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RAPID COMPUTATION OF SPECIFIC ENERGY LOSSES FOR ENERGETIC CHARGED PARTICLES

R. W. Peelle

Rec'd 5-27-65

ABSTRACT

A method is demonstrated for computing rapidly in a digital computer the specific energy loss of energetic charged particles, excluding electrons. For energies larger than an empirically determined cutoff TLIM, the computation is based on use of the usual Bethe-Bloch equation with a "shell correction" for nonparticipation of tightly bound electrons in the absorber atoms, but without a "density effect" correction which might be required for incident proton energies as high as 1 GeV. Rapid computation is achieved by interpolating a combined shell correction from a small table of values stored with the set of parameters peculiar to a given absorber material. The accuracy is limited to a few tenths of a percent by the coarseness of the interpolation procedure and by the accuracy of the combined shell corrections presently available to serve as a base for interpolation. For incident energies less than TLIM, a plausible value is computed based wholly on a few empirical parameters. The results are compared against published tabulations of specific energy loss and against a very small selection of experiments on relative energy loss and range. A computer subprogram which utilizes the described technique is listed in the IBM-7090 FORTRAN-II language, and brief instructions for its use are given.

Note:
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Note Added in Proof: Since preparation of this memorandum the literature has been enriched by the appearance of NAS-NRC 1133, Studies in Penetration of Charged Particles in Matter, which thoroughly covers in a series of papers the topics discussed here. The tables therein and in NASA SP-3013 in the paper by W. Barkas and M. Berger are presumably the most authoritative now available. Quick comparisons for aluminum and copper show differences between sample results to be as large as 0.4% for protons above 10 MeV, and larger at low energies.

1. INTRODUCTION

Processing the experimental data obtained in observing charged-particle reactions of 160-MeV protons on nuclei[1] has required computation of a very large number of proton energy losses in a variety of materials. Since in these experiments a given secondary proton passed through eight different materials, it seemed essential that the energy-loss computation be performed with the IBM 7090 used for data processing. The variance noted between published[2] energy-loss values suggested that an investigation would be required to assure a good interpolation among the existing experimental data.

Since all existing tables differ from experimental values at some energies by upwards of 1%, the criterion of rapid but precise computation did not require that the procedure reproduce the desired values to better than a few tenths percent, but it was necessary to include all the main features of a precise computation to avoid much larger errors.

Fano[3] recently described how the discrepancy between low- and high-energy experiments illuminated by Caldwell[4] may be removed within the assumption of an energy-independent average excitation potential by use of "shell corrections" for the inner electron shells, as given by Bichsel,[5]

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[1] R. W. Peelle, T. A. Love, N. W. Hill, and R. T. Santoro, Differential Cross Sections by Flight-Time Spectroscopy for Protons Produced by Interaction of 160-MeV Protons on Various Nuclei, ORNL-TM-1114, to be published.

[2] W. A. Aron, B. G. Hoffman, and F. C. Williams, Range Energy Curves, AECU-663 (1944); M. Rich and R. Madey, Range-Energy Tables, UCRL-2301 (1954); R. Sternheimer, Phys. Rev. 115, 137 (1959); C. Williamson and J. P. Boujot, Tables of Range and Rate of Energy Loss of Charged Particles of Energy of 0.5 to 150 MeV, Centre d'Etudes Nucleaires, Saclay, CEA-2189 (1962); H. Bichsel, in ref. 5.

[3] U. Fano, Ann. Rev. Nucl. Sci. 13, 1 (1963).

[4] D. O. Caldwell, Phys. Rev. 100, 291 (1955).

[5] H. Bichsel, Sect. 8C in American Institute of Physics Handbook, 2nd ed., McGraw-Hill, New York, 1963; see details in Bichsel, Higher Shell Corrections in Stopping Power, Technical Report 3, Linear Accelerator Group of University of Southern California.

larger than had previously been used. This explanation is consistent with the differences among the tabulations of ref. 2, most of which largely ignored the problem of shell corrections or approximated the values for the outer shells from the incomplete information available at the time each was produced.

The method described here is to interpolate a combined shell correction from a small table for each element prepared from a graph drawn by Turner.[6] This report summarizes the method of calculation, the input parameters chosen to represent the present information, and some comparisons with previously listed values of energy loss.

2. FORMULATION OF THE ENERGY LOSS PROBLEM

The basic energy dependence of the specific energy loss is taken from the Bethe-Bloch equation, which for most elements gives the experimental results within about 10% over three orders of magnitude in kinetic energy without any of the correction terms. This equation may be written

$$-\frac{dE}{d\xi} = \frac{4\pi\, m_e c^2\; r_o^2 N_o\; z^2 Z}{A\, \beta^2} \left[\ell n \frac{2\, m_e c^2\, \beta^2}{I(1 - \beta^2)} - \frac{\Sigma C_i}{Z} - \frac{\delta}{2} \right] , \qquad (1)$$

where all fundamental quantities have their usual definitions, and

ξ = surface density of absorber,

z = charge number of energetic incident particle,

Z = atomic number of stopping material,

A = gram-atomic weight of stopping material,

β = (incident particle velocity)/c,

I = the average excitation potential (sometimes called "average ionization potential") for the stopping material, the average being performed to allow the atomic number to remain outside the parentheses,

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[6] J. E. Turner, Fig. 6 in Ann. Rev. Nucl. Sci. **13**, 1 (1963); also, private communication, 1964.

C_i = shell correction for nonparticipation in the stopping process of atomic electrons in the ith atomic shell,

δ = density correction.

If energy loss is taken in MeV, I in eV, and ξ in g/cm^2, Eq. 1 reduces to the following when the density effect is ignored:[7]

$$-\frac{dE}{d\xi} = \frac{0.30718\, z^2}{\beta^2}\frac{Z_m}{A_m}\left[\ell n\,(1.02195 \times 10^6) - \ell n\, I + \ell n\,\frac{\beta^2}{1-\beta^2} - \frac{\Sigma C_i}{Z_m}\right] . \tag{2}$$

Equation 2 is written to symbolize some of the difficulties in treating molecules. In this case A_m becomes the molecular weight, Z_m the total number of nucleonic charges in the molecule, I an appropriately averaged excitation potential, and Z_{sh} the atomic number used to estimate a shell correction as described in the next section; Z_{sh} is not necessarily equal to Z_m.

