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## Supporting Information

### **Impact-Induced Mechanical and Chemical Responses of Cyclobutane Nitric Ester Isomers: A Reactive Molecular Dynamics Study**

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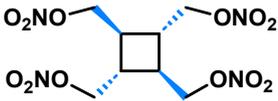
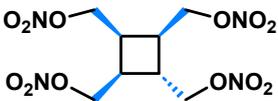
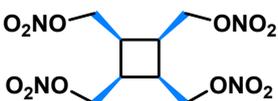
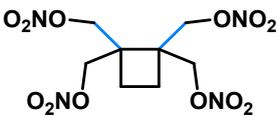
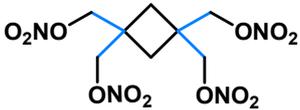
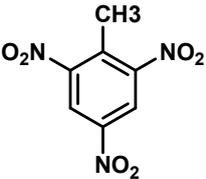
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**Table S1.** Modeling parameters of TNCBNE isomers

Isomer	Structural formula	Unit Cell Expansion	Total atoms
Iso-2		9×4×5	23328
Iso-3		10×7×6	30240
Iso-5		6×7×5	27204
Iso-6		12×3×4	29160
Iso-7		3×4×9	29180
TNT		4×4×10	25540

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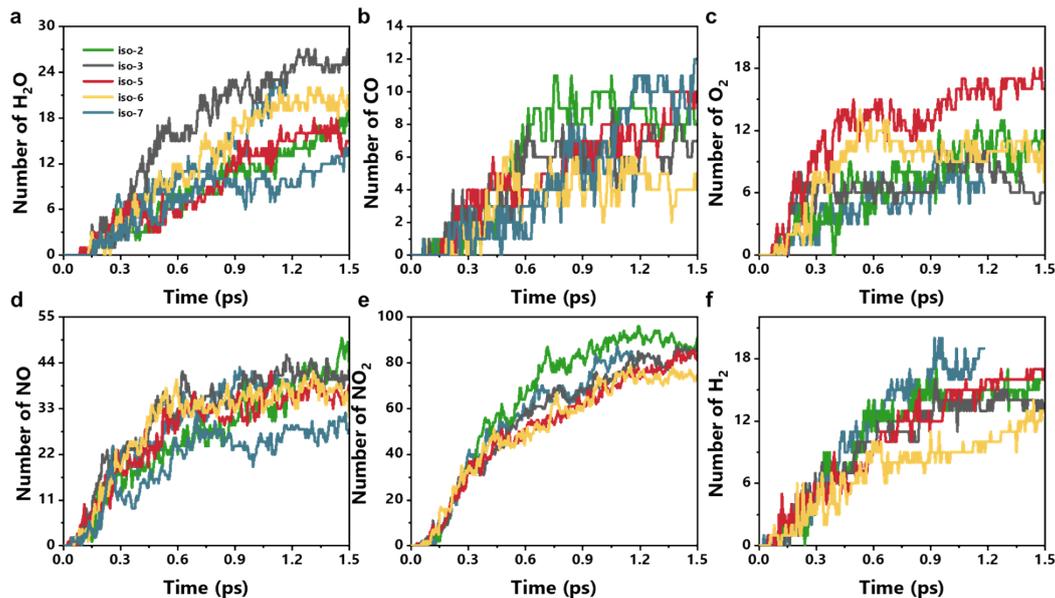
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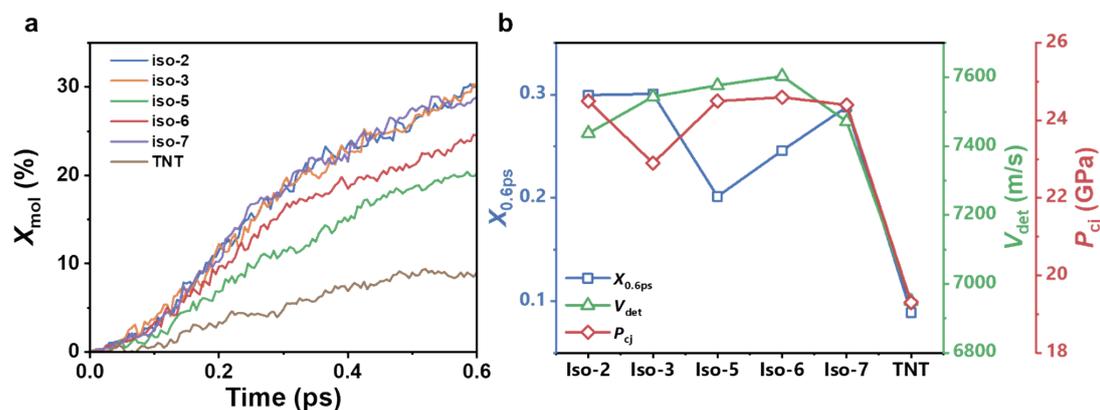
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40 **Fig. S1.** Temporal evolution of major decomposition products including (a) H<sub>2</sub>O, (b)  
 41 CO, (c) O<sub>2</sub>, (d) NO, (e) NO<sub>2</sub>, and (f) H<sub>2</sub> for different TNCBNE isomers.

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46 **Fig. S2.** (a) Time evolution of the total molecule generation rate ( $X_{mol}$ ) for different  
 47 isomers and TNT; (b) comparison of the molecule generation rate at 0.6 ps ( $X_{0.6}$ ),  
 48 detonation velocity<sup>1</sup> ( $V_{det}$ ), and Chapman–Jouguet pressure<sup>1</sup> ( $P_{CJ}$ ) among different  
 49 isomers and TNT.

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52 **Reference**

- 53 1. L. M. Barton, J. T. Edwards, E. C. Johnson, E. J. Bukowski, R. C. Sausa, E. F. C. Byrd, J. A.  
54 Orlicki, J. J. Sabatini and P. S. Baran, *Journal of the American Chemical Society*, 2019, **141**,  
55 12531-12535.  
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