CHEMICAL SYNTHESIS AND HIGH RESOLUTION SPECTROSCOPIC CHARACTERIZATION OF 1-AZA-ADAMANTANE-4-ONE $C_9H_{13}NO$ FROM THE MICROWAVE TO THE INFRARED

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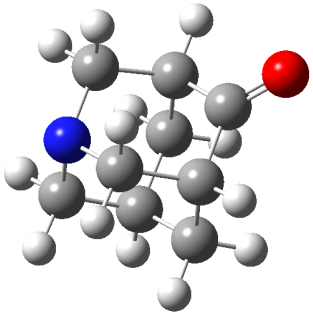

We have synthesized 1-aza-adamantane-4-one ($C_9H_{13}NO$) starting from commercial 1,4-cyclohexanedionemonoethylene acetal and tosylmethylisocianide and following a procedure described in details in the literature.[b] The high degree of sample purity was demonstrated by gas chromatography and mass spectrometric 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 distorsion 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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[b] Black, R. M. Synthesis, 1981, 829