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MCP Code Fluorescence-Routine Revision

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E. D. Cashwell

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MCP CODE FLUORESCENCE-ROUTINE REVISION

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ABSTRACT

A new method is described for treating fluorescence, which replaces the original subroutine of the Monte Carlo photon code (MCP), and eliminates its most undesirable features. The major changes include (a) elimination of the very inaccurate $1/E^3$ law for photoelectric cross section, (b) updating of relative intensities of K-fluorescence lines, (c) elimination of fluorescence from shells other than K and L, and (d) provision for secondary L-fluorescence. Except for the latter, the previous code is unchanged, as well as the storage format. However, the change in method is reflected in the new constants, which have been completely revised, and are included here in tabulated form.

I. INTRODUCTION

The revision of the original fluorescence treatment in the MCP code,[1] described below, is designed to eliminate its most unsatisfactory features, by a method involving only a slight addition to the previous routine, but an almost total replacement of the constants in "Z-section F" of the supporting library tape. The appended tables, now complete for all elements $12 \leq Z \leq 94$, are identical in format with the existing data of that section, except for some reductions in the length f for $Z \geq 70$. These reductions are due to the elimination of fluorescence from shells other than K and L. The probability of ejection from other shells, as well as the corresponding yields and fluorescent energies, are all comparatively small, and are greatest for high Z, where the p.e. cross section is enormous at the fluorescent energies. We therefore assume local absorption for such fluorescence.

Given a photoelectric event, the purpose of the present fluorescence subroutine is therefore to determine from which of the two shells, K or L, an electron is ejected (if either), and the fluorescent photon energy emitted (if any).

In Fig. 1, we give for easy reference an overview of the data to be discussed, and upon which Table I is based.

II. EDGE ENERGIES e

The single K-edge energy E_K is taken from Table II of Ref. 2, being identical with that of Ref. 3, which was used before. The L-edge energy (for $Z \geq 31$) is regarded as the simple average

$$\bar{E}_L = (E_{L1} + E_{L2} + E_{L3})/3$$

the individual E_{Li} being those in Table II of Ref. 2. The energies E_K, $\bar{E}_L$, compared with the incident photon energy E, serve to determine the possibility of K or L ejections. The L-shell is treated as a unit with respect to primary L-fluorescence.

III. FLUORESCENT ENERGIES F

Upon ejection of an electron from a shell of energy E_S by an incident photon ($E \geq E_S$) the vacancy created is filled by an electron transition from an "outer" shell of energy $E_T < E_S$. The photon, of energy $F = E_S - E_T$, created in the transition, may or may not escape the atom. In the former case, it is referred to as (primary) S-fluorescence.

Z	e	ϕ	Y	F	f
12-19	E_K	$\phi_o = \rho_K$	$Y_o = 0$	0	2
	E_K	$\phi_K = 1 - \rho_K$	Y_K	F_K	
20-30	E_K	$\phi_o = \rho_K$	$Y_o = 0$	0	4
	E_K		$Y_K p_1$	$FK\alpha_1$	
	E_K		$Y_K p_2$	$FK\alpha_2$	
	E_K	$\phi_K = 1 - \rho_K$	$Y_K p_3$	$FK\beta_1'$	
31-36	$\bar{E}_L$	$\phi_o = \rho_L$	$Y_o = 0$	0	5
	$\bar{E}_L$	$\phi_L = 1 - \rho_L$	Y_L	F_L	
	E_K		$Y_K p_1$	$FK\alpha_1$	
	E_K		$Y_K p_2$	$FK\alpha_2$	
	E_K	$\phi_K = \frac{1}{\rho_K} - 1$	$Y_K p_3$	$FK\beta_1'$	
37-94	$\bar{E}_L$	$\phi_o = \rho_L$	$Y_o = 0$	0	6
	$\bar{E}_L$	$\phi_L = 1 - \rho_L$	Y_L	F_L	
	E_K		$Y_K p_1$	$FK\alpha_1$	
	E_K		$Y_K p_2$	$FK\alpha_2$	
	E_K		$Y_K p_3$	$FK\beta_1'$	
	E_K	$\phi_K = \frac{1}{\rho_K} - 1$	$Y_K p_4$	$FK\beta_2'$	

Fig. 1. Overview of the data.

L-fluorescence is allowed only for $Z \geq 31$, and the single fluorescent energy F_L is taken as the $\bar{L}123$ in Table V of Ref. 2. This is an average of all energy gaps from edges Mj, Nk, ... to all Li edges, weighted by their relative intensities, as given in Tables IV and VI of Ref. 2.

The single value F_K given for $12 \leq Z \leq 19$ is the weighted average of the $K\alpha_1$, $K\alpha_2$ lines, given as $\bar{K}\alpha$ in Table V of Ref. 2.

For $20 \leq Z \leq 94$, the individual fluorescent energies $FK\alpha_1 > FK\alpha_2$ are taken from Table III of Ref. 2. These are pure lines resulting from the transitions L3 → K, L2 → K, respectively. For $20 \leq Z \leq 94$, the fluorescent energy $FK\beta_1'$ (M2 → K, M3 → K, M4 → K, composite) is also allowed and is taken as the weighted average of the three energy differences, computed from Tables III, VI of Ref. 2.

For $37 \leq Z \leq 94$, the tabulated energy $FK\beta_2'$ (N2 → K, N3 → K) is the corresponding weighted average of these two lines, obtained in the same way.

