

Curriculum Vitae

GAUTAM R. DESIRAJU

- **Affiliations:**

- Emeritus Professor, Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru.
- Distinguished Professor, University of Petroleum and Energy Studies, Dehradun.
- Distinguished Professor, Indian Institute of Technology, Mandi.
- Professor and Dean, SASTech, Rishihood University, Sonapat.

- **Web:** <http://desiraju.in>

- **Fellowships:** Indian Academy of Sciences (1993); The National Academy of Sciences, India (2000); Indian National Science Academy (2000); The World Academy of Sciences (2002).

- **Education**

- **B.Sc.** — St. Xavier's College, University of Bombay (1972)
- **M.S.** — School of Chemical Sciences, University of Illinois, Urbana-Champaign (1974)
- **Ph.D.** — School of Chemical Sciences, University of Illinois, Urbana-Champaign (1976) under Professors David Y. Curtin and Iain C. Paul

Research Evolution: From Reductionism to Holistic Architectures

Over a career spanning five decades, his scientific inquiry has evolved from a traditional, reductionist focus on isolated molecular structures and specific intermolecular interactions toward a holistic, systems-level perspective of molecular crystals and complex material systems.

- **Reductionist Phase (1970s–1990s):** Concentrated on identifying discrete structural building blocks, proving the viability of weak directional interactions (such as C-H...O and halogen bonds), and introducing the concept of the **supramolecular synthon** in 1995 to enable retrosynthetic design in crystal engineering.
- **Integrative & Holistic Transition (2000s–Present):** Shifted toward viewing molecular crystals as complex, holistic ensembles where crystal properties

emerge from non-additive, cooperative networks of interactions. This paradigm acknowledges that supramolecular structures are not merely linear combinations of functional groups, but emergent systems governed by structural landscapes, polymorphism, and phase behaviour. This epistemological shift extends beyond structural chemistry to comparative methodologies that juxtapose Western reductionist models with Indian Knowledge Systems (IKS), emphasising systems thinking across science, education, and societal organisation.

Research Interests

- Crystal Engineering and Supramolecular Chemistry
- Weak Intermolecular Interactions and Hydrogen Bonding
- Holistic Systems Thinking in Structural Chemistry & Materials
- Active Pharmaceutical Ingredients, Polymorphism, and Crystal Landscape Analysis
- Science Education Reform and Indian Knowledge Systems
- Civilisational Reawakening of Bhārat that is India

Positions Held

- **Research Scientist** — Eastman Kodak, Rochester (1976–1978)
- **Research Fellow** — Indian Institute of Science, Bengaluru (1978–1979)
- **Lecturer** — University of Hyderabad (1979–1984)
- **Reader** — University of Hyderabad (1984–1990)
- **Visiting Scientist** — E. I. DuPont de Nemours CR&D (1988–1989)
- **Professor** — University of Hyderabad (1990–2009)
- **Dean** — University of Hyderabad (1999–2002)
- **Professor** — Indian Institute of Science, Bengaluru (2009–present; now Emeritus Professor)
- **Distinguished Professor** — University of Petroleum and Energy Studies, Dehradun
- **Distinguished Professor** — Indian Institute of Technology, Mandi
- **Professor and Dean** — Rishihood University, Sonipat

Scientific Publications

4 books, 3 edited books, and ~425 research papers *h*-index = 105

Non-Scientific Publications

7 books

Honours and Distinctions

1. Erskine Professor, University of Canterbury, Christchurch, New Zealand, 1990.
2. Fellow, Indian Academy of Sciences, 1993.
3. Visiting Professor, University of Strasbourg, Strasbourg, France, 1997.
4. CHEMITO Award, 1999.
5. Fellow, The National Academy of Sciences, India, 2000.
6. Fellow, Indian National Science Academy, 2000.
7. Alexander von Humboldt Research Award, Forschungspreis, 2000.
8. Third World Academy of Sciences (TWAS) Award, 2000.
9. Ranbaxy Award for Pharmaceutical Sciences, 2000.
10. Millennium Medal of the Indian Science Congress, 2000.
11. Silver Medal for Excellence of the Chemical Research Society of India, 2000.
12. Prof. Priyadarajan Ray Memorial Award (Indian Chemical Society), 2000.
13. Fellow, Third World Academy of Sciences, 2002.
14. Michael Visiting Professor, Weizmann Institute of Science, Israel, 2002.
15. Senior Visiting Fellow, Institute of Advanced Study, University of Bologna, Italy, 2003.
16. Visiting Fellowship (Short Term), Japan Society for the Promotion of Science, 2003.
17. Goyal Prize in Chemistry, 2005.
18. J. C. Bose Fellowship, Department of Science and Technology, Government of India, 2006–2016.

19. Honorary Member, Hungarian Chemical Society, 2006.
20. Thomson Citation Laureate Award for Chemistry, 2006.
21. Chair, Gordon Research Conference in Crystal Engineering, 2010.
22. President, International Union of Crystallography, 2011-2014.
23. Crystal Growth & Design Virtual Special Issue in Honour of Prof. G. R. Desiraju, 2013.
24. PhD Honoris Causa, University of Cordoba, Argentina, 2014.
25. PhD Honoris Causa, Rayalaseema University, Kurnool, 2017.
26. ISA Award for Science, University of Bologna, 2018.
27. P. C. Ray Award for Science and Technology, University of Calcutta, 2018.
28. PhD Honoris Causa, Gulbarga University, Kalaburagi, 2022
29. Van der Waals Prize, ICNA, Strasbourg, 2024.
30. 14th Ewald Prize, International Union of Crystallography (Awarded March 2026, formally presented in Calgary, August 2026)

Selected Committee Memberships

1. Research Council, National Chemical Laboratory, Pune.
2. Research Council, Regional Research Laboratory, Thiruvananthapuram.
3. Research Council, Indian Institute of Chemical Biology, Kolkata.
4. Chairman, Program Advisory Committee for Organic Chemistry, Department of Science and Technology, New Delhi.
5. Appellate Authority, Andhra Pradesh Pollution Control Board, Hyderabad.
6. Commission for Structural Chemistry, International Union of Crystallography.
7. National Millennium Initiative for Technology Leadership Initiatives, High Power Committee, Council of Scientific and Industrial Research, New Delhi.
8. Research Council, National Institute for Pharmaceutical Education and Research, Chandigarh.
9. Executive Committee, International Union of Crystallography.

10. Book series Committee, International Union of Crystallography.
11. Research Grant Review Committee, Human Frontier Science Program, Strasbourg.
12. Council, Indian National Science Academy, New Delhi.
13. Board of Governors, Indian Institute of Science Education and Research, Kolkata.
14. Management Board, National Centre for Biological Research, Bangalore.

Current and Former Editorial Boards and Editorial Advisory Boards

1. *IUCrJ* (Main Editor for Chemistry and Crystal Engineering)
2. *Angewandte Chemie* (Wiley-VCH).
3. *Journal of the American Chemical Society* (American Chemical Society).
4. *Chemical Communications* (Royal Society of Chemistry).
5. *Accounts of Chemical Research* (American Chemical Society).
6. *Chemical Communications* (Royal Society of Chemistry).
7. *Acta Crystallographica* (International Union of Crystallography).
8. *Journal of Physical Organic Chemistry* (Wiley).
9. *Topics in Stereochemistry* (Wiley).
10. *Journal of Chemical Sciences* (Indian Academy of Sciences).
11. *Perspectives in Supramolecular Chemistry* (Wiley).
12. *Journal of Chemical Crystallography* (Kluwer).
13. *Current Opinion in Solid State and Materials Science* (Elsevier).
14. *Crystal Growth & Design* (American Chemical Society).
15. *CrystEngComm* (Royal Society of Chemistry).
16. *Chemistry: An Asian Journal* (Wiley-VCH).
17. *Chemical Science* (Royal Society of Chemistry).
18. *Polyhedron*, Editor-in-Chief (Elsevier).

Plenary and Keynote Lectures

1. 10th International Conference of the Chemistry of the Organic Solid State, Vancouver, Canada, 1991.
2. British Crystallographic Association Spring Meeting, Manchester, England, 1993 (keynote lecture).
3. Computational Methods in Chemical Design. Theory and Experiment (CMCD 4), Kloster Irsee, Germany, 1994.
4. Symposium on Organic Crystal Chemistry, Adam Mickiewicz University, Poznan-Rydzyna, Poland, 1994.
5. NATO-ARW workshop on Crystals as Supramolecular Materials, Sestri Levante, Italy, 1995.
6. 2nd Meeting of the Asian Crystallographic Association, Bangkok, Thailand, 1995 (plenary lecture).
7. NATO-ARW workshop on Self Assembly in Synthetic Chemistry, Val Morin, Québec, Canada, 1996.
8. Summer School on Supramolecular Chemistry, Ustroń, Poland, 1996.
9. International Union of Crystallography XVII Congress, Seattle, U.S.A., 1996 (keynote lecture).
10. XIII International Symposium on the Reactivity of Solids, Hamburg, Germany, 1996 (keynote lecture).
11. NATO-ASI school on Crystal Engineering, Digby, Nova Scotia, Canada, 1996.
12. Analysis and Design of Solid State Reactions, Tokyo Institute of Technology, Tokyo, Japan, 1996.
13. 36th IUPAC Congress, Geneva, Switzerland, 1997 (keynote lecture).
14. NATO-ARW on Large Supramolecular Assemblies, Athens, Greece, 1997.
15. NATO-ARW on Molecular Magnets and Conductors, Barcelona, Spain, 1998.
16. Royal Society of Chemistry Annual Congress (Symposium on Polymorphism), Durham, England, 1998.
17. International School of Crystallography and NATO-ARW: Implications of Molecular and Materials Structure for New Technologies, Ettore Majorana Centre for Scientific Culture, Erice, Sicily, Italy, 1998.

18. American Crystallographic Association Annual Meeting (Invited keynote speaker in the symposium to commemorate the 50th anniversary of the International Union of Crystallography), Arlington, VA, U.S.A., 1998.
19. Design and Assembly of Molecules and Networks: New Forms and Functions, Cursos de Verano Universidad Complutense, San Lorenzo de el Escorial, Spain, 1998.
20. Gordon Conference on Physical Organic Chemistry, Fukuoka, Japan, 1998.
21. 16th International CODATA Conference, New Delhi, India, 1998.
22. Sonderforschungsbereich programme in Supramolecular Chemistry (Universities of Essen and Bochum), Essen, Germany, 1998.
23. International School of Crystallography and Euroconference: Crystal Engineering: From Molecules and Crystals to Materials, Ettore Majorana Centre for Scientific Culture, Erice, Sicily, Italy, 1999.
24. International School of Crystallography: Data Mining in Crystallography, Ettore Majorana Centre for Scientific Culture, Erice, Sicily, Italy, 1999.
25. Drug Design and Small-molecule Crystallography, Technical University of Łódź, Łódź, Poland, 1999.
26. Royal Society of Chemistry Symposium on Crystal Engineering and Supramolecular Chemistry, London, England, 1999.
27. Indaba on Stereochemistry of Intermolecular Interactions, Kruger Park, Skukuza, South Africa, 2000.
28. Dalton Discussion Meeting 3 on Intermolecular Interactions, Bologna, Italy, 2000.
29. 13th International Conference of the Chemistry of the Organic Solid State, Mainz, Germany, 2001.
30. European Crystallographic Meeting, Cracow, Poland, 2001.
31. Foundation Day Lecture, National Institute of Immunology, New Delhi, 2001.
32. Indian Association for the Cultivation of Science, 125th Anniversary Lecture, IACS, Kolkata, 2001.
33. Department of Atomic Energy – C.V. Raman Lectureship, Institute of Science and St. Xavier's College, Mumbai, 2001.
34. American Chemical Society Annual Meeting (keynote lecture), Orlando, Florida, 2002.

35. German Crystallographic Association Annual Meeting (keynote lecture), Kiel, Germany, 2002.
36. American Crystallographic Association Annual Meeting (keynote lecture), San Antonio, Texas, 2002.
37. International Union of Crystallography XIX Congress, Geneva, Switzerland, 2002.
38. Third World Academy of Sciences Annual Meeting (award lecture), New Delhi, 2002.
39. Prof. Priyadarajan Ray Memorial Award Lecture (Indian Chemical Society), Nagarjuna University, 2002.
40. Foundation Day Lecture, Institute of Microbial Technology, Chandigarh, 2003.
41. American Chemical Society ProSpectives Series on Polymorphism, Invited Lecture, Tampa, Florida, 2003.
42. Foundation Day Lecture, Central Salt and Marine Chemicals Research Institute, Bhavnagar, 2003.
43. European Crystallographic Meeting, Durban, South Africa, 2003.
44. American Chemical Society ProSpectives Series on Polymorphism, Tampa, Florida, 2004.
45. Scientific Update Conference on Polymorphism, New Orleans, U.S.A., 2004.
46. O. P. Vig Endowment Lecture, Panjab University, Chandigarh, 2004.
47. American Crystallographic Association, Orlando, Florida, 2005.
48. Singapore International Chemical Conference, SICC-4 (plenary), Singapore, 2005.
49. Pacifichem 2005, Honolulu, Hawaii, 2005.
50. ACS CSIR meeting on Organic Chemistry and Chemical Biology, National Chemical Laboratory, Pune, 2006.
51. Indaba on Models, Mysteries and Magic of Molecules, Kruger Park, Berg-en-dal, South Africa, 2006.
52. IQPC Conference on Polymorphism and Crystallisation, London, 2007.
53. GVK-Wyeth Symposium on Organic Synthesis, Hyderabad, 2007.

54. Forschergruppe in Intermolecular Interactions (Universities of Bochum and Essen), Czochoa, Poland, 2008.
55. First China-India-Singapore Symposium on Crystal Engineering, National University of Singapore, Singapore, 2010.
56. International Symposium on Facets of Weak Interactions in Chemistry (plenary), University of Calcutta, Calcutta, India, 2011.
57. International Union of Crystallography XXII Congress (keynote), Madrid, Spain, 2011.
58. Indo-US Bilateral Meeting on The Evolving Role of Solid-State Chemistry in Pharmaceutical Science, Manesar, Delhi, India, 2012.
59. Gordon Research Conference on Crystal Engineering, Waterville Valley Resort, New Hampshire, USA, 2012.
60. Second China-India-Singapore Symposium on Crystal Engineering, Guangzhou, China, 2012.
61. ICMAT 2013 – the 7th Biennial International Conference on Materials for Advanced Technologies, Singapore, 2013.
62. ISXB1 - First International Symposium on Halogen Bonding (plenary), Porto Cesareo, Lecce, Italy, 2014.
63. XXV National Congress of the Italian Chemical Society (keynote), Cosenza, Italy, 2014.
64. 40th Mellanby Memorial Oration, Central Drug Research Institute, Lucknow, India, 2015.

Selected Plenary and Keynote Lectures on Crystal Engineering, Structural Complexity, and Noncovalent Interactions after 2015:

65. ISA Medal Lecture, Institute of Advanced Studies, University of Bologna, Bologna, Italy, 2018.
66. J. C. Bose Memorial Lecture, Bose Institute, Kolkata, 2022.
67. Keynote Lecture on Third Generation Crystal Engineering, European Crystallography Meeting (ECM), Belgrade, Serbia, 2024.
68. Ewald Prize Lecture, 27th International Union of Crystallography Congress, Calgary, Canada, 2026.

Summary of Research

Research is centred in the field of **Crystal Engineering**, with seminal, wide-ranging contributions at the international level. This interdisciplinary subject intersects organic and supramolecular chemistry, X-ray crystallography, and materials research. Crystal engineering encompasses three primary pillars: (1) Study of intermolecular interactions; (2) Development of strategies of crystal synthesis; and (3) Design of crystals with novel physical and chemical properties.

- **Intermolecular Interactions:** Work has expanded knowledge of the hydrogen bond, notably demonstrating that C–H groups can participate as donors in hydrogen bonds of the type C–H...O, establishing this interaction firmly in supramolecular chemistry. Extensive studies also cover halogen, sulfur, and transition metal atom interactions, highlighted by the co-authored volume *The Weak Hydrogen Bond in Structural Chemistry and Biology* (Oxford University Press, 1999).
- **Strategies of Crystal Synthesis:** Addressed the central challenge of crystal engineering—the lack of a direct correspondence between molecular and supramolecular structure—by introducing the concept of **structural insulation** and the **supramolecular synthon** in 1995. This framework enabled the application of retrosynthetic logic to crystal design, framing the molecular crystal as a holistic ensemble of intermolecular interactions.
- **Novel Properties and Systems Thinking:** Focused on achieving crystals for non-linear optics, organic reactivity, mechanochemistry, and polymorphism in active pharmaceutical ingredients (APIs). Recent theoretical extensions involve analysing structural landscapes, connecting reductionist structural metrics to overarching holistic and systems-level frameworks.

