Gautam R Desiraju

List of Publications by Year
in descending order

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302 papers	43,476 citations	4388 86 h-index	2280 200 g-index
322 all docs	322 docs citations	322 times ranked	21660 citing authors

#	Article	IF	Citations
1	Supramolecular Synthons in Crystal Engineeringâ€”A New Organic Synthesis. Angewandte Chemie International Edition in English, 1995, 34, 2311-2327.	4.4	4,495
2	Hydrogen Bridges in Crystal Engineering:â€‰ Interactions without Borders. Accounts of Chemical Research, 2002, 35, 565-573.	15.6	1,916
3	The Câ^'HÂ·Â·Â·O Hydrogen Bond:â€‰ Structural Implications and Supramolecular Design. Accounts of Chemical Research, 1996, 29, 441-449.	15.6	1,802
4	Definition of the halogen bond (IUPAC Recommendations 2013). Pure and Applied Chemistry, 2013, 85, 1711-1713.	1.9	1,554
5	Definition of the hydrogen bond (IUPAC Recommendations 2011). Pure and Applied Chemistry, 2011, 83, 1637-1641.	1.9	1,449
6	The C-H.cntdot..cntdot..cntdot.O hydrogen bond in crystals: what is it?. Accounts of Chemical Research, 1991, 24, 290-296.	15.6	1,327
7	Crystal Engineering: A Holistic View. Angewandte Chemie - International Edition, 2007, 46, 8342-8356.	13.8	1,285
8	Crystal Engineering: From Molecule to Crystal. Journal of the American Chemical Society, 2013, 135, 9952-9967.	13.7	1,239
9	Crystal Engineering and Organometallic Architecture. Chemical Reviews, 1998, 98, 1375-1406.	47.7	1,169
10	Defining the hydrogen bond: An account (IUPAC Technical Report). Pure and Applied Chemistry, 2011, 83, 1619-1636.	1.9	856
11	The nature of halogen.cntdot..cntdot..cntdot.halogen interactions: are short halogen contacts due to specific attractive forces or due to close packing of nonspherical atoms?. Journal of the American Chemical Society, 1989, 111, 8725-8726.	13.7	771
12	Polymorphs, Salts, and Cocrystals: Whatâ€™s in a Name?. Crystal Growth and Design, 2012, 12, 2147-2152.	3.0	767
13	Halogen Bonds in Crystal Engineering: Like Hydrogen Bonds yet Different. Accounts of Chemical Research, 2014, 47, 2514-2524.	15.6	741
14	Câ^'HÂ·Â·Â·F Interactions in the Crystal Structures of Some Fluorobenzenes. Journal of the American Chemical Society, 1998, 120, 8702-8710.	13.7	689
15	Chemistry beyond the molecule. Nature, 2001, 412, 397-400.	27.8	555
16	Supramolekulare Synthone fÃ¼r das Kristallâ€Engineering â€•eine neue organische Synthese. Angewandte Chemie, 1995, 107, 2541-2558.	2.0	537
17	Câ€“Hâ‹¯O and other weak hydrogen bonds. From crystal engineering to virtual screening. Chemical Communications, 2005, , 2995.	4.1	492
18	A Bond by Any Other Name. Angewandte Chemie - International Edition, 2011, 50, 52-59.	13.8	487

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19	The role of Cl.cntdot..cntdot..cntdot.Cl and C-H.cntdot..cntdot..cntdot.O interactions in the crystal engineering of 4-.ANG. short-axis structures. Accounts of Chemical Research, 1986, 19, 222-228.	15.6	420
20	Isostructurality, Polymorphism and Mechanical Properties of Some Hexahalogenated Benzenes: The Nature of Halogenâ‹…â‹…â‹…Halogen Interactions. Chemistry - A European Journal, 2006, 12, 2222-2234.	3.3	383
21	Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125.	1.8	371
22	Towards crystal structure prediction of complex organic compounds â€“ a report on the fifth blind test. Acta Crystallographica Section B: Structural Science, 2011, 67, 535-551.	1.8	358
23	From Molecules to Interactions to Crystal Engineering: Mechanical Properties of Organic Solids. Accounts of Chemical Research, 2018, 51, 2957-2967.	15.6	358
