Insights into energetic performance from structures: A density functional theory study on N_6

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1. Calculated section of N_6-1, N_6-2 and N_6-3

Table S1 Calculated heat of formation of three compounds.

Compd	E_0/au	ZPE/au	H_T/au	**H_f/kJ mol^{-1}**	**H_f/kJ g^{-1}**
N_6-1	-328.1017346	0.022863	0.004837	**1262.2**	**15.02**
N_6-2	-328.2386472	0.023822	0.005118	**978.7**	**11.65**
N_6-3	-328.2315394	0.020375	0.006499	**991.9**	**11.80**

Table S2 Calculated detonation performance of three compounds.

Compd	N	M	Q.10^{-3}	**D/m s^{-1}**	**P/GPa**
N_6-1	0.0357	28.00	3.590	**10653**	**47.6**
N_6-2	0.0357	28.00	2.783	**9756**	**39.0**
N_6-3	0.0357	28.00	2.821	**9423**	**35.0**

2. Boat conformation of N_6 (named N_6-2').

Table S3. The calculated results of **N6-2'.**

	E_0 au	ZPE au	H_T au	M_w g mol^{-1}	$\nu\sigma_{tot}^2$ kcal mol^{-1}
N_6-2'	-328.2944332	0.022224	0.00577	84.02	11.77

Table S4. The calculated energetic performance of **N_6-2** and **N_6-2'.**

	d g cm^{-3}	H_f (g, 298K) kJ mol^{-1}/ kJ g^{-1}	D m s^{-1}	P GPa	I_{sp} s	h_{50} cm
N_6-2	1.583	978.7/ 11.65	9756/ 10093	39.0/ 41.3	387.2	18
N_6-2'	1.578	829.7/ 9.88	9338/ 9739	35.6/ 37.7	362.7	16

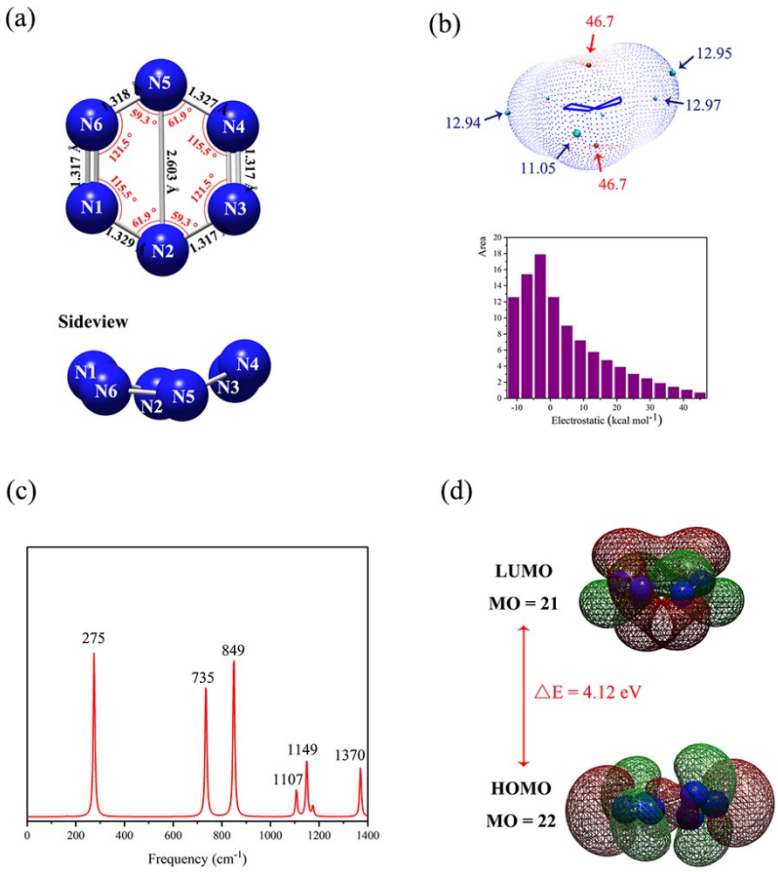

Figure S1. The optimized structure (a), surface electrostatic potentials (b), calculated IR spectra (c), and frontier molecular orbitals (d) of **N6-2'**.

According to the optimized structures and calculated results, the bonds lengths of **N_6-2'** are in the range of 1.317~2.603 Å, and the bond angles are in the range of 59.3°~121.5°. Viewing from the side, the compound exhibits a boat-like structure. The density of **N_6-2'** (d: 1.578 g cm^{-3}) is slightly lower than **N_6-2** (d: 1.583 g cm^{-3}), and the heats of formation of **N_6-2'** (H_f: 829.7 kJ mol^{-1}) also fall behind **N_6-2** (H_f: 978.7 kJ mol^{-1}). As a result, the detonation performance and specific impulse of **N_6-2'** are 9739 m s^{-1}, 37.7 GPa, 362.7 s, respectively, which are poorer than N_6-2. On the whole, the energetic performance of boat-like **N_6-2'** is slightly inferior to that of V-shaped **N_6-2**.

