

SUPPLEMENTARY MATERIAL

Theoretical studies on the new high-nitrogen explosives N14 and N18

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Table 1S. Standard orientations of every atom in N18

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1	1.337575	-0.299573	0.468483
2	0.928213	1.008563	0.468427
3	0.409368	-1.30817	0.468568
4	-0.409386	1.308159	0.468571
5	-1.337599	0.299565	0.468495
6	-0.928235	-1.008576	0.468443
7	0.142596	3.470521	-0.353447
8	-0.822135	2.627415	0.30345
9	-2.095696	2.770448	-0.352669
10	-2.934675	1.858953	-0.352449
11	-2.686513	0.601705	0.303935
12	-3.447501	-0.429661	-0.351847
13	-3.077545	-1.612004	-0.352
14	-1.864279	-2.025727	0.303617
15	-1.351464	-3.199794	-0.353351
16	-0.142574	-3.470495	-0.353485
17	0.822121	-2.627423	0.303455
18	2.095735	-2.770453	-0.352653
19	2.934679	-1.858922	-0.352423
20	2.686488	-0.601709	0.303893
21	3.44752	0.429665	-0.351784
22	3.077558	1.612015	-0.351934
23	1.864257	2.025712	0.30358
24	1.351483	3.199781	-0.353304

Table 2S. Standard orientations of every atom in N14

Center Number	Coordinates (Angstroms)		
	X	Y	Z
1	-0.655541	-0.006716	-0.027518
2	0.655552	0.006792	0.023897
3	3.312121	-0.11236	0.033419
4	2.707626	-1.207993	-0.016484
5	1.338963	-1.159683	-0.281979
6	0.640811	-2.327695	0.164945
7	-0.591417	-2.337358	0.153753
8	-1.310749	-1.175877	-0.404058
9	-3.31214	0.112654	-0.034569
10	-2.707473	1.208137	0.015977
11	-1.338983	1.159105	0.281596
12	-0.640861	2.328068	-0.161769
13	0.591449	2.337882	-0.150503

14	1.31082	1.174893	0.403925
15	2.663327	1.100079	-0.15009
16	-2.663472	-1.099949	0.149092
17	-3.229615	-1.800934	-0.318348
18	3.229396	1.801166	0.317296

Table 3S. NBO charges of atoms for four title compounds

N14				N18			
Atom	charge	Atom	charge	Atom	charge	Atom	charge
1	0.24	13	0.01	1	0.12	13	0.03
2	0.24	14	-0.18	2	0.10	14	-0.17
3	-0.03	15	-0.28	3	0.11	15	0.03
4	-0.02	16	-0.28	4	0.09	16	0.03
5	-0.16	17	0.39	5	0.23	17	-0.17
6	0.04	18	0.39	6	0.07	18	0.03
7	0.01			7	0.03	19	0.03
8	-0.19			8	-0.17	20	-0.17
9	-0.03			9	0.03	21	0.03
10	-0.02			10	0.03	22	0.03
11	-0.16			11	-0.20	23	-0.17
12	0.04			12	0.02	24	0.03

Table 4S. Calculation summaries of the Gaussian output parameters

	N14	N18
Job cpu time	1 hours 34 minutes 11.6 seconds	6 hours 46 minutes 21.1 seconds
Imaginary Freq	0	0
Charge	0	0

