

CrystEngComm

A journal at the forefront of the design and understanding of solid-state and crystalline materials

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Cover

See Užarević *et al.*, pp. 4291–4438.
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CrystEngComm, 2011, **13**, 4314.

EDITORIALS

4303

Dynamic behaviour in the solid state

Tomislav Friščić* and Graeme M. Day*

Welcome to this *CrystEngComm* themed issue on dynamic behaviour and reactivity in crystalline solids.

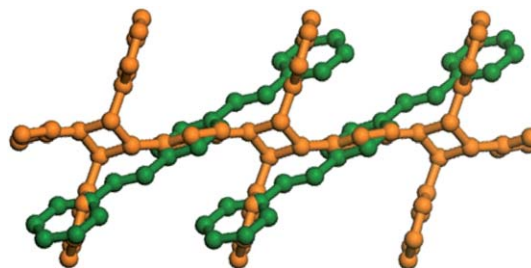


4304

Crystal engineering: origins, early adventures and some current trends

SirJohn Meurig Thomas*

An insight into the engineering of organic crystals.



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COMMUNICATIONS

4307

Surface nucleation in solid-state dimerisation of nitrosobenzenes promoted by sublimation

Ivan Halasz* and Hrvoj Vančik*

Nucleation on the surface during a solid state reaction is promoted by sublimation which possibly creates a defect rich environment.

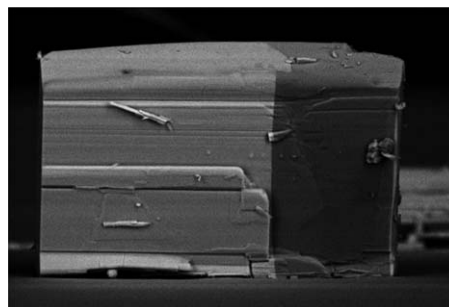


4311

Isostructural coordination polymers: epitaxis vs. solid solution

Matteo Lusi, Jerry L. Atwood, Leonard R. MacGillivray and Leonard J. Barbour*

Different synthetic conditions often afford different products and this is more evident for complex structures (*i.e.* solvates, polymorphs, co-crystals, solid solutions, *etc.*). We show how solution growth of a given set of components produces an epitaxial heterocrystal while mechanochemical synthesis yields a solid solution.



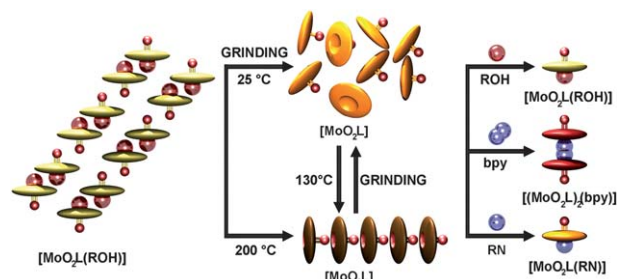
PAPERS

4314

Mechanosensitive metal–ligand bonds in the design of new coordination compounds

Krunoslav Užarević,* Mirta Rubčić,* Maja Radić, Andreas Puškarić and Marina Cindrić

The mechanochemical or thermal treatment of preorganised molybdenum complexes yields activated coordinatively unsaturated precursors for the highly efficient synthesis of various coordination compounds.

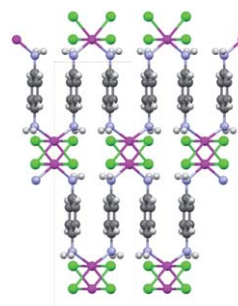


4324

Crystal synthesis of 1,4-phenylenediamine salts and coordination networks

Christopher J. Adams, Mairi F. Haddow, Matteo Lusi and A. Guy Orpen*

The solid-state syntheses of metal–organic salts and coordination networks containing 1,4-phenylenediamine have been investigated for zinc, cadmium and copper.



