160	1.147	1.144	1.201	1.069	1.410	1.335	1.500	1.333												
P2O5	1.101	1.126	1.112	1.147	1.134	1.129	1.185	0.917	1.049	1.324	1.481	1.339												
SO3	1.118	1.142	1.127	1.162	1.148	1.143	1.199	0.970	0.896	1.345	1.499	1.369												
Cl	1.095	1.098	1.067	1.088	1.065	1.046	1.087	0.774	0.654	1.317	1.363	1.566												
K2O	1.135	1.134	1.100	1.119	1.094	1.073	1.114	0.981	0.886	1.366	1.397	1.145												
CaO	1.164	1.164	1.130	1.151	1.126	1.105	1.147	1.069	0.984	1.401	1.439	0.730												
TiO2	1.000	1.028	1.098	1.115	1.089	1.066	1.106	1.131	1.050	1.202	1.387	0.901												
V2O3	0.975	1.000	0.989	1.100	1.070	1.041	1.074	1.164	1.071	1.171	1.350	0.910												
Cr2O3	0.815	1.011	1.000	1.032	1.087	1.054	1.086	1.222	1.119	0.747	1.365	0.966												
MnO	0.834	0.789	0.971	1.000	0.987	1.028	1.053	1.287	1.167	0.732	1.327	1.003												
FeO	0.885	0.853	0.776	1.014	1.000	1.045	1.067	1.358	1.220	0.803	1.346	1.071												
NiO	0.952	0.943	0.890	0.858	0.775	1.000	1.082	1.510	1.326	0.991	1.302	1.224												
ZnO	0.955	0.959	0.924	0.922	0.870	0.738	1.000	1.667	1.422	1.081	1.251	1.230												
SrO	0.969	0.966	0.935	0.948	0.923	0.897	0.922	1.000	1.902	1.164	1.157	1.414												
ZrO2	1.006	1.003	0.971	0.986	0.961	0.936	0.964	0.930	1.000	1.209	1.209	1.467												
BaO	0.834	0.839	0.902	0.937	0.908	0.843	0.837	1.546	1.299	1.000	1.063	0.964												
HfO2	0.888	0.870	0.826	0.818	0.773	0.786	0.794	1.887	1.543	1.029	1.000	1.383												
ThO2	0.929	0.931	0.893	0.872	0.823	0.760	0.749	1.207	1.084	1.115	0.951	1.000												

analyzed. Series of replicate analyses of each of the standards were performed under conditions described by Armstrong.¹¹ Results of the analyses are given in Fig. 3, which shows the percentage relative errors for the standards obtained from the new polynomial α -factors--or from the Armstrong/Love-Scott $\phi(\rho z)$ correction; both give the same results--against those obtained from the Albee and Ray⁴ α -factors. As can be seen, systematic errors produced by the

older α -factors are eliminated with the new polynomial expressions. Table 5 compares the best-fit α -factors determined by a multiple linear regression of the analytical data with those calculated from the new polynomial correction. The two sets of factors are very similar, which shows that the Armstrong/Love-Scott correction comes close to a best-fit correction for the data.

Conclusions

The conventional Bence-Albee α -factor correction produces significant deviations from the correction procedures on which it is based. Substitution of the composition-independent α -factor with a simple second-order polynomial function of concentration results in the procedure producing identical results to the ZAF, $\phi(\rho z)$, or Monte Carlo correction on which it is based. This new modified Bence-Albee expression results in significantly improved accuracy in the correction of silicate and oxide analyses, and is essentially as fast and straightforward a procedure as the initial Bence-Albee correction.

