

THE OPTICAL SPECTRUM OF THE DIAMANTANE RADICAL CATION

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Diamantoids are a class of stable, aliphatic molecules arranged in cage-like structures and serve as a link between small, cyclic hydrocarbons and bulk nanodiamonds. Similarities have been observed between the infrared spectra of diamantoids and unidentified infrared emission bands seen in the spectra of young stars with circumstellar disks.¹ It is also suggested that the radical cations of these molecules could contribute to features in the well-known but largely unassigned diffuse interstellar bands due to their low ionization energy and absorption in the visible range.² However, only the optical spectrum of the adamantane cation has been measured so far.³ Herein, we report the first optical spectrum of the diamantane radical cation ($C_{14}H_{20}^+$) between 400 and 1000 nm in the gas phase. Measurements were taken in a tandem mass spectrometer by photodissociation of mass-selected ions cooled in a cryogenic 22-pole ion trap held at 5 K. The optical spectrum reveals two broad and unresolved bands centered near 760 and 450 nm that are assigned to the $D_2(^2E_u) \leftarrow D_0(^2A_{1g})$ and $D_5(^2A_{2u}) \leftarrow D_0(^2A_{1g})$ transitions using time-dependent density function theory calculations. These calculations also assist to explain the lack of vibrational structure as the result of lifetime broadening and Franck-Condon congestion arising from large geometry changes.

Literature:

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