Supporting information for What are the roles of N_3 and N_5 rings in designing polynitrogen molecules?

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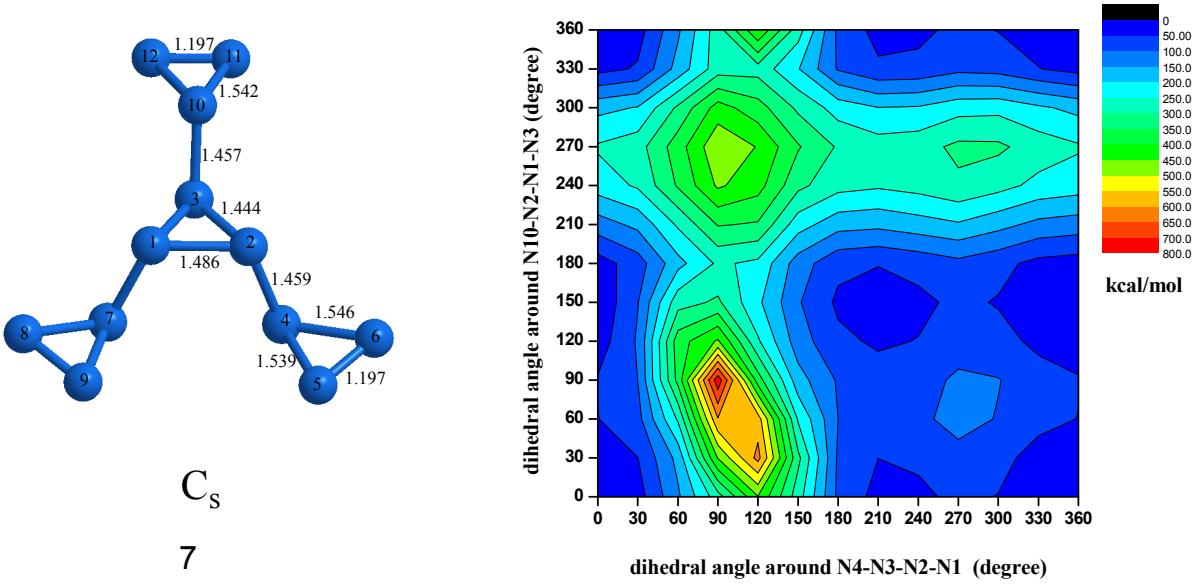

Fig. S-1 (a) Structure and bond lengths of N3(N3)3 (b) Contour plot showing the potential energy for N3(N3)3 as a function of the two dihedral angles, χ1 (N4-N2-N3-N1)and χ2 (N10-N3-N1-N2). DFT calculations at the B3LYP/cc-pVDZ level of theory were used to generate the energies for the plot for 30°increments of each dihedral angle.

Table S-1 Relative energy values of various points on potential energy surface with respect to the first point(χ1=0º, χ2=0º). These values are obtained by the relaxed potential energy (PER) scan along the two dihedral angles around N4-N2-N3-N1 (χ1) and N10-N3-N1-N2 (χ2) (kcal/mol) with 30º increasment in a range from 0º to 360º.

	0^o	30^o	60^o	90^o	120^o	150^o	180^o	210^o	240^o	270^o	300^o	330^o	360^o
0^o	0.0	15.5	54.0	70.2	34.6	4.7	5.6	49.6	128.8	190.6	103.4	23.7	0.0
30^o	17.2	31.7	69.8	88.1	53.2	22.8	23.2	67.5	147.6	209.3	122.5	41.9	17.2
60^o	49.1	62.5	98.9	118.3	85.6	55.6	57.5	104.6	180.8	241.2	153.9	73.8	49.1
90^o	54.0	67.8	103.6	120.2	89.0	61.8	72.9	117.7	182.0	243.3	154.7	77.1	54.0
120^o	24.9	40.0	77.4	92.6	59.3	34.8	45.9	80.0	151.1	214.3	124.8	47.6	24.9
150^o	8.0	24.0	61.7	75.4	41.4	14.3	16.1	56.9	137.1	199.5	107.2	30.3	8.0
180^o	26.65	41.0	77.8	94.5	61.3	31.5	31.8	75.3	156.8	216.9	128.0	50.7	26.7
210^o	125.8	139.0	175.3	195.5	162.8	131.9	131.4	172.3	255.5	311.9	229.1	151.9	125.8
240^o	223.7	237.6	273.8	294.2	260.7	230.2	229.8	268.4	354.3	402.7	324.7	248.9	223.7
270^o	255.9	271.5	308.7	324.0	289.6	260.7	262.0	302.6	381.1	439.1	351.5	277.5	255.9
300^o	185.0	202.1	240.4	251.4	216.2	188.2	190.5	234.5	309.2	371.7	281.9	205.6	185.0
330^o	32.5	48.9	87.6	101.2	65.5	36.4	38.0	82.1	159.8	220.8	133.2	54.9	32.5
360^o	0.0	15.5	54.1	70.2	34.6	4.7	5.6	49.6	128.8	190.6	103.4	23.7	0.0

Table S-2 Relative energies(kcal/mol) for N_6, N_{10} and N_8 isomers at different level of theory. The structure numbers listed here are corresponding to the structure numbers listed in the article.