PhD Students Mentored in Hyderabad and Bangalore

V. Aparna, R. Banerjee, S. Basavoju, P. M. Bhatt, K. Biradha, D. Das, A. Dey, R. Dubey, B. S. Goud, R. K. R. Jetti, K. V. Radha Kishan, T. S. R. Krishna, S. S. Kuduva, N. N. L. Madhavi, M. K. Mishra, A. Mukherjee, V. Nalini, P. K. Panigrahi, V. R. Pedireddi, C. M. Reddy, D. S. Reddy, J. A. R. P. Sarma, C. V. K. M. Sharma, R. Thaimattam, T. S. Thakur, V. R. Thalladi, P. K. Thallapally, S. Tothadi, V. R. Vangala

Books

1. *Organic Solid State Chemistry*, edited by G. R. Desiraju; Studies in Organic Chemistry 32; Elsevier: Amsterdam, 1987.
2. *Crystal Engineering: The Design of Organic Solids*, by G. R. Desiraju; Materials Science Monographs 54; Elsevier: Amsterdam, 1989.
3. *The Crystal as a Supramolecular Entity*, edited by G. R. Desiraju; Perspectives in Supramolecular Chemistry, Vol. 2; Wiley: Chichester, 1996.

4. *The Weak Hydrogen Bond in Structural Chemistry and Biology*, by G. R. Desiraju and T. Steiner; Oxford University Press: Oxford, 1999.
5. *Crystal Design: Structure and Function*, edited by G. R. Desiraju; Perspectives in Supramolecular Chemistry, Vol. 7; Wiley: Chichester, 2003.
6. *Crystal Engineering: A Textbook*, by G. R. Desiraju, J. J. Vittal, and A. Ramanan; World Scientific: Singapore, 2011.
7. *Crystal Engineering: Designing Complexity*; Lives in Chemistry. GNT, GDCh: Berlin, 2027.

Selected Reviews

1. The role of Cl $\cdots$ Cl and C–H $\cdots$ O interactions in the crystal engineering of 4-short-axis structures. J. A. R. P. Sarma and G. R. Desiraju, *Acc. Chem. Res.*, **1986**, 19, 222–228.
2. The C–H $\cdots$ O hydrogen bond in organic crystals. What is it? G. R. Desiraju, *Acc. Chem. Res.*, **1991**, 24, 290–296.
3. Supramolecular synthons in crystal engineering – A new organic synthesis. G. R. Desiraju, *Angew. Chem.*, **1995**, 107, 2541–2557; *Angew. Chem. Int. Ed. Engl.*, **1995**, 34, 2311–2327.
4. The C–H $\cdots$ O hydrogen bond: structural implications and supramolecular design. G. R. Desiraju, *Acc. Chem. Res.*, **1996**, 29, 441–449.
5. Chemistry beyond the molecule. G. R. Desiraju, *Nature*, **2001**, 412, 397–400.
6. Hydrogen bridges in crystal engineering. Interactions without borders. G. R. Desiraju, *Acc. Chem. Res.*, **2002**, 35, 565–573.
7. Chemistry. The Middle Kingdom. G. R. Desiraju, *Curr. Sci.*, **2005**, 88, 374–380.
8. Crystal engineering: A holistic view. G. R. Desiraju, *Angew. Chem. Int. Ed.*, **2007**, 46, 8342–8356.
9. Nanoindentation in crystal engineering: Quantifying mechanical properties of molecular crystals. S. Varughese, M. S. R. N. Kiran, U. Ramamurty, and G. R. Desiraju, *Angew. Chem. Int. Ed.*, **2013**, 52, 2701–2712.
10. Crystal engineering: From molecule to crystal. G. R. Desiraju, *J. Am. Chem. Soc.*, **2013**, 135, 9952–9967.

11. Halogen bonds in crystal engineering: Like hydrogen bonds yet different. A. Mukherjee, S. Tothadi, and G. R. Desiraju, *Acc. Chem. Res.*, **2014**, *47*, 2514–2524.
12. Crystal structure and prediction. T. S. Thakur, R. Dubey, and G. R. Desiraju, *Annu. Rev. Phys. Chem.*, **2015**, *66*, 21–42.
13. Crystal Engineering: An outlook for the future. A. K. Nangia and G. R. Desiraju, *Angew. Chem. Int. Ed.*, **2019**, *58*, 3700–3709.
14. Heterosynthons, solid form design and enhanced drug bioavailability. A. K. Nangia and G. R. Desiraju, *Angew. Chem. Int. Ed.*, **2022**, *61*, e202207484.

Key Publications

- The nature of halogen···halogen interactions: are short halogen contacts due to specific attractive forces or due to close packing of non-spherical atoms? G. R. Desiraju and R. Parthasarathy, *J. Am. Chem. Soc.*, **1989**, *111*, 8725–8726.
- Hydration in organic crystals. Prediction from molecular structure. G. R. Desiraju, *J. Chem. Soc., Chem. Commun.*, **1991**, 426–428.
- C–H···F interactions in the crystal structures of some fluorobenzenes. V. R. Thalladi, H.-C. Weiss, D. Bläser, R. Boese, A. Nangia, and G. R. Desiraju, *J. Am. Chem. Soc.*, **1998**, *120*, 8702–8710.
- Correspondence between molecular functionality and crystal structures. Supramolecular chemistry of a family of homologated aminophenols. V. R. Vangala, B. R. Bhogala, A. Dey, G. R. Desiraju, C. K. Broder, P. S. Smith, R. Mondal, and J. A. K. Howard, *J. Am. Chem. Soc.*, **2003**, *125*, 14495–14509.
- Structural studies of the system (Na⁺)(saccharinate[−])(H₂O)_n. A model for crystallisation. R. Banerjee, P. M. Bhatt, M. T. Kirchner, and G. R. Desiraju, *Angew. Chem. Int. Ed.*, **2005**, *44*, 2515–2520.
- Structural basis for bending of organic crystals. C. M. Reddy, R. C. Gundakaram, S. Basavoju, M. T. Kirchner, K. A. Padmanabhan, and G. R. Desiraju, *Chem. Commun.*, **2005**, 3945–3947.
- On the polymorphism of aspirin: Crystalline aspirin as intergrowths of two “polymorphic” domains. A. D. Bond, R. Boese, and G. R. Desiraju, *Angew. Chem. Int. Ed.*, **2007**, *46*, 618–622.
- Odd-even effect in the elastic moduli of α, ω -alkanedicarboxylic acids. M. K. Mishra, S. Varughese, U. Ramamurty, and G. R. Desiraju, *J. Am. Chem. Soc.*, **2013**, *135*, 8121–8124.
- Designing ternary cocrystals with hydrogen bonds and halogen bonds. S. Tothadi and G. R. Desiraju, *Chem. Commun.*, **2013**, *49*, 7791–7793.

- Four- and five-component molecular solids. Crystal engineering strategies based on lack of structural degeneracy. N. A. Mir, R. Dubey, and G. R. Desiraju, *IUCrJ*, **2016**, 3, 103–110.
- Looking at aniline-phenol recognition in molecular crystals: an evergreen endeavour. A. Sood and G. R. Desiraju, *Struct. Chem.*, **2016**, 28, 173–199.
- Hand-Twisted Helical Crystals as an Example of Third Generation Crystal Engineering. S. Saha and G. R. Desiraju, *J. Am. Chem. Soc.*, **2017**, 139, 1975–1983.
- New Cocrystals of Hydrochlorothiazide: Optimizing Solubility and Membrane Diffusivity. S. P. Gopi, M. Banik, and G. R. Desiraju, *Cryst. Growth Des.*, **2017**, 17, 308–316.
- Salts and Cocrystals of Antidiabetic Drugs, Gliclazide, Tolbutamide and Glipizide: Solubility Enhancements through Drug–Coformer Interactions. A. Samie and G. R. Desiraju, *Cryst. Growth Des.*, **2017**, 17, 2406–2417.
- σ -hole and π -hole Synthons Mimicry in Third Generation Crystal Engineering. Design of Elastic Crystals. S. Saha and G. R. Desiraju, *Chem. Eur. J.*, **2017**, 23, 4936–4943.
- Exploring the salt-cocrystal continuum with solid-state NMR using natural abundance samples: implications for crystal engineering. L. Rajput, M. Banik, J. R. Yarava, S. Joseph, M. K. Pandey, Y. Nishiyama, and G. R. Desiraju, *IUCrJ*, **2017**, 4, 466–475.
- Hand-twisted helical crystals based solely on hydrogen bonding. S. Saha and G. R. Desiraju, *Chem. Commun.*, **2017**, 53, 6371–6374.
- Approaches to crystal structure landscape exploration. G. R. Desiraju, *Acta Crystallogr. Sect. B*, **2017**, 73, 775–778.
- Crystal clear. Engineering complexity. G. R. Desiraju, *IUCrJ*, **2026**, 13(5).

Commentaries & General Articles

Odd-even carbon atom disparity in organic compounds. J. A. R. P. Sarma, A. Nangia, G. R. Desiraju, E. Zass, and J. D. Dunitz, *Nature*, 1996, 384, 320.

Even odder carbons. J. A. R. P. Sarma, A. Nangia, G. R. Desiraju, E. Zass, and J. D. Dunitz, *Nature*, 1997, 387, 464.

Crystal gazing: structure prediction and polymorphism. G. R. Desiraju, *Science*, 1997, 278, 404–405.

The All-Chemist (Millennium Essay). G. R. Desiraju, *Nature*, 2000, 408, 407.

Crystallography. Quo vadis? G. R. Desiraju, *Z. Krist.*, 2002, 217, 297–298.

‘Bond free’. G. R. Desiraju, *CrystEngComm*, 2002, 499.

Cryptic crystallography. G. R. Desiraju, *Nature Materials*, 2002, 1, 77–79.

Crystal: In search of clarity (Concept essay). G. R. Desiraju, *Nature*, 2003, 423, 485.

Crystal and co-crystal. G. R. Desiraju, *CrystEngComm*, 2003, 5, 466–467.

Counterpoint: What’s in a name? G. R. Desiraju, *Cryst. Growth Des.*, 2004, 4, 1089–1090.

Science Education and Research in India. G. R. Desiraju, *Economic and Political Weekly*, June 14, 2008, 37–43.

Science in a Changing World. G. R. Desiraju, *Angew. Chem. Int. Ed.*, 2011, 50, 5590–5591.

Policy: Bold strategies for Indian science. G. R. Desiraju, *Nature*, 2012, 484, 159–160.

Chemistry in India: Unlocking the potential. E. Arunan, R. Brakaspathy, G. R. Desiraju, and S. Sivaram, *Angew. Chem. Int. Ed.*, 2013, 52, 114–117.

Is a data deluge dampening our idea generation capability? (with Deekhit Bhattacharya). *The Innovation*, 2025, 6(7), 100883.

General Books

1. *Bhārat: India 2.0*, by G. R. Desiraju, Vitasta, Delhi, 2022.
2. *Delimitation and States Reorganization: For a Better Democracy in Bhārat*, by G. R. Desiraju and D. Bhattacharya, BluOne Ink, Delhi, 2025.
3. *India's Supply Chains in a World at War: Trade, Power, Conflict, and Entanglement among Empires in the New Global Order*, by G. R. Desiraju and D. Bhattacharya, BluOne Ink, Delhi, 2025.
4. *Fixing Science in India: A Socio-Economic Prescription*, by G. R. Desiraju and D. Bhattacharya, Vitasta, Delhi, 2025.
5. *India: Science, Politics, Geostrategy – A Thirty-Year Thought Journey*, by G. R. Desiraju, Garuda, Delhi, 2025.
6. *Indian Knowledge Systems: A Primer*, by G. R. Desiraju, A. Panda and D. Bhattacharya, Khanna Publishers, Delhi, 2026.
7. *Indian Knowledge Systems: A Text*, by G. R. Desiraju, A. Panda and D. Bhattacharya, Khanna Publishers, Delhi, 2027.

Full List of Publications

BOOKS

1. Organic Solid State Chemistry, edited by G. R. Desiraju, Studies in Organic Chemistry 32, Elsevier, Amsterdam, 1987: multi-author work with 16 chapters, 550 pages.
2. Crystal Engineering. The Design of Organic Solids by G. R. Desiraju, Materials Science Monographs 54, Elsevier, Amsterdam, 1989: 312 pages.
3. The Crystal as a Supramolecular Entity edited by G. R. Desiraju, Perspectives in Supramolecular Chemistry, 2, Wiley, Chichester, 1996: multi-author work with 6 chapters, 309 pages.
4. The Weak Hydrogen Bond in Structural Chemistry and Biology by G. R. Desiraju and T. Steiner, Oxford University Press, Oxford, 1999: 528 pages.
5. Crystal Design. Structure and Function edited by G. R. Desiraju, Perspectives in Supramolecular Chemistry, 7, Wiley, Chichester, 2003: multi-author work with 9 chapters, 408 pages.
6. Crystal Engineering. A Textbook by G. R. Desiraju, J. J. Vittal and A. Ramanan, World Scientific and IISc Press, Singapore and Bangalore, 2011, 216 pages.
7. Crystal Engineering: Designing Complexity by G. R. Desiraju. Lives in chemistry. GNT, GDCh, Berlin, 2027, 296 pages.

PAPERS

1. Conversion in the solid state of the yellow to the red form of 2-(4'-methoxyphenyl)-1,4-benzoquinone. X-ray crystal structures of the two forms and anisotropy of the rearrangement.
G. R. Desiraju, I. C. Paul and D. Y. Curtin
J. Am. Chem. Soc., 99, 1594-1601 (1977).
2. Crystal growth by non-aqueous gel diffusion.
G. R. Desiraju, D. Y. Curtin and I. C. Paul
J. Am. Chem. Soc., 99, 6148 (1977).
3. Synthesis and interconversion by hydrogen exchange of isomeric quinhydrone.
G. R. Desiraju, D. Y. Curtin and I. C. Paul
J. Org. Chem., 46, 4071-4075 (1977).

4. Resonance interactions in metal chelates of ortho-hydroxyazo compounds. Crystal growth, Structure and Spectra of 1-(2-Pyridylazo)-2-naphtholato-copper (II).
G. R. Desiraju, H. R. Luss and D. L. Smith
J. Am. Chem. Soc., 100, 6375-6382 (1978).
5. Structure studies of 1:1 quinone-hydroquinone complexes.
G. R. Desiraju, I. C. Paul and D. Y. Curtin
Mol. Cryst. Liq. Cryst., 52, 259-266 (1979).
6. Phase transition in malonic acid; an infrared study.
S. Ganguly, J. R. Fernandes, G. R. Desiraju and C. N. R. Rao
Chem. Phys. Lett., 69, 227-229 (1980).
7. Organic solid state chemistry-I. Topochemistry.
G. R. Desiraju
Indian J. Chem. Ed., 7(1), 1-8 (1980).
8. Organic solid state chemistry-II. Non-topochemical processes.
G. R. Desiraju
Indian J. Chem. Ed., 7(2), 1-6 (1980).
9. Phase transitions in solid hydrogen bonded p-chlorobenzamide, p-nitrophenol and an azo dye.
S. Ganguly and G. R. Desiraju
Indian J. Chem., 20A, 80-81 (1981).
10. Organic reactions in inorganic matrices-oxidation of hydroquinone to p-benzoquinone on solid MoO₃ surfaces.
G. R. Desiraju and B. P. Shastry
Proc. Indian Acad. Sci. (Chem. Sci.), 90, 243-246 (1981).
11. A mild transformation of γ -FeOOH to γ -Fe₂O₃ using organic reagents.
G. R. Desiraju and M. Rao
Mat. Res. Bull., 17, 443-449 (1982).
12. 6-Chloro-4-phenyl-1-methyl-2,1,3-benzothiadiazine-2,2'-dioxide.
G. R. Desiraju and R. Kamala
Acta Crystallogr., Section C, 39, 358-360 (1983).
13. Intermolecular proton transfers in the solid state: conversion of the hydroxyazo to the quinonehydrazone tautomer of 2-amino-3-hydroxy-6-phenylazopyridine. X-ray crystal structures of the two forms.
G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 1025-1030 (1983).