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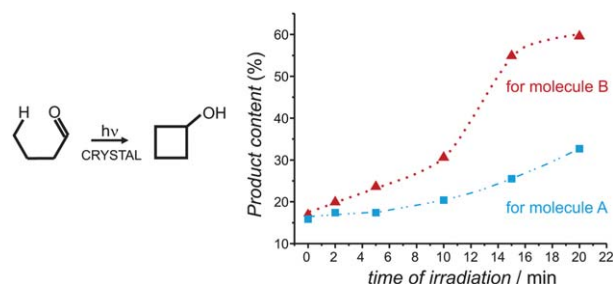
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PAPERS

4332

Photo-induced structural changes in two crystal forms with different numbers of independent moleculesJulia Bąkiewicz, Jacek Skarzewski
and Ilona Turowska-Tyrk*

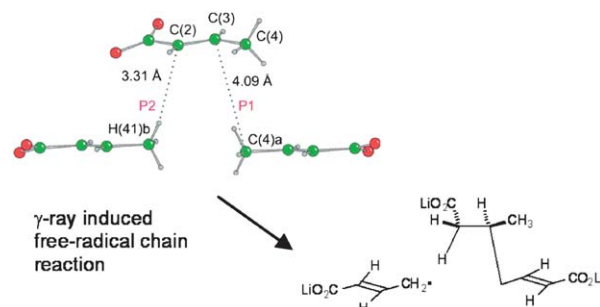
Two symmetrically independent molecules behave differently during the photochemical reaction; the cell parameters are influenced not only by the photoreaction.



4339

Chemo- and stereospecific solid-state dimerization of lithium *trans*-2-butenolate and lithium *trans*-2-butenolate formamide solvateWen Shang, Magali B. Hickey, Volker Enkelmann,
Barry B. Snider* and Bruce M. Foxman*

Exposure of solid lithium *trans*-2-butenolate salts to ^{60}Co γ -rays induces a chemo- and stereospecific dimerization, where hydrogen atom transfer is stereospecific, topochemical, and not part of a random process.

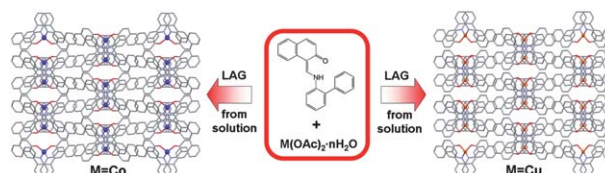


4351

Schiff base derived from 2-hydroxy-1-naphthaldehyde and liquid-assisted mechanochemical synthesis of its isostructural Cu(II) and Co(II) complexes

Dominik Cinčić* and Branko Kaitner

Two Schiff base complexes with Cu(II) and Co(II) have been obtained by a conventional solution-based method as well as by liquid-assisted grinding. Both complexes form 1D chains by weak C–H \cdots O and C–H \cdots C interactions.

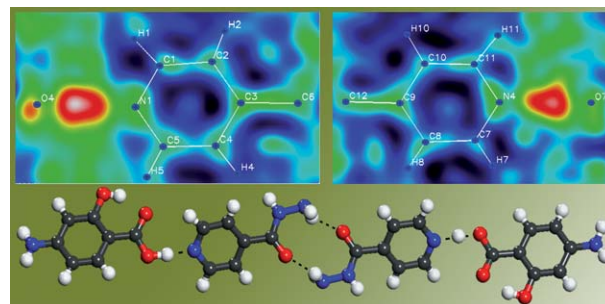


4358

Drug-drug co-crystals: Temperature-dependent proton mobility in the molecular complex of isoniazid with 4-aminosalicylic acid

Pawel Grobelny, Arijit Mukherjee and Gautam R. Desiraju*

The structures of two TB drug-drug co-crystals are reported and in one of them is observed the rare case of simultaneous existence of pure hydrogen bonded and partially ionic carboxylic acid \cdots nitrogen base synthons.



