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The Stopping Power of Matter for Positive Ions

Helmut Paul
Johannes Kepler University Linz,
Austria

1. Introduction

When a fast positive ion travels through matter, it excites and ionizes atomic electrons, losing energy. For a quantitative understanding of radiotherapy by means of positive ions, it is necessary to know the energy loss per unit distance of matter transversed, S, which is alternatively called stopping power or stopping force or linear energy transfer (LET)[1]. To avoid a trivial dependence of the linear stopping power S upon the density ρ, one often uses the mass stopping power S/ρ instead. In the following, we discuss experimental and theoretical stopping power data. Using our large collection[2] (Paul, 2011a) of experimental stopping data for ions from $_1H$ to $_{92}U$, the reliability of various stopping theories and stopping tables is estimated by comparing them statistically to these data. We consider here only the electronic (not the "nuclear") energy loss of ions in charge equilibrium.

We treat both gaseous and condensed targets (i.e., targets gaseous or condensed at normal temperature and pressure), and we treat them separately. Solid targets are assumed to be amorphous or polycrystalline. We treat elements, compounds and mixtures.

1.1 Tables and programs

The tables and computer programs used here are listed in Table 1. Program PASS (on which the tables in ICRU Report 73 are based) and the program by Lindhard and Sørensen (1996) (LS) are based on first principles only. The same is true for CasP (Grande & Schiwietz, 2004) and HISTOP (Arista & Lifshitz, 2004), except that they use empirical values (Schiwietz& Grande, 2001) for the ionic charge. The programs by Janni, by Hubert et al. and by Ziegler, and the program MSTAR are semi-empirical. Program LET is not further considered here since it is not independent, but based on Ziegler's programs.

To represent stopping for heavy ions at the highest energies correctly, it is necessary to use the non-perturbational LS theory which is fully relativistic and, in addition, assumes

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[1] While "stopping power" considers the energy reducing force of the material, the term "linear energy transfer (LET)" aims at the energy transferred to the surroundings by secondary electrons. If the energy transferred is restricted to electron energies below a certain threshold, this is then the "restricted linear energy transfer".

[2] See the "matrix" in (Paul, 2001a) for the availability of stopping data for various ions and targets.

Name, reference	Z_1	Z_2	(Specific) energy range	Remarks
ATIMA (Geissel et al., 2011)	1 - 92	1 – 92	≥10 MeV/u (as used here)	Based[3] on Lindhard-Sørensen above 30 MeV/u
BEST (Berger, Bichsel, 1994)	1 - 92	1 – 92; 180 compounds[4]	≥ 0.5 MeV/u	Bethe theory with corrections; bare ions
CasP v. 5.0 (Grande & Schiwietz, 2004)	1 - 92	1 – 92, any compound[5]	0.0001 – 200 MeV/u	Default settings used here for target ionization[6]
HISTOP (Arista and Lifshitz, 2004)	many	6	0.01 – 30 MeV/u	HISTOP for the valence electrons, SCA for the K shell of carbon
Hubert et al. (1990)	2 - 103	36 solid elements	2.5 – 500 MeV/u	
ICRU Report 49[7] (1993)	1, 2	25 elements, 48 compounds or mixtures	0.001-10000 MeV (p); 0.001-1000 MeV (α)	Programs NIST PSTAR, NIST ASTAR
ICRU Report 73 (2005)	3 – 18, 26	25 elements, 31 compounds	0.025 – 1000 MeV/u	Based on PASS
Janni (1982)	1	1 – 92; 63 compounds	0.001 – 10000 MeV	
LET (Zajic et al. (1999), Zajic (2001)	1 – 92	19 materials	0.2 – 1000000 MeV/u	Based on Ziegler's TRIM/SRIM programs (before 1999)
MSTAR (Paul, 2003)	3 - 18	31 elements, 48 compounds or mixtures	0.00025 – 250 MeV/u	Based on alpha stopping powers of ASTAR
PASS (Sigmund & Schinner, 2002)	many	many	Above 0.025 MeV/u	Binary Theory. Used for ICRU 73
SRIM[8] 2003 (Ziegler, 2004)	1 – 92	1 – 92, many compounds	1.1 eV – 10 GeV/u	SRIM stopping was not changed since 2003
Ziegler et al. (1985)	1 - 92	1 – 92; many other targets	0.1 – 100000 keV/u	First program to treat all ions, all targets

Table 1. Tables and computer programs for the stopping power of positive ions. "u" is the unified atomic mass unit, also called dalton.

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[3] Below 10 MeV/u, the values are based on an old version of SRIM (Ziegler et al., 1985). Between 10 and 30 MeV/u, the values are interpolated between SRIM and LS.

[4] Additional compounds may be calculated by entering a chemical formula

[5] Compounds are calculated according to chemical formula, assuming Bragg additivity.

[6] Target and projectile ionization must be calculated separately, and added.

[7] At high energy, the ICRU table was calculated using BEST

[8] SRIM was called TRIM in earlier times

projectile nuclei of finite size. For convenience, we have employed the program ATIMA (Geissel, Scheidenberger, et al., 2011) which is based on the LS program above 30 MeV/u and which includes shell, Barkas and Fermi-density effect corrections and in addition, a correction for projectile mean charge. But the use of the LS program will hardly be necessary for radiation therapy, since even for oxygen ions at 690 MeV/u, there is no difference between LS theory and Bethe theory (eq. 1) (Scheidenberger et al. 1994).

At high (but not too high) energies, where the ion has lost all electrons, the stopping power can be calculated by the relativistic Bethe theory without corrections (Bethe, 1932; ICRU Report 49):

$$S / \rho = (0.307075 \mathrm{MeVcm}^2 g^{-1}) \frac{Z_1^2}{\beta^2} \frac{Z_2}{A_2} L(\beta) \tag{1}$$

where Z_1 and v are charge number and velocity of the ion; Z_2 and A_2 are charge number and mass number of the target; $\beta = v/c$ (c = speed of light); and the stopping number L is given by

$$L(\beta) = \ln \frac{2mv^2}{I(1-\beta^2)} - \beta^2 \tag{2}$$

where m is the rest mass of the electron, and I is the mean ionization energy of the target. In this simple case, I is the only non-trivial constant that describes the stopping power. It can be deduced from optical or from stopping data. An earlier claim (Smith et al., 2006) that the results of these two methods may be in conflict, has been disproved (Paul et al., 2009a).

Lists of mean ionization energies I can be found in ICRU Report 49. The high energy parts of the stopping tables in this report were calculated using program BEST (Berger & Bichsel 1994). This program is also useful to calculate the stopping power eq. (1); normally, it uses the same I values as ICRU 49, but it also permits to enter a different value. BEST also includes the shell, Barkas, Bloch and Fermi-density effect corrections (see ICRU 49) not shown in eq. (2). It assumes a bare nucleus and is therefore not useful below about 1 MeV/nucleon.

At lower energies, the ion will carry electrons, and equilibrium between capture and loss of electrons will develop, leading to a certain mean charge of the ion, lower than Z_1e. Also, the Bethe eq. (1) must then be extended by the corrections mentioned.

1.2 Mixtures and compounds

For a mixture or, assuming Bragg's additivity rule (Bragg & Kleeman, 1905), for a compound, the mass stopping power is obtained by a linear combination of the constituent stopping powers (ICRU Report 49):

$$\frac{S}{\rho} = \sum_j w_j \left(\frac{S}{\rho} \right)_j \tag{3}$$

where w_j is the fraction by weight, and $(S/\rho)_j$ is the mass stopping power of the jth constituent. The corresponding relation for the mean ionization energy is

$$\ln I = \left(\sum w_j \frac{Z_{2j}}{A_{2j}} \ln I_j \right) \bigg/ \left\langle \frac{Z_2}{A_2} \right\rangle \tag{4}$$

where

$$\left\langle \frac{Z_2}{A_2} \right\rangle = \sum w_j \frac{Z_{2j}}{A_{2j}} . \tag{5}$$

A list of mean ionization energies I and other properties for 48 compounds and mixtures of interest to particle therapy can also be found in ICRU Report 49. To calculate the stopping power, I values different from those in the main list for elements were used, in an attempt to correct for the influence of binding and phase effects (see Table 2.11 of ICRU Report 49).

