

Pressure-stabilized solvates of xylazine hydrochloride

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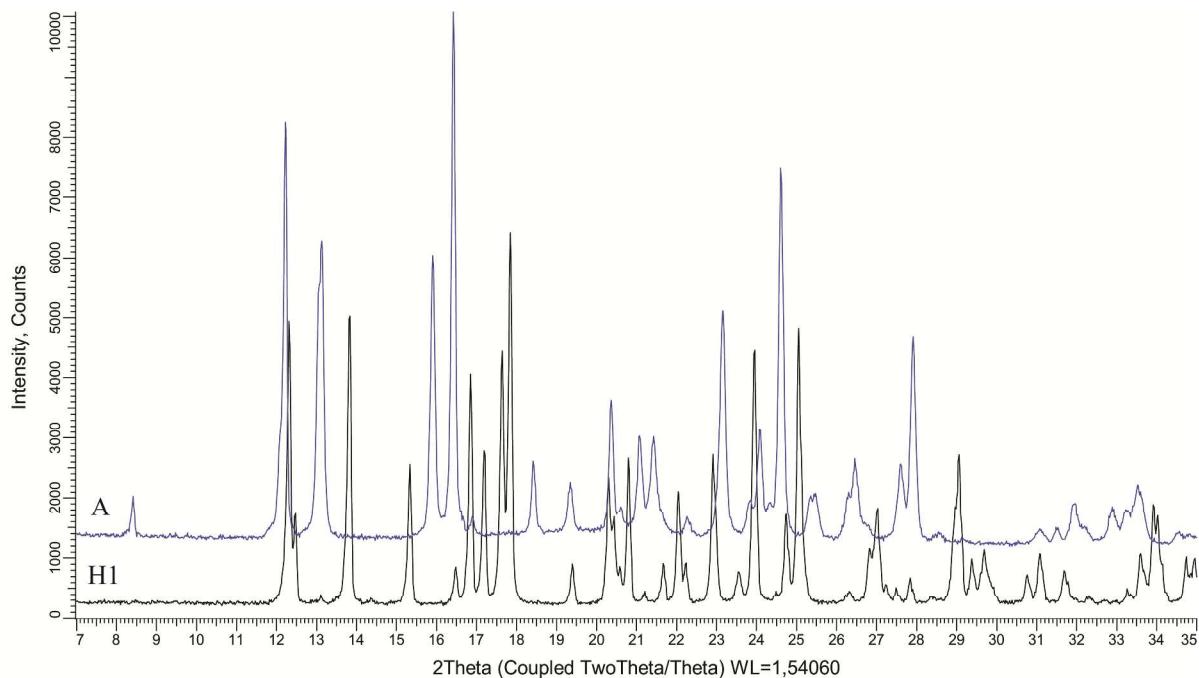


Figure S1. Powder patterns of XylHCl neat form A and its hydrate H1.

