Electronic Supplementary Material (ESI) for RSC Advances

Supporting Information

Computer-aided design of two novel and super-high energy cage explosives dodecanitrohexaprismane and hexanitrohexaazaprismane

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Table S1 Selected bond lengths (Å) of DNH1, DNH2, and ONC, and total energies (a.u.) of DNH1 and DNH2.

	DNH1	DNH2	ONC
C1-C2	1.562	1.568	1.568 (1.567[a], 1.563[b])
C2-C3	1.572	1.568	1.567
C3-C4	1.558	1.568	1.568
C1-C8	1.554	1.563	
C2-C9	1.585	1.563	
C3-C10	1.553	1.563	
C4-C11	1.593	1.563	
C1-N1	1.557	1.544	1.490 (1.482[a], 1.480[b])
C2-N2	1.538	1.544	1.490
C3-N3	1.550	1.544	1.490
C4-N4	1.534	1.544	1.490
Total energy	-2918.801	-2198.814	

[a] The values are from ref 50. [b] The values are from ref 51.

Table S2 Selected bond lengths (Å) and bond angles (°) of HNHAH.

Bond lengths		Bond angles	
N1-C2	1.474	N1C2N3	124.3
C2-N3	1.474	C2N3C4	115.4
N3-C4	1.473	N1C2N9	93.2
C4-N5	1.473	O1O2N1N3	75.9
N5-C6	1.473	O3O4N3N5	76.1
C6-N1	1.474	O5O6N5N1	76.0
C2-N13	1.518	O1O2N1N3	75.9
C4-N14	1.518	O7O8N9N7	75.8
C6-N15	1.518	O9O10N11N9	76.1
C8-N16	1.518	O11O12N7N11	76.0
C10-N17	1.518	O1O2N1N3	75.9
C12-N18	1.518		

Table S3 Unit cell parameters of the possible molecular packing of DNH2 in the ten possible space groups

Dreiding										
Space groups	$P2_1/c$	P-1	$P2_12_12_1$	Pbca	C2/c	$P2_1$	$Pna2_1$	C2	CC	Pbcn
Z	4	2	4	8	8	2	4	4	4	8
E[a]	251.37	251.31	249.99	251.59	251.38	252.47	252.23	253.39	251.32	252.38
ρ (g·cm^{-3})	1.932	1.937	1.958	1.917	1.939	1.913	1.926	1.878	1.908	1.925
a (Å)	29.77	9.99	10.03	16.64	16.83	9.85	11.65	17.26	15.72	31.28
b (Å)	9.92	9.99	10.14	20.17	18.89	13.11	15.66	10.12	11.80	11.61
c (Å)	19.47	15.10	23.21	14.37	17.59	9.81	13.17	14.31	13.07	13.23
α (deg)	90.0	81.5	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
β (deg)	155.4	98.6	90.0	90.0	121.4	72.7	90.0	80.2	89.2	90.0
γ (deg)	90.0	119.7	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0

[a]E in kJ·mol^{-1}·cell^{-1}.

Table S4 Unit cell parameters of the possible molecular packing of DNH1 in the ten possible space groups

