Electronic Supplementary Information

Host-guest Energetic Materials: a Promising Strategy of Incorporating Small Insensitive Molecule into the Lattice Cavities of 2, 4, 6, 8, 10, 12-Hexanitrohexaazaisowurtzitane to Enhance the Safety on the Premise of Maintaining the Excellent Energy Density

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Supplementary Figures and Tables

1 Figures

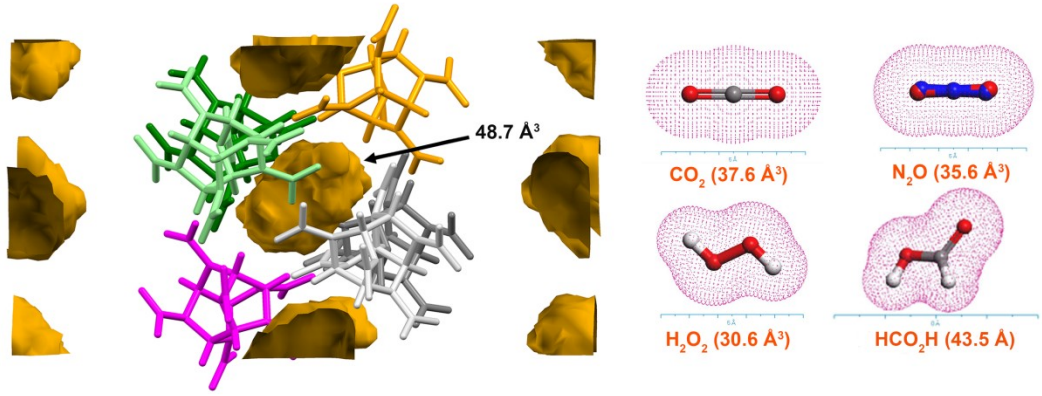

Figure S1. The excellent space matching between the guest molecules and the host explosives was proved by calculating the volume of lattice cavities in HNIW and the molecular volumes of guest molecules.

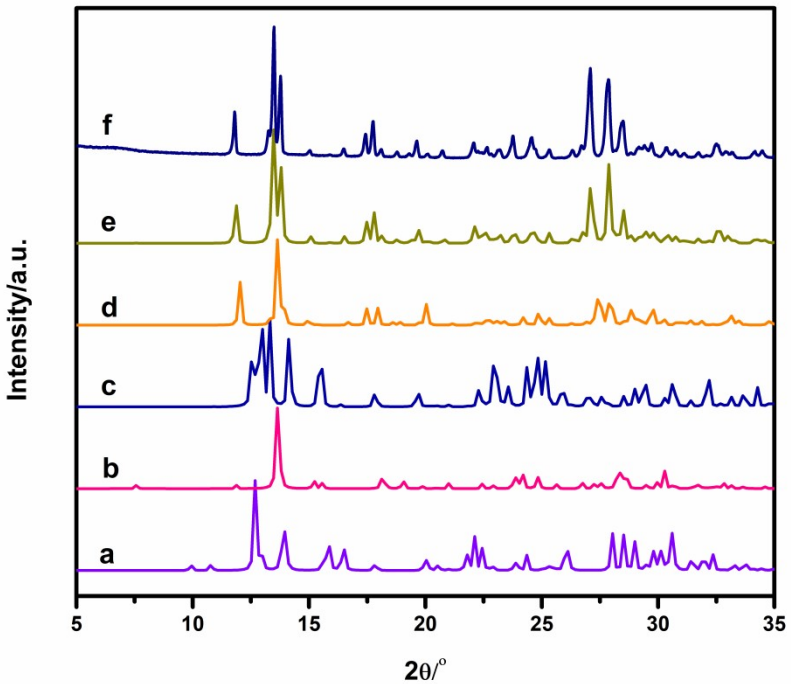

Figure S2. Powder X-ray diffraction patterns of HNIW-MA, α-HNIW, γ-HNIW, β-HNIW and ε-HNIW. a) simulated pattern of ε-HNIW; b) simulated pattern of β-HNIW; c) simulated pattern of γ-HNIW; d) simulated pattern of α-HNIW; e) simulated pattern of HNIW-MA; f) experimental pattern of HNIW-MA.