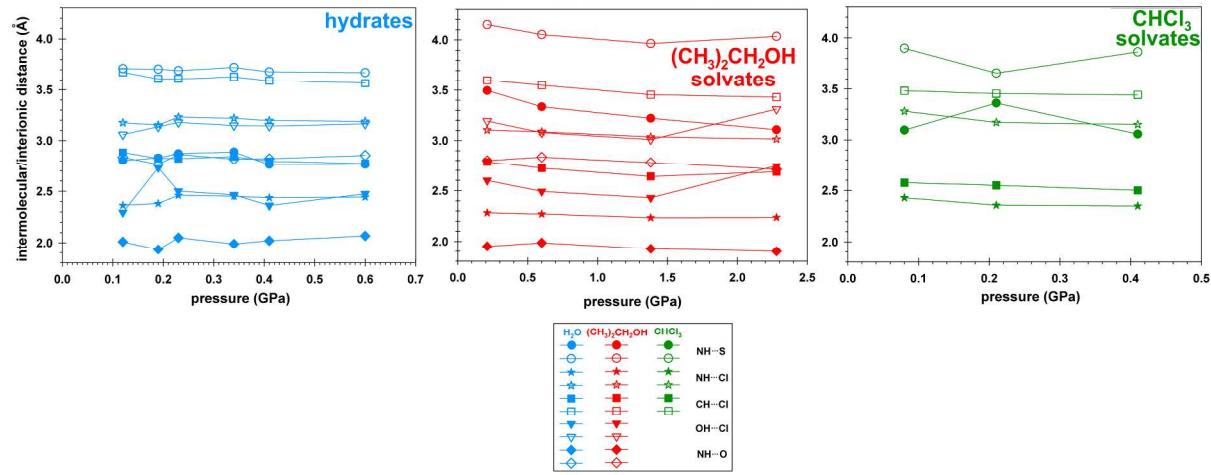


Figure S2. Intermolecular and interionic distances in XylHCl hydrates, $(\text{CH}_3)_2\text{CH}_2\text{OH}$ and CHCl_3 solvates as a function of pressure.

Table S1. The shortest intermolecular and interionic contacts ($\text{H}\cdots\text{acceptor/donor}\cdots\text{acceptor}$, Å) of XylHCl and its solvates.

XylHCl	0.11 GPa					
$\text{CH}\cdots\text{S}$	3.147(1)/ 4.144(6)					
$\text{NH}\cdots\text{Cl}$	2.255(1)/ 3.124(4)					
$\text{CH}\cdots\text{Cl}$	2.870(1)/ 3.749(6)					
XylHCl·CH ₃ Cl	0.08 GPa	0.21 GPa	0.41 GPa			
$\text{CH}\cdots\text{S}$	3.095(3)/ 3.90(5)	3.036(8)/ 3.66(3)	3.056(9)/ 3.65(10)			
$\text{NH}\cdots\text{Cl}$	2.429(12)/ 3.28(4)	2.357(15)/ 3.17(5)	2.349(12)/ 3.15(4)			
$\text{CH}\cdots\text{Cl}$	2.575(5)/ 3.48(2)	2.549(4)/ 3.452(19)	2.500(3)/ 3.439(14)			
XylHCl·(CH ₃) ₂ CH ₂ OH	0.21 GPa	0.60 GPa	1.38 GPa	2.38 GPa		
$\text{CH}\cdots\text{S}$	3.497(7)/ 4.15(3)	3.335(2)/ 4.053(11)	3.221(3)/ 3.65(14)	3.108(3)/ 4.035(3)		
$\text{NH}\cdots\text{Cl}$	2.282(4)/ 3.105(12)	2.270(5)/ 3.087(16)	2.234(5)/ 3.037(18)	2.237(4)/ 3.015(16)		
$\text{CH}\cdots\text{Cl}$	2.786(4)/ 3.60(2)	2.722(6)/ 3.55(3)	2.639(7)/ 3.45(3)	2.685(5)/ 3.43(3)		
$\text{OH}\cdots\text{Cl}$	2.599(14)/ 3.19(7)	2.493(9)/ 3.08(2)	2.429(10)/ 3.01(4)	2.745(11)/ 3.31(13)		
$\text{NH}\cdots\text{O}$	1.95(2)/ 2.80(2)	1.987(11)/ 2.836(18)	1.928(14)/ 2.78(2)	1.90(3)/ 2.71(3)		
XylHCl·(CH ₃) ₂ H ₂ O	0.12 GPa	0.19 GPa	0.23 GPa	0.34 GPa	0.41 GPa	0.60 GPa
$\text{CH}\cdots\text{S}$	2.804(7)/ 3.712(9)	2.830(3)/ 3.706(3)	2.873(9)/ 3.692(9)	2.889(7)/ 3.723(7)	2.762(5)/ 3.680(5)	2.763(3)/ 3.673(3)
$\text{NH}\cdots\text{Cl}$	2.364(3)/ 3.176(10)	2.382(3)/ 3.153(16)	2.461(5)/ 3.231(14)	2.452(4)/ 3.220(12)	2.437(4)/ 3.197(10)	2.443(2)/ 3.190(6)
$\text{CH}\cdots\text{Cl}$	2.884(4)/ 3.676(12)	2.825(3)/ 3.611(12)	2.823(3)/ 3.610(12)	2.843(3)/ 3.631(12)	2.796(2)/ 3.592(9)	2.775(1)/ 3.567(6)

OH···Cl	2.295(8)/ 3.06(3)	2.729(3)/ 3.136(15)	2.502(5)/ 3.179(17)	2.466(6)/ 3.149(14)	2.362(4)/ 3.143(12)	2.475(2)/ 3.164(8)
NH···O	2.010(14)/ 2.836(17)	1.934(8)/ 2.765(14)	2.050(15)/ 2.865(18)	1.989(11)/ 2.818(16)	2.021(11)/ 2.822(15)	2.068(8)/ 2.855(10)

Table S2. The torsion angles for XylHCl hydrates H1 and H2.

