MS34-2-2 Phase diagram P/T of resorcinol and the stabilization of high-pressure polymorphs by rational doping #MS34-2-2

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Abstract

Resorcinol, $C_6H_6O_2$, apart from being an important natural product and chemical agent of many applications [1,2], it was also the first compound, for which the structures of two polymorphs were determined in the 1930s [3,4]. These polymorphs α and β were puzzling, because they crystallized in the same space-group type $Pnc2_1$ and the high-temperature polymorph β was more dense than the low-temperature phase α. Moreover, the conformation of the molecules was different: anti-anti in polymorph α and anti-syn in polymorph β. Under high pressure resorcinol either transformed from phase α to β at about 0.5 GPa or no such a transformation was observed; at the same time new high-pressure phases γ and δ of resorcinol were postulated, but their structures were not determined [5]. Finally, a new polymorph ε of resorcinol, of space group $P2_12_12_1$ and Z=8, was obtained under ambient pressure by doping resorcinol with tartaric acid [6]. Most surprisingly, the density of polymorph ε was higher compared to those of polymorphs α and β. We grew single crystals of polymorph ε in a diamond-anvil cell (DAC), however these crystals could not be recovered to normal conditions, as they transformed back to form α below 0.2 GPa [7]. It showed that polymorph ε in its pure form is unstable in ambient pressure, where it was observed in the doped mixtures [6]. Above 0.7 GPa, we also obtained another polymorph ζ, monoclinic space group $P2_1/c$, Z=8 [7]. The outlined phase diagram of resorcinol explains its puzzling behaviour. The behaviour of resorcinol indicates the methods for stabilizing the high-pressure polymorphs of various compounds at ambient conditions. We also showed the preference for obtaining resorcinol solvates under high-pressure [8].

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