

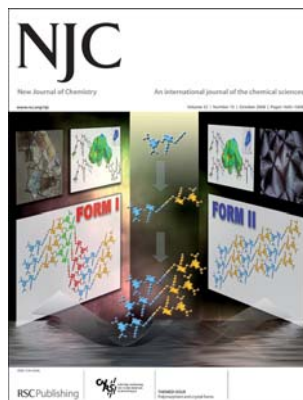
IN THIS ISSUE

ISSN 1144-0546 CODEN NJCHES 32(10) 1645-1808 (2008)



Cover

See Nicholas Blagden *et al.*, pp. 1659–1672. Melt co-crystallisation from the eutectic mixture of the components: isonicotinamide and benzoic acid. The 1 : 1 co-crystal phase is shown growing from the interface of the melted benzoic acid and melting isonicotinamide. Image reproduced with permission from Nicholas Blagden, David J. Berry, Andrew Parkin, Hafsa Javed, Asim Ibrahim, Pauline T. Gavan, Luciana L. De Matos and Colin C. Seaton from *New J. Chem.*, 2008, **32**, 1659.



Inside Cover

See Ulrich J. Griesser *et al.*, pp. 1677–1685. Two polymorphs of aprepitant differ only in alternatively stacked units (2D fragment) with molecular units of the same geometry, in spite of six freely rotatable bonds (packing polymorphism). Image reproduced with permission from Doris E. Braun, Thomas Gelbrich, Volker Kahlenberg, Gerhard Laus, Josef Wieser and Ulrich J. Griesser from *New J. Chem.*, 2008, **32**, 1677.

CHEMICAL SCIENCE

C73

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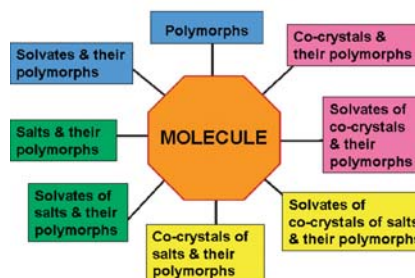
EDITORIAL

1657

Themed issue: Polymorphism and crystal forms

Common crystallization techniques, and mechanical and thermal treatments of the same molecule can generate a myriad of different crystalline forms, all of which can be "tainted" with polymorphism.

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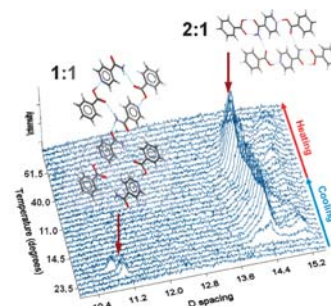
PERSPECTIVE

1659

Current directions in co-crystal growth

Nicholas Blagden,* David J. Berry, Andrew Parkin, Hafsa Javed, Asim Ibrahim, Pauline T. Gavan, Luciana L. De Matos and Colin C. Seaton

This perspective discusses co-crystallisation and is focused upon combining contemporary crystal growth and crystal engineering concepts along with phase equilibria to optimise functional materials design.



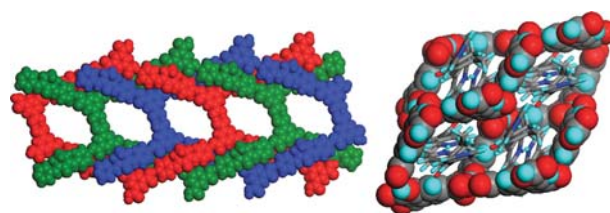
LETTER

1673

Crystal engineering with acid and pyridine heteromeric synthon: neutral and ionic co-crystals

Ramkinkar Santra, Nayan Ghosh and Kumar Biradha*

The crystal structure of the neutral form $H_3TMA \cdot 1$ (H_3TMA = trimesic acid, **1** = 2,6-bis(4-pyridylmethylene)cyclohexanone) exhibits a predictable triple interpenetrated (6,3)-hydrogen bond network, while the crystal structure containing ionic components exhibits an unpredictable double interpenetrated three-dimensional network containing an anionic (4,4) layer with the inclusion of cationic dimers.



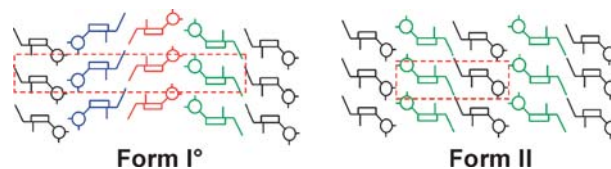
PAPERS

1677

Packing polymorphism of a conformationally flexible molecule (aprepitant)

Doris E. Braun, Thomas Gelbrich, Volker Kahlenberg, Gerhard Laus, Josef Wieser and Ulrich J. Griesser*

The two polymorphs of the NK_1 receptor antagonist aprepitant differ only in the packing of identical molecular units, a 2D packing fragment, which is a stack of 1D N-H...O bonded hydrogen ribbon chains. The minor structural differences may explain the fact that the two forms often crystallise concomitantly and also the high kinetic stability of the metastable form II.

