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Photoionization and photodissociation rates in solar and blackbody radiation fields

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ABSTRACT

Rate coefficients for ionization and dissociation have been calculated for over 140 atomic, molecular, and ionic species in the radiation fields of (1) the quiet and the active Sun at 1 AU heliocentric distance and (2) blackbodies at four selected temperatures in the range from $T=1000$ K to 1,000,000 K without factors for radiation dilution with distance from the source. The rate coefficients in units of transitions per second (s^{-1}) and associated excess energies of the photo products in eV are tabulated for about 265 ionization, dissociation, and dissociative ionization branches. Users can interactively access this information and plot and download cross sections and wavelength-binned results for various solar activities and blackbody temperatures on our website http://phidrates.space.swri.edu.

1. Introduction

Our database for photoionization of atoms, ions, and molecules and for photodissociation and dissociative photoionization of molecules of relevance to investigations of the planetary system has historic origins. It was originally developed for modeling comet comae and for interpreting observational data of comets (Huebner and Carpenter, 1979; Huebner et al., 1992). The new database has entries for over 140 mother species resulting in about 265 branches of products and has been expanded to include temperature-dependent blackbody radiation fields. Replacing old cross section data and thresholds with newer experimental and theoretical data and adding new species to our database have not only improved and expanded it, but also guaranteed that all photo rate coefficients are calculated consistently and uniformly with the same solar and blackbody sources for the radiation fields. Except for diatomic and many triatomic molecules, the products of photodissociation are not always well known and can vary strongly with dissociation channel, i.e., wavelength. We have improved on this situation whenever possible.

The unattenuated rate coefficient for the wavelength interval between λ_i and $\lambda_i+\Delta\lambda_i$ is

$$k_i=\int_{\lambda_i}^{\lambda_i+\Delta\lambda_i}\sigma(\lambda)\Phi(\lambda)\,d\lambda. \tag{1}$$

The integration is approximated by a sum

$$k=\sum_i k_i, \tag{2}$$

where

$$k_i=\sigma_i\Phi_i, \tag{3}$$

σ_i is the wavelength-averaged photo cross section in bin i of width $\Delta\lambda_i$, and, for the solar radiation field (SRF), Φ_i is the wavelength-integrated spectral photon flux at 1 AU heliocentric distance in the same bin. The spectral photon flux for the solar radiation field and its ratio for the active Sun to that of the quiet Sun, as used here, is the same as presented by Huebner et al. (1992).

For the blackbody radiation field (BBRF) the spectral photon flux (as opposed to the spectral energy flux) as a function of wavelength, without geometric dilution factor, is

$$\Phi(\lambda)=\frac{2\pi c}{4\lambda^4\left[\exp(hc/\lambda kT)-1\right]}, \tag{4}$$

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where c is the speed of light, h is the Planck constant, k is the Boltzmann constant, and λ is the wavelength of the radiation. For blackbody radiation we use the same wavelength grid as for the solar radiation field, but have added a few bins at long wavelengths for better resolution.

Rate coefficients for blackbody radiation are of interest in some models of planetary atmospheres, but in particular in laboratory experiments. Although the temperature range covers $T = 100$ K to more than 1,000,000 K, at the lower temperatures, in particular for $T < 1000$ K, the unattenuated and distance undiluted rate coefficients, k, for some species are so small that they are of little interest. Thus, we do not present values for $T < 1000$ K. Even at $T \approx 1000$ K some rate coefficients depend strongly on the cross sections at threshold and on the precise values of the threshold energies themselves. In these cases the rate coefficients are not very reliable; examples include Sc, Ti, V, Fe, Co, Xe, P^+, and Ca^+. In a few cases the wavelengths of the ionization thresholds are so short, e.g., $\lambda = 163.91$ Å for Li^+, 227.84 Å for He^+, and 262.20 Å for Na^+ that the photo rate coefficients for blackbody radiation are essentially zero even at $T = 2000$ K. Indeed, some lifetimes, $1/k$, are longer than the age of the solar system, which is about 10^{17} s. If a rate coefficient is less than $1 \times 10^{-99}\ s^{-1}$ the entry in the tables has been left blank.

Because of some steep gradients with respect to wavelength, we used more significant digits in all calculations. This brought about some small differences when comparing with our older results for solar radiation. These differences are mostly in the range of rounding errors and we will not dwell on them further. For the blackbody spectral photon flux see Fig. 1.