XylHCl·(CH ₃) ₂ ·H ₂ O	0.12 GPa	0.19 GPa	0.23 GPa	0.34 GPa	0.41 GPa	0.60 GPa
S(1)-C(2)-N(7)-C(8)	-5(1)	-11(3)	-11(3)	11(2)	1(2) 9(2)	3(1) 11(1)
N(3)-C(2)-N(7)-C(8)	-2(2)	-7(1)	3(2)	6(2)	6(1) 13(2)	2(1) 11(1)
C(2)-N(7)-C(8)C(13)	-93(1)	-92(2)	-95(2)	-94(2)	-95(1) 92(1)	94(1) 91(1)
C(2)-N(7)-C(8)-C(9)	88(1)	88(1)	88(2)	88(1)	-87(2) -88(2)	-89(1) -90(1)

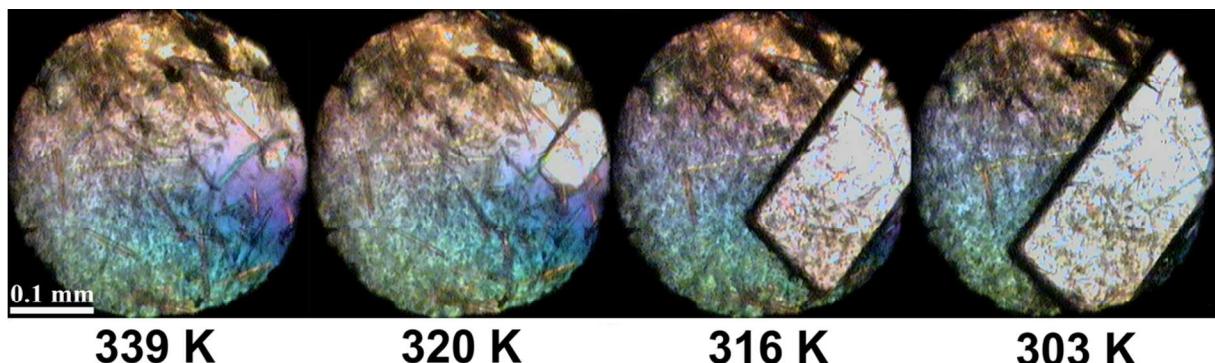


Figure S3. The single-crystal growth of the neat XylHCl form Z at 0.11 GPa.

