Supporting Information

The Co-crystal of TNT/CL-20 leads to Decreased Sensitivity toward Thermal Decomposition from First Principles Based Reactive Molecular Dynamics

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Table S_1. Bond order cut-off values for different atom pairs. *BondFrag* program uses these values as a default parameter set (can be adjusted by the user) to determine molecular fragments.

	C	H	O	N
C	0.55	0.40	0.80	0.30
H		0.55	0.40	0.55
O			0.65	0.55
N				0.45

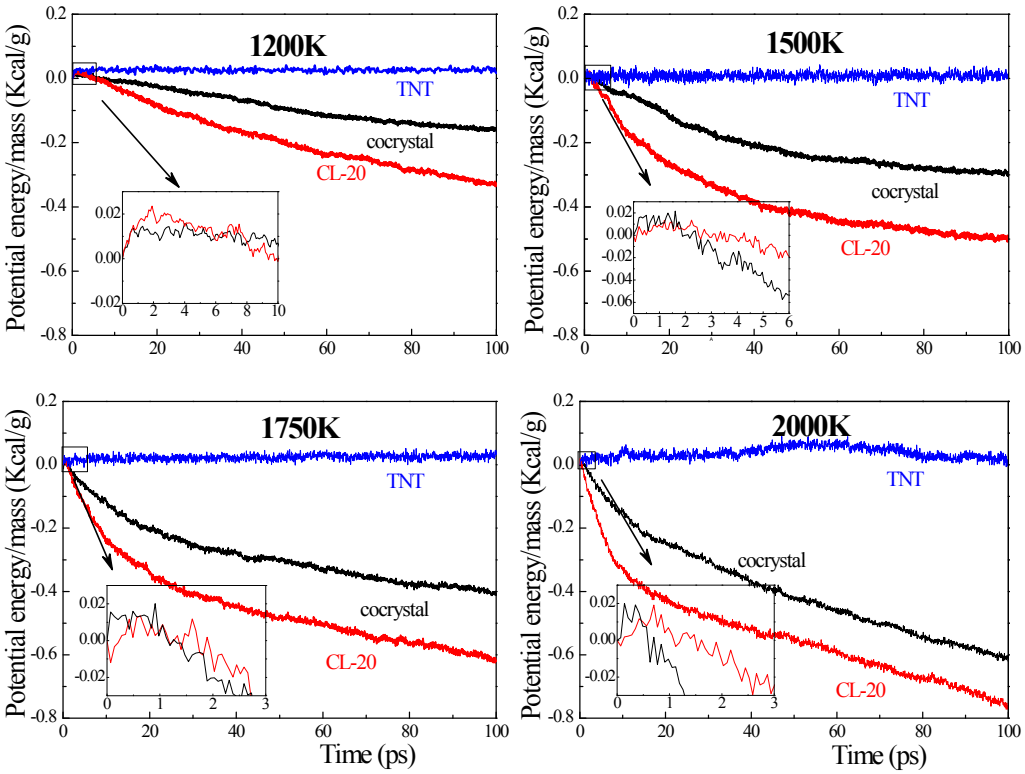

Figure S_1. Evolution of potential energy in the NVT MD simulations of CL-20, cocrystal and TNT. The initial potential energy is set to zero as a reference. For CL-20 and the cocrystal, the rate of potential energy decrease depends strongly on the temperature; whereas TNT does not react significantly under the conditions studied here. At each temperature, the energy release rate of CL-20 is faster than that of cocrystal, which is much faster than TNT.

