Theoretical study of hydroxamic acids

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Abstract

Ab initio molecular orbital calculations on formohydroxamic and acetohydroxamic acids give stabilities in the order: E-keto ≫ Z-keto ≫ Z-enol ≫ E-enol. However, on hydration the E-keto and Z-keto order is reversed, in agreement with NMR results. Methyl substituted forms are also considered, and the importance of hydrogen bonding is noted.