SPECTROSCOPIC CHARACTERIZATION OF PROPADIENYLIDENE ($H_2C{=}C{=}C{:}$)

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The electronic absorption spectrum of propadienylidene ($H_2C{=}C{=}C{:}$) (**1**) has been obtained under conditions of argon matrix isolation at 10 K. Calculations of the ground state and the three lowest singlet excited states of **1** using the equation-of-motion coupled-cluster method have been used to interpret the spectrum. The $\tilde{A}^1A_2 \leftarrow \tilde{X}^1A_1$ transition is only vibronically allowed, and gives rise to a series of weak absorptions beginning near 717 nm (1.73 eV). The $\tilde{B}^1B_1 \leftarrow \tilde{X}^1A_1$ transition (535 nm, 2.32 eV) and the $\tilde{C}^1A_1 \leftarrow \tilde{X}^1A_1$ transition (259 nm, 4.79 eV) display vibrational progressions associated with C$-$C stretching vibrations of ca. 1000 cm^{-1} and 900 cm^{-1}, respectively. The presence of highly-structured visible absorptions in the spectrum and the confirmed presence of propadienylidene and its homologs in the interstellar medium suggest that this family of compounds might be responsible for some of the mysterious diffuse interstellar bands.