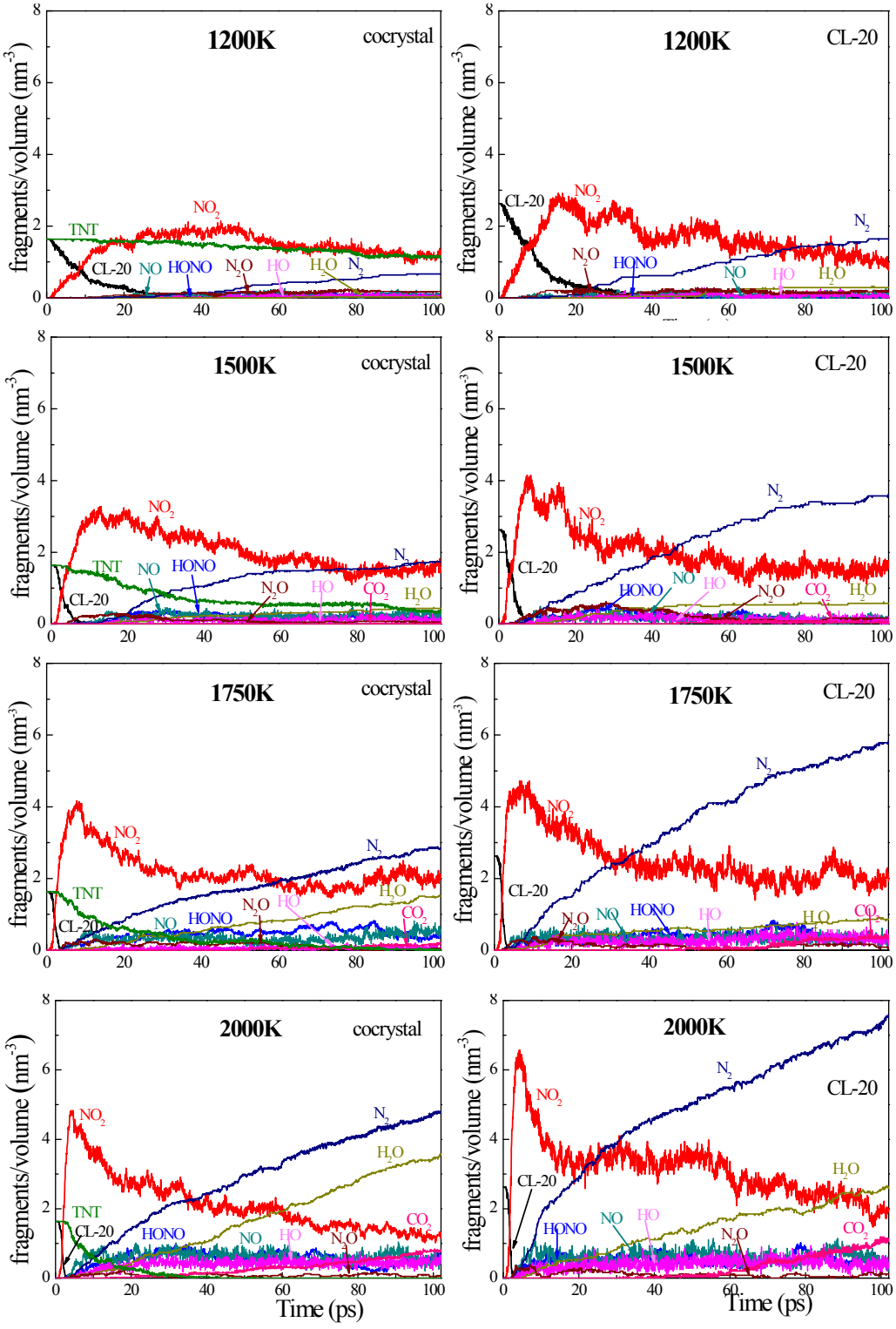

Figure S_2. Evolution of intermediate and secondary products of cocrystal and CL-20 of NVT MD. chemical reactions occur more intensely in CL-20 than in cocrystal at each temperature. NO_2 is the dominant products in the early stage of CL-20 dissociation.