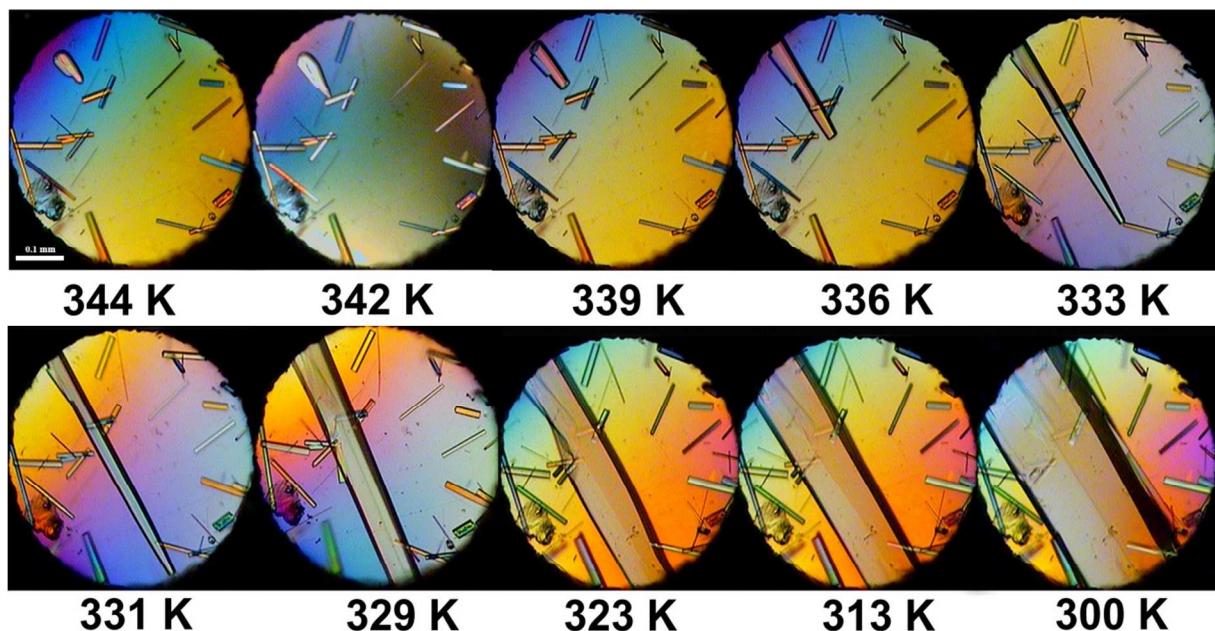


Figure S4. The single-crystal growth of the hydrate H1 form at 0.34 GPa.

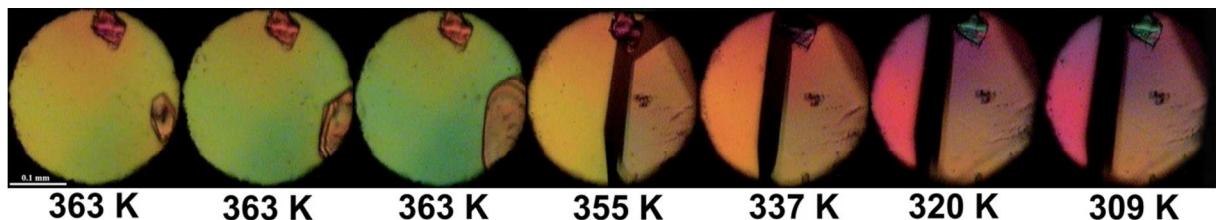


Figure S5. The single-crystal growth of the CHCl_3 solvate at 0.21 GPa.

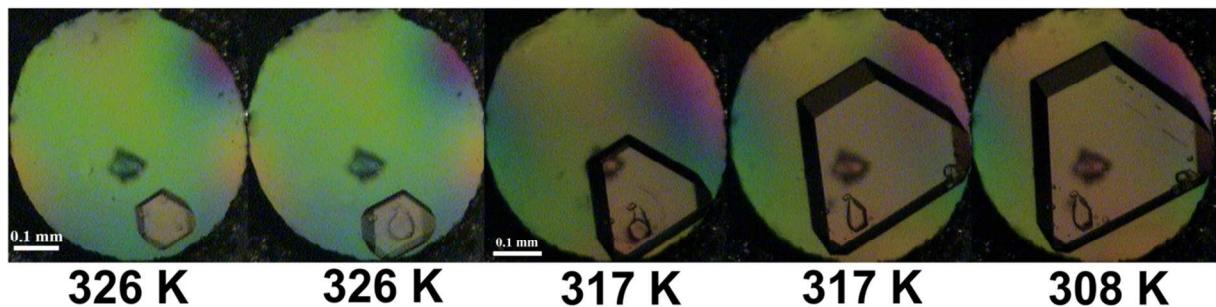


Figure S6. The single-crystal growth of the CH_2Cl_3 solvate at 0.13 GPa.

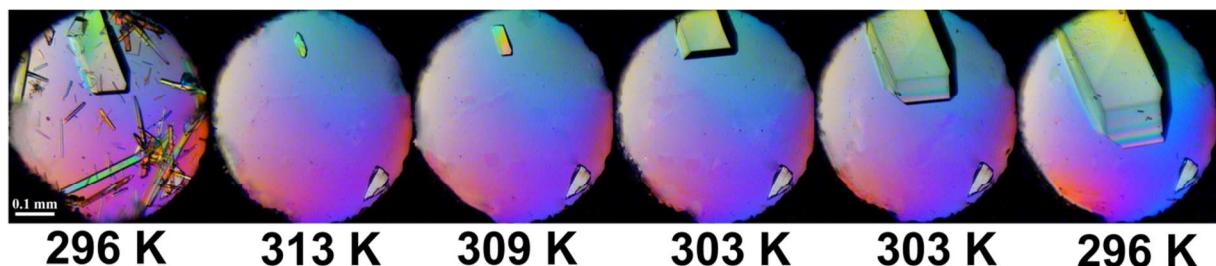


Figure S7. The single-crystal growth of the $(\text{CH}_3)_2\text{CHOH}$ solvate at 0.21 GPa.