species and their relative energies at different level of theory				
	1	**2**		
B3LYP/cc-pVDZ	0.0	81.6		
B3LYP/cc-pVTZ	0.0	83.9		
B3PW91/cc-pVDZ	0.0	76.2		
MP2/cc-pVDZ	0.0	88.5		
CCSD(T)/cc-pVDZ//MP2/cc-pVDZ	0.0	82.1		
	3	**4**	**5**	**6**
B3LYP/cc-pVDZ	0.0	4.4	249.2	64.2
B3LYP/cc-pVTZ	0.0	4.8	254.6	66.9
B3PW91/cc-pVDZ	0.0	4.2	246.6	66.0
MP2/cc-pVDZ	0.0	3.1	264.5	73.7
CCSD(T)/cc-pVDZ//MP2/cc-pVDZ	0.0	4.9	242.3	61.5
	7	**8**		
B3LYP/cc-pVDZ	0.0	18.0		
B3LYP/cc-pVTZ	-	-		
B3PW91/cc-pVDZ	0.0	21.5		
MP2/cc-pVDZ	0.0	16.1		
CCSD(T)/cc-pVDZ//MP2/cc-pVDZ	0.0	54.4		

Table S-3 Coordinates of all systems studied

Below are the xyz coordinates in Å of all systems studied. They are calculated at B3LYP/cc-pVDZ, B3PW91/cc-pVDZ, MP2/cc-pVDZ and B3LYP/cc-pVTZ level of theory, respectively.

B3LYP			
cyclic-N_3		-164.0947041	Hartrees
Atom	x	y	z
N	0.000000	0.613419	-0.440604
N	0.000000	-0.613419	-0.440604
N	0.000000	0.000000	0.881209

B3PW91			
cyclic-N_3		-164.0315709	Hartrees
Atom	x	y	z
N	0.000000	0.613123	-0.435900
N	0.000000	-0.613123	-0.435900
N	0.000000	0.000000	0.871800

B3LYP			
cyclic-N_5		-273.6326579	Hartrees
Atom	x	y	z
N	0.000000	0.758340	-0.878480
N	0.000000	1.132719	0.319729
N	0.000000	-0.758340	-0.878480
N	0.000000	0.000000	1.117502
N	0.000000	-1.132719	0.319729

B3PW91			
cyclic-N_5		-273.483768	Hartrees
Atom	x	y	z
N	0.000000	0.731192	-0.865911
N	0.000000	1.121008	0.320426
N	0.000000	-0.731192	-0.865911
N	0.000000	0.000000	1.090969
N	0.000000	-1.121008	0.320426

B3LYP			
N_3-N_3(1)		-328.2465755	Hartrees
Atom	x	y	z

B3PW91			
N_3-N_3(1)		-328.1214243	Hartrees
Atom	x	y	z

N	0.000000	1.735480	0.602430
N	0.000000	1.735480	-0.602430
N	-0.572491	0.463485	0.000000
N	0.572491	-0.463485	0.000000
N	0.000000	-1.735480	0.602430
N	0.000000	-1.735480	-0.602430

N	0.000000	1.718562	0.602691
N	0.000000	1.718562	-0.602691
N	-0.565347	0.464726	0.000000
N	0.565347	-0.464726	0.000000
N	0.000000	-1.718562	0.602691
N	0.000000	-1.718562	-0.602691

B3LYP			
N_3-N_3(2)		-328.1191267	Hartrees
Atom	x	y	z
N	0.000000	0.855292	0.761832
N	0.740705	-0.427646	-0.761832
N	-0.740705	-0.427646	0.761832
N	-0.740705	-0.427646	-0.761832
N	0.740705	-0.427646	0.761832
N	0.000000	0.855292	-0.761832

B3PW91			
N_3-N_3(2)		-328.0026252	Hartrees
Atom	x	y	z
N	0.000000	0.848951	0.756073
N	0.735213	-0.424476	-0.756073
N	-0.735213	-0.424476	0.756073
N	-0.735213	-0.424476	-0.756073
N	0.735213	-0.424476	0.756073
N	0.000000	0.848951	-0.756073

B3LYP			
N_5-N_5(3)		-547.3096703	Hartrees
Atom	x	y	z
N	0.000000	0.689071	2.630362
N	0.000000	1.118743	1.423621
N	0.000000	0.000000	0.676304
N	0.000000	-1.118743	1.423621
N	0.000000	-0.689071	2.630362
N	0.000000	0.000000	-0.676304
N	-1.118743	0.000000	-1.423621
N	-0.689071	0.000000	-2.630362
N	0.689071	0.000000	-2.630362
N	1.118743	0.000000	-1.423621

B3PW91			
N_5-N_5(3)		-547.1079283	Hartrees
Atom	x	y	z
N	0.000000	0.683088	2.618592
N	0.000000	1.113167	1.413439
N	0.000000	0.000000	0.673971
N	0.000000	-1.113167	1.413439
N	0.000000	-0.683088	2.618592
N	0.000000	0.000000	-0.673971
N	-1.113167	0.000000	-1.413439
N	-0.683088	0.000000	-2.618592
N	0.683088	0.000000	-2.618592
N	1.113167	0.000000	-1.413439

