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定常冲击波作用下六硝基六氮杂异伍兹烷(CL-20)/奥克托今(HMX)含能共晶初始分解机理研究

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Study on the Initial Decomposition Mechanism of Energetic Co-Crystal 2,4,6,8,10,12-Hexanitro-2,4,6,8,10,12-hexaazaiso-wurtzitane (CL-20)/1,3,5,7-Tetranitro-1,3,5,7-tetrazacy-clooctane (HMX) under a Steady Shock Wave

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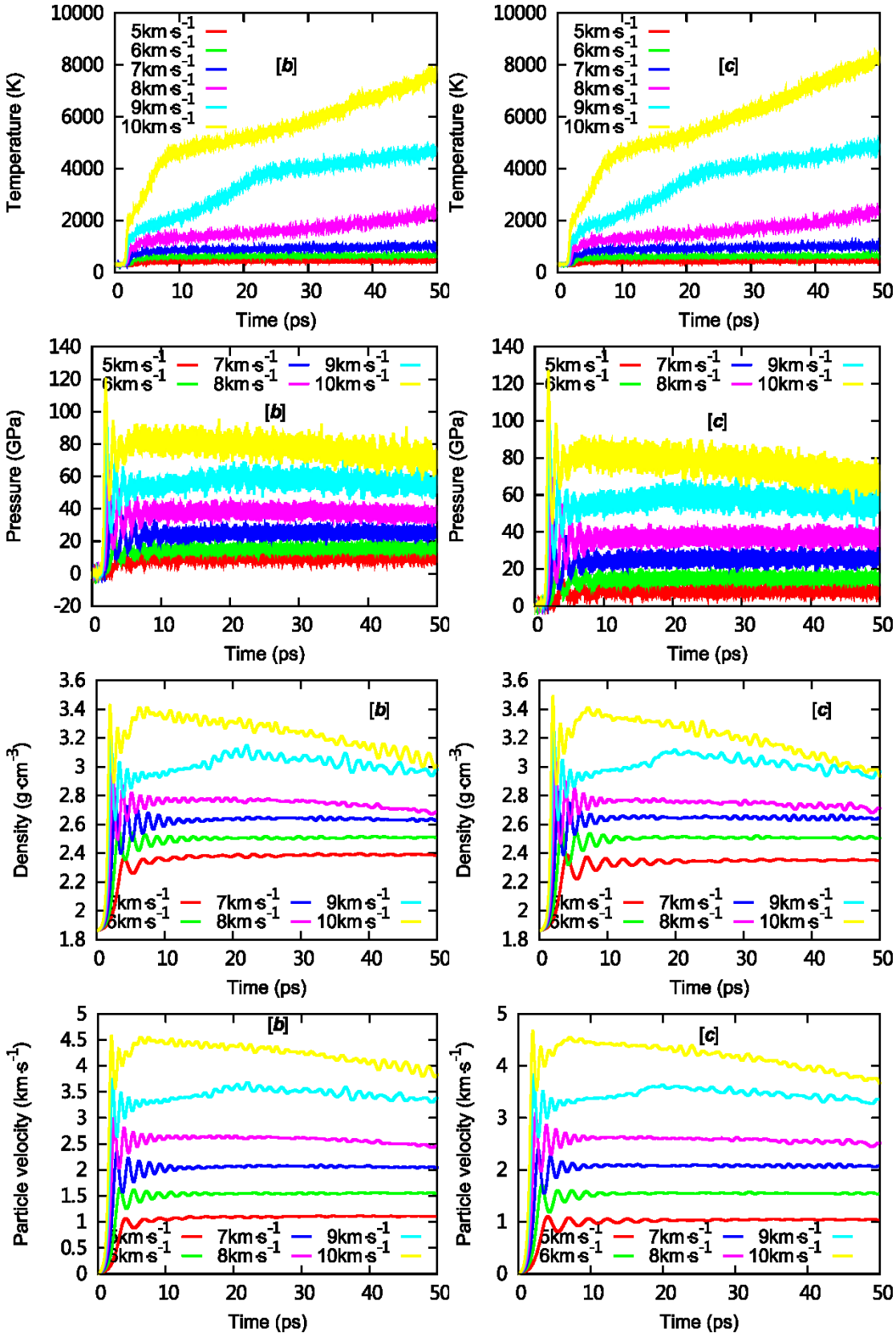
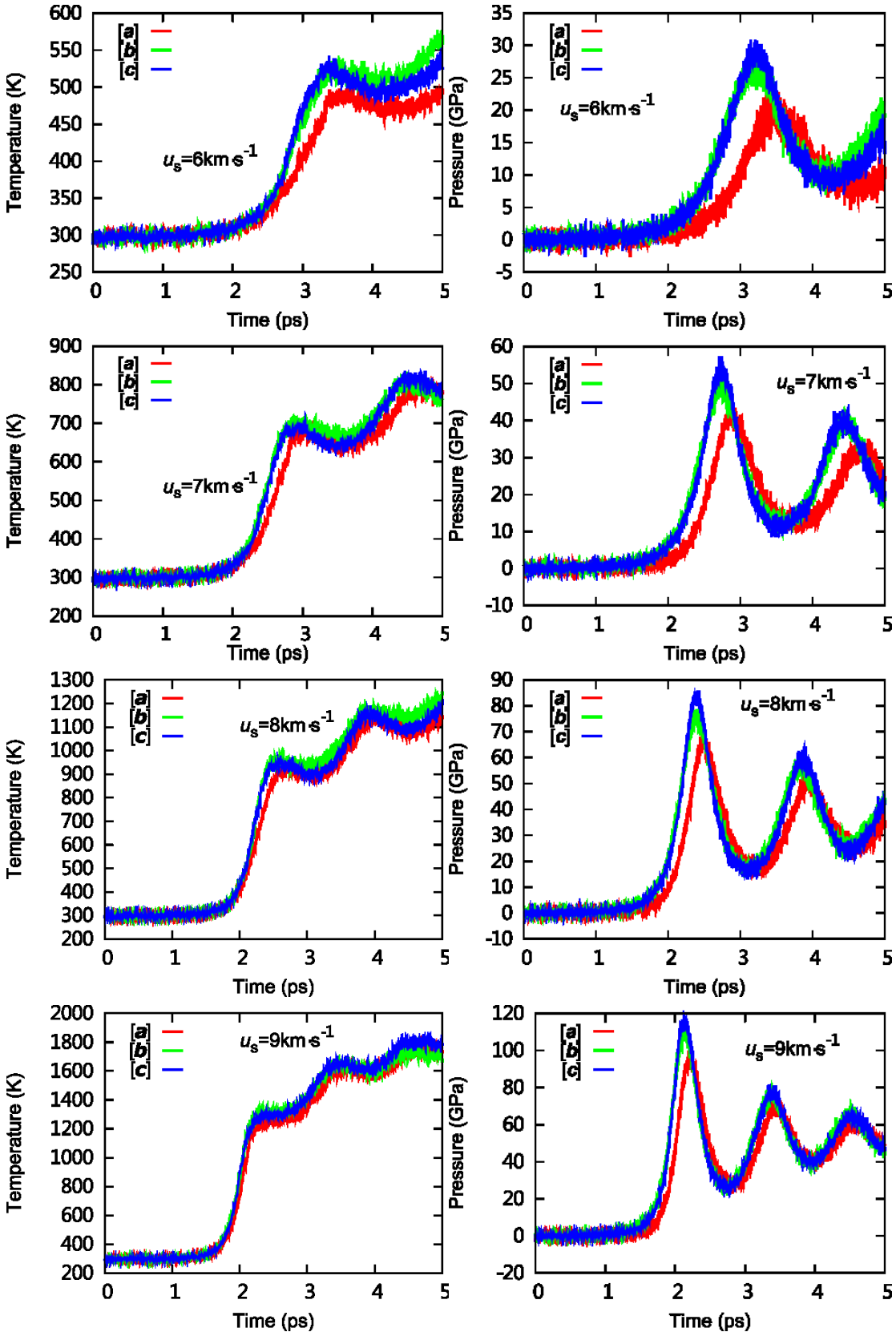

