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Atomic and Nuclear Properties of Materials

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ATOMIC AND NUCLEAR PROPERTIES OF MATERIALS

Abstract

Additional comments and background material are given for the table of "atomic and nuclear properties of materials" which is published by the Particle Data Group in their "Review of Particle Properties" (Rosenfeld Tables).

ATOM- UND KERNEIGENSCHAFTEN VON MATERIALIEN

Zusammenfassung

Es werden zusätzliche Kommentare und Hintergrundmaterial für die Tabelle "Atomic and nuclear properties of materials" zusammenge stellt, die von der Particle Data Gruppe in ihrer Übersicht von Teilcheneigenschaften (Rosenfeld-Tabellen) veröffentlicht wird.

In this note we give additional comments and background material to the table of "Atomic and Nuclear Properties of Materials" in the "Review of Particle Properties", as published by the Particle Data Group. The final compilation is shown in Table 1 and the following sections refer to the vertical columns of this table.

1. Nuclear Total Cross Section σ_T

The σ_T are mean values of neutron nuclei cross-section in the energy range 80-240 GeV. Experimentally well-established points are taken from Murthy et al⁽¹⁾ for H₂, D₂, Be, C, Al, Fe, Cu, W, Pb and U. To find cross-sections for atomic numbers that have not been measured two fits for interpolation are used:

- a) for elements heavier than Be the authors of Ref. 1 give

$$\sigma_T = 49.7 \times A^{0.77},$$

- b) for all nuclei a parametrization is used, which is derived from a simple optical model assuming that the absorption is proportional to the length of nuclear matter transversed. One finds⁽²⁾

$$\sigma_T = 2\pi R^2 \{ 1 - 1/2\kappa^2 |1 - (2\kappa + 1)e^{-2\kappa}| \} \text{ with } \kappa = R/x.$$

$R = r_0 A^{1/3}$ is the nuclear radius and x is the absorption length for neutrons in nuclear matter. A fit to the measured mean cross-sections gives $r_0 = 1.20$ fm and $x = 2.78$ fm. With these parameters the interpolation for the table was carried out, the values for all elements used are given in Table 2, column 4. The original values taken from the measurements are underlined.

A graphic presentation of the fit together with the measured cross-section is shown in Fig. 1 (upper curve). The fit agrees with the measured values within $\pm 1.5\%$.

A more precise interpolation is obtained when fitting the total cross-sections for each energy separately. The nuclear radius r_0 turns out to have the nearly energy independent value of 1.2 fm, which agrees satisfactorily with the value obtained from electron scattering. The nuclear absorption χ has a clear energy dependence as shown in Fig. 2, which has to be taken into account if an energy dependent interpolation is needed.

2. Nuclear Inelastic Cross Section σ_I

The σ_I are mean values of neutron nuclei cross-sections in the energy range 60-375 GeV taken from Roberts et al⁽³⁾. The inelastic cross-section is obtained from the total cross-section by subtracting a) the coherent elastic scattering σ_E and b) the quasi-elastic scattering σ_Q , i.e. scattering wherein the nucleus is disrupted but there are no meson produced:

$$\sigma_I = \sigma_{\text{Tot}} - \sigma_E - \sigma_Q$$

This inelastic cross-section is of practical interest in many applications as attenuation length in matter, nuclear absorption, punch-through calculation, etc. Like for the total cross-section interpolation was done with an exponential $\sigma_I = 39.64 \times A^{0.715}$ as given by the authors of Ref. 3 for elements heavier than Be and by the optical model formula. The measured and fitted values agree within $\pm 2\%$ as shown in Fig. 1 (lower curve). The interpolated cross-sections are given in column 5 of Table 2.

Inelastic cross-sections for charged mesons π^+ , π^- , k^+ , k^- and for protons and antiprotons can be found in Carroll et al⁽⁴⁾.

3. Energy Loss for Minimum-Ionizing Particles

A) ΔE is the stopping power or the mean energy loss per path length of 1 g/cm² for particles heavier than electrons. The numbers are taken from Ref. 5 and plotted in Fig. 3. Values other than

calculated are found by interpolation following the two curves for gases (full line) and solids (dashed line). The two curves differ as the result of the density correction term. The values for ΔE are given in column 6 of Table 2, the calculated values are underlined. For compounds and mixtures with an atomic number A_{1+2} the values are calculated according to

$$\underline{\Delta E}(A_{1+2}) = (\underline{\Delta E}(A_1) \times A_1 + \underline{\Delta E}(A_2) \times A_2)/A_{1+2}$$

This relation holds within a few percent (Bragg rule) - see Ref. 6. The values for various compounds are given in Table 3.

