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Polarity and structure of 2-(1-methylbenzimidazol-2-yl)-1-phenyl- and -1,2-diphenyl-1-nitroethenes

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Abstract

Polarity of 2-(1-methylbenzimidazol-2-yl)-1-phenyl- and -1,2-diphenyl-1-nitroethenes was determined and their structure was studied using electronic and ^1H , ^{13}C NMR spectroscopy, dipole moments measuring, XRD analysis, and quantum-chemical calculations. It was shown that the 2-(1-methylbenzimidazol-2-yl)-1-nitro-1-phenylethene has Z-configuration both in crystal and solution. The nitro group and benzimidazole substituent in its molecule are removed from the plane of the double bond. For 1,2-diphenyl-1-nitroethene E-structure is typical. © 2012 Pleiades Publishing, Ltd.

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