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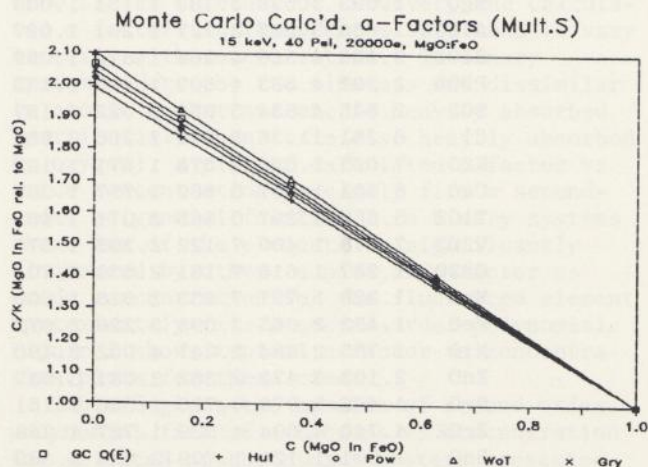


FIG. 1.--Plot of C/K vs C for Mg K α in MgO:FeO, calculated from Monte Carlo multiple-scattering calculations from various ionization cross section expressions.

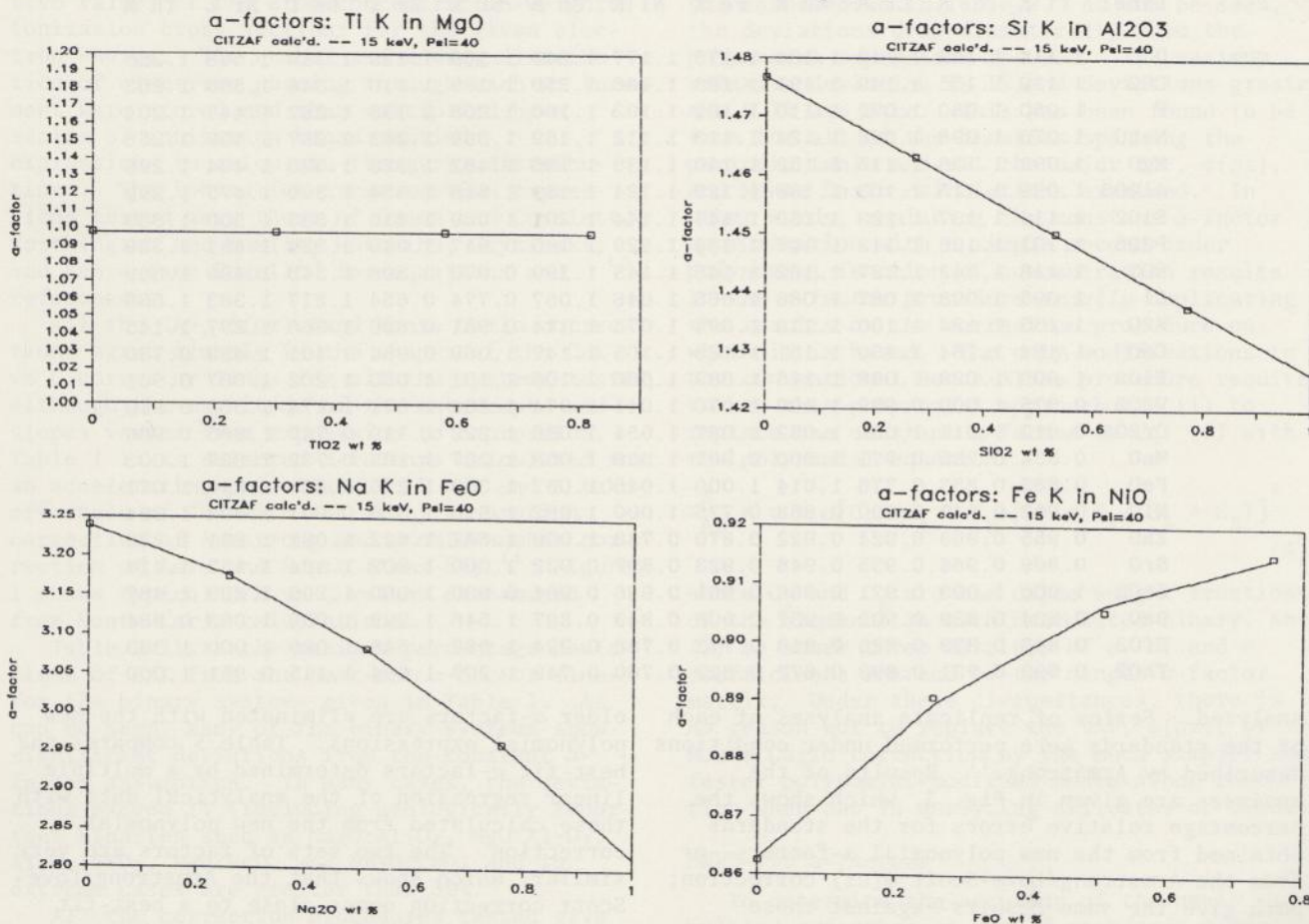


FIG. 2.--Plots of calculated α -factor vs concentration, in oxide weight fraction, for (a) Ti K α in TiO₂:MgO, (b) Si K α in SiO₂:Al₂O₃, (c) Na K α in Na₂O:FeO, (d) Fe K α in FeO:NiO.

TABLE 2.--Maximum % deviations from linear fit of C/K vs C for α -factors in Table 1.

Emitting																								
Line:	O	K	C	K	F	K	Na	K	Mg	K	Al	K	Si	K	P	K	S	K	Cl	K	K	K	Ca	K
O	0.0	0.0	36.2	2.7	0.7	0.2	0.1	0.1	0.0	0.0	0.1	0.1	0.1	0.1	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
CO2	3.5	0.0	27.6	1.6	0.4	0.1	0.1	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
F	0.9	1.5	0.0	4.9	1.5	0.5	0.3	0.1	0.1	0.1	0.3	0.1	0.1	0.1	0.3	0.2	0.1	0.3	0.2	0.1	0.2	0.1	0.1	0.1
Na2O	0.8	6.8	4.3	0.0	3.9	1.6	0.6	0.3	0.1	0.3	0.1	0.3	0.1	0.3	0.1	0.3	0.2	0.3	0.1	0.2	0.1	0.1	0.1	0.1
MgO	1.5	8.2	10.0	0.3	0.0	2.0	0.8	0.4	0.2	0.3	0.4	0.2	0.3	0.1	0.2	0.3	0.2	0.3	0.1	0.2	0.1	0.1	0.1	0.1
Al2O3	2.4	9.8	14.3	0.1	0.4	0.0	1.1	0.5	0.2	0.4	0.2	0.3	0.1	0.5	0.2	0.3	0.2	0.4	0.2	0.1	0.1	0.1	0.1	0.1
SiO2	3.5	11.0	18.0	0.4	0.2	0.5	0.0	0.6	0.3	0.4	0.2	0.3	0.1	0.6	0.3	0.4	0.2	0.4	0.2	0.1	0.1	0.1	0.1	0.1
P2O5	4.6	11.8	20.7	0.6	0.0	0.3	0.5	0.0	0.4	0.6	0.3	0.4	0.0	0.4	0.6	0.2	0.6	0.2	0.1	0.1	0.1	0.1	0.1	0.1
S03	6.0	12.5	23.3	0.9	0.1	0.1	0.3	0.7	0.0	0.6	0.3	0.7	0.0	0.6	0.6	0.2	0.6	0.2	0.1	0.1	0.1	0.1	0.1	0.1