Temperature (K)
Time (ps)
[b]
[c]
5km·s-1
6km·s-1
7km·s-1
8km·s-1
9km·s-1
10km·s-1
Pressure (GPa)
Density (g·cm-3)
Particle velocity (km·s-1)

(a)


Temperature (K)
Pressure (GPa)
Time (ps)
[a]
[b]
[c]
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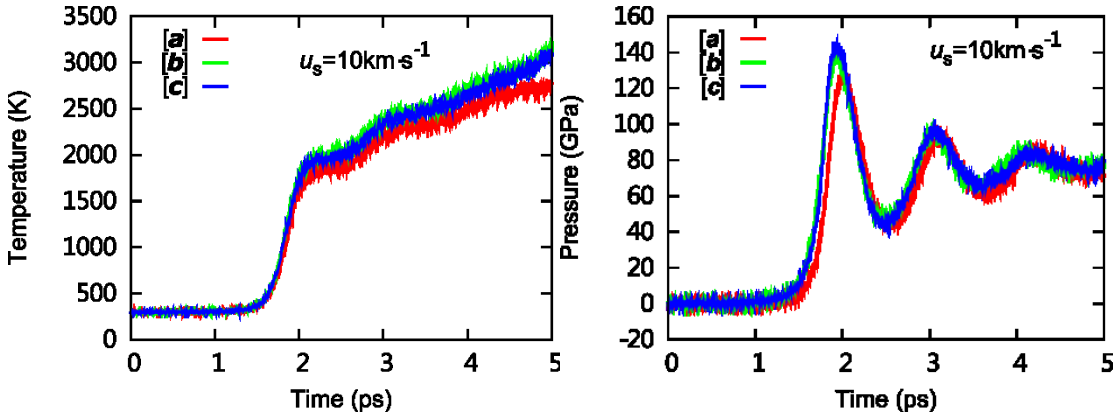
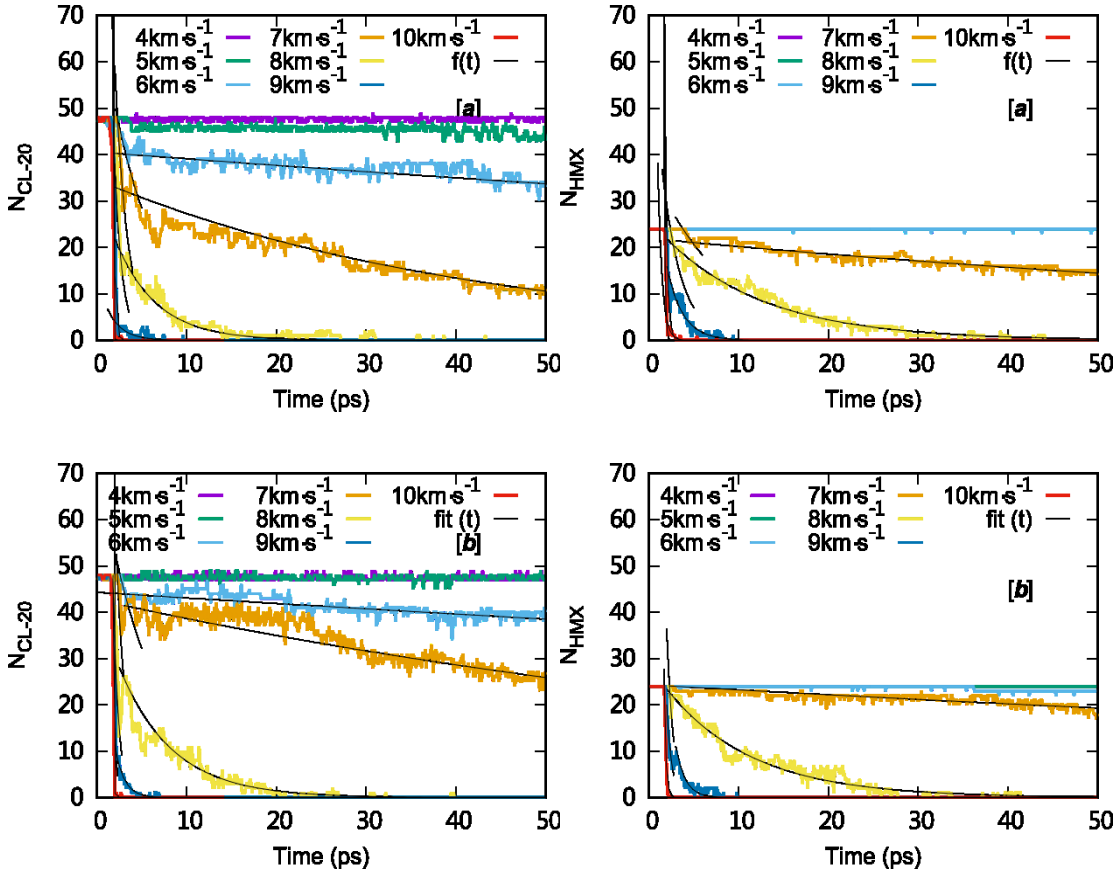
u_s=7km·s^{-1}
u_s=8km·s^{-1}
u_s=9km·s^{-1}



(b)

图 S1　*b*，*c* 晶格矢量方向的热力学演化路径及 6–10 km·s^{-1} (a)与冲击波速度条件下前 5 ps 的系统温度和压力演化曲线(b)

Fig. S1　Thermodynamic evolution paths along *b*, *c* lattice vector direction (a) and system temperature and pressure evolution curve at early 5 ps under the condition of 6–10 km·s^{-1} shock wave velocity (b).



