MS27-2-11 Intermolecular Interactions, Polymorphism and Properties of Primary Amines at High Pressure #MS27-2-11

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Abstract

A series of the simplest primary amines: ethylamine (EA), propylamine (PA), butylamine (BA), and pentylamine (PEA), has been studied at high pressure by single-crystal X-ray diffraction. EA is gaseous, while PA, BA, and PEA are liquids at ambient conditions. They represent an important class of compounds, used in organic chemistry, and their crystal structures have been previously determined only at ambient pressure and low temperature.[1] We have obtained single crystals of particular amines in a diamond-anvil cell (DAC) in the range between their freezing pressures at ambient temperature to *ca*. 6 GPa. EA at high pressure crystallizes in phase II of space group $P2_1/c$. For the series from PA to PEA six new polymorphs at high pressure have been found: two of PA (phases II and III, both in $P2_1/c$ space group), two of BA (phases II and III, space group $Pbc2_1$), and two of PEA (phase II and III, space group $Pbc2_1$ and $P2_1cn$). We have explained the structural transformations of primary amines at high pressure by analysing the NH···N and CH···N intermolecular interactions. We have also found the structure-symmetry relations for new polymorphs and we have correlated them with the melting temperature, freezing pressure, and molecular symmetries. Phase diagrams of studied amines have been also outlined up to *ca*. 6 GPa.

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References

1.Maloney, A. G. P.; Wood, P. A.; Parsons, S. Competition between Hydrogen Bonding and Dispersion Interactions in the Crystal Structures of the Primary Amines. CrystEngComm 2014, 16, 3867−3882