Adenine, a DNA base, has been complexed with a single magnesium atom within superfluid helium droplets. The N9H stretch, symmetric and asymmetric NH2 stretching modes have been measured and compared to the adenine monomer. It was found that three separate isomers exist in the helium droplets environment, specifically, magnesium binds to the N1, N3 and N7 sites on the adenine. Vibrational bands are unambiguously characterized using vibrational transition moment angle (VTMA) analysis.