高压下 $\beta$-HMX 热分解机理的 ReaxFF 反应分子动力学模拟

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Thermal Decomposition Mechanism of $\beta$-HMX under High Pressures via ReaxFF Reactive Molecular Dynamics Simulations

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图S1  $T$=2500K 时不同压缩态 $\beta$-HMX 晶体中平均每个 HMX 分子的分解产物 $\text{H}_2\text{CO}$ (a), HCON (b) 和 HCN (c) 的数量随时间的变化

Fig. S1  Evolution of quantities of $\text{H}_2\text{CO}$ (a), HCON (b), and HCN (c) per HMX molecule for $\beta$-HMX crystals with different densities at $T$=2500 K
Fig.S2  $T=2500$ K时不同压缩态$\beta$-HMX晶体中平均每个HMX分子的分解产物O$_2$(a)和HO(b)的数量随时间的变化

Evolution of quantities of O$_2$ (a) and HO (b) per HMX molecule for $\beta$-HMX crystals with different densities at $T=2500$ K
图S3  $T=2500$ K时不同压缩态$\beta$-HMX晶体中平均每个HMX分子的分解产物H$_2$O(a)、N$_2$(b)和CO$_2$(c)的数量随时间的变化

**Fig.S3** Evolution of quantities of H$_2$O (a), N$_2$ (b), and CO$_2$ (c) per HMX molecule for $\beta$-HMX crystals with different densities at $T=2500$ K

表S1 不同压缩态晶体中$\beta$-HMX分子的键长

**Table S1** Bond length in $\beta$-HMX molecule for crystals with different densities

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<th>Bond length/nm</th>
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表S2 不同压缩态晶体中β-HMX分子的二面角

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<th>Dihedral angle</th>
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