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CASIM Input Parameters for Various Materials

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1 Introduction:

During the past year, the computer program CASIM [1] has been placed in a common area from which copies can be obtained by a wide array of users. The impetus for this arrangement was the need to have a standard code that could be maintained and transported to other platforms. In addition, an historical record would be kept of each version as the program evolved.

CASIM requires a series of parameters (input by the user) that describe the medium in which the cascade develops. Presently a total of 9 materials can be defined. Occasions arise when one needs to know the properties of materials (elements, compounds, and mixtures) that have not been defined. Because it is desirable to have a uniform set of values for all CASIM users, this note presents a methodology for obtaining the input parameters for an arbitrary material. The parameter names and units are listed in TABLE 1. They are read in by the Subroutine CASIM_PROG from the user supplied file CASIM.DAT.

TABLE 1

Parameter	Name	Unit
Atomic Number	ZT	---
Atomic Weight	AT	amu
Density	RHO	gm/cm^3
Ionization Potential	VIP	electron volts
Radiation Length	RALG	cm
Nuclear Radius	RFM	fermi
Elastic Cross Section	SIGL	barn

2 Material Parameters:

In typical cases, the density ρ and chemical composition $C_iD_jE_k$ (where the capital letters represent dummy element symbols) of the material are known. For mixtures the fraction by weight w_m of each of the constituent elements **m** is also known. Using ρ, $C_iD_jE_k$, w_m and **m**, one can obtain a set of input parameters for an arbitrary material.

(a) Atomic Weight and Atomic Number--**AT** and **ZT**.
For an element, AT = A
ZT = Z

For a compound or mixture containing **n** constituent elements,

$$AT = \sum_{m=1}^{n} w_m * A(m) \quad \cdots\cdots\cdots \quad 1$$

$$ZT = \sum_{m=1}^{n} w_m * Z(m) \quad \cdots\cdots\cdots \quad 2$$

Note that for a compound such as $C_iD_jE_k$,

$$w_m = w_c = \frac{i * AT(C)}{i * AT(C) + j * AT(D) + k * AT(E)}$$

(b) Ionization Potential, Radiation Length, Nuclear Radius and Elastic Cross Section--**VIP**, **RALG**, **RFM**, and **SIGL**.

All of these are obtained as functions of **AT** and **ZT**.

The semi-empirical formula given by Segre[2] is used for the ionization potential,

$$VIP = 9.1 * ZT(1.+1.9 * (ZT)^{-2/3}) \quad \cdots\cdots\cdots \quad 3$$

This representation is plotted along with the data from the Radiological Health Handbook[3] in Figure 1.

The radiation length is calculated from a formula in the Particle Properties Data Booklet[4] that approximates the values tabulated by Tsai[5].

$$X_0(g/cm^2) = \frac{716.4 * AT}{ZT * (ZT+1) * \ln\left(287/\sqrt{ZT}\right)}$$

$$RALG = X_0/\rho \qquad \cdots\cdots\cdots \quad 4$$

Nuclear radii as measured in proton-nucleus scattering at 20 GeV by Bellettini *et al.*[6], are compared with those determined in electron-nucleus scattering [7] in Figure 2. As pointed out in ref.[6], agreement is quite good for the lighter elements, but radii obtained in proton scattering are larger by about 0.5 fermi for the heaviest nuclei. For **AT** between 6 and 12 the nuclear radius is approximated by a constant. For masses of 12 and greater, the solid line is a fit of the Bellettini (proton) data to the customary relation **RFM**=$r_0A^{1/3}$.

$$RFM = 3.4 \qquad 6 \le AT < 12 \qquad \cdots\cdots\cdots \quad 5$$

$$RFM = 1.3 * (AT)^{1/3} \qquad AT \ge 12 \qquad \cdots\cdots\cdots \quad 6$$

The elastic cross section (shown in Figure 3) is obtained by taking the difference between the total and inelastic cross sections from ref.[8]. Fig 1 in ref.[9] shows that the correction for quasi-elastic scattering is small. A power law fit to the data in Figure 3 gives a determination of **SIGL** as,

$$SIGL = 0.0099 * (AT)^{0.91} \qquad \cdots\cdots\cdots \quad 7$$

(c) Examples:

Element--molybdenum (Mo).

AT = 96
ZT = 42
RHO = 10.2
VIP = 442.
XO = 10.0
RALG = 0.98
RFM = 5.95
SIGL = 0.630

Compound--beryllium oxide (BeO).

