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AUSTRALIAN ATOMIC ENERGY COMMISSION

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LUCAS HEIGHTS

TABLES OF CORRECTION FACTORS FOR USE IN THE PEAK/BACKGROUND RATIO METHOD OF X-RAY SPECTROCHEMICAL ANALYSIS

by

K.P. CHAMPION
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ABSTRACT

The tables provide factors for the K_α lines of elements Z23 to Z42.

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CONTENTS

1. INTRODUCTION

It has been shown (Champion et al. 1966) that under certain conditions the concentration C, of an element i in a sample x, can be related to a standard s, by the relationship

$$C_x = C_s \cdot \frac{(P/B)_x}{(P/B)_s} \cdot S \qquad \ldots(1)$$

where C_x = concentration of element in sample
C_s = concentration of element in standard
$(P/B)_x$ = peak to background ratio of sample
$(P/B)_s$ = peak to background ratio of standard
S = the ratio of sample scattering factor to the water scattering factor

thus $S = (K_s)_i / (K_s)_{H_2O}$. $\qquad \ldots(2)$

The value S has been tabulated in this report to assist in the ready application of this method.

The scattering factor functions were calculated from the relation (2) and

$$(K_s)_i = \left[F_i^2 + r\,(Z_i - f_i^2) \right] / A_i \qquad \ldots(3)$$

where K_s = scattering factor
F = atomic scattering power
f^2 = incoherent scattering power
Z = atomic number
r = recoil factor
A = atomic weight .

Values for F and f^2 were obtained from Lonsdale (1962) for a scattering angle of 98° which is about the geometry of a Philips (Eindhoven) Type PW1540 X-ray spectrometer.

2. FORM OF TABLES

The tables are arranged according to the K_α lines of the element to be determined over the range of general applicability of the peak/background method. The matrix elements are the first twenty-six elements of the periodic table.

Although the factors are quoted to three decimal places such accuracy is not implied but is included to allow for computer round off.

The values obtained from Lonsdale (1962), were for seven specific wave-lengths.

The intermediate values used in equation (3) were obtained by simple linear interpolation of these values.

For a matrix m of n components

$$S_m = \sum_{i=1}^{n} \left[C_i \cdot S_i \right] \quad . \qquad \ldots(4)$$

The appendix gives an example of the calculation for a specific sample using equation (4) and the table of factors.

The factors have been calculated relative to water because of the ease in preparing aqueous standard solutions.

To obtain factors relative to a standard other than water, let

S_m = scattering factor of sample relative to water
S_s = scattering factor of standard relative to water .

Then the scattering factor of the sample (S_R) relative to the new standard is

$$S_R = S_m/S_s \quad . \qquad \ldots(5)$$

3. REFERENCES

Champion, K.P., Taylor, J.C. and Whittem, R.N. (1966). - Anal. Chem., 38, 109.

Champion, K.P. and Whittem, R.N. (1968). - Analyst, 92, 124.

David, D.J. (1969). - Analyst, 94, 884.

Lonsdale, K. (1962). - ed., "International Tables for X-ray Crystallography" Vol. III, Chap. 3, Kynock, Birmingham.

APPENDIX

Calculation of the scattering factor for oyster flesh ash at Zn K_α line. $\lambda = 1.437$.

Element	a Weight Fraction	b S. Factor	a x b
Na	0.10	1.458	0.15
Si	0.02	2.241	0.04
Cl	0.15	2.439	0.37
Ca	0.12	2.710	0.33
K	0.08	2.550	0.20
Al	0.15	1.971	0.30
P	0.05	2.319	0.12
O	0.33	0.956	0.32
	1.00		S=1.83

Results obtained for organic matrices are given by Champion and Whittem (1968) and have been confirmed by David (1969).

SCATTERING FACTORS RELATIVE TO WATER

ELEMENT VERSUS WAVELENGTH IN ANGSTROMS

ELEMENT	V	CR	MN	FE	CO	NI	CU
	2.505	2.291	2.103	1.937	1.791	1.659	1.542
H	0.761	0.843	0.932	1.029	1.116	1.201	1.288
HE	0.498	0.530	0.566	0.604	0.637	0.667	0.698
LI	0.462	0.500	0.540	0.585	0.618	0.647	0.676
BE	0.467	0.510	0.556	0.607	0.648	0.685	0.723
B	0.521	0.555	0.593	0.634	0.672	0.710	0.748
C	0.636	0.658	0.682	0.708	0.739	0.773	0.808
N	0.813	0.817	0.822	0.827	0.837	0.850	0.863
O	1.030	1.020	1.009	0.996	0.985	0.975	0.964
F	1.229	1.117	0.994	0.860	0.821	0.831	0.841
NE	1.607	1.575	1.541	1.503	1.449	1.386	1.321
NA	1.773	1.763	1.753	1.741	1.690	1.616	1.541
MG	1.956	1.982	2.009	2.039	2.004	1.933	1.860
AL	1.964	2.019	2.080	2.145	2.142	2.102	2.060
SI	2.055	2.133	2.216	2.308	2.333	2.323	2.314
P	2.030	2.108	2.193	2.286	2.329	2.346	2.364
S	2.143	2.216	2.296	2.382	2.440	2.483	2.527
CL	2.130	2.181	2.237	2.297	2.347	2.392	2.439
AR	2.191	2.218	2.247	2.279	2.300	2.315	2.331
K	2.574	2.584	2.596	2.608	2.604	2.592	2.580
CA	2.848	2.855	2.862	2.870	2.847	2.806	2.765
SC	2.827	2.821	2.814	2.807	2.769	2.715	2.658
TI	2.998	2.996	2.994	2.992	2.942	2.866	2.787
V	3.170	3.165	3.160	3.154	3.092	2.997	2.901
CR	3.538	3.515	3.491	3.465	3.376	3.252	3.126
MN	3.716	3.708	3.699	3.689	3.598	3.462	3.323
FE	4.078	4.074	4.069	4.063	3.960	3.802	3.641