Some of the I-values in ICRU 49 are probably outdated, and a commission of the ICRU is working to improve the values for water and graphite. Comparisons with newer values of ionization energies are shown by Paul and Berger (1995), and by Paul et al. (2007a). The particular case of water is discussed in sect. 5 below.

BEST will also calculate the stopping of any compound defined by a chemical formula, and in particular, for 180 numbered compounds and mixtures[9] identified by three-digit ID numbers.

The file compound.dat in the SRIM program contains information for many compounds, including those covered by ICRU Report 49. Compound.dat also includes corrections for a deviation[10] from Bragg additivity (Ziegler & Manoyan, 1988) that becomes noticeable below 1 MeV/nucleon. In addition, it contains instructions on how to add more compounds to the SRIM program. To produce the data in table 6 below, we have added the properties of many compounds contained in our data base. Properties of compounds are also given by Janni (1988), and by Moyers et al. (2010).

1.3 Statistical comparisons

For statistical comparisons between experimental data and tables, we use our program "Judge", v. 3.19 (Paul & Schinner, 2001). This program calculates the normalized differences

$$\delta = (S_{ex} - S_{tab}) / S_{ex} \tag{6}$$

for every data point. Here, S_{ex} is the experimental value, and S_{tab} the corresponding table value for the same ion, same target and same energy. In every range of specific energy, i.e., energy per nucleon, it then determines the average normalized difference:

$$\Delta = \langle \delta \rangle \tag{7}$$

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[9] For only 48 of these, where experimental low-energy stopping data were available, stopping tables are given in ICRU Report 49. The properties of all the 180 substances can be found in program NIST ESTAR for electron stopping powers.

[10] These corrections are only applied for H and He ions. The absolute values of the non-zero Bragg corrections amount to about 3 %, on the average (Paul & Schinner, 2006). An attempt to test the accuracy of those corrections statistically is shown in the same paper.

and its standard deviation

$$\sigma = \sqrt{\langle \delta^2 \rangle - \langle \delta \rangle^2} \tag{8}$$

The averages are unweighted, except that obviously discrepant data are rejected (Paul, 2011a). A small Δ usually signifies good agreement between table and experimental data; in such a case, σ is related to the mean experimental accuracy, and σ may be taken as a measure of the accuracy of the table, as determined from experiment.

2. Hydrogen and helium ions

2.1 Hydrogen and helium ions in elements

In Tables 2 and 3, the reliability of various stopping power tables for H and He ions in solid elements is given in terms of $\Delta \pm \sigma$. Here, E is the energy of the ion. These tables were originally published by Paul & Schinner (2005), but many new data have since been added. This has not changed the results much, but it adds to the reliability.

E/A_1 (MeV)	0.01-0.1	0.1 – 1	1 – 10	10 - 100	0.01 -100
Number of points	*1357*	*2492*	*1212*	*225*	*5286*
Janni, 1982	2.1 ± 11	-1.1 ± 7.1	-0.9 ± 3.6	-0.3 ± 0.5	-0.2 ± 7.7
Ziegler et al., 1985	-1.3 ± 11	-3.1 ± 7.8	-0.4 ± 4.2	0.4 ± 2.2	-1.9 ± 8.2
ICRU, 1993	0.8 ± 11	-0.7 ± 7.0	-0.3 ± 4.0	-0.1 ± 0.5	-0.2 ± 7.5
SRIM, 2003	0.6 ± 10.3	-0.9 ± 6.7	-0.6 ± 3.7	-0.2 ± 0.6	-0.4 ± 7.2

Table 2. Mean normalized deviations $\Delta \pm \sigma$ (in %) for H ions in 17 solid elements covered by the ICRU Table, compared to various tables.

E/A_1 (MeV)	0.01-0.1	0.1 – 1	1 – 10	10 - 100	0.01 -100
Number of points	*1036*	*1913*	*400*	*11*	*3360*
Ziegler et al., 1985	3.2 ± 8.7	0.6 ± 5.6	-0.8 ± 3.3	0.8 ± 2.4	1.2 ± 6.7
ICRU, 1993	2.6 ± 8.3	0.2 ± 5.6	0.1 ± 3.3	0.9 ± 0.9	0.9 ± 6.4
SRIM, 2003	3.5 ± 8.2	0.6 ± 5.2	-0.3 ± 3.1	0.2 ± 0.9	1.4 ± 6.3

Table 3. Mean normalized deviations $\Delta \pm \sigma$ (in %) for He ions in 16 solid elements covered by the ICRU Table.

One can see that σ always decreases with increasing energy, due to the higher accuracy of measurements at high energy. The numbers of experimental points averaged is also shown, to give an idea of the accuracy. To provide a fair comparison with the smaller number of targets in the ICRU table, we compare only with the targets of that table, even though we have many more targets in our files (Paul, 2011a). We see that generally, σ has decreased and hence, the overall agreement has improved in time, with the exception of (Ziegler et al., 1985); but this was the first table capable of treating all ions and all targets.

Table 4 gives results for H ions in elemental gases. Here, we exclude measurements for low energy H ions in helium (Golser & Semrad, 1991; Schiefermüller et al., 1993; Raiola et al., 2001). Due to the threshold effect (Fermi & Teller, 1947) these data would produce a very

large Δ and thus obscure any other discrepancy. Except for the tables by Ziegler et al. (1985) (due to large discrepancies for H and He targets), the gas measurements appear here more reliable than those on solids.

E/A_1 (MeV)	0.001 - 0.01	0.01 - 0.1	0.1 - 1.0	1 - 10	10 - 100	0.001 - 100
No. of points	*124*	*335*	*535*	*303*	*11*	*1308*
Janni, 1982	-0.9 ± 9.2	-0.0 ± 4.6	0.5 ± 3.9	0.9 ± 3.2	3.2 ± 0.6	0.4 ± 4.7
Ziegler et al., 1985	22 ± 14	22 ± 11	0.4 ± 6.8	-1.1 ± 1.7	-1.0 ± 0.5	7.7 ± 14
ICRU, 1993	-0.6 ± 6.7	-1.2 ± 5.0	-1.2 ± 3.7	-0.8 ± 1.6	-0.2 ± 0.5	-1.0 ± 4.1
SRIM, 2003	2.1 ± 5.2	-0.1 ± 4.7	-0.4 ± 3.6	-0.2 ± 1.6	0.2 ± 0.3	-0.1 ± 3.9

Table 4. Mean normalized difference Δ ± σ (in %) for H ions in all elemental gases except F, Cl, Rn

Table 5 shows results for He ions in elemental gases. Again, the agreement with the data is much better than for solids, and we can observe a gradual improvement in time.

E/A_1 (MeV)	0.001 - 0.01	0.01 - 0.1	0.1 - 1.0	1 – 10	0 - 10
No. of points	*5*	*267*	*863*	*238*	*1373*
Ziegler et al., 1985	7.2 ± 13	2.5 ± 5.9	3.0 ± 4.9	-0.5 ± 2.5	2.3 ± 5.0
ICRU, 1993	0.5 ± 6.8	-1.0 ± 4.2	0.1 ± 4.2	0.7 ± 2.3	0.0 ± 4.0
SRIM, 2003	-5.4 ± 6.1	0.3 ± 3.9	0.1 ± 3.8	-0.2 ± 2.2	0.1 ± 3.7

Table 5. Mean normalized difference Δ ± σ (in %) for He ions in all elemental gases except F, Cl, Rn

2.2 Hydrogen and helium ions in compounds

Data for compounds have been treated in (Paul & Schinner, 2006). In our data base (Paul, 2011a), we have data for 150 different compounds. Table 6 shows results for hydrogen and helium ions in these compounds, compared to SRIM. Because of the different low energy limit chosen[11], some of the results appear somewhat better than for elements. Again, the errors σ tend to be smaller for gases than for solids.

