Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Hydrate Smaller than the Anhydrate

*Witold Zieliński and Andrzej Katrusiak**
Department of Materials Chemistry Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-614 Poznań, Poland
**Corresponding author e-mail: katran@amu.edu.pl*

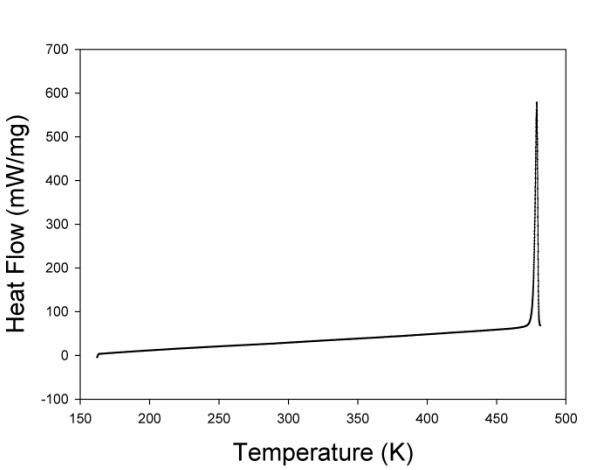

Figure S1. Differential scanning calorimetry for 56dMBzIm in range of temperatures from 163.15 K to 483.15 K.

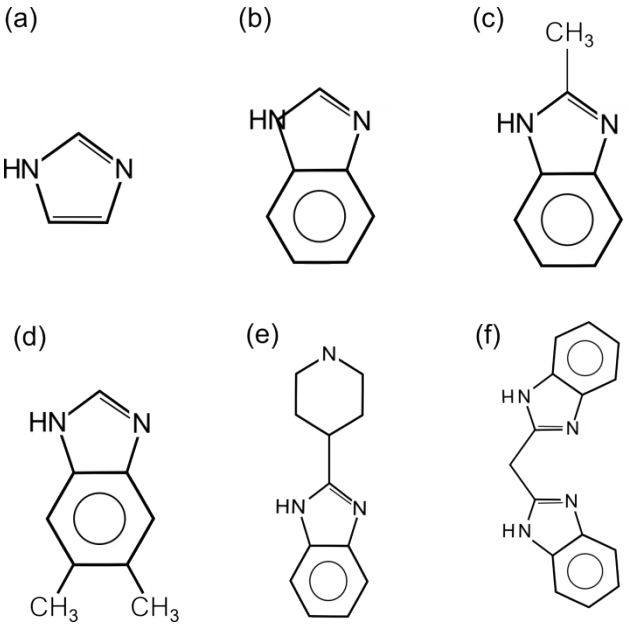

Figure S2. Structural formulas of (a) imidazole (b) benzimidazole (BzIm) (c) 2-methylbenzimidazole (2MBzIm) (d) 5,6-dimethylobenzimidazole (dMBzIm) (e) 2-(4-pyridyl)benzimidazole (PyrBzIm) (f) bis(benzimidazole-2-yl) methane (bBzImM).

