**Thermal decomposition mechanisms of energetic CL-20-based co-crystals: quantum molecular dynamics simulation**

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**Fig. S1** Molecular conformations and crystal structures of (a) *β*-CL-20, (b) *γ*-CL-20 and (c) *ε*-CL-20



**Fig. S2** Crystal structures and phases of CL-20 in CL-20:DNP and CL-20:DNG co-crystals

**Table S1** Bond type and bond cutoff radius in the fragment analysis of the DFTB-MD trajectory

|  |  |  |  |
| --- | --- | --- | --- |
| Bond type | Cutoff radius(Å) | Bond type | Cutoff radius(Å) |
| C−C | 2.31 | H−O | 1.50 |
| C−H | 1.63 | H−N | 1.61 |
| C−O | 2.15 | O−O | 2.22 |
| C−N | 2.20 | O−N | 2.10 |
| H−H | 1.11 | N−N | 2.17 |

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