Electronic Supplementary Material for CrystEngComm

Supplementary Materials

Table S1: Additional high pressure structures mined from the CSD using the search conditions: high pressure (≥ 0.1 GPa), room temperature, only organic compounds with at least one H or D atom, R-factor > 10%, no disorder, must have 3D coordinates. The CSD refcodes are given along with the pressure each crystal structure was collected at, the year of the publication and the first author listed in the publication. The data in the original set of compression studies was also removed to avoid duplication.

CSD Refcodes	No. of CIFs	Compound	Pressure(s) (GPa)	Reference
ACETAC09	1	Acetic Acid	0.46	Dawson, 2004
BENZEN04, 11	2	Benzene	2.5, 0.7	Fourme, 1971, Budzianowski, 2006
BISMEV04	1	Piracetam	0.4	Pulham, 2005
DATREV01	1	bis(Ethylenedithio)-tetrathiafulvalene tri-iodide	0.95	Molchanov, 1986
DCLMET11, 12	2	Dichloromethane	0.7	Podsiadlo, 2005
FACRIK03, 04	2	1,3-Cyclohexanedione	1.14,1.9	Katrusiak, 1990
FIGYID01	1	Cyclopropylamine	1.2	Lozano-Casal, 2005
GLYCIN36, 41, 44-47, 50, 61, 65-68	12	Glycine	0.95, 7.1, 5.1, 4.38, 3.63, 3.12, 1.39, 6.47, 0.5, 1.3, 1.9, 4.3	Boldyreva, 2005 & Dawson, 2005
GUHHAS01-03	3	Chlorotrimethylsilane	0.23, 0.3, 0.58	Gajda, 2006
HEGHUX	1	Cyclopentanol	1.5	Moggach, 2005a
KETVEK03	1	Cyclobutanol	1.3	McGregor, 2005
LCYSTN24, 25, 27	3	L-Cysteine	2.6, 4.2, 1.8	Moggach, 2006
LSERIN11-16	6	L-Serine	0.3, 1.4, 2.9, 4.1, 4.8, 5.4	Moggach, 2005b
NAGHOT, 02, 03	3	2,5-bis(4-Nitrophenyl)-(1,3,4)-oxadiazole	2.9, 1.1, 2.0	Orgzall, 1999
NAPHTA12	1	Naphthalene	0.51	Alt, 1982
PHENOL11	1	Phenol	0.16	Allan, 2002
PRONAC02	1	Propionic Acid	1.4	Allan, 2000
QAMTUU01	1	3-Fluorophenol	0.12	Oswald, 2005
QAMVEG01	1	3-Chlorophenol	0.1	Oswald, 2005
THIOUR19	1	Thiourea	0.97	Asahi, 2000
TTFTCG06	1	Tetradeutero-tetrathiafulvene	0.46	Filhol, 1981
WAFNAT	1	Paracetamol dihydrate	1.1	Fabbiani, 2004
WANMUU01	1	2-Chlorophenol	0.12	Oswald, 2005

Table S2: PIXEL dimer interaction energies for methane collinear C-H…H-C contact at varying H…H separation. Distances are in Å, energies are in kJ mol^{-1}. The energies for each component and the total are rounded to the nearest 0.05 kJ mol^{-1}.

H…H Distance	Coulombic	Dispersion	Repulsion	Polarisation	Total
4.0	0.00	-0.10	0.00	0.00	-0.05
3.8	0.00	-0.10	0.00	0.00	-0.10
3.6	0.00	-0.15	0.00	0.00	-0.10
3.4	0.00	-0.20	0.00	0.00	-0.15
3.2	0.05	-0.25	0.05	0.00	-0.20
3.0	0.05	-0.35	0.05	0.00	-0.25
2.9	0.05	-0.45	0.10	0.00	-0.30
2.8	0.05	-0.50	0.15	0.00	-0.35
2.7	0.00	-0.60	0.25	-0.05	-0.35
2.6	0.00	-0.70	0.40	-0.05	-0.40
2.5	-0.05	-0.85	0.60	-0.10	-0.40
2.4	-0.10	-1.00	0.85	-0.15	-0.40
2.3	-0.20	-1.20	1.30	-0.25	-0.30
2.2	-0.30	-1.40	1.95	-0.40	-0.15
2.1	-0.50	-1.65	2.80	-0.65	0.00
2.0	-0.75	-1.95	3.95	-0.95	0.30
1.9	-1.10	-2.25	6.05	-1.50	1.20
1.8	-1.65	-2.65	8.60	-2.35	2.05
1.7	-2.20	-3.05	12.20	-3.30	3.65
1.6	-3.40	-3.45	16.90	-5.30	4.75