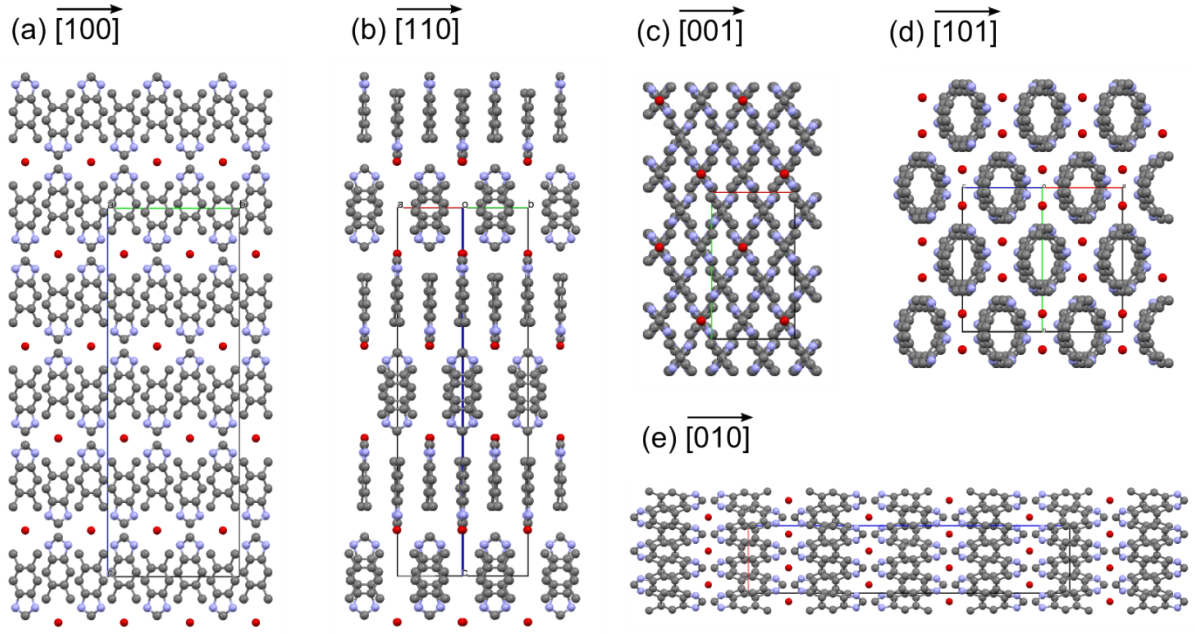

Figure S3. Molecular packing of 5,6-dimethylbenzimidazole hemihydrate vieved along different crystallographic directions. Hydrogen atoms has been removed for clearyty.

Table S1. The high-pressure crystal data and experimental details of 5,6-dimethybenzimidazole hemihydrates.

$C_9H_{10}N_2 \cdot ½H_2O$						
Pressure (GPa)		0.0001 (2)	0.54(2)	0.70 (2)	1.10(2)	1.49(2)
Temperature (K)		296(2)	296(2)	296(2)	296(2)	296(2)
Formula weight		309.39	309.39	309.39	309.39	309.39
Crystal colour		yellow	yellow	yellow	yellow	yellow
Crystal size (mm)		0.15x0.15x0.10	0.15x0.15x0.10	0.15x0.15x0.10	0.15x0.15x0.10	0.15x0.15x0.10
Crystal system		Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic	Orthorhombic
Space group		*Fddd*	*Fddd*	*Fddd*	*Fddd*	*Fddd*
Unit cell dimensions (Å)	*a* =	7.5684(10)	7.2661(15)	7.173(3)	7.040(2)	6.9376(16)
	b =	12.432(2)	12.407(8)	12.383(5)	12.334(4)	12.228(3)
	c =	34.803(4)	34.550(5)	34.439(4)	34.323(3)	34.174(2)
Volume ($Å^3$)		3274.5(8)	3115(2)	3059.0(16)	2980.3(15)	2899.1(10)
Z		8	8	8	8	8
D_x (mg cm^{-3})		1.255	1.320	1.344	1.379	1.418
Wavelength MoKα, λ (Å)		0.71073	0.71073	0.56087	0.71073	0.71073
Absorption coefficient (m/mm^{-1})		0.081	0.085	0.056	0.089	0.091
F(000) (e)		1320.0	1320.0	1320.0	1320.0	1320.0
2θ max (°)		53.044	54.32	49.384	54.75	56.28
Min./Max. indices h,k,l		-8/9,-15/15,-43/42	-8/8,-8/8,-41/41	-8/8,-14/14,-50/51	-6/6,-11/11,-43/44	-6/6,-12/12,-45/45
Reflections collected/unique		3718/798	3831/486	5885/693	3870/398	4816/421
R_{int}		0.1387	0.1459	0.2197	0.1105	0.0826
Data/parameters		798/58	486/58	693/58	398/59	421/58
Goodness of fit on F^2		1.077	1.027	1.014	1.029	1.086
Final R_1/wR_2 indices (I>4σ(I))		0.0772/0.1505	0.0848/0.2067	0.0933/0.2169	0.0696/0.1817	0.0695/0.1839
R_1/wR_2 indices (all data)		0.1719/0.1999	0.1586/0.2753	0.2145/0.2891	0.1290/0.2223	0.1104/0.2223
$\Delta\sigma_{max}$, $\Delta\sigma_{min}$ ($eÅ^{-3}$)		0.20/-0.23	0.20/-0.21	0.23/-0.23	0.25/-0.21	0.23/-0.23
Weighting scheme: x; y[a]		0.845;0	0.158;0	0.136/0	0.1374;0	0.117;6.935
Extinction coefficient		–	–	–	–	–
Absorption corrections		DAC, gasket and sample crystal	DAC, gasket and sample crystal	DAC, gasket and sample crystal	DAC, gasket and sample crystal	DAC, gasket and sample crystal
DAC transmission min/max		0.93/0.99	0.92/0.99	0.92/0.99	0.91/0.99	0.92/0.99
Gasket shadowing min/max		0.75/0.98	0.79/0.98	0.75/0.96	0.70/0.98	0.73/0.97
Sample transmission min/max		0.98/0.98	0.989/0.988	0.986/0.988	0.985/0.988	0.986/0.987

