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Dipole moments and quantum chemical study of the structure of furan-containing gem-bromonitroethenes

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Abstract

© 2015 Pleiades Publishing, Ltd. As shown by the dipole moment method and quantum chemical calculations, 1-(furan-2-yl)-2-nitroethene and 1-nitro-2-(5-nitrofuran-2-yl)ethenes exist in solution as E-s-trans isomers while 1-bromo-2-(5-bromofuran-2-yl)-1-nitroethene and 1-bromo-1-nitro-2-(5-nitrofuran-2-yl)ethene have Z-s-cis configuration.

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