High P-T phase Diagram of Solid Benzene, and Transformation to an Extended Amorphous State

Mario Santoro[a], Lucia Ciabini[a,b], Federico A. Gorelli[a,c], Roberto Bini[a,b], Vincenzo Schettino[a,b], Mohammed Mezouar[d], [a]*LENS, European Laboratory for Non-linear Spectroscopy and INFM, Via Carrara 1, I-50019 Sesto Fiorentino, Firenze, Italy.* [b]*Dipartimento di Chimica dell'Universita' di Firenze, Via della Lastruccia 3, I-50019 Sesto Fiorentino, Firenze, Italy.* [c]*INFM-CRS SOFT, Universit'a di Roma La Sapienza, P.zza A. Moro 2, I-00185, Roma, Italy.* [d]*European Synchrotron Research Facility, BP220, F38043 Grenoble, France.* E-mail: santoro@lens.unifi.it

The high pressure structural properties of solid benzene have been investigated in the P-T range where the chemical reaction does occur, e.g. above 15-40 GPa depending on temperature, by x-ray diffraction and infrared absorption techniques. Sample annealing above 500 K produces pure phase II crystals (monoclinic $P2_1/c$). X-ray diffraction patterns collected at 540 K on these crystals allowed the equation of state of benzene to be obtained. These results indicate the stability of phase II up the pressure where benzene reacts and no evidences of the III and III' crystal structures is gained. On these bases the existing thermodynamic phase diagram of benzene was reinterpreted and a simplified new one is proposed [1]. Unique features of the high pressure transformation to the extended amorphous state of this important model system were unveiled by observing, *in situ*, the pressure evolution of the Bragg peaks. Indeed the crystalline pattern merges, at high pressure, into a broad amorphous-like diffraction profile related to the static structure factor S(Q) of the final product.

[1] Ciabini L., Gorelli F.A., Santoro M., Bini R., Schettino V., Mezouar M., *High temperature equation of state and phase diagram of solid benzene*, *submitted to PRB*.

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