physico-chemical properties.

NN414 is a very weak acid with pKₐ = 8.5, log P = 1.6, and molar weight M₀ = 291.8 g/mol. Two true polymorphs, A and B, of this compound have been identified. Polymorph A crystallizes in needle-shaped crystals with a triclinic unit cell by precipitation from a variety of solvents such as acetic acid, acetonitrile, diluted ammonia, methanol, N-methyl-pyrolidone, 1-propanol, or 2-propanol [1]. Polymorph B forms prismatic crystals by precipitation from methanol or ethanol, and this unit cell is rhombohedral [1]. Mixtures of A and B can also be obtained. Both polymorphs are highly crystalline. Polymorph A melts at approximately 257°C whereas polymorph B melts at approximately 269°C [1].

To establish the thermodynamic relationship between A and B, different experiments concerning crystallization, density of mass, solubility and melting behaviour were carried out using hot stage microscopy, He-pycnometry, intrinsic solubility, and differential scanning calorimetry [2]. The results of these experiments unambiguously point to an enantiotropic relationship between A and B, with A being thermodynamically stable at ambient conditions, and B being the stable polymorph at elevated temperatures. A transition point temperature between A and B has been estimated to Ttrans = 215°C ± 15°C from the differences in melting enthalpies.

The title compounds, 1-methyl-1-phenyl-3-[1-hydroxyimino-2-(1,4-diaryl)-phenyl]cyclobutyl)-2-morpholin-4-yl-ethanone oxime, C₁₇H₂₄N₂O₂, (I), and 1-(3-methyl-3-phenylcyclobutyl)-2-morpholin-4-yl-ethane oxime, C₁₇H₂₀N₂O₃, (II), crystallize in space group P2₁/c, [1]. Each compound contains a cyclobutane ring, an oxime group and a benzene ring [2]. The molecules in (I) are connected by O–H...O hydrogen bonds and crystal packing is governed by weak intermolecular C–H...O hydrogen bonds and π–π stacking.

Keywords: polymorphism, phase transition, drug molecule

P.06.10.13

Epimerization of α-amino Nitriles to Single Stereoisomers in the Solid State
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Enantiomeric or diastereomeric enrichment to a single isomer has had only limited success to date. We have found that a diastereomeric mixture of α-amino nitriles, which was prepared by the diastereo-selective Strecker reaction using the amino alcohol as a chiral auxiliary, thermally epimerizes to a single stereoisomer in the solid state. X-ray structure analyses have shown that the α-amino nitrile, [1S,2R(SR)]=C=O-N-(cyano)(phenyl)methyl-1-aminoodindan-2-ol, epimerizes at 65 °C to give a single diastereomer with an (S)-configuration ([S]-isomer) at the α position to the nitrite moiety. Namely the (R)-isomer is thermally unstable and the (S)-isomer is stable in the solid state. In DMSO solution, the diastereomerically pure (S)-isomer epimerizes at room temperature to give a 1 : 1 mixture of the (S)- and (R)-isomers. Therefore the cause of thermal unstability of (R)-isomer in the solid state should be ascribed to the crystal structure. In the (R)-isomer crystal there are two hydrogen bonds, an intramolecular N–H...O and an intermolecular C–N...HO bonds which promote dissociation of the cyanide anion. On the other hand, the intramolecular O–H...N bond in the (S)-isomer crystal retards the dissociation of the cyanide anion. As a result, the (R)-isomer selectively epimerizes to the (S)-counterpart via an iminium or imine intermediate.

Keywords: epimerization, solid state isomerization, diastereomeric enrichment

P.06.10.14

Two Oxime Derivatives Including Succinimid and Morpholin Groups
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The title compounds, 1-methyl-1-phenyl-3-[1-hydroxyiminino-2-succinimidido] ethyl cyclobutane, C₁₇H₂₃N₂O₂, (I), and 1-(3-methyl-3-phenylcyclobutyl)-2-morpholin-4-yl-ethane oxime, C₁₇H₂₀N₂O₂, (II), crystallize in space group P2₁/c, [1]. Each compound contains a cyclobutane ring, an oxime group and a benzene ring [2]. The cyclobutane ring in (II) is more puckered than in (I). In (II), morpholin ring adopts a chair conformation. Although the oxime moiety in (I) has an E configuration, the oxime moiety in (II) has a Z configuration. The molecules in (I) are linked by O–H...O and C–H...π(benzene) interactions, forming a two-dimensional network, while the molecules in (II) are connected by O–H...N interaction.

Keywords: crystal structures, organic molecule, drug action

P.06.10.15

3-Methoxy-5-(4-methylphenyl)azetidin-2-one and 3-methoxy-5-(2-methylphenyl)azetidin-2-one
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The two title molecules, both C₁₇H₂₀N₂O₂, are roughly planar and display a trans conformation with respect to the N–N–double bond, as found for other diazene derivatives. In both compounds, there are intramolecular O–H...O hydrogen bonds and the crystal packing is governed by weak intermolecular C–H...O hydrogen bonds and π–π stacking.

Keywords: azo groups, π–π stacking, aromatic ring

P.06.10.16

Crystal Structure of 2-cyclohexyl-5-formyl-6-(4-bromophenyl) Imidazo[2,1-b][1,3,4] Thiadiazole
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1,3,4-thiadiazole nucleus is associated with a broad spectrum of biological activities, possibly due to built in toxophoric thioamide (S=C=N-) unit. Biosteric nature with biologically significant thiazole moiety and its non-carcinogenic nature. A lot of work on the synthesis and biological activities of condensed imidazo(b) thiadiazoles has been reported since the discovery of novel broad spectrum anthelmintic, Tetramisole. The trend has been shifted to explore the drugs containing biosteric thiadiazole ring in place of thiazole ring of tetramisole viz., imidazo (2,1-b)-1,3,4-thiadiazoles and their derivatives. The title compound screens them for their pharmacological activities.