In Eq. 2 I is intended to parameterize the energy loss in the energy region sufficiently high that the bound electron velocity is always small compared with that of the incident particle, but sufficiently low that the density effect is not important. At low β the C_i's must go very negative to prevent the Bethe-Bloch prediction (the $\ell n\, \beta^2$ term) from yielding a negative result in the conceptually simple case that the electrons in the ith atomic shell are quite bound with respect to the slowly moving primary particle. These electrons give no contribution to the actual stopping power, but a large negative C_i correction in Eq. 2 is required to approximate this condition. Nevertheless, there is an energy of incident particle, called TLIM, below which Eq. 2 cannot easily give reliable results simply because the C_i's are no longer small but instead are much larger than the

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[7] The density correction is ignored because this computation was expected to be used only at energies below about 500 MeV. From R. M. Steinheimer (*Phys. Rev.* **103**, 511, 1956) one may obtain the following approximate value of the relative importance of the density effect for 1-GeV protons: Be, 1.7%; graphite, 1.3%; polystyrene, 0.6%; Al, 1.1%; Cu, 0.2%; Ag, 0.1%; Pb, < 0.3%. At lower energies the effect becomes smaller; for instance, the effect is estimated to be 0.3% in Be for 300-MeV protons.

net value of the term in square brackets. For such low energies a scheme based on simply obtained approximate values of C_i cannot function. For practical computation it was desired that plausible energy loss values be computed even for values of incident particle kinetic energy less than TLIM, and for incident particle charges greater than unity (which lead to higher values of TLIM). In the latter case deionization of the incident particle becomes increasingly important in producing discrepancies between Eq. 2 and experiment, since the C_i's are supposed not to depend on the incident charge. To provide approximate values of energy loss for kinetic energy T less than TLIM, the following formulation was employed:

For $T \geq$ TLIM, use Eq. 2.

For TPEAK $\leq T <$ TLIM, use the straight-line interpolation between $\frac{dE}{d\xi}$ (TLIM) and $\frac{dE}{d\xi}$ (TPEAK).

For $T <$ TPEAK, $\frac{dE}{dx}(T) = \frac{dE}{dx}(\mathrm{TPEAK})\ [-\ T^2 + 2T(\mathrm{TPEAK})]$.

Values of TPEAK and $\frac{dE}{dx}$ (TPEAK) are estimated as well as possible from experimental values,[8] and have proved adequate to give sensible path-length integrals for protons in the neighborhood of a few MeV. For this case useful values of TLIM vary from 150 keV for light elements to 350 keV for copper to 1 MeV for the heaviest elements. If precise values of energy losses in the low-energy region (below 5 MeV) were the dominant consideration, the suitability of the calculational scheme given here would be in doubt.

If repetitive computations are made with Eq. 2, not all parts of the formula need be computed for each entry, as, for instance, β need not be recomputed for calculations for a new stopping material at the same energy.

If μ is the incident particle mass in MeV, $\beta^2/(1 - \beta^2)$ is computed as $T(2T + \mu)/\mu^2$, and β^2 in turn is computed from this quantity.

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[8] Particularly useful has been: W. Whaling, p. 193 in Handbuch der Physic, Vol. 34/2, Springer, Berlin, 1958; also S. K. Allison and S. D. Warshaw, Revs. Mod. Phys. **25**, 779 (1953).

3. INTERPOLATION OF THE NONPARTICIPATION CORRECTIONS C_i

Two basic approaches have been used by investigators to estimate the shell corrections C_i to account for nonparticipation in the stopping process of the more tightly bound electrons in the absorber atoms. One is the microscopic approach, which has been popular until recently and depends on published estimates[9] based on the use of hydrogen-like wave functions with appropriate corrections. In this scheme corrections are estimated for each shell thought likely to make a significant correction at the energy in question. If one considers the stopping contribution from electrons in a single shell, the contribution nicely goes to zero at low incident velocities, and comparison with Eq. 1 allows corrections to be estimated. Figures 1 and 2 show theoretical relative K-shell and L-shell corrections to the stopping power for a few elements. With the exception of the L-shell correction for aluminum, which was taken from Bischel *et al.*,[10] these corrections are based on interpolations from the works cited in ref. 9. (Note the scale change in each plot.) It can be seen that the estimated maximum relative corrections are appreciable in some cases. The form of the curves for low velocities is what might be expected on the basis of the discussion in the previous section, and does not imply that electrons in the inner shells add energy to the incident particle for low particle velocities.

The second approach is more macroscopic and is known to have been employed by Bichsel[5] and Turner,[6] and is discussed in the review paper of Fano.[3] By this approach one hopes to determine the values of the corrections by direct comparison of the predictions of the Bethe-Bloch equation against the results of experiment for the elements most studied. In the process, calculated corrections like those in Figs. 1 and 2 can be used for the inner shells, with the details of the shapes of similar functions left free for the higher shells. In this way, like Turner,[6] one may attempt to judge from the combined results of experiment what the sum of the corrections

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[9] L. M. Brown, *Phys. Rev.* **79**, 297 (1950); M. C. Walske, *Phys. Rev.* **88**, 1283 (1952) and *Phys. Rev.* **101**, 940 (1956); H. A. Bethe and J. Ashkin, p. 166 in *Experimental Nuclear Physics* (E. Segrè, ed.), Vol. 1, Wiley, New York, 1951.

[10] H. Bichsel, R. Mozley, and W. Aron, *Phys. Rev.* **105**, 1788 (1957).

