Creation of crystalline supramolecular assemblies using a C–H···O/O–H···N pair-wise hydrogen bond coupling

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The systematic construction of various supramolecular motifs using a cyclic coupling involving both a strong and a weak hydrogen bond is described.

Supramolecular chemistry involves the efficient creation of molecular assemblies by means of specific intermolecular (*i.e.* non-covalent) interactions.[1] Its success requires a knowledge of the types of interactions which may be reliably used, with the appropriate choice meeting both geometric as well as energetic considerations.[2] In building up supramolecular assemblies there is an analogy with conventional (covalent) synthetic chemistry. In the same way that efficient chemical synthesis requires judicial choice of reactants and a chosen strategy (*e.g.* reaction type) the construction of molecular arrays *via* non-covalent linkages requires the careful coupling of molecules through the non-covalent bonding of appropriate functional groups.

The hydrogen bond, with well characterised geometry and robustness, is frequently used in designing supramolecular arrays.[3,4] Specific interactions (couplings) based on hydrogen bonding which are frequently used are shown as **I–VIII** in Scheme 1. Unlike **I–VII**, which are constructed from either strong (*e.g.* O–H···O, N–H···O, N–H···N, **I–V**) or weak (*e.g.* C–H···O, **VII**) hydrogen bonds, couplings **VIII** and **IX** consist of both a weak and a strong hydrogen bond, although neither has previously been used to systematically design co-crystals.† In this communication we use **IX** to create various arrays.

Compounds capable of forming assemblies with $-CO_2H$ and utilizing coupling **IX** are N-heterocycles and a supramolecular array **3a** based on this coupling results when a mixture of 3,5-dinitrobenzoic acid **2** and **1** (in 2 : 1 mol ratio) are co-crystallised from MeOH.‡ Within the structure (Fig. 1) acid **2** recognises **1** through the formation of coupling **IX**, with the short H···N [1.75(4) Å, 166(3)°] and H···O [2.36(3) Å, 161(2)°] contacts confirming the affinity of the $-CO_2H$ group to form this type of coupling. Fig. 1 also indicates that molecules of **1** themselves self-recognise through C–H···N [H···N, 2.55(3) Å, 166(2)°] hydrogen bonds. The result is a unit consisting of two molecules of both **1** and **2**. (This four-membered unit then acts as the building unit for the assembly *via* a herringbone arrangement of **3a**). We note that an alternative recognition pattern (Scheme 2) involving a 2 : 1 complex is not formed.

Within complex **3a** the aromatic hydrogen at the *para* position in **2** does not participate in the formation of C–H···O hydrogen bonds as is generally observed in the crystal structures of dinitrobenzoic acid derivatives.[6] Within the crystal structure of pure **2** one of the $-NO_2$ group is twisted by 23° from the plane of the phenyl ring, perhaps to facilitate the formation of C–H···O hydrogen bonds. In the complex **3a**, however, both $-NO_2$ groups are essentially planar with the phenyl rings. As a result the *para*-H atom is completely enclosed between bulky NO_2 groups and is most likely shielded and therefore excluded from hydrogen bond formation. If this shielding effect could, by appropriate substitution, be removed an infinite molecular tape might result.

To explore this point, 3,5-dinitro-4-methylbenzoic acid, **4**, was co-crystallised with **1** (from a 2 : 1 ratio in solution) to yield complex **3b**. Our rationalisation for this is that the hydrogens of the methyl group would now be sufficiently removed from the NO_2 groups to participate in hydrogen bonding, particularly in the formation of C–H···O hydrogen bonds.[7]

The crystal structure determination of complex **3b**‡ revealed that the recognition pattern *via* coupling **IX** is similar to that in complex **3a**, although **3b** crystallises in a 1 : 2 ratio with each molecule of **1** connected to two acid molecules **4** (Fig. 2). In