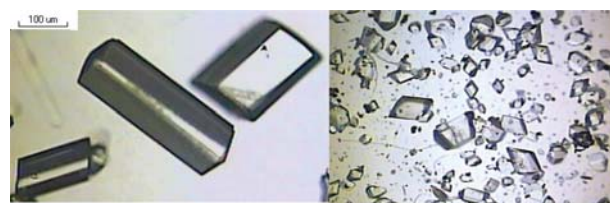


1686

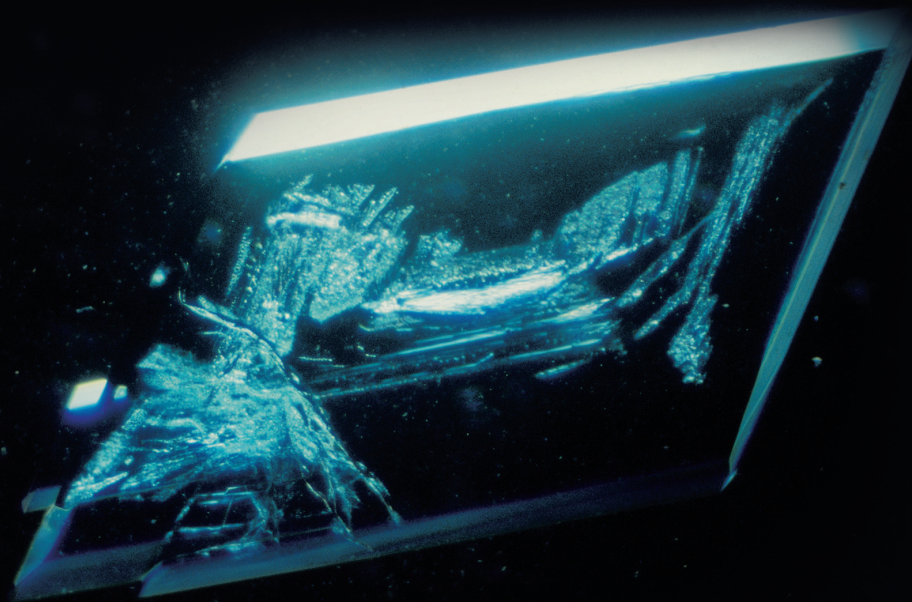
The crystallisation and stability of a polymorphic salt, ethylene diammonium dinitrobenzoate

Roger J. Davey and Helen P. Jones

Ostwald's law is not always obeyed: crystallisation control of the triclinic and monoclinic forms of a polymorphic molecular salt.



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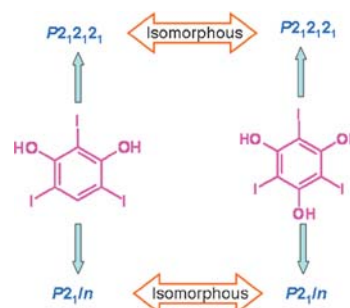
PAPERS

1693

Isostructural polymorphs of triiodophloroglucinol and triiodoresorcinol

Naba K. Nath, Binoy K. Saha and Ashwini Nangia*

The orthorhombic and monoclinic polymorphs of triiodoresorcinol and triiodophloroglucinol establish a structural link in the crystal structure series from triiodobenzene ($P2_12_12_1$) to trifluorotriiodobenzene ($P2_1/n$).

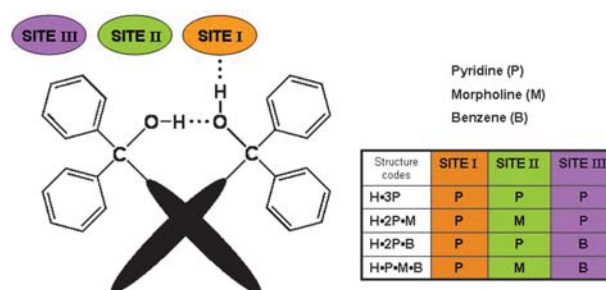


1702

Polymorphism, isostructurality and variability in the inclusion chemistry of a diol host compound

Luigi R. Nassimbeni,* Hong Su and Edwin Weber

The title diol-host forms a series of isostructural inclusion compounds with pyridine, morpholine and benzene, in which the guests are interchangeable and located at fixed sites.

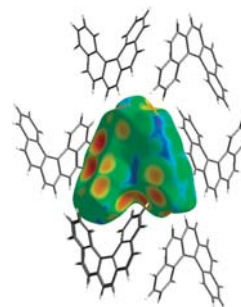


1710

Synthesis, crystal structure and crystal packing of diaza[5]helicenes

Cristina Bazzini, Tullio Caronna, Francesca Fontana, Piero Macchi,* Andrea Mele, Isabella Natali Sora, Walter Panzeri and Angelo Sironi

The *isomorphism* and *polymorphism* of carbo- and aza[5]helicenes in the solid state.

