

OPTICAL SPECTRA OF N-SUBSTITUTED ADAMANTANE CATIONS

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Diamantoids are a class of aliphatic molecules arranged in cage-like structures and serve as a link between small, cyclic hydrocarbons and bulk nanodiamonds. They are well-known for their interesting optical properties, as they typically exhibit large optical band gaps of around 6 eV or higher.¹ Their radical cations, however, are predicted to display transitions in the visible and, due to their favorable structural and optical properties, may be viable candidates as carriers of the diffuse interstellar bands.² So far, only the optical spectra of adamantane and diamantane cations have been measured, which exhibit broad and mostly vibronically unresolved features.^{3,4} To explore the effects of functionalization, we report the first optical spectra of N-substituted adamantane cations, namely 1-cyanoadamantane ($C_{11}H_{15}N^+$) and urotropine ($(CH)_6N_4^+$) between 260 and 1200 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 experimental results are compared to photoelectron spectra and time-dependent DFT calculations for interpretation.

Literature:

¹ L. Landt et al., PRL, 103, 047402 (2009).

² M. Steglich et al., ApJ, 729, 91 (2011).

³ P. Crandall et al., ApJL, 900, L20 (2020).

⁴ P. Crandall et al., ApJ, 940, 104 (2022).