- B) E_p is the most-probable energy deposited on a path length of 1 cm. For calculation Landau's formula with the modification of Maccabee and Papworth⁽⁷⁾ is used

$$E_p = \frac{Ax}{\beta^2} \left| \ln \left(\frac{2mc^2}{I^2} \times \frac{(\beta\gamma)^2}{\beta^2} \times Ax \right) + 0.198 - \beta^2 - \delta \right|$$

$$A = 0.153 \times Z/A \times \rho \text{ with } \rho = \text{density in g/cm}^3$$

For minimum ionization $\beta = 0.96$ and $\gamma = 3.4$ are taken, the density correction has been neglected (it would amount to approximately 3% for light and 1% for heavy nuclei).

The calculated values for E_p together with the mean excitation energy I used are given in Table 2. The values of I follow the expression $I/Z = 9.76 + 58.8 Z^{-1.19}$ as given by Sternheimer⁽⁸⁾. A more recent best guess can be found in Ref. 9.

For compounds the mean excitation energy is given as

$$\ln I = \sum_k f_k I_k$$

where f_k is the fractional number of electrons in the k^{th} atomic species with excitation potential I_k . The mean value of Z/A is

given by

$$Z/A = \sum_k n_k (Z/A)_k,$$

where n_k is the partial density of the k^{th} atomic component. Experimental results for E_p agree within the experimental uncertainties with the values calculated by the formula - see, e.g., for NaI the measurements of Bellamy et al⁽¹⁰⁾ and for gases the article of Cobb et al⁽¹¹⁾.

The values for compounds are given in Table 3.

4. Radiation Length

The values given in the tables are from the most recent calculation of Y.S. Tsai⁽¹²⁾. The figures refer to the infinite energy limit. A correction table for finite energy can be found in Tsai's article, the corrections amount to 5-10% at 1 GeV.

For chemical compounds or mixtures of molecules with the atomic weight $A_{12} = A_1 + A_2$ the formula

$$\frac{A_{12}}{X_{12}} = \frac{A_1}{X_1} + \frac{A_2}{X_2}$$

was used. The values of Tsai refer strictly only to free atoms; effects of molecular bindings, crystal structures, polarization of the medium, etc. are ignored. Calculations for molecules have been performed for H_2 by Bernstein and Panofsky⁽¹³⁾, who find a 2.8% decrease of the radiation length and for N_2 and O_2 by Genannt and Pilkuhn⁽¹⁴⁾, who find a 5.3% and 4.4% decrease. For the values for H_2 , D_2 , N_2 , O_2 and air quoted in the tables these reduction factors have been applied to the values of Tsai. For a discussion of effects in crystal structures see the review in the book of Ter-Mikaelian⁽¹⁵⁾.

5. Density and Refractive Index

- Values can be found in a variety of standard works and encyclopaedias. For the compilation the following handbooks were used:
 - Handbook of Chemistry and Physics, 61st edition, CRC-Press 1980-81
 - American Institute of Physics Handbook, 3rd edition, McGraw-Hill, 1972
 - Landolt-Börnstein, 6th edition, Springer Verlag, Berlin, Heidelberg, New York, 1972
 - D'Ans-Lax, Taschenbuch für Chemiker und Physiker, 3rd edition, Springer Verlag, Berlin, Heidelberg, New York, 1967
 - Gas Encyclopaedia, Elserier, Amsterdam, 1976
- Deuteron values are given in:
Advances of Cryogenics Engineering 15 (1970) 65
- H₂ and H-Ne mixtures in~
R.W. Newport, "Bubble chamber technology", Proc. Int. Conf. on Bubble Chamber Techniques, June 1970, ANL.
- Propane values in:
R.P. Shutt, "Bubble and Spark Chambers", Vol. I, pg. 167, Academic Press 1967
- Information on bubble chamber operation and physical constants of liquids by:
G. Harigel, CERN-BEBC,
- on standard shielding by:
K. Göbel, CERN-SPS.

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- (13) D. Bernstein and W.K.H. Panofsky, Phys. Rev. 102 (1962) 522
- (14) R. Genannt and H. Pilkuhn, Proceedings 13th Int. Cosmic Ray Conf. (Denver 1973) pg. 2434
- (15) M.L. Ter-Mikaelian, "High-Energy Electromagnetic Processes in Condensed Media", Wiley-Interscience, New York 1972

Figures and Table Captions

Figure 1: Neutron nuclei total and inelastic cross-sections.