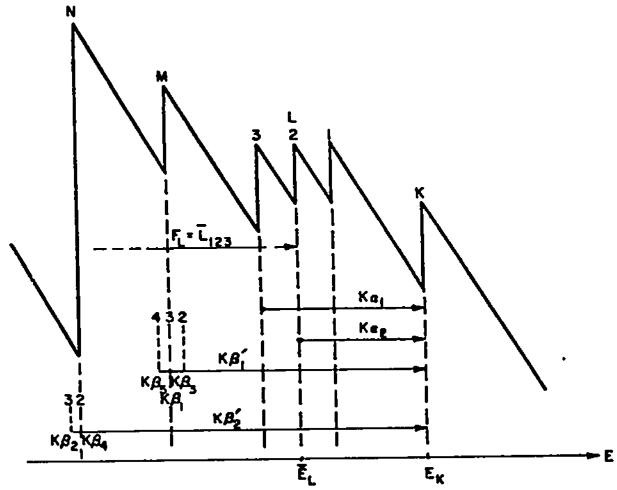

Fig. 2. Fluorescent "Lines".

Note the order of tabulation in Fig. 1 and the relations

$$12 \leq Z \leq 19. \quad \bar{K}\alpha = \text{Av.}(K\alpha_1, K\alpha_2)$$

$$20 \leq Z \leq 30. \quad K\alpha_1,\ K\alpha_2,\ K\beta_1'$$

$$31 \leq Z \leq 36. \quad \bar{L}_{123}\ \text{Av.},\ K\alpha_1,\ K\alpha_2,\ K\beta_1'$$

$$37 \leq Z \leq 94. \quad \bar{L}_{123}\ \text{Av.},\ K\alpha_1,\ K\alpha_2,\ K\beta_1',\ K\beta_2'$$

$$F_L < FK\alpha_2 < FK\alpha_1 < FK\beta_1' < FK\beta_2'$$

The fluorescent "lines" provided for are indicated very schematically in Fig. 2.

IV. THE YIELDS Y

The yield Y_S for a shell S is the total probability of fluorescent emission accompanying electron transition from all outer shells to a vacancy in shell S, however created (Cf. Part VII).

The data for Y_L in Ref. 4 ($Z \geq 31$) are very spotty; and the values now used, from Table VIII of Ref. 3, seem not too bad a compromise between those of Ref. 4 and those of Ref. 5, which were used previously.

The total yield Y_K is that used before, furnished by Israel and Storm as an updated version of Table VIII of Ref. 3. For this, we have no published reference. (No yields are included in Ref. 2.) We note that the update is in general accord with Table II of Ref. 4 and for $Z > 60$ is identical with Ref. 3, but is higher for $Z \leq 60$.

As noted in Part III, K-fluorescence was assumed to consist of the three lines $K\alpha_1$, $K\alpha_2$, $K\beta_1'$ for $20 \leq Z \leq 36$ and for $Z > 36$ of the additional line $K\beta_2'$. These assumptions were made before, but the relative intensities of the lines were based on Ref. 6. We now use the intensities given in Table VI of Ref. 2, which were based on the calculations of Scofield and are considered to be nearer the truth. From these data, the probabilities p_1, p_2, p_3 $(20 \leq Z \leq 36)$ and $p_1, \ldots, p_4$ $(Z > 36)$ of the components of the yield Y_K were obtained, and thus the individual yields as indicated in Fig. 1.

V. RELATIVE PROBABILITIES ϕ OF K, L EJECTION

A. For $12 \leq Z \leq 30$

Only K-fluorescence is considered and can occur only for $E \geq E_K$. For such an incident E, it is assumed (cf. Ref. 2, p. 569) that the probability of a K-ejection has the constant value

$$\phi_K = (\sigma_K - \sigma_K')/\sigma_K = 1 - \rho_K$$

where $\rho_K = \sigma_K'/\sigma_K$ is the ratio of the p.e. cross section at bottom and top of the K-edge, as indicated in Fig. 3. Here and elsewhere, σ' and σ are taken from Table I of Ref. 2. Note that ϕ_K is the entry σ_K(photo)/σ(photo) given in Table VIII. Referring to Fig. 1, it is clear that $\phi_K Y_K$ is the probability of fluorescence F_K for $12 \leq Z \leq 19$, while, for example, $\phi_K Y_K p_1$ is the probability of $FK\alpha_1$ fluorescence if $20 \leq Z \leq 30$, assuming a p.e. went at $E \geq E_K$.

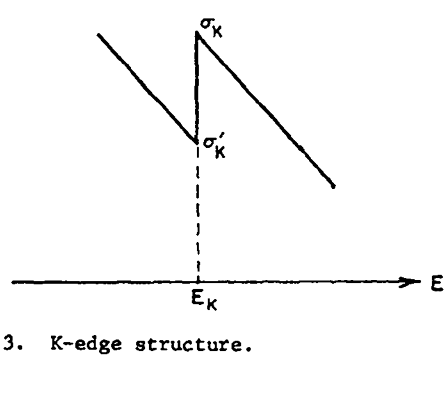

Fig. 3. K-edge structure.

B. For $31 \leq Z \leq 94$

Both L and K ejections are considered; and in order to follow the scheme of Ref. 5 used before, with no change in code, we require three numbers

$$\phi_K, \ \phi_L, \ \phi_0$$

which will determine the relative probabilities of K, L, and outer shell ejection for p.e. events at $E \geq E_K$, and such that ϕ_L, ϕ_0 also define the chances of L or outer shell ejection for $\bar{E}_L \leq E < E_K$.

Our basic assumption here is that the relative contribution of any edge to the total p.e. σ at that edge is $(\sigma - \sigma')/\sigma = 1 - \sigma'/\sigma$, and that this contribution remains constant up to the next edge of higher energy (if any). If we define $\rho_i = \sigma_i'/\sigma_i$, $i = 1,2,3$ (see Fig. 4), it is then easy to show that

$$\rho_L \equiv \rho_1\rho_2\rho_3 \qquad \text{and} \qquad 1 - \rho_L \tag{1}$$

are the probabilities of outer and L shell ejections at the L_I edge. (The latter appears in Column 2 of Table VIII of Ref. 2, with some minor discrepancies.)

