Supplemental material for

Flexible-molecule force field to model and study Hexanitrohexaazoisowurzitane (CL-20) – Polymorphism under extreme conditions

X. Bidault and S. Chaudhuri

Department of Civil and Materials Engineering, University of Illinois at Chicago, Chicago, Illinois 60607, United States



1. Model/experiment comparison of pressure-induced variations of ε-CL20 lattice parameters

FIG. S1. Evolution of ε -CL20 lattice parameters with pressure: MD simulations using SB-CL20 without and with CCNN dihedral add-on, and comparison with experiments (see main text for simulation details and references).

2. Distributions of wag angles δ and mean values in other polymorphs than ϵ -CL20



FIG. S2. Left: Wag angle (δ) distributions in γ -CL20. Right: experimental conformation from .cif file (ref. 117778 on CCDC). Bottom: Experimental δ and mean values extracted from the distributions.



ζ-CL20 at 3.3 GPa

 δ from exp. .cif file

δ - MD SB-CL20	-30.2	+37.6	+45.5	5 +43.7	+46.8	-43.5
δ - MD SB-CL20 + CCNN	-30.7	+41.4	+45.9	+42.9	+47.7	-44.1
FIG. S3. Left: Wag ang	le (δ) distributions	in ζ-CL20.	Right:	experimental	conformation	from .cif file

+32.1

+41.8

+41.6

+42.2

-44.0

-37.3

(ref. 765864 on CCDC). Bottom: Experimental δ and mean values extracted from the distributions.

α-CL20



* From experimental structure containing water, whereas simulations are without water.

FIG. S4. Left: Wag angle (δ) distributions in α -CL20. Right: experimental conformation from .cif file (ref. 117776 on CCDC). Bottom: Experimental δ and mean values extracted from the distributions.



FIG. S5. Left: Wag angle (δ) distributions in β -CL20. Right: experimental conformation from .cif file (ref. 117777 on CCDC). Bottom: Experimental δ and mean values extracted from the distributions.

3. Replication-induced defects in supercell-framed ε-CL20 at 30 GPa (SB-CL20 + CCNN FF)



FIG. S6. Defects in supercell-framed ε-CL20 at 30 GPa (SB-CL20 + CCNN FF). Only mol. sym. #1 is shown. Left: defects due to odd replication 15x9x9 (AA or BB instead of AB or BA alternation) – blue: defects along "2c" lattice parameter – red: defects along "2a" lattice parameter. Right: even initial replication 14x8x8 and no supercell defect.

4. Density and pressure during the decompression of the γ sample up to its disintegration



FIG. S7. Density and pressure during the decompression of the γ sample modeled with SB-CL20 + CCNN FF, up to its disintegration.