The curves show the optical model fit as described in the text.

Figure 2: The parameter r_0 and x (= attenuation length in nuclear matter) of the optical model fit. The values for 11, 14 and 21 GeV are taken from Ref. 2.

Figure 3: The energy loss for minimum-ionizing particles heavier than electrons as taken from Ref. 5. The interpolation lines are hand drawn, the solid line connects values for gases and the dashed line connects values for liquids and solids.

Table 1: Final compilation

Table 2: Compilation for elements including in the lower part elements occurring only in compounds of Table 1. The underlined cross-sections are measured values. The underlined values for ΔE and I are taken from Ref. 5.

Table 3: Compilation for compounds. The underlined values for ΔE and I are taken from Ref. 5.

Material	Z	A	Nuclear ^{a)} total cross-section σ_t [barn]	Nuclear ^{b)} inelastic cross-section σ_i [barn]	Nuclear ^{c)} length of interaction λ_T	Nuclear ^{c)} length of interaction λ_I	dE/dx min ^{d)} [MeV/g/cm ²] for gas	Ep [keV/cm]	Radiation length ^{e)} l_{rad} [g/cm ²]	Density ^{f)} [g/cm ³] (ρ) is for gas	Refractive Index ^{g)} (n) is for gas for gas ($n-1$) $\times 10^6$	
H ₂	1	1.01	0.0387	0.033	43.3	50.8	4.12	(0.19)	61.28	865	0.0708(0.090)	1.112 (140)
D ₂	1	2.01	0.073	0.061	45.7	53.7	2.07	(0.17)	122.6	764	0.162 (0.177)	1.28
He	2	4.00	0.133	0.102	49.9	65.1	1.94	(0.16)	94.32	755	0.125 (0.178)	1.024 (35)
Li	3	6.94	0.211	0.157	54.6	73.4	1.58	0.70	82.76	155	0.534	-
Be	4	9.01	0.268	0.199	55.8	75.2	1.61	2.61	65.19	35.3	1.848	-
C	6	12.01	0.331	0.231	60.2	86.3	1.78	3.57	42.70	18.8	2.265 ^{g)}	-
H ₂ O	7	14.01	0.379	0.265	61.4	87.8	1.82	(0.93)	35.97	44.5	0.808(1.25)	1.205(300)
O ₂	8	16.00	0.420	0.292	63.2	91.0	1.82	(1.31)	32.73	28.7	1.14 (1.43)	1.22 (266)
Ne	10	20.18	0.507	0.347	66.1	96.6	1.73	(0.75)	28.94	24.0	1.207(0.90)	1.092(67)
Al	13	26.98	0.634	0.421	70.6	106.4	1.62	3.81	24.01	8.9	2.70	-
Ar	18	39.95	0.868	0.566	76.4	117.2	1.51	1.30	19.55	14.0	1.40 (1.78)	1.233(283)
Fe	26	55.85	1.120	0.703	82.8	131.9	1.48	10.7	13.84	1.76	7.87	-
Cu	29	63.54	1.232	0.782	85.6	134.9	1.44	11.85	12.86	1.43	8.96	-
Sn	50	118.69	1.967	1.21	100.2	163.	1.26	8.3	8.82	1.21	7.31	-
Xe	54	131.30	2.120	1.29	102.8	169.	1.24	(3.57)	8.48	2.88	3.057(5.89)	(705)
W	74	183.85	2.767	1.65	110.3	185.	1.16	21.1	6.76	0.35	19.3	-
Pb	82	207.19	2.960	1.77	116.2	194.	1.13	11.7	6.37	0.56	11.35	-
U	92	238.03	3.378	1.98	117.0	199.	1.09	19.3	6.00	≈0.32	≈18.95	-
Air (20°C)				62.0	90.0	1.82	(1.12)	34.84	28993	0.001205	1.000273	
H ₂ O				60.1	84.9	2.03	1.72	36.08	36.1	(1.29)	(293)	
Shielding Concrete ^{h)}				67.4	99.9	1.70	3.68	26.7	10.7	1.00	1.33	
SiO ₂ (quartz)				67.0	99.2	1.72	3.28	27.05	12.3	2.5	-	
SiO ₂ (bubble chamber 26°K)				43.3	50.8	4.12	0.20	61.28	≈1000	≈0.063 ^{j)}	1.112	
D ₂ (bubble chamber 31°K)				45.7	53.7	2.07	0.22	122.6	≈ 900	≈0.140 ^{j)}	1.110	
H-Ne mixture (50 mole percent) ^{j)}				65.0	94.5	1.84	0.59	29.70	73.0	0.407	1.092	
Propane (C ₃ H ₈) ^{k)}				56.5	77.2	2.25	(2.54)	45.38	111	0.41 (2.0)	1.25(1005)	
Ilford emulsion G5				82.0	134	1.44	4.79	11.0	2.89	3.815	-	
NaI				94.8	152	1.32	4.13	9.49	2.59	3.67	1.775	
LiF				62	89.2	1.63	3.78	39.25	14.9	2.64	1.394	
BGO (Bi ₄ Ge ₃ O ₁₂)				97.4	156	1.27	8.07	7.98	1.12	7.1	2.15	
Polystyrene, scintillator (CH) ^{f)}				58.4	82.0	1.95	1.72	43.8	42.4	1.032	1.581	
Lucite, Plexiglas (C ₅ H ₈ O ₂)				59.2	83.6	1.95	1.98	40.55	≈ 34.4	1.16 - 1.20	≈1.49	
Polyethylene (CH ₂)				56.9	78.8	2.09	1.68	44.8	≈ 47.9	0.92 - 0.95	-	
Mylar (C ₅ H ₄ O ₂)				60.2	85.7	1.86	2.24	39.95	28.7	1.39	-	
Borosilicate glass (Pyrex) ^{m)}				66.2	97.6	1.72	3.32	28.3	12.7	2.23	1.474	
CO ₂				62.4	90.5	1.82	(1.92)	36.2	20220.	1.977	(410)	
Methane CH ₄				54.7	74.0	2.41	(0.91)	46.5	64850.	0.423	(444)	
Isobutane C ₄ H ₁₀				56.3	77.4	2.22	(3.43)	45.2	16930.	{0.717}	(1270)	
Freon 12 (CCl ₂ F ₂) ⁿ⁾				70.6	106	1.62	(4.49)	23.7	4810.	{2.67}	(1080)	
Freon 13 (CClF ₃) ⁿ⁾				68.1	101	1.64	(3.91)	27.1	6370.	(4.93)	(720)	
Silica Aerogel ^{o)}				65.5	95.7	1.83	0.28	29.85	≈150.	(4.26)	1.0+0.25 ρ	
Spark or proportional chamber ^{p)}				0.028%	0.020%	-	0.034	0.067%	0.019			