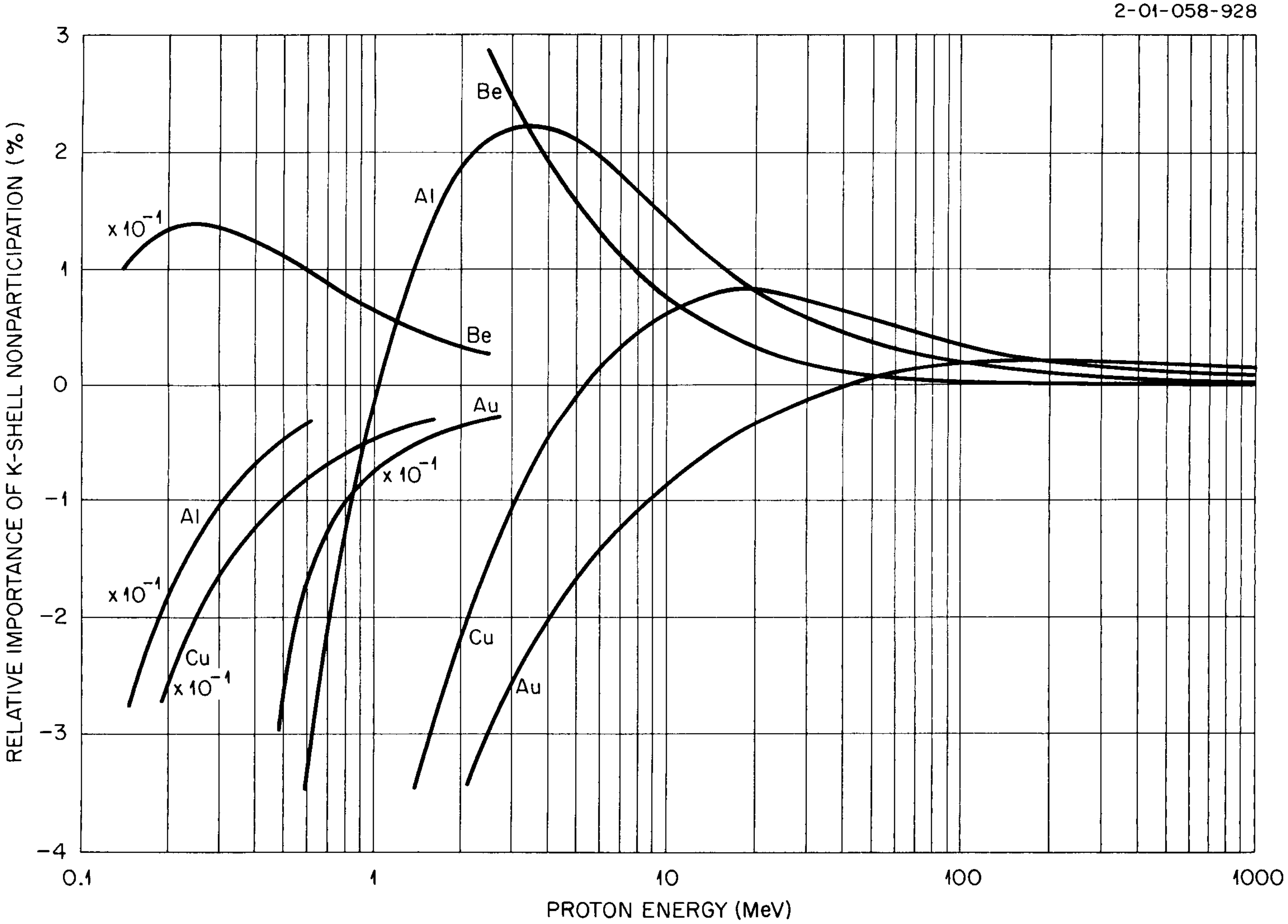

Fig. 1. Computed Relative Importance of K-Shell Nonparticipation.