AT = (9/25)*9 + (16/25)*16 = 13.5
ZT = (9/25)*4 + (16/25)*8 = 6.6
RHO = 2.85
VIP = 92.
X0 = 40.9
RALG = 14.3
RFM = 3.10
SIGL = 0.106

Mixture--heavy concrete[10], (silicon 0.7%, iron 62.9%, calcium 3.3%, oxygen 32.2%).

AT = 0.007*28 + 0.629*56 + 0.033*40 + 0.322*16 = 41.9
ZT = 0.007*14 + 0.629*26 + 0.033*20 + 0.322*8 = 19.7
RHO = 4.27
VIP = 226.
X0 = 17.7
RALG = 4.13
RFM = 4.52
SIGL = 0.296

Mixture--ordinary concrete[10], (silicon 10.2%, iron 1.6%, calcium 21.1%, magnesium 6.5%, carbon 7.3%, and oxygen 51.5%).

AT = 22.9
ZT = 11.4
RHO = 2.4
VIP = 143.
X0 = 26.1
RALG = 10.9
RFM = 3.69
SIGL = 0.171

Mixture--moist soil[10], (silicon 22.8%, aluminum 5.5%, iron 2.9%, calcium 6.1%, magnesium 2.1%, carbon 3.3%, and oxygen 55.0%).

AT = 21.6
ZT = 10.7
RHO = 2.25
VIP = 135.
X0 = 27.6
RALG = 12.3
RFM = 3.62
SIGL = 0.162

3 Other Applications:

CASIM has been benchmarked with measurements to a factor of 2 or 3 so that for most applications, the calculation of parameters as given in Section 2 will be adequate. However, other situations arise outside of CASIM where more accurate values are required. Such examples are multiple scattering, target length determinations, and particle production fluxes. This section gives guidelines to obtain more accurate values for the radiation length and the interaction length than what would be obtained by substituting **ZT** and **AT** into the approximate formulas.

For elements listed in the Particle Properties Data Booklet[8], **ZT**, **AT**, X_0, and λ_I should be taken directly. For compounds and mixtures a more accurate value can be obtained by using TABLE 2 and the chemical compositions. Thus,

$$\frac{1}{X_0} = \sum_{m=1}^{n} \frac{w_m}{X_0} \qquad \text{......... } 8$$

For example the radiation length for mylar ($C_5H_4O_2$) would be,

$$\frac{i*A(C)+j*A(D)+k*A(E)}{X_0(mylar)} = \frac{i*A(C)}{X_0(C)} + \frac{j*A(D)}{X_0(D)} + \frac{k*A(E)}{X_0(E)}$$

$$\frac{96}{X_0(mylar)} = \frac{5*12}{42.6983} + \frac{4*1}{63.0470} + \frac{2*16}{34.2381}$$

$$X_0(mylar) = 39.95 \quad g/cm^2$$

For a mixture like air, assuming 76.9% nitrogen, 21.8% oxygen, and 1.3% argon,

$$\frac{1}{X_0} = \frac{.769}{37.9879} + \frac{.218}{34.2381} + \frac{.013}{19.5489}$$

$$X_0 = 36.66 \quad g/cm^2$$

Note that for these compounds/mixtures, the calculated values agree with those given in ref.[8].

At present, CASIM calculates the interaction length, λ_I by taking the atomic weight (**AT**) and interpolating from four materials--beryllium, aluminum, copper, and lead--(9, 85.), (27, 113.), (64, 141.) and (208, 197.). (Note for historical purposes, that the CASIM printout calls λ_I "Collision Length for Nucleons." The CASIM "collision length" is the "nuclear interaction length" given in ref.[8] modified by incoherent elastic scattering from the individual nucleons in the nuclei (quasi-elastic scattering)). The same method can be applied to find λ_I for compounds and mixtures by substituting λ_I for X_0 in equation 8.

X_0 and λ_I for the elements are listed in TABLE 2 in the columns **X0** and **L**. Both are in units of gm/cm^2. X_0 is taken from Tsai[5], as are **ZT** and **AT**. λ_I comes from two sources: (1) the Particle Properties Data Booklet[8] when available, and (2) a supplemental calculation **AT/(N*CS)**. **N** is Avogadro's number and **CS** is the inelastic cross section which was parameterized by Carroll[9] as **CS**(barn) = 0.038***AT****0.72.