Cl	25.2	20.3	10.2	0.2	0.2	0.3	0.6	1.3	2.4	0.0	0.4	0.1	0.1	2.4	0.0	0.4	0.1	0.4	0.1	0.1	0.1	0.1	0.1	0.1
K2O	30.3	0.5	18.8	0.5	0.1	0.1	0.1	0.3	0.6	2.6	0.1	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1	0.1
CaO	30.6	0.4	24.6	1.1	0.1	0.0	0.1	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1	0.1
TiO2	26.2	0.2	32.2	2.7	0.7	0.2	0.0	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1
V2O3	33.8	0.3	33.8	3.6	1.0	0.2	0.0	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1
Cr2O3	0.2	0.1	32.8	4.4	1.3	0.3	0.0	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1
MnO	0.4	0.2	33.8	5.9	1.8	0.5	0.1	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1
FeO	0.3	0.5	1.7	7.0	2.3	0.7	0.2	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1	0.1
NiO	0.4	1.5	2.0	9.9	3.8	1.4	0.4	0.1	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1
ZnO	1.4	3.1	2.6	5.7	6.3	2.6	0.9	0.3	0.0	0.1	0.3	0.6	2.6	0.1	0.1	0.3	0.6	2.6	0.0	0.4	0.1	0.1	0.1	0.1
SrO	10.7	4.8	8.0	0.1	0.2	0.2	0.1	1.6	0.9	1.1	0.2	0.0	0.0	1.1	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ZrO2	13.2	4.2	13.1	0.7	0.0	0.1	0.1	0.1	0.8	1.2	0.2	0.0	0.0	1.2	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
BaO	1.7	2.4	0.5	2.5	2.4	1.8	0.8	0.6	0.4	0.4	0.2	0.0	0.0	0.4	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HfO2	2.1	5.3	3.2	0.1	0.1	0.3	1.6	0.9	0.6	1.3	0.3	0.1	0.1	0.6	1.3	0.3	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1
ThO2	4.2	2.8	3.5	1.1	0.5	0.8	0.7	0.8	0.7	0.6	0.4	0.1	0.1	0.6	1.3	0.3	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1