Ions	Targets	E/A_1 (MeV)	0.025-0.25	0.25 – 2.5	2.5 - 30	0.025 – 30
H	cond.	*No. of points*	*412*	*946*	*232*	*1590*
		Δ ± σ	-1.3 ± 8.2	1.4 ± 6.3	-0.1 ± 4.0	0.5 ± 6.7
	gas	*No. of points*	*508*	*378*	*24*	*910*
		Δ ± σ	-0.9 ± 4.3	0.1 ± 3.3	-0.9 ± 2.1	-0.5 ± 3.9
He	cond.	*No. of points*	*472*	*1460*	*14*	*1946*
		Δ ± σ	0.4 ± 6.8	-0.5 ± 4.3	-2.0 ± 3.1	-0.3 ± 5.1
	gas	*No. of points*	*997*	*1742*	*0*	*2739*
		Δ ± σ	-2.6 ± 7.2	1.1 ± 2.9		-0.3 ± 5.2

Table 6. Mean normalized deviations Δ ± σ (in %) for H and He ions in condensed or gaseous compounds, as compared to SRIM (2003).

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[11] This is to avoid large deviations due to the threshold effect in LiF (Markin et al., 2009)

Table 7 shows a comparison between SRIM 2003 and ICRU Report 49, for the smaller number of compounds covered by the latter table, for H and He ions together (Paul & Schinner, 2006). For this restricted number of targets, ICRU Report 49 is clearly better than SRIM.

E/A_1 (MeV)	0 – 0.03	0.03 – 0.3	0.3 – 3.0	3 – 30	0 – 30
Number of points	*116*	*1036*	*1237*	*135*	*2524*
ICRU, 1993	0.2 ± 8.9	1.4 ± 5.9	1.3 ± 5.2	1.0 ± 4.4	1.3 ± 5.7
SRIM, 2003	-7.8 ± 12	-1.0 ± 6.4	0.4 ± 5.6	-0.6 ± 4.0	-0.6 ± 6.6

Table 7. Mean normalized deviations $\Delta \pm \sigma$ (in %) for H and He ions in 23 (solid or gaseous) compounds covered by ICRU Report 49 (1993)

Moyers et al. (2010) have recently measured the linear stopping powers for protons at 135, 175, and 225 MeV in many compounds of interest to particle therapy, relative to a water target. They compared their results to the Janni (1988) or LET tables (Zajic, 2001), finding agreement within 1 to 3 %. As examples, Fig. 1 shows a few results by Moyers et al., compared to the Janni, BEST and SRIM tables. The BEST calculation uses the *I*-values of ICRU Report 49, except that $I = 78$ eV was taken for water (cf. Sect. 5 below). It should be noted that in this energy region, corrections to eq. (2) are small[12], hence eq. (2) would also suffice in place of BEST.
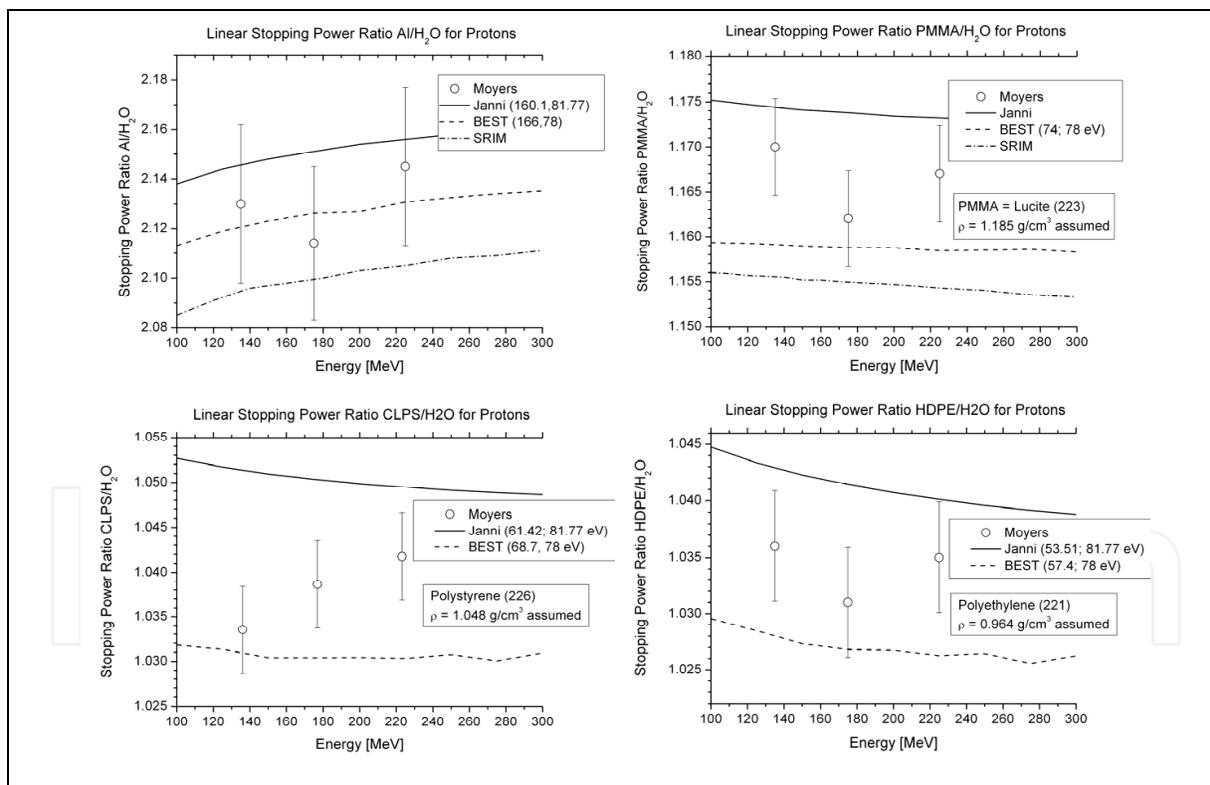

Fig. 1. The linear stopping power of Al, polymethyl methacrylate (PMMA), clear polystyrene (CLPS) and high density polyethylene (HDPE), for protons relative to water, compared to the tables Janni, BEST, and SRIM. The 3-digit ID numbers from ICRU 49 are shown in parentheses. For the curves, the *I* values for both substances are shown in parentheses, where available. Experimental data are from Moyers et al. (2010) and Moyers (2011).

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[12] In the case of p in Al, e.g., corrections are below 0.2 %.

Inspection of Fig. 1 shows that the curves are essentially determined by the *I* values. In particular, the Janni curves are always above the BEST curves because of the rather high *I* value for water and the rather low *I* values for the other substances. Evidently, BEST agrees best with the Al measurements. For the compounds, BEST appears slightly low; this might point to slight errors of the I values used.

2.3 Application to particle therapy

Inspection of Tables 2 and 4 shows that, for protons in elements, in the range 10 – 100 MeV, the value of Δ is negligible for the ICRU and SRIM tables, and σ is 0.5 %, on the average. Hence, in this energy range important for therapy, the ICRU and SRIM tables can be expected to be accurate to 0.5 %. And the same accuracy may be expected up to 1000 MeV, if the ICRU or SRIM tables are extended[13] using the pure Bethe theory eq. (1), since the corrections to Bethe are minimal (cf. Fig. 8 below). The same holds for the Janni table for elemental solids (not for gases).

For protons in compounds, the highest energy range (Table 6) goes only up to 30 MeV, and σ is larger (2 – 4 %). Hence, the predictive quality of SRIM appears worse for compounds. On the other hand, since Bragg additivity holds at high energy, the stopping power of compounds at high energy may be calculated using eq. (3), and in this way, the accuracy could be improved somewhat.

