

High pressure phase transitions in ZnSiO₃ pyroxene by molecular dynamics simulation

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High pressure structural behavior of ZnSiO₃ pyroxene at 300K was studied by molecular dynamics simulation. During decompression, a transition from HP C2/c to LP C2/c phase was observed. During compression, a transition from LP C2/c to P21/c phase was observed, and it was reversible. No transition from P21/c to HP C2/c was observed, however, LP C2/c to HP C2/c transition was realized when compressed quickly. They suggest that observed LP C2/c in real experiment is retrograde phase of either HP C2/c or P21/c.