Emitting																								
Line:	Ti	K	V	K	Cr	K	Mn	K	Fe	K	Ni	K	Zn	K	Sr	L	Zr	L	Ba	L	Hf	L	Th	M
O	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.3	0.2	0.6	0.5	1.0	0.6	0.5	0.9	0.5	0.5	0.9	0.9
CO2	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.2	0.2	0.8	0.6	1.5	0.6	0.5	1.5	0.6	0.5	1.5	1.5
F	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.1	0.8	0.6	1.5	0.6	0.5	1.5	0.6	0.5	1.5	1.5	1.5
Na2O	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.1	0.1	1.3	0.8	1.3	0.8	0.7	0.5	1.3	0.7	0.5	1.3	1.3
MgO	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	1.3	0.8	1.3	0.8	0.7	0.5	1.3	0.7	0.5	1.3	1.3
Al2O3	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	1.6	1.0	1.6	1.0	0.6	0.4	1.3	0.6	0.4	1.3	1.3
SiO2	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	1.0	0.6	1.0	0.6	0.4	1.2	0.6	0.4	1.2	1.2	1.2
P2O5	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	4.1	0.1	4.1	0.1	0.6	0.4	1.4	0.6	0.4	1.4	1.4
S03	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	3.4	4.5	3.4	4.5	0.6	0.4	1.3	0.6	0.4	1.3	1.3
Cl	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	5.3	7.8	5.3	7.8	0.6	0.3	2.0	0.6	0.3	2.0	2.0
K2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.9	3.0	1.9	3.0	0.6	0.3	0.5	0.6	0.3	0.5	0.5
CaO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	1.1	1.9	1.1	1.9	0.6	0.2	11.2	0.6	0.2	11.2	11.2
TiO2	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.5	0.3	0.5	0.3	0.3	6.5	0.3	0.3	6.5	6.5	
V2O3	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.1	0.2	0.2	0.2	0.2	0.3	0.4	5.5	0.3	0.4	5.5	5.5
Cr2O3	3.0	0.0	0.0	0.0	0.1	0.1	0.1	0.0	0.2	0.1	0.1	0.0	0.2	0.1	9.9	0.3	4.7	9.9	0.3	4.7	9.9	0.3	4.7	4.7
MnO	1.7	3.4	0.0	0.0	0.0	0.0	0.0	0.0	0.5	0.2	0.1	0.0	0.5	0.2	9.6	0.3	2.9	9.6	0.3	2.9	9.6	0.3	2.9	2.9
FeO	1.0	2.3	3.6	0.0	0.0	0.0	0.0	0.0	0.6	0.2	0.1	0.0	0.6	0.2	8.8	0.3	1.9	8.8	0.3	1.9	8.8	0.3	1.9	1.9
NiO	0.3	0.8	1.5	3.1	4.6	0.0	0.0	0.0	0.9	0.4	0.1	0.0	0.9	0.4	4.7	0.0	0.4	4.7	0.0	0.4	4.7	0.0	0.4	0.4
ZnO	0.0	0.1	0.4	1.0	1.7	4.2	0.0	0.0	1.6	0.7	0.1	0.0	1.6	0.7	1.7	0.1	0.5	1.7	0.1	0.5	1.7	0.1	0.5	0.5
SrO	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.9	2.5	0.0	0.9	0.9	0.0	0.0	0.9	0.9
ZrO2	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	2.5	0.0	0.9	2.5	0.0	0.9	0.9	0.0	0.0	0.9	0.9
BaO	0.3	0.3	0.1	0.1	0.0	0.1	0.0	0.1	1.1	0.5	0.1	0.0	1.1	0.5	0.0	0.0	1.5	1.1	0.5	1.5	0.0	0.0	1.5	1.5
HfO2	0.4	0.4	0.4	0.4	0.3	0.0	0.1	2.4	1.2	0.2	0.0	0.1	2.4	1.2	0.2	0.0	1.5	1.2	0.2	1.5	0.0	0.0	1.5	1.5
ThO2	0.3	0.3	0.2	0.1	0.0	0.0	0.0	0.5	0.4	0.1	0.0	0.0	0.5	0.4	0.1	0.0	1.5	0.4	0.1	1.5	0.0	0.0	1.5	1.5

