New Phases Discovery of ε-CL-20 under High Pressure up to 60 GPa

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Among the numerous nitramines explosives, energetic material CL-20 possess high density, high heat of formation, and high explosive power due to the caged molecular structure, six N-NO_2 groups in the polycyclic structure and high oxygen balance. The information during the explosion or chemical reaction is the key to understanding the performance of the explosive, and it is difficult to be characterized due to the ultrafast and damaging process. An alternative method is to observe more physical processes under hydrostatic pressure.

The pressure-induced structural phase transitions of ε-CL-20 were studied by using the Raman and Mid-infrared spectra up to 60 GPa. A phase transition of ε-form to γ-form starts at 0.9 GPa and completed at 4.4 GPa. Compared to the literature, its starting pressure point is about 4 GPa in advance, which truly clarified the pressure stability of ε-phase. Moreover, the slight cage distortion was observed in the pressure range of 6.9-8.4 GPa in γ-phase under higher pressure. This may correspond to a new conformation similar to γ-phase, named as η-phase. As the pressure increases to 28 GPa and 50 GPa, two more new phases distinct from the high pressure ζ-phase appear, named as φ- and ι-phase, respectively. Infrared and Raman results are in good agreement, both indicate similar phase regions for CL-20 under high pressure.

In addition, high-pressure experiments with γ-form as the starting phase at room temperature were performed. There are definite changes in the Raman and IR spectra with the increase of pressure at about 1.3 GPa, which can be identified as high-pressure ζ-phase that have been reported by Russell, Gump and Millar et al. No significant changes were observed as the pressure was further increased up to around 20 GPa. After comparing the high pressure studies of different initial phases, it can be concluded that there are profound distinction in the process and mechanism of phase transition.

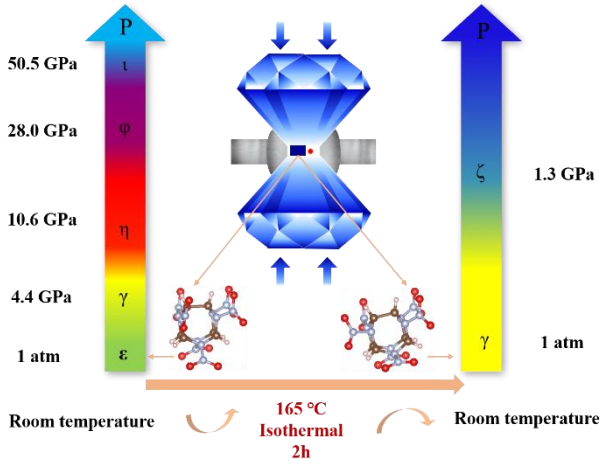

Figure 1. Phase diagram for Cl-20 crystals showing the conditions of several phase transitions

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