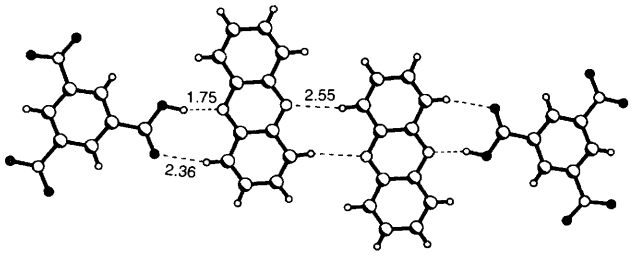
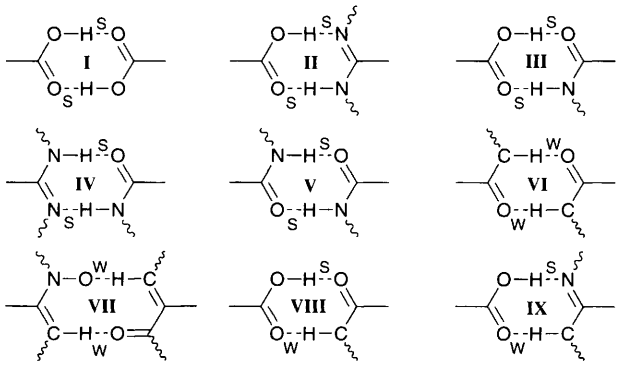
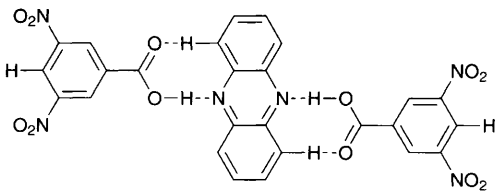


Fig. 1 Supramolecular unit in the complex **3a**; coupling **IX** is identified between phenazine **1** and 3,5-dinitrobenzoic acid **2**. Molecules of **1** interact *via* C–H···N hydrogen bonds.



Scheme 1 s = strong, w = weak



Scheme 2

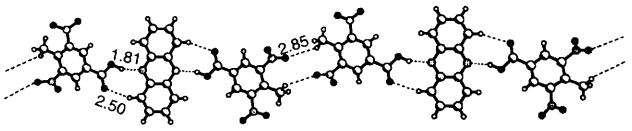
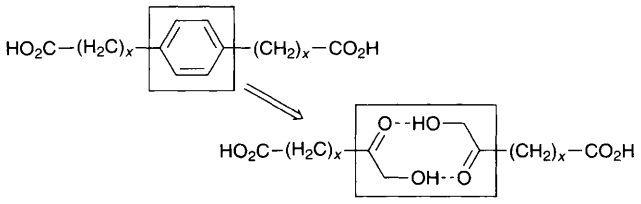


Fig. 2 Molecular tape generated in complex **3b** involving coupling **IX**

particular, Fig. 2 illustrates that indeed the expected centrosymmetric C–H···O bonds [H···O 2.85(3) Å, 110(2)°] between the $-NO_2$ and $-CH_3$ groups of the acid molecules, **4**, are formed.§ As a result the building motif is extended into a chain. The hydrogen-bond distances involved in **IX** in **3b** [H···N, 1.81(3) Å, 161(3)°; H···O, 2.50(3) Å, 159(2)°] are longer than the corresponding distances in **3a** [H···N 1.75(4) Å, H···O 2.36(3) Å] possibly suggesting that the $-CH_3$ group, in addition to forming C–H···O hydrogen bonds, may also modify the strength of the coupling by its electron-donating nature.

The molecular tape formed in **3b** involves the use of two couplings. To create a tape in which only **IX** was utilised we considered co-crystallisation of **1** with a dicarboxylic acid (such as terephthalic acid, **5**). Attempts to co-crystallise **1** and **5** were not successful, however, because of the differences in their solubility. We therefore sought to create a non-covalent analogue to **5** which would enable the molecular tape to be created.[8] This is illustrated in Scheme 3 where a non-covalent analogue of **5** is generated using two aliphatic acid molecules *via* coupling **I**. This approach was confirmed by complex **3c** which was obtained between **2** and malonic acid **6** from a 2 : 1 solution in MeOH.

Complex **3c** crystallises with the formation of coupling **IX** between **1** and **6** in a 2 : 1 ratio (Fig. 3).‡ Again, the hydrogen-bond distances observed in the coupling are significantly short [H···O 1.72(4) Å, 167(3)°; H···O 2.33(2) Å, 154(2)°]. A particularly interesting feature, revealed in Fig. 3, is that a molecular tape results through coupling **I** [H···O 1.60(4) Å, 177(4)°] between the second $-CO_2H$ group on the adjacent molecules of **6** rather than through the formation of the coupling **IX**. This suggests that selection of appropriate phenyldicarboxylic acids would also result in the formation of molecular tapes exclusively *via* the formation of coupling **IX**. The formation of complex **3c** may be regarded as a further example indicating the interchange of covalent and non-covalent linkages in the formation of supramolecular assemblies.



