physico-chemical properties.

NN414 is a very weak acid with pK_a = 8.5, log P = 1.6, and molar weight M_w = 291.8 g/mol. Two true polymorphs, A and B, of this compound have been identified. Polymorph A crystallizes in needleshaped crystals with a triclinic unit cell by precipitation from a variety of solvents such as acetic acid, acetonitrile, diluted ammonia, methanol, N-methyl-pyrrolidone, 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 257ºC whereas polymorph B melts at approximately 269ºC [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 unanimously 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 T_{trans}= 215°C ± 15°C from the differences in melting enthalpies.

[1] Jensen A.F., Junager F., Jessen C. U., Kornø H. T., *International Patent Application*, 2004, WO2004005299. [2] Bernstein J., Davey R. J., Henck J.-O., *Ang. Chem. Intl. Ed*., 1999, **38**, 3440-3461.

Keywords: polymorphism, phase transition, drug molecule

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Epimerization of α-amino Nitriles to Single Stereoisomers in the Solid State

Akira Uchida[a], Rumiko Sakurai[b], Tetsutaro Hattori[b], Masanori Yamaura[c], [a]*Toho University.* [b]*Tohoku University.* [c]*Iwaki Meisei University.* E-mail: auchida@biomol.sci.toho-u.ac.jp

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, [1*S*,2*R*,(*SR*)]-N-cyano(phenyl)methyl-1-aminoindan-2-ol, epimerizes at 65 °C to give a single diastereomer with an (*S*)-configureation ((*S*)-isomer) at the α position to the nitrile 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 CN…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

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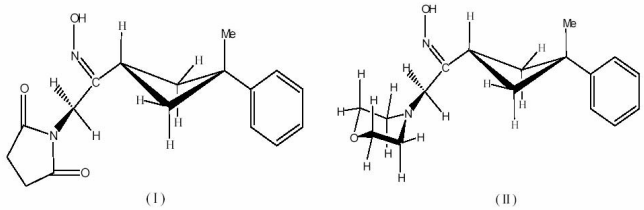
Two Oxime Derivatives Including Succinimid and Morpholin Groups

Muharrem Dinçer[a], Namık Özdemir[a], İbrahim Yılmaz[b], Alaaddin Çukurovalı[b], [a]*Dep. of Physics, Ondokuz Mayıs Univ., 55139, Samsun, Turkey.* [b]*Dep. of Chem., Fırat Univ., 23119, Elazığ, Turkey*. E-mail: mdincer@omu.edu.tr

The title compounds, 1-methyl-1-phenyl-3-[1-hydroxyimino-2-succinimido) ethyl] cyclobutane, $C_{17}H_{20}N_2O_3$, (I), and 1-(3-methly-3-phenylcyclobutyl)-2-morpholin-4-yl-ethanone oxime, $C_{17}H_{24}N_2O_2$, (II), crystallize in space group $P2_1/c$, [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.



(I) (II)

[1] Özdemir N., Dinçer M., Yılmaz İ., Çukurovalı A., *Acta Cryst*., 2004, **E60**, o145-o147. [2] Ahmedzade M., Çukurovalı A., Koparır M., *J. Chem. Soc. Pak*., 2003, **25**, 51-55.

Keywords: crystal structures, organic molecule, drug action

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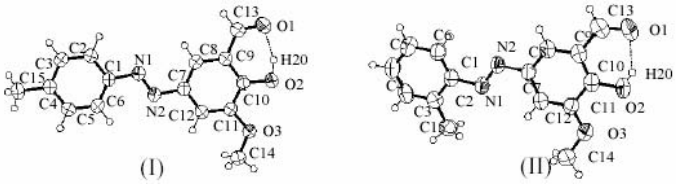
3-Methoxy-5-(4-methylphenyldiazenyl)salicylaldehyde and 3-methoxy-5-(2-methylphenyldiazenyl)salicylaldehyde

Ahmet Erdönmez[a], Cem Cüneyt Ersanlı[a], Çiğdem Albayrak[b], Mustafa Odabaşoğlu[b], Canan Kazak[a], [a]*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Samsun, Turkey.* [b]*Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, TR-55139 Samsun, Turkey*. E-mail: erdonmez@omu.edu.tr

The two title molecules, both $C_{15}H_{14}N_2O_3$, 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.



(I) (II)

The structures of both (I) and (II) (Figs. 1 and 2) contain two essentially planar fragments, *viz*. one monosubstituted (C1-C6) and one trisubstituted phenyl ring (C7-C12). The aromatic rings are in a *trans* conformation with respect to the azo double bond. The C14–O3 bond length [1.413(2)Å in (I) and 1.429(4)Å in (II)] is approximately equal to that usually associated with a methyl C–O bond in a methoxy group attached to an aromatic ring (1.424Å; Allen *et al*., 1987).

[1] Allen F. H., Kennard O., Watson D. G., Brammer L., Orpen A. G., *J. Chem. Soc. Perkin Trans*., 1987, **2**, S1-19.

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

P.06.10.16

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Crystal Structure of 2-cyclohexyl-5-formyl-6-(4-bromophenyl) Imidazo[2,1-b] [1,3,4] Thiadiazole

K.V. Arjuna Gowda[a], G.D. Kolavi[b], I.M. Khazi[b], [a]*Department of Physics, MVJ College of Engineering, Bangalore-560 067, India.* [b]*Department of Chemistry, Karnataka university, Dharwad-580 003, India.* E-mail: arjunagowda@indiainfo.com

1,3,4-thiadizole 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) thiazoles 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., imdizo (2,1-b) -1,3,4-thiadizoles and their derivaties. The title compound screens them for their pharmacological activities.