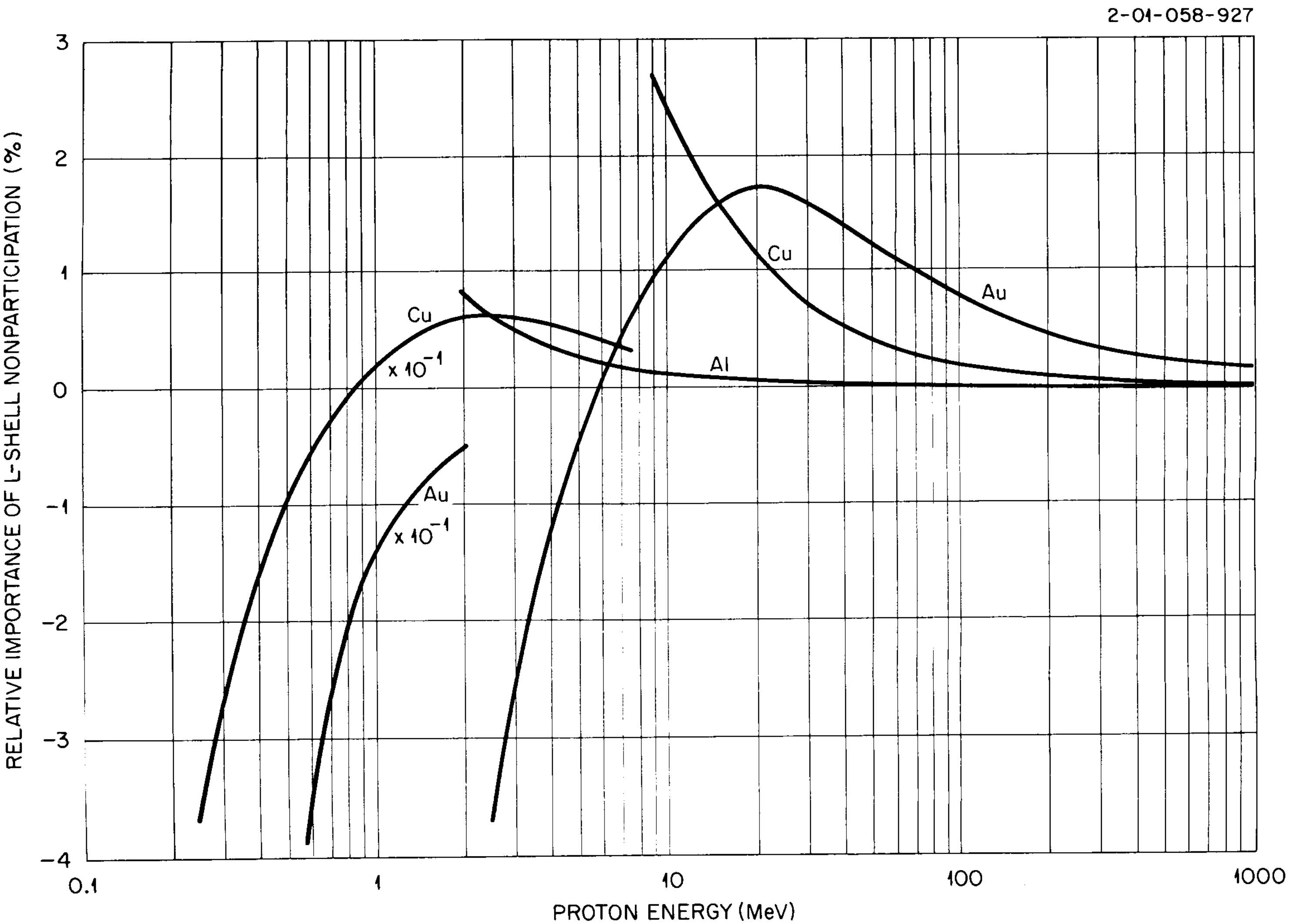

Fig. 2. Computed Relative Importance of L-Shell Nonparticipation.

must be. The chosen correction just compensates for any difference between Eq. 1 and experiment, whatever the conceptual origin of the disagreement, although the form of the correction is somewhat restricted.

The method used in the present practical calculations consists of taking shell corrections from the graph of Turner, shown in Fig. 3, and then hand-interpolating among the curves to estimate the behavior for intermediate elements, a difficult procedure for the lighter elements. The abscissa in Fig. 3 is $x = \ell n(T_{keV}/25Z_{sh})$, where T is the kinetic energy of the incident particle. For each absorber for which calculated values were desired, values of $\Sigma\, C_i/Z_{sh}$ were tabulated for integral values of $\ell n\, x$ between -1 and 6, it being assumed that all the curves of Fig. 3 reach zero ordinate by $\ell n\, x = 7$ and remain there. Considering the accuracy of the basic data at this time, it was felt that a linear interpolation between adjacent values would be adequate.

The eight parameters thus determined, the average excitation potential I, the three parameters which specify the behavior at low energies, and other miscellaneous material properties are stored for machine calculation by the subprogram utilized for a series (up to 12 in the present version) of absorber-incident particle combinations. This procedure is clumsy in that input information containing the above must be supplied to the subprogram and the interpolations among atomic numbers must be performed by hand for each case. The advantage is the relative simplicity in updating the accuracy of the results as better values of the combined shell correction become available from any source.

The parameters used for computing specific energy losses for various materials are shown in Table 1. For hydrogen compounds, the expected departure of the stopping effect of hydrogen from the Bethe-Bloch equation was ignored.

4. THE AVERAGE EXCITATION POTENTIAL

Equation 1 was chosen to make the average excitation potential I the single parameter on which the calculation most seriously depends. The calculations reported here have thus far employed the values listed by Fano[3] and in NBS Handbook 79,[11] supplemented by average values for various

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[11] Stopping Power Study Group of the National Committee on Radiation Protection and Measurements, NBS Handbook 79 (1961).

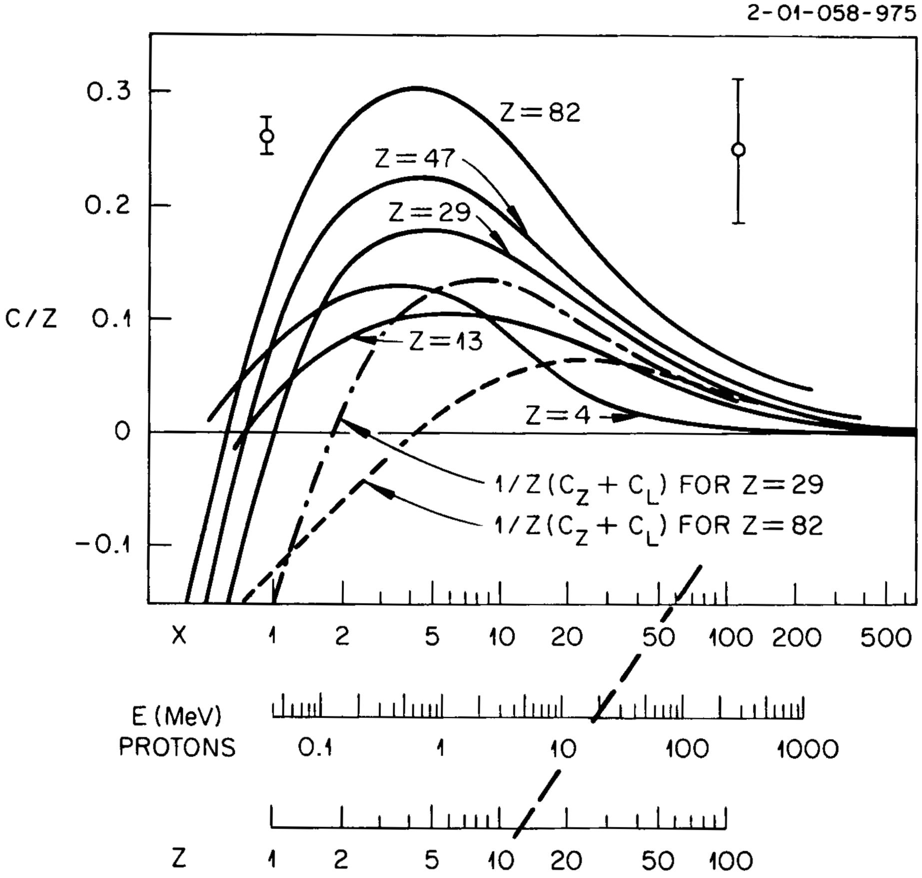

Fig. 3. Combined Shell Correction for Various Metals as a Function of x = ln $(T_{keV}/25Z_{sh})$. The error bars represent the approximate effect of 1% error in the stopping power at the respective abscissas for all elements. The example of nomogram used shows that x = 59 for 20-MeV protons in aluminum. (Reprint permission granted by J. E. Turner, ORNL, and Annual Reviews, Inc.; illustration previously published in article by U. Fano, Annual Review of Nuclear Science, Volume 13.)

