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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, $S(v)$:

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

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

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

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

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

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]

$$\ln I_0=\frac{\int\frac{df}{dE}\ln E\,dE}{\int\frac{df}{dE}dE} \tag{4}$$

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

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

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

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

leading to the stopping power of the mixture:

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

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

	I0 (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 poly-atomic ions as well [5,12-14].

Some representative examples include CH^+, OH^-, SH^+, CN^-, and 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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