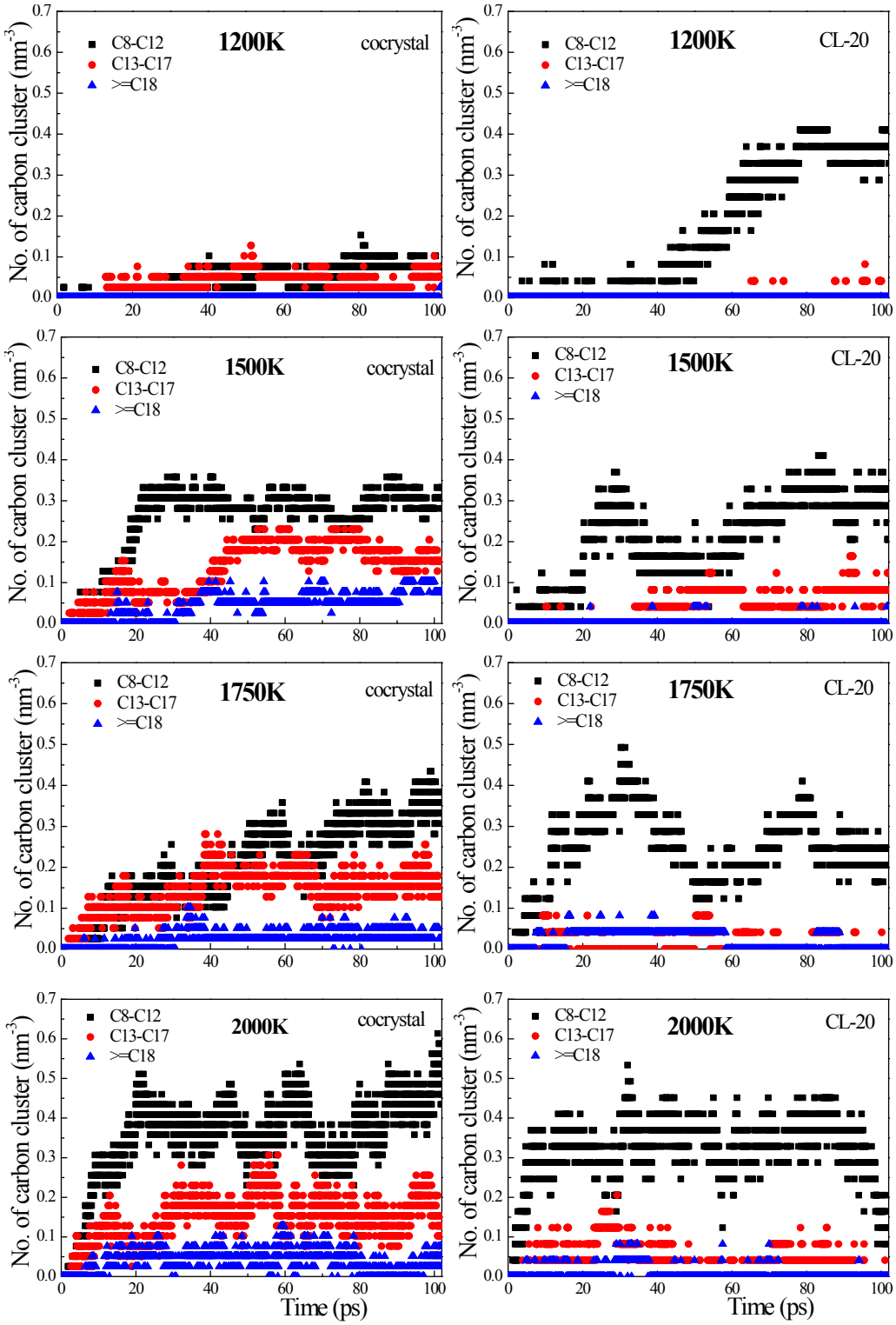

Figure S3. Time evolution of three types of carbon clusters formed for cocrystal and CL-20 during NVT-MD simulation. More and larger carbon-rich aggregates are observed in cocrystal than CL-20, leading to a slower chemical reaction process.