* Table revised March 82 by J. Engler. For details see Report KfK 3386B, Kernforschungszentrum D 75 Karlsruhe, P.O. Box 3640.

a) σ_{total} at 80-240 GeV for neutrons ($\approx \sigma$ for protons) from Murthy et al., Nucl. Phys. B92(1975) 269.

b) σ_{inelastic} = σ_{total} - σ_{elastic} at 60-375 GeV for neutrons from Roberts et al., Nucl. Phys. B159(1979) 56 and for protons from Carroll et al., Nucl. Phys. Lett. 80B(1979) 319. σ_T(p)=σ_T(n), for other particles see Carroll et al.

c) Mean free path between collision (λ_T) or inelastic interaction (λ_I), calculated λ = A/(Nσ_T).

d) For minimum-ionizing protons and pions. ΔE is energy loss per g/cm² from Barkas and Berger, Tables of Energy Losses and Ranges of Heavy Charged Particles, NASA-SP-3013(1964), for electrons see Penetration of Charged Particles in Matter, NAS-NS39(1964). Ep is the most probable deposited energy per cm, in MeV for solids and liquids, in keV for gases.

e) From Y.S. Tsai, Rev. Mod. Phys. 46(1974) 815. Corrections for molecular binding applied for H₂, D₂, N₂, O₂ and air.

f) Values for solids, or the liquid phase at boiling point. Values in parentheses for gaseous phase STP(0°C, 1 atm), except where noted. Refr. active index for sodium D line.

g) For pure graphite, industrial graphite density may vary 2.1 - 2.3 g/cm³.

h) Standard shielding blocks, typical composition O₂ 52%, Si 32.5%, Ca 6%, Na 1.5%, Fe 2%, Al 4% plus reinforcing iron bars.

i) Attenuation length λ = 115 ± 5 g/cm², also valid for earth (typical ρ = 2.15) from CERN-LRL-RHEL Shielding exp. UCRL 17841(1968).

j) Density may vary about ±3%, depending on operation conditions.

k) Values for typical working condition with H₂ target; 50 mole percent, 29°C, 7 atm.

l) Values for typical chamber working conditions: Propane ~ 57°C, 8-10 atm. Freon 13B1 ~ 28°C, 8-10 atm.