Scheme 3

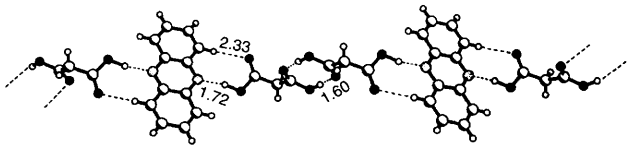


Fig. 3 Representation of molecular tape in complex **3c** through coupling **I** and **IX**; the malonic acid units form a centrosymmetric pair with the topology suggested in Scheme 3

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Footnotes

† This conclusion is based on a search performed on the CSD [version 5.09 (April, 1995 release), F. H. Allen and O. Kennard, *Chemical Design Automation News*, 1993, **8**, 1, 31]. We have found that although the coupling **IX** is present in various crystal structures (the majority of them for biologically active molecules), the original papers do not consider the weak hydrogen bond as part of a cyclic motif or discuss the possible use of **IX** as a potential coupling unit in the design of supramolecular arrays.

‡ *Crystal data*: **3a** $C_7H_4N_2O_6{\cdot}C_{12}H_8N_2$, M = 392.33, monoclinic, space group, $P2_1/n$, a = 5.845(2), b = 11.928(2), c = 24.642(3) Å, β = 93.17(2)°, U = 1715.4(7) Å^3, Z = 4, D_c = 1.519 Mg m^{-3}, R_1 = 0.037, wR_2 = 0.088, residual electron density: min., max. −0.221, 0.193 e Å^{-3}. **3b** $2(C_8H_6N_2O_6){\cdot}C_{12}H_8N_2$, M = 632.50, monoclinic, space group $P2_1/n$, a = 8.727(1), b = 11.245(2), c = 14.123(2) Å, β = 101.99(1), U = 1355.7(3) Å^3, Z = 2, D_c = 1.549 Mg m^{-3}, R_1 = 0.034, wR_2 = 0.086, residual electron density: min., max. −0.151, 0.157 e Å^{-3}. **3c** $2(C_3H_3O_4){\cdot}C_{12}H_8N_2$, M = 388.33, triclinic, space group $P\bar{1}$, a = 5.583(1), b = 6.535(1), c = 12.410(2) Å, α = 82.01(3), β = 89.69(3), γ = 75.16(3)°, U = 433.2(1) Å^3, Z = 1, D_c = 1.488 Mg m^{-3}, R_1 = 0.038, wR_2 = 0.098, residual electron density: min., max. −0.169, 0.148 e Å^{-3}. Atomic coordinates, bond lengths and angles, and thermal parameters have been deposited at the Cambridge Crystallographic Data Centre (CCDC). See Information for Authors, Issue No. 1. Any request to the CCDC for this material should quote the full literature citation and the reference number 182/37.

§ Since C–H···O hydrogen bonds are electrostatic in nature, falling off much more slowly with distance than other intermolecular forces such as van der Waals or dispersive forces (ref. 2), the H···O distance of 2.85 Å observed here is well within a range acceptable for C–H···O hydrogen bonds.

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8 See for example H. Nakanishi, W. Jones, J. M. Thomas, H. Hasegawa and W. L. Rees, *Proc. R. Soc. London A.*, 1980, **369**, 307 in the comparison between α-*trans*-cinnamic acid and α-distyrylpyrazine.

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Contact: American Chemical Society, Meetings, PO Box 18598, 20th St Station, Washington, DC 20036 8598, USA.

13th IUPAC International Conference on Physical Organic Chemistry
Seoul, Korea August 25-29
Contact: Professor J Suh, Department of Chemistry, Seoul National University, Seoul 151-742, Republic of Korea.
Tel +82 2 8805456. Fax +82 2 8891568.

10th International Biotechnology Symposium
Sydney, Australia August 25-30
Contact: 10th IBS '96 Symposium Secretariat, PO Box 128, Sydney, NSW 2001, Australia. Tel +61 (2) 2622277.
Fax +61 (2) 2622323. E-mail veckels@tourhosts.com.au

14th IUPAC Conference on Chemical Thermodynamics
Osaka, Japan August 25-30
Contact: Professor M Sorai, Executive Secretary of ICCT-96. Microcalorimetry Reasearch Center, Faculty of Science. Osaka University, Toyonaka, Osaka 560, Japan.
Tel +81 (6) 8505523. Fax +81 (6) 850 5526 or 5288.
E-mail icct96@chem.sci.osaka-u.ac.jp