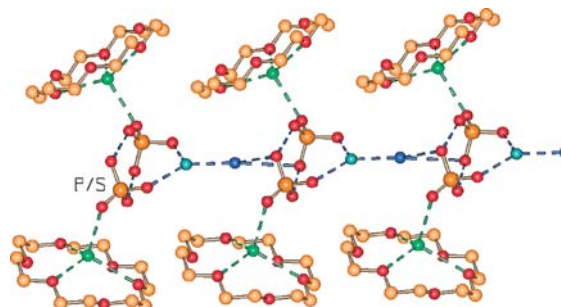


1718

Crystal forms of highly “dynamic” 18-crown[6] complexes with $M[HSO_4]$ and $M[H_2PO_4]$ ($M^+ = NH_4^+, Rb^+, Cs^+$): thermal behaviour and solid-state preparation

Dario Braga, Enrico Modena, Marco Polito,* Katia Rubini and Fabrizia Grepioni*

The dehydration and decomplexation of 18-crown[6] complexes prepared *via* solid-state reactions are investigated by DSC, TGA and variable temperature X-ray powder diffraction.



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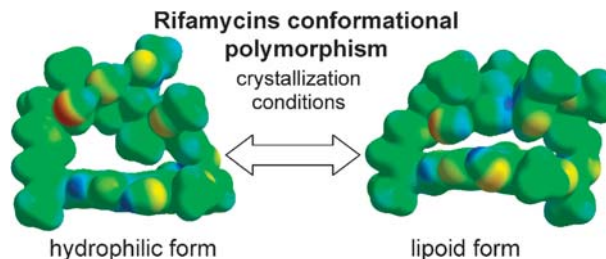
PAPERS

1725

Sampling rifamycin conformational variety by cruising through crystal forms: implications for polymorph screening and for biological models

Alessia Bacchi,* Mauro Carcelli and Giancarlo Pelizzi

A new conformer of rifamycin S has been isolated in the solid state by planning the crystallization conditions; implications on the models used to explain the activity of rifamycins are discussed. The first X-ray structure of rifaximin is also determined and discussed.

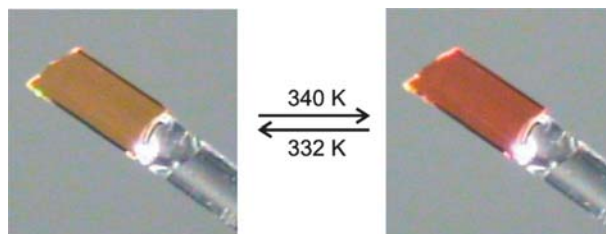


1736

Synthesis, characterization and phase transitions of the inorganic–organic layered perovskite-type hybrids $[(C_nH_{2n+1}NH_3)_2PbI_4]$ ($n = 12, 14, 16$ and 18)

David G. Billing* and Andreas Lemmerer

The reversible and thermochromic phase transitions of the inorganic–organic layered perovskite-type hybrids $[(C_nH_{2n+1}NH_3)_2PbI_4]$ ($n = 12, 14, 16$ and 18) are investigated *via* single-crystal diffraction.

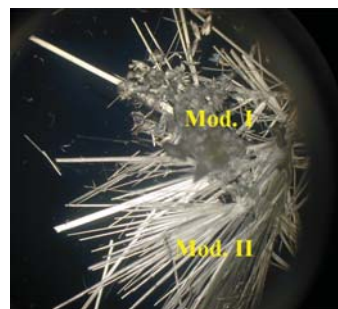


1747

The study of the polymorphic system of 2-chloro-4-nitrobenzoic acid

Inna Barsky, Joel Bernstein,* Peter W. Stephens and Kevin H. Stone

Two concomitant polymorphs of 2-chloro-4-nitrobenzoic acid have been characterized by spectroscopic, structural and thermal methods, including synchrotron PXRD that demonstrated a very strong thermal expansion anomaly of Modification I around 90 °C upon heating.

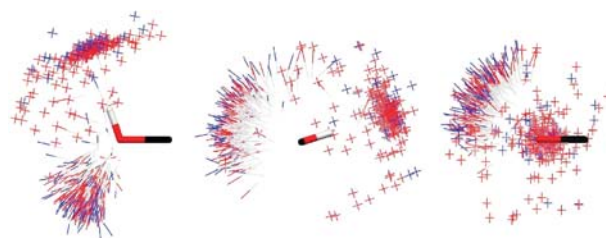


1754

A study of methanol solvates using the Cambridge structural database

Monika Brychczynska, Roger James Davey and Elna Pidcock

An analysis of methanol in solvated crystal structures reveals the relative occurrence of different hydrogen bonding environments.