24	Definition of the chalcogen bond (IUPAC Recommendations 2019). Pure and Applied Chemistry, 2019, 91, 1889-1892.	1.9	322
25	From molecular to crystal structure; polynuclear aromatic hydrocarbons. Journal of the Chemical Society Chemical Communications, 1989, , 621.	2.0	319
26	Hydrogen Bonding in Organometallic Crystals. 6.â€Xâˆ’H---M Hydrogen Bonds and M---(Hâˆ’X) Pseudo-Agostic Bonds. Organometallics, 1997, 16, 1846-1856.	2.3	309
27	Crystal and co-crystal. CrystEngComm, 2003, 5, 466.	2.6	304
28	The nature of halogen ? halogen interactions and the crystal structure of 1,3,5,7-tetraiodoadamantane. Journal of the Chemical Society Perkin Transactions II, 1994, , 2353.	0.9	294
29	Nanoindentation in Crystal Engineering: Quantifying Mechanical Properties of Molecular Crystals. Angewandte Chemie - International Edition, 2013, 52, 2701-2712.	13.8	290
30	Hydrogen Bonding in Organometallic Crystals. 2. C-H.cntdot. .cntdot. .cntdot.O Hydrogen Bonds in Bridged and Terminal First-Row Metal Carbonyls. Journal of the American Chemical Society, 1995, 117, 3156-3166.	13.7	265
31	On the presence of multiple molecules in the crystal asymmetric unit (Zâ€² > 1). CrystEngComm, 2007, 9, 91-92.	2.6	248
32	Cubanecarboxylic Acids. Crystal Engineering Considerations and the Role of Câˆ’HÂ·Â·Â·O Hydrogen Bonds in Determining Oâˆ’HÂ·Â·Â·O Networks. Journal of the American Chemical Society, 1999, 121, 1936-1944.	13.7	246
33	Crystal engineering. From molecules to materials. Journal of Molecular Structure, 2003, 656, 5-15.	3.6	240
34	Nï£¿Hâ€¦O, Oï£¿Hâ€¦O, and Cï£¿Hâ€¦O hydrogen bonds in protein-ligand complexes: Strong and weak interactions in molecular recognition. Proteins: Structure, Function and Bioinformatics, 2003, 54, 247-259.	2.6	240
35	Innovation in crystal engineeringÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂÂ. CrystEngComm, 2002, 4, 500-509.	2.6	235
36	On the Polymorphism of Aspirin: Crystalline Aspirin as Intergrowths of Two â€œPolymorphicâ€•Domains. Angewandte Chemie - International Edition, 2007, 46, 618-622.	13.8	233

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37	Cryptic crystallography. Nature Materials, 2002, 1, 77-79.	27.5	230
38	Structureâ^'Property Correlations in Bending and Brittle Organic Crystals. Crystal Growth and Design, 2006, 6, 2720-2731.	3.0	228
39	Saccharin Salts of Active Pharmaceutical Ingredients, Their Crystal Structures, and Increased Water Solubilities. Crystal Growth and Design, 2005, 5, 2299-2309.	3.0	222
40	Cocrystals of Hydrochlorothiazide: Solubility and Diffusion/Permeability Enhancements through Drugâ€"Coformer Interactions. Molecular Pharmaceutics, 2015, 12, 1615-1622.	4.6	218
41	Structural basis for bending of organic crystals. Chemical Communications, 2005, , 3945.	4.1	214
42	Designing Elastic Organic Crystals: Highly Flexible Polyhalogenated Nâ€Benzylideneanilines. Angewandte Chemie - International Edition, 2015, 54, 2674-2678.	13.8	213
43	Crystal Engineering of Some 2,4,6-Triaryloxy-1,3,5-triazines:â€‰ Octupolar Nonlinear Materials. Journal of the American Chemical Society, 1998, 120, 2563-2577.	13.7	211
44	Hydrogen bonds and other intermolecular interactions in organometallic crystalsâ€Šâ€. Dalton Transactions RSC, 2000, , 3745-3751.	2.3	208
45	Strong and weak hydrogen bonds in the protein-ligand interface. Proteins: Structure, Function and Bioinformatics, 2007, 67, 128-141.	2.6	201
46	Crystal Engineering of Hand-Twisted Helical Crystals. Journal of the American Chemical Society, 2017, 139, 1975-1983.	13.7	199
