MS30-P112 - LATE | STRUCTURAL SIMILARITIES OF 2D AND 3D WATER FRAMEWORKS IN 3,3DIMETHYL-2-BUTYLAMINE, TERT-AMYLAMINE AND AZEPANE HYDRATES

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The presence of water molecules in the structure can play an important role in the stability and property of the crystals. However the resulting structure is still hard to predict. Herein we present crystalline hydrates of racemic mixture of 3,3-dimethyl-2-butylamine (**1**), chiral (S)-3,3-dimethyl-2-butylamine (**1***), *tert*-amylamine (**2**) and azepane (**3**). All these phases were grown under ambient pressure using IR laser assisted *is situ* method.

Amines (**1**), (**1***) and (**2**) forms dihydrates. These structures crystallize in different space groups. Moreover dihydrate of (**1***) undergoes reversible $P2_1 \leftrightarrow P1$ phase transition. Nevertheless all these crystal structures contain the same water layers denoted as L4(4)8(8) composed of 4- and 8-membered rings. With a moderate water amount (**3**) forms trihydrate containing L4(6)5(7)6(8) [2] layered water motif. In addition all these amines form hydrates with higher amount of water. In the case of (**1***), (**2**) and (**3**) undecahydrate with the same 3D water framework topology is observed. These structures contain channels occupied by the amine interacting with H_2O species. In these structures empty $4^3 5^6$ cages are also present. Surprisingly the amine (**1**) which is a racemate of (**1***) behaves differently and crystallizes as heksadekahydrate. Here the amine is trapped in large $6^8 5^{10}$ water cages but unlike in clathrate hydrates forms strong hydrogen bonds with H_2O.