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TABLE 3.--Calculated oxide polynomial α -factor expressions from Love-Scott correction; for each oxide, line 1 contains c factors, line 2, d factors; line 3, e factors.

		EO = 15 KEV, PSI = 40 DEGREES											
Emitting													
Line:	Na K	Mg K	Al K	Si K	K K	Ca K	Ti K	V K	Cr K	Mn K	Fe K	Ni K	
Na2O	1.000	2.047	1.593	1.327	1.086	1.042	1.070	1.099	1.088	1.125	1.114	1.112	
	0.000	-0.169	-0.069	-0.030	-0.007	-0.006	-0.002	-0.003	-0.004	-0.005	-0.005	-0.006	
	0.000	-0.016	-0.003	0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.000	-0.001	-0.001	
MgO	1.153	1.000	1.727	1.417	1.120	1.073	1.098	1.126	1.115	1.152	1.141	1.139	
	0.025	0.000	-0.086	-0.037	-0.007	-0.005	0.000	-0.002	-0.003	-0.004	-0.005	-0.006	
	-0.017	0.000	-0.007	-0.001	0.000	-0.000	0.000	0.000	0.000	0.000	-0.000	-0.001	
Al2O3	1.261	1.025	1.000	1.477	1.118	1.068	1.089	1.116	1.103	1.139	1.128	1.125	
	0.001	0.026	0.000	-0.050	-0.008	-0.006	-0.002	-0.003	-0.003	-0.004	-0.005	-0.006	
	-0.008	-0.015	0.000	-0.001	0.000	-0.000	0.000	0.000	-0.000	-0.000	-0.000	-0.001	
SiO2	1.373	1.098	1.014	1.000	1.145	1.092	1.110	1.137	1.124	1.160	1.147	1.144	
	-0.014	0.012	0.032	0.000	-0.008	-0.006	0.000	0.000	-0.003	-0.003	-0.004	-0.005	
	-0.005	-0.007	-0.017	0.000	0.000	0.000	0.000	0.000	0.000	0.000	-0.000	-0.001	
K2O	1.572	1.199	1.073	0.988	1.000	1.204	1.135	1.134	1.100	1.119	1.095	1.073	
	-0.017	0.004	0.005	0.008	0.000	-0.010	0.000	0.000	0.000	0.000	-0.002	-0.002	
	-0.013	-0.002	-0.001	-0.002	0.000	-0.000	0.000	0.000	0.000	0.000	0.000	0.000	
CaO	1.760	1.309	1.153	1.050	0.841	1.000	1.164	1.165	1.130	1.151	1.126	1.105	
	-0.041	-0.004	0.000	0.004	0.334	0.000	-0.002	-0.002	0.000	0.000	-0.002	-0.002	
	-0.019	-0.003	0.000	-0.001	-0.238	0.000	-0.000	-0.000	0.000	0.000	0.000	0.000	
TiO2	2.078	1.465	1.235	1.093	0.925	0.847	1.000	1.028	1.098	1.115	1.089	1.066	
	-0.108	-0.027	-0.006	0.000	0.119	0.184	0.000	0.000	-0.003	-0.004	-0.004	-0.004	
	-0.040	-0.007	-0.002	0.000	-0.083	-0.126	0.000	0.000	0.000	0.000	0.000	-0.000	
V2O3	2.303	1.577	1.294	1.122	0.929	0.858	0.975	1.000	0.989	1.101	1.070	1.041	
	-0.129	-0.035	-0.008	0.000	0.068	0.110	0.000	0.000	0.000	-0.004	-0.003	-0.003	
	-0.069	-0.014	-0.004	0.000	-0.043	-0.068	0.000	0.000	0.000	0.000	0.000	0.000	
Cr2O3	2.540	1.707	1.377	1.177	0.962	0.898	0.803	1.011	1.000	1.032	1.087	1.054	
	-0.151	-0.046	-0.012	0.000	0.040	0.067	0.212	0.000	0.000	0.000	-0.003	-0.003	
	-0.099	-0.021	-0.005	0.000	-0.024	-0.039	-0.123	0.000	0.000	0.000	0.000	0.000	
MnO	2.924	1.904	1.485	1.235	0.960	0.899	0.828	0.774	0.971	1.000	0.987	1.028	
	-0.168	-0.057	-0.016	-0.000	0.020	0.034	0.118	0.244	0.000	0.000	0.000	-0.002	
	-0.178	-0.043	-0.012	-0.004	-0.011	-0.017	-0.062	-0.143	0.000	0.000	0.000	0.000	
FeO	3.239	2.076	1.593	1.305	0.990	0.931	0.881	0.843	0.761	1.014	1.000	1.045	
	-0.184	-0.069	-0.023	-0.004	0.010	0.018	0.071	0.163	0.258	0.000	0.000	0.000	
	-0.238	-0.059	-0.016	-0.004	-0.006	-0.009	-0.036	-0.091	-0.150	0.000	0.000	0.000	
NiO	4.016	2.497	1.848	1.465	1.034	0.975	0.951	0.939	0.884	0.845	0.755	1.000	
	-0.212	-0.101	-0.043	-0.014	0.000	0.000	0.018	0.056	0.105	0.222	0.333	0.000	
	-0.423	-0.115	-0.032	-0.008	0.000	0.000	-0.009	-0.029	-0.056	-0.133	-0.205	0.000	