47	Evidence for O-H.cntdot..cntdot..cntdot.C and N-H.cntdot..cntdot..cntdot.C hydrogen bonding in crystalline alkynes, alkenes, and aromatics. Journal of the American Chemical Society, 1993, 115, 4868-4869.	13.7	195
48	Pseudopolymorphism: occurrences of hydrogen bonding organic solvents in molecular crystals. Chemical Communications, 1999, , 605-606.	4.1	195
49	Crystal engineering: A brief overview. Journal of Chemical Sciences, 2010, 122, 667-675.	1.5	186
50	Halogen bonds in some dihalogenated phenols: applications to crystal engineering. IUCrJ, 2014, 1, 49-60.	2.2	184
51	Cyano-halogen interactions and their role in the crystal structures of the 4-halobenzonitriles. Journal of the American Chemical Society, 1989, 111, 6757-6764.	13.7	174
52	Supramolecular Synthons in Crystal Engineering. 4. Structure Simplification and Synthon Interchangeability in Some Organic Diamondoid Solids1. Journal of the American Chemical Society, 1996, 118, 4090-4093.	13.7	174
53	Crystal Engineering: An Outlook for the Future. Angewandte Chemie - International Edition, 2019, 58, 4100-4107.	13.8	171
54	Interaction anisotropy and shear instability of aspirin polymorphs established by nanoindentation. Chemical Science, 2011, 2, 2236.	7.4	151

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55	Reflections on the Hydrogen Bond in Crystal Engineering. Crystal Growth and Design, 2011, 11, 896-898.	3.0	150
56	Co-Crystals of the Anti-HIV Drugs Lamivudine and Zidovudine. Crystal Growth and Design, 2009, 9, 951-957.	3.0	148
57	Crystal Engineering and Correspondence between Molecular and Crystal Structures. Are 2- and 3-Aminophenols Anomalous?. Journal of the American Chemical Society, 1997, 119, 3477-3480.	13.7	146
58	Drug-drug co-crystals: Temperature-dependent proton mobility in the molecular complex of isoniazid with 4-aminosalicylic acid. CrystEngComm, 2011, 13, 4358.	2.6	146
59	Dual Stress and Thermally Driven Mechanical Properties of the Same Organic Crystal: 2,6-Dichlorobenzylidene-4-fluoro-3-nitroaniline. Journal of the American Chemical Society, 2015, 137, 9912-9921.	13.7	140
60	On the Polymorphism of Aspirin. Angewandte Chemie - International Edition, 2007, 46, 615-617.	13.8	139
61	Polymorphism: The Same and Not Quite the Same. Crystal Growth and Design, 2008, 8, 3-5.	3.0	139
62	First Neutron Diffraction Analysis of an Oâ^'HÂ·Â·Â·Ï€ Hydrogen Bond:Â 2-Ethynyladamantan-2-ol. Journal of the American Chemical Society, 1996, 118, 4081-4084.	13.7	137
63	Hydration in organic crystals: prediction from molecular structure. Journal of the Chemical Society Chemical Communications, 1991, , 426.	2.0	136
64	Salt and Cocrystals of Sildenafil with Dicarboxylic Acids: Solubility and Pharmacokinetic Advantage of the Glutarate Salt. Molecular Pharmaceutics, 2013, 10, 4687-4697.	4.6	131
65	Mechanical Anisotropy in Crystalline Saccharin: Nanoindentation Studies. Crystal Growth and Design, 2010, 10, 4650-4655.	3.0	130
66	Polymorphism of 1,3,5-Trinitrobenzene Induced by a Trisindane Additive. Angewandte Chemie - International Edition, 2004, 43, 1149-1155.	13.8	125
67	Synthon polymorphism and pseudopolymorphism in co-crystals. The 4,4â€²-bipyridineâ€“4-hydroxybenzoic acid structural landscape. Chemical Communications, 2011, 47, 4090.	4.1	124
68	Synthon Modularity in Cocrystals of 4-Bromobenzamide with n-Alkanedicarboxylic Acids: Type I and Type II HalogenÂ·Â·Â·Halogen Interactions. Crystal Growth and Design, 2013, 13, 3242-3254.	3.0	116
69	The Supramolecular Synthon Approach to Crystal Structure Prediction. Crystal Growth and Design, 2002, 2, 93-100.	3.0	110