3. Ions from $_3$Li to $_{18}$Ar

In tables 8 to 10, MSTAR v.3 (Paul, 2003), SRIM (2003), and ICRU Report 73 (2005) are compared to experimental data. To provide a fair comparison between MSTAR and SRIM, we compare both tables to the same data; not all of these are covered by ICRU 73. These comparisons are based upon our earlier analyses (Paul, 2006) but contain many newer data. This has hardly changed the results, but it adds credibility.

E/A_1 (MeV)	0.025 - 0.1	0.1- 1	1 – 10	10 - 100	100-1000	0.025-1000
No. of points	*1426*	*3821*	*1370*	*190*	*11*	*6818*
MSTAR	2.3 ± 9.6	0.3 ± 6.5	1.1 ± 4.9	0.2 ± 2.1	0.7 ± 1.4	0.9 ± 7.0
SRIM, 2003	1.3 ± 8.8	-0.5 ± 5.8	-0.1 ± 4.8	-1.5 ± 2.8	-0.1 ± 1.6	-0.1 ± 6.4
ICRU Rep. 73	-11.7 ± 20	-6.3 ± 11	-2.9 ± 5.8	-0.9 ± 2.9	-0.8 ± 1.9	-6.6 ± 13

Table 8. Mean normalized deviations $\Delta \pm \sigma$ (in %) for ions from $_3$Li to $_{18}$Ar in all the elemental solids covered by MSTAR. The number of points refers to MSTAR and SRIM; for ICRU 73, it is slightly smaller since that table does not cover B, Zr, Gd, and Ta targets.

Table 8 shows the reliability of the tables in terms of $\Delta \pm \sigma$ for ions from $_3$Li to $_{18}$Ar in solid elements. Similarly, Table 9 gives the reliability of the same tables for the 10 compounds for which we have data. Finally, Table 10 shows results for all gases covered by MSTAR and ICRU Report 73 for which we have data. We find that MSTAR and SRIM describe the data about equally well, and that ICRU 73 is too high at low energy, on the average. Fig. 2 shows an extreme example: the stopping power of Ag for Li ions, where ICRU 73 is too high, and

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[13] In the case of ICRU, this simply means using the ICRU table up to 1000 MeV.

E/A_1 (MeV)	0.025 – 0.1	0.1 – 1	1- 10	10 - 100	0.025-100
No. of points	*180*	*775*	*554*	*16*	*1525*
MSTAR	4.8 ± 10.1	0.8 ± 6.4	5.4 ± 4.3	0.8 ± 2.4	3.0 ± 6.7
SRIM, 2003	-2.2 ± 9.4	-0.5 ± 6.0	0.1 ± 5.0	-1.5 ± 2.5	-0.5 ± 6.2
ICRU Rep. 73	-11 ± 11	-2.6 ± 7.4	-1.1 ± 5.0	-0.8 ± 1.7	-3.1 ± 7.9

Table 9. Mean normalized deviations Δ ± σ (in %) for ions from $_3$Li to $_{18}$Ar in 10 condensed compounds[14]. The number of points refers to MSTAR and SRIM; for ICRU 73, it is slightly smaller since that table does not cover polypropylene and toluene.

E/A_1 (MeV)	0.025 – 0.1	0.1 – 1	1- 10	10 - 100	0.025-100
No. of points	*163*	*190*	*574*	*189*	*1116*
MSTAR	-2.5 ± 10.4	-2.1 ± 12	0.1 ± 3.8	0.7 ± 2.4	-0.5 ± 7.2
SRIM, 2003	3.2 ± 10.1	-7.6 ± 12	-1.0 ± 5.9	-2.2 ± 3.9	-1.7 ± 8.2
ICRU Rep. 73	-50 ± 28	-3.1 ± 16	-1.9 ± 10.3	-0.1 ± 3.8	-8.8 ± 23

Table 10. Mean normalized deviations Δ ± σ (in %) for ions from $_3$Li to $_{18}$Ar in all (elemental and compound) gases covered by MSTAR and ICRU 73 for which we have data.
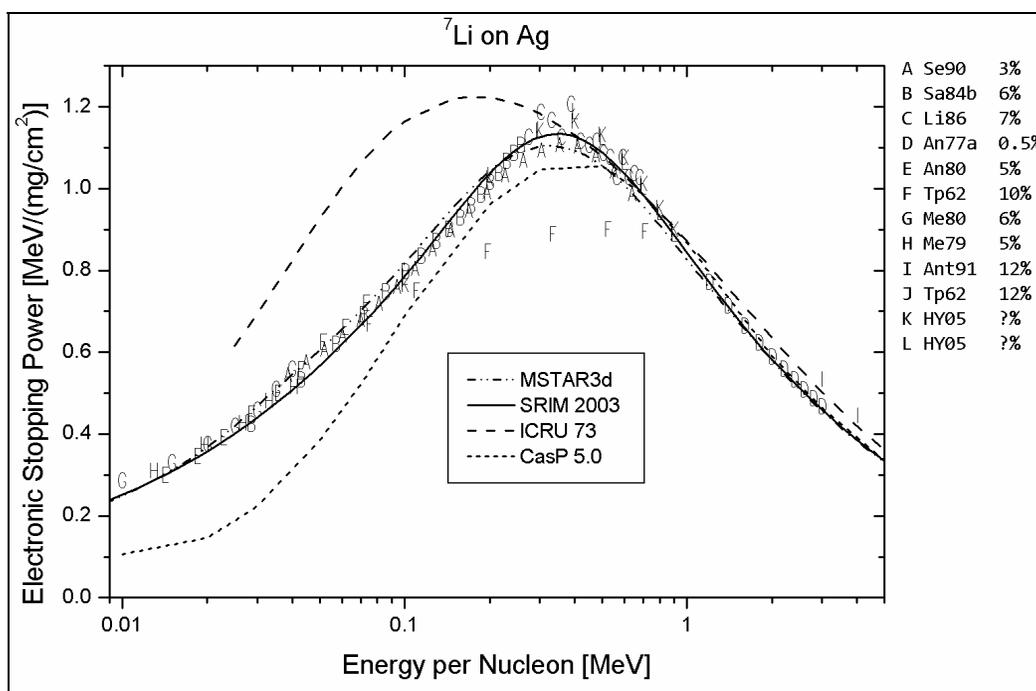
Fig. 2. Electronic stopping power as a function of specific energy for Li ions in Ag, compared to various tables. Experimental points are marked by letters; the references corresponding to the reference codes given in the margin can be found in (Paul, 2011a).

CasP is too low at low energy. Table 10 shows that the overall agreement is here not better for gases than for solids. The agreement of ICRU 73 with the data for gases at low energy is noticeably worse than for solids. This could be related to the fact that PASS uses the same ionic charge for gases as for solids.

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[14] Aluminum oxide, kapton polyimide, polycarbonate (makrolon), polyethylene, polyethylene terephthalate (mylar), polypropylene, polyvinyl chloride, silicon dioxide, toluene, water (liquid)

3.1 In particular: Carbon ions

We consider carbon ions especially because of their importance for medical therapy. As an example, Fig. 3 shows stopping powers for carbon ions in carbon. Here, there is good agreement between the experimental data and the MSTAR, SRIM, HISTOP and ICRU 73 tables in most energy regions, while CasP is too low at low energy[15].

Table 11 shows the reliability of MSTAR, SRIM and ICRU 73 for C ions in elemental solids. The overall agreement for MSTAR and SRIM is slightly better than in Table 7 for all ions (Li to Ar), but the highest energy range goes only up to 100 MeV/nucleon. Here, the accuracy in the highest range (10 – 100 MeV/nucleon) is only about 3 % for MSTAR and SRIM, much worse than for protons.