Table 1. Parameters Employed to Compute Specific Energy Losses for Various Materials

									$\Sigma C_i/Z_{sh}$							
									For ℓn x of							
Material	I (eV)	TLIM (MeV)	ELLIM (MeV cm^2 g^{-1})	TPEAK (MeV)	ELPK (MeV cm^2 g^{-1})	Z_m	A_m	Z_{sh}	-1	0	1	2	3	4	5	6
H	19.0	0.150	2469.	0.070	3885.	1.0	1.0	1.0	-0.150	0.600	0.460	0.200	0.020	-0	-0	-0
He	42.0	0.150	873.	0.090	1114.	2.0	4.0	2.0	-0	0.150	0.240	0.170	0.030	0.007	-0	-0
Li	39.0	0.150	821.	0.080	800.	3.0	6.9	3.0	-0.010	0.100	0.170	0.140	0.035	0.010	-0	-0
Be	64.0	0.150	652.	0.080	640.	4.0	9.0	4.0	-0.024	0.077	0.134	0.117	0.044	0.011	0.003	-0
C	80.0	0.150	646.	0.080	650.	6.0	12.0	6.0	-0.038	0.060	0.113	0.101	0.054	0.022	0.006	0.001
Mg	151.0	0.150	365.	0.080	460.	12.0	24.3	12.0	-0.087	0.038	0.100	0.106	0.081	0.041	0.012	0.001
Al	163.0	0.150	331.	0.075	440.	13.0	27.0	13.0	-0.093	0.031	0.098	0.104	0.086	0.043	0.014	0.004
Si	172.0	0.180	334.	0.080	420.	14.0	28.1	14.0	-0.113	0.031	0.100	0.110	0.088	0.046	0.015	0.003
Ca	228.0	0.250	265.	0.100	340.	20.0	40.1	20.0	-0.225	0.020	0.125	0.130	0.105	0.055	0.020	0.006
Cr	266.0	0.300	215.	0.120	280.	24.0	52.0	24.0	-0.295	0.016	0.143	0.143	0.114	0.063	0.022	0.007
Co	295.0	0.350	193.	0.160	250.	27.0	58.9	27.0	-0.330	0.018	0.160	0.155	0.119	0.067	0.024	0.008
Cu	315.0	0.350	185.	0.160	230.	29.0	63.5	29.0	-0.340	0.017	0.179	0.172	0.121	0.066	0.026	0.010
Zr	420.0	0.500	124.	0.180	170.	40.0	91.2	40.0	-0.293	0.065	0.207	0.196	0.136	0.076	0.032	0.012
Ag	471.0	0.500	106.	0.200	140.	47.0	107.9	47.0	-0.270	0.102	0.230	0.211	0.136	0.076	0.033	0.014
In	489.0	0.600	99.	0.190	130.	49.0	114.8	49.0	-0.260	0.105	0.236	0.218	0.145	0.080	0.036	0.015
Ta	738.0	0.900	58.	0.180	97.	73.0	180.9	73.0	-0.205	0.165	0.290	0.270	0.170	0.090	0.050	0.022
Au	761.0	1.000	56.	0.180	92.	79.0	197.0	79.0	-0.195	0.170	0.305	0.282	0.182	0.095	0.052	0.024
Pb	788.0	1.000	53.	0.200	90.	82.0	207.2	82.0	-0.190	0.174	0.305	0.289	0.187	0.096	0.051	0.025
Bi	797.0	1.000	53.	0.200	90.	83.0	209.0	83.0	-0.190	0.174	0.310	0.290	0.187	0.096	0.051	0.025
Air	85.0	0.150	624.	0.085	740.	7.2	14.4	7.2	-0.045	0.055	0.107	0.100	0.060	0.026	0.007	0.001
H_2O	70.0	0.150	806.	0.090	920.	10.0	18.0	8.0	-0.053	0.050	0.105	0.100	0.065	0.030	0.008	0.002
D_2O	70.0	0.150	725.	0.090	830.	10.0	20.0	8.0	-0.053	0.050	0.105	0.100	0.065	0.030	0.008	0.002
NaI	432.0	0.600	112.	0.190	130.	64.0	149.9	53.0	-0.250	0.117	0.247	0.228	0.149	0.083	0.039	0.017
CsI	555.0	0.600	84.	0.200	120.	54.0	129.9	54.0	-0.250	0.120	0.250	0.230	0.150	0.083	0.039	0.016
CH_2	54.0	0.150	961.	0.060	3000.	8.0	14.0	6.0	-0.038	0.060	0.113	0.101	0.054	0.022	0.006	0.001
C_6H_{10}	59.0	0.150	961.	0.060	1100.	58.0	106.2	48.0	-0.038	0.060	0.113	0.101	0.054	0.022	0.006	0.001
C_6H_8	60.0	0.150	941.	0.060	1100.	50.0	92.1	42.0	-0.038	0.060	0.113	0.101	0.054	0.022	0.006	0.001
C_6H_6	60.2	0.150	847.	0.060	1000.	7.0	13.0	6.0	-0.038	0.060	0.113	0.101	0.054	0.022	0.006	0.001
Ne	59.4	0.500	450.	0.060	1090.	7.2	13.2	6.0	-0.038	0.060	0.113	0.101	0.054	0.022	0.006	0.001

compounds based on these sources together with the work of Thompson[12] on the effect of chemical binding. In applying the latter work to various organic compounds not directly studied by Thompson, rather arbitrary identifications of chemical binding were made which are untested by comparison with experimental values. Table 1 lists the values of the average ionization potential employed thus far, along with the corresponding values of the other parameters used for computing proton stopping power.

It should be noted that the values of the mean excitation potential given in Table 1 are rather different from those employed in the tabulations by Sternheimer[2] and by Williamson.[2] The reason seems to be that the values they used weighed rather heavily the experimental results in the tens of MeV, using shell corrections based on the work of ref. 9. Both earlier and later work depend on values which weigh more heavily the experimental work above 200 MeV, the resulting difficulty at lower energy now being compensated for by somewhat larger shell corrections.