B3LYP			
N_5-N_5(4)		-547.3025581	Hartrees
Atom	x	y	z
N	0.000000	0.679503	2.634659
N	0.000000	1.116699	1.417245
N	0.000000	0.000000	0.685435
N	0.000000	-1.116699	1.417245
N	0.000000	-0.679503	2.634659
N	0.000000	0.000000	-0.685435
N	0.000000	-1.116699	-1.417245
N	0.000000	-0.679503	-2.634659
N	0.000000	0.679503	-2.634659
N	0.000000	1.116699	-1.417245

B3PW91			
N_5-N_5(4)		-547.1010323	Hartrees
Atom	x	y	z
N	0.000000	0.675021	2.622698
N	0.000000	1.111562	1.408086
N	0.000000	0.000000	0.682345
N	0.000000	-1.111562	1.408086
N	0.000000	-0.675021	2.622698
N	0.000000	0.000000	-0.682345
N	0.000000	-1.111562	-1.408086
N	0.000000	-0.675021	-2.622698
N	0.000000	0.675021	-2.622698
N	0.000000	1.111562	-1.408086

B3LYP			
N_5-N_5(5)		-546.9088055	Hartrees
Atom	x	y	z

B3PW91			
N_5-N_5(5)		-546.7113186	Hartrees
Atom	x	y	z

N	0.000000	1.275046	0.760134
N	-1.212641	0.394011	0.760134
N	1.212641	0.394011	0.760134
N	0.749453	-1.031534	0.760134
N	-0.749453	-1.031534	0.760134
N	-0.749453	-1.031534	-0.760134
N	0.749453	-1.031534	-0.760134
N	1.212641	0.394011	-0.760134
N	0.000000	1.275046	-0.760134
N	-1.212641	0.394011	-0.760134

N	0.000000	1.265570	0.754491
N	-1.203629	0.391083	0.754491
N	1.203629	0.391083	0.754491
N	0.743884	-1.023868	0.754491
N	-0.743884	-1.023868	0.754491
N	-0.743884	-1.023868	-0.754491
N	0.743884	-1.023868	-0.754491
N	1.203629	0.391083	-0.754491
N	0.000000	1.265570	-0.754491
N	-1.203629	0.391083	-0.754491

B3LYP			
N_5-N_5(6)		-547.160051	Hartrees
Atom	x	y	z
N	0.000000	0.000000	1.084453
N	1.152671	0.665495	0.465222
N	-1.152671	0.665495	0.465222
N	0.000000	-1.330990	0.465222
N	0.613973	1.703512	-0.413353
N	1.782271	-0.320040	-0.413353
N	-0.613973	1.703512	-0.413353
N	-1.782271	-0.320040	-0.413353
N	-1.168299	-1.383472	-0.413353
N	1.168299	-1.383472	-0.413353

B3PW91			
N_5-N_5(6)		-546.954513	Hartrees
Atom	x	y	z
N	0.000000	0.000000	1.079097
N	1.143959	0.660465	0.457419
N	-1.143959	0.660465	0.457419
N	0.000000	-1.320930	0.457419
N	0.613802	1.690264	-0.408559
N	1.770713	-0.313564	-0.408559
N	-0.613802	1.690264	-0.408559
N	-1.770713	-0.313564	-0.408559
N	-1.156911	-1.376700	-0.408559
N	1.156911	-1.376700	-0.408559

B3LYP			
N_3-N_5 (7)		-437.776935	Hartrees
Atom	x	y	z
N	0.000000	1.110002	1.262685
N	0.000000	0.669594	0.000000
N	0.000000	-1.110002	1.262685
N	0.000000	0.000000	1.981628
N	0.000000	-0.669594	0.000000
N	0.000000	-1.110002	-1.262685
N	0.000000	0.000000	-1.981628
N	0.000000	1.110002	-1.262685

B3PW91			
N_3-N_5 (7)		-437.617015	Hartrees
Atom	x	y	z
N	0.000000	1.105524	1.255321
N	0.000000	0.667055	0.000000
N	0.000000	-1.105524	1.255321
N	0.000000	0.000000	1.971865
N	0.000000	-0.667055	0.000000
N	0.000000	-1.105524	-1.255321
N	0.000000	0.000000	-1.971865
N	0.000000	1.105524	-1.255321

B3LYP			
N_3-N_5(8)		-437.7815432	Hartrees
Atom	x	y	z
N	0.518458	1.909316	0.685551
N	0.518458	1.909316	-0.685551
N	0.041159	0.793112	-1.112574
N	-0.247830	0.101922	0.000000
N	0.041159	0.793112	1.112574
N	-0.953720	-1.096252	0.000000
N	0.041159	-2.205263	-0.591452

B3PW91			
N_3-N_5(8)		-437.6173073	Hartrees
Atom	x	y	z
N	0.497825	1.906483	0.677084
N	0.497825	1.906483	-0.677084
N	0.038339	0.780807	-1.105842
N	-0.231101	0.096272	0.000000
N	0.038339	0.780807	1.105842
N	-0.917907	-1.120151	0.000000
N	0.038339	-2.175351	-0.596298

