Toward Low-sensitive and High-energetic Cocrystal II: Structural, Electronic and Energetic Features of CL-20 Polymorphs and the Observed CL-20-based Energetic-energetic Cocrystals

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Electronic supplementary information (ESI)

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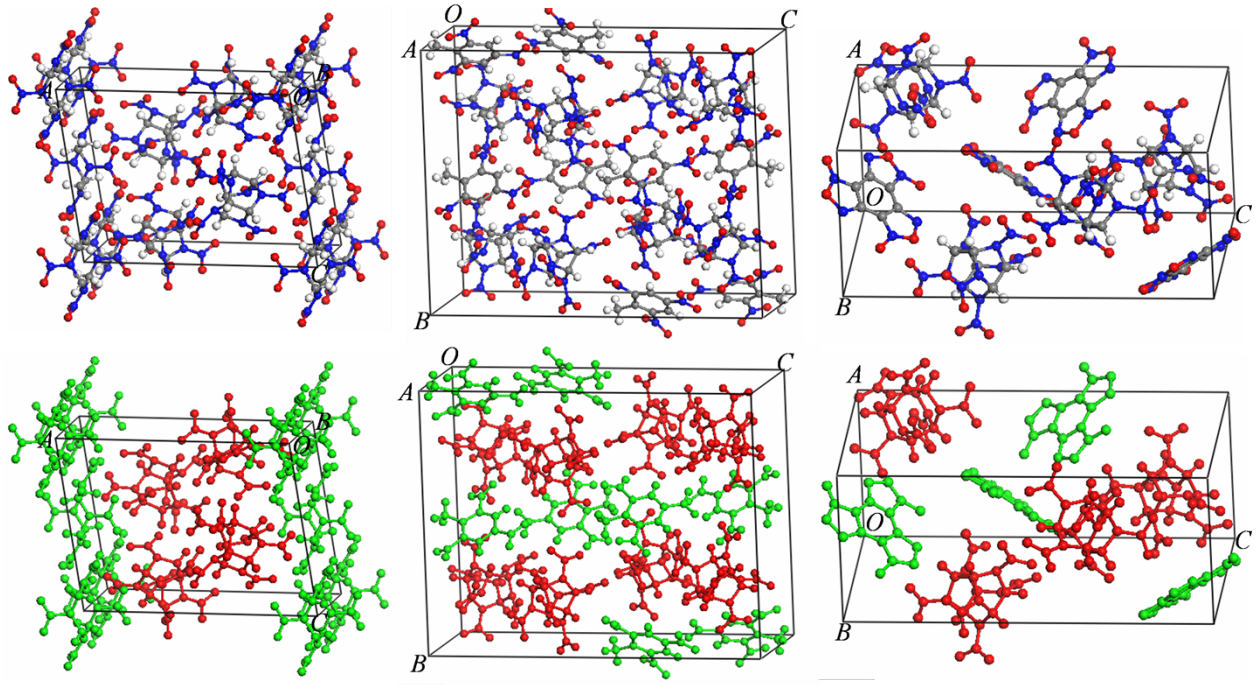
S1. Crystal packing of three CL-20-based EECCs.



(a) CL-20/HMX (b) CL-20/TNT (c) CL-20/BTF

Figure s1. Crystal packing of three CL-20-based EECCs. In the bottom arrow, two kinds of energetic molecules are distinguished by different colors.

S2. Relative energy of three formed conformers of CL-20 is gaseous state and solutions.

The geometries of α (γ), β, and ε-formed CL-20 conformations in gaseous state and solvents and all solvent molecules were fully optimized at the B3LYP/6-311++G** level of density functional theory.

