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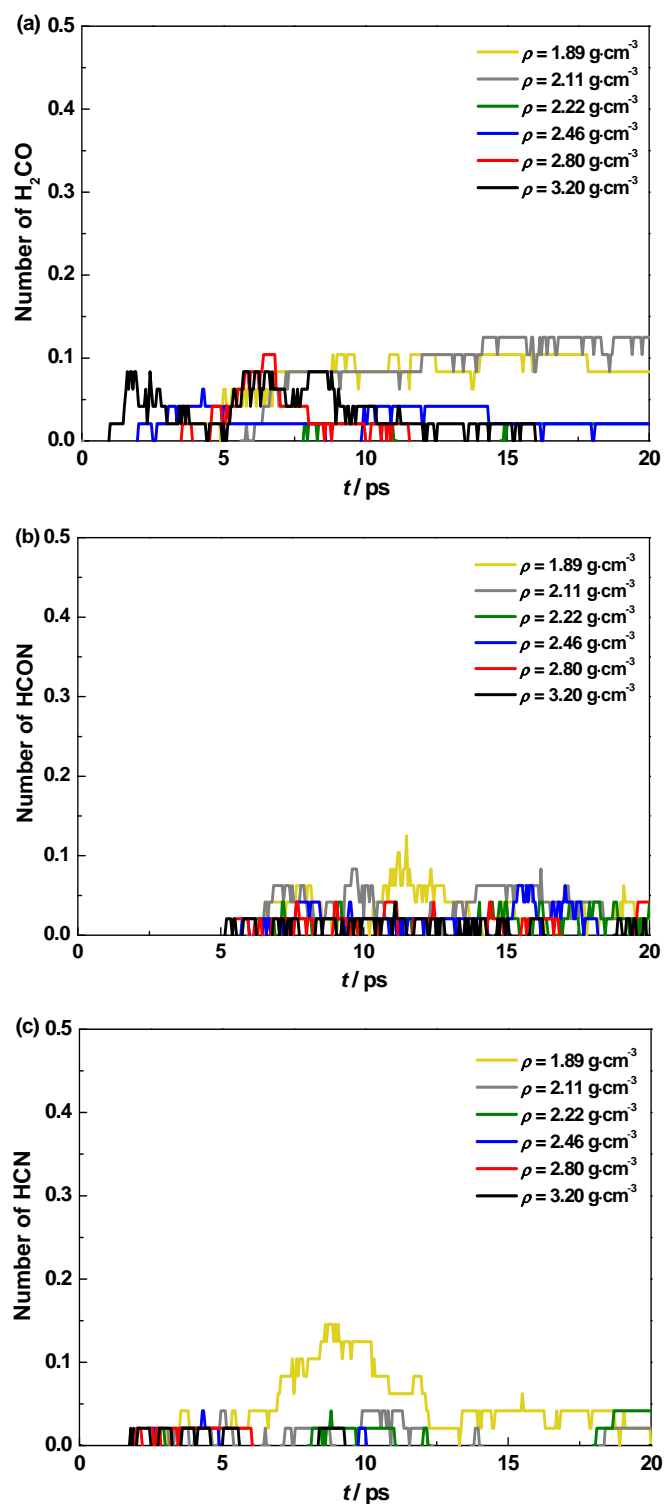
## 高压下 $\beta$ -HMX 热分解机理的 ReaxFF 反应分子动力学模拟