N	0.041159	-2.205263	0.591452

N	0.038339	-2.175351	0.596298

B3LYP

$N_3(N_3)_3(9)$		-656.4743353	Hartrees
Atom	x	y	z
N	-2.227010	-1.738645	0.121189
N	-1.437782	-2.634964	0.037070
N	-0.931297	-1.318151	-0.595915
N	-0.111752	-0.743109	0.465318
N	-0.111751	0.743109	0.465318
N	0.918630	0.000000	-0.220754
N	2.091236	-0.000001	0.644751
N	3.202906	0.598728	-0.239661
N	3.202906	-0.598730	-0.239661
N	-0.931296	1.318152	-0.595915
N	-1.437780	2.634965	0.037070
N	-2.227009	1.738646	0.121189

B3PW91

$N_3(N_3)_3(9)$		-656.226573	Hartrees
Atom	x	y	z
N	-0.136171	-2.200111	1.764549
N	-0.009533	-1.386632	2.636847
N	0.585129	-0.947992	1.306344
N	-0.463818	-0.120529	0.733892
N	-0.463818	-0.120529	-0.733892
N	0.223913	0.903166	0.000000
N	-0.634573	2.073554	0.000000
N	0.229723	3.166904	-0.599915
N	0.229723	3.166904	0.599915
N	0.585129	-0.947992	-1.306344
N	-0.009533	-1.386632	-2.636847
N	-0.136171	-2.200111	-1.764549

B3LYP

$N_3(N_5)_3(10)$		-985.0610569	Hartrees
Atom	x	y	z
N	-0.859579	-0.007610	0.284747
N	-0.220275	-0.704324	-0.825891
N	-0.214506	0.827495	-0.691324
N	-3.028409	-0.077157	1.213615
N	-4.219823	-0.032973	0.737085
N	-2.239168	0.012190	0.134459
N	-4.161840	0.081696	-0.632783
N	-2.934199	0.110175	-1.009300
N	2.736627	-2.332201	-0.413730
N	2.157306	-2.560439	0.802363
N	1.959122	-1.588312	-1.125429
N	1.025187	-1.950336	0.867917
N	0.920159	-1.340654	-0.323988
N	1.591159	2.314652	-0.873435
N	0.929862	1.396392	-0.152345
N	2.563255	2.675716	-0.117563
N	1.494196	1.189752	1.055328
N	2.500925	1.985938	1.070274

B3PW91

$N_3(N_5)_3(10)$		-984.6995139	Hartrees
Atom	x	y	z
N	-0.857109	-0.011048	0.288924
N	-0.219098	-0.689748	-0.820638
N	-0.211280	0.814761	-0.682503
N	-3.015790	-0.077416	1.208353
N	-4.203671	-0.029913	0.728112
N	-2.230476	0.010811	0.136490
N	-4.141772	0.085210	-0.630386
N	-2.914752	0.111448	-1.003136
N	2.737985	-2.288778	-0.409510
N	2.137611	-2.572410	0.771282
N	1.969254	-1.526560	-1.108799
N	0.997050	-1.980308	0.834282
N	0.916702	-1.329036	-0.325583
N	1.562447	2.322903	-0.847987
N	0.928327	1.382654	-0.146460
N	2.538683	2.673174	-0.095632
N	1.504828	1.148919	1.039606
N	2.501061	1.955336	1.063582

B3LYP

$N_5(N_5)_5(11)$		-1641.8050604	Hartrees
Atom	x	y	z
N	0.251653	-1.014665	0.884212
N	-1.106223	-0.667523	0.682876
N	0.914331	0.222381	0.600597
N	0.229505	0.722562	-0.656680

B3PW91

$N_5(N_5)_5(11)$		-1641.2015012	Hartrees
Atom	x	y	z
N	-0.418859	-0.437045	-1.134279
N	0.537643	-1.170265	-0.439222
N	-0.237083	0.941290	-0.648816
N	0.428884	0.842066	0.668845

N	-1.169772	0.386880	-0.310933	N	0.849946	-0.494463	0.784236
N	-0.054927	2.963088	0.294006	N	2.683491	1.517382	0.050642
N	0.358128	2.100577	-0.655620	N	1.515841	1.694780	0.667822
N	0.279376	4.113173	-0.156924	N	3.360978	2.561461	0.353435
N	0.946893	2.725371	-1.691062	N	1.461813	2.840521	1.346677
N	0.902430	3.966762	-1.382647	N	2.605131	3.381163	1.142901
N	-1.692111	-0.253395	1.863160	N	1.656938	-1.389490	-1.212681
N	-2.776009	-0.884834	2.344443	N	2.256980	-2.579559	-1.217754
N	-1.299743	0.764290	2.649795	N	2.214199	-0.524492	-2.060625
N	-3.052333	-0.260605	3.427831	N	3.209797	-2.443504	-2.062737
N	-2.138620	0.757658	3.617573	N	3.175227	-1.183561	-2.591235
N	2.265486	0.160543	0.466249	N	-1.390232	1.655819	-0.577355
N	3.067188	0.885157	1.285153	N	-1.556358	2.757012	-1.329505
N	2.988543	-0.530559	-0.453658	N	-2.435897	1.445462	0.244770
N	4.249377	0.634765	0.886394	N	-2.694751	3.209697	-0.985101
N	4.201042	-0.243692	-0.192354	N	-3.237878	2.400548	-0.010601
N	-2.628552	0.824296	-2.103476	N	0.871355	-2.081850	2.518832
N	-1.850158	-0.044077	-1.438937	N	0.246336	-1.099831	1.878652
N	-3.147226	0.130944	-3.049763	N	0.085005	-2.366039	3.494306
N	-1.906566	-1.280520	-1.959720	N	-0.900820	-0.749259	2.453418
N	-2.713789	-1.170889	-2.950809	N	-0.993098	-1.537159	3.463073
N	1.052885	-3.238528	0.739212	N	-2.553538	-0.922247	-1.992218
N	0.632205	-2.116348	0.123096	N	-1.686825	-0.976855	-0.978419
N	1.358419	-4.031419	-0.215068	N	-3.574921	-1.567610	-1.569286
N	0.697064	-2.221069	-1.218983	N	-2.156308	-1.676932	0.057152
N	1.141503	-3.400323	-1.427962	N	-3.322997	-2.047041	-0.314927