[a] $w = 1/(\sigma^2(F_o^2)+x^2P^2+yP)$, where $P=(\mathrm{Max}(F_o^2, 0)+2F_c^2)/3$.

Table S2. The high-pressure crystal data and experimental details of 5,6-dimethybenzimidazole.

$C_9H_{10}N_2$					
Pressure (GPa)	0.11 (2)	0.22(2)	0.28 (2)	0.33(2)	0.64 (2)
Temperature (K)	296(2)	296(2)	296(2)	296(2)	296(2)
Formula weight	146.19	146.19	146.19	146.19	146.19
Crystal colour	yellow	yellow	yellow	yellow	yellow
Crystal size (mm)	0.15x0.15x0.10	0.15x0.15x0.10	0.15x0.15x0.10	0.15x0.15x0.10	0.15x0.15x0.10
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space group	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$	$P2_1/c$
a =	6.5122(6)	6.4776(7)	6.5011(10)	6.538(3)	6.487(2)
b =	27.61(2)	27.51(3)	27.23(2)	26.99(14)	26.63(12)
c =	14.0669(13)	14.0381(15)	13.949(2)	13.930(5)	13.831(4)
β =	102.550(9)	102.456(10)	102.615(15)	102.68(4)	102.50(3)
Volume (Å^3)	2469(2)	2443(3)	2410(2)	2398(13)	2333(11)
Z	12	12	12	12	12
D_x (mg cm^{-3})	1.180	1.192	1.209	1.215	1.249
Wavelength MoKα, λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073
Absorption coefficient (m/mm^{-1})	0.072	0.073	0.074	0.075	0.077
F(000) (e)	936.0	936.0	936.0	936.0	936.0
2θ max (^{o})	48.684	46.596	55.074	56.158	56.21
Min./Max. indices h,k,l	-8/8,-10/10,-18/18	-9/9,-10/10,-19/19	-8/8,-15/14,-17/17	-8/8,-7/7,-18/18	-8/8,-6/6,-18/18
Reflections collected/unique	15179/ 1896	16405/ 1961	14463/2331	14260/1358	12153/1174
R_{int}	0.1493	0.1360	0.2093	0.2049	0.1634
Data/parameters	1896/304	1961/304	2331/304	1358/303	1174/304
Goodness of fit on F^2	1.187	1.197	1.010	1.008	1.042
Final R_1/wR_2 indices (I>4σ(I))	0.1192/0.3185	0.1177/0.3170	0.1163/0.2809	0.0883/0.2049	0.0730/0.1559
R_1/wR_2 indices (all data)	0.2578/0.4008	0.2476/0.3922	0.2814/0.3944	0.2291/0.2909	0.1776/0.2103
$\Delta\sigma_{max}$, $\Delta\sigma_{min}$ (eÅ^{-3})	0.20/-0.20	0.19/-0.20	0.19/-0.23	0.11/-0.12	0.09/-0.10
Weighting scheme: x; y[a]	1.14;0	2.205;0	6.005;0	2.203;0	2.555;0
Extinction coefficient	–	–	–	–	–
Absorption corrections	DAC, gasket and sample crystal	DAC, gasket and sample crystal	DAC, gasket and sample crystal	DAC, gasket and sample crystal	DAC, gasket and sample crystal
DAC transmission min/max	0.94/0.99	0.93/0.99	0.92/0.99	0.90/0.99	0.93/0.99
Gasket shadowing min/max	0.79/0.98	0.80/0.98	0.75/0.96	0.80/0.98	0.79/0.97
Sample transmission min/max	0.98/0.98	0.98/0.99	0.986/0.988	0.98/0.99	0.97/0.99

[a] $w = 1/(\sigma^2(F_o^2)+x^2P^2+yP)$, where $P=(\mathrm{Max}(F_o^2, 0)+2F_c^2)/3$.