14. Crystal engineering via donor-acceptor interactions. X-ray crystal structure and solid state reactivity of the 1:1 complex 3,4-dimethoxycinnamic acid-2,4-dinitrocinnamic acid.
J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 45-46 (1983).
15. Structural mimicry and the photoreactivity of organic solids.
W. Jones, C. R. Theocharis, J. M. Thomas and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1443-1444 (1983).
16. Crystal engineering via non-bonded interactions involving oxygen. X-ray crystal structures of 3,4-methylenedioxycinnamic acid and 3,4-dimethoxycinnamic acid.
G. R. Desiraju, R. Kamala, B. H. Kumari and J. A. R. P. Sarma
J. Chem. Soc., Perkin Transac. 2, 181-189 (1984).
17. Crystal engineering via Cl...Cl non-bonded interactions. The novel 2:1 complex 6-chloro-3,4-methylenedioxycinnamic acid - 2,4-dichlorocinnamic acid. Topochemical conversion to an unsymmetrical cyclobutane and kinetics of the reaction.
J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 145-147 (1984).
18. Organic solid state chemistry – some perspectives.
G. R. Desiraju
Proc. Indian Acad. Sci. (Chem. Sci.), 93, 407-419 (1984).
19. An NMR method to distinguish between truxinic and truxillic dimers of some trans-cinnamic acids.
J. A. R. P. Sarma and G. R. Desiraju
Indian J. Chem., B23, 658-659 (1984).
20. The use of mixed crystals for engineering organic solid state reactions: applications to benzylbenzylidenecyclopentanones.
C. R. Theocharis, G. R. Desiraju and W. Jones
J. Am. Chem. Soc., 106, 3606-3609 (1984).
21. An investigation into the role of chloro-substituents in hydrogen bonded crystals: the crystal structures of the dichlorophenols.
N. W. Thomas and G. R. Desiraju
Chem. Phys. Lett., 110, 99-102 (1984).
22. Carrying out organic chemistry within crystalline solids
G. R. Desiraju
Endeavour, 8, 201-206 (1984).

23. Determination of an organic crystal structure with the aid of topochemical and related considerations: correlation of the molecular and crystal structures of α -benzylidene- γ -butyrolactone and 2-benzylidenecyclopentanone with their solid state photoreactivity.
S. K. Kearsley and G. R. Desiraju
Proc. Roy. Soc. London Ser.A, 397, 157-181 (1985).
24. The chloro-substituent as a steering group : a comparative study of non-bonded interactions and hydrogen bonding in crystalline chloro-aromatics.
J. A. R. P. Sarma and G. R. Desiraju
Chem. Phys. Lett., 117, 160-164 (1985).
25. Organische Chemie in kristallinen Festkörpern.
G. R. Desiraju
Die Umschau, 413-417 (1985).
26. The novel 1:1 donor acceptor complex 3,4-dimethoxycinnamic acid – 2,4-dinitrocinnamic acid. Crystal engineering, structure and anomalous lack of solid state topochemical reactivity.
J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 1905-1912 (1985).
27. Some chemical implications of database derived crystallographic information.
G. R. Desiraju
Indian J. Chem., B25, 1-8 (1986).
28. What is the maximum yield in the solid state cinnamic acid dimerisation? A combinatorial mathematical approach.
G. R. Desiraju and V. Kannan
Proc. Indian Acad. Sci. (Chem. Sci.), 96, 351-362 (1986).
29. Crystal engineering and chemical reactivity of organic molecular solids.
G. R. Desiraju
Proc. Indian Natnl. Sci. Acad., 52A, 379-399 (1986).
30. The chloro-methyl exchange rule and its violations in the packing of organic molecular solids.
G. R. Desiraju and J. A. R. P. Sarma
Proc. Indian Acad. Sci. (Chem. Sci.), 96, 599-605 (1986).
31. Molecular discrimination in the formation of mixed crystals of some substituted chlorocinnamic acids.
J. A. R. P. Sarma and G. R. Desiraju
J. Am. Chem. Soc., 108, 2791-2793 (1986).
32. Recent studies on the formation and properties of quinhydrone complexes.
A. O. Patil, W. T. Pennington, G. R. Desiraju, D. Y. Curtin and I. C. Paul,

- Mol. Cryst. Liq. Cryst., 134, 279-304 (1986).
33. The role of non-bonded interactions involving sulphur in the crystal engineering of 4Å-short axis structures. Unusual topochemical reactivity of 4-(4-chlorophenyl)thiazole-2(1H)-thione.
V. Nalini and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1030-1032 (1986).
 34. The role of Cl...Cl and C-H...O interactions in the crystal engineering of 4Å - short axis structures.
J. A. R. P. Sarma and G. R. Desiraju
Acc. Chem. Res., 19, 222-228 (1986).
 35. Hydrogen bonding and phase transitions in pentachlorophenol – hexachlorobenzene solid solutions.
Md. A. Masood and G. R. Desiraju
Chem. Phys. Lett., 130, 199-202 (1986).
 36. Dipole-dipole interactions and the inversion motif in the crystal structures of planar chloro aromatics: the unusual packings of 1,2,3-trichlorobenzene and 1,2,3,7,8,9-hexachlorodibenzo-p-dioxin.
G. R. Desiraju, J. A. R. P. Sarma and T. S. R. Krishna
Chem. Phys. Lett., 131, 124-128 (1986).
 37. Interstack and intrastack forces in molecular solids: a new look at donor-acceptor complexes and organic metals.
G. R. Desiraju
Curr. Sci. (India), 55, 1009-1012 (1986).
 38. Structure of 3-hydroxy-6-(4'-methyl)phenylazopyridine.
T. S. R. Krishna and G. R. Desiraju
Acta Crystallogr., Section C, 42, 1246-1248 (1986).
 39. Crystal engineering, X-ray crystallography and organic solid state chemistry
G. R. Desiraju
Indian J. Phys., 61A, 43-50 (1987).
 40. The crystal and molecular structure of 3,4-dihydroxy-trans-cinnamic acid, C₉H₈O₄, caffeic acid and its lack of solid state topochemical reactivity.
S. Garcia-Granda, G. Beurskens, P. T. Beurskens, T. S. R. Krishna and G. R. Desiraju
Acta Crystallogr., Section C, 43, 683-685 (1987).
 41. Crystal engineering through non-bonded contacts to sulphur. Structure and solid state photoreactivity of 4-(4'-chloro)phenyl-Δ-4-thiazolene-2-thione.
V. Nalini and G. R. Desiraju
Tetrahedron, 43, 1313-1320 (1987).

42. Gas-solid reaction of 4-phenylthiazole-2(1H)-thione.
V. Nalini and G. R. Desiraju
J. Chem. Soc., Chem. Commun. , 1046-1048 (1987).
43. Crystal engineering a 4 Å-short axis for planar chloro aromatics:
G. R. Desiraju in Organic Solid State Chemistry, Ed. G. R. Desiraju, Elsevier, Amsterdam (1987), pp 519-546.
44. Correlation between crystallographic and spectroscopic properties for C–H...O bonds in terminal acetylenes.
G. R. Desiraju and B. N. Murty
Chem. Phys. Lett., 139, 360-361 (1987).
45. Mixed crystals of 6-chloro-3,4-methylenedioxycinnamic acid with 2,4- and 3,4-dichlorocinnamic acids. Structure, topochemistry and intermolecular interactions.
J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 1187-1193 (1987).
46. C–H...O interactions and the adoption of 4Å-short axis structures by oxygenated aromatic compounds.
J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 1195-1202 (1987).
47. Designing organic crystals.
G. R. Desiraju
Prog. Solid State Chem., 17, 295-353 (1987)
48. Crystal engineering a solid state Diels-Alder reaction.
K. V. R. Kishan and G. R. Desiraju
J. Org. Chem., 52, 4640-4641 (1987).
49. Structure and photochemical reactivity of some chlorocinnamic acid molecular complexes.
G. R. Desiraju
Izv. Sib. Otd. Akad. Nauk SSSR, Ser. Khim. Nauk, 15-21 (1987).
50. Structure of (4 SR, 6a RS)-4-[-2-methyl-1,3-dioxalan-2-yl]ethyl]-4,5,6,6a-tetrahydro-5,5,6a-trimethyl-2(1H)-pentalenone.
V. Nalini and G. R. Desiraju
Acta Crystallogr., Section C, 44, 510-512 (1988).
51. The crystal and molecular structures of 4-hydroxy-3-methoxycinnamic acid, C₁₀H₁₀O₄, ferulic acid.
M. Nethaji, V. Pattabhi and G. R. Desiraju
Acta Crystallogr., Section C, 44, 275-277 (1988).

52. Prediction of non-centrosymmetric packing for 1,3-disubstituted nitro aromatics. Crystal and molecular structure of 3-hydroxy- 6-(3'-nitro)-phenylazopyridine.
G. R. Desiraju and T. S. R. Krishna
Mol. Cryst. Liq. Cryst., 159, 277-287 (1988).
53. Non-centrosymmetry in organic crystals: a study of molecular conformation in some substituted tolans.
G. R. Desiraju and T. S. R. Krishna
J. Chem. Soc., Chem. Commun., 192-194 (1988).
54. A systematic analysis of packing energies and other packing parameters for fused-ring aromatic hydrocarbons.
A. Gavezzotti and G. R. Desiraju
Acta Crystallogr., Section B, 44, 427-434 (1988).
55. A convenient preparation of 2,5-dibenzylidenecyclopent-3-ene-1-ones.
G. R. Desiraju and K. V. R. Kishan
Indian J. Chem., B27, 953-954 (1988).
56. Distance dependence of C-H...O interactions in some chloroalkyl compounds.
G. R. Desiraju
J. Chem. Soc., Chem. Commun., 179-180 (1989).
57. From molecular to crystal structure: polynuclear aromatic hydrocarbons.
G. R. Desiraju and A. Gavezzotti
J. Chem. Soc., Chem. Commun., 621-623 (1989).
58. Structure of 4-phenylthiazole-2(1h)-thione and 4-chlorophenacyl disulphide, the product obtained on its gas-solid chlorination.
V. Nalini and G. R. Desiraju
Acta Crystallogr., Section C, 45, 1525-1527 (1989).
59. Tautomerism in the thiazole thiones. Crystal and molecular structure of 4-(3'-nitro)-phenylthiazole-2(1H)-thione.
V. Nalini and G. R. Desiraju
Acta Crystallogr., Section C, 45, 1528-1530 (1989).
60. Crystal chemistry of some alkoxyphenylpropionic acids. the role of oxygen and hydrogen atoms in determining stack structures of planar aromatic compounds.
G. R. Desiraju and K. V. R. Kishan
J. Am. Chem. Soc., 111, 4838-4843 (1989).
61. Crystal structure and solid state photoreactivity of 2,5-dibenzylidenecyclopent-3-ene-1-one and its tetrachloro derivative.
G. R. Desiraju, J. Bernstein, K. V. R. Kishan and J. A. R. P. Sarma

- Tetrahedron Lett., 30, 3029-3032 (1989).
62. Crystal structures of polynuclear aromatic hydrocarbons. classification, rationalisation and prediction from molecular structure.
G. R. Desiraju and A. Gavezzotti
Acta Crystallogr., Section B, 45, 473-482 (1989).
 63. Solid state dimerisation of β -nitrostyrene: a disordered photoreactive crystal.
G. R. Desiraju and V. R. Pedireddi
J. Chem. Soc., Chem. Commun., 1112-1113 (1989).
 64. Cyano...halogen interactions and their role in the crystal structures of the 4-halobenzonitriles.
G. R. Desiraju and R. L. Harlow
J. Am. Chem. Soc., 111, 6757-6764 (1989).
 65. The nature of halogen...halogen interactions: are short halogen contacts due to specific attractive forces or due to close packing of non-spherical atoms?
G. R. Desiraju and R. Parthasarathy
J. Am. Chem. Soc., 111, 8725-8726 (1989).
 66. Clathrate compound of a new host material: 3-hydroxy-6-(4'-nitro) phenylazopyridine.
P. Ramachandra, T. S. R. Krishna and G. R. Desiraju
Proc. Indian Acad. Sci., (Chem. Sci.), 101, 329-334 (1989).
 67. Strength and linearity of C-H...O bonds in molecular crystals: a database study of some terminal alkynes.
G. R. Desiraju
J. Chem. Soc., Chem. Commun., 454-455 (1990).
 68. Structure of L-lanthionine.
G. R. Desiraju and D. R. Rao
Acta Crystallogr., Section C, 46, 627-629 (1990).
 69. Structure of perhydrotriphenylene.
R. L. Harlow and G. R. Desiraju
Acta Crystallogr., Section C, 46, 1054-1055 (1990).
 70. Unexpected hydrogen bonding in the crystal structure of 4-chloro-phenylpropionic acid. The role of C-H...O hydrogen bonds in determining O...H...O networks.
G. R. Desiraju, B. N. Murty and K. V. R. Kishan
Chem. Mater., 2, 447-449 (1990).
 71. Organic compounds and materials science.
G. R. Desiraju
Curr. Sci. (India), 59, 452-455 (1990).

72. Database analysis of crystal structure determining interactions involving sulphur. Implications for the design of organic metals.
G. R. Desiraju and V. Nalini
J. Mater. Chem., 1, 201-203 (1991).
73. Hydration in organic crystals. Prediction from molecular structure.
G. R. Desiraju
J. Chem. Soc., Chem. Commun., 426-428 (1991)
74. Pseudo-inversion centres in the space group P1-bar and a redetermination of the crystal structure of 3,4-dimethoxycinnamic acid. A study of non-crystallographic symmetry.
G. R. Desiraju, J. C. Calabrese and R. L. Harlow,
Acta Crystallogr., Section B, 47, 77-86 (1991).
75. C-H...O hydrogen bonding and topochemistry in crystalline 3,5-dinitrocinnamic acid and its 1:1 donor-acceptor complex with 2,5-dimethoxycinnamic acid.
G. R. Desiraju and C. V. K. M. Sharma
J. Chem. Soc., Chem. Commun., 1239-1241 (1991).
76. Unusual 2 + 2 topochemical cycloadditions of 3-cyano and 4-cyanocinnamic acids. Temperature dependent solid state photochemical reactions.
M. S. K. Dhurjati, J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1702-1703 (1991).
77. The C-H...O hydrogen bond in organic crystals. What is it?
G. R. Desiraju
Acc.Chem.Res., 24, 290-296 (1991).
78. C-H...O interactions and the deliberate design of organic crystal structures.
G. R. Desiraju
Mol. Cryst. Liq. Cryst., 211, 63-74 (1992).
79. Crystal engineering and solid state chemistry of some β -nitrostyrenes.
V. R. Pedireddi, J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 311-320 (1992).
80. Molecular recognition via C $\equiv$ H...O hydrogen bonding. Crystal structure of the 1:1 complex 4-nitrobenzoic acid - 4-(N,N-dimethylamino)benzoic acid.
C. V. K. M. Sharma, K. Panneerselvam, T. Pilati and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 832-833 (1992).
81. A crystallographic scale of carbon acidity.
V. R. Pedireddi and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 988-990 (1992).

82. Database analysis of Au...Au interactions.
S. S. Pathaneni and G. R. Desiraju
J. Chem. Soc., Dalton Transac., 319-322 (1993).
83. Structure of (4-bromophenyl)propionic acid and its unusual hydrogen bonding pattern.
B. S. Goud and G. R. Desiraju
Acta Crystallogr., Section C, 49, 292-294 (1993).
84. Structure of 4-iodo-trans-cinnamic acid and a study of carboxyl group conformation and disorder.
B. S. Goud, S. S. Pathaneni and G. R. Desiraju
Acta Crystallogr., Section C, 49, 1107-1111 (1993).
85. C-H...O packing motifs in some cyclopenta[a]phenanthrenes.
G. R. Desiraju, S. Kashino, M. M. Coombs and J. P. Glusker
Acta Crystallogr., Section B, 49, 880-892 (1993).
86. Determination of the crystal structure of 4-iodo- β -nitrostyrene with the aid of packing considerations: a study of halogen...nitro interactions.
G. R. Desiraju, V. R. Pedireddi, J. A. R. P. Sarma and D. E. Zacharias
Acta Chim. Hungarica – Models in Chemistry, 130, 451-465 (1993).
[Kitaigorodskii Memorial Issue]
87. Evidence for O-H...C and N-H...C hydrogen bonding in crystalline alkynes, alkenes and aromatics.
M. A. Viswamitra, R. Radhakrishnan, J. Bandekar and G. R. Desiraju
J. Am. Chem. Soc., 115, 4868-4869 (1993).
88. Molecular tapes based on C $\equiv$ N...Cl interactions.
D. S. Reddy, K. Panneerselvam, T. Pilati and G. R. Desiraju.
J. Chem. Soc., Chem. Commun., 661-662 (1993).
89. C-H...N mediated hexagonal network in the crystal structure of the 1:1 molecular complex 1,3,5-tricyanobenzene – hexamethylbenzene.
D. S. Reddy, B. S. Goud, K. Panneerselvam and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 663-664 (1993).
90. Database studies of halide ion pairs with bridging H₂O and NH₂ amino molecules.
S. S. Pathaneni and G. R. Desiraju
J. Chem. Soc., Dalton Transac., 2505-2508 (1993).
91. Solid state supramolecular assembly via C-H...O hydrogen bonds: crystal structures of the complex of 1,3,5-trinitrobenzene with dibenzylideneacetone and 2,5-dibenzylidenecyclopentanone.