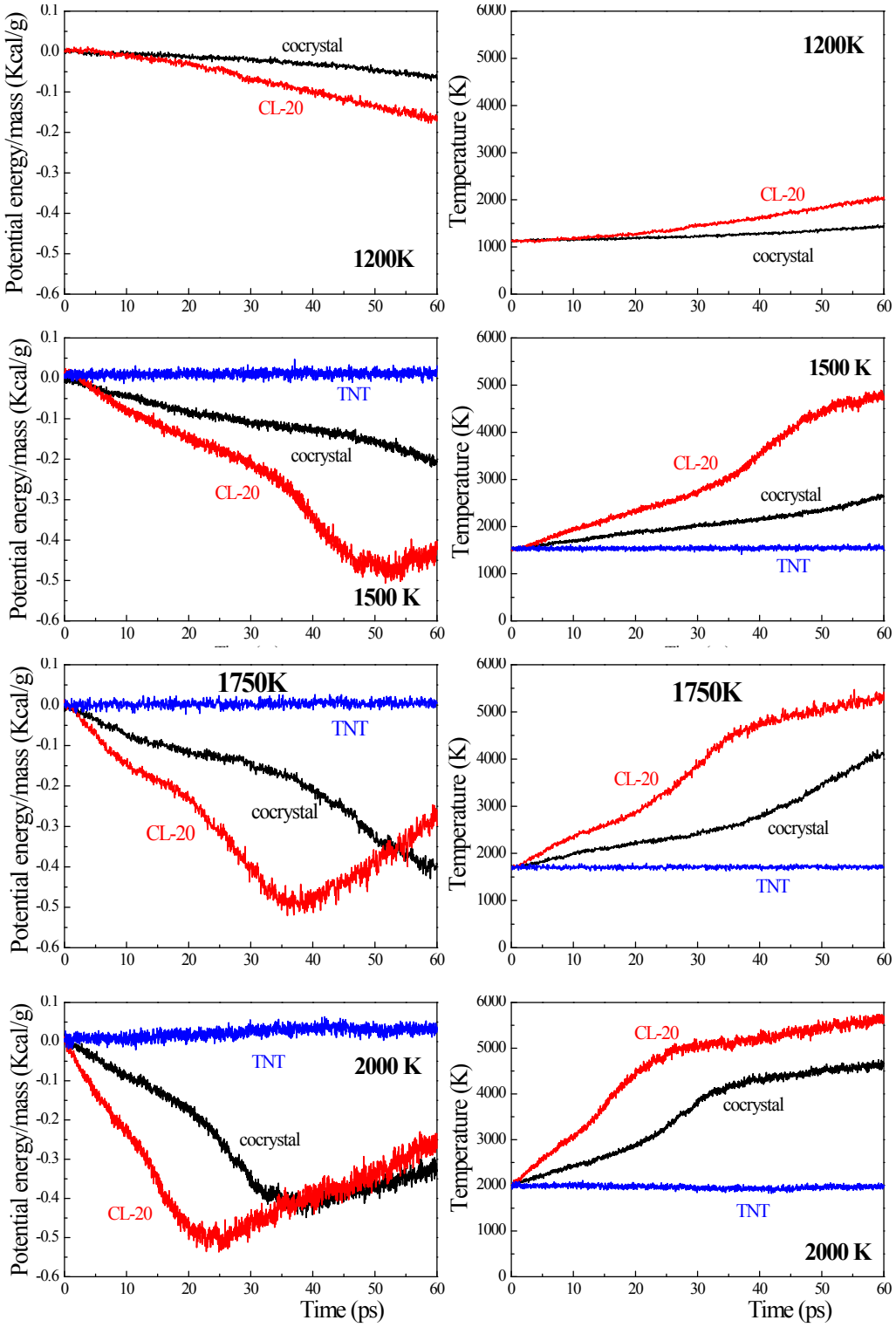

Figure S4. Normalized potential energy and temperature as a function of time during the NVE-MD with initial temperatures T = 1200, 1500, 1750 and 2000 K. The initial potential energy is set to zero as a reference.