5. COMPUTED RESULTS

The appendix lists the Fortran program used to materialize the method described above, along with minimum instructions for its operation. In the program's main application no results were printed out, but for test purposes a special program was used to produce tabulated path length and specific energy loss estimates. Specific-energy-loss values obtained in the present calculation are compared in Table 2 with those obtained by other investigators. The values for I are given in each case, since most of the differences are simply the result of the variety of assumptions used -- all authors can compute uncorrected values from Eq. 1 with no difficulty. Since simple values of shell corrections employed are seldom given, it is difficult to trace the differences at low energies. It was believed that when the same I value was used the results of the present computation would agree reasonably well with those of Bichsel, except where the interpolation approximations of the present method cause small errors, since his work was

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[12] T. J. Thompson, The Effect of Chemical Structure on Stopping Powers for High Energy Protons, UCRL-1910 (1952).

Table 2. Comparison of Typical Computed Values of Specific Energy Loss, -dE/dξ

Investigator[a]	Mean Excitation Potential (eV)	-dE/dξ (MeV cm^2 g^{-1}) for 0.5 MeV	1 MeV	2 MeV	3 MeV	6 MeV	10 MeV	20 MeV	30 MeV	60 MeV	100 MeV	200 MeV	500 MeV	1000 MeV
						Beryllium								
Rich	46		247	145.9	106	60.7	39.9	22.5	16.12	9.20	6.19	3.80	2.31	1.856
Williamson	64	348	212	128.6	95.3	56.0	37.3	21.3	15.34	8.80	5.95			
Sternheimer	64			131.9	97.5	56.7	37.6	21.4	15.34	8.79	5.93	3.65	2.215	1.767
Peelle (Preliminary)	64		211.6	130.5	96.5	56.3	37.4	21.4	15.34	8.80	5.94	3.66	2.23	1.795
Bichsel	64			134	98.4	57.0	37.7	21.4	15.38	8.81	5.95	3.66	2.23	1.798
Present Calculation	64	347	220	134	98.3	57.0	37.7	21.4	15.38	8.81	5.95	3.66	2.23	1.798
						Graphite								
Rich	69		241.8	149.7	109.8	63.5	42.0	23.9	17.14	9.83	6.64	4.09	2.49	2.01
Williamson	78.1	379	236	140.3	103.0	60.4	40.4	23.2	16.73	9.64	6.52			
Sternheimer	78			140.6	104.4	61.3	40.9	23.3	16.79	9.65	6.53	4.02	2.448	1.960
Peelle (Preliminary)	78	357	226	139.7	103.8	61.0	40.7	23.3	16.80	9.66	6.53	4.03	2.46	1.986
Present Calculation	80	360	231	142	104.7	61.2	40.8	23.2	16.74	9.62	6.51	4.01	2.45	1.979
						Aluminum								
Rich	150			115	86.2	51.2	34.5		14.56	8.46	5.76	3.58	2.20	1.785
Williamson	169.3	259	177.8	113.1	84.8	50.3	33.8	19.56	14.21	8.29	5.66			
Sternheimer	166			110.8	83.2	49.8	33.8	19.7	14.31	8.33	5.67	3.52	2.17	1.754
Peelle (Preliminary)	166	267	176.8	110.8	83.0	49.8	33.7	19.66	14.29	8.32	5.67	3.53	2.18	1.766
Bichsel	166			110.7	83.2	50.0	33.9	19.76	14.36	8.36	5.70	3.54	2.18	1.771
Present Calculation	163	256	173.3	110.7	83.4	50.1	33.9	19.77	14.36	8.36	5.70	3.54	2.18	1.771
						Copper								
Rich	333.5					40.5	27.8	16.4	12.02	7.07	4.85	3.04	1.891	1.545
Williamson	377.6	139.3	115.4	80.6	62.8	39.2	27.0	16.00	11.71	6.90	4.74			
Sternheimer	371			78.9	61.8	38.7	26.8	15.91	11.68	6.91	4.76	2.99	1.863	1.522
Peelle (Preliminary)	371	176	120.5	78.0	60.1	37.7	26.3	15.76	11.61	6.89	4.75	2.99	1.86	1.525
Bichsel	322			81.1	62.6	39.1	27.1	16.23	11.94	7.07	4.86	3.05	1.90	1.552
Present Calculation	315	169	122.7	80.7	62.8	39.3	27.3	16.27	11.96	7.08	4.87	3.06	1.90	1.555

Table 2 (Cont.)

Investigator	Mean Excitation Potential (eV)	$-dE/dx$ (MeV cm^2 g^{-1}) for 0.5 MeV	1 MeV	2 MeV	3 MeV	6 MeV	10 MeV	20 MeV	30 MeV	60 MeV	100 MeV	200 MeV	500 MeV	1000 MeV
Silver														
Aron	540					33.72	23.49	14.12	10.42	6.20	4.28	2.70	1.693	1.391
Williamson	612	79.2	79.8	61.7	49.7	32.3	22.7	13.73	10.16	6.06	4.18			
Peelle (Preliminary)	611	131.5	101.8	69.2	53.4	33.2	23.2	13.97	10.33	6.18	4.28	2.71	1.70	1.397
Bichsel	485			63.9	50.6	32.5	23.0	14.04	10.41	6.25	4.33	2.74	1.72	1.41
Present Calculation	471	106	91.1	64.6	50.5	32.7	23.1	14.08	10.45	6.26	4.34	2.74	1.72	1.41
Lead														
Rich	943		61.8	47.0	38.5	25.5	18.21	11.21	8.36	5.05	3.52	2.24	1.420	1.175
Williamson	1068	36.4	42.0	40.1	34.5	24.0	17.39	10.83	8.11	4.93	3.44			
Sternheimer	1070			41.1	34.6	23.7	17.18	10.73	8.05	4.90	3.42	2.19	1.390	1.153
Peelle (Preliminary)	1070	32.4	52.0	44.0	36.4	24.3	17.36	10.68	7.99	4.86	3.40	2.18	1.388	1.152
Bichsel	800			45.14	36.36	24.12	17.53	10.98	8.29	5.09	3.57	2.29	1.451	1.201
Present Calculation	988	(76)	53.4	43.9	36.0	23.9	17.42	10.94	8.27	5.07	3.56	2.28	1.447	1.197

a. Methods used for shell correcting are as follows:

Aron: combined overall correction based on graph of Turner.[6]

Rich and Madey: followed Aron et al.[2] in making some correction through the M shell.