E/A_1 (MeV)	0.025 - 0.1	0.1- 1	1 – 10	10 - 100	0.025-100
No. of points	202	632	229	8	1071
MSTAR	-1.6 ± 9.6	0.6 ± 5.8	0.9 ± 5.1	0.0 ± 2.8	0.2 ± 6.6
SRIM, 2003	0.4 ± 8.3	-0.5 ± 5.3	-0.6 ± 5.2	1.0 ± 3.0	-0.3 ± 6.0
ICRU Rep. 73	-13.0 ± 12	-9.2 ± 11	-2.6 ± 5.8	-0.6 ± 3.8	-8.5 ± 11

Table 11. Mean normalized deviations $\Delta \pm \sigma$ (in %) for C ions in 15 elemental solids covered by MSTAR. The number of points refers to MSTAR and SRIM; for ICRU 73, it is slightly smaller since that table does not cover Gd and Ta targets.
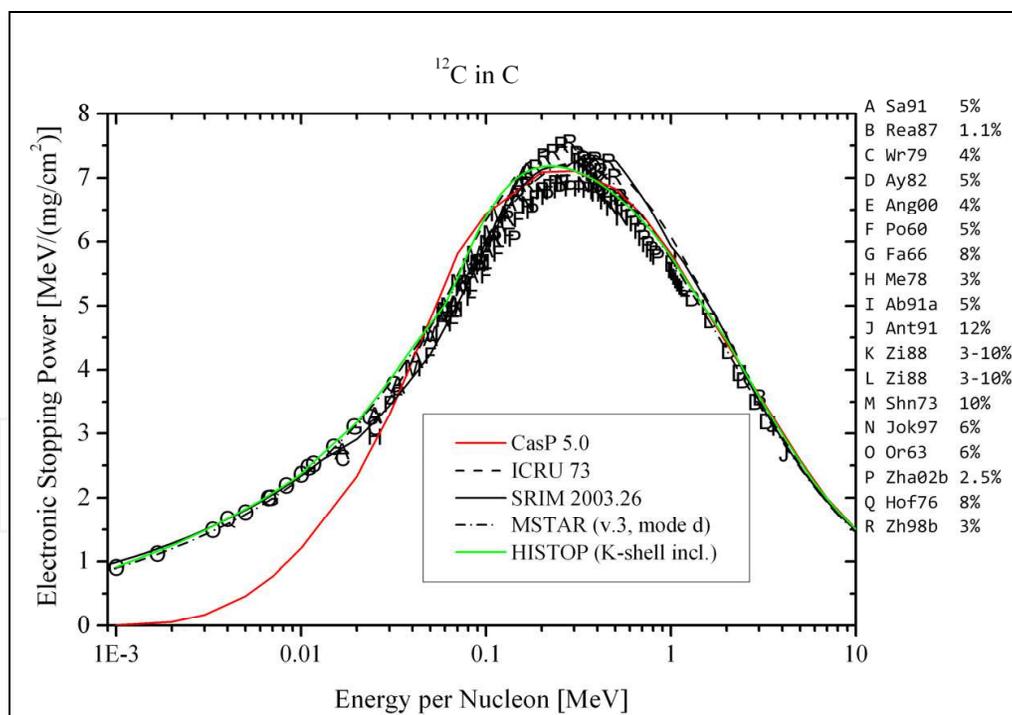

Fig. 3. Like Fig. 2, for C ions in amorphous carbon[16].

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[15] This discrepancy has not changed much from CasP v. 3.1 to v. 5.0

[16] The CasP calculation was done using oscillator strengths for carbon, and adding projectile ionization to target ionization.

4. Ions from $_{19}$K to $_{92}$U

In Table 12 (Paul, 2010), the reliability of stopping tables for ions $_{19}$K to $_{92}$U in elemental solids is given numerically. We find that, at the highest energy, only the non-perturbational Lindhard-Sørensen theory (calculated using ATIMA) is correct. Between 2.5 and 100 MeV/nucleon, the Hubert table is best. SRIM is fairly good everywhere, except near the maximum (2.5 – 30 MeV/n). By detailed analysis, it can be shown, that on the average, for heavy ions in solid elemental targets, SRIM is 6 % high in heavy targets and 5 % low in light targets at the maximum, as has been noted already by Randhawa & Virk (1996). For examples, see the graphs for U in Au (Fig. 4) and for Pb in C (Fig. 5).
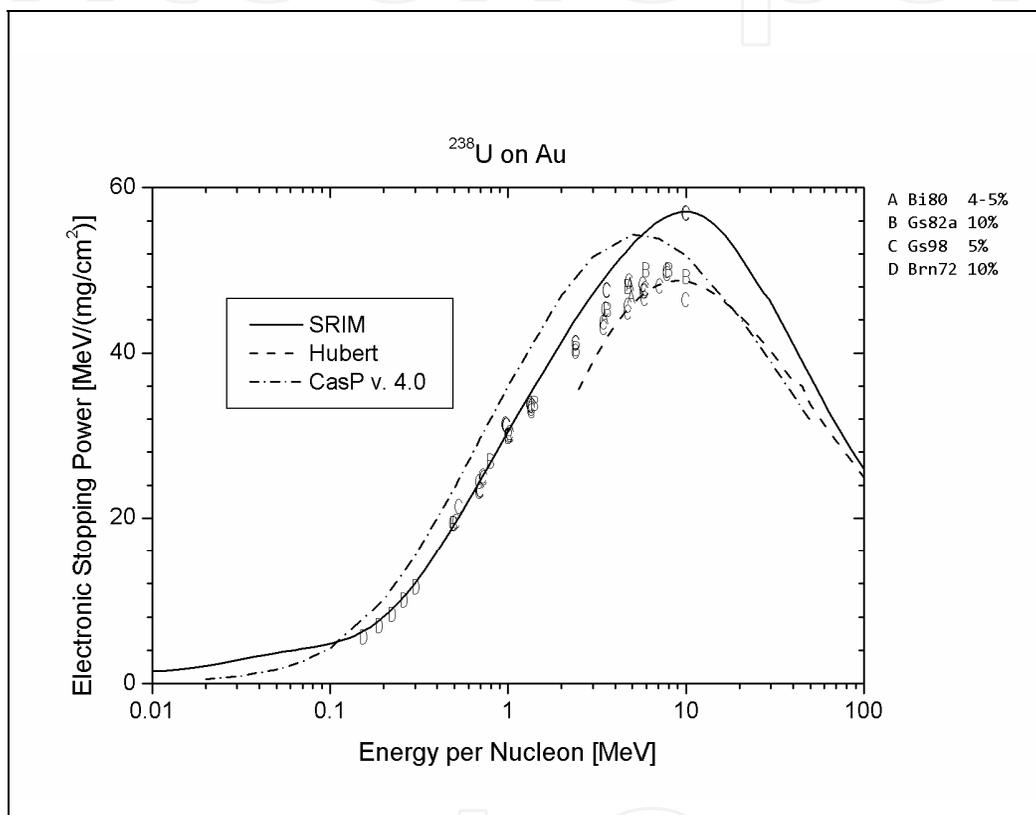
Fig. 4. Electronic stopping power as a function of specific energy for U ions in Au. The data points are indicated by letters; corresponding references can be found in (Paul, 2011a).

Fig. 6 (Paul, 2011b) shows the stopping power for U ions at 10 MeV/nucleon in elements, versus target atomic number Z_2. One can see the well known positive solid-gas difference due to the high collision frequency of fast ions in solids (Geissel et al., 1982; Paul, 2009b) which is well described by CasP 4.0 (due to the different ionic charge states used by CasP for solids and gases) but not by SRIM[17]; SRIM is too high for heavy ions in gaseous elements (see Table 13). For gaseous compounds, SRIM is also too high, especially for the heaviest ions at the maximum (see, e.g., the graph for U ions in Butane in (Paul, 2011a) and Table 14).