Similarly, with $\rho_K \equiv \sigma_K'/\sigma_K$, one sees that $\rho_L\sigma_K'/\sigma_K = \rho_L\rho_K$, $(1 - \rho_L)\sigma_K'/\sigma_K = (1 - \rho_L)\rho_K$, $(\sigma_K - \sigma_K')/\sigma_K = 1 - \rho_K$ are the probabilities of outer, L, and K ejections at the K-edge. The proportional numbers

$$\phi_0 = \rho_L, \ \phi_L = 1 - \rho_L, \ \phi_K = \frac{1}{\rho_K} - 1 \tag{2}$$

also define these probabilities, when normed by their sum $1/\rho_K$, and moreover the first two are precisely

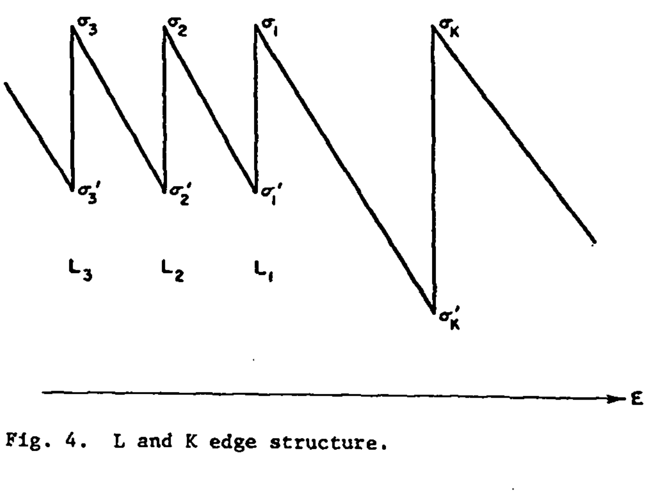

Fig. 4. L and K edge structure.

the probabilities in (1). The numbers (2) therefore satisfy our requirements and appear in the ϕ column of Fig. 1 for $Z \geq 31$.

The basic assumptions adopted above constitute a radical departure from the method of Ref. 5, used before. The latter involved essentially the same procedure, but supposed the minimal σ_t' value at an edge t given by $\sigma_t' = \sigma_{t+1}E_{t+1}^3/E_t^3$, where t + 1 is the next edge of lower energy. The underlying $1/E^3$ law is very inaccurate, and it seems that the present method is superior, insofar as the values of σ', σ are correct in Table I of Ref. 2.

VI. THE FINAL TABULATED ϕ AND Y

In order to facilitate computation, the values listed as ϕ and Y in the final appended tables were derived from the entries in Fig. 1 as indicated in Fig. 5. The tabulation for $37 \leq Z \leq 94$ is the exact analogue of that for $31 \leq Z \leq 36$, and is omitted.

Two examples, for $31 \leq Z \leq 36$, should make the method clear: (1) for a p.e. event at $E \geq E_K$, a random number between $Y_4/(\phi_o + \phi_L + \phi_K)$ and $Y_3/(\phi_o + \phi_L + \phi_K)$ implies a $FK\alpha_2$ fluorescence; (2) for $E_L \leq E < E_K$, a random number between $Y_2/(\phi_o + \phi_L)$ and $Y_1/(\phi_o + \phi_L)(= 0)$ implies an F_L fluorescence.

VII. SECONDARY L-FLUORESCENCE

The fluorescence thus far discussed is primary, in the sense that it arises from the transition of an electron from an outer shell to a shell in which a vacancy has been created by ejection of an electron from that shell by the initial incident photon. Thus, we have allowed for K-fluorescenct following a K-ejection, and for L-fluorescence following an L-ejection. Only such primary fluorescence was considered in the original code.

In this final section, we attempt to show roughly why secondary L-fluorescence may be of the same order of importance as primary L-fluorscence, and then describe how the present code provides for it, in a necessarily approximate fashion.

We stipulate a p.e. event on an element $Z \geq 31$, at an incident energy $E \geq E_K$. Then the probability of an L-ejection is ϕ_L/Σ, where $\Sigma = \phi_o + \phi_L + \phi_K$, and, as already stated, the overall probability of primary L-fluorescence is given by

$$P' = \frac{\phi_L}{\Sigma} \cdot Y_L \qquad (3)$$

On the other hand, there is a probability ϕ_K/Σ of a K-ejection. In this event, the K-vacancy may be filled by an $L3 \rightarrow K$ or $L2 \rightarrow K$ transition, say with probabilities P_{L3K}, P_{L2K}, thus creating a vacancy in

Z	e	ϕ	Y		F
12-19	E_K	$\phi_o = \rho_K$	$\phi_o Y_o$		0
	E_K	$\phi_o + \phi_K = 1$	$\phi_o Y_o + \phi_K Y_K$		F_K
20-30	E_K	$\phi_o = \rho_K$	$\phi_o Y_o$		0
	E_K		$\phi_o Y_o + \phi_K Y_K p_1$		$FK\alpha_1$
	E_K		$\phi_o Y_o + \phi_K Y_K p_1 + \phi_K Y_K p_2$		$FK\alpha_2$
	E_K	$\phi_o + \phi_K = 1$	$\phi_o Y_o + \phi_K Y_K p_1 + \phi_K Y_K p_2 + \phi_K Y_K p_3$		$FK\beta_1'$
31-36	$\bar{E}_L$	$\phi_o = \rho_L$	$\phi_o Y_o = 0$	$= Y_1$	0
	$\bar{E}_L$	$\phi_o + \phi_L = 1$	$\phi_o Y_o + \phi_L Y_L$	$= Y_2$	F_L
	E_K		$\phi_o Y_o + \phi_L Y_L + \phi_K Y_K p_1$	$= Y_3$	$FK\alpha_1$
	E_K		$\phi_o Y_o + \phi_L Y_L + \phi_K Y_K p_1 + \phi_K Y_K p_2$	$= Y_4$	$FK\alpha_2$
	E_K	$\phi_o + \phi_L + \phi_K = \frac{1}{\rho_K}$	$\phi_o Y_o + \phi_L Y_L + \phi_K Y_K p_1 + \phi_K Y_K p_2 + \phi_K Y_K p_3$	$= Y_5$	$FK\beta_1'$