- K. Biradha, C. V. K. M. Sharma, K. Panneerselvam, L. Shimoni, H. L. Carrell, D. E. Zacharias and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1473-1475 (1993).
92. Molecular recognition involving an interplay of O-H...O, C-H...O and $\pi\cdots\pi$ interactions. The anomalous crystal structure of the 1:1 complex 3,5-dinitrobenzoic acid - 4-(N,N-dimethylamino)benzoic acid.
C. V. K. Sharma, K. Panneerselvam, T. Pilati and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 2209-2216 (1993).
93. N...Br mediated diamondoid network in the crystalline complex, carbon tetrabromide:hexamethylenetetramine.
D. S. Reddy, D. C. Craig, A. D. Rae and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1737-1738 (1993).
94. Molecular and crystal structure of 1-(8-carboxyoctyl)-1,3,5,7-tetraazaadamantan-1-ium bromide and 1-(6-bromohexyl)-1,3,5,7-tetraazaadamantan-1-ium bromide.
D. S. Reddy, K. Panneerselvam, L. Shimoni, H. L. Carrell and G. R. Desiraju
J. Mol. Str., 327, 113-120 (1994).
[C. N. R. Rao Commemoration Issue]
95. 3-(3',5'-Dinitrophenyl)-4-(2',5'-dimethoxyphenyl)cyclobutane-1,2-dicarboxylic acid. Engineered topochemical synthesis, molecular and supramolecular properties.
C. V. K. Sharma, K. Panneerselvam, L. Shimoni, H. Katz, H. L. Carrell and G. R. Desiraju
Chem. Mater., 6, 1282-1292 (1994).
[Etter Memorial Issue]
96. Organic alloys. Diamondoid networks in crystalline complexes of 1,3,5,7-tetrabromoadamantane, hexamethylenetetramine and carbon tetrabromide.
D. S. Reddy, D. C. Craig and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1457-1458 (1994).
97. C-H...O hydrogen bond patterns in crystalline nitro compounds. Studies in solid state molecular recognition.
C. V. K. Sharma and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 2345-2352 (1994).
98. The nature of halogen...halogen interactions and the crystal structure of 1,3,5,7-tetraiodoadamantane.
V. R. Pedireddi, D. S. Reddy, B. S. Goud, D. C. Craig, A.D.Rae and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 2353-2360 (1994).
99. Towards inorganic supramolecular chemistry.
G. R. Desiraju

Proc. Indian Acad. Sci. (Chem. Sci.), 106, 593-597 (1994).

100. Hydrogen bonding in organometallic crystals – 1. From carboxylic acids and alcohols to carbonyl compounds.
D. Braga, F. Grepioni, P. Sabatino and G. R. Desiraju
Organometallics, 13, 3532-3543 (1994).
101. Molecular recognition via iodo...nitro and iodo...cyano interactions: crystal structures of the 1:1 complexes of 1,4-diiodobenzene with 1,4-dinitrobenzene and 7,7,8,8-tetracyanoquinodimethane (TCNQ).
F. H. Allen, B. S. Goud, V. J. Hoy, J. A. K. Howard and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 2729-2730 (1994).
102. Intramolecular Michael-type addition in the solid state.
B. S. Goud, K. Panneerselvam, D. E. Zacharias and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 325-330 (1995).
103. Topological equivalences between organic and inorganic crystal structures: 1,3,5,7-tetrahydroxyadamantane and caesium chloride.
D. S. Reddy, D. C. Craig and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 339-340 (1995).
104. Hexagonal supramolecular networks in the crystal structure of the 1:1 molecular complex trimethylisocyanurate – 1,3,5-trinitrobenzene.
V. R. Thalladi, K. Panneerselvam, C. J. Carrell, H. L. Carrell and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 340-341 (1995).
105. Hydrogen bonding in organometallic crystals – 2. C–H...O hydrogen bonds in bridged and terminal first row metal carbonyls.
D. Braga, F. Grepioni, K. Biradha, V. R. Pedireddi and G. R. Desiraju
J. Am. Chem. Soc., 117, 3156-3166 (1995).
106. 4,6-Dimethyl-2-(4-nitrobenzylidene)-3(2H)-benzofuranone.
B. S. Goud, K. Panneerselvam, D. E. Zacharias and G. R. Desiraju
Acta Crystallogr., Section C, 51, 265-267 (1995).
107. 1:1 Molecular complex of 2,3,4,5,6-pentafluoro-trans-cinnamic acid and 4-(N,N-dimethylamino)-trans-cinnamic acid.
B. S. Goud, P. K. Reddy, K. Panneerselvam and G. R. Desiraju
Acta Crystallogr., Section C, 51, 683-685 (1995).
108. Methyl 3,5-dinitro-trans-cinnamate.
C. V. K. Sharma, K. Panneerselvam, T. Pilati and G. R. Desiraju
Acta Crystallogr., Section C, 51, 1364-1366 (1995).
109. Supramolecular synthons in crystal engineering – a new organic synthesis.
G. R. Desiraju

- Angew. Chem., 107, 2541-2557 (1995); Angew. Chem. Int. Ed. Engl., 34, 2311-2327 (1995).
110. Solid state nuclear bromination of some phenols by N-bromosuccinimide.
B. S. Goud and G. R. Desiraju
J.Chem.Res.(S), 244-245 (1995).
 111. (4-Dimethylaminopyridine)₅(benzoic acid)₃(H₂O)₁₀ : a two-dimensional clathrate hydrate.
K. Biradha, R. E. Edwards, G. J. Foulds, W. T. Robinson and G. R. Desiraju
J. Chem. Soc., Chem. Commun., 1705-1707 (1995).
 112. 1,3,5-Tricyanobenzene.
D. S. Reddy, K. Panneerselvam, G. R. Desiraju, C. J. Carrell and H. L. Carrell.
Acta Crystallogr., Section C, 51, 2352-2354 (1995).
 113. The supramolecular concept as a bridge between organic, inorganic and organometallic crystal chemistry.
G. R. Desiraju
J. Mol. Str., 374, 191-198 (1996).
 114. Hydrogen bonding in organometallic crystals – 3. Transition metal complexes containing amido groups.
K. Biradha, G. R. Desiraju, D. Braga and F. Grepioni.
Organometallics, 15, 1284-1295 (1996).
 115. Supramolecular synthons in crystal engineering. Structure simplification, synthon robustness and supramolecular retrosynthesis.
V. R. Thalladi, B. S. Goud, V. J. Hoy, F. H. Allen, J. A. K. Howard and G. R. Desiraju
Chem. Comm., 401-402 (1996).
 116. First neutron diffraction analysis of an O-H... π hydrogen bond. 2-Ethynyladamantan-2-ol
F. H. Allen, J. A. K. Howard, V. J. Hoy, G. R. Desiraju, D. S. Reddy and C.C.Wilson
J. Am. Chem. Soc., 118, 4081-4084 (1996).
 117. Supramolecular synthons in crystal engineering. 3 – Solid state architecture and synthon robustness in some 2,3-dicyano-5,6-dichloro-1,4-dialkoxybenzenes.
D. S. Reddy, Y. E. Ovchinnikov, O. V. Shishkin, Y. T. Struchkov and G. R. Desiraju
J. Am. Chem. Soc., 118, 4085-4089 (1996).
 118. Supramolecular synthons in crystal engineering. 4 – Structure simplification and synthon interchangeability in some organic diamondoid solids.
D. S. Reddy, D. C. Craig and G. R. Desiraju
J. Am. Chem. Soc., 118, 4090-4093 (1996).

119. Crystal engineering and molecular recognition – twin facets of supramolecular chemistry: G. R. Desiraju and C. V. K. Sharma in *The Crystal as a Supramolecular Entity* Ed. G. R. Desiraju, *Perspectives in Supramolecular Chemistry*, 2, Wiley, Chichester, 1996, pp 31-61.
120. Correlation of biological activity in β -lactam antibiotics with Woodward and Cohen structural parameters – A Cambridge Database study
A. Nangia, K. Biradha and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 943-954 (1996).
121. Review of general principles: G. R. Desiraju in *Comprehensive Supramolecular Chemistry*, Eds. D. D. MacNicol, R. Bishop, F. Toda, Volume 6, “Crystal Engineering”, Pergamon, New York, 1996, pp 1-22.
122. Organic solid state reactivity – past, present and future: G. R. Desiraju and B.S.Goud in *Solid State Reactivity – Past, Present and Future*, Ed. V. V. Boldyrev, Blackwell, Oxford, 1996, pp 223-236.
123. Hydrogen bonding in organometallic crystals. 4. M-H...O hydrogen bonding interactions.
D. Braga, F. Grepioni, E. Tedesco, K. Biradha and G. R. Desiraju
Organometallics, 15, 2692-2699 (1996).
124. Agostic interactions in organometallic compounds. A Cambridge Structural Database study.
D. Braga, F. Grepioni, K. Biradha and G. R. Desiraju
J. Chem. Soc., Dalton Trans., 3925-3930 (1996)
125. The C-H...O hydrogen bond: structural implications and supramolecular design
G. R. Desiraju
Acc.Chem.Res. 29, 441-449 (1996).
126. The hydrogen bond C-H donor and π -acceptor characteristics of three-membered rings
F. H. Allen, J. P. M. Lommerse, V. J. Hoy, J. A. K. Howard and G. R. Desiraju
Acta Crystallogr., Section B 52, 734-745 (1996).
127. Odd-even carbon atom disparity in organic compounds
J. A. R. P. Sarma, A. Nangia, G. R. Desiraju, E. Zass and J. D. Dunitz
Nature (London), 384, 320 (1996).
128. 2,6-Dibenzoylhydroquinone
K. Biradha, A. K. Katz, H. L. Carrell and G. R. Desiraju
Acta Crystallogr., Section C, 52, 2839-2841 (1996).

129. Design of a SHG-active crystal, 4-iodo-4'-nitrobiphenyl. The role of supramolecular synthons.
J. A. R. P. Sarma, F. H. Allen, V. J. Hoy, J. A. K. Howard, R. Thaimattam, K. Biradha, and G. R. Desiraju
Chem. Comm., 101-102 (1997).
130. 2,4-Dinitro-trans-cinnamic acid
V. R. Thalladi, C. V. K. Sharma and G. R. Desiraju
Acta Crystallogr., Section C, 53, 227-229 (1997).
131. Crystal engineering and correspondence between molecular and crystal structures. Are 2- and 3-aminophenol anomalous?
F. H. Allen, V. J. Hoy, J. A. K. Howard, V. R. Thalladi and G. R. Desiraju
J. Am. Chem. Soc., 119, 3477-3480 (1997)
132. Hydrogen bonding in organometallic crystals. 6. X-H...M hydrogen bonds and M... (H-X) pseudo-agostic bonds
D. Braga, F. Grepioni, E. Tedesco, K. Biradha and G. R. Desiraju
Organometallics, 16, 1846-1856 (1997).
133. Even odder carbons
J. A. R. P. Sarma, A. Nangia, G. R. Desiraju, E. Zass and J. D. Dunitz
Nature (London), 387, 464 (1997).
134. C-H...O hydrogen bonded multi-point recognition in molecular assemblies of dibenzylideneketones and 1,3,5-trinitrobenzenes.
K. Biradha, A. Nangia, G. R. Desiraju, C. J. Carrell and H. L. Carrell
J. Mater.Chem., 1111-1122 (1997)
135. Crystal engineering: solid state supramolecular synthesis
G. R. Desiraju
Curr. Opin. Solid State & Materials Science, 2, 451-454 (1997)
136. Designer crystals: intermolecular interactions, network structures and supramolecular synthons
G. R. Desiraju
Chem. Comm., 1475-1482 (1997)
137. Engineering of an octupolar non-linear optical crystal: tribenzyl isocyanurate
V. R. Thalladi, S. Brasselet, D. Bläser, R. Boese, J. Zyss, A. Nangia and G. R. Desiraju
Chem. Comm., 1841-1842 (1997).
138. Evidence for the characterisation of the C-H... π interaction as a weak hydrogen bond: toluene and chlorobenzene solvates of 2,3,7,8-tetraphenyl-1,9,10-anthridine
N. N. L. Madhavi, A. K. Katz, H. L. Carrell, A. Nangia and G. R. Desiraju

Chem. Comm., 1953-1954 (1997)

139. Crystal gazing: structure prediction and polymorphism
G. R. Desiraju
Science, 278, 404-405 (1997)
140. Reactivity of organic solids – retrospect and prospect
G. R. Desiraju
Solid State Ionics, 101-103, 839-842 (1997).
141. 2,6-Dibenzoyl-1,4-benzoquinone
K. Biradha, M. J. Zaworotko, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section C, 53, 1653-1655 (1997).
142. The halogen...O(nitro) supramolecular synthon in crystal engineering: a combined crystallographic database and ab initio molecular orbital study
F. H. Allen, J. P. M. Lommerse, V. J. Hoy, J. A. K. Howard, G. R. Desiraju
Acta Crystallogr., Section B, 53, 1006-1016 (1997).
143. Hydrogen bonding in organometallic crystals – a survey
D. Braga, F. Grepioni and G. R. Desiraju
J. Organomet. Chem., 548, 33-43 (1997).
144. Molecular networks in the crystal structures of tetrakis-(4-iodophenyl)methane and (4-iodophenyl)triphenylmethane
R. Thaimattam, D. S. Reddy, F. Xue, T. C. W. Mak, A. Nangia and G. R. Desiraju
New J. Chem., 22, 143-148 (1998).
145. 4-(Triphenylmethyl) benzoic acid: a supramolecular wheel-and-axle host
R. K. R. Jetti, S. S. Kuduva, D. S. Reddy, F. Xue, T. C. W. Mak, A. Nangia, G. R. Desiraju.
Tetrahedron Lett., 39, 913-916 (1998)
146. Crystal engineering: some further strategies.
A. Anthony, G. R. Desiraju, R. K. R. Jetti, S. S. Kuduva, N. N. L. Madhavi, A. Nangia, R. Thaimattam, V. R. Thalladi.
Crystal Engineering, 1, 1-18 (1998).
147. Trimethylisocyanurate and triethylisocyanurate
V. R. Thalladi, A. K. Katz, H. L. Carrell, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section C, 54 86-89 (1998).
148. Crystal engineering of some 2,4,6-triaryloxy-1,3,5-triazines: octupolar non-linear materials
V. R. Thalladi, S. Brasselet, H. -C. Weiss, D. Bläser, A. K. Katz, H. L. Carrell, R. Boese, J. Zyss, A. Nangia and G. R. Desiraju

- J. Am. Chem. Soc., 120, 2563-2577 (1998).
149. Distinction between the weak hydrogen bond and the van der Waals interaction
T. Steiner and G. R. Desiraju
Chem. Comm., 891-892 (1998).
150. Supramolecular synthons and pattern recognition
A. Nangia and G. R. Desiraju
Topics in Current Chemistry, Design of Organic Solids, Vol. 198 (ed. E. Weber)
57-95 (1998).
151. Crystal engineering and organometallic architecture
D. Braga, F. Grepioni and G. R. Desiraju,
Chem. Rev., 98, 1375-1405 (1998).
152. Octupolar versus dipolar crystalline structures for nonlinear optics: a dual
crystalline and propagative engineering approach
J. Zyss, S. Brasselet, V. R. Thalladi, G. R. Desiraju
J. Chem. Phys. 109, 658-669 (1998)
153. Interplay of strong and weak hydrogen bonding in molecular complexes of some
4,4'-disubstituted biphenyls with urea, thiourea and water
R. Thaimattam, D. S. Reddy, F. Xue, T. C. W. Mak, A. Nangia and
G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 1783-1789 (1998).
154. Synthesis, X-ray crystal structures and biological evaluation of some mono- and
bicyclic 1,3-diazetid-2-ones
P. S. Chandrakala, A. K. Katz, H. L. Carrell, P. R. Sailaja, A. R. Podile,
A. Nangia and G. R. Desiraju,
J. Chem. Soc., Perkin Transac. 1, 2597-2609 (1998).
155. C-H...F interactions in the crystal structures of some fluorobenzenes
V. R. Thalladi, H. -C. Weiss, D. Bläser, R. Boese, A. Nangia and
G. R. Desiraju
J. Am. Chem. Soc., 120, 8702-8710 (1998).
156. Isostructurality in crystalline oxa-androgens. A case of C-O-H...O and C-H...O
interaction mimicry and solid solution formation.
A. Anthony, M. Jaskólski, A. Nangia and G. R. Desiraju
Chem. Comm., 2537-2538 (1998).
157. Supramolecular structures – reason and imagination
A. Nangia and G. R. Desiraju
Acta Crystallogr., Section A, 54, 934-944 (1998).

