Self-assembly of amides of *endo*-3-(3-methylthio-1*H*-1,2,4-triazol-5-yl)bicyclo[2.2.1]hept-5-ene-2-carboxylic acid directed by *N*-amide substituents.

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Streszczenie

The condensation of endo-S-methyl-N′-(bicyclo[2.2.1]hept-5-ene-2,3-dicarbonyl) isothiosemicarbazide with 12 primary amines was investigated. The molecular structure of all new products (3a–3l) was confirmed by spectroscopic methods, including 1D/2D NMR, IR spectroscopy and mass spectrometry, and an X-ray crystallography of three selected representative amide crystals. The 2,3-disubstitution of norbornene (endo-bicyclo[2.2.1]hept-5-ene) unit stabilizes overall cisoid orientation of substituents. Spectroscopic and structural analyses indicate that for the series of 12 derivatives the rigid molecular part is endo-bicyclo[2.2.1]hept-5-ene-2-carboxamide fragment. The specific orientation of the 3-(methylthio)-1H-1,2,4-triazole unit, second substituent to the norbornene skeleton, is correlated with the chemical character of N-amide substituents. Phenyl derivatives stabilize transoid orientation of the N–Htriazole and C=Oamide bonds, whereas the alkyl (methylene or methine) spacer promotes cisoid orientation of these bonds and provides possibility for an intramolecular hydrogen bonding. The solid-state IR spectra and X-ray analysis indicate three patterns of intermolecular association in this series of crystals. Hydrogen bonds observed in crystals influence positions of vibrational bands corresponding to νNH (3322–3180 cm−1), νC=O (1634–1676 cm−1), and δNH (1600–1500 cm−1).

Słowa kluczowe

norbornene, atom, molecule, 4-triazole, crystal structure, IR spectra, 1D/2D NMR experiments, Hydrogen bond

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