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

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

Fig. S2  The decaying curves of the amount of CL-20 and HMX molecules and the corresponding fitted curves.
Fig. S3  The evolution curves of reactants decay and products formation under shock wave along lattice vector $b, c$. 

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