70	Oddâ€“Even Effect in the Elastic Modulii of Î±,Ï‰-Alkanedicarboxylic Acids. Journal of the American Chemical Society, 2013, 135, 8121-8124.	13.7	109
71	Crystal engineering: solid state supramolecular synthesis. Current Opinion in Solid State and Materials Science, 1997, 2, 451-454.	11.5	108
72	Synthon evolution and unit cell evolution during crystallisation. A study of symmetry-independent molecules (Zâ€² > 1) in crystals of some hydroxy compounds. Chemical Communications, 2006, , 555-557.	4.1	107

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73	Designing ternary cocrystals with hydrogen bonds and halogen bonds. Chemical Communications, 2013, 49, 7791.	4.1	107
74	Tuning Mechanical Properties of Pharmaceutical Crystals with Multicomponent Crystals: Voriconazole as a Case Study. Molecular Pharmaceutics, 2015, 12, 889-897.	4.6	107
75	Hydrogen Bonding in Organometallic Crystals. 1. From Carboxylic Acids and Alcohols to Carbonyl Complexes. Organometallics, 1994, 13, 3532-3543.	2.3	105
76	Cocrystal and Salt Forms of Furosemide: Solubility and Diffusion Variations. Crystal Growth and Design, 2016, 16, 5418-5428.	3.0	105
77	Hydrogen bonding in organometallic crystals â€" a survey. Journal of Organometallic Chemistry, 1997, 548, 33-43.	1.8	103
78	Obtaining Synthon Modularity in Ternary Cocrystals with Hydrogen Bonds and Halogen Bonds. Crystal Growth and Design, 2014, 14, 5293-5302.	3.0	102
79	Inclusion Compounds of Tetrakis(4-nitrophenyl)methane:Â Câ^'HÂ·Â·Â·O Networks, Pseudopolymorphism, and Structural Transformations. Journal of the American Chemical Society, 2001, 123, 4432-4445.	13.7	101
80	AcidÂ·Â·Â·Amide Supramolecular Synthon in Cocrystals: From Spectroscopic Detection to Property Engineering. Journal of the American Chemical Society, 2018, 140, 6361-6373.	13.7	101
81	Synthon identification in co-crystals and polymorphs with IR spectroscopy. Primary amides as a case study. CrystEngComm, 2013, 15, 4640.	2.6	96
82	Câ€"Hâ‹¯Fâ€"C hydrogen bonding in 1,2,3,5-tetrafluorobenzene and other fluoroaromatic compounds and the crystal structure of alloxan revisited. CrystEngComm, 2010, 12, 2079.	2.6	95
83	Correspondence between Molecular Functionality and Crystal Structures. Supramolecular Chemistry of a Family of Homologated Aminophenols. Journal of the American Chemical Society, 2003, 125, 14495-14509.	13.7	93
84	Polymorphs, Pseudopolymorphs, and Co-Crystals of Orcinol: Exploring the Structural Landscape with High Throughput Crystallography. Crystal Growth and Design, 2011, 11, 2637-2653.	3.0	92
85	Diamondoid and Square Grid Networks in the Same Structure. Crystal Engineering with the IodoÂ·Â·Â·Nitro Supramolecular Synthon. Crystal Growth and Design, 2001, 1, 103-106.	3.0	88
86	Sorting of polymorphs based on mechanical properties. Trimorphs of 6-chloro-2,4-dinitroaniline. Chemical Communications, 2005, , 2439.	4.1	88
87	Counterpoint:â€‰ What's in a Name?. Crystal Growth and Design, 2004, 4, 1089-1090.	3.0	87
88	Shape and size mimicry in the design of ternary molecular solids: towards a robust strategy for crystal engineering. Chemical Communications, 2011, 47, 12080.	4.1	87
89	A Drugâ€"Drug Salt Hydrate of Norfloxacin and Sulfathiazole: Enhancement of in Vitro Biological Properties via Improved Physicochemical Properties. Molecular Pharmaceutics, 2016, 13, 3590-3594.	4.6	86
90	Crystal Structure Prediction of Aminols:Â Advantages of a Supramolecular Synthon Approach with Experimental Structures. Journal of the American Chemical Society, 2005, 127, 10545-10559.	13.7	85