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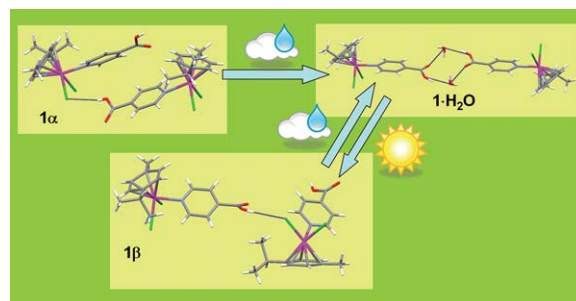
PAPERS

4365

Water vapour uptake and extrusion by a crystalline metallorganic solid based on half-sandwich Ru(II) building-blocks

Alessia Bacchi,* Giulia Cantoni, Michele R. Chierotti, Alberto Girlando, Roberto Gobetto, Giuseppe Lapadula, Paolo Pelagatti,* Angelo Sironi and Matteo Zecchini

Water uptake transforms **1 α** into the hydrated form (**1 \cdot H₂O**). Thermal treatment of **1 \cdot H₂O** does not restore **1 α** but rather its polymorph **1 β** , which gives **1 \cdot H₂O** back upon water uptake.

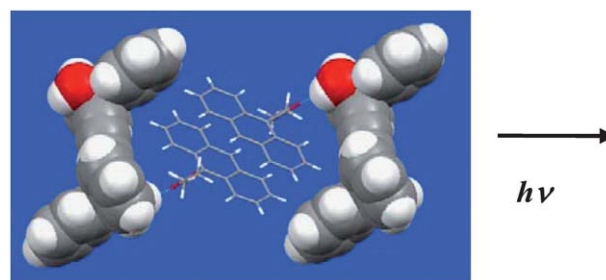


4376

Photodimerization of anthracene derivatives in their neat solid state and in solid molecular compounds

I. Zouev, Den-Ke Cao, T. V. Sreevidya, M. Telzhensky, M. Botoshansky and M. Kaftory*

Comparison of irradiation of crystals of neat compounds and crystals of their molecular compounds.

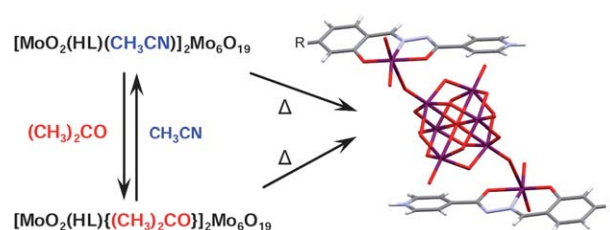


4382

Hybrid organic–inorganic compounds based on the Lindqvist polyoxomolybdate and dioxomolybdenum(vI) complexes

Višnja Vrdoljak,* Biserka Prugovečki, Dubravka Matković-Čalogović and Jana Pisk

The lability of the solvent molecule in [MoO₂(HL)(CH₃CN)]₂Mo₆O₁₉ allows the formation of a desolvated active intermediate which can interact with a weak donor substrate or with the Lindqvist polyoxomolybdate moiety.

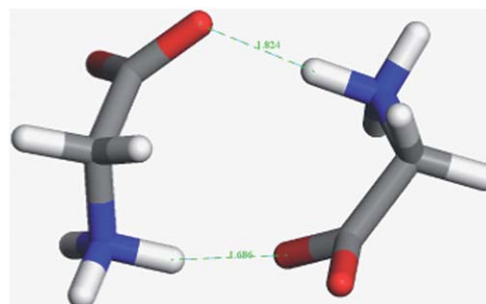


4391

Are glycine cyclic dimers stable in aqueous solution?

Said Hamad* and C. Richard A. Catlow

We have used *ab initio* molecular dynamics in an extensive study of the dynamics of glycine dimers in aqueous glycine solutions, investigating the effect of several variables, such as the presence of deuterated water or the presence of Cl[−] and Na⁺ ions. We have not found evidences of stable, long-lived cyclic dimers.





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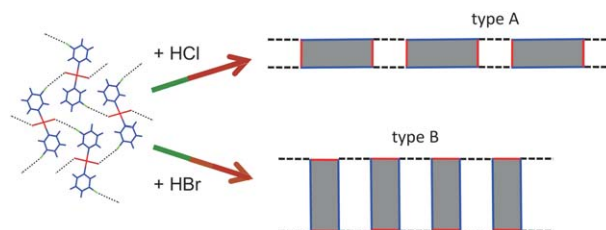
PAPERS

4400

Different structural destinations: comparing reactions of $[\text{CuBr}_2(3\text{-Brpy})_2]$ crystals with HBr and HCl gas

Guillermo Mínguez Espallargas, Alastair J. Florence, Jacco van de Streek and Lee Brammer*

A solid–gas reaction with aqueous HCl or HBr vapour results in chemically similar but structurally dissimilar crystalline products.