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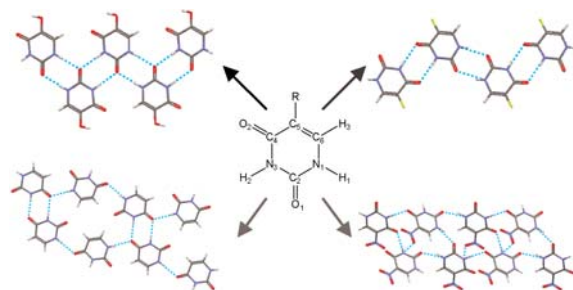
PAPERS

1761

The observed and energetically feasible crystal structures of 5-substituted uracils

Sarah A. Barnett, Ashley T. Hulme, Nizar Issa, Thomas C. Lewis, Louise S. Price, Derek A. Tocher and Sarah L. Price*

The observed and computed low energy structures of twelve 5-substituted uracils demonstrate the significant effect of any substituent on the range of uracil hydrogen bonding motifs.

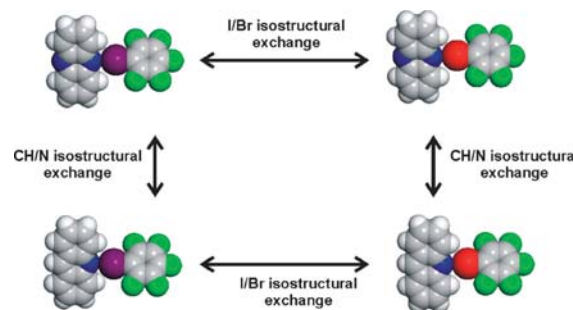


1776

A cocrystallisation-based strategy to construct isostructural solids

Dominik Cinčić, Tomislav Friščić and William Jones*

The structural equivalences of CH and N moieties and of halogen-bonded Br and I groups has been utilised to systematically construct a set of altogether four isostructural halogen-bonded cocrystals.

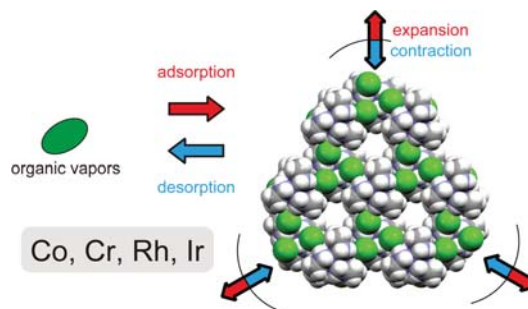


1782

Gas-adsorbing ability of tris-ethylenediamine metal complexes (M = Co(III), Cr(III), Rh(III), Ir(III)) as transformable ionic single crystal hosts

Satoshi Takamizawa,* Masa-aki Kohbara, Takamasa Akatsuka and Ryosuke Miyake

Single crystals of $[M^{III}(\text{en})_3]\text{Cl}_3$ (M = Co, Cr, Rh, Ir) show gas adsorbency for various organic vapors accompanying channel expansion in their crystal structures.

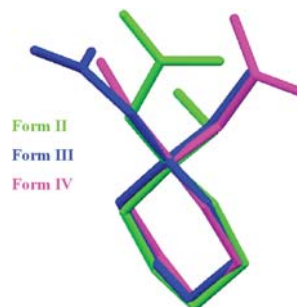


1788

Polymorphic gabapentin: thermal behaviour, reactivity and interconversion of forms in solution and solid-state

Dario Braga, Fabrizia Grepioni,* Lucia Maini, Katia Rubini, Marco Polito, Roberto Brescello, Livius Cotarca, M. Teresa Duarte,* Vânia André and M. Fátima M. Piedade

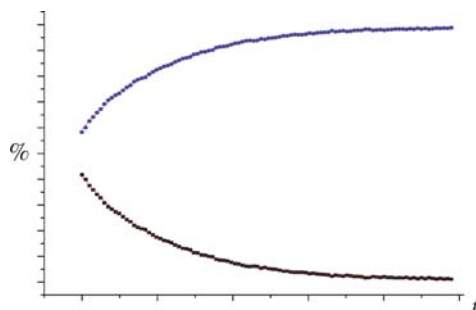
Polymorphic forms of gabapentin were investigated by DSC, HSM and PXRD.



PAPER



1796



Structural characterisation of two pharmaceutically important steroids by solid-state NMR

Abdullah Othman, Robin K. Harris,* Paul Hodgkinson, Elizabeth A. Christopher and Robert W. Lancaster

Magic-angle spinning NMR provides an essential tool, complementary to diffraction, for studying the crystallography and molecular-level mobility of organic polymorphs and solvates, as illustrated by two steroids.

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