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[17] The „Gas Tgt" button in SRIM does, however, describe the *negative* solid-gas difference due to polarization screening in the solid, found at low energy, see ref. (Paul 2009b).
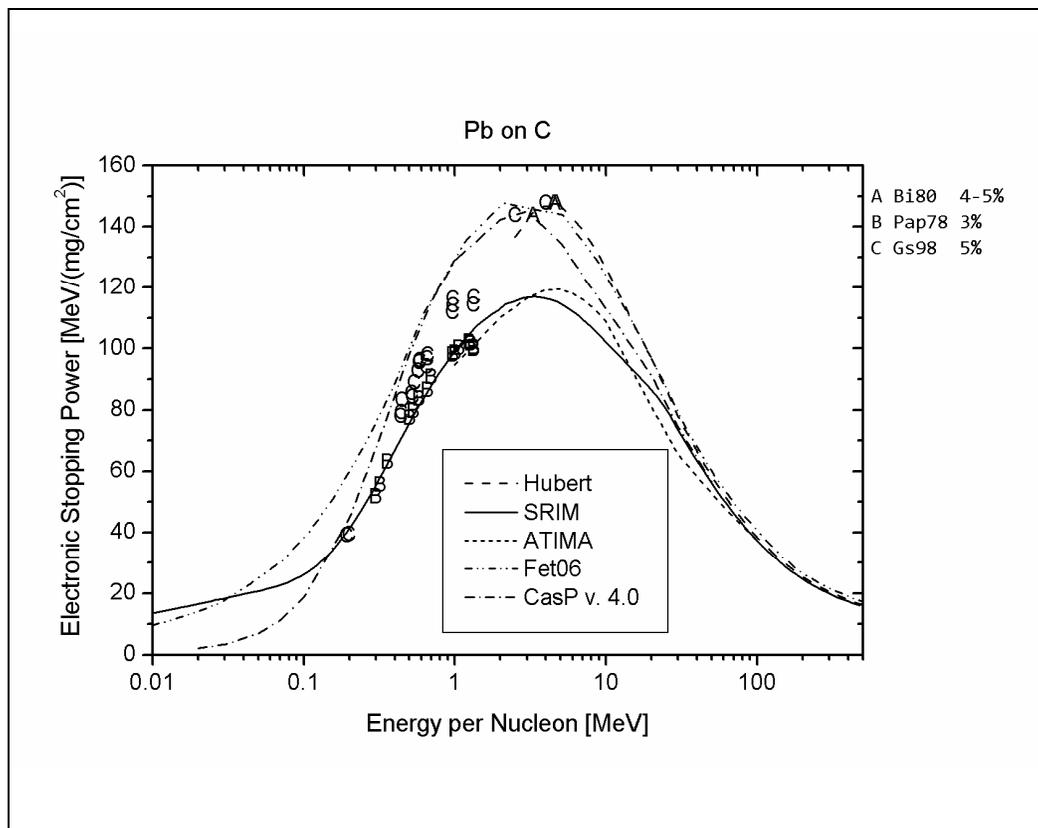
Fig. 5. Electronic stopping power of carbon for Pb ions, versus specific energy. Measured points are indicated by letters; the corresponding references are found in (Paul, 2011a). The curve designations are explained in Table 1, except for Fet06 (Fettouhi et al.). This curve is based on PASS, but incorporating a realistic mean charge of the ion.

E/A_1 (MeV)	0.025-0.25	0.25 – 2.5	2.5 - 30	30 - 100	100 - 500	500 - 1000	Total range
No. of pts. SRIM	*655* 2.0 ± 19	*3025* 1.8 ± 6.6	*1058* -2.0 ± 9.0	*65* -0.3 ± 3.4	*43* 5.0 ± 2.4	*13* 7.5 ± 2.2	*4859* 1.0 ± 9.9
No of pts. Hubert			*934* 0.8 ± 5.1	*65* 1.1 ± 3.2	*43* 4.6 ± 2.5		*1042* 1.0 ± 5.0
No. of pts. ATIMA				*65* 2.3 ± 4.0	*43* 1.2 ± 1.5	*13* 0.9 ± 0.8	*121* 1.7 ± 3.1

Table 12. Mean normalized deviations $\Delta \pm \sigma$ of experimental data for 31 ions from $_{19}K$ to $_{92}U$ in all 54 solid elemental targets for which we have data, in various ranges of specific energy.

E/A_1 (MeV)	0.25 – 2.5	2.5 - 30	30 - 100	Total Range
Number of points	*276*	*459*	*38*	*773*
SRIM	1.4 ± 6.9	-6.0 ± 10.3	-7.2 ± 5.9	-3.4 ± 9.7

Table 13. $\Delta \pm \sigma$ (in %) for SRIM, for ions from $_{19}K$ to $_{92}U$ in all elemental gas targets for which we have experimental data in (Paul, 2011a).
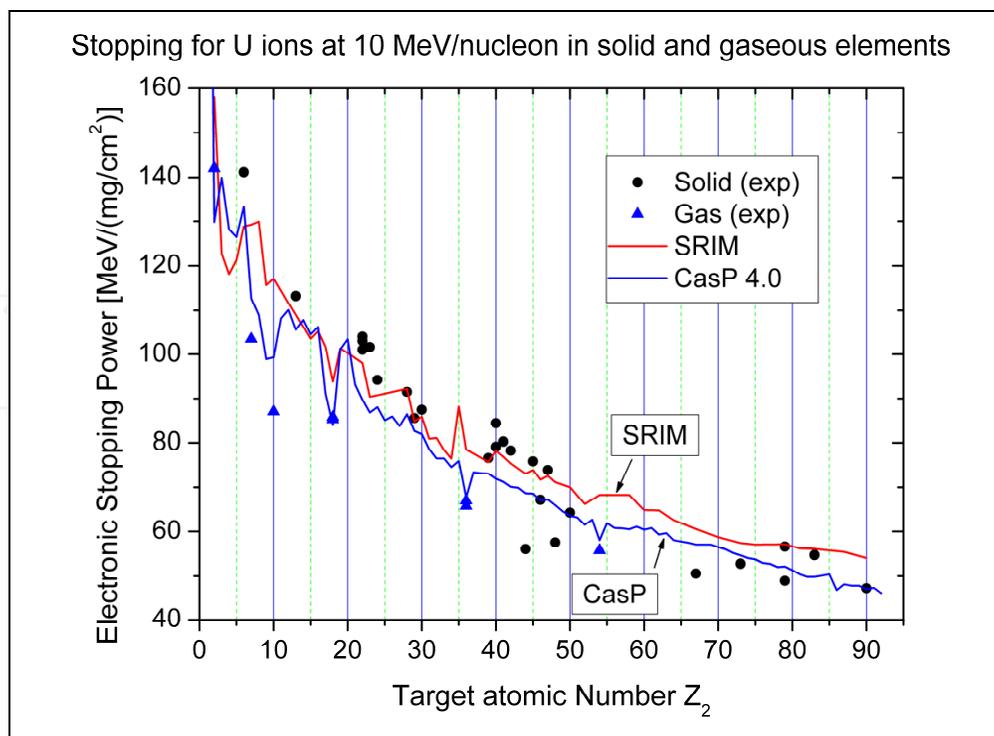
Fig. 6. The stopping power of elements for U ions at 10 MeV/nucleon, as a function of target atomic number. The graph shows the well-known positive solid-gas difference.

E/A$_1$ (MeV)	0.025-0.25	0.25 – 2.5	2.5 – 30	30 – 100	Total Range
No. of points	*21*	*112*	*195*	*15*	*343*
SRIM	-1.6 ± 9.5	-4.8 ± 5.3	-9.9 ± 7.7	-0.9 ± 7.3	-7.4 ± 7.8

Table 14. Δ ± σ (in %) for SRIM, for ions from $_{19}$K to $_{92}$U in all gaseous compounds for which we have data in (Paul, 2011a): butane, CF_4, methane, CO_2, and C_3F_8 (Freon-218).