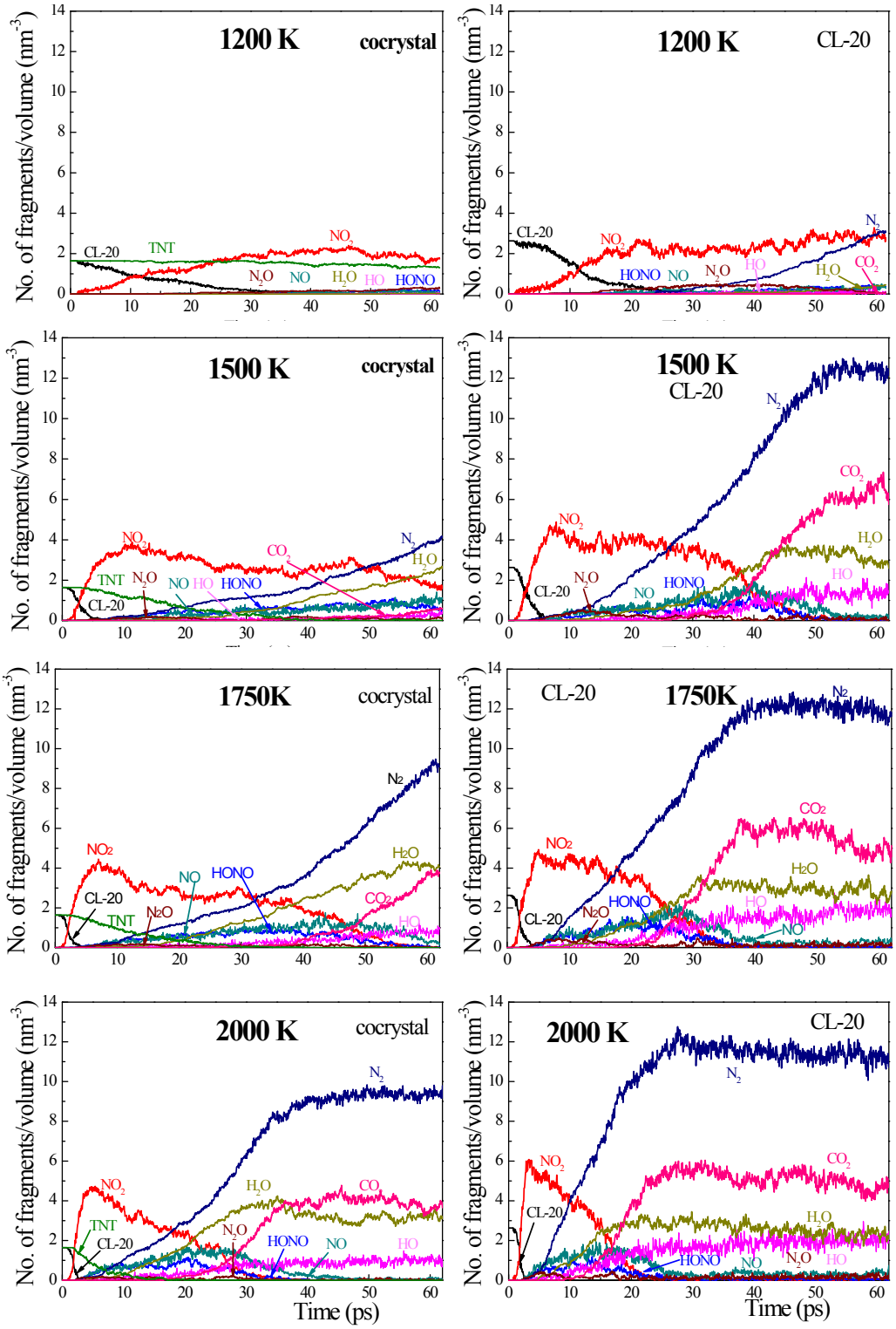

Figure S5. Time evolution of chemical products during the NVE-MD after heating to1200, 1500, 1750 and 2000 K.