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91	Strategy and Methodology in the Synthesis of Multicomponent Molecular Solids: The Quest for Higher Cocrystals. Accounts of Chemical Research, 2019, 52, 2210-2220.	15.6	85
92	Ïƒâ€Hole and Ï€â€Hole Synthon Mimicry in Thirdâ€Generation Crystal Engineering: Design of Elastic Crystals. Chemistry - A European Journal, 2017, 23, 4936-4943.	3.3	84
93	Nature and strength of Câ€“Hâ‹¯O interactions involving formyl hydrogen atoms: computational and experimental studies of small aldehydes. Physical Chemistry Chemical Physics, 2011, 13, 14076.	2.8	83
94	Using structural modularity in cocrystals to engineer properties: elasticity. Chemical Communications, 2016, 52, 7676-7679.	4.1	83
95	Theoretical investigation of Câ€“Hâ‹¯M interactions in organometallic complexes: A natural bond orbital (NBO) study. Computational and Theoretical Chemistry, 2007, 810, 143-154.	1.5	82
96	Combinatorial Exploration of the Structural Landscape of Acidâ€“Pyridine Cocrystals. Crystal Growth and Design, 2014, 14, 1375-1385.	3.0	82
97	Supramolecular Synthons in Crystal Engineering. 3. Solid State Architecture and Synthon Robustness in Some 2,3-Dicyano-5,6-dichloro-1,4-dialkoxybenzenes1. Journal of the American Chemical Society, 1996, 118, 4085-4089.	13.7	81
98	Solid Solution Hardening of Molecular Crystals: Tautomeric Polymorphs of Omeprazole. Journal of the American Chemical Society, 2015, 137, 1794-1797.	13.7	81
99	Câ€“H â‹¯ N mediated hexagonal network in the crystal structure of the 1 : 1 molecular complex 1,3,5-tricyanobenzeneâ€“hexamethylbenzene. Journal of the Chemical Society Chemical Communications, 1993, , 663-664.	2.0	80
100	Searching for a Polymorph: Second Crystal Form of 6-Amino-2-Phenylsulfonylimino-1,2-Dihydropyridine. Angewandte Chemie - International Edition, 2003, 42, 1963-1967.	13.8	79
101	Solubility-Hardness Correlation in Molecular Crystals: Curcumin and Sulfathiazole Polymorphs. Crystal Growth and Design, 2014, 14, 3054-3061.	3.0	79
102	Mechanical property design of molecular solids. Current Opinion in Solid State and Materials Science, 2016, 20, 361-370.	11.5	78
103	The chloro-methyl exchange rule and its violations in the packing of organic molecular solids. Journal of Chemical Sciences, 1986, 96, 599-605.	1.5	77
104	Six-Component Molecular Solids: ABC[D_{1â€“(x+y)}E_xF_y]₂. Journal of the American Chemical Society, 2018, 140, 2309-2315.	13.7	77
105	Crystal Structure Prediction of a Co-Crystal Using a Supramolecular Synthon Approach: 2-Methylbenzoic Acidâˆ’2-Amino-4-methylpyrimidine. Crystal Growth and Design, 2008, 8, 4031-4044.	3.0	75
106	Long-range synthon Aufbau modules (LSAM) in crystal structures: systematic changes in C₆H_{6âˆ’n}F_n (0 â‰¤ n â‰¤ 6) fluorobenzenes. CrystEngComm, 2010, 12, 817-833.	2.6	75
107	Molecular Complexation as a Design Tool in the Crystal Engineering of Noncentrosymmetric Structures. Ideal Orientation of Chromophores Linked by Oâˆ’HÂ·Â·Â·O and Câˆ’HÂ·Â·Â·O Hydrogen Bonds for Nonlinear Optics. Chemistry of Materials, 2001, 13, 1473-1479.	6.7	74
108	Structure-Based Design of DevR Inhibitor Active against Nonreplicating Mycobacterium tuberculosis. Journal of Medicinal Chemistry, 2009, 52, 6324-6334.	6.4	74

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109	Studying Microstructure in Molecular Crystals With Nanoindentation: Intergrowth Polymorphism in Felodipine. Angewandte Chemie - International Edition, 2014, 53, 13102-13105.	13.8	72
110	New Solid State Forms of the Anti-HIV Drug Efavirenz. Conformational Flexibility and High Zâ€² Issues. Crystal Growth and Design, 2010, 10, 3191-3202.	3.0	71