Fig. 5. Final ϕ, Y tabulation.

the L3 or L2 subshell, and at the same time producing a photon $K\alpha_1$, or $K\alpha_2$. If we denote by Q_{L3K}, Q_{L2K} the chances of the latter photons escaping the atom (as fluorescence), then clearly, as part of the K-yield,

$$P_{L3K}Q_{L3K} + P_{L2K}Q_{L2K} = Y_K p_1 + Y_K p_2 \tag{4}$$

in our previous notation.

But, regarding the L3, L2 subshells as separate entities, we may expect (secondary) L3 or L2 fluorescence with yield probabilities Y_{L3}, Y_{L2}, due to the now existing vacancies created by $L \rightarrow K$ transition. Hence, the probability of this secondary L-fluorescence is given by

$$P'' = \frac{\phi_K}{\Sigma} \cdot (P_{L3K}Y_{L3} + P_{L2K}Y_{L2}). \tag{5}$$

Apparently none of the probabilities in parentheses are known. Making the assumption

$$Y_{L3} = Y_{L2} = Y_{L1} = Y_L/3 \tag{6}$$

(5) becomes

$$P'' = \frac{\phi_K}{\Sigma} (P_{L3K} + P_{L2K}) \; Y_L/3. \tag{7}$$

But from (7) and (4) we see that, for the secondary L-fluorescence,

$$P'' \geq \frac{\phi_K}{\Sigma} (Y_K p_1 + Y_K p_2) \; Y_L/3 \equiv P^* \tag{8}$$

and even P^* may exceed the primary probability P'.

For example, one finds from the appended tables (for Z = 79),

$$P' = \frac{.282}{4.859} = .058 < P^* = \frac{3.213-.282}{4.859} \cdot \frac{.282}{.759} \cdot \frac{1}{3}$$

$$\cong .075 \leq P''.$$

Thus, it would appear that secondary L-fluorescence should be included for the sake of consistency and accuracy.

Guided by the relation (8), we therefore make the following presumably inadequate provision in the revised code. In case of a p.e. event,on $Z \geq 31$ at $E \geq E_K$, which is followed by $K\alpha_1$ or $K\alpha_2$ fluorescence, we assume secondary L3 or L2 fluorescence emitted, each with probability $Y_L/3$, and take F_L as the fluorescent energy in either case.

We include in Fig. 6 a flow diagram for the fluorescence subroutine. The only change from the previous one is the by-pass FS for banking secondary fluorescence, and the Bank exit from (N).

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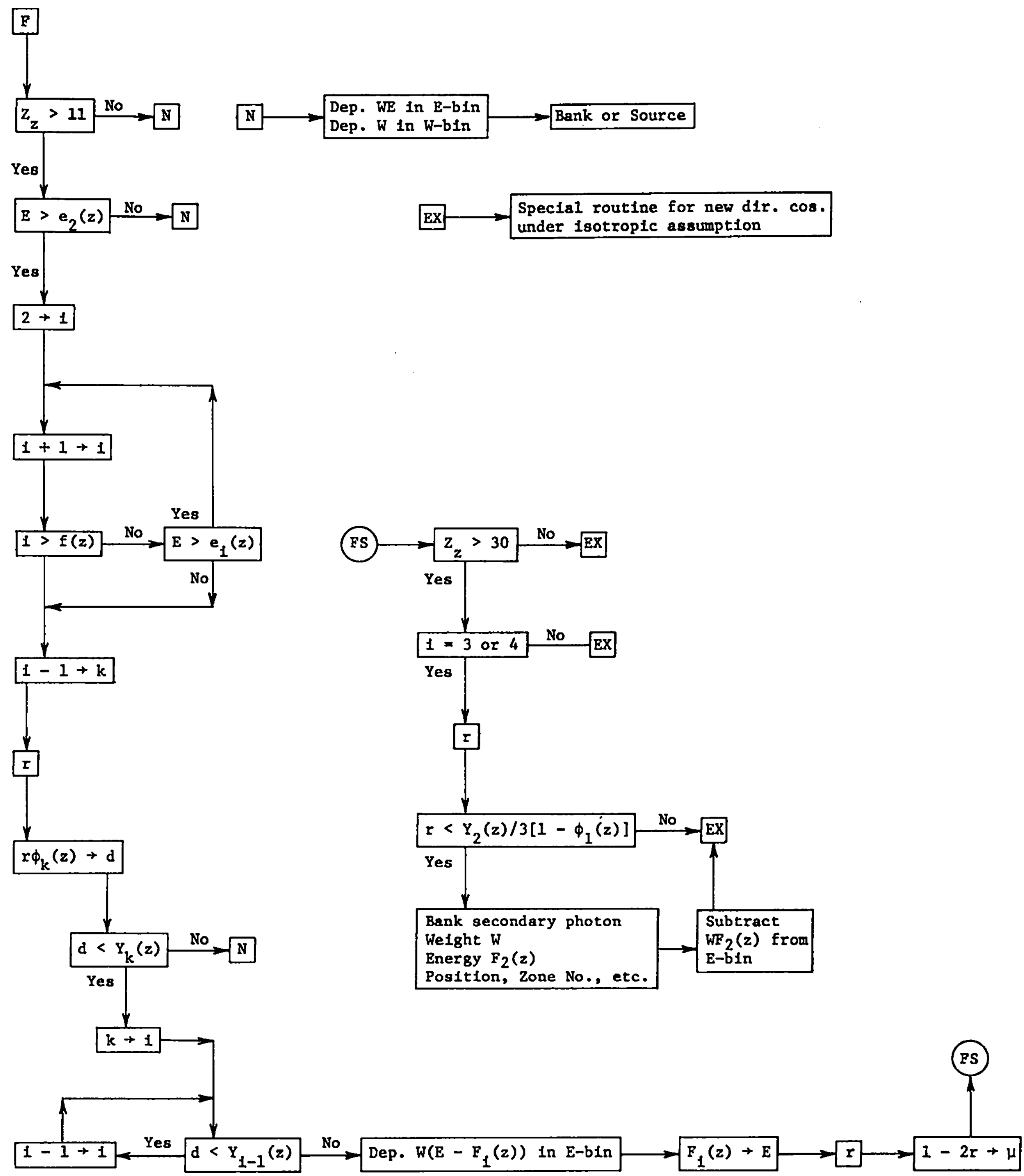