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

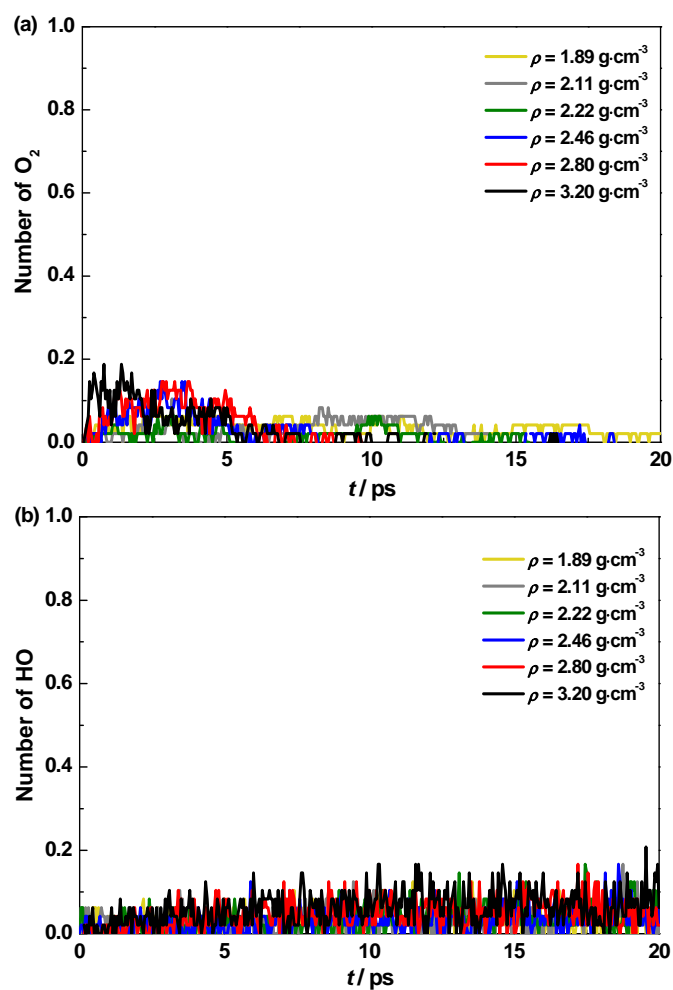
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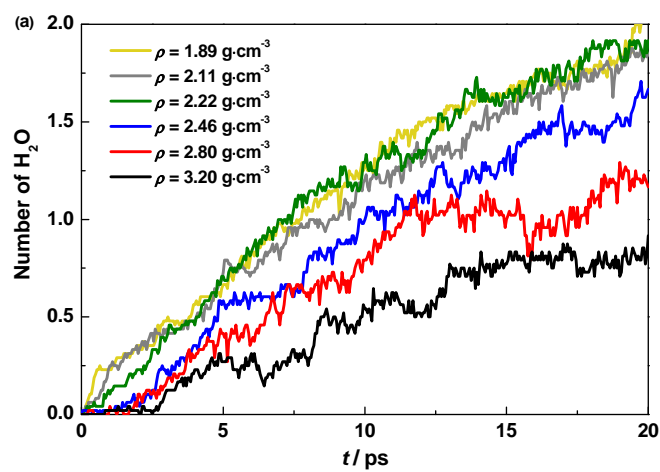
图S1  $T=2500\text{K}$ 时不同压缩态 $\beta$ -HMX晶体中平均每个HMX分子的分解产物  $\text{H}_2\text{CO}$ (a)、HCON(b)和HCN(c)的数量随时间的变化