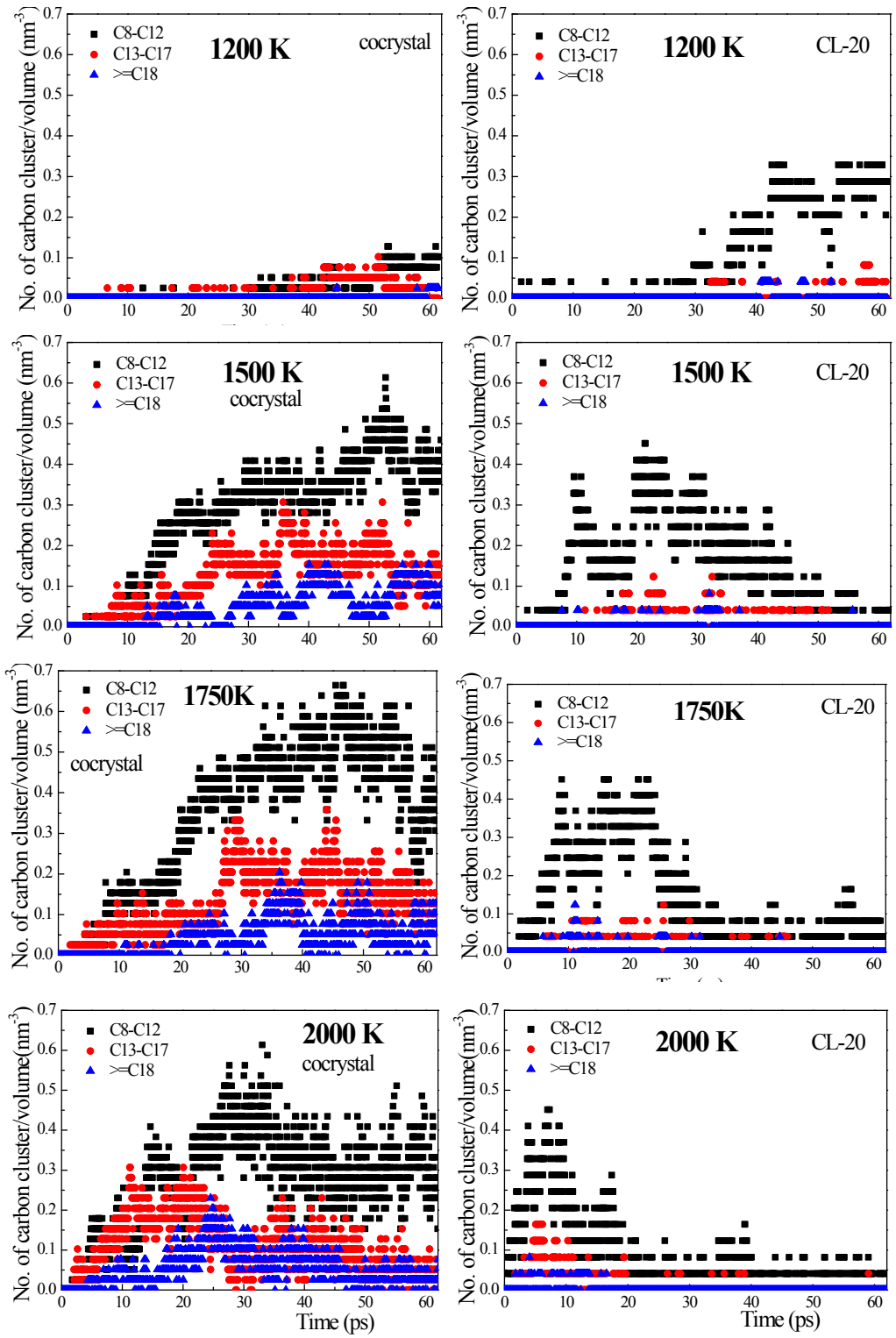

Figure S$_6$. Time evolution of three types of carbon cluster formed during NVE-MD for cocrystal and CL-20.