Fig. 6. Flow diagram.

TABLE I

MCP CODE FLUORESCENCE UPDATE

Z	e	ϕ	Y	F	f
12	.001305	0.0784	0.0	0.0	2
Mg	.001305	1.0	0.0258	0.001255	
13	.001560	0.0839	0.0	0.0	2
Al	.001560	1.0	0.0347	0.001487	
14	.001839	0.0888	0.0	0.0	2
Si	.001839	1.0	0.0465	0.001739	
15	.002144	0.0927	0.0	0.0	2
P	.002144	1.0	0.0599	0.002014	
16	.002472	0.0966	0.0	0.0	2
S	.002472	1.0	0.0732	0.002307	
17	.002824	0.1000	0.0	0.0	2
Cl	.002824	1.0	0.0873	0.002622	
18	.003203	0.104	0.0	0.0	2
Ar	.003203	1.0	0.1066	0.002957	
19	.003607	0.108	0.0	0.0	2
K	.003607	1.0	0.1267	0.003312	
20	.004037	0.110	0.0	0.0	4
Ca	.004037	0.644	0.0892	0.003691	
	.004037	0.915	0.1345	0.003687	
	.004037	1.0	0.1487	0.004012	
21	.004491	0.113	0.0	0.0	4
Sc	.004491	0.643	0.1007	0.004090	
	.004491	0.913	0.1520	0.004085	
	.004491	1.0	0.1687	0.004459	
22	.004966	0.116	0.0	0.0	4
Ti	.004966	0.642	0.1162	0.004510	
	.004966	0.910	0.1754	0.004504	
	.004966	1.0	0.1953	0.004931	
23	.005465	0.117	0.0	0.0	4
V	.005465	0.642	0.1297	0.004952	
	.005465	0.910	0.1959	0.004944	
	.005465	1.0	0.2184	0.005427	
24	.005989	0.120	0.0	0.0	4
Cr	.005989	0.642	0.1441	0.005414	
	.005989	0.908	0.2175	0.005405	
	.005989	1.0	0.2429	0.005947	
25	.006539	0.122	0.0	0.0	4
Mn	.006539	0.642	0.1544	0.005899	
	.006539	0.907	0.2331	0.005888	
	.006539	1.0	0.2607	0.006492	
26	.007112	0.124	0.0	0.0	4
Fe	.007112	0.642	0.1673	0.006404	
	.007112	0.907	0.2529	0.006391	
	.007112	1.0	0.2833	0.007059	
27	.007709	0.126	0.0	0.0	4
Co	.007709	0.643	0.1810	0.006930	
	.007709	0.907	0.2734	0.006915	
	.007709	1.0	0.3063	0.007649	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
28	.008332	0.127	0.0	0.0	4
Ni	.008332	0.642	0.1942	0.007478	
	.008332	0.906	0.2937	0.007461	
	.008332	1.0	0.3291	0.008265	
29	.008981	0.129	0.0	0.0	4
Cu	.008981	0.642	0.2083	0.008048	
	.008981	0.905	0.3151	0.008028	
	.008981	1.0	0.3537	0.008907	
30	.009659	0.130	0.0	0.0	4
Zn	.009659	0.642	0.2217	0.008639	
	.009659	0.905	0.3356	0.008616	
	.009659	1.0	0.3772	0.009572	
31	.001186	0.118	0.0	0.0	5
Ga	.001186	1.0	0.0088	0.001129	
	.010367	4.861	1.808	0.009252	
	.010367	6.844	2.732	0.009225	
	.010367	7.588	3.079	0.010263	
32	.001293	0.125	0.0	0.0	5
Ge	.001293	1.0	0.0140	0.001221	
	.011104	4.814	1.921	0.009887	
	.011104	6.780	2.904	0.009856	
	.011104	7.531	3.280	0.010981	
33	.001404	0.129	0.0	0.0	5
As	.001404	1.0	0.0183	0.001317	
	.011867	4.754	2.015	0.010544	
	.011867	6.689	3.044	0.010508	
	.011867	7.450	3.451	0.011725	
34	.001520	0.137	0.0	0.0	5
Se	.001520	1.0	0.0233	0.001416	
	.012658	4.693	2.128	0.011224	
	.012658	6.603	3.217	0.011183	
	.012658	7.367	3.653	0.012495	
35	.001643	0.141	0.0	0.0	5
Br	.001643	1.0	0.0275	0.001519	
	.013474	4.624	2.192	0.011923	
	.013474	6.495	3.309	0.011877	
	.013474	7.259	3.765	0.013288	
36	.001774	0.147	0.0	0.0	5
Kr	.001774	1.0	0.0333	0.001631	
	.014323	4.570	2.282	0.012648	
	.014323	6.420	3.448	0.012596	
	.014323	7.187	3.931	0.014110	
37	.001911	0.152	0.0	0.0	6
Rb	.001911	1.0	0.0373	0.001745	
	.015200	4.452	2.312	0.013395	
	.015200	6.245	3.494	0.013337	
	.015200	6.999	3.991	0.014958	
	.015200	7.078	4.043	0.015185	
38	.002054	0.155	0.0	0.0	6
Sr	.002054	1.0	0.0414	0.001864	
	.016105	4.380	2.356	0.014165	
	.016105	6.139	3.561	0.014098	
	.016105	6.893	4.077	0.015832	
	.016105	6.983	4.138	0.016085	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
39	.002202	0.161	0.0	0.0	6
Y	.002202	1.0	0.0461	0.001987	
	.017038	4.327	2.402	0.014959	
	.017038	6.058	3.628	0.014883	
	.017038	6.814	4.164	0.016735	
	.017038	6.908	4.231	0.017013	
40	.002354	0.166	0.0	0.0	6