TABLE 4.--Maximum % deviations from polynomial fit of C/K vs C for α -factors in Table 3.

Emitting																							
Line:	O	K	C	K	F	K	Na	K	Mg	K	Al	K	Si	K	P	K	S	K	Cl	K	K	Ca	K
O	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
F	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Na2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MgO	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SiO2	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
P2O5	0.0	0.2	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO3	0.0	0.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cl	0.4	2.3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
K2O	0.6	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0
CaO	0.5	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.4	0.0	0.0	0.0	0.0
TiO2	0.3	0.0	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1
V2O3	0.6	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.1	0.1	0.1
Cr2O3	0.0	0.0	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MnO	0.0	0.0	0.7	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
FeO	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
NiO	0.0	0.0	0.0	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ZnO	0.0	0.1	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SrO	0.0	0.7	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ZrO2	0.2	0.4	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
BaO	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
HfO2	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
ThO2	0.2	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

Emitting																								
Line:	Ti	K	V	K	Cr	K	Mn	K	Fe	K	Ni	K	Zn	K	Sr	L	Zr	L	Ba	L	Hf	L	Th	M
O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1
CO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
F	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1
Na2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
MgO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Al2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SiO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
P2O5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
SO3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.4	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Cl	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.4	0.5	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
K2O	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
CaO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	1.0
TiO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.7
V2O3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.6	0.6
Cr2O3	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.5	0.5	
MnO	0.1	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.3	0.3	
FeO	0.0	0.1	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.7	0.0	0.0	0.0	0.2	0.2	
NiO	0.0	0.0	0.1	0.2	0.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.3	0.0	0.0	0.0	0.0	0.0	
ZnO	0.0	0.0	0.0	0.0	0.1	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	
SrO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
ZrO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
BaO	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
HfO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	
ThO2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	