m) Main components: 80% SiO₂ + 12% B₂O₃ + 5% Na₂O.

n) Used in Cerenkov counters, values at 26°C and 1 atm. Indices of refraction from E.R. Hayes, R.A. Schluter, and A. Tamosaitis, ANL-6916 (1964).

o) n(SiO₂) + 2n(H₂O) used in Cerenkov counters, ρ = density in g/cm³. From M. Cantin et al., Nucl. Instr. Meth. 118, 177(1974).

p) Values for typical construction: 2 layers 50 μm Cu/Be wires, 8 mm gap, 60% isobutane or CO₂, 2 layers 50 μm Mylar/Aclar foils.

Element	Z	A	σ_T barn	σ_I barn	dE/dx (Min)		I (eV)	Radiation Length (g/cm ²)
					ΔE MeV/gcm ⁻²	E_p MeV/cm (keV/cm)		
H ₂	1	1.01	<u>0.0387</u>	<u>0.033</u>	<u>4.12</u>	(0.190)	<u>18.7</u>	61.28
D ₂	1	2.01	<u>0.073</u>	<u>0.061</u>	<u>2.07</u>	(0.165)	<u>18.7</u>	122.6
He	2	4.00	<u>0.132</u>	0.102	<u>1.94</u>	(0.159)	<u>42.0</u>	94.32
Li	3	6.94	0.211	0.157	1.58	0.70	50.3	82.76
Be	4	9.01	<u>0.268</u>	<u>0.199</u>	<u>1.61</u>	2.61	<u>60.0</u>	65.19
C	6	12.01	<u>0.331</u>	<u>0.231</u>	<u>1.78</u>	3.57	<u>78.0</u>	42.70
N ₂	7	14.01	0.378	0.265	1.82	(0.925)	90.7	35.97
O ₂	8	16.00	0.421	0.292	1.82	(1.314)	100.9	32.73
Ne	10	20.18	0.507	0.347	<u>1.73</u>	(0.747)	<u>131.</u>	28.94
Al	13	26.98	<u>0.634</u>	<u>0.421</u>	<u>1.62</u>	3.81	<u>163.</u>	24.01
Ar	18	39.95	0.868	0.566	<u>1.51</u>	(1.295)	<u>210.</u>	19.55
Fe	26	55.85	<u>1.113</u>	<u>0.703</u>	<u>1.48</u>	10.7	<u>273.</u>	13.84
Cu	29	63.54	<u>1.232</u>	<u>0.782</u>	<u>1.44</u>	11.85	<u>314.</u>	12.86
Sn	50	118.69	<u>1.120</u>	1.21	1.26	8.27	516.	8.82
Xe	54	131.30	2.120	1.29	<u>1.24</u>	(3.57)	<u>555.</u>	8.48
W	74	183.85	<u>2.767</u>	<u>1.65</u>	1.16	21.1	748.	6.76
Pb	82	207.19	<u>2.960</u>	<u>1.77</u>	<u>1.13</u>	11.7	<u>826.</u>	6.37
U	92	238.03	<u>3.378</u>	<u>1.98</u>	<u>1.09</u>	19.3	<u>923.</u>	6.00
B	5	10.8	0.305	0.219	1.67		75.	52.69
F	9	19.0	0.484	0.332	1.65		120.	32.93
Na	11	22.99	0.563	0.381	1.63		140.	27.74
Si	14	28.09	0.660	0.440	1.67		170.	21.82
Cl	17	35.45	0.792	0.520	1.58		198.	19.28
Ca	20	40.08	0.871	0.567	1.63		228.	16.14
Ge	32	72.6	1.368	0.861	1.37		345.	12.25
Br	35	79.91	1.470	0.920	1.35		374.	11.42
Kr	36	83.8	1.523	0.951	<u>1.35</u>		<u>381.</u>	11.37
Ag	47	107.8	1.835	1.13	<u>1.32</u>		<u>487.</u>	8.97
I	53	126.9	2.067	1.26	1.23		547.	8.48
Au	79	197.0	2.842	1.71	<u>1.15</u>		<u>797.</u>	6.46
Bi	83	209	2.964	1.78	1.13		835.	6.29

Table 2: Compilation for elements including in the lower part elements occurring only in compounds of Table 1. The underlined cross-sections are measured values. The underlined values for ΔE and I are taken from Ref. 5.

