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From mono-rings to bridged bi-rings to caged bi-rings: A promising design strategy for all-nitrogen high-energy-density materials N_{10} and N_{12}

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Table S1 Calculated heat of formation of seven compounds.

Compd	E_0/au	ZPE/au	H_t/au	**Hf/kJ mol^{-1}**	**Hf/kJ g^{-1}**
N_6	-328.290297	0.021717	0.026052-0.021274	**836.67**	**9.96**
N_6^+	-327.8902749	0.020016	0.025427-0.019607	**1885.20**	**22.44**
N_6^-	-328.3896022	0.022049	0.026950-0.021599	**578.32**	**6.88**
bridged-N_{10}	-547.2833042	0.046555	0.053366-0.045605	**1070.78**	**7.64**
brideged-N_{12}	-656.5689841	0.050356	0.059341-0.049328	**1720.72**	**10.24**
caged-N_{10}	-546.8753837	0.042505	0.047911-0.041638	**2127.24**	**15.19**
caged-N_{12}	-656.170148	0.048069	0.055590-0.047088	**2757.90**	**16.41**

Table S2 Calculated detonation performance of four compounds.

Compd	N	M	Q.10^{-3}	**D/m s^{-1}**	**P/GPa**
Bridege-N_{10}	0.0357	28.01	1.827	**9251**	**36.79**
Bridged-N_{12}	0.0357	28.01	2.447	**9992**	**45.11**
Caged-N_{10}	0.0357	28.01	3.630	**11559**	**60.05**
Caged-N_{12}	0.0357	28.01	3.922	**12010**	**65.85**

Distributions of electrostatic potentials

Note: Area unit is in Angstrom^2

Begin	End	Center	Area	%
-20.0000	-15.0000	-17.5000	4.1848	2.8560
-15.0000	-10.0000	-12.5000	13.2651	9.0532
-10.0000	-5.0000	-7.5000	14.1220	9.6380
-5.0000	0.0000	-2.5000	27.1630	18.5382
0.0000	5.0000	2.5000	24.7010	16.8579
5.0000	10.0000	7.5000	15.1391	10.3322
10.0000	15.0000	12.5000	11.6134	7.9259
15.0000	20.0000	17.5000	9.5765	6.5358
20.0000	25.0000	22.5000	8.3203	5.6785
25.0000	30.0000	27.5000	9.0078	6.1476
30.0000	35.0000	32.5000	6.0740	4.1454
35.0000	40.0000	37.5000	2.8976	1.9775
40.0000	45.0000	42.5000	0.4595	0.3136
45.0000	50.0000	47.5000	0.0000	0.0000
50.0000	55.0000	52.5000	0.0000	0.0000
55.0000	60.0000	57.5000	0.0000	0.0000
60.0000	65.0000	62.5000	0.0000	0.0000
Sum:			146.5241	100.0000

Figure S1. Distributions of electrostatic potentials of bridged-N_{10}.

Note: Area unit is in Angstrom^2

Begin	End	Center	Area	%
-20.0000	-15.0000	-17.5000	0.0000	0.0000
-15.0000	-10.0000	-12.5000	1.6062	1.2721
-10.0000	-5.0000	-7.5000	26.4352	20.9365
-5.0000	0.0000	-2.5000	26.8485	21.2639
0.0000	5.0000	2.5000	25.8144	20.4448
5.0000	10.0000	7.5000	14.6341	11.5901
10.0000	15.0000	12.5000	9.5876	7.5933
15.0000	20.0000	17.5000	6.6281	5.2494
20.0000	25.0000	22.5000	5.0282	3.9823
25.0000	30.0000	27.5000	3.8159	3.0221
30.0000	35.0000	32.5000	2.0319	1.6092
35.0000	40.0000	37.5000	1.2116	0.9596
40.0000	45.0000	42.5000	0.9917	0.7854
45.0000	50.0000	47.5000	0.8213	0.6505
50.0000	55.0000	52.5000	0.6631	0.5252
55.0000	60.0000	57.5000	0.1458	0.1155
60.0000	65.0000	62.5000	0.0000	0.0000
Sum:			126.2637	100.0000

Figure S2. Distributions of electrostatic potentials of caged-N_{10}.

Note: Area unit is in Angstrom^2

Begin	End	Center	Area	%
-20.0000	-15.0000	-17.5000	6.5616	3.9897
-15.0000	-10.0000	-12.5000	16.2679	9.8916
-10.0000	-5.0000	-7.5000	25.8955	15.7457
-5.0000	0.0000	-2.5000	26.0290	15.8268
0.0000	5.0000	2.5000	22.9600	13.9607
5.0000	10.0000	7.5000	14.4497	8.7861
10.0000	15.0000	12.5000	11.0763	6.7349
15.0000	20.0000	17.5000	8.6829	5.2796
20.0000	25.0000	22.5000	7.2902	4.4328
25.0000	30.0000	27.5000	5.9930	3.6440
30.0000	35.0000	32.5000	5.6901	3.4598
35.0000	40.0000	37.5000	5.2745	3.2071
40.0000	45.0000	42.5000	3.8256	2.3261
45.0000	50.0000	47.5000	4.4649	2.7149
50.0000	55.0000	52.5000	0.0000	0.0000
55.0000	60.0000	57.5000	0.0000	0.0000
60.0000	65.0000	62.5000	0.0000	0.0000
Sum:			164.4610	100.0000

Figure S3. Distributions of electrostatic potentials of bridged-N_{12}.

Note: Area unit is in Angstrom^2

Begin	End	Center	Area	%
-20.0000	-15.0000	-17.5000	0.0000	0.0000
-15.0000	-10.0000	-12.5000	2.6641	1.8757
-10.0000	-5.0000	-7.5000	31.3847	22.0973
-5.0000	0.0000	-2.5000	33.3961	23.5135
0.0000	5.0000	2.5000	23.7694	16.7355
5.0000	10.0000	7.5000	15.1874	10.6931
10.0000	15.0000	12.5000	9.9056	6.9743
15.0000	20.0000	17.5000	7.1639	5.0439
20.0000	25.0000	22.5000	5.3604	3.7742
25.0000	30.0000	27.5000	3.7456	2.6372
30.0000	35.0000	32.5000	2.0391	1.4357
35.0000	40.0000	37.5000	1.7481	1.2308
40.0000	45.0000	42.5000	1.5171	1.0682
45.0000	50.0000	47.5000	1.4189	0.9990
50.0000	55.0000	52.5000	1.1802	0.8309
55.0000	60.0000	57.5000	1.0072	0.7092
60.0000	65.0000	62.5000	0.5418	0.3814
Sum:			142.0296	100.0000

Figure S4. Distributions of electrostatic potentials of caged-N_{12}.