Table 15 shows a statistical comparison for solid compounds. The deviation between SRIM and experiments is larger than for elements, and SRIM is too low, on the average. An example is the case for Ni ions in SiC (see the figure in (Paul, 2011a)).

E/A$_1$ (MeV)	0.025-0.25	0.25-2.5	2.5-30	30-100	Total Range
No. of points	*239*	*211*	*86*	*10*	*546*
SRIM	8.1 ± 12	4.6 ± 9.2	8.5 ± 9.8	5.9 ± 5.8	6.8 ± 10.7

Table 15. Δ ± σ (in %) for ions from $_{19}$K to $_{92}$U in all solid compounds (Al_2O_3, Formvar, Havar, Mylar, NE111 Plastic Scintillator, Polycarbonate, Polyethylene naphthalate, Polypropylene, Polystyrene, SiC, Silicon Nitride, ZrO_2) for which we have data in (Paul, 2011a) and which are calculable, compared to SRIM.

5. Water as a target

Water as a target is especially important for medical physics. Fig. 7 gives an overview of experimental and tabulated values of the stopping power of solid and liquid water for

protons. Fig. 8 shows the same data again, but divided by the values of ICRU 49 (to make small differences apparent), and only the high energy part which is most important for radiation physics. Because corrections to the simple Bethe formula, eqs. (1 & 2), are smaller than 0.68 % beyond 10 MeV, the value of the stopping power is essentially given by the value of the mean ionization energy in this entire region.
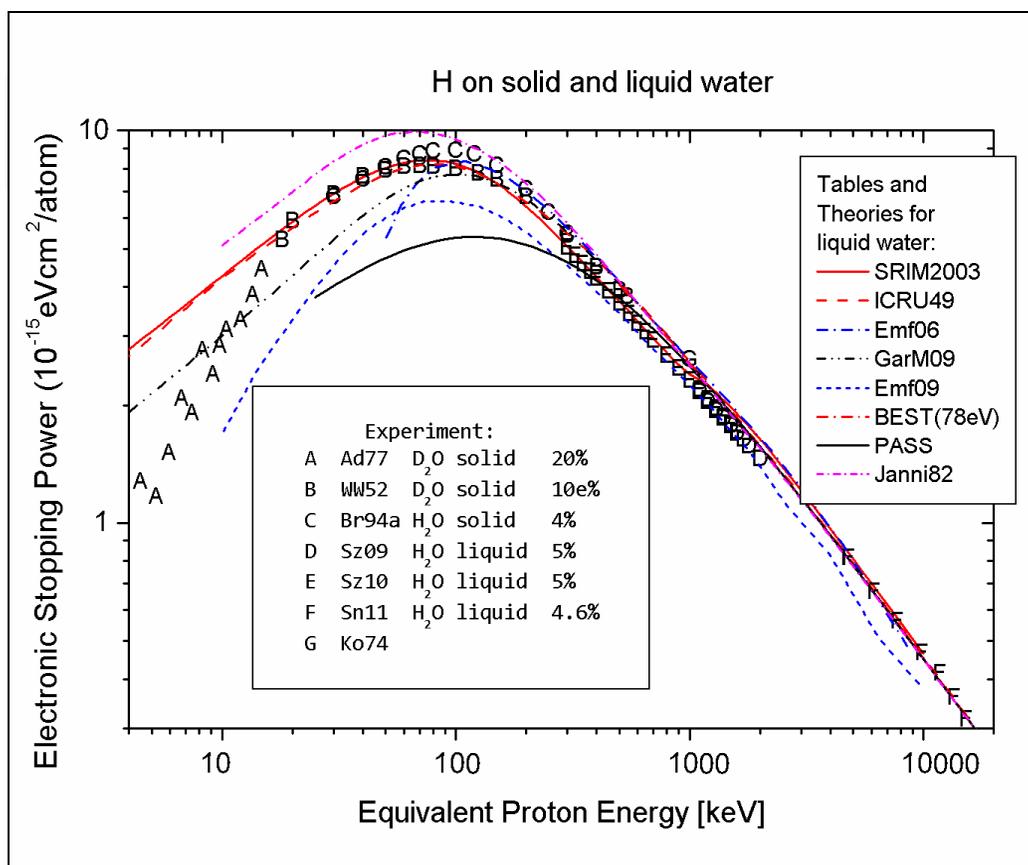

Fig. 7. Electronic stopping power of solid and liquid water for protons, versus energy. The file designations for experiments are explained in Paul (2011a). The table and theory designations are explained in Table 1, except for the following: Emf06 (Emfietzoglou et al, 2006), Emf09 (Emfietzoglou et al., 2009), GarM09 (Garcia-Molina et al., 2009), PASS (Sigmund & Schinner, 2002; Sigmund, 2010)

Table 16 gives an overview of calculated and measured values of the mean ionization energy of liquid water[18] (Paul et al., 2007a). On the basis of the data available in 1984, the value I = 75.0 was chosen in ICRU 37 (1984) and again in ICRU 49 (1993). But evidently, all the more recent determinations indicate a larger value.

Recently, there have been measurements of the stopping power of liquid water for protons by two groups: the Kyoto group (Shimizu et al., 2009, 2010) using a liquid water jet in vacuum, and the Jyväskylä group (Siiskonen, et al., 2011) using a thin water sheet (enclosed within two thin copper sheets) in transmission. The results are shown as points D, E and F in Figs. 7 and 8.

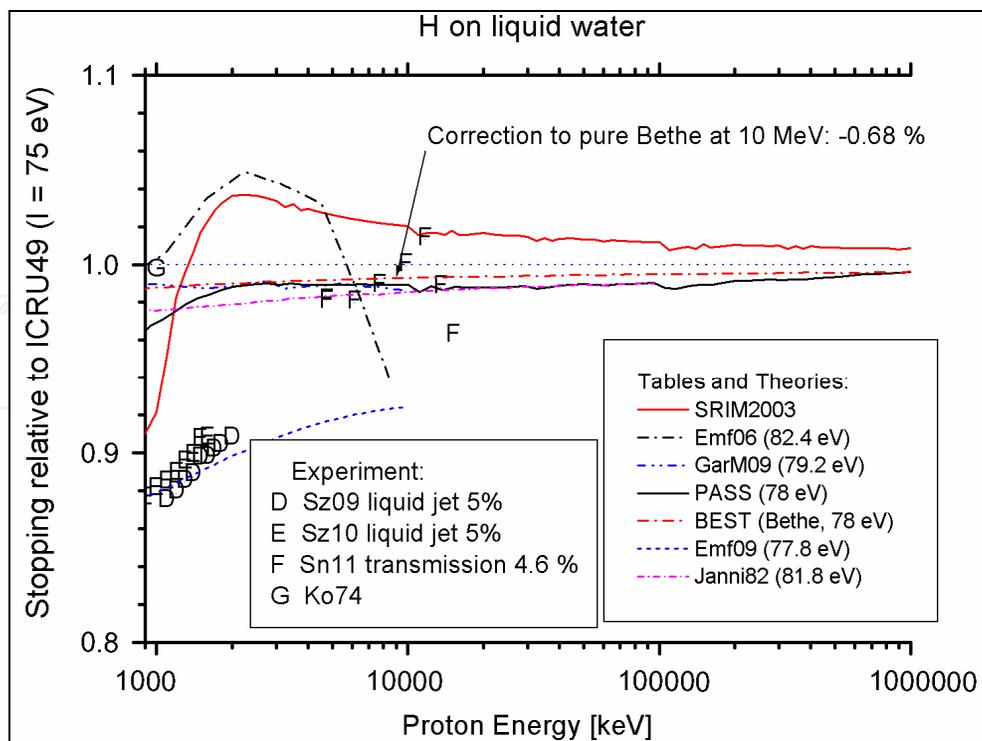[18] We assume that the I-values for solid and liquid water are equal.

Fig. 8. Stopping power of liquid water for protons, normalized by the table ICRU 49. The designations for tables and for experimental points are as in Fig. 7. *I*-values are shown in parentheses.

