A MODEL OF ELECTRONICALLY-EXCITED STATES OF N_2 AND ITS EXTREME-ULTRAVIOLET SPECTRUM.

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The nitrogen molecule is a long-studied and difficult problem in molecular spectroscopy, and many important details of its interaction with radiation remain unexplained. A principal problem of continuing interest concerns the resonant photoabsorption and resultant predissociation of N_2 when exposed to extreme-ultraviolet radiation.

A model of the relevant excited states of N_2 has been developed in order to quantify their interactions and reproduce photoabsorption and photodissociation cross sections between 100 000 and 118 500 cm^{-1} (100 and 84 nm). This solves the radial Schrödinger equation within a coupled-channels formulation for new diabatic potential-energy curves, homogeneous and heterogeneous state mixing, and electronic transition moments for the optically allowed transitions. The accidental predissociation of $^1\Pi_u$ states between 100 000 and 112 500 cm^{-1} has been quantitatively modelled by spin-orbit coupling these to a set of $^3\Pi_u$ and $^3\Sigma_u^+$ states which includes unbound members.

Following reference to a large experimental database, the model is both accurate and comprehensive and may be used to simulate synthetic cross sections for any temperature or isotopologue. These are suitable for use in high-resolution photochemical models of atmospheric and astrophysical environments.