10th Conference of the European Society of Biomechanics
Leuven, Belgium August 28-31
Contact: Dr J Vander Sloten, Executive Secretary, 10th Conference of the European Society of Biomechanics, Katholieke Universiteit Leuven, Division of Biomechanics and Engineering Design, Celestijnenlaan 200A, B-3001 Heverlee, Belgium.
Tel +32 16 32 70 96. Fax +32 16 29 27 16.
E-mail jos.vandersloten@mech.kuleuven.ac.be

Supramolecular Chemistry: Molecular Recognition and Drug–Receptor Interactions
Salamanca, Spain August 29-September 3
Contact: Dr J Hendekovic, European Science Foundation, 1 quai Lezay-Marnésia, 67080 Strasbourg Cedex, France.
Tel +33 88 76 71 35. Fax +33 88 36 69 87.
E-mail euresco@esf.org

September 1996

NSW Southern Highlands Conference on Heterocyclic Chemistry
Bowral, Australia September 1-3
Contact: Professor David St C Black, School of Chemistry, University of New South Wales, Sydney, NSW 2052, Australia.
Tel +61 2 385 4712. Fax +61 2 662 2835.
E-mail D.Black@unsw.edu.au

8th FECHEM Conference on Heterocycles in Bio-organic Chemistry
Villa Olmo, Como, Italy September 1-4
Contact: Professor Bruno Danieli, Dipartimento di Chimica Organica e Industriale, Università di Milano, Via Golgi 19, I-20133 Milano, Italy.

ECME 96, Third European Conference on Molecular Electronics
Leuven, Belgium September 1-6
Contact: Professor F C De Schryver, Department of Chemistry, KU. Leuven, Celestijnenlaan 200 F, B-3001 Heverlee, Belgium.

XIth International Symposium on Organosilicon Chemistry
Montpellier, France September 1-6
Contact: Professor R J P Corriu, Laboratoire des Precurseurs Organométalliques de Materiaux, UMR CNRS 44, Université de Montpellier II, Place E. Bataillon, CC 007, F34095 Montpellier Cedex 5, France. Fax +33 67 14 38 88.

11th European Symposium on Quantitative Structure-Activity Relationships: Computer-assisted Lead Finding and Optimization
Lausanne, Switzerland September 1-6
Contact: Dr Han van de Waterbeemd, c/o F, Hoffmann-La Roche Ltd, Dept. PRPC 65/314, CH-4002 Basel, Switzerland.
Tel +41 61 688 8421. Fax +41 61 688 1075.
E-mail johannes.van_de_waterbeemd@roche.com

†*Contact:* Dr J F Gibson, The Royal Society of Chemistry, Burlington House, London, UK W1V 0BN. Tel +44 (0) 171 437 8656. Fax +44 (0) 171 8883.

5th International Conference on Chemical Synthesis of Antibiotics and Related Microbial Products
Debrecen, Hungary September 1-6
Contact: The Congress Center, L. Kossuth University, 5th ICSA, H-4010 Debrecen, PO Box 68, Hungary. Fax +36 52 310936. E-mail antibiotics@tigris. klte.hu

RSC 3rd International Symposium: Transition Metals in Organic Synthesis
London, UK September 4-6
Contact: RSC†

Biocoordination Chemistry and Framework Structures
Odense, Denmark September 6-11
Contact: Professor H Toftlund, Kenusk Institut, Department of Chemistry, Odense Universitet, Campusvej 55, DK-5230 Odense M, Denmark.

9th International Symposium on Molecular Recognition and Inclusion (ISMRI9)
Lyon, France September 7-12
Contact: Dr A W Coleman, Institute de Chimie et Biologie des Protéines, CNRS UPR 417, 7 Passage du Vercors, F-69376 Lyon Cedex 07, France. Tel +33 72 72 26 40. Fax +33 72 72 26 01.

XIVth International Symposium on Medicinal Chemistry
Maastricht, The Netherlands September 8-12
Contact: H Timmerman, Leiden/Amsterdam Centre for Drug Research (LACDR), Department of Pharmacochemistry, Vrije University, De Boelelaan 1083, NL-1081-HV Amsterdam, The Netherlands. Tel +31 (0) 20 44 47580. Fax +31 (0) 20 44 47610. E-mail bijloo@chem.vu.nl

4th International Symposium on Heterogeneous Catalysis and Fine Chemicals
Basel, Switzerland September 8-12
Contact: 4th International Symposium on HCFC '96, c/o AKM Congress Service, PO Box, CH-4005 Basel, Switzerland.
Tel +41 61 691 51 11. Fax +41 61 691 81 89.