158. Supramolecular synthons mediated by weak hydrogen bonding. Forming linear molecular arrays via $C\equiv C-H\cdots N\equiv C$ and $C\equiv C-H\cdots O_2N$ recognition.
R. Thaimattam, P. J. Langley, J. Hulliger and G. R. Desiraju
New J. Chem. 1307-1309 (1998).
159. 17,17-Ethylenedioxyandrost-4-ene-3,6-dione and 17,17-ethylenedioxyandrosta-1,4-diene-3,6-dione
A. Anthony, M. Jaskólski, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section C, 54 1894-1898 (1998).
160. 5 β -Androstan-3,17-dione
A. Anthony, M. Jaskólski, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section C, 54 1898-1900 (1998).
161. Some current challenges in crystal engineering
A. Nangia and G. R. Desiraju, in Supramolecular Engineering of Synthetic Metallic Materials: Conductors and Magnets, Eds. J. Veciana, C. Rovira, D.B. Amabilino, NATO ASI Series, Kluwer, Dordrecht, 1999, pp 1-21.
162. Weak hydrogen bonds in supramolecular synthesis
A. Nangia and G. R. Desiraju, in Current Challenges on Large Supramolecular Assemblies, Ed. G. Tsoucaris, NATO ARW Series, Kluwer, Dordrecht, 1999, pp 193-208.
163. Axial and equatorial conformations of penicillins, their sulfoxides and sulfones: The role of $N-H\cdots S$ and $C-H\cdots O$ hydrogen bonds
A. Nangia and G. R. Desiraju
J. Mol. Str., 474, 65-79 (1999).
164. Cubane carboxylic acids. Crystal engineering considerations and the role of $C-H\cdots O$ hydrogen bonds in determining $O-H\cdots O$ networks
S. S. Kuduva, D. C. Craig, A. Nangia and G. R. Desiraju
J. Am. Chem. Soc., 121, 1936-1944 (1999).
165. Crystal structure of sodium glutacetaldehyde tetrahydrate, $Na_2(C_5H_5O_2)_2 \cdot 4H_2O$
M. Muthuraman, Y. le Fur, J. -F. Nicoud, R. Masse and G. R. Desiraju
Z. Kristallogr. NCS, 214, 283-284 (1999).
166. Pseudopolymorphism. Occurrences of hydrogen bonding organic solvents in molecular crystals
A. Nangia and G. R. Desiraju
Chem. Comm., 605-606 (1999).
167. Tri-p-tolyl-1,3,5-triazine
V. R. Thalladi, M. Muthuraman, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section C, 55 698-700 (1999).

168. Pseudopolymorphs of 3,5-dinitrosalicylic acid
V. R. Senthil Kumar, S. S. Kuduva and G. R. Desiraju
J. Chem. Soc., Perkin Transac. 2, 1069-1073 (1999).
169. Current challenges in crystal engineering
G. R. Desiraju, in Implications of Molecular and Materials Structure for New Technologies, Eds. J. A. K. Howard, F. H. Allen and G. P. Shields, Kluwer, Dordrecht, 1999, pp 321-339.
170. Steering non-centrosymmetry into the third dimension. Crystal engineering of an octupolar nonlinear optical crystal.
V. R. Thalladi, R. Boese, S. Brasselet, I. Ledoux, J. Zyss, R. K. R. Jetti and G. R. Desiraju
Chem. Comm., 1639-1640 (1999).
171. When is a polymorph not a polymorph? Helical trimeric O-H...O synthons in trans-1,4-diethynyl-1,4-cyclohexanediol.
C. Bilton, J. A. K. Howard, N. N. L. Madhavi, A. Nangia, G. R. Desiraju and F. H. Allen
Chem. Comm., 1675-1676 (1999).
172. Sodium 4-nitrophenolate 4-nitrophenol dihydrate crystal: a new herringbone structure for quadratic nonlinear optics
M. Muthuraman, M. Bagieu-Beucher, R. Masse, J. -F. Nicoud and G. R. Desiraju
J. Mater. Chem., 1471-1474 (1999).
173. Engineering of nonlinear optical crystals displaying a quasi perfect polar alignment of chromophores
M. Muthuraman, Y. Le Fur, M. Bagieu-Beucher, R. Masse, J. -F. Nicoud and G. R. Desiraju
J. Mater. Chem., 2233-2239 (1999).
174. 4-(Triphenylmethyl)phenol-Triphenylphosphine oxide (1/1)
R. K. R. Jetti, H.-C. Weiss, V. R. Thalladi, R. Boese, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section C, 55, 1530-1533 (1999).
175. Polymorphism and Pseudopolymorphism in Organic Crystals. A Cambridge Structural Database Study
J. A. R. P. Sarma and G. R. Desiraju, in Crystal Engineering. The Design and Applications of Functional Solids, Eds. K. R. Seddon and M. Zaworotko, Kluwer, Dordrecht, 1999, pp 325-356.
176. Diversity and certainty – Database research in crystal engineering

- G. R. Desiraju, in *Crystal Engineering: From molecules and crystals to materials*, Eds. D. Braga et al., Kluwer, Dordrecht, 1999, pp 229-241.
177. The indecisive role of the C–F group in crystal packing—an analysis of the crystal structures of the tetrahalogenated hydroquinones and γ -hydroquinone
V. R. Thalladi, H.-C. Weiss, R. Boese, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section B, 55 1005-1013 (1999).
 178. The even/odd disparity in organic compounds
G. R. Desiraju, J. D. Dunitz, A. Nangia, J. A. R. P. Sarma and E. Zass
Helv. Chim. Acta, 83, 1-15 (2000).
 179. Establishing structural repetitivity in systems with interaction interference: crystal engineering in the gem-alkynol family
N. N. L. Madhavi, C. Bilton, J. A. K. Howard, F. H. Allen, A. Nangia and G. R. Desiraju
New J. Chem., 24, 1-4 (2000).
 180. Molecular dynamics study of the solid state photoreactivity of 3- and 4-cyano-trans-cinnamic acids.
J. A. R. P. Sarma, B. Chaudhuri and G. R. Desiraju
Indian. J. Chem., Sect. A, 39, 253-261 (2000).
 181. C–H...O and C–H...N hydrogen bond networks in the crystal structures of some 1,2-dihydro-N-aryl-4,6-dimethylpyrimidin-2-ones
M. Muthuraman, Y. Le Fur, M. Bagieu-Beucher, R. Masse, J. -F. Nicoud, S. George, A. Nangia and G. R. Desiraju
J. Solid State Chem., 152, 221-228 (2000).
 182. The supramolecular synthon in crystal engineering
G. R. Desiraju in, *Stimulating concepts in chemistry*, Eds. S. Shibasaki, J. F. Stoddart, F. Vögtle, Wiley, Chichester, 2000, pp. 293-308.
 183. tris-(2-Cyanoethyl) isocyanurate
P. K. Thallapally and G. R. Desiraju
Acta Crystallogr., Section C, 56, 572-573 (2000).
 184. Three dimensional Quantitative Structural Activity Relation (3D QSAR) studies of some 1,5-diarylpyrazoles: Analogue based design of selective cyclooxygenase-2 inhibitors.
G. R. Desiraju, B. Gopalakrishnan, R. K. R. Jetti, D. Raveendra, J. A. R. P. Sarma and H. S. Subramanya
Molecules, 5, 945-955 (2000).
 185. Shape and size effects in the crystal structures of complexes of 1,3,5-trinitrobenzene with some trigonal donors: the benzene–thiophene exchange rule.

- P. K. Thallapally, K. Chakraborty, H. L. Carrell, S. Kotha and G. R. Desiraju
Tetrahedron, 56, 6721-6728 (2000).
186. Benzyltriphenylphosphonium glutacetaldehyde
M. Muthuraman, J. -F. Nicoud, R. Masse and G. R. Desiraju
Acta Crystallogr., Section C, 56 986-988 (2000).
 187. Hydrogen bonding and other intermolecular interactions in organometallic crystals
G. R. Desiraju
J. Chem. Soc., Dalton Transac., 3745-3752 (2000).
 188. Melting points of meta and para isomers of 4-anisylpinacolone
S. S. Kuduva, J. A. R. P. Sarma, A. K. Katz, H. L. Carrell and G. R. Desiraju
J. Phys. Org. Chem. 13, 719-728, (2000).
 189. 4-Ethynyl-4-hydroxy-cyclohexanone and 4-ethynyl-4-hydroxy-2,3,4,5-tetramethylcyclohexa-2,5-diene-1-one
C. Bilton, J. A. K. Howard, N. N. L. Madhavi, G. R. Desiraju and F. H. Allen
Acta Crystallogr., Section C, 56, 1356-1358 (2000).
 190. Racemic 1,2-diphenyl-3-butyn-2-ol
N. N. L. Madhavi, G. R. Desiraju, C. Bilton, J. A. K. Howard and F. H. Allen
Acta Crystallogr., Section C, 56, 1359-1360 (2000)
 191. Crystal engineering in the gem-alkynol family: interplay between strong and weak interactions in structures of 2,3,5,6-tetrahalo[F,Cl,Br]-trans-1,4-diethynyl-cyclohexa-2,5-diene-1,4-diols
N. N. L. Madhavi, G. R. Desiraju, C. Bilton, J. A. K. Howard and F. H. Allen
Acta Crystallogr., Section B, 56, 1063-1070, (2000).
 192. Crystal engineering in the gem-alkynol family: synthon repetitivity and topological similarity in diphenylethynylmethanols: structures that lack O-H...O hydrogen bonds
C. Bilton, J. A. K. Howard, N. N. L. Madhavi, A. Nangia, G. R. Desiraju, F. H. Allen and C. C. Wilson
Acta Crystallogr., Section B, 56, 1071-1079, (2000).
 193. Halogen trimer synthons in crystal engineering: low temperature X-ray and neutron diffraction study of the 1:1 complex of 2,4,6-tris(4-chlorophenoxy)-1,3,5-triazine with tribromobenzene
C. K. Broder, J. A. K. Howard, D. A. Keen, C. C. Wilson, F. H. Allen, R. K. R. Jetti, A. Nangia and G. R. Desiraju
Acta Crystallogr., Section B, 56, 1080-1084, (2000).
 194. The All-Chemist (Millennium Essay)
G. R. Desiraju

Nature (London), 408, 407 (2000).

195. Crystallisation of pseudopolymorphs of some gamboge pigments. Pyridine, dimethylformamide and dimethylsulfoxide solvates of morellic acid, gambogic acid and guttiferic acid.
A. Anthony and G. R. Desiraju
Supramolecular Chemistry, 13, 11-23 (2001)
196. Hydrogen bonding in two tetracyclic indole alkaloids
A. K. Varma, A. Nangia, G. R. Desiraju, V. S. Giri and P. Jaisankar
Acta Crystallogr., Section C, 57, 97-99 (2001)
197. Crystal engineering of primary cubanecarboxamides. Repetitive formation of an unexpected N-H...O hydrogen bonded network
S. S. Kuduva, D. Bläser, R. Boese and G. R. Desiraju
J. Org. Chem., 66, 1621-1626 (2001).
198. Diamond and square grid networks in the same structure. Crystal engineering with the iodo · · · nitro supramolecular synthon.
R. Thaimattam, C. V. K. M. Sharma, A. Clearfield and G. R. Desiraju
Cryst. Growth Des., 1, 103-106 (2001).
199. Nonlinear optical crystals designed with 4-nitrophenolate chromophores: An engineering route using a multipdipolar chromophore, 3-hydroxy-2,4,6-trinitrophenolate.
M. Muthuraman, J. -F. Nicoud, R. Masse and G. R. Desiraju
Mol. Cryst. Liq. Cryst., 356, 1-13 (2001).
200. Area correction of multiatom acceptor hydrogen bond frequency distributions.
Z. Ciunik and G. R. Desiraju
Chem. Comm., 703-704 (2001).
201. Molecular Complexation as a design tool in the crystal engineering of non-centrosymmetric structures. Ideal orientation of chromophores linked by O-H...O and C-H...O hydrogen bonds for nonlinear optics
M. Muthuraman, R. Masse, J. -F. Nicoud and G. R. Desiraju
Chem. Mater., 13, 1473-1479 (2001)
202. Inclusion compounds of tetrakis-(4-nitrophenyl)methane: C-H...O networks, pseudopolymorphism and structural transformations
R. Thaimattam, X. Feng, J. A. R. P. Sarma, T. C. W. Mak and G. R. Desiraju
J. Am. Chem. Soc., 123, 4432-4445 (2001).
203. Crystal structures and packing of 4-cyanocubane carboxylic acid, its ethyl ester and the solid solution of 1,4-dicyanocubane and 1,4-dibromocubane
S. S. Kuduva, D. Bläser, R. Boese and G. R. Desiraju
Struct. Chem., 12, 259-266 (2001).

204. Matching of molecular and supramolecular symmetry. An exercise in crystal engineering.
P. K. Thallapally, K. Chakraborty, A. K. Katz, H. L. Carrell, S. Kotha and G. R. Desiraju
CrystEngComm, 31, (2001).
205. Chemistry beyond the molecule
G. R. Desiraju,
Nature (London), 412, 397-400 (2001).
206. Computer aided design of selective COX-2 inhibitors: comparative molecular field analysis and docking studies of some 3,4-diaryloxazolone derivatives
G. R. Desiraju, J. A. R. P. Sarma, D. Raveendra, B. Gopalakrishnan, R. Thilagavathi, M. E. Sobhia and H. S. Subramanya
J. Phys. Org. Chem., 14, 481-487 (2001).
207. Crystal engineering in the gem-alkynol family. The key role of water in the structure of 2,3,5,6-tetrabromo-trans-1,4-diethynyl-cyclohexa-2,5-diene-1,4-diol monohydrate
C. Bilton, J. A. K. Howard, N. N. L. Madhavi, G. R. Desiraju, F. H. Allen, D. A. Keen and C. C. Wilson
Acta Crystallogr., Section B, 57, 560-566 (2001).
208. Crystal structure of N,N'-di-5-nitrosalicylidene-(R,R)-1,2-cyclohexanediamine, $C_{20}H_{20}N_4O_6$
M. Muthuraman, J. -F. Nicoud, R. Masse and G. R. Desiraju
Z. Kristallogr. NCS, 216, 381-382 (2001).
209. Crystal structure of N,N'-di-5-nitrosalicylidene-(R,S)-1,2-cyclohexanediamine, $C_{20}H_{20}N_4O_6$
M. Muthuraman, J. -F. Nicoud, R. Masse and G. R. Desiraju
Z. Kristallogr. NCS, 216, 383-384 (2001).
210. Crystal engineering. Outlook and prospects.
G. R. Desiraju
Curr. Sci., 81, 1038-1042 (2001).
211. Steroidal aromatase inhibitors. Model receptor surfaces and 3D QSAR.
R. K. R. Jetti, A. Anthony, A. Nangia and G. R. Desiraju
Ind. J. Chem. Section B, 40, 1054-1062 (2001).
[Ghatak Commemoration Issue]
212. Unusually long cooperative chain of seven hydrogen bonds. An alternative packing type for symmetrical phenols.
P. K. Thallapally, A. K. Katz, H. L. Carrell and G. R. Desiraju
Chem. Comm. 344-345 (2002).

213. 3D-QSAR Studies of some [[1-Aryl(or Benzyl)-1-(benzenesulphonamido)methyl] phenyl] alkanoic acid derivatives as Thromboxane A2 Receptor Antagonists
K. V. V. M. Sairam, J. A. R. P. Sarma and G. R. Desiraju
Drug Design and Discovery, 18, 45-49 (2002).
214. Topological Equivalences between Organic and Coordination Polymer Crystal Structures: An organic ladder formed with three-connected molecular and supramolecular synthons
S. Aitipamula, P. K. Thallapally, R. Thaimattam, M. Jaskolski and G. R. Desiraju
Org. Lett., 4, 921-924 (2002)
215. The supramolecular synthon approach to crystal structure prediction
J. A. R. P. Sarma and G. R. Desiraju
Cryst. Growth Des., 2, 93-100 (2002)
216. 1,3-Dibromo-2,4,6-trinitrobenzene (DBTNB). Crystal engineering and perfect polar alignment of two-dimensional hyperpolarizable chromophores
P. K. Thallapally, G. R. Desiraju, M. Bagieu-Beucher, R. Masse, C. Bourgogne and J. F. Nicoud
Chem. Comm. 1052-1053 (2002).
217. Hydrogen bridges in crystal engineering. Interactions without borders.
G. R. Desiraju
Acc. Chem. Res., 35, 565-573 (2002)
218. Supramolecular synthons based on N-H...N and C-H...O hydrogen bonds. Crystal engineering of a helical structure with 5,5-diethylbarbituric acid.
P. Vishweshwar, R. Thaimattam, M. Jaskolski and G. R. Desiraju
Chem. Comm. 1830-1831 (2002).
219. Crystallography. Quo vadis?
G. R. Desiraju
Z. Krist., 217, 297-298 (2002).
[125 Year Commemoration Issue]
220. 'Bond free'.
G. R. Desiraju
CrystEngComm, 4, 499 (2002).
221. Innovation in crystal engineering
D. Braga, G. R. Desiraju, J. S. Miller, A. G. Orpen and S. L. Price
CrystEngComm, 4, 500-509 (2002).

