Supplementary Information

High Pressure Used for Producing a New Solvate of 1,4-Diazabicyclo[2.2.2]octane Hydroiodide

Anna Olejniczak, Marcin Podsiadło and Andrzej Katrusiak*

Faculty of Chemistry, Adam Mickiewicz University, Umultowska 89b, 61-614 Poznań, Poland

*Corresponding author: katran@amu.edu.pl

Table S1. Crystal data and structure-refinements details for high-pressure measurements of dabcoHI·H_2O·CH_3OH.

	dabcoHI·H_2O·CH_3OH
Formula	$[C_6H_{13}N_2]^+I^-\cdot H_2O\cdot CH_3OH$
Pressure (GPa)	3.10(2)
Temperature (K)	296(2)
Formula weight	290.14
Wavelength (Å)	0.71073
Crystal system	Monoclinic
Space group	*C*2/*c*
Unit cell dimensions (Å,°)	
a	10.966(3)
b	7.4850(12)
c	23.09(2)
β	100.94(5)
Volume (Å^3)	1860.6(18)
Z, *Z*′	8, 1
Calculated density (g/cm^3)	2.072
Absorption coefficient (mm^{-1})	3.408
F(000)	1152
Crystal size (mm)	0.23/0.14/0.09
θ-range for data collection (°)	3.31 to 26.40
Min/max indices: h, k, l	-13/13, -9/9, -7/7
Reflect. collected/unique	2065/323
R_{int}	0.0756
Refinement method	Full-matrix least-squares on F^2
Completeness (%)	16.9
Data/restrains/parameters	323/17/42
Goodness-of-fit on F^2	1.086
Final R_1/wR_2 ($I>2\sigma_1$)	0.0459/0.1170
R_1/wR_2 (all data)	0.0920/0.1544
Weighting parameters w_1, w_2 [a)]	0.0597, 30.57
Largest diff. peak/hole (e·Å^{-3})	0.364/-0.346

[a)] $w=1/(\sigma^2F_o^2+w_1^2*P^2+w_2*P)$, where $P=(\mathrm{Max}(F_o^2,0)+2*F_c^2)/3$

Table S2. The shortest intermolecular and interionic interactions in dabcoHI·H_2O·CH_3OH structure at 3.10 GPa/296 K.

DH···A	H···A (Å)	D···A (Å)	DH···A (°)	Symmetry code
O(9)-H(9a)···N(2)	1.79(1)	2.74(2)	166	x,y,z
O(8)-H(8)···N(2)	2.60(1)	3.27(3)	140	x,y,z
O(8)-H(8)···O(9)	2.49(1)	3.10(3)	132	x,y,z
N(1)-H(1)···O(8)	2.49(1)	3.10(4)	125	x,y-1,z
N(1)-H(1)···O(9)	2.00(2)	2.80(2)	146	x,y-1,z
O(9)-H(9b)···I(1)	2.38(1)	3.35(4)	166	x,y,z
O(8)-H(8)···I(2)	2.71(1)	3.25(6)	125	x,y,z
C(2)-H(2A)···O8	2.44(3)	3.22(3)	138	x,y-1,z
C(3)-H(3B)···O8	2.50(3)	3.04(3)	114	0.5+x,y-0.5,z
C(4)-H(4A)···O9	2.54(2)	3.02(2)	111	x-0.5,y-0.5,z
C(3)-H(3B)···O9	2.56(2)	3.04(2)	110	x-0.5,y-0.5,z

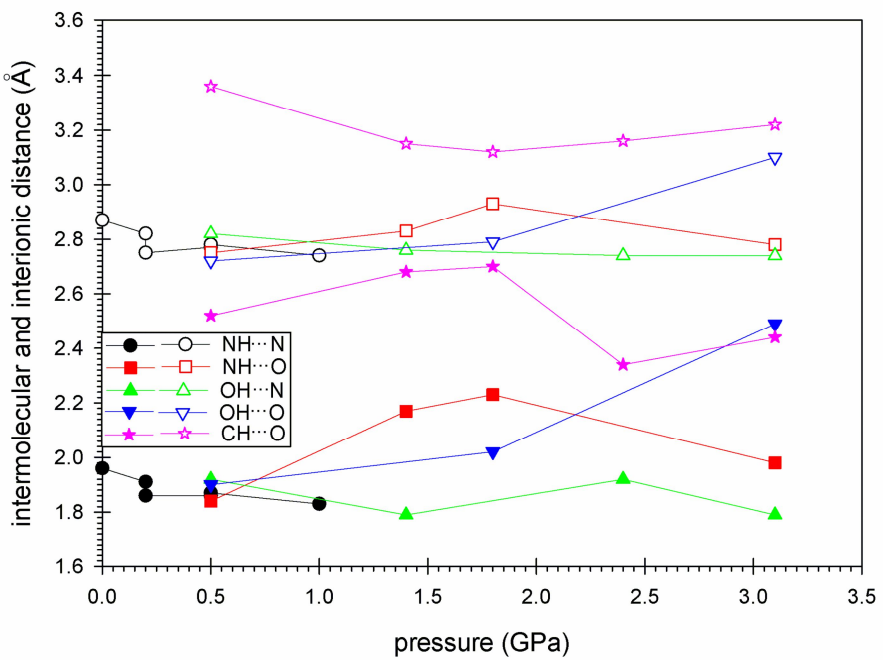

Figure S1. Pressure dependence of hydrogen-bond distances in the dabcoHI polymorphs (black symbols), dabcoHI hydrates, methanol solvates of disalt dabco2HI·3CH_3OH and N-methylated dabcoCH_3I·2CH_3OH , as well as in mixed solvate dabcoHI·H_2O·CH_3OH. The lines are for guiding the eye, as they link the points representing distances in different polymorphs and solvates. Full and open symbols denote the corresponding H···acceptor and H-donor···acceptor distances, respectively. Standard deviations are equal or smaller than the size of the symbols (*cf.* Table S2).