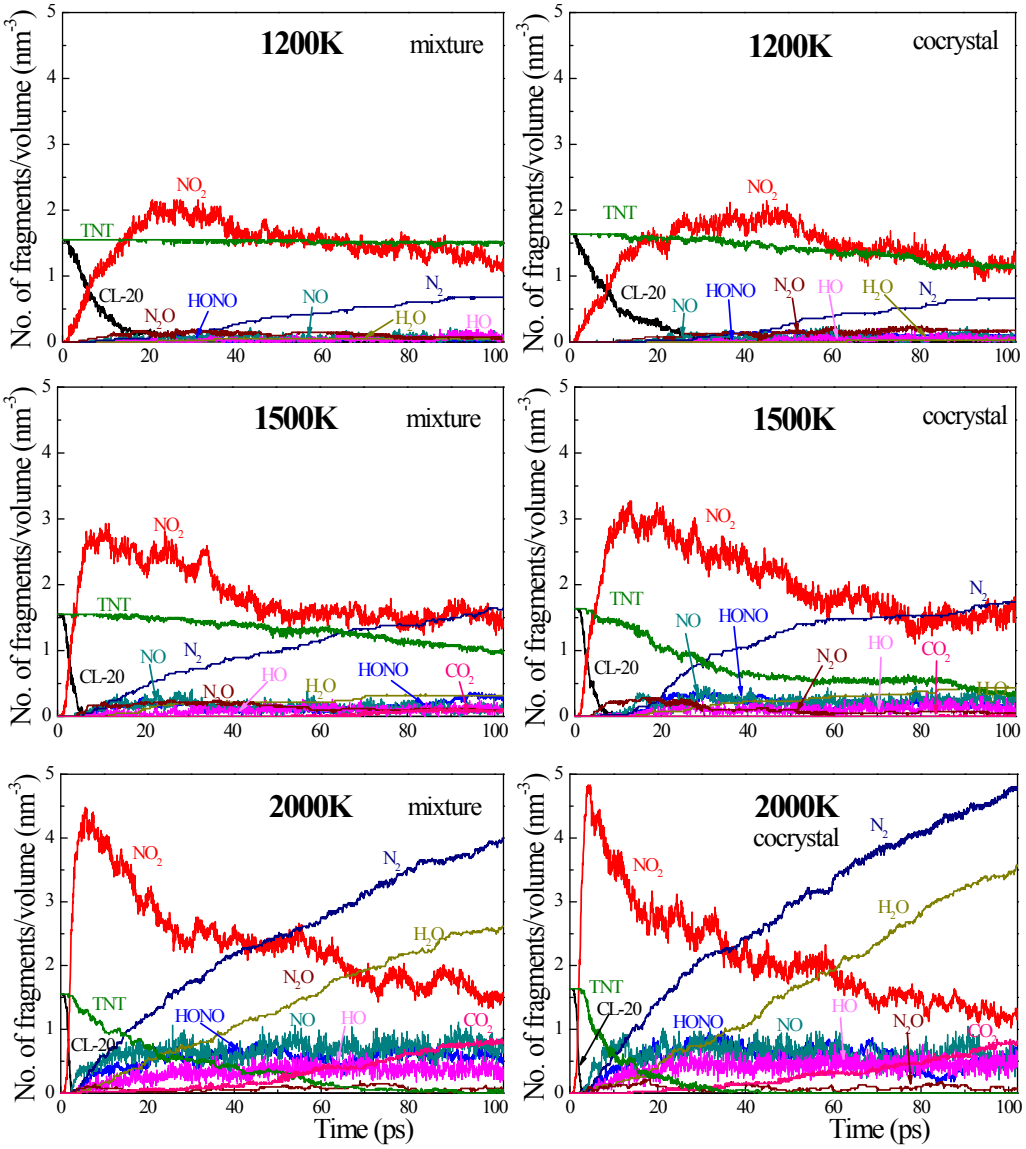

Figure S7. Evolution of intermediate and secondary products of mixture and cocrystal during NVT-MD simulations.