222. Crystal structures and packing of 2,4,6-tris(4-fluorophenoxy)-1,3,5-triazine and 2,4,6-tris(3,4-dimethylphenoxy)-1,3,5-triazine. New materials for octupolar nonlinear optics.
R. Boese, G. R. Desiraju, R. K. R. Jetti, M. T. Kirchner, I. Ledoux, V. R. Thalladi, and J. Zyss
Struct. Chem. 13, 321-328 (2002).
[Mackay Commemorative Issue]
223. Cryptic crystallography
G. R. Desiraju
Nature Materials, 1, 77-79 (2002).
224. A 1:1 molecular complex of bis(4-aminophenyl)disulfide and 4-aminothiophenol
V. R. Vangala, G. R. Desiraju, R. K. R. Jetti, D. Bläser and R. Boese
Acta Crystallogr., Section C, 58, o635-o636 (2002).
225. 3,5-Dinitrosalicylic acid–phenazine (1/1)
V. S. Senthil Kumar, S. S. Kuduva and G. R. Desiraju
Acta Crystallogr., Section E, 58, o865-o866 (2002).
226. Computer aided design of selective COX-2 inhibitors: Comparative Molecular Field Analysis (CoMFA), Comparative Similarity Indices Analysis (CoMSIA) and docking studies of some 1,2-diarylimidazole derivatives.
G. R. Desiraju, B. Gopalakrishnan, R. K. R. Jetti, A. Nagaraju, D. Raveendra, J. A. R. P. Sarma, M. E. Sobhia and R. Thilagavathi,
J. Med. Chem. 45, 4847-4857 (2002).
227. C–H...O Hydrogen Bonds in Molecular Complexes of 1,3,5-Trinitrobenzene with some N-Heterocycles.
P. K. Thallapally, A. K. Katz, H. L. Carrell, G. R. Desiraju
CrystEngComm, 5, 87-92 (2003)
228. Crystal engineering. Retrospect and prospect.
G. R. Desiraju
J. Ind. Chem. Soc., 80, 151-155 (2003)
229. Searching for a polymorph. Second form of 6-amino-2-phenylsulfonylimino-1,2-dihydropyridine.
R. K. R. Jetti, R. Boese, J. A. R. P. Sarma, L. S. Reddy, P. Vishweshwar and G. R. Desiraju
Angew. Chem. Int. Ed., 42, 1963-1967 (2003)
230. Crystal: In search of clarity (Concept essay)
G. R. Desiraju
Nature, 423, 485 (2003)

231. Dilemmas in crystallisation. The 'unusual' behaviour of 1,5-dichloro-trans-9,10-diethynyl-9,10-dihydroanthracene-9,10-diol and the more 'normal' behaviour of its pseudopolymorphs with dipolar aprotic solvents.
R. Banerjee, G. R. Desiraju, R. Mondal, A. S. Batsanov, C. K. Broder and J. A. K. Howard
Helv. Chim. Acta, 86, 1339-1351 (2003)
[Dunitz Commemoration Issue]
232. Supramolecular equivalence of halogen, ethynyl and hydroxy groups. A comparison of the crystal structures of some 4-substituted anilines
A. Dey, R. K. R. Jetti, R. Boese and G. R. Desiraju
CrystEngComm 5, 248-252 (2003)
233. Crystal engineering. From molecules to materials.
G. R. Desiraju
J. Mol. Str., 656, 5-15 (2003)
[Achim Müller Commemoration Issue]
234. Coupling octupoles in crystals: the case of the 1,3,5-trinitrobenzene-triphenylene 1:1 molecular co-crystal
J. Zyss, I. Ledoux-Rak, H. -C. Weiss, D. Bläser, R. Boese, P. K. Thallapally, V. R. Thalladi and G. R. Desiraju
Chem. Mater., 15, 3063-3073 (2003)
235. Stereoelectronic effects of substituent groups in the solid state. Crystal chemistry of some cubanecarboxylic and phenylpropionic acids.
D. Das, R. K. R. Jetti, R. Boese and G. R. Desiraju
Cryst. Growth Des., 3, 675-681 (2003)
236. Design of EGFR Kinase Inhibitors: A Ligand Based Approach and its Confirmation with Structure Based Studies.
A. Vema, S. K. Panigrahi, G. Rambabu, B. Gopalakrishnan, J. A. R. P. Sarma and G. R. Desiraju
Bioorg. Med. Chem., 11, 4643-4653 (2003).
237. Square Networks based on the Br...NO₂ Supramolecular Synthon
P. K. Thallapally, S. Basavoju, G. R. Desiraju, M. Bagieu-Beucher, R. Masse, and J. -F. Nicoud
Curr. Sci., 85, 995-1001 (2003)
[Ramaseshan Commemorative Issue]
238. Five new pseudopolymorphs of sym-trinitrobenzene
R. K. R. Jetti, R. Boese, P. K. Thallapally, and G. R. Desiraju
Cryst. Growth Des. 3, 1033-1040 (2003)
239. Multiple molecules in the crystallographic asymmetric unit. An alternative mode of close packing of networks of rigid hydrogen bonded molecules.

- S. Aitipamula, G. R. Desiraju, M. Jaskólski, A. Nangia, and R. Thaimattam
CrystEngComm, 5, 447-450 (2003)
240. Crystal and co-crystal
G. R. Desiraju
CrystEngComm, 5, 466-467 (2003)
 241. Correspondence between molecular functionality and crystal structures.
Supramolecular chemistry of a family of homologated aminophenols
V. R. Vangala, B. R. Bhogala, A. Dey, G. R. Desiraju, C. K. Broder, P. S. Smith, R. Mondal, and J. A. K. Howard
J. Am. Chem. Soc. 125, 14495-14509 (2003).
 242. Database study of N–H...O, O–H...O and C–H...O hydrogen bonds in protein–ligand complexes
S. Sarkhel and G. R. Desiraju
Proteins: Structure, Function and Bioinformatics, 54, 247-259 (2004)
 243. Polymorphism of 1,3,5-trinitrobenzene induced by trisindane additive
P. K. Thallapally, R. K. R. Jetti, A. K. Katz, H. L. Carrell, K. Singh, K. Lahiri, S. R. Kotha, R. Boese and G. R. Desiraju
Angew. Chem. Int. Ed. 43, 1149-1155 (2004).
 244. Gauche and staggered forms of diethylamine in solvates of 1,5-dichloro-cis-9,10-diethynyl-9,10-dihydroanthracene-9,10-diol. A case of conformational pseudopolymorphism?
R. Mondal, J. A. K. Howard, R. Banerjee, G. R. Desiraju
Chem. Comm., 644-645 (2004)
 245. Homology modelling in protein structure prediction: Epidermal Growth Factor Receptor kinase domain
S. K. Panigrahi and G. R. Desiraju
Natnl. Acad. Sci. Lett., 27, 1-12 (2004).
 246. Host-guest and network structures of some tetraphenylmethane derivatives
S. Basavoju, S. Aitipamula, G. R. Desiraju
CrystEngComm., 6, 120-125 (2004).
 247. A 1:1 molecular complex of 4-aminocyclohexanol and (4-hydroxycyclohexyl)-carbamic acid
A. Dey, G. R. Desiraju, R. Mondal, J. A. K. Howard
Acta Crystallogr., Sect. E, 60, o857-o859 (2004).
 248. Hydrogen Bonding
G. R. Desiraju
Encyclopaedia of Supramolecular Chemistry (Eds. J. L. Atwood and J. Steed)
Marcel Dekker, New York, 2004, 1, pp 658-665.

249. Organic chlorine as a hydrogen bridge acceptor. Evidence for the existence of intramolecular O–H...Cl–C interactions in some gem-alkynols.
R. Banerjee, G. R. Desiraju, R. Mondal, J. A. K. Howard
Eur. J. Chem., 10, 3373-3383 (2004).
250. A novel saturated hydrogen bridge architecture in supraminols
B. R. Bhogala, V. R. Vangala, P. S. Smith, J. A. K. Howard, G. R. Desiraju
Cryst. Growth Des., 4, 647-649 (2004).
251. Structural variations and polymorphism of some derivatives of 6-amino-2-phenylsulfonylimino-1,2-dihydropyridine
M. T. Kirchner, L. S. Reddy, G. R. Desiraju, R. K. R. Jetti, R. Boese
Cryst. Growth Des., 4, 701-709 (2004).
252. Midsummer madness (Turning Point Essay)
G. R. Desiraju
Nature, 431, 25 (2004)
253. Proton transfer and N(+)–H...S(–) hydrogen bonds in the crystal structure of 4-aminothiophenol
R. K. R. Jetti, R. Boese, T. S. Thakur, V. R. Vangala, G. R. Desiraju
Chem. Comm., 2526-2527 (2004)
254. Crystal engineering in the aminophenol family. Novel carborundum network in a supramolecular homologous series.
A. Dey, G. R. Desiraju, R. Mondal, J. A. K. Howard
Chem. Comm., 2528-2529 (2004)
255. Counterpoint: What's in a name?
G. R. Desiraju
Cryst. Growth Des., 4, 1089-1090 (2004).
256. Supramolecular equivalence of ethynyl, chloro, bromo and iodo groups. A comparison of the crystal structures of some 4-phenoxyanilines.
A. Dey and G. R. Desiraju
CrystEngComm., 6, 642-646 (2004).
257. Dianiline–diphenol molecular complexes based on supraminol recognition
V. R. Vangala, R. Mondal, C. K. Broder, J. A. K. Howard, G. R. Desiraju
Cryst. Growth Des., 5, 99-104 (2005).
258. Chemistry. The Middle Kingdom.
G. R. Desiraju
Curr. Sci., 88, 374-380 (2005).

259. Saccharin as a salt former. Enhanced solubilities of saccharinates of active pharmaceutical ingredients.
P. M. Bhatt, N. V. Ravindra, R. Banerjee and G. R. Desiraju
Chem. Comm., 1073-1075 (2005).
260. 2-Methylsulfanylnicotinic acid
S. Basavoju, C. M. Reddy and G. R. Desiraju
Acta Crystallogr., Sect. E, 61, o822-o823 (2005).
261. Structural studies of the system $(\text{Na}^+)(\text{saccharinate}^-)(\text{H}_2\text{O})_n$. A model for crystallization.
R. Banerjee, P. M. Bhatt, M. T. Kirchner and G. R. Desiraju.
Angew. Chem. Int. Ed., 44, 2515-2520 (2005).
[VIP]
262. Virtual Screening of 4-Anilinoquinazoline Analogs as EGFR Kinase Inhibitors: Importance of Hydrogen Bonds in the Evaluation of Poses and Scoring Functions.
V. Aparna, G. Rambabu, S. K. Panigrahi, J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Inf. Model., 45, 725-738 (2005).
263. Sorting of polymorphs based on mechanical properties. Trimorphs of 6-chloro-2,4-dinitroaniline.
C. M. Reddy, S. Basavoju and G. R. Desiraju
Chem. Comm., 2439-2441 (2005).
264. Correlation between molecular dipole moment and centrosymmetry in some crystalline diphenyl ethers
A. Dey and G. R. Desiraju
Chem. Comm., 2486-2488 (2005).
265. Rare syn-anti catemer in 4-nitrophenylpropionic acid
D. Das, G. R. Desiraju, R. K. R. Jetti and R. Boese
Acta Crystallogr., Sect. E, 61, o1588-o1589 (2005).
266. The C–H...O and other weak hydrogen bonds. From crystal engineering to virtual screening.
G. R. Desiraju
Chem. Comm., 2995-3001 (2005).
[Focus article to commemorate 40 years of the journal]
267. Structural basis for bending of organic crystals
C. M. Reddy, R. C. Gundakaram, S. Basavoju, M. T. Kirchner, K. A. Padmanabhan and G. R. Desiraju
Chem. Comm., 3945-3947 (2005).
268. Rational Design of TMP Kinase Inhibitors as Antitubercular agents based on docking, pharmacophore and 3D QSAR studies

- B. Gopalakrishnan, V. Aparna, J. Jeevan, M. Ravi, G. R. Desiraju
J. Chem. Inf. Model., 45, 1101-1108 (2005).
269. Crystal Structure Prediction of Aminols: Advantages of a Supramolecular Synthon Approach with Experimental Structures
A. Dey, M. T. Kirchner, V. R. Vangala, G. R. Desiraju, R. Mondal and J. A. K. Howard
J. Am. Chem. Soc., 127, 10545-10559 (2005)
270. Saccharin salts of active pharmaceutical ingredients, their crystal structures and increased water solubilities.
R. Banerjee, P. M. Bhatt, N. V. Ravindra, and G. R. Desiraju
Cryst. Growth Des., 5, 2299-2309 (2005).
271. Five varieties of hydrogen bonds in 1-formyl-3-thiosemicarbazide: An electron density study.
P. Munshi, T. S. Thakur, T. N. Guru Row and G. R. Desiraju
Acta Crystallogr. Sect B, 62, 118-127 (2006).
272. 3D-QSAR studies on antitubercular thymidine monophosphate kinase inhibitors based on different alignment methods
V. Aparna, J. Jeevan, M. Ravi, G. R. Desiraju and B. Gopalakrishnan
Bioorg. Med. Chem. Lett., 16, 1014-1020 (2006).
273. Isostructurality, Polymorphism and Mechanical Properties of Some Hexahalogenated Benzenes. The Nature of Halogen...Halogen Interactions
C. M. Reddy, M. T. Kirchner, R. C. Gundakaram, K. A. Padmanabhan, and G. R. Desiraju
Chem. Eur. J., 12, 2222-2234 (2006).
274. Misassigned C–H...Cu agostic interaction in a copper (II) ephedrine derivative is actually a weak, multicentred hydrogen bond
T. S. Thakur and G. R. Desiraju
Chem. Comm. 552-554 (2006).
275. Synthon evolution and unit cell evolution during crystallisation. A study of symmetry-independent molecules ($Z' > 1$) in crystals of some hydroxy compounds
D. Das, R. Banerjee, R. Mondal, J. A. K. Howard, R. Boese and G. R. Desiraju
Chem. Comm., 555-557 (2006).
276. Synthon Robustness and Solid State Architecture in Substituted gem-Alkynols
R. Banerjee, R. Mondal, J. A. K. Howard and G. R. Desiraju
Cryst. Growth Des., 6, 999-1009 (2006).
277. A 1:1 molecular complex of 4-methylpyridine N-oxide and saccharin
B. K. Saha, R. Banerjee, A. Nangia and G. R. Desiraju

- Acta Crystallogr., Sect. E, 62, o2283-o2284 (2006).
278. Solid state architecture of saccharin salts of some diamines.
R. Banerjee, B. K. Saha and G. R. Desiraju
Acta Crystallogr., Sect. C, 62, o346-o349 (2006).
279. Ligand coordinate analysis of SC-558 from the active site to the surface of COX-2: A molecular dynamics study
K. V. V. M. Sairam, G. Rambabu, J. A. R. P. Sarma and G. R. Desiraju
J. Chem. Inf. Model., 46, 1784-1794 (2006).
280. Form 1 of desloratadine, a tricyclic antihistamine
P. M. Bhatt and G. R. Desiraju
Acta Crystallogr., Sect. C, 62, o362-o363 (2006).
281. Dimorphs of 4'-amino-4-hydroxy-2'-methylbiphenyl: Assessment of likelihood of polymorphism in flexible molecules
A. Dey and G. R. Desiraju
CrystEngComm., 8, 478-482 (2006).
282. Packing modes in some mono- and disubstituted phenylpropionic acids. Repeated occurrence of the rare syn,anti-catemer.
D. Das and G. R. Desiraju
Chem. Asian J., 1, 231-244 (2006).
[VIP]
283. Solvates of sildenafil saccharinate. A new host material.
R. Banerjee, P. M. Bhatt and G. R. Desiraju
Cryst. Growth Des, 6, 1468-1478 (2006).
284. Effects of the substituent on the formation of dimers and catemers in phenylpyruvic acids
CrystEngComm, 8, 674-679 (2006).
285. Synthons robustness in saccharinate salts of some substituted pyridines
R. Banerjee, B. K. Saha and G. R. Desiraju
CrystEngComm, 8, 680-685 (2006).
286. Intellect and intuition (Retrospect essay)
G. R. Desiraju
Nature, 443, 398 (2006).
287. Crystal structure prediction with the supramolecular synthon approach: experimental structures of 2-amino-4-ethylphenol and 3-amino-2-naphthol and comparison with prediction
A. Dey, N. N. Pati and G. R. Desiraju
CrystEngComm, 8, 751-755 (2006).