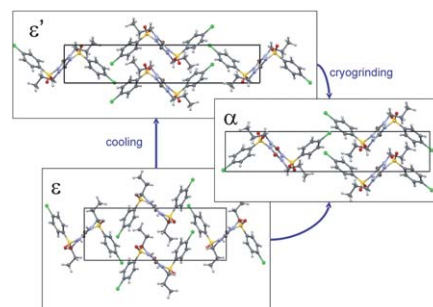


4405

'Hedvall effect' in cryogrinding of molecular crystals. A case study of a polymorphic transition in chlorpropamide

Tatiana N. Drebuschak, Anna A. Ogienko and Elena V. Boldyreva*

A phase transition, induced by low temperature, facilitates another one, induced by mechanical treatment.

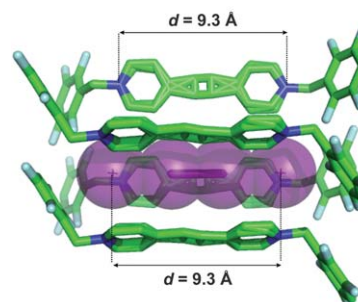


4411

Dimensional caging of polyiodides: cation-templated synthesis using bipyridinium salts

Marcos D. García,* Javier Martí-Rujas, Pierangelo Metrangolo,* Carlos Peinador, Tullio Pilati, Giuseppe Resnati,* Giancarlo Terraneo and Maurizio Ursini

Cation-templated synthesis and size-matching approach drive the formation of polyiodides into supramolecular cages.

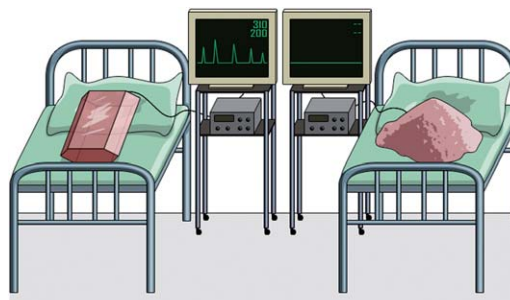


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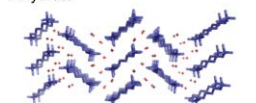
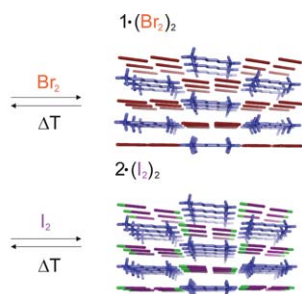
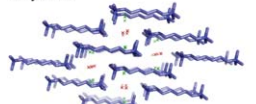
Decreasing particle size helps to preserve metastable polymorphs. A case study of DL-cysteine

Vasily S. Minkov,* Valery A. Drebuschak, Andrey G. Ogienko and Elena V. Boldyreva*

The interconversion between high-temperature and low-temperature polymorphs of DL-cysteine is no longer observed after larger crystals are ground to powder.



4427

Hexamethonium Bromide ($1 \cdot (\text{H}_2\text{O})_2$)
DihydrateHexamethonium Chloride ($2 \cdot (\text{H}_2\text{O})_2$)
Dihydrate

Solid-state synthesis of mixed trihalides *via* reversible absorption of dihalogens by non porous onium salts

Lorenzo Meazza, Javier Martí-Rujas, Giancarlo Terraneo,*
Chiara Castiglioni, Alberto Milani, Tullio Pilati,
Pierangelo Metrangolo* and Giuseppe Resnati*

1,6-Bis(trimethylammonium)hexane bis(trihalides) and mixed bis(trihalides) have been synthesized by treating the corresponding dihydrated halides with molecular dihalogens under gas–solid and solution conditions.

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