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Title:	Azine-Hydrazone Tautomerism of Guanylhydrazones: Evidence for the Preference Toward the Azine Tautomer
Authors:	Khullar, S. (/jspui/browse?type=author&value=Khullar%2C+S.) Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Guanylhydrazones Chemistry Medicinal Organic synthesis
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Citation:	Journal of Organic Chemistry, 81(17), pp.7574-7583.
Abstract:	Guanylhydrazones have been known for a long time and have wide applications in organic synthesis, medicinal chemistry, and material science; however, little attention has been paid toward their electronic and structural properties. Quantum chemical analysis on several therapeutically important guanylhydrazones indicated that all of them prefer the azine tautomeric state (by about 3–12 kcal/mol). A set of simple and conjugated azines were designed using quantum chemical methods, whose tautomeric preference toward the azine tautomer is in the range of 3–8 kcal/mol. Twenty new azines were synthesized and isolated in their neutral state. Variable temperature NMR study suggests existence of the azine tautomer even at higher temperatures with no traces of the hydrazone tautomer. The crystal structures of two representative compounds confirmed that the title compounds prefer to exist in their azine tautomeric form.
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