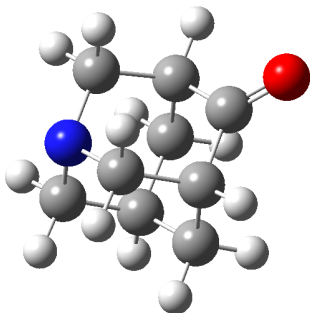


CHEMICAL SYNTHESIS AND HIGH RESOLUTION SPECTROSCOPIC CHARACTERIZATION OF 1-AZA-ADAMANTANE-4-ONE C₉H₁₃NO FROM THE MICROWAVE TO THE INFRARED

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We have synthesized 1-aza-adamantane-4-one (C₉H₁₃NO) starting from commercial 1,4-cyclohexanedione monoethylene acetal and tosylmethylisocyanide and following a procedure described in details in the literature.^b The high degree of sample purity was demonstrated by gas chromatography and mass spectrometric measurements, and its structure evidenced by ¹H and ¹³C NMR spectroscopy. We present a thorough spectroscopic characterization of this molecule by gas phase vibrational and rotational spectroscopy. Accurate vibrational frequencies have been determined by infrared and far-infrared spectra. The pure rotational spectrum of the molecule has been recorded both by cavity-based Fourier-transform microwave spectroscopy in the 2-20 GHz region, by supersonically expanding the vapor pressure of the warm sample, and by room-temperature absorption spectroscopy in the 140-220 GHz range. Quantum-chemical calculations have enabled a fast analysis of the spectra. Accurate sets of rotational and centrifugal distortion parameters of 1-aza-adamantane-4-one in its ground state and five vibrationally excited states have been derived from these measurements.

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^bBlack, R. M. *Synthesis*, 1981, 829