References

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[2] E. Segre, Nuclei and Particles, 2nd ed., (Reading, Massachusetts: The Benjamin/Cummings Publishing Company, Inc., 1977), 31.

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[5] Y. S. Tsai, "Pair production and bremsstrahlung of charged leptons", Reviews of Modern Physics 46 (1974), 815.

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[7] R. Herman and R. Hofstadter, High-Energy Electron Scattering Tables, (Stanford, CA: Stanford University Press, 1960), 61.

[8] Ibid., Physical Review D45, III.5.

[9] A. S. Carroll *et al.*, "Absorption Cross Section of Pi$^\pm$, Ka$^\pm$, p and pbar on Nuclei Between 60 and 280 GeV/c", Physics Letters, 80B (1979), 319.

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TABLE 2: Radiation Length(X0) and Interaction Length(L) of the Elements

ZT	AT	X0(g/sq. cm)	CS(barn)	L (g/sq. cm)
1	1.008	63.047	0.033	50.7
2	4.003	94.322	0.102	65.2
3	6.939	82.756	0.157	73.4
4	9.012	65.190	0.199	75.2
5	10.811	52.687	0.213	84.4
6	12.011	42.698	0.231	86.3
7	14.007	37.988	0.265	87.8
8	15.999	34.238	0.292	91.0
9	18.998	32.930	0.319	98.9
10	20.183	28.937	0.347	96.6
11	22.990	27.736	0.366	104.4
12	24.312	25.039	0.381	106.0
13	26.982	24.011	0.421	106.4
14	28.086	21.823	0.440	106.0
15	30.974	21.205	0.453	113.5
16	32.064	19.495	0.465	114.6
17	35.453	19.278	0.499	117.9
18	39.948	19.549	0.566	117.2
19	39.102	17.317	0.536	121.2
20	40.080	16.144	0.546	122.0
21	44.956	16.546	0.592	126.0
22	47.900	16.174	0.637	124.9
23	50.942	15.842	0.648	130.5
24	51.996	14.944	0.658	131.3
25	54.938	14.640	0.684	133.3
26	55.847	13.839	0.703	131.9
27	58.933	13.617	0.720	136.0
28	58.710	12.682	0.718	135.8
29	63.540	12.862	0.782	134.9
30	65.370	12.427	0.776	140.0
31	69.720	12.473	0.812	142.5
32	72.590	12.246	0.858	140.5
33	74.922	11.940	0.855	145.4
34	78.960	11.908	0.888	147.6
35	79.909	11.423	0.896	148.1
36	83.800	11.372	0.927	150.1
37	85.470	11.027	0.940	150.9
38	87.620	10.762	0.957	152.0
39	88.905	10.410	0.967	152.6
40	91.220	10.195	0.985	153.7
41	92.906	9.922	0.999	154.5
42	95.940	9.803	1.022	155.9
43	99.000	9.688	1.045	157.3
44	101.070	9.482	1.061	158.2
45	102.905	9.265	1.075	159.0
46	106.400	9.202	1.101	160.5

TABLE 2: Radiation Length(X0) and Interaction Length(L) of the Elements

ZT	AT	X0(g/sq. cm)	CS(barn)	L (g/sq. cm)
47	107.870	8.970	1.112	161.1
48	122.400	8.994	1.217	167.0
49	114.820	8.849	1.163	164.0
50	118.690	8.817	1.210	162.9
51	121.750	8.724	1.213	166.7
52	127.600	8.827	1.254	168.9
53	126.904	8.480	1.249	168.7
54	131.300	8.482	1.290	169.0
55	132.905	8.305	1.292	170.9
56	137.340	8.307	1.323	172.4
57	138.910	8.138	1.333	173.0
58	140.120	7.956	1.342	173.4
59	140.907	7.758	1.347	173.7
60	144.240	7.705	1.370	174.8
61	145.000	7.519	1.375	175.1
62	150.350	7.573	1.411	176.9
63	151.960	7.438	1.422	177.4
64	157.250	7.483	1.458	179.1
65	158.924	7.356	1.469	179.7
66	162.500	7.320	1.493	180.8
67	164.930	7.233	1.509	181.5
68	167.260	7.145	1.524	182.3
69	168.934	7.032	1.535	182.8
70	173.040	7.021	1.562	184.0
71	174.970	6.924	1.574	184.6
72	178.490	6.891	1.597	185.6
73	180.948	6.818	1.613	186.3
74	183.850	6.763	1.650	185.0
75	186.200	6.690	1.646	187.8
76	190.200	6.676	1.671	189.0
77	192.200	6.594	1.684	189.5
78	195.090	6.543	1.708	189.7
79	196.967	6.461	1.714	190.8
80	200.590	6.437	1.737	191.8
81	204.370	6.418	1.760	192.8
82	207.190	6.369	1.770	194.4
83	208.980	6.290	1.788	194.0
84	210.000	6.191	1.795	194.3
85	210.000	6.065	1.795	194.3
86	222.000	6.283	1.868	197.4
87	223.000	6.187	1.874	197.6
88	226.000	6.148	1.892	198.4
89	227.000	6.056	1.898	198.6
90	232.038	6.073	1.928	199.8
91	231.000	5.932	1.922	199.6
92	238.030	5.999	1.980	199.6