288. Crystallographic studies of supramolecular synthons in amine solvates of trans-1,5-dichloro-9,10-diethynyl-9,10-dihydroanthracene-9,10-diol
R.Mondal, J. A. K. Howard, R. Banerjee and G. R. Desiraju
Cryst. Growth Des, 6, 2507 - 2516 (2006).
289. Bending and brittle organic crystals: structure-property correlations
C. M. Reddy, K. A. Padmanabhan and G. R. Desiraju
Cryst. Growth Des, 6, 2720-2731 (2006).
290. On the occurrence of multiple molecules in the crystal asymmetric unit ($Z' > 1$)
G. R. Desiraju
CrystEngComm, 9, 91-92 (2006)
291. On the polymorphism of aspirin
A. D. Bond, R. Boese and G. R. Desiraju
Angew. Chem. Int. Ed. 46, 615-617 (2007).
292. On the polymorphism of aspirin: crystalline aspirin as intergrowths of two “polymorphic” domains
A. D. Bond, R. Boese and G. R. Desiraju
Angew. Chem. Int. Ed. 46, 618-622 (2007).
293. 5,5-Dibenzylbarbituric acid monohydrate
P. M. Bhatt and G. R. Desiraju
Acta Crystallogr., Sect. E, 63, o771-o772 (2007).
294. Hexaiodobenzene: a redetermination at 100 K
S. Ghosh, C. M. Reddy and G. R. Desiraju
Acta Crystallogr., Sect. E, 63, o910-o911 (2007).
295. Strong and weak hydrogen bonds in the protein–ligand interface
S. K. Panigrahi and G. R. Desiraju
Proteins, 67, 128-141 (2007).
296. Theoretical investigation of C–H $\cdots$ M interactions in organometallic complexes: A natural bond orbital (NBO) study.
T. S. Thakur and G. R. Desiraju
J. Mol. Str. (THEOCHEM), 810, 143-154 (2007).
297. Tautomeric polymorphism in omeprazole
P. M. Bhatt and G. R. Desiraju
Chem. Comm, 2057-2059 (2007).
298. What is a polymorph? Aspirin as a case study.
A. D. Bond, R. Boese and G. R. Desiraju
Am. Pharm. Rev. May-June issue, 1-4 (2007)

299. Crystal structure of $\text{Na}_4\text{Li}_4(\text{saccharinate})_8 \cdot 14\text{H}_2\text{O}$ and its comparison with other alkali metal saccharinates
P. M. Bhatt and G. R. Desiraju
J. Mol. Str., 871, 73-79 (2007).
300. Insights into ligand selectivity in nitric oxide synthase isoforms: a molecular dynamics study
V. Aparna, G. R. Desiraju and B. Gopalakrishnan,
J. Mol. Graphics Model., 26, 457-470 (2007).
301. Strong and weak hydrogen bonds in drug–DNA complexes: a statistical analysis
S. K. Panigrahi and G. R. Desiraju
J. Biosciences, 32, 677-691 (2007).
302. Crystal Engineering : A holistic approach
G. R. Desiraju
Angew. Chem. Int. Ed., 46, 8342-8356 (2007).
303. Polymorphism. The same and not quite the same
G. R. Desiraju
Cryst. Growth. Des., 8, 3-5 (2008).
304. Van der Waals and polar distances in crystals. Quantifying supramolecular synthons.
P. Ganguly and G. R. Desiraju
Chem. Asian J., 3, 868-880 (2008).
305. Crystal structure prediction of a co-crystal using a supramolecular synthon approach: 2-methylbenzoic acid - 2-amino-4-methylpyrimidine
T. S. Thakur and G. R. Desiraju
Cryst. Growth Des., 8, 4031-4044 (2008).
306. Co-crystal formation and the determination of absolute configuration
P. M. Bhatt and G. R. Desiraju
CrystEngComm, 10, 1747-1749 (2008).
307. Co-crystals of the anti-HIV Drugs lamivudine and zidovudine
P. M. Bhatt, Y. Azim, T. S. Thakur and G. R. Desiraju
Cryst. Growth Des. 9, 951-957 (2009).
308. Additive induced polymorphism. The Pentafluorophenol–Pentafluoroaniline system.
M. T. Kirchner, D. Bläser, R. Boese and G. R. Desiraju
CrystEngComm, 11, 229-231 (2009).

309. Significant progress in predicting the crystal structures of small organic molecules - a report on the fourth blind test
G. M. Day, T. G. Cooper, A. J. Cruz-Cabeza, K. E. Hejczyk, H. L. Ammon, S. X. M. Boerrigter, J. S. Tan, R. G. Della Valle, E. Venuti, J. Jose, S. R. Gadre, G. R. Desiraju, T. S. Thakur, B. P. van Eijck, J. C. Facelli, V. E. Bazterra, M. B. Ferraro, D. W. M. Hofmann, M. A. Neumann, F. J. J. Leusen, J. Kendrick, S. L. Price, A. J. Misquitta, P. G. Karamertzanis, G. W. A. Welch, H. A. Scheraga, Y. A. Arnautova, M. U. Schmidt, J. van de Streek, A. K. Wolf and B. Schweizer.
Acta Crystallogr., B65, 107-125 (2009).
310. The nature of halogen...halogen Interactions : A model derived from experimental charge density analysis
T. T. T. Bui, S. Dahaoui, C. Lecomte, G. R. Desiraju and E. Espinosa
Angew. Chem. Int. Ed., 48, 3838-3841 (2009).
311. Structure-based design of DevR inhibitor active against non-replicating *Mycobacterium tuberculosis*
R. K. Gupta, T. S. Thakur, G. R. Desiraju and J. S. Tyagi
J. Med Chem., 52, 6324-6334 (2009)
312. 1,3-Difluorobenzene
M. T. Kirchner, D. Bläser, R. Boese, T. S. Thakur and G. R. Desiraju
Acta Crystallogr., E65, o2668-o2669 (2009).
313. 1,2,3-Trifluorobenzene
M. T. Kirchner, D. Bläser, R. Boese, T. S. Thakur and G. R. Desiraju
Acta Crystallogr., E65, o2670 (2009).
314. Long-Range synthon Aufbau modules (LSAM) and crystal structures: Systematic changes in $C_6H_{6-n}F_n$ ($0 < n < 6$) fluorobenzenes
P. Ganguly and G. R. Desiraju
CrystEngComm, 12, 817-833 (2010).
315. N-H...O and C-H...O Interaction mimicry in the 1:1 molecular complexes of 5,5-diethylbarbituric acid with urea and acetamide
T. S. Thakur, Y. Azim, T. Srinu and G. R. Desiraju
Curr. Sci. 98, 793-802 (2010)
316. Molecular and crystal structure of 4-ethynylcyanobenzene. An example of C-H...N hydrogen bonding.
S. Mahapatra, Y. Azim and G. R. Desiraju
J. Mol. Str., 976, 200-204 (2010)
317. New Solid State Forms of the Anti-HIV Drug Efavirenz. Conformational Flexibility and High Z' Issues
S. Mahapatra, T. S. Thakur, S. Joseph, S. Varughese and G. R. Desiraju
Cryst. Growth Des., 10, 3191-3202 (2010)

318. C–H...F–C Hydrogen bonding in 1,2,3,5-tetrafluorobenzene and other fluoroaromatic compounds and the crystal structure of alloxan revisited.
T. S. Thakur, M. T. Kirchner, D. Bläser, R. Boese and G. R. Desiraju
CrystEngComm 12, 2079-2085 (2010)
319. Using Water as a Design Element in Crystal Engineering. Host-Guest Compounds of Hydrated 3,5-Dihydroxybenzoic acid
S. Varughese and G. R. Desiraju
Cryst. Growth Des., 10, 4184-4196 (2010)
320. Co-crystals of alprazolam with carboxylic acids, boric acid, boronic acids and phenols. Evaluation of supramolecular heterosynthons mediated by a triazole ring.
S. Varughese, Y. Azim and G. R. Desiraju
J. Pharm. Sci., 99, 3743-3753 (2010).
321. Crystal engineering. A brief overview.
G. R. Desiraju
J. Chem. Sci., 122, 667-675 (2010)
322. Quinoxaline, Z' = 1 form.
R. Sathishkumar, S. Mahapatra, T. S. Thakur and G. R. Desiraju
Acta Crystallogr., E66, o2789 (2010)
323. Mechanical Anisotropy in Crystalline Saccharin: Nanoindentation Studies
M. S. R. N. Kiran, S. Varughese, C. Malla Reddy, U. Ramamurty and G. R. Desiraju
Cryst. Growth Des., 10, 4650-4655 (2010)
324. Third polymorph of phenylacetylene.
T. S. Thakur, R. Sathishkumar, A. G. Dikundwar, T. N. Guru Row and G. R. Desiraju
Cryst. Growth Des., 10, 4246-4249 (2010)
325. Dimorphism and structural modulation in quinoxaline.
R. Sathishkumar, S. Mahapatra, T. S. Thakur and G. R. Desiraju
Curr. Sci., 99, 1807-1810 (2010)
326. A Bond by any other name
G. R. Desiraju
Angew. Chem. Int. Ed., 50, 52-59 (2011)
327. Transferability of multipole charge density parameters for supramolecular synthons: A new tool for quantitative crystal engineering.
V. R. Hathwar, T. S. Thakur, T. N. Guru Row and G. R. Desiraju
Cryst. Growth Des., 11, 616-623 (2011)

328. Drug-drug co-crystals. Temperature-dependent proton mobility in the molecular complex of isoniazid with 4-aminosalicylic acid.
P. Grobelny, A. Mukherjee and G. R. Desiraju
CrystEngComm, 13, 4358-4364 (2011)
329. Synthron polymorphism and pseudopolymorphism in co-crystals. The 4,4'-bipyridine – 4-hydroxybenzoic acid structural landscape.
A. Mukherjee and G. R. Desiraju
Chem. Comm. 47, 4090-4092 (2011)
330. Reflections on the hydrogen bond in crystal engineering.
G. R. Desiraju
Cryst. Growth Des., 11, 896-898 (2011)
331. Polymorphs, pseudopolymorphs and co-crystals of orcinol: Exploring the structural landscape with high throughput crystallography.
A. Mukherjee, P. J. Grobelny, T. S. Thakur, and G. R. Desiraju
Cryst. Growth Des., 11, 2637-2653 (2011).
332. Defining the hydrogen bond: An account.
E. Arunan, G. R. Desiraju, R. A. Klein, J. Sadlej, S. Scheiner, I. Alkorta, D. C. Clary, R. H. Crabtree, J. J. Dannenberg, P. Hobza, H. G. Kjaergaard, A. C. Legon, B. Mennucci and D. J. Nesbitt
Pure Appl. Chem., 83, 1619-1636 (2011)
333. Definition of the hydrogen bond.
E. Arunan, G. R. Desiraju, R. A. Klein, J. Sadlej, S. Scheiner, I. Alkorta, D. C. Clary, R. H. Crabtree, J. J. Dannenberg, P. Hobza, H. G. Kjaergaard, A. C. Legon, B. Mennucci and D. J. Nesbitt
Pure Appl. Chem., 83, 1637-1641 (2011)
334. The nature and strength of C–H...O interactions involving formyl hydrogen atoms: Computational and experimental studies of small aldehydes.
T. S. Thakur, M. T. Kirchner, D. Bläser, R. Boese and G. R. Desiraju
Phys. Chem. Chem. Phys., 13, 14076-14091 (2011)
335. Structural variability in the monofluoroethynylbenzenes mediated through interactions involving 'organic' fluorine.
A. G. Dikundwar, R. Sathishkumar, T. N. Guru Row and G. R. Desiraju
Cryst. Growth Des., 11, 3954-3963 (2011)
336. Halogen bonding and structural modularity in 2,3,4- and 3,4,5-trichlorophenol
A. Mukherjee and G. R. Desiraju
Cryst. Growth Des., 11, 3735-3739 (2011)
337. Interaction anisotropy and shear instability of aspirin polymorphs established by nanoindentation.

- S. Varughese, M. S. R. N. Kiran, K. Solanko, A. D. Bond, U. Ramamurty and G. R. Desiraju
Chem. Sci., 2, 2236-2242 (2011)
338. C–H...O hydrogen bonds in anisaldehyde, salicylaldehyde and cinnamaldehyde
M. T. Kirchner, D. Bläser, R. Boese, T. S. Thakur and G. R. Desiraju
Acta Cryst., C, 67, O387-O390 (2011)
 339. Shape and size mimicry in the design of ternary molecular solids: Towards a robust strategy for crystal engineering
S. Tothadi, A. Mukherjee and G. R. Desiraju
Chem. Comm. 47, 12080-12082 (2011)
 340. Crystal Packing and Melting Temperatures of Small Oxalate Esters: The Role of C–H...O Hydrogen Bonding
S. Joseph, R. Sathishkumar, S. Mahapatra and G. R. Desiraju
Acta Cryst. Sect B, 67, 525-534 (2011)
 341. Towards crystal structure prediction of pharmaceutically relevant organic molecules — a report on the fifth blind test
D. A. Bardwell, C. S. Adjiman, Y. A. Arnautova, E. Bartashevich, S. X. M. Boerrigter, D. E. Braun, A. J. Cruz-Cabeza, G. M. Day, R. G. Della Valle, G. R. Desiraju, B. P. van Eijck, J. C. Facelli, M. B. Ferraro, D. Grillo, M. Habgood, D. W. M. Hofmann, F. Hofmann, K. V. J. Jose, P. G. Karamertzanis, A. V. Kazantsev, J. Kendrick, L. N. Kuleshova, F. J. J. Leusen, A. V. Maleev, A. J. Misquitta, S. Mohamed, R. J. Needs, M. A. Neumann, D. Nikylov, A. M. Orendt, R. Pal, C. C. Pantelides, C. J. Pickard, L. S. Price, S. L. Price, H. A. Scheraga, J. van de Streek, T. S. Thakur, S. Tiwari, E. Venuti and I. K. Zhitkov
Acta Cryst. Sect B, 67, 535-551 (2011)
 342. Phenylboronic acids in crystal engineering. Utility of the energetically unfavourable syn,syn-conformation in co-crystal design
S. Varughese, S. B. Sinha and G. R. Desiraju
Science China Chem. 54, 1909-1919 (2011)
 343. Probing water assisted self-assembly and dehydration in sodium saccharin dihydrate with nanoindentation
M. S. R. N. Kiran, S. Varughese, U. Ramamurty and G. R. Desiraju
CrystEngComm, 14, 2489-2493 (2011)
 344. Pharmaceutical salts and co-crystals. Retrospect and prospect
G. R. Desiraju
In Pharmaceutical Salts and Co-Crystals, eds. J. Wouters and L. Quere, Royal Society of Chemistry, 2011, pp 1-8.
 345. Triclabendazole: An Intriguing Case of Co-existence of Conformational and Tautomeric Polymorphism

- S. Tothadi, B. R. Bhogala, A. R. Gorantla, T. S. Thakur, R. K. R. Jetti and G. R. Desiraju
Chem. Asian J. 7, 330-342 (2011)
346. Extending the supramolecular synthon based fragment approach (SBFA) for transferability of multipole charge density parameters to monofluorobenzoic acids and their co-crystals with isonicotinamide: Importance of C–H...O, C–H...F and F...F intermolecular regions.
V. R. Hathwar, T. S. Thakur, R. Dubey, M. S. Pavan, T. N. Guru Row and G. R. Desiraju
J. Phys. Chem., 115, 12852-12863 (2011)
347. Unusual co-crystal of isonicotinamide. The structural landscape in crystal engineering
S. Tothadi and G. R. Desiraju
Philos. Trans. R. Soc., 370, 2900-2915 (2012)
348. Polymorphs, Salts, and Cocrystals: What's in a Name?
S. Aitipamula, R. Banerjee, A. K. Bansal, K. Biradha, M. L. Cheney, A. R. Choudhury, G. R. Desiraju, A. G. Dikundwar, R. Dubey, N. Duggirala, P. P. Ghogale, S. Ghosh, P. K. Goswami, N. R. Goud, R. K. R. Jetti, P. Karpinski, P. Kaushik, D. Kumar, V. Kumar, B. Moulton, A. Mukherjee, G. Mukherjee, A. S. Myerson, V. Puri, A. Ramanan, T. Rajamannar, C. M. Reddy, N. Rodriguez-Hornedo, R. D. Rogers, T. N. G. Row, P. Sanphui, N. Shan, G. Shete, A. Singh, C. C. Sun, J. A. Swift, R. Thaimattam, T. S. Thakur, R. K. Thaper, S. P. Thomas, S. Tothadi, V. R. Vangala, N. Variankaval, P. Vishweshwar, D. R. Weyna and M. J. Zaworotko
Cryst. Growth Des., 12, 2147-2152 (2012)
349. Structural landscape of benzoic acid: using experimental crystal structures of fluorobenzoic acids as a probe
R. Dubey, M. S. Pavan and G. R. Desiraju
Chem. Commun., 48, 9020-9022 (2012)
350. Nanoindentation as a Probe for Mechanically Induced Molecular Migration in Layered Organic Donor-Acceptor Complexes
S. Varughese, M. S. R. N. Kiran, U. Ramamurty and G. R. Desiraju
Chem. Asian J. 7, 2118-2125 (2012)
351. Polymorphs and hydrates of Etoricoxib, a selective COX-2 inhibitor
P. Grobelny, A. Mukherjee and G. R. Desiraju
CrystEngComm, 14, 5785-5794 (2012)
352. Synthon modularity in 4-hydroxybenzamide– α,ω -dicarboxylic acid cocrystals
S. Tothadi and G. R. Desiraju
Cryst. Growth Des., 12, 6188-6198 (2012)

353. Nanoindentation in Crystal Engineering: Quantifying Mechanical Properties of Molecular Crystals
S. Varughese, M. S. R. N. Kiran, U. Ramamurty and G. R. Desiraju
Angew. Chem. Int. Ed., 52, 2701-2712 (2013)
354. Synthon identification in co-crystals and polymorphs with IR spectroscopy. Primary amides as a case study.
A. Mukherjee, S. Tothadi, S. Chakraborty, S. Ganguly and G. R. Desiraju
CrystEngComm. 15, 4640-4654 (2013)
355. Odd-even effect in the elastic moduli of α,ω -alkanedicarboxylic acids
M. K. Mishra, S. Varughese, U. Ramamurty and G. R. Desiraju
J. Am. Chem. Soc., 135, 8121-8124 (2013)
356. Crystal Engineering. From Molecule to Crystal
G. R. Desiraju
J. Am. Chem. Soc., 135, 9952-9967 (2013)
357. Synthon Modularity in Cocrystals of 4-Bromobenzamide with n-Alkanedicarboxylic Acids: Type-I and Type-II Halogen...Halogen Interactions
S. Tothadi, S. Joseph and G. R. Desiraju
Cryst. Growth Des., 13, 3242-3254 (2013).
358. New Solid Forms of the Anti-HIV Drug Etravirine: Salts, Cocrystals and Solubility
L. Rajput, P. Sanphui and G. R. Desiraju
Cryst. Growth Des., 13, 3681-3690 (2013).
359. Designing Ternary Cocrystals with Hydrogen Bonding and Halogen Bonding.
S. Tothadi and G. R. Desiraju
Chem. Commun. 49, 7791-7793 (2013).
360. Definition of the halogen bond (IUPAC Recommendations 2013)
G. R. Desiraju, P. S. Ho, L. Kloo, A. C. Legon, R. Marquardt, P. Metrangolo, P. Politzer, G. Resnati and K. Rissanen
Pure Appl. Chem. 85, 1711-1713 (2013).
361. Halogen bonds in some dihalogenated phenols. Applications to crystal engineering.
A. Mukherjee and G. R. Desiraju
IUCrJ, 1, 49-60 (2014).
362. Crystal Landscape in the Orcinol:4,4'-Bipyridine System: Synthon Modularity, Polymorphism and Transferability of Multipole Charge Density Parameters
R. Dubey, M. S. Pavan, T. N. Guru Row and G. R. Desiraju
IUCrJ, 1, 8-18 (2014).

