Solution Structures of Purine Base Analogues 9-deazaguanine and 9-deazahypoxanthine

Vishakha Karnawat and Mrinalini Puranik^{*}

¹Indian Institute of Science Education and Research, Pune-411008, India

Supplementary Information

Manuscript submitted to: Journal of Biomolecular Structure and Dynamics

*Corresponding Author:

Dr. Mrinalini Puranik, Mendeleev Building, Indian Institute of Science Education and Research,
Pune-411008, Maharashtra, India

Phone: +91-735 069 4600; Email: mrinalini@iiserpune.ac.in

Figure S1: DFT (B3LYP/6-31G (d, p) computed spectra of (a) neutral 9DAG, (b) N3 protonated, (c) N1 deprotonated, (d) N7 deprotonated. N7 deprotonated shows weak carbonyl stretch at 1813 cm^{-1} whereas in N1 deprotonated, the carbonyl stretch is completely disappeared.

Figure S2: Normal mode vectors of neutral 9-deazaguanine. Structure of 9-deazaguanine was computed using dispersion corrected density functional theory in Gaussian 09. WB97XD/6-31G (d, p) level of theory was used for the purpose. Wavenumber calculations were performed on the optimized structure using same level of theory.*represents the wavenumber obtained in UVRR experiment.

Figure S3: Lorentzian fits to the Raman bands at 1540 cm⁻¹ and 1551 cm⁻¹. (a) The spectrum in the range 1530-1560 cm⁻¹ is fitted with two Lorentzian bands. The experimental spectrum is shown in grey, the fitted spectrum is shown in solid black and the deconvoluted fits to contributing bands are shown in dashed lines. (b) Upon isotopic labeling of hydrogen with deuterium, the band at 1551 cm⁻¹ downshifts to 1545 cm⁻¹ while the band at 1540 cm⁻¹ shifts much lower to 1156 cm⁻¹, out of this range.

Figure S4: DFT (B3LYP/6-31G (d, p)) computed spectra of (a) neutral 9DAH, (b) N3 protonated, (c) N1 deprotonated, (d) N7 deprotonated. N7 deprotonated shows weak carbonyl stretch at 1810 cm⁻¹ whereas in N1 deprotonated, the carbonyl stretch is completely disappeared.

Figure S5: Normal mode vectors of 9-deazahypoxanthine. Structure of 9-deazahypoxanthine was computed using dispersion corrected density functional theory in Gaussian 09. WB97XD/6-31G (d, p) level of theory was used for the purpose. Wavenumber calculations were performed on the optimized structure using same level of theory.*represents the wavenumber obtained in UVRR experiment.

Figure S6: Lorentzian fits to the Raman bands in 1400 cm⁻¹ to 1500 cm⁻¹ region. The experimental spectrum is shown in grey, the fitted spectrum is shown in solid black and the deconvoluted bands are shown in dashed lines.