Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information

The Anisotropic Structure Deformation of β-Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine under High Pressure: A Vibration Spectra Calculation and Resolving Based on AIMD Simulation

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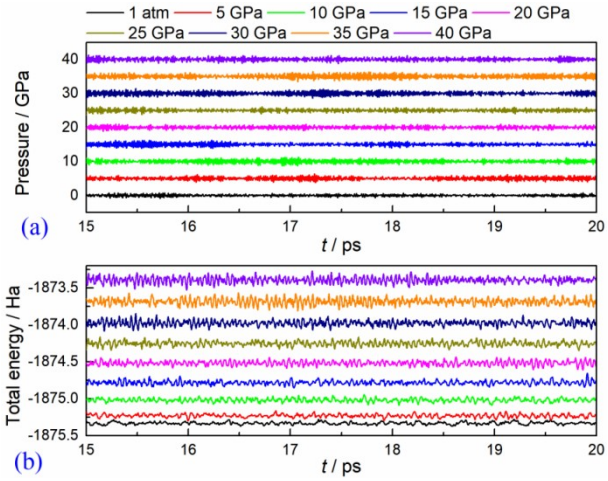

Fig. S1 Pressure and total energy evolution versus simulation time.

Tab. 1 Vibrational modes for Raman frequencies.

Raman	Vibration mode	Raman	Vibration mode
118	τ(ring)	1028	τ(ring)
143	τ(ring)+τ(NO_2)	1059	τ(ring)+γ($NO_{2\text{-axial}}$)
155		1128	τ(ring)+ ρ(CH_2)
181		1170	τ(ring)
211	τ(ring)	1179	τ(ring)+ν($NO_{2\text{-axial}}$)
221	τ(ring)+γ(NO_2)	1202	ν($NO_{2\text{-equatorial}}$)+ ρ(CH_2)
285		1251	ν(ring)+γ(NO_2)+ δ(CH_2)
295	τ/ν(ring)	1324	
354		1401	
428		1451	ν_{as}($NO_{2\text{-equatorial}}$)+ω(CH_2)
460	γ(NO_2)	1532	ν_{as}(NO_2)
493	τ(ring)+γ(NO_2)	1623	
603		1683	τ(ring)+γ(NO_2)
642	γ(NO_2)	1900	ν_{as}($NO_{2\text{-axial}}$)
702	τ(ring)+γ(NO_2)	1926	
783	τ(ring)+γ(NO_2)+γ(CH_2)	3109	ν_s(CH_2)
829	τ(ring)+ν($NO_{2\text{-axial}}$)	3163	ν_{as}(CH_2)
879	τ(ring)	3222	
902	τ(ring)+γ(NO_2)		

ν: stretching vibration; δ: deformation vibration; τ: torsional vibration; γ: ring structural deformation and combined with adjacent non-ring bond; ω: wag out of plane; ρ: rocking in plane; as: anti-symmetric; s: symmetric.