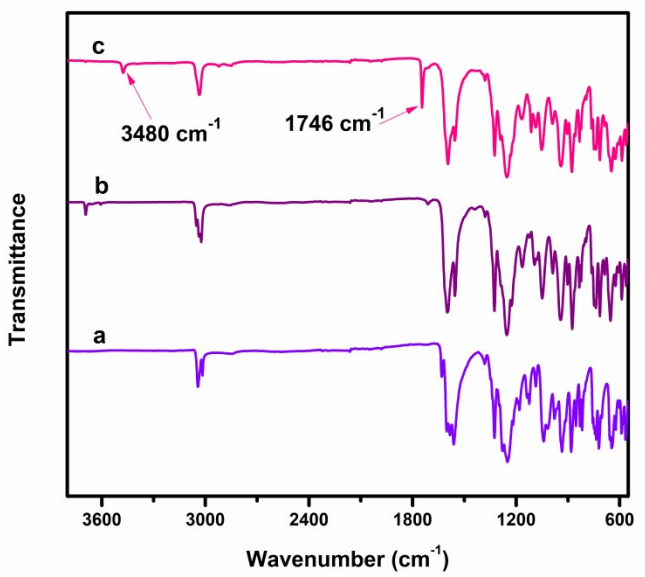

Figure S3. The IR spectroscopy of ε-HNIW, α-HNIW and HNIW-MA. a) ε-HNIW; b) ε-HNIW; c) HNIW-MA.

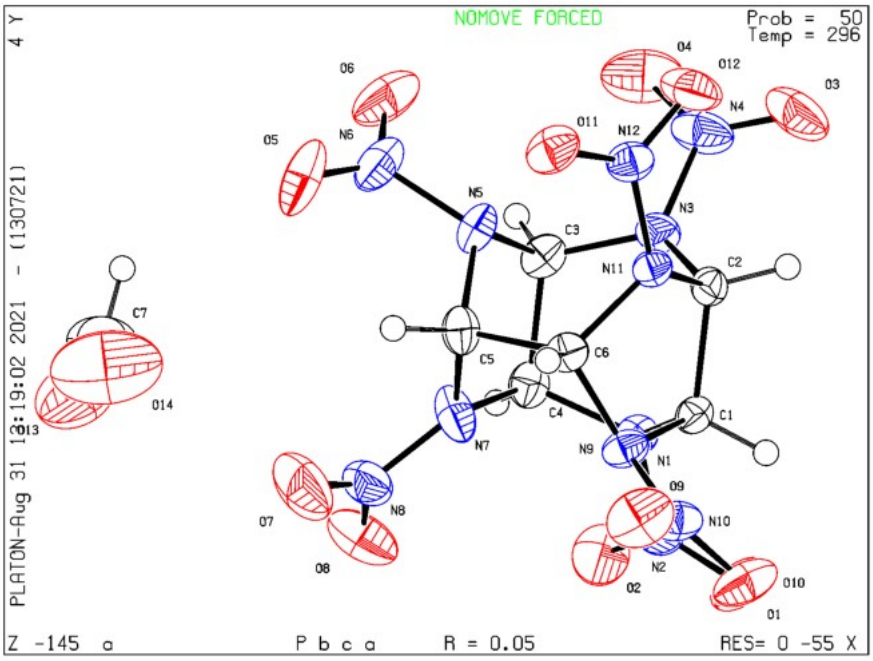

Figure S4. ORTEP diagram for HNIW-MA collected at 296 K with thermal ellipsoids of 50% probability.

2 Tables

Table S1. The calculated packing coefficient value of HNIW-MA.

Materials	V (cell)/Å^3	V_m(HNIW)/Å^3	V_m (guest)/Å^3	packing coefficient/%
HNIW-MA	3059.9	292.18	43.75	82.11 %

Table S2. Hydrogen bond lengths (Å) and bond angles (°) for HNIW-MA.

	D–H···A	d(H···A)	d(D···A)	Angle(D–H···A)

HNIW-HA	C(4)-H(4)···O(14)	2.35 Å	2.89 Å	114°
	C(3)-H(3)···O(14)	2.49 Å	2.97 Å	110°
	C(7)-H(7)···O(5)	2.45 Å	3.13 Å	131°
	O(13)-H(13)···O(2)	2.81 Å	3.42 Å	132°

Table S3. Summary of the various interactions contributions to the Hirshfeld surface area of HNIW-MA, α-HNIW and ε-HNIW.

Interactions	**Materials**		
	ε-HNIW	**HNIW-CO_2**	**HNIW-MA**
C…C	0	0	0
C…O	0.1	1.9	0.6
C…H	0	0	0.1
C…N	0	0	0
H…H	1.6	1.4	3.2
H…O	36.8	32.4	37.3
H…N	0.8	0.6	1.4
O…O	41.4	44.1	39.4
O…N	19.2	19.2	17.9
N…N	0.1	0.4	0.3

Table S4. The detonation parameters were predicted with EXPLO5 V5.05 and mechanical sensitivity were experimentally determined.

Sample	**$\Delta_f H$ (kJ/mol)**	**Dv (km/s)**	**P (GPa)**	**H_{50}(cm)**
HNIW-MA	159.0	9466	41.86	20.8
ε-HNIW	365.4	9436	45.32	<14.1
α-HNIW	7.2	9217	39.81	14.8