Williamson: fitted Walske's[9] K correction for $\eta_K > 0.5$ and ignored L-shell correction and effects for small η_K.

Sternheimer: used K-shell correction of Walske,[9] and also his L-shell correction for Pb and Cu; used $C_L = 0.685/T_p$ for Al; and made corrections for density effect.

Peelle's preliminary calculations: intended to include the K- and L-shell corrections given by Walske and others.[9]

Bichsel's data include fitted shell corrections for all shells.[5]

consulted in producing Turner's graph. This expectation seems to be realized except for low energies in lead.

In the "preliminary" data computed by the author, the values were obtained by a program (not described here) which interpolated K- and L-shell corrections from the works of ref. 9. Since at points these papers are difficult to follow, it is possible that the authors' intentions were not followed precisely in every case. These preliminary energy-loss values are included for comparison with those of Williamson and of Sternheimer, which were computed for similar I values. The discrepancies further illustrate the variety of results which may readily be computed.

6. COMPARISON WITH EXPERIMENT

No extensive direct comparison with experiment has been performed with specific energy losses computed by the method described here. Table 3 compares for a few materials the predicted path lengths corresponding to experiments of Bichsel, Mozley, and Aron[10] and of Mather and Segrè.[13] In each case the experimental value is the path length given by the experimenter after correction for multiple scattering -- there is no guarantee that the methods of correction used were consistent. The computed path-length integrals were obtained by a suitable Gauss quadrature, using energy losses based on the parameters of Table 1. At neighboring energies, where possible, the range values are compared with the recently published compilation of Bichsel.[5] Table 4 compares computed relative energy losses by the author and by Bichsel[5] at 20 MeV against the experimental ones of Burkig and MacKenzie.[14] Agreement is fairly satisfactory except for tantalum.

7. CONCLUSION

On the basis of the comparisons made in the preceding sections it appears that a rather simple program to calculate specific energy loss

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[13] R. Mather and E. Segrè, Phys. Rev. 84, 191 (1951).

[14] V. C. Burkig and K. R. MacKenzie, Phys. Rev. 106, 848 (1957).

Table 3. Comparison of Integrated Path Length Against Experimental Results

Absorber	Experimental Path Length (g/cm^2)	Proton Energy (MeV)	Computed Path Length (g/cm^2)	
			This Paper	Bichsel[a]
Be	0.1379	9.578[b]	0.1370	
		10.0	0.1480	0.1479
	0.400	17.34[b]	0.3985	
		18.0	0.4264	0.4263
	76.7	339.7[c]	77.4	
		300	63.1	63.1
Al	0.0734	6.15[b]	0.0734	
		6.00	0.0704	0.0702
	0.2273	11.82[b]	0.2269	
		12.0	0.2330	0.2329
	0.3440	14.791[b]	0.3433	
		14.0	0.3051	0.3051
	0.4687	17.836[b]	0.4673	
		18.0	0.4749	0.4748
	78.6	338.5[c]	79.7	
		300	65.4	65.5
Cu	0.218	9.938[b]	0.2166	
		10.0	0.2189	0.2201
	0.595	17.893[b]	0.588	
		18.0	0.5943	0.5966
	91.8	337.9[b]	92.2	
		300	76.0	76.2
Ag	0.268	10.022[b]	0.268	
		10.0	0.2672	0.265
	0.7048	17.923[b]	0.7006	
		18.0	0.706	0.704
Au	0.3418	9.698[b]	0.3402	
	0.883	17.549[b]	0.878	

a. H. Bichsel, Sect. 8C in American Institute of Physics Handbook, 2d ed., McGraw-Hill, New York, 1963.

b. H. Bichsel, R. Mozley, and W. Aron, Phys. Rev. 105, 1788 (1957). Errors are stated to be less than 0.14% in energy and 0.1% in range, plus a substantial uncertainty in the multiple-scattering correction applied.

c. R. Mather and E. Segrè, Phys. Rev. 84, 191-3 (1951). A 1% uncertainty in the beam energy is felt by the authors to be dominant.

Table 4. Spot-Check Test Against the Relative Energy-Loss Measurements of Burkig and MacKenzie

Element	Relative Energy Loss[a]		
	Burkig and MacKenzie[b]	This Paper[b]	Bichsel[c]
Al	1.000	1.000	1.000
Be	1.073 ± 0.005	1.083	1.083
Ca	1.008 ± 0.02	0.967	
Cu	0.821 ± 0.002	0.823	0.821
As	0.715 ± 0.003	0.712	0.710
In	0.693 ± 0.002	0.690	
Ta	0.597 ± 0.005	0.579	
Au	0.576 ± 0.003	0.568	
Pb	0.556 ± 0.003	0.553	0.555

a. Compared to aluminum: $(dE/d\xi)_{\text{element}}/(dE/d\xi)_{\text{Al}}$.

b. At 19.8-MeV proton energy.

c. At 20-MeV proton energy.

can be made to reproduce values obtained from more complex computations at an apparent accuracy well within that of most of the experiments on which any computation must be based. The question remains whether a method of the type presented here is superior to other schemes designed for similar purposes. One such method, mentioned by Fano[3] and employed by Berger and Barkas,[15] is based on interpolation formulas of reasonable form directly fitted to the data. This scheme was kindly made available to the author, but slightly too late to be utilized. Also, a calculation much more rapid than the present one for highly repetitive computations could be performed by using interpolation from a table of a hundred or more values, provided that a source of tabulated information is available for all the stopping materials to be employed.

Thus the relatively crude interpolation of the shell correction in the present method gives satisfactory results, but has not been shown to be superior to some other schemes of computation either in accuracy, utility, storage space, or computation speed. It is, however, my belief that for favorable combinations of requirements this intermediate approach, based directly on the Bethe-Bloch equation, is apt to be superior to the other methods mentioned.

---

[15] M. Berger and W. Barkas, private communication (1964). This work is expected to be published in NAS-NRC 1133, the result of a committee to study the status of energy loss computation.