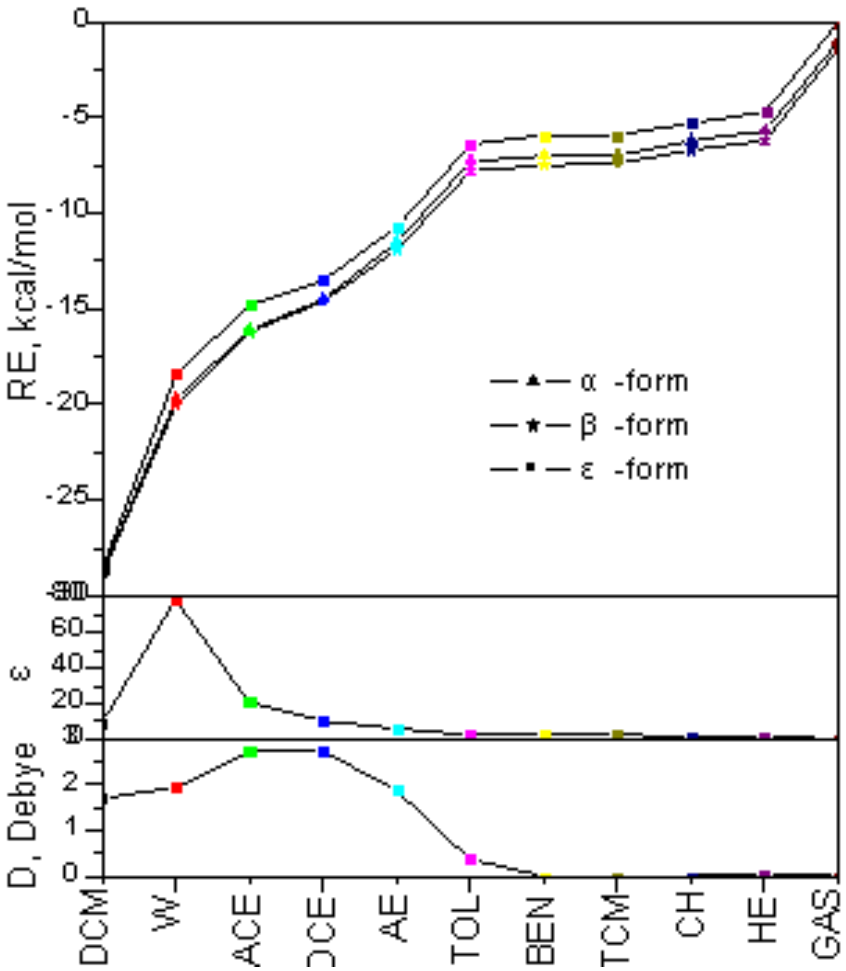


Figure s2. Relative energies of three interested CL-20 conformations in the ten solvents to the ε-formed one in gaseous state, dielectric constants (ε) and dipole moments (D) of the solvents. Ten solvents with a large range of dielectric constants (ε) within 1.92-78.39, heptane (HE), cyclohexane (CH), carbontetrachloride (TCM), benzene (BEN), toluene (TOL), acetic ether (AE), dichloromethane (DCM), dichloroethane (DCE), acetone (ACE) and water (W).

S3. Dihedrals in β-CL-20, CL-20/TNT, CL-20/HMX and CL-20/BTF.

Table s1. Dihedrals in β-CL-20, CL-20/TNT, CL-20/HMX and CL-20/BTF.

	β-CL-20	CL-20/TNT	CL-20/HMX	CL-20/BTF
C27-N17-N18-O5	-23.7	-38.9	-15.3 (γ)/(β)	19.1
C30-N13-N14-O1	-26.3	-15.7	20.1	21.3
C27-N19-N20-O7	-15.1	-17.3	22.9	17.7
C30-N23-N24-O12	-28.1	-33.0	24.7	16.8

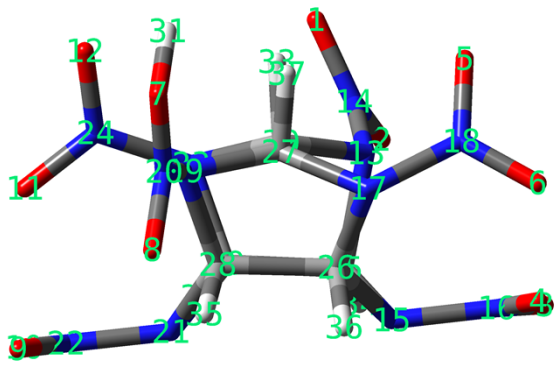


Figure s3. Atomic numbering of β-CL-20.

S4. Crystal packing of TATB.

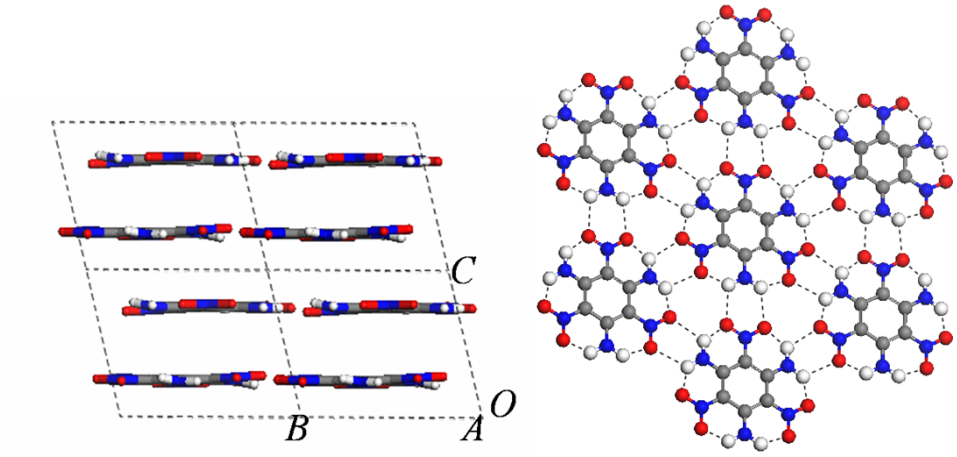


Figure s4. Layered crystal packing of TATB (left) and hydrogen bonds in a layer represented by dash (right).