

Abstract

Highly correlated icMRCI wavefunctions are used to calculate the potential energy and spin-orbit coupling functions for several of the lowest electronic states of the CO^{2+} dication. Using these functions, the positions and lifetimes of the corresponding vibronic states are evaluated by means of both stabilisation and complex-scaling methods within the framework of multichannel Schrödinger analysis. Since the predicted lifetimes agree well with the measure values, exactly the same procedure based on the *ab initio* calculations can be used to determinate the positions and widths of the isoelectronic system CS^{2+} . The computed lifetimes of several vibronic states of CS^{2+} are in the range $1 \text{ ps} < \tau \ll 1 \mu\text{s}$, therefore these states govern the second step in the sequential pathway $\text{CS}_2^{3+} \rightarrow \text{S}^+ + \text{CS}^{2+} \rightarrow \text{S}^+ + \text{C}^+ + \text{S}^+$ of the overall three-body Coulomb explosion of CS_2^{3+} .

In terms of the foregoing calculations, an attempt to determine both Vis and IR emission and absorption spectra of CO^{2+} is made. Radiative lifetimes found for transition moment matrix elements and Einstein A coefficients are evaluated using the complex-scaling method. Unfortunately, when emission is concerned, the radiative lifetimes of $\text{A}^3\Sigma^+$ and $\text{b}^1\Pi$ electronic states in CO^{2+} are longer than the rate of predissociation from these states, which makes it impossible for emission to occur. The absorption spectra of $\text{A}^3\Sigma^+ \leftarrow \text{X}^3\Pi$ and $\text{b}^1\Pi \leftarrow \text{a}^1\Sigma^+$ are determined and their absolute intensities are calculated. Also the rotational structure (energy positions and widths) for these transitions is evaluated.