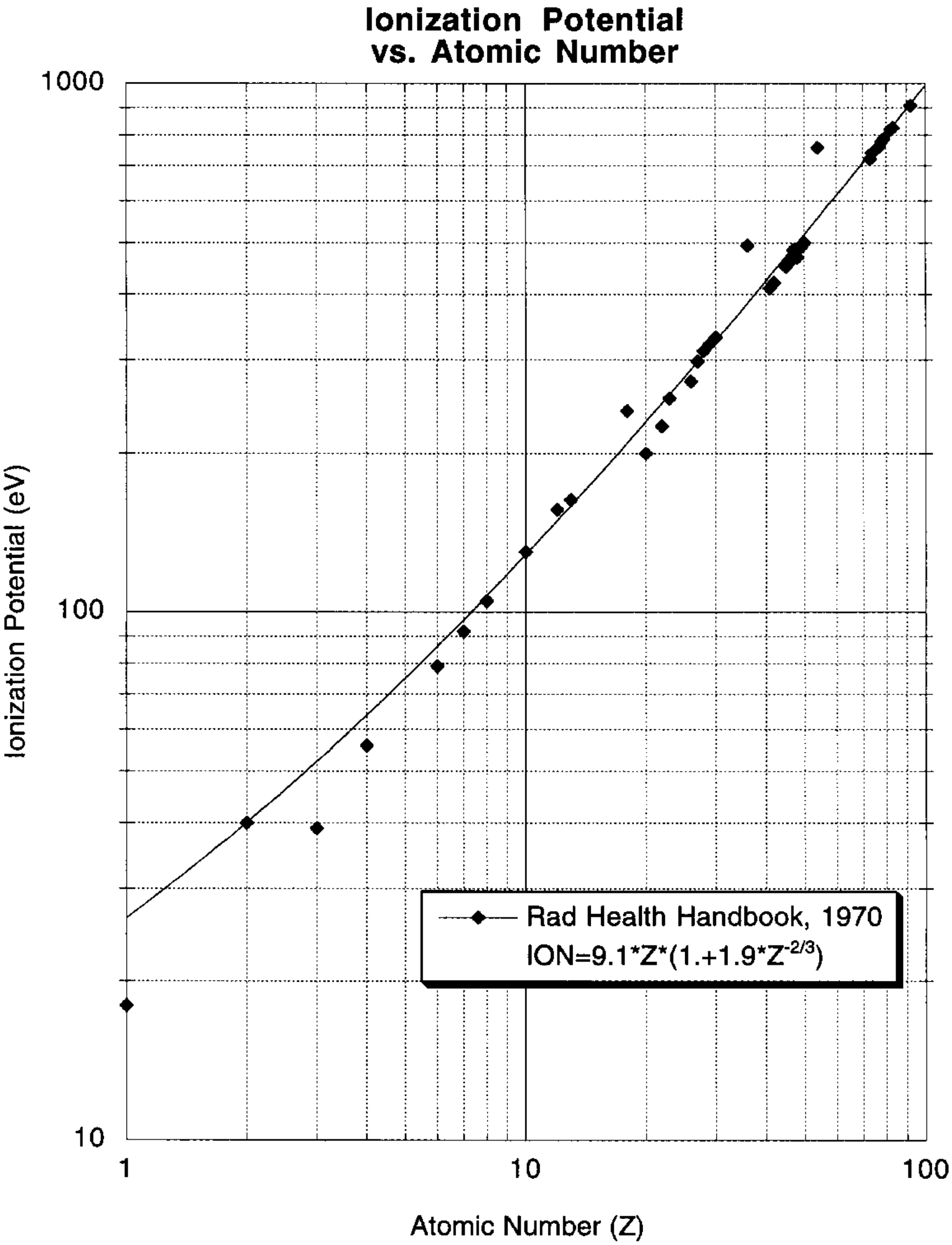
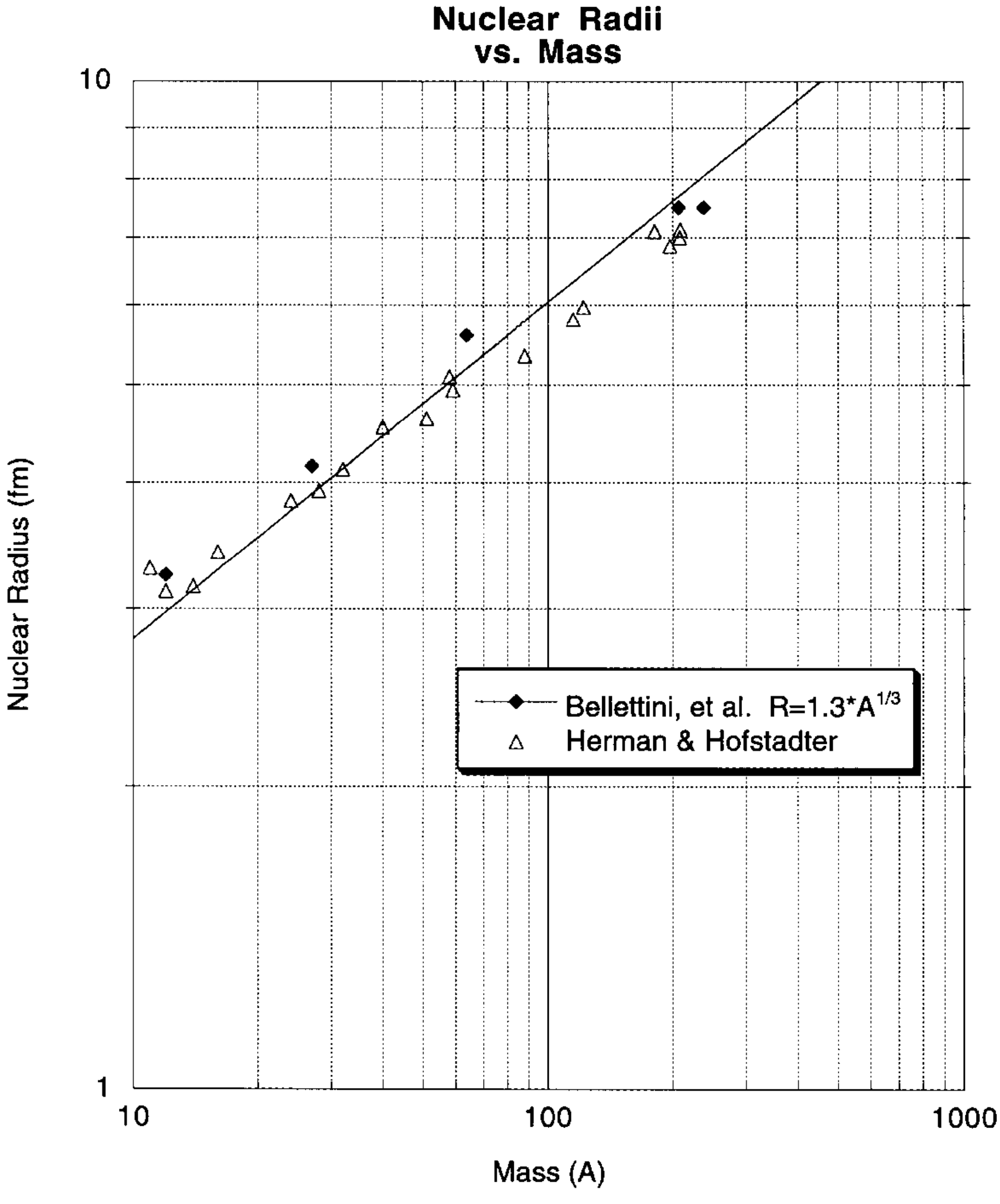
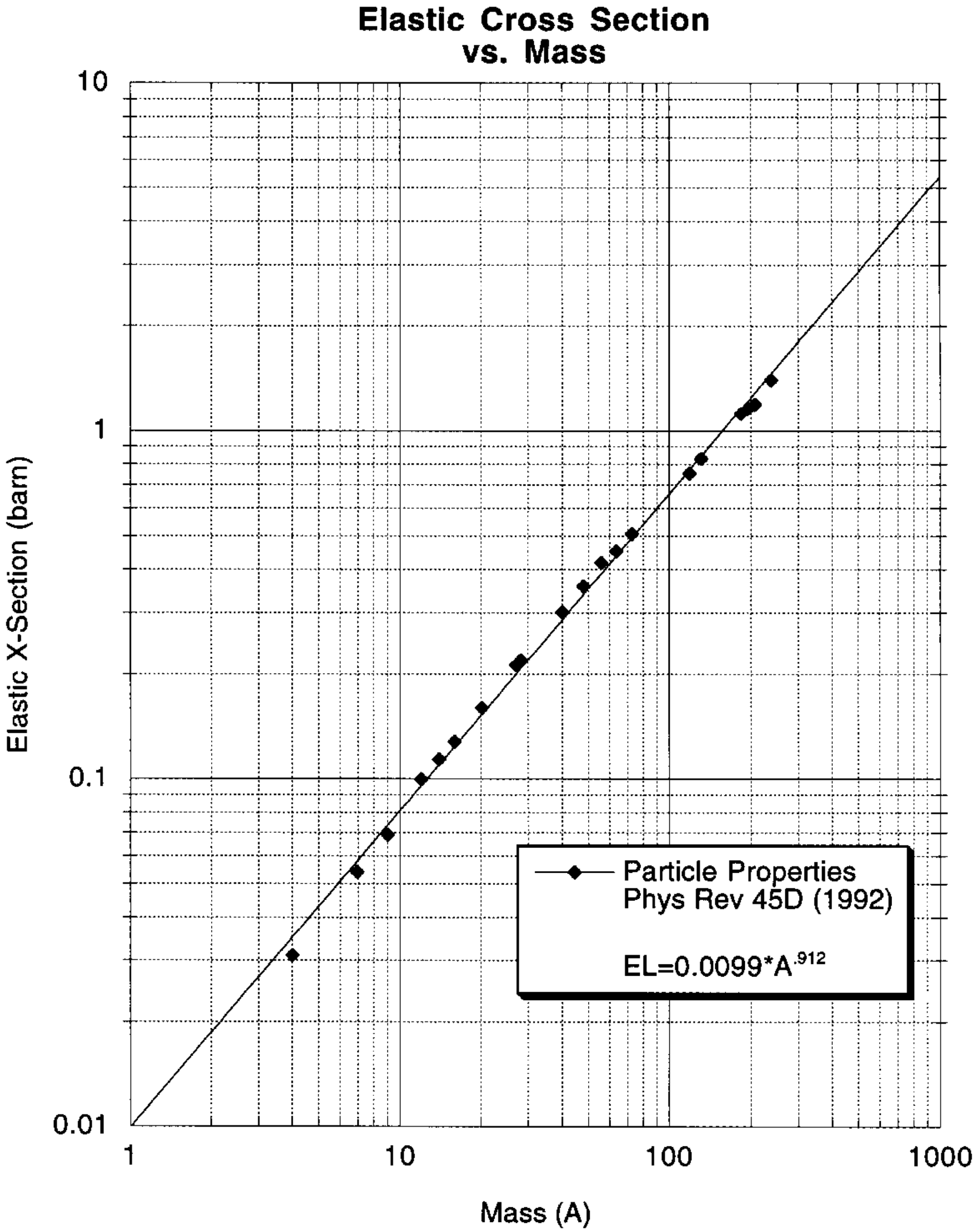

Ionization Potential
vs. Atomic Number
1000
100
10
Ionization Potential (eV)
1
10
100
Atomic Number (Z)
Rad Health Handbook, 1970
ION=9.1*Z*(1.+1.9*Z^-2/3)

Figure 1



Nuclear Radii
vs. Mass
10
1
10
100
1000
Nuclear Radius (fm)
Mass (A)
Bellettini, et al. R=1.3*A^1/3
Herman & Hofstadter

Figure 2



Elastic Cross Section
vs. Mass
10
1
0.1
0.01
Elastic X-Section (barn)
1
10
100
1000
Mass (A)
Particle Properties
Phys Rev 45D (1992)
EL=0.0099*A^.912

Figure 3