Zr	.002354	1.0	0.0500	0.002113	
	.017998	4.280	2.444	0.015775	
	.017998	5.996	3.697	0.015691	
	.017998	6.757	4.253	0.017663	
	.017998	6.857	4.326	0.017969	
41	.002511	0.171	0.0	0.0	6
Nb	.002511	1.0	0.0547	0.002244	
	.018986	4.217	2.458	0.016616	
	.018986	5.901	3.716	0.016522	
	.018986	6.662	4.285	0.018620	
	.018986	6.766	4.363	0.018954	
42	.002671	0.175	0.0	0.0	6
Mo	.002671	1.0	0.0594	0.002378	
	.020000	4.193	2.495	0.017479	
	.020000	5.873	3.777	0.017375	
	.020000	6.644	4.365	0.019602	
	.020000	6.753	4.448	0.019965	
43	.002838	0.178	0.0	0.0	6
Tc	.002838	1.0	0.0641	0.002517	
*	.021044	4.134	2.502	0.018367	
	.021044	5.783	3.785	0.018251	
	.021044	6.554	4.385	0.020612	
	.021044	6.667	4.473	0.021006	
44	.003010	0.183	0.0	0.0	6
Ru	.003010	1.0	0.0678	0.002669	
	.022117	4.075	2.510	0.019279	
	.022117	5.696	3.797	0.019150	
	.022117	6.459	4.403	0.021649	
	.022117	6.570	4.491	0.022075	
45	.003187	0.184	0.0	0.0	6
Rh	.003187	1.0	0.0726	0.002820	
	.023220	4.018	2.506	0.020216	
	.023220	5.615	3.793	0.020074	
	.023220	6.372	4.403	0.022716	
	.023220	6.487	4.496	0.023173	
46	.003370	0.188	0.0	0.0	6
Pd	.003370	1.0	0.0771	0.002976	
	.024350	3.958	2.500	0.021176	
	.024350	5.523	3.782	0.021020	
	.024350	6.273	4.396	0.023809	
	.024350	6.397	4.498	0.024298	
47	.003560	0.190	0.0	0.0	6
Ag	.003560	1.0	0.0810	0.003136	
	.025514	3.927	2.510	0.022163	
	.025514	5.482	3.801	0.021990	
	.025514	6.233	4.424	0.024933	
	.025514	6.362	4.531	0.025456	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
48	.003761	0.192	0.0	0.0	6
Cd	.003761	1.0	0.0856	0.003301	
	.026711	3.911	2.534	0.023174	
	.026711	5.463	3.839	0.022984	
	.026711	6.223	4.478	0.026084	
	.026711	6.351	4.586	0.026646	
49	.003969	0.195	0.0	0.0	6
In	.003969	1.0	0.0902	0.003472	
	.027940	3.880	2.538	0.024210	
	.027940	5.413	3.841	0.024002	
	.027940	6.171	4.485	0.027264	
	.027940	6.304	4.598	0.027866	
50	.004183	0.198	0.0	0.0	6
Sn	.004183	1.0	0.0946	0.003647	
	.029200	3.820	2.529	0.025271	
	.029200	5.326	3.829	0.025044	
	.029200	6.077	4.477	0.028472	
	.029200	6.213	4.594	0.029114	
51	.004404	0.200	0.0	0.0	6
Sb	.004404	1.0	0.0984	0.003828	
	.030491	3.777	2.508	0.026359	
	.030491	5.266	3.800	0.026110	
	.030491	6.013	4.448	0.029710	
	.030491	6.152	4.569	0.030392	
52	.004631	0.202	0.0	0.0	6
Te	.004631	1.0	0.1029	0.004014	
	.031814	3.744	2.501	0.027473	
	.031814	5.221	3.792	0.027202	
	.031814	5.967	4.444	0.030978	
	.031814	6.110	4.569	0.031701	
53	.004866	0.204	0.0	0.0	6
I	.004866	1.0	0.1067	0.004206	
	.033170	3.720	2.498	0.028613	
	.033170	5.186	3.787	0.028318	
	.033170	5.932	4.443	0.032276	
	.033170	6.074	4.568	0.033041	
54	.005110	0.205	0.0	0.0	6
Xe	.005110	1.0	0.1113	0.004402	
	.034561	3.679	2.479	0.029779	
	.034561	5.129	3.761	0.029459	
	.034561	5.872	4.418	0.033605	
	.034561	6.017	4.546	0.034415	
55	.005362	0.206	0.0	0.0	6
Cs	.005362	1.0	0.1159	0.004603	
	.035985	3.637	2.463	0.030973	
	.035985	5.062	3.731	0.030625	
	.035985	5.799	4.387	0.034965	
	.035985	5.947	4.519	0.035820	
56	.005619	0.208	0.0	0.0	6
Ba	.005619	1.0	0.1196	0.004811	
	.037441	3.602	2.446	0.032194	
	.037441	5.013	3.707	0.031818	
	.037441	5.748	4.364	0.036356	
	.037441	5.900	4.500	0.037257	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
57	.005880	0.209	0.0	0.0	6
La	.005880	1.0	0.1250	0.005022	
	.038925	3.551	2.416	0.033441	
	.038925	4.937	3.661	0.033034	
	.038925	5.659	4.309	0.037775	
	.038925	5.813	4.447	0.038728	
58	.006145	0.211	0.0	0.0	6
Ce	.006145	1.0	0.1278	0.005237	
*	.040443	3.532	2.412	0.034720	