B3LYP			
$N_5(N_5)_2$		-820.902052	Hartrees
Atom	x	y	z
N	1.410255	0.249386	-3.577063
N	1.192449	-0.069052	-2.356427
N	-0.139572	0.073933	-2.208751
N	-0.736973	0.480857	-3.337426
N	0.218756	0.589418	-4.184876
N	-0.829416	-0.161273	-1.052741
N	-0.829417	-1.516141	-0.618307
N	-0.829417	-1.516141	0.618307
N	-0.829416	-0.161273	1.052741
N	-0.572181	0.705719	0.000000
N	-0.139572	0.073933	2.208751
N	-0.736973	0.480857	3.337426
N	0.218756	0.589418	4.184876
N	1.410255	0.249386	3.577063
N	1.192449	-0.069052	2.356427

B3PW91			
$N_5(N_5)_2$		-820.599196	Hartrees
Atom	x	y	z
N	-1.036912	0.954852	3.588109
N	-1.041713	0.573832	2.367820
N	0.151191	-0.012102	2.204232
N	0.888251	0.008484	3.314047
N	0.151191	0.607203	4.172350
N	0.589188	-0.571549	1.044633
N	-0.121406	-1.708358	0.618220
N	-0.121406	-1.708358	-0.618220
N	0.589188	-0.571549	-1.044633
N	0.840420	0.295280	0.000000
N	0.151191	-0.012102	-2.204232
N	0.888251	0.008484	-3.314047
N	0.151191	0.607203	-4.172350
N	-1.036912	0.954852	-3.588109
N	-1.041713	0.573832	-2.367820

B3LYP

$N_5(N_5)_3$		-1094.511423	Hartrees
Atom	x	y	z
N	-1.151642	2.842904	-0.970600
N	-0.364840	1.900584	-0.591168
N	-0.947601	1.397521	0.507203
N	-2.092131	2.018476	0.804023
N	-2.222144	2.912693	-0.111688
N	-0.453761	0.319649	1.323019
N	-0.559062	-1.012130	0.637316
N	0.542956	-1.133168	-0.225852
N	1.353486	-0.337004	0.375784
N	0.967724	0.432359	1.384450
N	2.668850	-0.325961	0.003106
N	3.435634	-1.429469	-0.050928
N	4.581282	-0.984998	-0.414016
N	4.520275	0.382410	-0.573692
N	3.335327	0.796279	-0.313136
N	-1.756713	-1.300875	0.069472
N	-2.588164	-2.222438	0.590092
N	-3.600561	-2.221831	-0.190893
N	-3.400080	-1.303166	-1.206164
N	-2.268834	-0.731834	-1.046330

B3PW91

$N_5(N_5)_3$		-1094.109271	Hartrees
Atom	x	y	z
N	-1.087114	2.854025	-0.963799
N	-0.327591	1.889790	-0.590112
N	-0.926489	1.396830	0.493237
N	-2.048227	2.040771	0.792725
N	-2.150278	2.943916	-0.114788
N	-0.459554	0.310361	1.302859
N	-0.569131	-0.989499	0.610897
N	0.522498	-1.114356	-0.250458
N	1.337427	-0.342601	0.366319
N	0.953953	0.402138	1.388468
N	2.648785	-0.340111	0.003157
N	3.391650	-1.447698	-0.079631
N	4.544104	-1.010148	-0.423104
N	4.505337	0.350908	-0.540150
N	3.327252	0.775102	-0.273394
N	-1.767992	-1.284959	0.065853
N	-2.573132	-2.217438	0.587367
N	-3.597022	-2.216637	-0.175511
N	-3.425339	-1.290716	-1.173558
N	-2.299137	-0.709679	-1.026375

B3LYP

$N_5(N_5)_4$		-1368.158004	Hartrees
Atom	x	y	z
N	-0.547063	-3.514037	1.483810
N	-0.648041	-2.509114	0.692454
N	0.295311	-1.656178	1.116215
N	0.980677	-2.128000	2.167450
N	0.460444	-3.278906	2.393478
N	0.580924	-0.409774	0.582652
N	0.942159	-0.569332	-0.827006
N	0.000040	0.000016	-1.656825
N	-0.942300	0.569283	-0.827212
N	-0.581026	0.410334	0.582472
N	-2.230714	0.167711	-1.116665
N	-3.239176	1.050374	-1.146037
N	-4.267460	0.351231	-1.456771
N	-3.887700	-0.963914	-1.636963
N	-2.631693	-1.082825	-1.421283
N	2.230710	-0.168353	-1.116578
N	2.632259	1.082015	-1.421156
N	3.888201	0.962537	-1.636878