111	Stereoelectronic Effects of Substituent Groups in the Solid State. Crystal Chemistry of Some Cubanecarboxylic and Phenylpropiolic Acids. Crystal Growth and Design, 2003, 3, 675-681.	3.0	69
112	Using Water as a Design Element in Crystal Engineering. Hostâ^'Guest Compounds of Hydrated 3,5-Dihydroxybenzoic Acid. Crystal Growth and Design, 2010, 10, 4184-4196.	3.0	68
113	New Cocrystals of Hydrochlorothiazide: Optimizing Solubility and Membrane Diffusivity. Crystal Growth and Design, 2017, 17, 308-316.	3.0	68
114	New Solid Forms of the Anti-HIV Drug Etravirine: Salts, Cocrystals, and Solubility. Crystal Growth and Design, 2013, 13, 3681-3690.	3.0	67
115	Organic Chlorine as a Hydrogen-Bridge Acceptor: Evidence for the Existence of Intramolecular Oï¿Hâ‹…â‹…â‹…Clï¿C Interactions in Somegem-Alkynols. Chemistry - A European Journal, 2004, 10, 3373-3383.	3.3	65
116	Transferability of Multipole Charge Density Parameters for Supramolecular Synthons: A New Tool for Quantitative Crystal Engineering. Crystal Growth and Design, 2011, 11, 616-623.	3.0	65
117	Designing Elastic Organic Crystals: Highly Flexible Polyhalogenated Nâ€Benzylideneanilines. Angewandte Chemie, 2015, 127, 2712-2716.	2.0	65
118	Crystal Structure and Prediction. Annual Review of Physical Chemistry, 2015, 66, 21-42.	10.8	65
119	The use of mixed crystals for engineering organic solid-state reactions: application to benzylbenzylidenecyclopentanones. Journal of the American Chemical Society, 1984, 106, 3606-3609.	13.7	63
120	Intermolecular atomâ€“atom bonds in crystals â€“ a chemical perspective. IUCrJ, 2015, 2, 159-160.	2.2	63
121	Hydrogen Bonding in Organometallic Crystals. 3.1Transition-Metal Complexes Containing Amido Groups. Organometallics, 1996, 15, 1284-1295.	2.3	62
122	Topological Equivalences between Organic and Coordination Polymer Crystal Structures:â€‰ An Organic Ladder Formed with Three-Connected Molecular and Supramolecular Synthons. Organic Letters, 2002, 4, 921-924.	4.6	61
123	Shape and Size Effects in the Crystal Structures of Complexes of 1,3,5-Trinitrobenzene with some Trigonal Donors: The Benzeneâ€“Thiophene Exchange Rule. Tetrahedron, 2000, 56, 6721-6728.	1.9	60
124	Exploring the saltâ€“cocrystal continuum with solid-state NMR using natural-abundance samples: implications for crystal engineering. IUCrJ, 2017, 4, 466-475.	2.2	60
125	Conversion in the solid state of the yellow to the red form of 2-(4'-methoxyphenyl)-1,4-benzoquinone. X-ray crystal structures and anisotropy of the rearrangement. Journal of the American Chemical Society, 1977, 99, 1594-1601.	13.7	58
126	3-(3',5'-Dinitrophenyl)-4-(2',5'-dimethoxyphenyl)cyclobutane-1,2-dicarboxylic Acid: Engineered Topochemical Synthesis and Molecular and Supramolecular Properties. Chemistry of Materials, 1994, 6, 1282-1292.	6.7	58

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127	Hydrogen Bonding in Organometallic Crystals. 4.â€Mâ^'H-Â-Â-O Hydrogen-Bonding Interactions. Organometallics, 1996, 15, 2692-2699.	2.3	57
128	Extending the Supramolecular Synthon Based Fragment Approach (SBFA) for Transferability of Multipole Charge Density Parameters to Monofluorobenzoic Acids and their Cocrystals with Isonicotinamide: Importance of Câ€"HÂ·Â·Â·O, Câ€"HÂ·Â·Â·F, and FÂ·Â·Â·F Intermolecular Regions. Journal of Physical Chemistry A, 2011, 115, 12852-12863.	2.5	57
129	Four- and five-component molecular solids: crystal engineering strategies based on structural inequivalence. IUCrJ, 2016, 3, 96-101.	2.2	57
130	Effects of the substituent on the formation of dimers and catemers in phenylpyruvic acids. CrystEngComm, 2006, 8, 674.	2.6	55
