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## Topochemical polymerization under high pressure: threshold distance and selectivity

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Unsaturated molecular crystal can polymerize into extended carbon structure like diamond nanothread and graphene nanoribbon under external pressure, which is called pressure-induced polymerization (PIP). PIP has an obvious topochemical feature, with the structure of the polymeric product similar with the reactant. By analyzing the crystal structures of many reactants, we conclude that alkynes have a threshold distance of  $\sim 3.0$  Å before the PIP. For acetylene, the distance include an intrinsic threshold of 2.3 Å and thermal displacement of  $\sim 0.8$  Å. The threshold distance also depends on the reaction path. To realize a perfect topochemical PIP, an ordered doping of “inert” atom and a suitable intermolecular stacking with strong intermolecular interaction are necessary.

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