Poster

Resorcinol polymorphism: the lattice energy and conformers

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Resorcinol, 1,3-benzediol, $C_6H_6O_2$, is a common building block in the synthesis of numerous polymers and a fundamental compound in the realm of material science due to its extensive application in resins, dyes and pharmaceuticals [1]. It was also for resorcinol that the first structural determinations of polymorphs were performed by Robertson and Ubbelohde in the 1930s [2,3].

The exploration of molecular polymorphism under extreme conditions offers insights into the background of properties of substances at the atomic level [4]. Our study presents an in-depth analysis of resorcinol polymorphs, emphasizing their preferred configurations under various conditions and the lattice energy changes.

The recent research conducted in a diamond anvil cell (DAC) expanded our understanding of resorcinol polymorphism under pressure. The high pressure provides a unique insight to the conformational flexibility of resorcinol. We explore the energy landscape of resorcinol polymorphs to understand the thermodynamic preferences for conformers. The main focus of this study are the transformation between the syn-syn, anti-syn and anti-anti conformers (Figure 1).

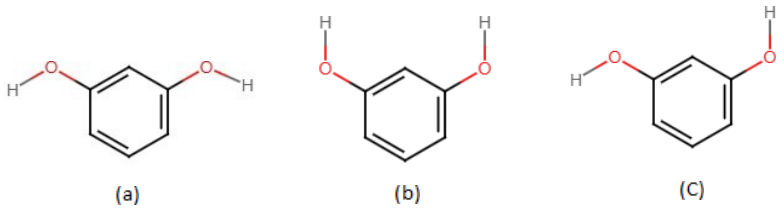

Figure 1. Resorcinol conformers: (a) anti-anti, (b) syn-syn and (c) anti-syn.

[1] Dressler, H. (1994). Resorcinol: its uses and derivatives, *Springer*.

[2] Robertson, J. (1936). *Proc.R.Soc.London,Ser.A.*, **157**, 79.

[3] Robertson, J.M. and Ubbelohde, A.R. (1938). *Proc.R.Soc.London,Ser.A.*, **167**, 122.

[4] Guerain, M.. (2020). *Journal of Pharmaceutical Sciences.*, **9**, 2640-2653.