

AVVISO DI SEMINARIO

Lunedì 23 ottobre 2023 alle ore 14.30 presso l'Aula IV del Dipartimento di Chimica "Giacomo Ciamician" in via F. Selmi 2, il Professor Andrzej Katrusiak, Adam Mickiewicz University, Poznan, Polonia, terrà un seminario, nell'ambito dei Dipartimenti d'Eccellenza, dal titolo:

CAN WE APPLY HIGH-PRESSURE POLYMORPHS AT AMBIENT CONDITIONS? PHASE DIAGRAM OF RESORCINOL AND THE METHOD OF STABILIZING ITS HIGH-PRESSURE PHASES

La S. V. è invitata a partecipare.

Sarà possibile seguire il seminario da remoto, collegandosi al link TEAMS.

Per informazioni: Dr. Simone d'Agostino, Prof. Dario Braga.





DIPARTIMENTO DI CHIMICA "G. CIAMICIAN"

CAN WE APPLY HIGH-PRESSURE POLYMORPHS AT AMBIENT CONDITIONS? PHASE DIAGRAM OF RESORCINOL AND THE METHOD OF STABILIZING ITS HIGH-PRESSURE PHASES

Abstract

High pressure efficiently generates new phases: only few compounds are known to resist the effect of pressure.

However, the high-pressure phases transform back when the pressure is released. Therefore, the high-pressure phases are regarded useless at ambient conditions. This attitute can change, owing to one-century long studies of resorcinol, $C_6H_6O_2$. This first organic compound for which the crystal structures of two polymorphs, α and β , were determined in 1936 and 1938 by Robertson and Ubbelohde, has confused Materials Chemists for decades.

Both polymorphs α and β have the same space-group symmetry Pna2₁, and the low-temperature phase α is less dense than the high-temperature phase β . New high-pressure phases γ and δ were postulated, but their structures were not determined. In 2016, Prof. Kahr and co-workers reported a new phase ϵ and its structure (space group P2₁2₁2₁) under normal conditions. We determined its high-pressure dependence and found yet another polymorph ζ of space group P2₁/c.

Based on recrystallization experiments, we outlined the phase diagram of resorcinol and suggested a method for stabilizing the high- pressure polymorphs [1]. This method of rational doping generates the internal strain mimicking the high-pressure conditions under ambient conditions. We approved this method also for other compounds, so it opens a new way of improving the properties of materials for pharmaceutical and other applications.

[1] Safari, F.; Katrusiak, A. High-Pressure Polymorphs Nucleated and Stabilized by Rational Doping under Ambient Conditions. *J. Phys. Chem. C* **2021**, *125*, 23501–23509.