B3PW91

$N_5(N_5)_4$		-1367.655016	Hartrees
Atom	x	y	z
N	-0.527322	-3.475075	1.519469
N	-0.634659	-2.481732	0.717345
N	0.300693	-1.627301	1.128017
N	0.987758	-2.078319	2.176839
N	0.473368	-3.226936	2.416585
N	0.575697	-0.391066	0.581719
N	0.937610	-0.557021	-0.812099
N	0.002425	0.000290	-1.645344
N	-0.943695	0.554404	-0.822856
N	-0.580603	0.418745	0.572465
N	-2.221894	0.139464	-1.109811
N	-3.233929	1.005719	-1.132385
N	-4.250289	0.295501	-1.450402
N	-3.855291	-1.001125	-1.642229
N	-2.599481	-1.105286	-1.426120
N	2.222756	-0.171416	-1.104554
N	2.628612	1.065200	-1.418831
N	3.881165	0.932701	-1.636943

N	4.267366	-0.352796	-1.456750
N	3.238778	-1.051473	-1.145995
N	-0.295401	1.656971	1.115486
N	-0.980555	2.129146	2.166699
N	-0.460376	3.280193	2.392138
N	0.546876	3.515063	1.482120
N	0.647759	2.509830	0.691145

N	4.246743	-0.373381	-1.448463
N	3.215208	-1.060443	-1.129538
N	-0.305609	1.666577	1.091549
N	-0.983857	2.135704	2.138167
N	-0.472732	3.291463	2.348753
N	0.516667	3.526272	1.435600
N	0.620659	2.517064	0.653065

MP2/cc-pVDZ			
N_3-N_3(1)		-327.376176	Hartrees
Atom	x	y	z
N	0.000000	1.727046	0.619289
N	0.000000	1.727046	-0.619289
N	-0.580346	0.456610	0.000000
N	0.580346	-0.456610	0.000000
N	0.000000	-1.727046	0.619289
N	0.000000	-1.727046	-0.619289

B3LYP/cc-pVTZ			
N_3-N_3(1)		-328.311608	Hartrees
Atom	x	y	z
N	0.000000	1.737460	0.596692
N	0.000000	1.737460	-0.596692
N	-0.569961	0.459259	0.000000
N	0.569961	-0.459259	0.000000
N	0.000000	-1.737460	0.596692
N	0.000000	-1.737460	-0.596692

MP2/cc-pVDZ			
N_3-N_3(2)		-327.235127	Hartrees
Atom	x	y	z
N	0.000000	0.866917	0.767115
N	0.750772	-0.433458	-0.767115
N	-0.750772	-0.433458	0.767115
N	-0.750772	-0.433458	-0.767115
N	0.750772	-0.433458	0.767115
N	0.000000	0.866917	-0.767115

B3LYP/cc-pVTZ			
N_3-N_3(2)		-328.177965	Hartrees
Atom	x	y	z
N	0.000000	0.853647	0.759739
N	0.739280	-0.426824	-0.759739
N	-0.739280	-0.426824	0.759739
N	-0.739280	-0.426824	-0.759739
N	0.739280	-0.426824	0.759739
N	0.000000	0.853647	-0.759739

MP2/cc-pVDZ			
N_5-N_5(3)		-545.834865	Hartrees
Atom	x	y	z
N	0.000000	0.681214	2.643669
N	0.000000	1.127430	1.405652
N	0.000000	0.000000	0.678563
N	0.000000	-1.127430	1.405652
N	0.000000	-0.681214	2.643669
N	0.000000	0.000000	-0.678563
N	-1.127430	0.000000	-1.405652
N	-0.681214	0.000000	-2.643669
N	0.681214	0.000000	-2.643669
N	1.127430	0.000000	-1.405652

B3LYP/cc-pVTZ			
N_5-N_5(3)		-547.402615	Hartrees
Atom	x	y	z
N	0.000000	0.686835	2.621696
N	0.000000	1.111618	1.419791
N	0.000000	0.000000	0.674813
N	0.000000	-1.111618	1.419791
N	0.000000	-0.686835	2.621696
N	0.000000	0.000000	-0.674813
N	-1.111618	0.000000	-1.419791
N	-0.686835	0.000000	-2.621696
N	0.686835	0.000000	-2.621696
N	1.111618	0.000000	-1.419791

MP2/cc-pVDZ			
N_5-N_5(4)		-545.829897	Hartrees

B3LYP/cc-pVTZ			
N_5-N_5(4)		-547.394887	Hartrees

Atom	x	y	z
N	0.000000	0.676786	2.648757
N	0.000000	1.128703	1.405436
N	0.000000	0.000000	0.685084
N	0.000000	-1.128703	1.405436
N	0.000000	-0.676786	2.648757
N	0.000000	0.000000	-0.685084
N	0.000000	-1.128703	-1.405436
N	0.000000	-0.676786	-2.648757
N	0.000000	0.676786	-2.648757
N	0.000000	1.128703	-1.405436