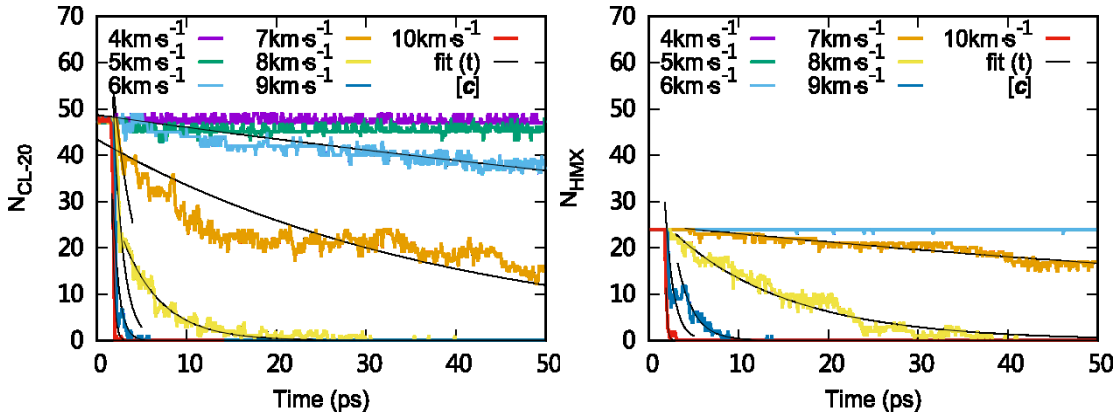
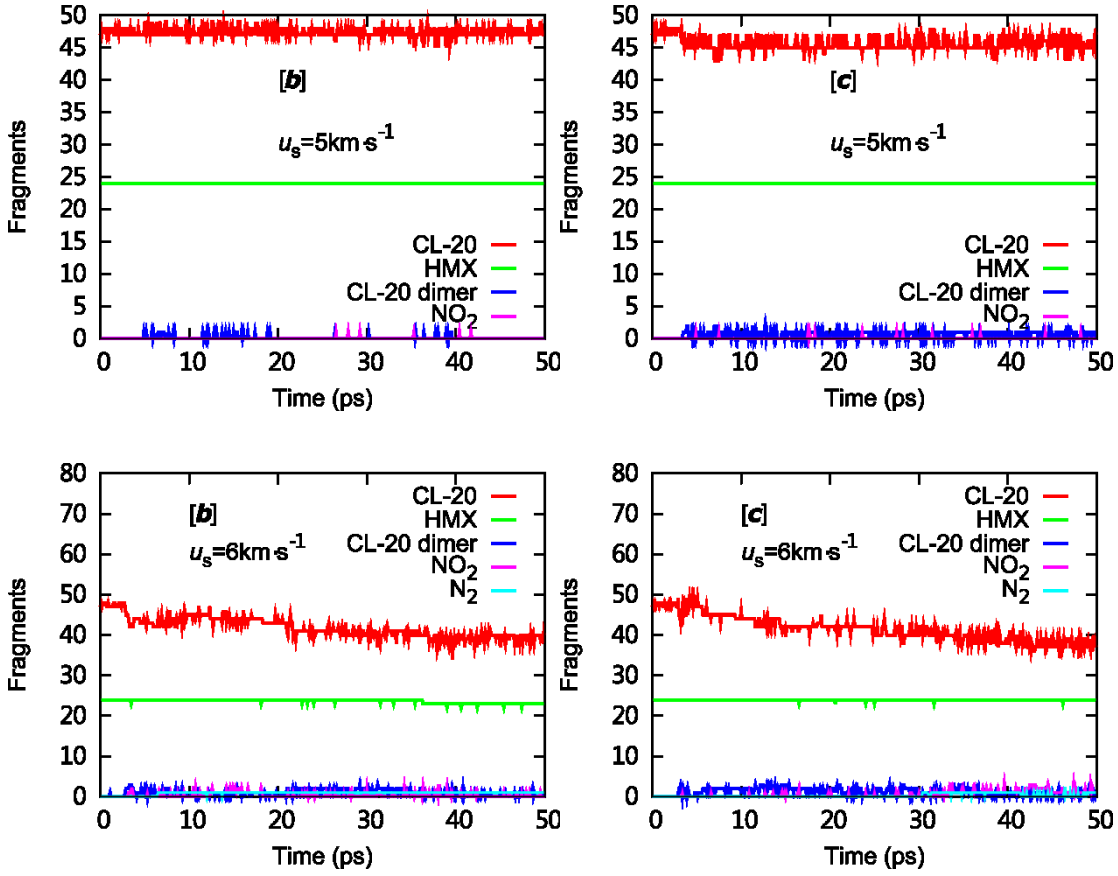