	.040443	4.918	3.662	0.034279	
	.040443	5.642	4.315	0.039229	
	.040443	5.795	4.453	0.040233	
59	.006413	0.211	0.0	0.0	6
Pr	.006413	1.0	0.1333	0.005450	
*	.041991	3.491	2.387	0.036027	
	.041991	4.857	3.623	0.035551	
	.041991	5.575	4.273	0.040718	
	.041991	5.726	4.410	0.041769	
60	.006686	0.213	0.0	0.0	6
Nd	.006686	1.0	0.1362	0.005684	
	.043569	3.461	2.376	0.037361	
	.043569	4.813	3.606	0.036847	
	.043569	5.529	4.258	0.042237	
	.043569	5.679	4.394	0.043335	
61	.006967	0.215	0.0	0.0	6
Pm	.006967	1.0	0.1413	0.005917	
*	.045184	3.452	2.377	0.038725	
	.045184	4.802	3.608	0.038171	
	.045184	5.517	4.260	0.043790	
	.045184	5.671	4.400	0.044939	
62	.007255	0.216	0.0	0.0	6
Sm	.007255	1.0	0.1450	0.006154	
*	.046834	3.410	2.353	0.040118	
	.046834	4.742	3.573	0.039522	
	.046834	5.452	4.223	0.045376	
	.046834	5.609	4.367	0.046579	
63	.007549	0.216	0.0	0.0	6
Eu	.007549	1.0	0.1497	0.006396	
	.048519	3.382	2.341	0.041542	
	.048519	4.701	3.554	0.040901	
	.048519	5.408	4.204	0.046995	
	.048519	5.563	4.347	0.048253	
64	.007849	0.219	0.0	0.0	6
Gd	.007849	1.0	0.1539	0.006642	
*	.050239	3.360	2.330	0.042996	
	.050239	4.673	3.541	0.042309	
	.050239	5.375	4.188	0.048649	
	.050239	5.529	4.330	0.049959	
65	.008158	0.220	0.0	0.0	6
Tb	.008158	1.0	0.1576	0.006896	
*	.051996	3.329	2.315	0.044482	
	.051996	4.628	3.518	0.043744	
	.051996	5.327	4.165	0.050336	
	.051996	5.479	4.306	0.051703	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
66	.008472	0.223	0.0	0.0	6
Dy	.008472	1.0	0.1624	0.007155	
	.053788	3.305	2.303	0.045998	
	.053788	4.595	3.501	0.045208	
	.053788	5.294	4.150	0.052058	
	.053788	5.450	4.295	0.053482	
67	.008795	0.222	0.0	0.0	6
Ho	.008795	1.0	0.1665	0.007420	
*	.055618	3.274	2.283	0.047546	
	.055618	4.554	3.475	0.046700	
	.055618	5.245	4.118	0.053817	
	.055618	5.399	4.261	0.055297	
68	.009125	0.223	0.0	0.0	6
Er	.009125	1.0	0.1709	0.007691	
*	.057486	3.249	2.272	0.049128	
	.057486	4.517	3.456	0.048222	
	.057486	5.206	4.100	0.055611	
	.057486	5.359	4.243	0.057151	
69	.009460	0.225	0.0	0.0	6
Tm	.009460	1.0	0.1744	0.007966	
	.059390	3.225	2.259	0.050742	
	.059390	4.482	3.437	0.049773	
	.059390	5.169	4.081	0.057441	
	.059390	5.320	4.222	0.059039	
70	.009803	0.225	0.0	0.0	6
Yb	.009803	1.0	0.1782	0.08250	
*	.061332	3.196	2.240	0.052389	
	.061332	4.446	3.414	0.051354	
	.061332	5.131	4.057	0.059308	
	.061332	5.281	4.198	0.060965	
71	.010156	0.227	0.0	0.0	6
Lu	.010156	1.0	0.1832	0.008540	
*	.063316	3.159	2.215	0.054071	
	.063316	4.390	3.373	0.052967	
	.063316	5.065	4.008	0.061213	
	.063316	5.217	4.151	0.062931	
72	.010524	0.229	0.0	0.0	6
Hf	.010524	1.0	0.1866	0.008839	
	.065345	3.131	2.194	0.055785	
	.065345	4.349	3.341	0.054606	
	.065345	5.020	3.973	0.063153	
	.065345	5.170	4.114	0.064942	
73	.010899	0.229	0.0	0.0	6
Ta	.010899	1.0	0.1912	0.009142	
	.067416	3.110	2.183	0.057536	
	.067416	4.322	3.327	0.056280	
	.067416	4.988	3.956	0.065132	
	.067416	5.137	4.097	0.066991	
74	.011281	0.231	0.0	0.0	6
W	.011281	1.0	0.2253	0.009454	
	.069525	3.084	2.196	0.059321	
	.069525	4.284	3.331	0.057984	
	.069525	4.947	3.958	0.067147	
	.069525	5.094	4.097	0.069078	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
75	.011673	0.232	0.0	0.0	6
Re	.011673	1.0	0.2427	0.009775	
	.071676	3.060	2.196	0.061142	
	.071676	4.248	3.322	0.059719	
	.071676	4.909	3.949	0.069205	
	.071676	5.055	4.087	0.071206	
76	.012075	0.232	0.0	0.0	6
Os	.012075	1.0	0.2565	0.010103	
	.073871	3.020	2.173	0.063000	
	.073871	4.194	3.287	0.061486	
	.073871	4.845	3.905	0.071304	
	.073871	4.993	4.045	0.073377	
