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Title:	Ring-chain isomerism in conjugated guanyldiazones: Experimental and theoretical study
Authors:	Mandal, S.K. (/jspui/browse?type=author&value=Mandal%2C+S.K.)
Keywords:	Ring-chain DFT Isomerism Guanyldiazone NMR
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Citation:	Tetrahedron, 74(23), pp. 2857-2864
Abstract:	<p>Treatment of 1,3-diaryl-propene-2-one with aminoguanidine under acidic conditions for a short reaction period (1 h) delivers - in accordance with a literature report - the corresponding guanyldiazones. However, when the reaction time was increased to 12 h, formation of the ring annulated product 4,5-dihydro-1H-pyrazole-1-carboximidamide was observed. This is the first case of ring-chain isomerism in conjugated guanyldiazones. The acyclic conjugated guanyldiazone and the corresponding annulated product (4,5-dihydro-1H-pyrazole-1-carboximidamide) could be clearly distinguished by means of UV and NMR spectroscopy. The formation of the ring isomer was further confirmed by single crystal XRD analysis. The time-dependent ¹H NMR study indicated the gradual transformation of the open-chain compound into the cyclic one. The mechanistic insights into the formation of these two products were explored using quantum chemical methods which revealed that the ring isomer is thermodynamically more stable than the open-chain isomer by 6–11 kcal/mol and the barrier for cyclization was found to be 31.37 kcal/mol.</p>
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