XIIIth International Symposium on the Reactivity of Solids
Hamburg, Germany September 8-12
Contact: Secretary XIIIth ISRS, Institute of Inorganic and Applied Chemistry, University of Hamburg, Martin-Luther-King-Platz 6, 20146 Hamburg, Germany. Tel +49 40 41 23 60 86.
Fax +49 40 41 23 63 48.

RSC 24th Symposium of the European Peptide Society
Edinburgh, UK September 8-13
Contact: RSC†

Advances in Chemistry of Crop Protection
Cambridge, UK September 9-11
Contact: Conference Secretariat, SCI, 14/15 Belgrave Square, London, UK SW1X 8PS.
Tel +44 (0) 171 235 3681. Fax +44 (0) 171 823 1698.

14th International Symposium on Gas Kinetics
Leeds, UK September 9-12
Contact: RSC†

RSC Autumn Meeting
Uxbridge, UK September 10-13
Contact: RSC†

Reactivity in Organised Microstructures: Chemical Reactions and Physical Processes in Compartmentalized Systems
Santiago de Compostela, Spain September 10-15
Contact: Dr J Hendekovic, European Science Foundation, 1 quai Lezay-Mamésia, 67080 Strasbourg Cedex, France.
Tel +33 88 76 71 35. Fax +33 88 36 69 87.
E-mail euresco@esf.org WWW http://www.esf.org/euresco

COPS-IV 4th International Symposium on the Characterisation of Porous Solids
Bath, UK September 15-18
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, UK BS19 2FQ.
Tel & Fax +44 (0) 1275 853311.

20th IUPAC Symposium on the Chemistry of Natural Products
Chicago, USA September 15-20
Contact: IUPAC Symposium Headquarters, 5999 Butterfield Road, Hillside, IL 60162, USA. E-mail IUPAC@searle.monsanto.com
www http://www.a2z.com/iupac20/index.hml

3rd International Medicinal Chemistry Symposium
Bath, UK September 22-24
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Nailsea, Bristol, UK BS19 2FQ.
Tel & Fax +44 (0) 1275 853311.
E-mail i.s.blagbrough@bath.ac.uk and m.d.threadgill@bath.ac.uk

23rd Annual Conference of the Federation of Analytical Chemistry and Spectroscopic Societies, FACSS XXIII
Kansas City, USA September 29-October 4
Contact: FACSS National Office, 201-B Broadway St., Frederick, MD 21701-6501 USA.
Tel +1 301 846 4797. Fax +1 301 694 6860.

October 1996

XVIIth European Colloquium of Heterocyclic Chemistry
Regensburg, Germany October 6-9
Contact: Professor G Märkl, Institut für Organische Chemie, Universität Regensburg, D-93040 Regensburg, Germany.
Tel +49 941 943 4631. Fax +49 941 943 4505.

Joint RSC Fine Chemicals and Medicinals Group-SCI Cardiovascular Meeting
Edinburgh, UK October 20-22
Contact: RSC†

Recent Advances in Drugs for the Treatment of Cardiovascular Disease
Edinburgh, UK October 20-22
Contact: Elaine Wellingham, Conference Secretariat, Field End House, Bude Close, Nailsea, Bristol, UK BS19 2FQ.
Tel & Fax +44 (0) 1275 853311.

December 1996

Fifth Eurasia Conference on Chemical Sciences
Guangzhou, China December 10-14
Contact: Professor Liang-Nian Ji, Biotechnology Research Center, Zhongshan (Sun Yatsen) University, Guangzhou, Canton 510275, China. Tel +86 (20) 418 5461. Fax +86 (20) 418 9173.
E-mail leiy@bepc2.ihep.ac.cn

January 1997

International Symposium on Chemical and Biological Thermodynamics
Amritsar, India January 5-8
Contact: Professor D V S Jain, Department of Chemistry, Panjab University, Chandigarh 160014, India. Tel +91 (172) 541435.
Fax +91 (172) 541409. E-mail dvs-jain@imtech.ernet.in

April 1997

Spring ACS National Meeting
San Francisco, USA April 13-17
Contact: American Chemical Society, Meetings, PO Box 18598, 20th St Station, Washington, DC 20036-8598, USA.

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