131	Solvates of Sildenafil Saccharinate. A New Host Material. Crystal Growth and Design, 2006, 6, 1468-1478.	3.0	55
132	Crystal chemistry and photomechanical behavior of 3,4-dimethoxycinnamic acid: correlation between maximum yield in the solid-state topochemical reaction and cooperative molecular motion. IUCrJ, 2015, 2, 653-660.	2.2	55
133	Structural mimicry and the photoreactivity of organic solids. Journal of the Chemical Society Chemical Communications, 1983, , 1443.	2.0	54
134	Effect of dehydration on the mechanical properties of sodium saccharin dihydrate probed with nanoindentation. CrystEngComm, 2012, 14, 2489-2493.	2.6	54
135	Trimorphs of 4-bromophenyl 4-bromobenzoate. Elastic, brittle, plastic. Chemical Communications, 2018, 54, 6348-6351.	4.1	54
136	Supramolecular equivalence of halogen, ethynyl and hydroxy groups. A comparison of the crystal structures of some 4-substituted anilines. CrystEngComm, 2003, 5, 248.	2.6	53
137	Dianiline-Diphenol Molecular Complexes Based on Supraminol Recognition. Crystal Growth and Design, 2005, 5, 99-104.	3.0	53
138	Halogen Bonding and Structural Modularity in 2,3,4- and 3,4,5-Trichlorophenol. Crystal Growth and Design, 2011, 11, 3735-3739.	3.0	53
139	Supramolecular synthons mediated by weak hydrogen bonding: forming linear molecular arrays via Cî€,Câ€"HÂ·Â·Â·Nî€,C and Cî€,Câ€"HÂ·Â·Â·O2N recognition. New Journal of Chemistry, 1998, 22, 1307-1309.	2.8	52
140	Five New Pseudopolymorphs of sym-Trinitrobenzene. Crystal Growth and Design, 2003, 3, 1033-1040.	3.0	52
141	Anilineâ€"phenol recognition: from solution through supramolecular synthons to cocrystals. IUCrJ, 2014, 1, 228-239.	2.2	52
142	A hand-twisted helical crystal based solely on hydrogen bonding. Chemical Communications, 2017, 53, 6371-6374.	4.1	52
143	Area correction of multi-atomâ€"acceptor hydrogen bond frequency distributions. Chemical Communications, 2001, , 703-704.	4.1	51
144	Structural landscape of benzoic acid: using experimental crystal structures of fluorobenzoic acids as a probe. Chemical Communications, 2012, 48, 9020.	4.1	51

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145	Synthon Robustness and Solid-State Architecture in Substitutedgem-Alkynols. Crystal Growth and Design, 2006, 6, 999-1009.	3.0	49
146	Synthon Modularity in 4-Hydroxybenzamideâ€“Dicarboxylic Acid Cocrystals. Crystal Growth and Design, 2012, 12, 6188-6198.	3.0	49
147	Strong and weak hydrogen bonds in drug-DNA complexes: A statistical analysis. Journal of Biosciences, 2007, 32, 677-691.	1.1	48
148	Designing Ternary Co-crystals with Stacking Interactions and Weak Hydrogen Bonds. 4,4â€²-Bis-hydroxyazobenzene. Crystal Growth and Design, 2014, 14, 2571-2577.	3.0	48
149	Database analysis of crystal-structure-determining interactions involving sulphur: implications for the design of organic metals. Journal of Materials Chemistry, 1991, 1, 201.	6.7	47
150	Unusual co-crystal of isonicotinamide: the structural landscape in crystal engineering. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2012, 370, 2900-2915.	3.4	47
151	Crystal Engineering of Primary Cubanecarboxamides. Repetitive Formation of an Unexpected Nâ^'HÂ·Â·Â·O Hydrogen-Bonded Network. Journal of Organic Chemistry, 2001, 66, 1621-1626.	3.2	45
152	Co-crystal formation and the determination of absolute configuration. CrystEngComm, 2008, 10, 1747.	2.6	45
153	Nanoindentation as a Probe for Mechanicallyâ€Induced Molecular Migration in Layered Organic Donorâ€“Acceptor Complexes. Chemistry - an Asian Journal, 2012, 7, 2118-2125.	3.3	45
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