363. Salt and cocrystals of sildenafil with dicarboxylic acids: Solubility and pharmacokinetic advantage of the glutarate salt
P. Sanphui, S. Tothadi, S. Ganguly and G. R. Desiraju
Mol. Pharm, 10, 4687-4697 (2014).
364. Structural landscape of the 1:1 benzoic acid–isonicotinamide cocrystal
R. Dubey and G. R. Desiraju
Chem. Commun. 50, 1181-1184 (2014).
365. Synthron transferability probed with IR spectroscopy: cytosine salts as models for salts of lamivudine
S. Chakraborty, S. Ganguly and G. R. Desiraju
CrystEngComm. 16, 4732-4741 (2014).
366. Some themes in chemical crystallography pertinent to the Indian contribution
G. R. Desiraju
J. Indian Inst. Sci. 94, 1-8 (2014).
367. Combinatorial exploration of structural landscape of acid–pyridine cocrystals
A. Mukherjee and G. R. Desiraju
Cryst. Growth Des. 14, 1475-1485 (2014).
[ACS Editors' Choice]
368. Designing ternary co-crystals with stacking interactions and weak hydrogen bonds. 4,4'-bis-Hydroxyazobenzene
S. Chakraborty, L. D. Rajput and G. R. Desiraju
Cryst. Growth Des. 14, 2571-2577 (2014).
369. Aniline–phenol recognition. From solution through supramolecular synthons to cocrystals
A. Mukherjee, K. Dixit, S. P. Sarma and G. R. Desiraju
IUCrJ 1, 228-239 (2014).
370. Solubility-Hardness Correlation in Molecular Crystals: Curcumin and Sulfathiazole Polymorphs
M. K. Mishra, P. Sanphui, U. Ramamurty and G. R. Desiraju
Cryst. Growth Des. 14, 3054-3061 (2014).
371. Obtaining synthron modularity in ternary cocrystals with hydrogen bonds and halogen bonds
S. Tothadi, P. Sanphui and G. R. Desiraju
Cryst. Growth Des. 14, 5293-5302 (2014).
372. Combinatorial Crystal Synthesis: Structural Landscape of Phloroglucinol:1,2-bis(4-pyridyl)ethylene and Phloroglucinol:Phenazine
R. Dubey and G. R. Desiraju
Angew. Chem. Int. Ed. 53, 13178-13182 (2014).

373. Halogen Bonds in Crystal Engineering: Like Hydrogen Bonds yet Different
A. Mukherjee, S. Tothadi and G. R. Desiraju
Acc. Chem. Res. 47, 2514-2524 (2014).
374. Graded IR-filters: Distinguishing between single and multipoint NO₂...I
halogen bonded supramolecular synthons (P, Q, R synthons)
S. Saha, S. Ganguly and G. R. Desiraju
Aust. J. Chem. 67, 1840-1848 (2014).
375. Studying Microstructure in Molecular Crystals with Nanoindentation: Intergrowth
Polymorphism in Felodipine.
M. K. Mishra, G. R. Desiraju, U. Ramamurty and A. D. Bond
Angew. Chem. Int. Ed. 53, 13102-13105 (2014).
376. Crystal Structure and Prediction
T. S. Thakur, R. Dubey and G. R. Desiraju
Ann. Rev. Phys. Chem. 66, 21-42 (2015).
377. IR Spectroscopy as a probe for C–H...X hydrogen bonded supramolecular
synthons
S. Saha, L. Rajput, S. Joseph, M. K. Mishra, S. Ganguly and G. R. Desiraju
CrystEngComm, 17, 1273-1290 (2015).
378. Exploring the crystal structure landscape with a heterosynthon module:
Fluorobenzoic acid:1,2-bis(4-pyridyl)ethylene 2:1 cocrystals
R. Dubey and G. R. Desiraju
Cryst. Growth Des. 15, 489-496 (2015).
379. Tuning mechanical properties of pharmaceutical crystals with multicomponent
crystals: Voriconazole as a case study
P. Sanphui, M. K. Mishra, U. Ramamurty and G. R. Desiraju
Mol. Pharm. 12, 889-897 (2015).
380. Designing elastic organic crystals: Highly flexible polyhalogenated N-
benzylideneanilines
S. Ghosh, M. K. Mishra, S. Kadambi, U. Ramamurty and G. R. Desiraju
Angew. Chem. Int. Ed. 54, 2674-2678 (2015).
381. Solid solution hardening of molecular crystals: tautomeric polymorphs of
omeprazole
M. K. Mishra, U. Ramamurty and G. R. Desiraju
J. Am. Chem. Soc., 137, 1794-1797 (2015).
382. Bimodal nanoindentation response of the (001) face in crystalline sodium
saccharin dihydrate
M. K. Mishra, U. Ramamurty and G. R. Desiraju

- Macedonian J. Chem. Chem. Engg. 34, 51-55 (2015).
383. Cocrystals of Hydrochlorothiazide: Solubility and diffusion/permeability enhancements through drug-coformer interactions
P. Sanphui, V. Kusum Devi, D. Mathew, N. Malviya, S. Ganguly and G. R. Desiraju
Mol. Pharm. 12, 1615-1622 (2015).
384. Hardness Alternation in α,ω -Alkanedicarboxylic Acids
M. K. Mishra, U. Ramamurty and G. R. Desiraju
Chem. Asian J. 10, 2176-2181 (2015).
385. Combinatorial selection of molecular conformations and supramolecular synthons in quercetin cocrystal landscapes. A route to ternary cocrystals
R. Dubey and G. R. Desiraju
IUCrJ, 2, 402-408 (2015).
386. Dual Stress and Thermally Driven Mechanical Properties of the Same Organic Crystal: 2,6-Dichlorobenzylidene-4-fluoro-3-nitroaniline
S. Ghosh, M. K. Mishra, S. Ganguly and G. R. Desiraju
J. Am. Chem. Soc., 137, 9912-9921 (2015).
387. Combinatorial crystal synthesis of ternary solids based on 2-methylresorcinol
N. A. Mir, R. Dubey, S. Tothadi and G. R. Desiraju
CrystEngComm, 17, 7866-7869 (2015).
388. Crystal chemistry and photomechanical behavior of 3,4-dimethoxycinnamic acid: Correlation between maximum yield in the solid state topochemical reaction and cooperative molecular motion
M. K. Mishra, A. Mukherjee, U. Ramamurty and G. R. Desiraju
IUCrJ, 2, 653-660 (2015).
389. Four- and five-component molecular solids. Crystal engineering strategies based on lack of structural degeneracy
N. A. Mir, R. Dubey and G. R. Desiraju
IUCrJ, 3, 96-101 (2016).
390. Quaternary cocrystals. Combinatorial synthetic strategies based on long-range synthon Aufbau modules (LSAM)
R. Dubey, N. A. Mir and G. R. Desiraju
IUCrJ, 3, 102-107 (2016).
391. New multi-component solid forms of an anti-cancer drug erlotinib: Role of auxiliary interactions in determining a preferred conformation
P. Sanphui, L. D. Rajput, S. P. Gopi and G. R. Desiraju
Acta Crystallogr., Sect. B, 72, 291-300 (2016).

392. Using structural modularity in cocrystals to engineer properties: elasticity
S. Saha and G. R. Desiraju
Chem. Commun. 52, 7676-7679 (2016).
393. Cocrystal and salt forms of furosemide: solubility and diffusion variations
M. Banik, S. P. Gopi, S. Ganguly and G. R. Desiraju
Cryst. Growth Des. 16, 5418-5428 (2016).
394. Use of the term "Crystal Engineering" in the regulatory and patent literature of pharmaceutical solid forms. Some comments.
G. R. Desiraju and A. Nangia
Cryst. Growth Des. 16, 5585-5587 (2016).
395. Mechanical property design of molecular solids
M. K. Mishra, U. Ramamurty and G. R. Desiraju
Curr. Opin. Solid State & Materials Science 20, 361-370 (2016).
396. A drug-drug salt hydrate of norfloxacin and sulfathiazole: Enhancement of in vitro biological properties via improved physicochemical properties
S. P. Gopi, S. Ganguly and G. R. Desiraju
Mol. Pharm. 13, 3590-3594 (2016).
397. Looking at aniline-phenol recognition in molecular crystals: an evergreen endeavour
A. Sood and G. R. Desiraju
Struct. Chem. 28, 173-199 (2016).
398. Hand-Twisted Helical Crystals as an Example of Third Generation Crystal Engineering.
S. Saha and G. R. Desiraju
J. Am. Chem. Soc. 139, 1975-1983 (2017).
399. New Cocrystals of Hydrochlorothiazide: Optimizing Solubility and Membrane Diffusivity
S. P. Gopi, M. Banik and G. R. Desiraju
Cryst. Growth Des. 17, 308-316 (2017).
400. Salts and Cocrystals of Antidiabetic Drugs, Gliclazide, Tolbutamide and Glipizide: Solubility Enhancements through Drug-Coformer Interactions
A. Samie and G. R. Desiraju
Cryst. Growth Des. 17, 2406-2417 (2017).
401. σ -hole and π -hole Synthons Mimicry in Third Generation Crystal Engineering. Design of Elastic Crystals
S. Saha and G. R. Desiraju
Chem. Eur. J. 23, 4936-4943 (2017).

402. Exploring the salt-cocrystal continuum with solid-state NMR using natural abundance samples: implications for crystal engineering
L. Rajput, M. Banik, J. R. Yarava, S. Joseph, M. K. Pandey, Y. Nishiyama and G. R. Desiraju
IUCrJ, 4, 466-475 (2017).
403. Hand-twisted helical crystals based solely on hydrogen bonding
S. Saha and G. R. Desiraju
Chem. Commun. 53, 6371-6374 (2017).
404. Approaches to crystal structure landscape exploration
G. R. Desiraju
Acta Crystallogr. Sect. B, 73, 775-778 (2017).
405. Six-component Molecular Solids, $ABC[D_{1-(x+y)}E_xF_y]_2$
M. Paul, S. Chakraborty and G. R. Desiraju
J. Am. Chem. Soc. 140, 2309-2315 (2018).
406. Exploring the structural landscape with 'partial' fluoro-substitution as a probe
S. Chakraborty and G. R. Desiraju
CrystEngComm, 20, 2793-2805 (2018).
407. Probing the crystal structure landscape by doping: 4-bromo, 4-chloro and 4-methylcinnamic acids
S. Chakraborty, S. Joseph and G. R. Desiraju
Angew. Chem. Int. Ed, 57, 9279-9283 (2018).
408. C–H...F hydrogen bonds in solid solutions of benzoic acid and 4-fluorobenzoic acid
S. Chakraborty and G. R. Desiraju
Cryst. Growth Des., 18, 3607-3615 (2018).
409. Acid...Amide Supramolecular Synthons in Cocrystals: From Spectroscopic Detection to Property Engineering
S. Saha and G. R. Desiraju
J. Am. Chem. Soc. 140, 6361-6373 (2018).
410. Trimorphs of 4-bromophenyl 4-bromobenzoate. Elastic, brittle, plastic.
S. Saha and G. R. Desiraju
Chem. Comm. 54, 6348-6351 (2018).
411. From Molecules to Interactions to Crystal Engineering: Mechanical Properties of Organic Solids
S. Saha, M. K. Mishra, C. M. Reddy and G. R. Desiraju
Acc. Chem. Res. 51, 2957-2967 (2018).

412. Crystal Engineering. An Outlook for the Future
A. K. Nangia and G. R. Desiraju
Angew. Chem. Int. Ed, 58, 4100-4107 (2019).
413. Science and Society. What do they owe each other?
G. R. Desiraju
Angew. Chem. Int. Ed, 58, 3232-3234 (2019).
414. From a Binary to a Quaternary Cocrystal: An Unusual Supramolecular Synthon
M. Paul and G. R. Desiraju
Angew. Chem. Int. Ed, 58, 12027-12031 (2019).
415. Strategy and Methodology in the Synthesis of Multicomponent Molecular Solids:
The Quest for Higher Cocrystals
N. A. Mir, R. Dubey and G. R. Desiraju
Acc. Chem. Res., 52, 2210-2220 (2019).
416. Strong and Weak Hydrogen Bonds in Protein-Ligand Recognition
G. Bulusu and G. R. Desiraju
J. Ind. Inst, Sci., 100, 31-41 (2020).
417. Drug-Drug Binary Solids of Nitrofurantoin and Trimethoprim: Crystal Engineering
and Pharmaceutical Properties.
D. K. Maity, R. K. Paul and G. R. Desiraju
Mol. Pharm., 17, 4435-4442 (2020)
418. Quaternary and Quinary Solids Based on Structural Inequivalence and
Combinatorial Approaches: 2-Nitroresorcinol and 4,6-Dichlororesorcinol
M. Rajkumar and G. R. Desiraju.
IUCrJ, 8, 178-185 (2021)
419. Synthetic Approaches to Halogen Bonded Ternary Cocrystals
H. Jain, D. Sutradhar, S. Roy and G. R. Desiraju
Angew. Chem. Int. Ed, 60, 12841-12846 (2021).
420. Cocrystal Hydrate of Bandrowski's Base and Clotrimazole: A Prospective
Ingredient for Hair Dye Formulations
CrystEngComm, 23, 5421-5424 (2021).
421. Heterosynthons, Solid Form Design and Enhanced Drug Bioavailability
A. K. Nangia and G. R. Desiraju
Angew. Chem. Int. Ed, 61, e202207484 (2022).
422. Synthetic Strategies toward Higher Cocrystals of some Resorcinols
S. Roy, R. Gaur, M. Paul, M. Rajkumar and G. R. Desiraju
Cryst. Growth Des., 22, 7578-7589 (2022).

423. Definition of the Pnictogen Bond (IUPAC Recommendations 2023)
G. Resnati, D. L. Bryce, G. R. Desiraju, A. Frontera, I. Krossing, A. C. Legon, P. Metrangolo, F. Nicotra, K. Rissanen, S. Scheiner and G. Terraneo
Pure Appl. Chem., 96, 135-145 (2024).
424. Pharmaceutical Solid Form Screening and Selection. Which Form Emerges?
P. Chappa, R. N. Jenjeti, J. Klijn, S. Mittapalli, A. Pichler and G. R. Desiraju
Cryst. Growth Des., 25, 4783-4794 (2025).
425. Is a Data Deluge Dampening our Idea Generation Capability?
G. R. Desiraju and D. Bhattacharya
The Innovation, 6, 100883 (2025).
426. Crystal Clear: Engineering Complexity
G. R. Desiraju
IUCrJ, 13, 527-540 (2026).
-