APPENDIX. FUNCTION SUBPROGRAM DEDX(T,L)

The FORTRAN-II subprogram DEDX(T,L) has been utilized on an IBM 7090 to compute the absolute (always positive) value of the specific energy loss in MeV cm^2 g^{-1} for a given incident particle of kinetic energy T (MeV) on material number L. The subprogram must be initialized prior to use to define the important parameters of the Lth material and to inform the routine of the properties of the incident particle. These initializations may be modified at any time by means of the same procedure. As written, the parameters of 12 materials may be stored at a given time in the subroutine storage, though this may be readily modified. As listed, the program with its storage requires 644 memory locations.

The calling program initializes the incident particle by calling DUMMY = DEDX(-XMUAMU, -KZ), where KZ is the integral charge number and XMUAMU is the mass of the incident particle in atomic mass units, physical. (1 amu is taken as 931.14 MeV.) These parameters remain in the program until it is again called with both arguments negative.

The list of material parameters for the Lth absorber is provided by calling DUMMY = DEDX(PARMA, -L), where PARMA is a one-index array of 20 values, including atomic number, atomic mass, average excitation potential, and values for the interpolation of the inner shell nonparticipation correction. These quantities need not be changed for various incident particles, but PARMA also contains the parameters TPEAK, ELPK, TLIM, and ELLIM, which define the low-energy behavior of the returned value of DEDX. These do depend on the identity of the incident particle; so if DEDX values at low energies below TLIM are desired, a different material index must be used for the parameters which give the appropriate low-energy behavior for each incident particle. The definition of the PARMA parameters is contained in the program list on comment cards.

```
 DEDX FOR CALPROT AND GENERAL USE. R. PEELLE.  6-2-64 , REVISED
C
             FUNCTION DEDX( T2, L2)
C
C*    T2 IS PARTICLE KINETIC ENERGY FOR POSITIVE L2
C**      L2 IF POSITIVE IDENTIFIES STOPPING MATERIAL.
C*  L2 AND T2 NEGATIVE SET INCIDENT PARTICLE CHARGE AND MASS IN AMU(PHYS).
C                                MATERIAL SPEC. MUST ACCOUNT LOW ENERGY EFFECTS.
C**     L2 NEGATIVE AND T2 POSITIVE MAKES T2 THE L2 TH MATERIAL COLUMN ARRAY
C
       DIMENSION T2(13), PAR(20, 12)
       TI# T2
       LI # L2
       IF(LI) 51, 1101, 101
   51  IF(TI) 52, 61, 61
   52  ZIN # -LI
       XLN106 # LOGF(1021952.0)
       XMU # -TI* 931.141
       CONST # ZIN**2 • 0.307181
       L # 0
       T # 0.0
C*          NOW INITIALIZED
       RETURN
   61    LM # -LI
        DO 62 L # 1,20
   62    PAR(L,  LM) # T2(L)
       PAR(5, LM) # LOGF( PAR(5, LM) )
       PAR(18, LM) # PAR(8, LM)/ PAR(6, LM)
       PAR(19,LM) # PAR(6, LM)/ PAR(7, LM)
       I #0
       LL#0
       RETURN
C*            THIS STORES ALL PARAMETERS FOR ONE MATERIAL. ROW CODE BELOW
C*     FIRST FOUR PARAMETERS MAY CHANGE FOR EACH NEW INCIDENT PARTICLE
C*       1  TLIM                     8     Z FOR SHELL CORRECTIONS
C        2  ELLIM                    9-17   C/Z INTERPOLATION VALUES AT Z
C        3  TPEAK                   20  ELEMENT NAME
C        4  ELPK                    18  ZSHELL/ZMOLEC
C        5  XI , LOGF(XI)           19   ZMOLEC/ MOLWT
C        6  ZMOLEC
C        7  MOLECULAR WEIGHT
  101  IF(TI - PAR(1,LI))102, 111, 111
  102  IF(TI) 1101, 1101, 1102
 1101    DEDX# 0.0
         GO TO 201
 1102  IF(LL- LI) 103, 104, 103
  103  LL # LI
       ELLIM # PAR(2,LL)
       TPEAK # PAR(3,LL)
       ELPK # PAR(4,LL)
  104  TIMTP # TI- TPEAK
       IF(TIMTP   ) 105, 105, 106
  105  DEDX # ELPK • (1.0-(  TIMTP/TPEAK)**2)
       GO TO 201
  106  RHOHI # (TIMTP   )/(PAR(1,LL) - TPEAK)
       DEDX # RHOHI * ELLIM+(1.0- RHOHI) • ELPK
```

```
 DEDX FOR CALPROT AND GENERAL USE. R. PEELLE.  6-2-64 , REVISED

      GO TO 201
  111 IF(T-T1) 112, 113, 112
  112 T # T1
      E # T+ XMU
      POMUSQ # T* (E+XMU) /XMU**2
      BETASQ # POMUSQ/(1.0 + POMUSQ)
C**       PARTICLE MASS MUST BE PROPERLY SET ELSEWHERE
      XNUM1 # LOGF(POMUSQ) - BETASQ + XLN106
  113 IF(L-L1) 114, 115, 114
  114 L # L1
       ZSHELL # PAR(8, L)
      CONST1 # CONST* PAR(19, L)
      ZRAT # PAR(18, L)
      XLNI #      PAR(5, L)
  115 XLNX # LOGF(BETASQ* 18780.92/ ZSHELL )
C*          NOW INTERPOLATE COZ BETWEEN INDEX+10 AND INDEX+11
      IF(XLNX- 7.0) 119. 120, 120
  120    COZ # 0.0
         GO TO 121
  119 IF(XLNX + 1.0) 122, 122, 123
  122    INDEX # -1
        GO TO 124
  123 INDEX # XLNX
  124 RHOHI # XLNX- FLOATF(INDEX)
      COZ # RHOHI * PAR(INDEX+11, L) + (1.0- RHOHI) * PAR(INDEX+10, L)
      COZ # COZ *  ZRAT
  121 XNUM # XNUM1 - XLNI - COZ
      DEDX # CONST1 * XNUM/BETASQ
  201  RETURN
     END(1,1,0,0,0,0,1,0,0,1,0,0,0,0,0)
```

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