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# On the Need for the Mean Excitation Energies of Polyatomic Ionic Systems

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There are many cases where energy is deposited by fast hadrons into a gaseous target consisting of a variety of components. Examples include, but are not restricted to, planetary atmospheres [1], reactor plasmas [2,3], liquid crystals [4], and intergalactic space [5]. In all of these systems, although they differ widely in density ( $n$ ), the incoming projectile will deposit energy into some mixture of atoms, molecules, their ions, and electrons.

To understand the energy deposition process, one needs to know the stopping power, or energy loss of the projectile with velocity  $v$  per unit track length:  $-dE(v)/dx$ . The stopping power of a substance is frequently normalized with regard to the density and referred to as the target cross section,  $S(v)$ :

$$S(v) = \frac{1}{n} \frac{dE(v)}{dx} \quad (1)$$

In the simplest case, that of Bethe stopping [1], the stopping cross section of each component  $i$  can be written:

$$S_i(v) = \frac{4\pi e^2 Z_1^2 Z_2^2}{mv^2} L_i(v) \quad (2)$$

Where  $Z_1$  is the projectile charge and  $Z_2$  is the target electron number.  $L_i(v)$  is the stopping number of component  $i$ , given by

$$L_i(v) = \ln \frac{2mv^2}{I_0^i} - \frac{C(v)}{Z_2} \quad (3)$$

Here the second term is the shell corrections. The mean excitation energy of component  $i$ ,  $I_0^i$  measures the ability of substance  $i$  to absorb energy from the projectile. At this level of approximation, this key quantity is the first energy weighted moment of the dipole oscillator strength distribution (DOSD) of each component of the target [6]

$$\ln I_0 = \frac{\int \frac{df}{dE} \ln E dE}{\int \frac{df}{dE} dE} \quad (4)$$

The stopping power of a target containing a mixture of components is then given, according to the Bragg rule [7] as a sum of the stopping powers of the target components

$$\left( -\frac{dE}{dx} \right)_{mix} = \sum_{i=components} \left( -\frac{dE}{dx} \right)_i \quad (5)$$

In terms of the stopping cross sections of the components, this becomes

$$\left( -\frac{dE}{dx} \right)_{mix} = \frac{4\pi e^4 Z_1^2}{mv^2} \sum_i n_i Z_i \ln \frac{2mv^2}{I_0^i} \quad (6)$$

leading to the stopping power of the mixture:

$$\left( -\frac{dE}{dx} \right)_{mix} = \frac{4\pi e^4 Z_1^2}{mv^2} \sum_i n_i Z_i \ln \frac{2mv^2}{I_0^i} \quad (7)$$

Thus, the mean excitation energy and thus the stopping cross sections of each of the components must be known.

The stopping power and mean excitation energy of the electron gas is well known [8].

Similarly, stopping powers and mean excitation energies of neutral atoms [9] and some molecules [10] are also well known, from theory or experiment, or both.

The mean excitation energies of target ions and molecules, as would be expected in space and some plasmas, are much lesser known. In a recent paper [11], the mean excitation energies for all ions of some small atoms have been calculated using the aug-cc-pCV5Z basis set. Representative results for Ne are shown in the following table.

Calculated  $I_0$  (eV) of Ne and its Ions

	$I_0$ (eV)
Ne	137.2
Ne1+	165.2
Ne2+	196.9
Ne3+	235.2
Ne4+	282.8
Ne5+	352.6
Ne6+	475.0
Ne7+	696.8
Ne8+	1409.2
Ne9+	1498.4

A previous calculation for the neutral Ne atom [9] gave  $I_0 = 137.3$  eV, but there is no comparable data for the other ions.

Thus, information is available, or at least obtainable, for determination of the stopping properties of atoms, atomic ions, neutral molecules and electrons, so contribution to energy deposition by energetic hadrons in these systems can be determined. However, planetary atmospheres, deep space, and various plasmas contain polyatomic ions as well [5,12-14].

Some representative examples include  $\text{CH}^+$ ,  $\text{OH}^-$ ,  $\text{SH}^+$ ,  $\text{CN}^-$ , and  $\text{HCO}^+$ . Thus, in order to understand the interaction of fast hadrons in space, the mean excitation energies of such ions must be available, and calculation of them is suggested here.

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## References

1. Fox JL, Garland MI, Johnson RE (2008) Energy Deposition in Planetary Atmospheres by Charged Particles and Solar Photons. *Space Sci Rev* 139: 3-62.
2. Rostoker N, Binderbauer M, Monkhorst HJ (1996) Fusion Reactors Based on Colliding Beams in a Field Reversed Configuration Plasma. *Fusion Tech* 30: 1395-1402.
3. Rostoker N, Binderbauer MW, Monkhorst HJ (1997) Colliding beam fusion reactor *Science* 278: 1419-1422.
4. Mincher BJ, Wishart JF (2014) The Radiation Chemistry of Ionic Liquids: A Review. *Solv Extr Ion Exch* 32: 363-383.
5. Martinez O Jr, Snow TP, Bierbaum VM (2008) Ion Chemistry in the Interstellar Medium. *Proc IAU Symposium No 251*: 139-140, eds. S Kwok and S Sandford.
6. Bethe H (1930) Zue Theorie des Durchgangs Schneller Korpuskularstrahlen durch Materie. *Ann Phys* 397: 325-400.
7. Bragg WH, Kleeman H (1905) On the Alpha Particles of Radium and their Loss of Range in Passing through Various Atoms and Molecules. *Philos Mag* 10: 318-340.
8. Lindhard J, Winther Aa (1964) Stopping power of Electron Gas and Equipartition Rule. *Mat Fys Medd Dan Vid Selsk* 34: 1-22.
9. Oddershede J, Sabin JR (1984) Orbital and Whole-Atom Stopping Power and Shell Corrections for some Atoms with  $Z \leq 36$ . *At Data Nuc Data Tables* 31: 275-297.
10. Sauer SPA, Sabin JR, Oddershede J (1995) Calculated Molecular Mean Excitation Energies for Some Small Molecules. *Nuc Inst Meth B* 100: 458-463.
11. Sauer SPA, Oddershede J, Sabin JR (2015) The Mean Excitation Energy of Atomic Ions. *Adv Quantum Chem* 71: In press.
12. Roth B, Blythe P, Daerr H, Patacchini L, Shiller S (2006) Production of Iltracold, Diatomic and Triatomic Molecular Ions of Spectroscopic and Astrophysical Interest. *J Phys B: At Mol Opt Phys* 39: S1241-S1258.
13. Singh M, Chaturvedi JP (1989) Polyatomic Molecules, Molecular Ions, and Radicals of Astrophysical Interest, I. *Astrophys Space Sci* 162: 251-278.
14. Singh M, Chaturvedi JP (1989) Polyatomic Molecules, Molecular Ions, and Radicals of Astrophysical Interest, II. *Astrophys Space Sci* 162: 287-296.

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