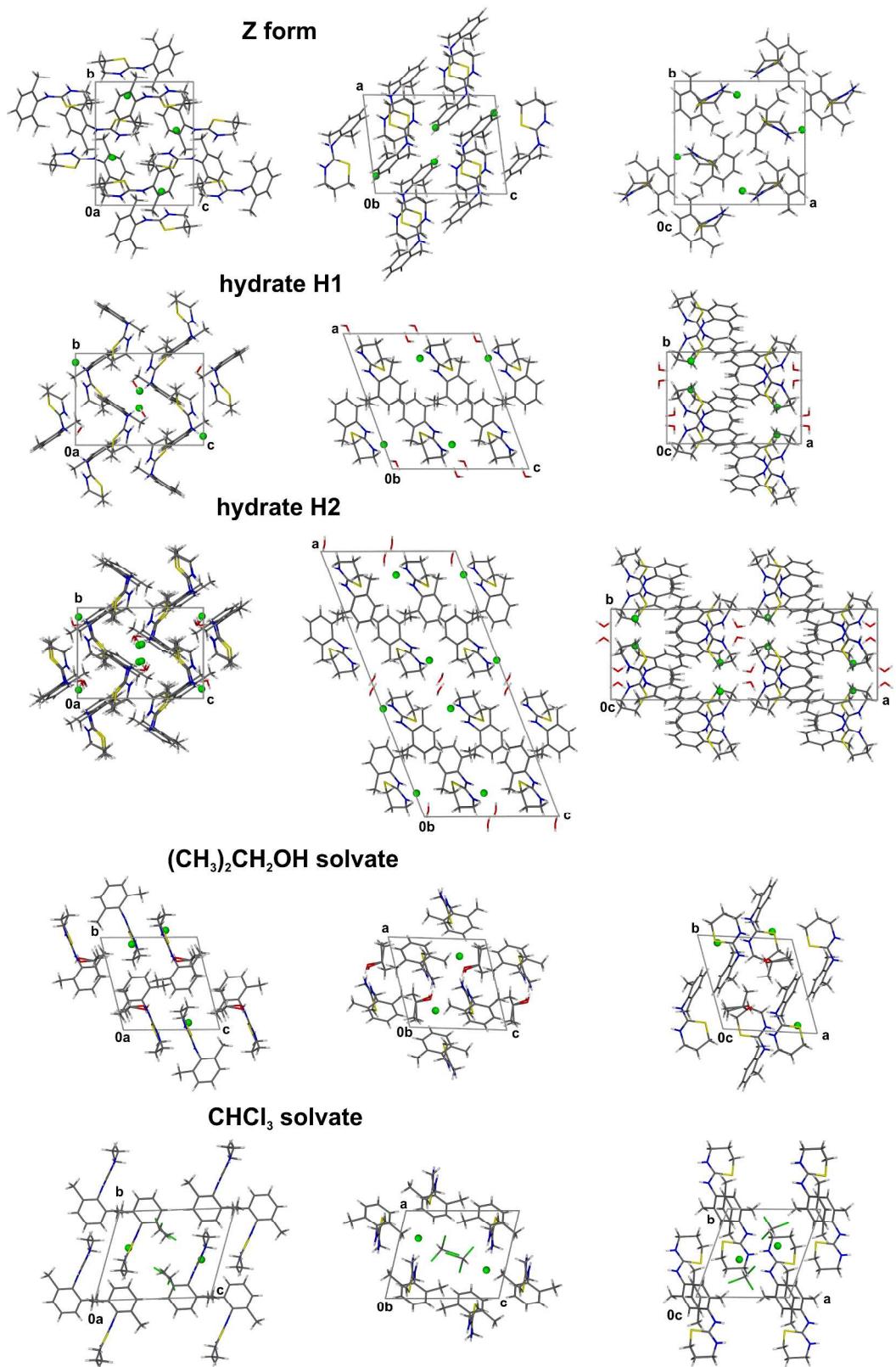


Figure S8. Unit-cell packing of XylHCl neat form and its solvates.