Material	Z/A	λ_T g/cm ²	λ_I g/cm ²	dE/dx (min)		I eV	Radiation Length g/cm ²
				ΔE MeV/gcm ⁻²	E_p MeV/cm (keV/cm)		
Air	.50	62.0	90.0	<u>1.82</u>	(1.12)	<u>86.8</u>	34.84
H ₂ O	.555	60.1	84.9	<u>2.03</u>	1.72	<u>65.1</u>	36.08
Concrete	0.5	67.4	99.9	1.70	3.3	128	26.7
SiO ₂ (quartz)	.50	67.0	99.2	1.72	3.28	128.7	27.05
H ₂ (26° K)	1.0	43.3	50.8	4.12	0.198	18.7	61.28
D ₂ (31° K)	.5	45.7	53.7	2.07	0.221	18.7	122.6
H-Ne(50%)	.524	65.0	94.5	1.84	0.588	110.	29.7
Propane	.591	56.5	77.2	2.25	(2.54)	50.3	45.38
Emulsion	.454	82.0	134.	<u>1.44</u>	4.79	307.	11.0
NaI	.427	94.8	152.	<u>1.32</u>	4.13	<u>433.</u>	9.49
LiF	.463	62.	89.2	<u>1.63</u>	3.78	96.5	39.25
BGO	.420	97.4	156.	1.27	8.07	482.	7.98
Scintillator	.538	58.4	82.0	1.95	1.72	63.6	43.8
Lucite	.540	59.2	83.6	<u>1.95</u>	1.98	<u>65.6</u>	40.55
Polyethylene	.571	56.9	78.8	<u>2.09</u>	1.68	<u>54.6</u>	44.8
Mylar	.521	60.2	85.7	1.86	2.24	75.5	39.95
Pyrex	.50	66.2	97.6	1.72	3.32	128.	28.3
CO ₂	.50	62.4	90.5	<u>1.82</u>	(1.92)	<u>85.9</u>	36.2
Methane	.625	54.7	74.0	<u>2.41</u>	(0.91)	44.1	46.5
Isobutane	.586	56.3	77.4	2.22	(3.43)	51.2	45.2
Freon 12	.480	70.6	106.	1.62	(4.49)	154.	23.7
Freon 13	.479	68.1	101.	1.64	(3.91)	135.	27.1
Silica Aerogel	.520	65.5	95.7	1.83	0.28	98.	29.85

Table 3: Compilation for compounds. The underlined values for ΔE and I are taken from Ref. 5.