图 S2　共晶中 CL-20 及 HMX 分子数量衰减及拟合曲线

Fig. S2　The decaying curves of the amount of CL-20 and HMX molecules and the corresponding fitted curves.



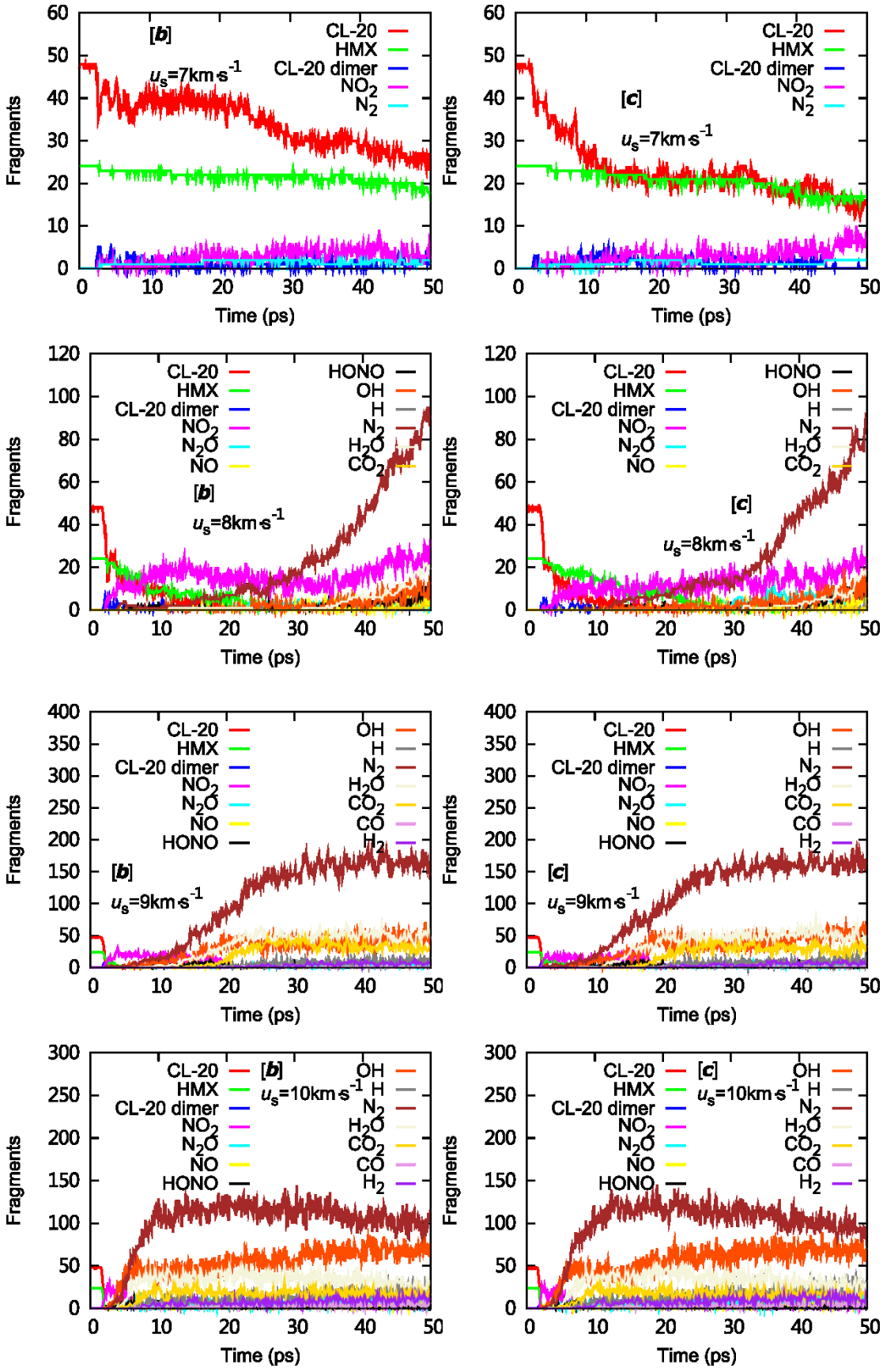


图 S3　沿晶格矢量 *b*，*c* 冲击作用下反应物衰减及产物形成演化曲线

Fig. S3　The evolution curves of reactants decay and products