Dreiding										
Space groups	$P2_1/c$	P-1	$P2_12_12_1$	Pbca	C2/c	$P2_1$	$Pna2_1$	C2	CC	Pbcn
Z	2	2	4	8	8	2	4	4	4	8
E^a	260.09	260.08	261.50	262.53	260.91	261.63	261.30	261.63	262.42	263.0
ρ (g·cm^{-3})	2.138	2.143	2.068	2.053	2.123	2.083	2.085	2.083	2.077	2.073
a (Å)	16.11	9.27	14.26	13.27	16.11	9.35	15.04	9.35	15.91	32.90
b (Å)	9.26	9.27	16.96	33.10	9.27	14.88	9.23	15.95	11.92	9.98
c (Å)	18.58	15.91	9.25	10.26	39.04	9.25	15.97	17.58	19.27	13.58
α (deg)	90.0	96.3	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
β (deg)	128.7	66.2	90.0	90.0	131.7	120.4	90.0	122.1	142.5	90.0
γ (deg)	90.0	119.7	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
Compass										
Space groups	$P2_1/c$	P-1	$P2_12_12_1$	Pbca	C2/c	$P2_1$	$Pna2_1$	C2	CC	Pbcn
Z	2	2	4	8	8	2	4	4	4	8
E^a	-517.4	-519.5	-513.9	-514.5	-516.7	-515.9	-515.8	-516.3	-517.6	-513.8
ρ (g·cm^{-3})	2.595	2.574	2.360	2.490	2.565	2.470	2.460	2.477	2.588	2.381
a (Å)	12.64	7.17	29.68	16.97	16.65	9.11	15.37	17.93	9.06	35.91
b (Å)	15.54	9.12	9.35	8.90	8.72	16.45	7.09	7.11	15.76	7.11
c (Å)	16.96	14.47	7.06	24.59	24.95	6.98	17.24	15.19	13.18	15.21
α (deg)	90.0	89.5	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
β (deg)	147.7	89.5	90.0	90.0	85.0	62.6	90.0	105.4	71.6	90.0
γ (deg)	90.0	105.7	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0

[a] E in kJ·mol^{-1}·cell^{-1}.

Table S5 Unit cell parameters of the possible molecular packing of HNHAH in the ten possible space groups

Dreiding										
Space groups	$P2_1/c$	P-1	$P2_12_12_1$	Pbca	C2/c	$P2_1$	$Pna2_1$	C2	CC	Pbcn
Z	4	2	4	8	8	2	4	4	4	8
E[a]	177.39	176.46	180.55	180.68	177.15	178.30	179.41	177.76	177.92	181.39
ρ (g·cm^{-3})	2.068	2.057	1.929	1.926	2.034	1.982	1.948	2.016	2.058	1.881
a (Å)	12.64	9.22	7.32	7.72	12.25	7.37	7.65	12.21	7.34	30.30
b (Å)	28.53	7.30	15.45	29.61	7.76	13.12	13.26	7.79	28.81	12.96
c (Å)	7.41	14.46	13.17	13.04	40.25	9.44	14.52	15.74	7.40	7.77
α (deg)	90.0	107.1	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0
β (deg)	148.7	117.7	90.0	90.0	132.5	127.5	90.0	108.0	117.0	90.0
γ (deg)	90.0	54.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0	90.0

[a]E in kJ·mol^{-1}·cell^{-1}.

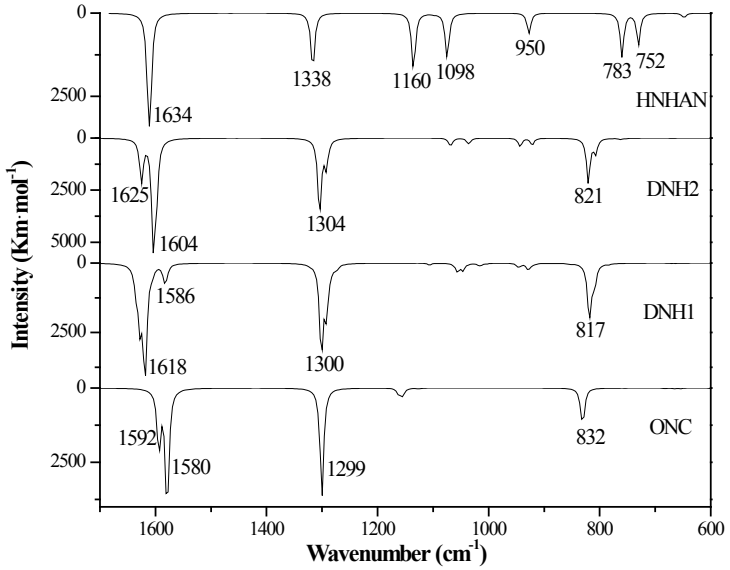

Fig. S1 Calculated IR spectrums for DNH1, DNH2, HNHAH, and ONC.