Atom	x	y	z
N	0.000000	0.676978	2.626955
N	0.000000	1.109782	1.414124
N	0.000000	0.000000	0.684678
N	0.000000	-1.109782	1.414124
N	0.000000	-0.676978	2.626955
N	0.000000	0.000000	-0.684678
N	0.000000	-1.109782	-1.414124
N	0.000000	-0.676978	-2.626955
N	0.000000	0.676978	-2.626955
N	0.000000	1.109782	-1.414124

MP2/cc-pVDZ			
N_5-N_5(5)		-545.413345	Hartrees

Atom	x	y	z
N	0.000000	1.281130	0.767040
N	-1.218427	0.395891	0.767040
N	1.218427	0.395891	0.767040
N	0.753029	-1.036456	0.767040
N	-0.753029	-1.036456	0.767040
N	-0.753029	-1.036456	-0.767040
N	0.753029	-1.036456	-0.767040
N	1.218427	0.395891	-0.767040
N	0.000000	1.281130	-0.767040
N	-1.218427	0.395891	-0.767040

B3LYP/cc-pVTZ			
N_5-N_5(5)		-546.996961	Hartrees

Atom	x	y	z
N	0.000000	1.271333	0.757888
N	-1.209109	0.392863	0.757888
N	1.209109	0.392863	0.757888
N	0.747271	-1.028530	0.757888
N	-0.747271	-1.028530	0.757888
N	-0.747271	-1.028530	-0.757888
N	0.747271	-1.028530	-0.757888
N	1.209109	0.392863	-0.757888
N	0.000000	1.271333	-0.757888
N	-1.209109	0.392863	-0.757888

MP2/cc-pVDZ			
N_5-N_5(6)		-545.717364	Hartrees

Atom	x	y	z
N	0.000000	0.000000	1.100943
N	1.160897	0.670244	0.483588
N	-1.160897	0.670244	0.483588
N	0.000000	-1.340489	0.483588
N	0.623102	1.695278	-0.425285
N	1.779705	-0.308017	-0.425285
N	-0.623102	1.695278	-0.425285
N	-1.779705	-0.308017	-0.425285
N	-1.156603	-1.387261	-0.425285
N	1.156603	-1.387261	-0.425285

B3LYP/cc-pVTZ			
N_5-N_5(6)		-547.295983	Hartrees

Atom	x	y	z
N	0.000000	0.000000	1.075219
N	1.149110	0.663439	0.462526
N	-1.149110	0.663439	0.462526
N	0.000000	-1.326878	0.462526
N	0.609726	1.702749	-0.410466
N	1.779487	-0.323336	-0.410466
N	-0.609726	1.702749	-0.410466
N	-1.779487	-0.323336	-0.410466
N	-1.169761	-1.379413	-0.410466
N	1.169761	-1.379413	-0.410466

MP2/cc-pVDZ			
N_5-N_3(7)		-436.63571	Hartrees

Atom	x	y	z

B3LYP/cc-pVTZ			
N_5-N_3(7)		-437.890322	Hartrees

Atom	x	y	z

N	0.000000	1.124448	1.263106
N	0.000000	0.685049	0.000000
N	0.000000	-1.124448	1.263106
N	0.000000	0.000000	1.995184
N	0.000000	-0.685049	0.000000
N	0.000000	-1.124448	-1.263106
N	0.000000	0.000000	-1.995184
N	0.000000	1.124448	-1.263106

N	0.000000	1.104665	1.256086
N	0.000000	0.665705	0.000000
N	0.000000	-1.104665	1.256086
N	0.000000	0.000000	1.974239
N	0.000000	-0.665705	0.000000
N	0.000000	-1.104665	-1.256086
N	0.000000	0.000000	-1.974239
N	0.000000	1.104665	-1.256086

MP2/cc-pVDZ			
N_5-N_3(8)		-436.609984	Hartrees
Atom	x	y	z
N	0.536065	1.908356	0.677540
N	0.536065	1.908356	-0.677540
N	0.033657	0.768098	-1.121610
N	-0.254687	0.099915	0.000000
N	0.033657	0.768098	1.121610
N	-0.952073	-1.123316	0.000000
N	0.033657	-2.164754	-0.614548
N	0.033657	-2.164754	0.614548

B3LYP/cc-pVTZ			
N_5-N_3(8)			Hartrees
Atom	x	y	z

MP2/cc-pVDZ			
$N_3(N_3)_3$(9)		-654.7693968	Hartrees
Atom	x	y	z
N	-0.091694	-2.253887	1.556990
N	-0.073765	-1.517985	2.546385
N	0.605402	-0.902625	1.294231
N	-0.472806	-0.073911	0.752985
N	-0.472806	-0.073911	-0.752985
N	0.238789	0.949942	0.000000
N	-0.647901	2.112561	0.000000
N	0.237418	3.217156	-0.616625
N	0.237418	3.217156	0.616625
N	0.605402	-0.902625	-1.294231
N	-0.073765	-1.517985	-2.546385
N	-0.091694	-2.253887	-1.556990

B3LYP/cc-pVTZ			
$N_3(N_3)_3$(9)		-656.596485	Hartrees
Atom	x	y	z
N	-0.126509	-2.214191	1.798238
N	-0.026692	-1.411572	2.662905
N	0.596841	-0.929943	1.323752
N	-0.459638	-0.127042	0.745299
N	-0.459638	-0.127042	-0.745299
N	0.208140	0.907147	0.000000
N	-0.651616	2.071160	0.000000
N	0.237737	3.193595	-0.592114
N	0.237737	3.193595	0.592114
N	0.596841	-0.929943	-1.323752
N	-0.026692	-1.411572	-2.662905
N	-0.126509	-2.214191	-1.798238