SCATTERING FACTORS RELATIVE TO WATER

ELEMENT VERSUS WAVELENGTH IN ANGSTROMS

ELEMENT	ZN 1.437	GA 1.341	GE 1.256	AS 1.177	SE 1.106	BR 1.041	KR 0.981
H	1.353	1.408	1.461	1.494	1.526	1.549	1.565
HE	0.723	0.745	0.766	0.777	0.787	0.795	0.800
LI	0.694	0.706	0.718	0.722	0.726	0.727	0.726
BE	0.749	0.769	0.788	0.791	0.795	0.794	0.789
B	0.778	0.802	0.826	0.836	0.845	0.847	0.846
C	0.836	0.860	0.883	0.897	0.910	0.918	0.921
N	0.875	0.886	0.897	0.904	0.911	0.916	0.919
O	0.956	0.949	0.942	0.938	0.934	0.931	0.929
F	0.847	0.852	0.856	0.856	0.857	0.861	0.868
NE	1.260	1.200	1.143	1.099	1.056	1.025	1.002
NA	1.458	1.370	1.286	1.215	1.147	1.095	1.053
MG	1.764	1.658	1.556	1.450	1.351	1.269	1.201
AL	1.971	1.861	1.754	1.632	1.515	1.415	1.327
SI	2.241	2.141	2.043	1.908	1.781	1.661	1.548
P	2.319	2.246	2.174	2.048	1.928	1.804	1.678
S	2.507	2.460	2.413	2.296	2.186	2.058	1.919
CL	2.439	2.418	2.396	2.303	2.216	2.102	1.972
AR	2.318	2.292	2.265	2.193	2.124	2.032	1.927
K	2.550	2.513	2.475	2.407	2.343	2.256	2.155
CA	2.710	2.649	2.590	2.516	2.445	2.360	2.267
SC	2.594	2.527	2.461	2.388	2.319	2.243	2.162
TI	2.694	2.594	2.498	2.408	2.323	2.241	2.164
V	2.785	2.662	2.544	2.437	2.336	2.246	2.165
CR	2.986	2.841	2.701	2.571	2.448	2.343	2.253
MN	3.158	2.983	2.814	2.658	2.510	2.387	2.284
FE	3.444	3.233	3.030	2.842	2.665	2.518	2.394

SCATTERING FACTORS RELATIVE TO WATER

ELEMENT VERSUS WAVELENGTH IN ANGSTROMS

	RB	SR	Y	ZR	NB	MO
	0.927	0.877	0.831	0.788	0.748	0.710
ELEMENT						
H	1.580	1.595	1.607	1.614	1.621	1.627
HE	0.806	0.811	0.815	0.817	0.819	0.821
LI	0.726	0.725	0.724	0.724	0.723	0.722
BE	0.785	0.782	0.778	0.773	0.769	0.765
B	0.844	0.843	0.840	0.835	0.829	0.824
C	0.923	0.926	0.927	0.923	0.918	0.914
N	0.921	0.924	0.926	0.924	0.922	0.920
O	0.927	0.926	0.924	0.923	0.922	0.922
F	0.874	0.880	0.884	0.881	0.878	0.875
NE	0.980	0.960	0.943	0.935	0.927	0.920
NA	1.015	0.978	0.947	0.931	0.915	0.901
MG	1.139	1.079	1.028	1.003	0.979	0.956
AL	1.246	1.168	1.100	1.059	1.020	0.983
SI	1.442	1.342	1.253	1.193	1.137	1.082
P	1.562	1.451	1.351	1.274	1.201	1.131
S	1.790	1.667	1.553	1.454	1.359	1.268
CL	1.852	1.737	1.630	1.537	1.448	1.363
AR	1.828	1.735	1.645	1.555	1.470	1.387
K	2.061	1.972	1.885	1.789	1.699	1.611
CA	2.180	2.098	2.015	1.911	1.812	1.717
SC	2.087	2.016	1.943	1.853	1.766	1.683
TI	2.091	2.023	1.954	1.873	1.795	1.720
V	2.090	2.018	1.948	1.874	1.803	1.735
CR	2.170	2.090	2.015	1.943	1.875	1.808
MN	2.188	2.096	2.012	1.942	1.875	1.811
FE	2.278	2.168	2.069	1.995	1.925	1.858