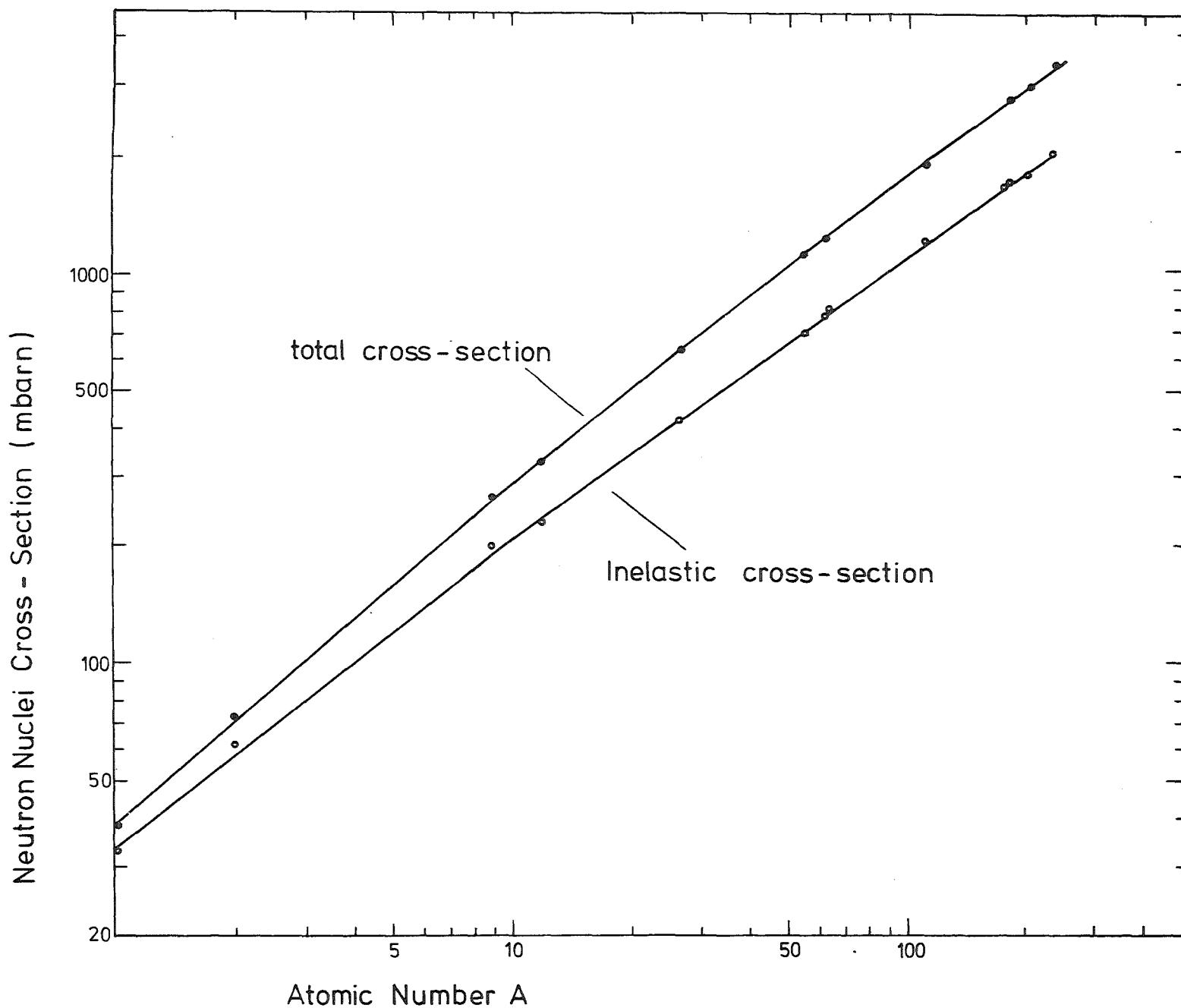


Figure 1: Neutron nuclei total and inelastic cross-sections.
The curves show the optical model fit as described
in the text.

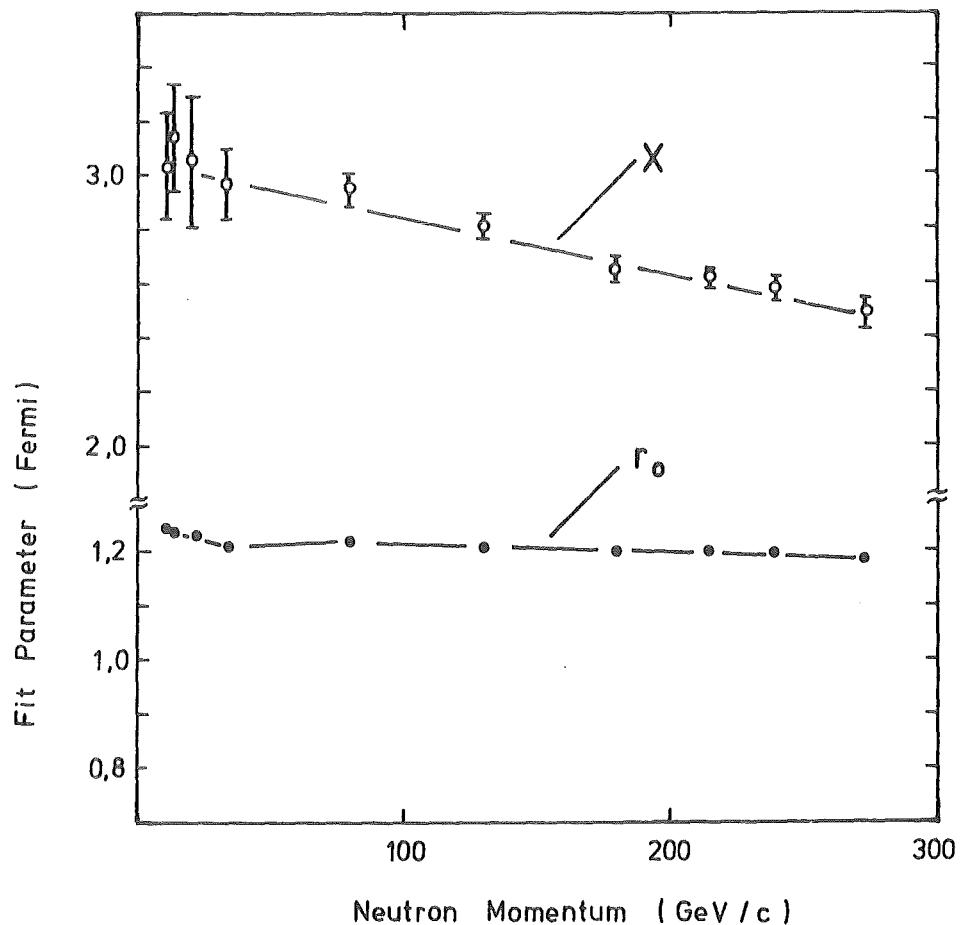


Figure 2: The parameter r_0 and x (= attenuation length in nuclear matter) of the optical model fit. The values for 11, 14 and 21 GeV are taken from Ref. 2.