77	.012486	0.235	0.0	0.0	6
Ir	.012486	1.0	0.2670	0.010436	
	.076111	2.999	2.166	0.064896	
	.076111	4.163	3.272	0.063287	
	.076111	4.812	3.889	0.073442	
	.076111	4.958	4.028	0.075590	
78	.012906	0.236	0.0	0.0	6
Pt	.012906	1.0	0.2758	0.010776	
	.078395	2.964	2.144	0.066831	
	.078395	4.114	3.238	0.065122	
	.078395	4.753	3.846	0.075624	
	.078395	4.897	3.983	0.077846	
79	.013335	0.241	0.0	0.0	6
Au	.013335	1.0	0.2823	0.011125	
	.080725	2.941	2.130	0.068806	
	.080725	4.079	3.213	0.066991	
	.080725	4.712	3.816	0.077848	
	.080725	4.859	3.956	0.080146	
80	.013778	0.240	0.0	0.0	6
Hg	.013778	1.0	0.2903	0.011480	
	.083102	2.908	2.108	0.070819	
	.083102	4.035	3.182	0.068893	
	.083102	4.660	3.778	0.080112	
	.083102	4.809	3.920	0.082491	
81	.014233	0.241	0.0	0.0	6
Tl	.014233	1.0	0.2968	0.011815	
	.085530	2.879	2.090	0.072874	
	.085530	3.991	3.151	0.070833	
	.085530	4.611	3.742	0.082422	
	.085530	4.758	3.882	0.084883	
82	.014699	0.242	0.0	0.0	6
Pb	.014699	1.0	0.3032	0.012217	
	.088004	2.854	2.074	0.074969	
	.088004	3.957	3.127	0.072804	
	.088004	4.570	3.712	0.084777	
	.088004	4.715	3.850	0.087320	
83	.015175	0.244	0.0	0.0	6
Bi	.015175	1.0	0.3084	0.012598	
	.090526	2.832	2.059	0.077106	
	.090526	3.924	3.103	0.074812	
	.090526	4.535	3.687	0.087179	
	.090526	4.678	3.824	0.089805	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
84	.015665	0.246	0.0	0.0	6
Po	.015665	1.0	0.3122	0.012987	
*	.093105	2.801	2.036	0.079291	
	.093105	3.883	3.071	0.076861	
	.093105	4.486	3.648	0.089627	
	.093105	4.631	3.787	0.092350	
85	.016163	0.248	0.0	0.0	6
At	.016163	1.0	0.3166	0.013383	
	.095730	2.778	2.020	0.081516	
	.095730	3.852	3.049	0.078945	
	.095730	4.448	3.620	0.092120	
	.095730	4.592	3.758	0.094937	
86	.016670	0.249	0.0	0.0	6
Rn	.016670	1.0	0.3207	0.013784	
*	.098404	2.744	1.992	0.083785	
	.098404	3.799	3.003	0.081067	
	.098404	4.385	3.564	0.094661	
	.098404	4.530	3.703	0.097573	
87	.017191	0.250	0.0	0.0	6
Fr	.017191	1.0	0.3232	0.014196	
*	.101137	2.719	1.972	0.086107	
	.101137	3.765	2.975	0.083233	
	.101137	4.344	3.530	0.097256	
	.101137	4.487	3.667	0.100264	
88	.017722	0.250	0.0	0.0	6
Ra	.017722	1.0	0.3278	0.014618	
	.103922	2.699	1.959	0.088476	
	.103922	3.735	2.954	0.085438	
	.103922	4.312	3.508	0.099902	
	.103922	4.454	3.644	0.102999	
89	.018266	0.251	0.0	0.0	6
Ac	.018266	1.0	0.3288	0.015049	
*	.106759	2.676	1.938	0.090889	
	.106759	3.705	2.926	0.087676	
	.106759	4.276	3.474	0.102599	
	.106759	4.420	3.612	0.105783	
90	.018820	0.252	0.0	0.0	6
Th	.018820	1.0	0.3321	0.015489	
	.109651	2.651	1.917	0.093351	
	.109651	3.676	2.901	0.089958	
	.109651	4.241	3.443	0.105348	
	.109651	4.383	3.579	0.108616	
91	.019384	0.254	0.0	0.0	6
Pa	.019384	1.0	0.3335	0.015939	
*	.112601	2.625	1.894	0.095868	
	.112601	3.639	2.867	0.092287	
	.112601	4.196	3.402	0.108155	
	.112601	4.336	3.536	0.111522	
92	.019959	0.254	0.0	0.0	6
U	.019959	1.0	0.3350	0.016398	
	.115606	2.602	1.875	0.098436	
	.115606	3.604	2.838	0.094658	
	.115606	4.158	3.370	0.111015	
	.115606	4.296	3.503	0.114485	

TABLE I (Cont'd)

Z	e	ϕ	Y	F	f
93	.020547	0.257	0.0	0.0	6
Np	.020547	1.0	0.3358	0.016867	
*	.118670	2.575	1.851	0.101057	
	.118670	3.562	2.800	0.097070	
	.118670	4.111	3.328	0.113931	
	.118670	4.247	3.459	0.117503	
94	.021147	0.256	0.0	0.0	6
Pu	.021147	1.0	0.3378	0.017348	
	.121797	2.539	1.819	0.103734	
	.121797	3.509	2.752	0.099527	
	.121797	4.046	3.269	0.116905	
	.121797	4.180	3.398	0.120583	

*Element omitted in previous version.

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