Fig. 2 compares the solar spectral photon flux (number of photons per square centimeter per second per angstrom) at 1 AU heliocentric distance for the quiet Sun with that of the active Sun. The binned values of the spectral flux for the quiet Sun and the binned spectral flux ratios for the active Sun to that of the quiet Sun have already been presented by Huebner et al. (1992). Also shown is the blackbody spectral photon flux at $T = 5770$ K, which simulates the solar spectral flux above $\lambda = 4000$ Å when diluted by the square of the ratio of the radius of the Sun ($R = 6.955 \times 10^5$ km) to that of the Earth's mean orbital radius ($r = 1$ AU $= 1.496 \times 10^8$ km): $(R/r)^2 = 2.16 \times 10^{-5}$. However, the blackbody flux deviates markedly from that of the Sun below $\lambda = 4000$ Å and becomes negligibly small, which is not surprising because that is the region where most of the strong atomic

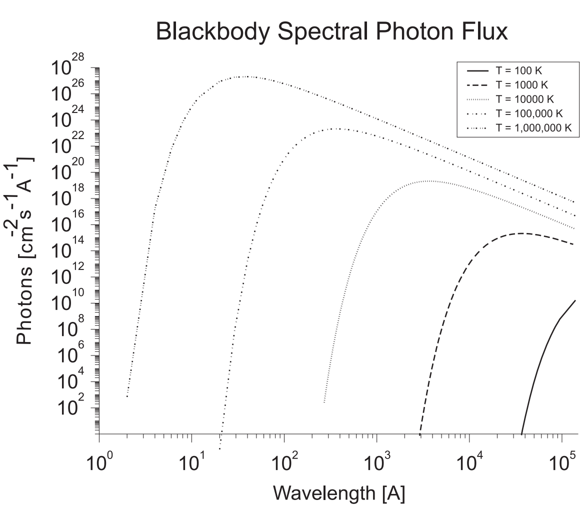

Fig. 1. Comparison of blackbody spectral fluxes (without radiation dilution factor) vs. wavelength of radiation and as a function of blackbody temperatures from $T = 10^2$ K (far right) to $T = 10^6$ K (far left). Note that for low temperatures the blackbody flux is very small in the wavelength range below dissociation or ionization thresholds of most atoms and molecules.

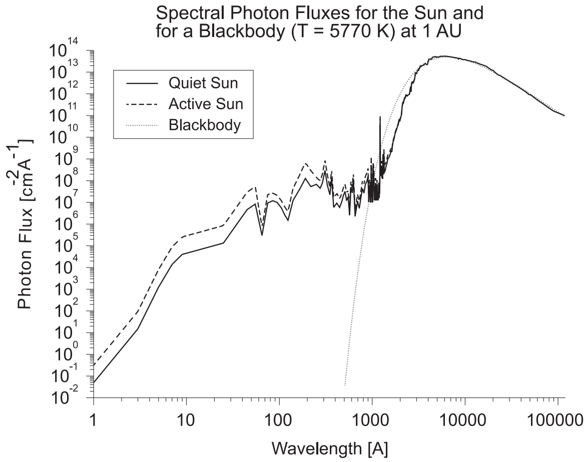

Fig. 2. A comparison of the spectral photon fluxes from the quiet Sun (full curve), active Sun (dashed curve), and a blackbody source at $T = 5770$ K (dotted curve) using the same radiation dilution factor as for the Sun at 1 AU. Note the significant contribution to the spectral photon flux of the Sun below $\lambda \approx 1000$ Å.

and molecular emission lines are in hot plasmas such as in the Sun or other stars. This is an important fact to keep in mind when simulating stellar or interstellar radiation fields by blackbody radiation.

Rate coefficients for ionization, dissociation, and dissociative ionization and the corresponding excess energies of the photo products can be calculated interactively on our website, http://phidrates.space.swri.edu, for various conditions ranging from the quiet to the active Sun and for various temperatures of the blackbody radiation field (BBRF). We have improved the website to make it consistent with modern web standards and to make it easier to download cross section data by including a download link after each cross section display. Rate coefficients for photoionization, photodissociation, and dissociative photoionization in units of s^{-1} and associated average excess energies in eV can be obtained for various levels of solar activity, ranging from the quiet Sun (activity=0) to the active Sun (activity=1), or blackbody temperatures in the range from about 100 K to over 10^6 K. The rate coefficients can also be viewed and downloaded in preset wavelength or photon energy bins. When temperature-dependent blackbody radiation fields are considered, the list allows the user to cross compare rate coefficients under various conditions.

The excess energy is the photon energy above the dissociation or ionization threshold (i.e., binding energy) that is converted into kinetic energy of the given photo products. The mean excess energy of photolysis products for a particular bound state j is

$$E^j = \frac{\int_0^{\lambda_{th}^j} hc\left(\frac{1}{\lambda} - \frac{1}{\lambda_{th}^j}\right)\sigma^j(\lambda)\Phi(\lambda)\,d\lambda}{\int_0^{\lambda_{th}^j} \sigma^j(\lambda)\Phi(\lambda)\,d\lambda}, \quad (\lambda \le \lambda_{th}^j)$$
$$\approx \sum_i hc\left[\frac{\lambda_i + \Delta\lambda_i/2}{\lambda_i(\lambda_i + \Delta\lambda_i)} - \frac{1}{\lambda_{th}^j}\right]\frac{k_i^j}{k^j}, \tag{5}$$

where $\sigma^j(\lambda)$ is the partial photodissociation or photoionization cross section for bound state j having a threshold wavelength $\lambda_{(th)}^j = hc/E^j$, where h is Planck's constant, c is the speed of light, and k^j is the rate coefficient as given in Eq. (2). The mean value of the excess energy is then

$$E = \sum_i E^j. \tag{6}$$

The summation over i in Eq. (5) is over all wavelength bins. Thus, the most tightly bound components of a molecule or