3. Distributions of electrostatic potentials

Begin	End	Center	Area	%
-11.0000	-8.1333	-9.5667	8.1236	8.5088
-8.1333	-5.2667	-6.7000	10.9406	11.4593
-5.2667	-2.4000	-3.8333	10.9451	11.4641
-2.4000	0.4667	-0.9667	11.1585	11.6876
0.4667	3.3333	1.9000	12.6446	13.2442
3.3333	6.2000	4.7667	8.9260	9.3492
6.2000	9.0667	7.6333	7.6892	8.0537
9.0667	11.9333	10.5000	7.2953	7.6412

11.9333	14.8000	13.3667	5.1546	5.3990
14.8000	17.6667	16.2333	3.7266	3.9033
17.6667	20.5333	19.1000	3.0975	3.2443
20.5333	23.4000	21.9667	2.1681	2.2708
23.4000	26.2667	24.8333	1.5774	1.6522
26.2667	29.1333	27.7000	1.3104	1.3725
29.1333	32.0000	30.5667	0.7157	0.7496
			95.4732	100.0000

Table S3. Distributions of electrostatic potentials of **N_6-1**.

Begin	End	Center	Area	%
-12.0000	-9.2000	-10.6000	4.9101	4.9666
-9.2000	-6.4000	-7.8000	7.5902	7.6777
-6.4000	-3.6000	-5.0000	10.7137	10.8371
-3.6000	-0.8000	-2.2000	10.7262	10.8498
-0.8000	2.0000	0.6000	11.1381	11.2665
2.0000	4.8000	3.4000	11.9503	12.0880
4.8000	7.6000	6.2000	13.7098	13.8678
7.6000	10.4000	9.0000	7.6607	7.7490
10.4000	13.2000	11.8000	5.7641	5.8305
13.2000	16.0000	14.6000	4.8460	4.9018
16.0000	18.8000	17.4000	4.2223	4.2709
18.8000	21.6000	20.2000	2.7466	2.7782
21.6000	24.4000	23.0000	2.0185	2.0418
24.4000	27.2000	25.8000	0.6607	0.6683
27.2000	30.0000	28.6000	0.2038	0.2061
			98.8611	100.0000

Table S4. Distributions of electrostatic potentials of **N_6-2**.

Begin	End	Center	Area	%
-14.0000	-11.9333	-12.9667	1.6625	1.5688
-11.9333	-9.8667	-10.9000	2.6506	2.5012
-9.8667	-7.8000	-8.8333	2.6293	2.4811
-7.8000	-5.7333	-6.7667	4.9093	4.6326
-5.7333	-3.6667	-4.7000	10.1634	9.5906
-3.6667	-1.6000	-2.6333	10.3401	9.7573
-1.6000	0.4667	-0.5667	10.9147	10.2995
0.4667	2.5333	1.5000	12.9948	12.2624
2.5333	4.6000	3.5667	12.5097	11.8046
4.6000	6.6667	5.6333	9.5146	8.9783
6.6667	8.7333	7.7000	8.2334	707694
8.7333	10.8000	9.7667	6.6732	6.2971
10.8000	12.8667	11.8333	4.8481	4.5748
12.8667	14.9333	13.9000	5.4392	5.1326
14.9333	17.0000	15.9667	2.4899	2.3495
			105.9729	100.0000

Table S5. Distributions of electrostatic potentials of **N_6-3**.

Begin	End	Center	Area	%
-13.0000	-9.0000	-11.0000	12.5560	12.6279
-9.0000	-5.0000	-7.0000	15.4018	15.4900
-5.0000	-1.0000	-3.0000	17.8692	17.9715
-1.0000	3.0000	1.0000	12.5625	12.6344
3.0000	7.0000	5.0000	9.0124	9.0640
7.0000	11.0000	9.0000	7.1756	7.2167
11.0000	15.0000	13.0000	5.7452	5.7782
15.0000	19.0000	17.0000	4.7203	4.7474
19.0000	23.0000	21.0000	3.8776	3.8998
23.0000	27.0000	25.0000	3.0130	3.0302
27.0000	31.0000	29.0000	2.4682	2.4824
31.0000	35.0000	33.0000	1.8782	1.8889
35.0000	39.0000	37.0000	1.1400	1.4180
39.0000	43.0000	41.0000	1.0418	1.0478
43.0000	47.0000	45.0000	0.6987	0.7027
			99.4304	100.0000

Table S6. Distributions of electrostatic potentials of **N_6-2'.**