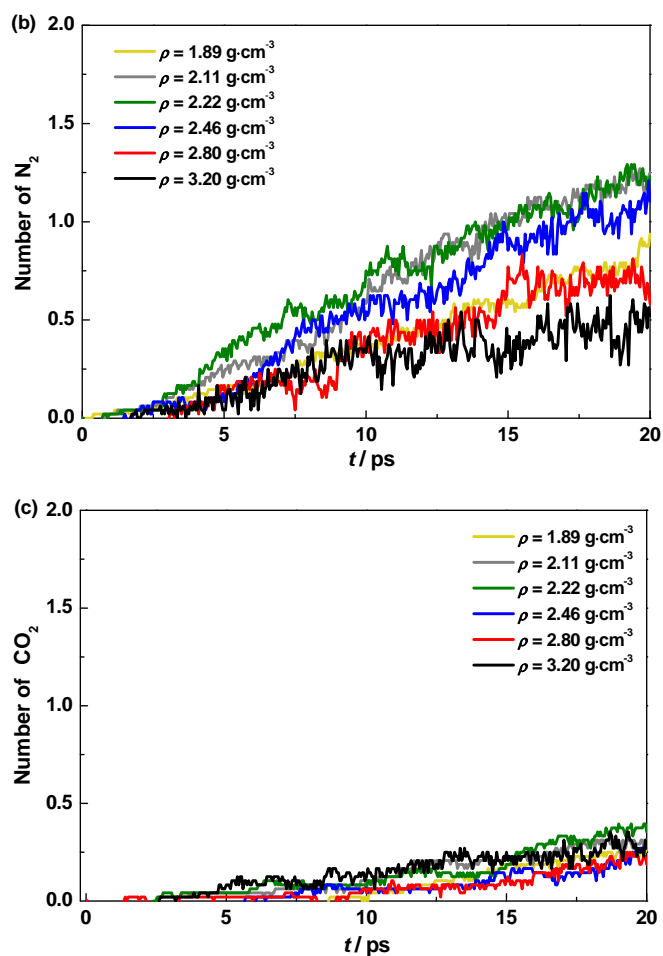
Fig.S1 Evolution of quantities of  $\text{H}_2\text{CO}$  (a), HCON (b), and HCN (c) per HMX molecule for  $\beta$ -HMX crystals with different densities at  $T=2500 \text{ K}$



图S2  $T=2500 \text{ K}$ 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

Fig.S2 Evolution of quantities of  $O_2$  (a) and HO (b) per HMX molecule for  $\beta$ -HMX crystals with different densities at  $T=2500 \text{ K}$





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  
 $\text{H}_2\text{O}$ (a)、 $\text{N}_2$ (b)和 $\text{CO}_2$ (c)的数量随时间的变化

Fig.S3 Evolution of quantities of  $\text{H}_2\text{O}$  (a),  $\text{N}_2$  (b), and  $\text{CO}_2$  (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

Bond length/nm	Density/( $\text{g}\cdot\text{cm}^{-3}$ )					
	1.89	2.11	2.22	2.46	2.80	3.20
N1-N2	0.1354	0.1304	0.1279	0.1236	0.1167	0.1063
N3-N4	0.1373	0.1331	0.1307	0.1253	0.1202	0.1146
N2-C2	0.1472	0.1417	0.1394	0.1357	0.1313	0.1331
C2-N3	0.1437	0.1384	0.1358	0.1313	0.1239	0.1128
N3-C1	0.1455	0.1403	0.1382	0.1362	0.1319	0.1363
C1-N2	0.1448	0.1392	0.1364	0.1299	0.1234	0.1123
C1-H1	0.1110	0.1083	0.1064	0.1021	0.0977	0.0923
C1-H2	0.1091	0.1044	0.1026	0.0996	0.0958	0.0950
C2-H3	0.1101	0.1046	0.1023	0.0976	0.0930	0.0867
C2-H4	0.1094	0.1075	0.1061	0.1035	0.1006	0.1029
N1-O1	0.1233	0.1185	0.1166	0.1134	0.1097	0.1109
N1-O2	0.1221	0.1188	0.1167	0.1120	0.1072	0.1016
N4-O3	0.1209	0.1167	0.1150	0.1134	0.1099	0.1138
N4-O4	0.1205	0.1159	0.1137	0.1103	0.1043	0.0967

表S2 不同压缩态晶体中 $\beta$ -HMX分子的二面角

Table S2 Dihedral angle in  $\beta$ -HMX molecule for crystals with different densities

Dihedral angle/ $^{\circ}$	Density/(g·cm $^{-3}$ )					
	1.89	2.11	2.22	2.46	2.80	3.20
H2-C1-N2-N1	13.671	13.913	13.978	14.047	14.311	15.035
H3-C2-N3-N4	32.692	33.297	33.480	34.082	34.465	36.088
C1-N2-C2-N3	18.097	18.144	18.190	18.224	18.612	19.966
N2-C2-N3-C1	101.683	103.758	104.438	106.837	108.385	115.987
C2-N3-C1-N2	-117.116	-118.661	-118.910	-119.404	-119.428	-119.201
N3-C1-N2-C2	43.334	43.082	42.786	41.150	40.372	35.437