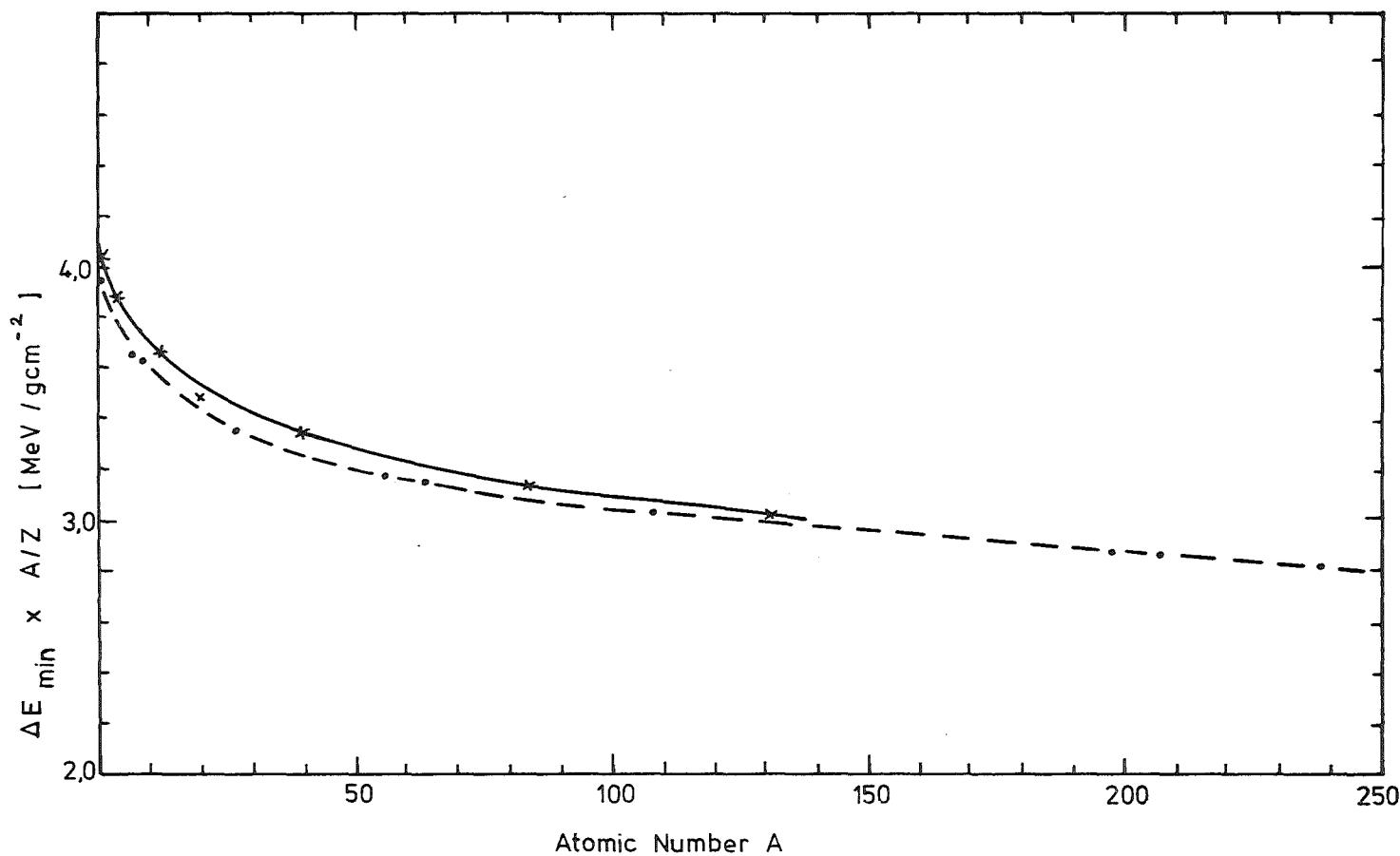


Figure 3: The energy loss for minimum-ionizing particles heavier than electrons as taken from Ref. 5. The interpolation lines are hand drawn, the solid line connects values for gases and the dashed line connects values for liquids and solids.