I (eV)	Reference	Method or remark
75.4 ± 1.9[19]	Thompson, 1952	Range, 340 – 200 MeV p, assuming I_{Cu} = 322 eV
74.6 ± 2.7	Nordin et al., 1979	Stopping power, 60 MeV pions
75	Ritchie et al., 1978	Dielectric response function
75.4	Ashley, 1982	Dielectric response function
81.77	Janni, 1982	Averaging data for H and O
79.7 ± 2	Bichsel et al., 1992	Ionization curves, 70 MeV p
81.8	Dingfelder et al., 1998	Dielectric response function
80.0	Bichsel et al., 2000	C ions, 290 MeV/u
77	Kramer et al., 2000	Depth dose curves for C ions
78.4	Kumazaki et al., 2007	Depth dose curves for protons
78	Schardt et al., 2008	Bragg curves for H, He, Li, C, and O ions
75.0 ± 3	Chosen in ICRU 37, 49	
78.0 ± 2	Chosen in Sigmund et al. (2009)	Replaces the value 67.2 eV in ICRU Report 73

Table 16. *I* values for liquid water.

This brings up a problem (Paul, 2010). The Bethe equation (i.e., BEST) is generally reliable (Paul & Schinner, 2005) and depends only on *I* and on the shell correction in this energy region, and the latter correction is quite small here. The GarM09 curve and the PASS curve are very close to BEST, about 1 % below ICRU 49 (i.e., unity) due to the higher *I*-value. Hence it appears that the Emf09 curve (and also the Shimizu measurements) may be low by about 10 %.

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[19] The data were analyzed by Berger (ICRU Report 37)

It appears that at present, the most precise measurements of the mean ionization energy of water are the range measurements made in Darmstadt (Schardt et al., 2008), leading to I = 78 eV. And this value has also been assumed for the corrected table of ICRU 73 (Sigmund et al., 2009). Evidently, the recent Jyväskylä measurements are in very good agreement with BEST and PASS (using I = 78 eV): the points F yield an average of 0.986 ± 0.005, very close to the relative value of BEST: 0.993. But the Jyväskylä results alone would not yield a precise I value; it is the range measurements (Schardt et al., 2008) that give a clear distinction between various values.

6. Some remarks concerning the physics of radiation therapy

In radiation therapy, water is used as tissue reference medium (Schardt et al., 2010). Rules for the application of proton therapy have been defined in ref. (ICRU, 2007).

For the dosimetry of fast heavy ions, following a recommendation of the International Atomic Energy Agency (Andreo, 2000), air filled ionization chambers should be used. To convert the absorbed dose in air thus determined to the dose in water (Paul, Geithner and Jäkel, 2007a, 2007b), the first approximation is to use the ratio of mass stopping powers

$$\frac{(S(E) / \rho)_w}{(S(E) / \rho)_{air}} \tag{9}$$

where $(S(E)/\rho)_m$ denotes the mass stopping power of medium m evaluated at the energy E.

This ratio is essentially determined by the mean ionization energies I of water and air. It should be sufficiently accurate from about 5 MeV/nucleon up to (but not beyond) the primary ion energy.

To obtain a more accurate correspondence between the measurement in air and its application to water, it is necessary to use Monte Carlo calculations to take into account all physical processes, especially the effect of fragments produced by nuclear reactions. One defines the 'stopping power ratio' (Andreo, 2000) (as opposed to the simple ratio of stopping powers defined above), i.e., the fluence-weighted average ratio of stopping powers

$$s_{w,air} = \frac{\sum_i \int_0^\infty \Phi_{E,i,w}(S_i(E) / \rho)_w \, dE}{\sum_i \int_0^\infty \Phi_{E,i,w}(S_i(E) / \rho)_{air} \, dE} \tag{10}$$

where $S_i(E)/\rho$ is the mass stopping power for a (primary or secondary) particle i with energy E in water or air, and $\Phi_{E,i,w}$ is the particle spectrum differential in energy, at a particular depth in water, for particles of type i.

For carbon ions of 400 MeV/nucleon and assuming an increased mean ionization energy I_{water} = 80.8 eV for water, it was shown (Paul et al., 2007b) that $s_{w,air}$ still fits[20] into the range $s_{w,air}$ = 1.13 ± 0.02 adopted for heavy ion beams by the IAEA Code of Practice (Andreo, 2000). This would probably hold also for the more realistic value I_{water} = 78 eV adopted by ICRU 73.

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[20] For lower ion energies, the limit 1.15 might be exceeded, however.

7. Conclusion

For a quantitative understanding of radiotherapy by positive ions, one needs information about stopping powers. In this chapter, we discuss stopping power tables and programs, and we compare them statistically to our large collection of experimental data. In this way, the reliability of various tables can be estimated. We describe it by $\Delta \pm \sigma$, where Δ is the average normalized difference between experimental and tabulated values, and σ is its standard deviation. A small Δ usually signifies good agreement; in this case, σ may be taken as a measure of the accuracy of the table. We treat both condensed and gaseous targets, and we consider elements, compounds and mixtures. We give an overview of relevant tables and programs, and of the basic formulas of Bethe theory.

We find that σ always decreases with increasing energy, and that in general, the agreement between tables and experimental data has improved in time. For H ions in elements, in the highest range of specific energy (10 – 100 MeV/nucleon), we find that $\sigma = 0.5$ %, on the average. For H and He ions in elements, σ is always smaller than 1 % in that energy range, except for He ions in elemental gases, where we have data only up to 10 MeV/nucleon. The SRIM tables and the tables from ICRU Report 49 are equally good in general, but the SRIM tables describe many more targets. For H and He ions, the gas measurements appear more reliable than those on solids. For compounds, results are similar to those for elements, except that experimental data go only up to 30 MeV/nucleon, so that σ is larger (2 – 4 %) in the highest energy range.

For ions from $_3$Li to $_{18}$Ar in elemental solid targets compared to SRIM and MSTAR, we find that σ is about 1.5 % in the highest specific energy range (100 – 1000 MeV/nucleon) and that the energy-dependent accuracy is comparable in condensed compounds, except that data go only up to 100 MeV/nucleon in that case. ICRU Report 73 is too high at low energy, particularly for gases. For ions from $_3$Li to $_{18}$Ar, the overall agreement is not better for gases than for solids.

For carbon ions in particular, the overall agreement is slightly better than for all ions (Li to Ar), but the accuracy in the highest energy range (10 – 100 MeV/nucleon) is only about 3 %, much worse than for protons.

For ions from $_{19}$K to $_{92}$U, the ATIMA, Hubert and SRIM tables are best in different ranges of specific energy. The positive gas-solid difference due to the high collision frequency of fast ions in solids is well described by the CasP program but not by SRIM.

Precise values of the mean ionization energy of a substance, I, deduced from range measurements, could often be more useful at high energy than measurements of stopping power. It is shown that the value $I = 75$ eV that has long been accepted for water, should be increased to $I = 78$ eV, following the very precise range measurements of Schardt et al. Recent stopping power measurements for water at Jyväskyläa are in good agreement with this value, but the measurements by the Kyoto group are probably too low by about 10 %. The I-value of water is also discussed in relation with the validity of the IAEA Code of Practice for heavy ions.

8. Acknowledgments

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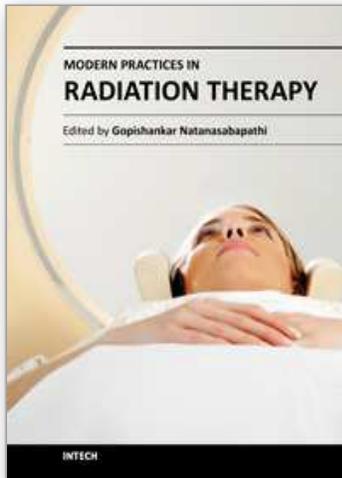
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