MP2/cc-pVDZ			
$N_3(N_5)_3$(10)		-982.4962496	Hartrees
Atom	x	y	z
N	0.901308	0.034451	0.326420
N	0.298077	0.680307	-0.869121
N	0.278488	-0.864614	-0.635678
N	3.075044	0.139667	1.220994

B3LYP/cc-pVTZ			
$N_3(N_5)_3$(10)		-985.223065	Hartrees
Atom	x	y	z
N	-0.860909	-0.010226	0.284576
N	-0.216032	-0.697976	-0.827774
N	-0.206820	0.825762	-0.677895
N	-3.024634	-0.078800	1.205164

N	4.286114	0.047939	0.709448	N	-4.211026	-0.028137	0.733856
N	2.281981	-0.017137	0.152550	N	-2.237013	0.014837	0.133475
N	4.204504	-0.155728	-0.633471	N	-4.152632	0.095153	-0.630883
N	2.937576	-0.198832	-1.001655	N	-2.930068	0.122255	-1.002561
N	-2.858195	1.920061	-0.401942	N	2.757698	-2.276278	-0.399957
N	-2.218930	2.454060	0.666332	N	2.119019	-2.630971	0.745607
N	-2.014877	1.172105	-1.097071	N	2.001774	-1.489813	-1.080966
N	-0.959979	2.050806	0.689472	N	0.971488	-2.057841	0.795861
N	-0.878106	1.273674	-0.399861	N	0.917625	-1.345967	-0.329691
N	-1.650767	-2.180247	-0.803493	N	1.562720	2.346796	-0.832689
N	-0.912654	-1.321807	-0.081461	N	0.931565	1.397105	-0.138278
N	-2.702934	-2.391508	-0.042191	N	2.540167	2.695284	-0.088955
N	-1.471486	-0.976264	1.095288	N	1.523247	1.156613	1.041906
N	-2.595164	-1.666932	1.105439	N	2.513831	1.962204	1.069204

MP2/cc-pV DZ				B3LYP/cc-pV TZ			
$N_5(N_5)_5(11)$		-1637.534696	Hartrees	$N_5(N_5)_5(11)$		-1642.067468	Hartrees
Atom	x	y	z	Atom	x	y	z
N	-0.013907	-0.557141	-1.301928	N	0.000000	0.000000	0.000000
N	1.279602	-0.452749	-0.726512	N	1.410669	0.000000	0.000000
N	-0.687252	0.576895	-0.701823	N	-0.294405	1.396628	0.000000
N	-0.261349	0.501410	0.760988	N	0.662233	1.971545	1.017944
N	1.157320	0.150717	0.601884	N	1.870878	1.204105	0.658205
N	0.434514	2.839993	0.787720	N	1.324363	3.790419	-0.471688
N	-0.317972	1.811707	1.212825	N	0.863396	3.296467	0.686846
N	-0.026729	3.855469	1.487963	N	1.347124	5.050991	-0.295485
N	-1.236230	2.145324	2.134557	N	0.604495	4.262329	1.577255
N	-1.044064	3.436321	2.296356	N	0.896971	5.344822	0.974422
N	2.066298	0.369362	-1.509614	N	1.915214	-0.082358	-1.279804
N	3.245028	-0.080824	-1.970442	N	2.754039	-1.066615	-1.618809
N	1.777120	1.628691	-1.875773	N	1.664032	0.742607	-2.302251
N	3.708355	0.940834	-2.654564	N	3.020497	-0.853048	-2.846311
N	2.819106	1.976278	-2.600754	N	2.342203	0.267316	-3.271056
N	-2.055854	0.469930	-0.746147	N	-1.583529	1.745604	0.225062
N	-2.780497	1.451329	-1.323657	N	-2.271513	2.456901	-0.693593
N	-2.813611	-0.508077	-0.200292	N	-2.337840	1.504023	1.321571
N	-4.017963	1.062280	-1.145553	N	-3.414138	2.636796	-0.180874
N	-4.040125	-0.126985	-0.465235	N	-3.456437	2.042389	1.073974
N	0.861895	-0.826370	2.759131	N	3.670035	1.657408	2.093132
N	1.387412	-0.886797	1.541205	N	2.609233	0.904480	1.787049
N	1.426142	-1.866925	3.369646	N	4.152924	1.124164	3.146685
N	2.272778	-1.859088	1.347752	N	2.448812	-0.108589	2.643759
N	2.270684	-2.484109	2.524144	N	3.405335	0.022261	3.478316
N	-1.298881	-2.461555	-1.850954	N	-1.299476	-1.822814	0.752458

N	-0.560065	-1.796323	-0.950602	N	-0.532464	-0.759757	1.034551
N	-1.740108	-3.498373	-1.171747	N	-1.648968	-2.278364	1.886843
N	-0.538300	-2.364950	0.264269	N	-0.424529	-0.557833	2.355085
N	-1.273345	-3.446274	0.107155	N	-1.107797	-1.490910	2.882829