formation under shock wave along lattice vector *b*, *c*.

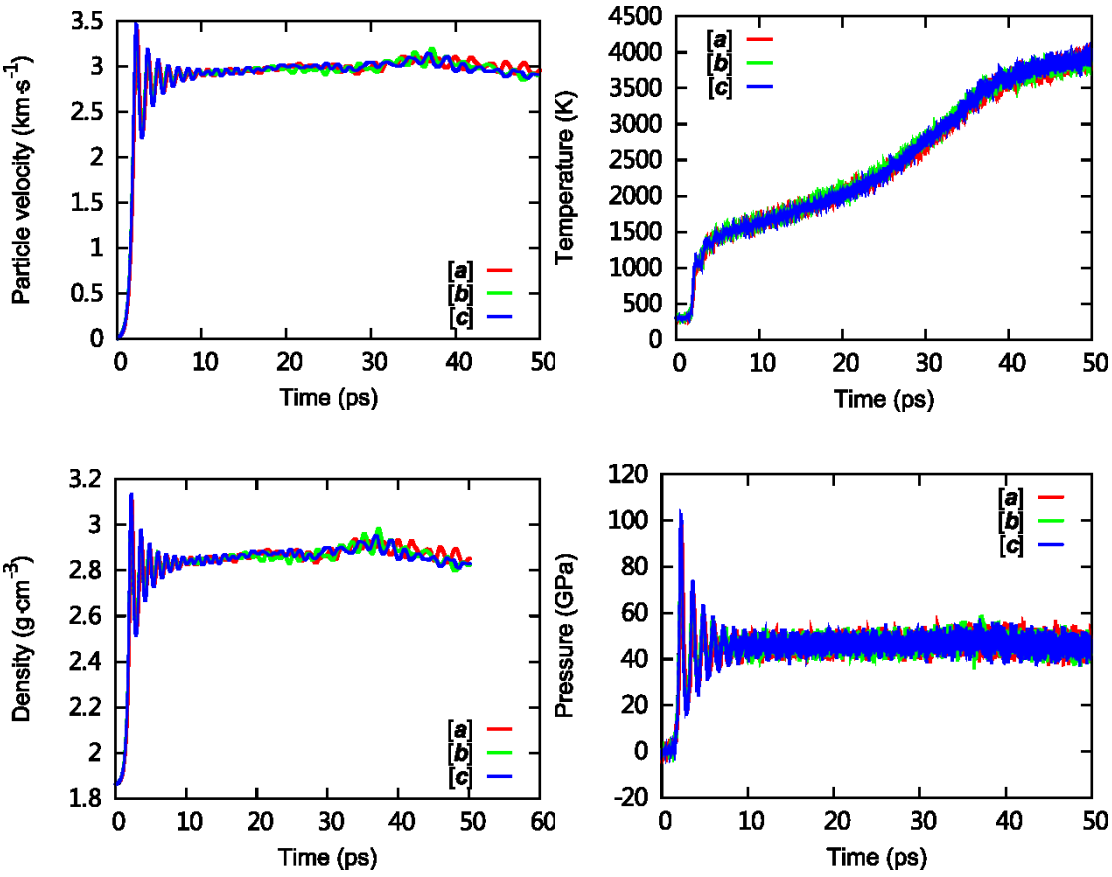


图 S4　8.5 km·s^{-1} 定常冲击波速度入射至 CL-20/HMX 含能共晶后的系统热力学演化路径

Fig. S4　Thermodynamic evolution paths of 8.5 km·s^{-1} steady shock wave velocity incident on CL-20/HMX energetic co-crystal.