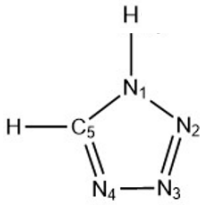
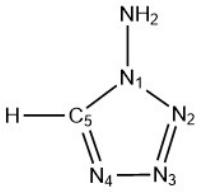
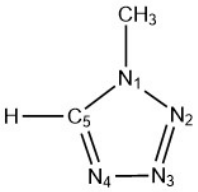
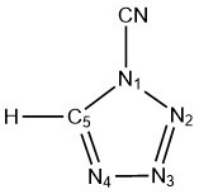
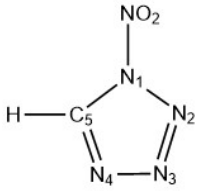
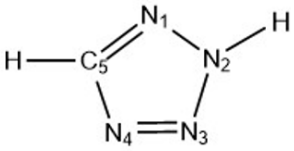
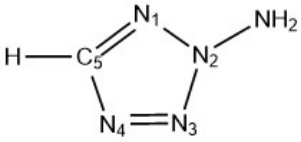
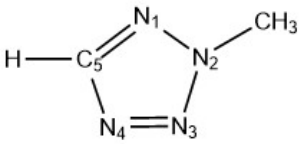
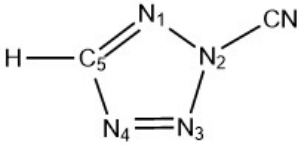
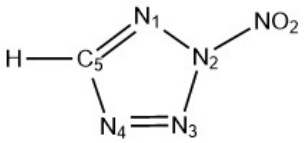
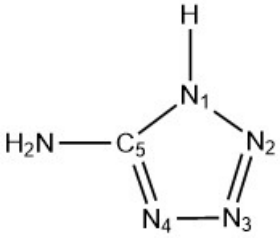
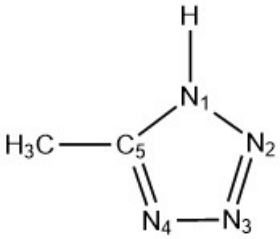
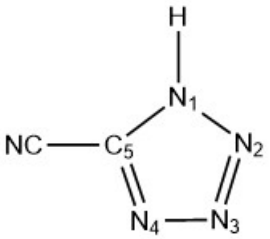
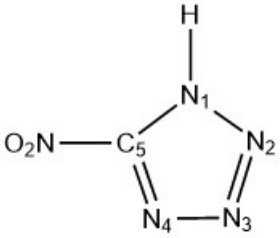
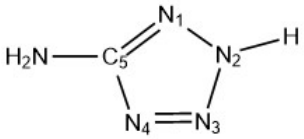
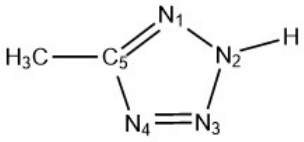
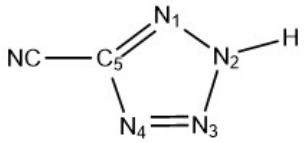
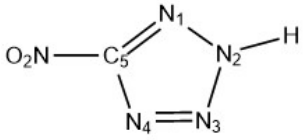
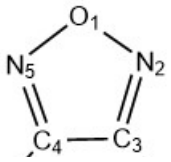
Electronic supplementary information (ESI) for "*A theoretical library of N1s core binding energies of polynitrogen molecules and ions in the gas phase*" by Du et al.

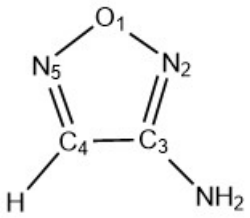
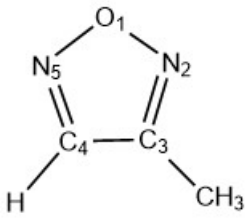
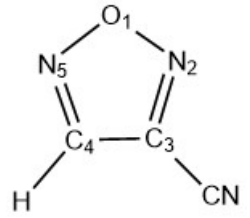
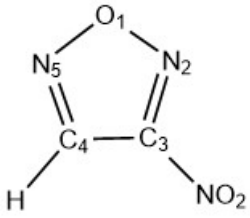
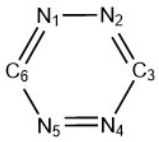
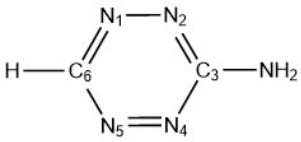
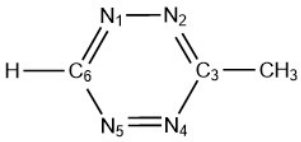
Table S1. Simulated N1s ionic potentials (IPs) in eV for 59 molecules. IP was computed by the ΔKS method with the BP86 functional, based on geometry optimized at M06-2X/ aug-cc-pVTZ level.

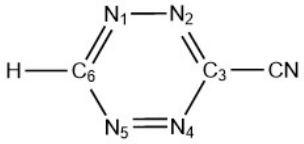
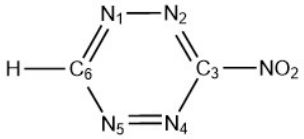
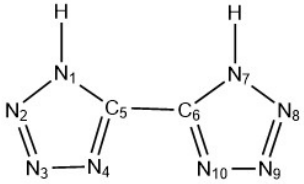
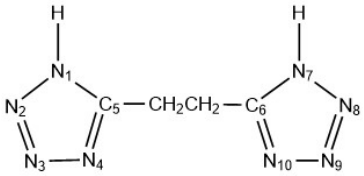
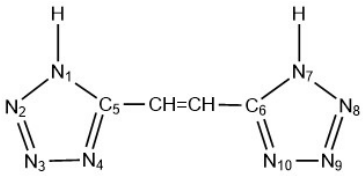
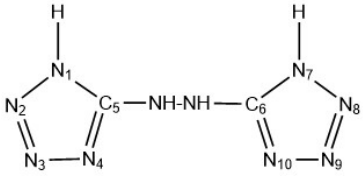
No.	Structure	Name	Atom	IP
1		1H-tetrazole	N_1	408.08
			N_2	407.00
			N_3	406.54
			N_4	405.82
2		1-aminotetrazole	N_1	408.42
			N_2	406.59
			N_3	406.29
			N_4	405.56
			N	407.44
3		1-methyltetrazole	N_1	407.73
			N_2	406.48
			N_3	406.08
			N_4	405.42
4		1-cyanotetrazole	N_1	409.44
			N_2	407.79
			N_3	407.35
			N_4	406.56
			N	406.15

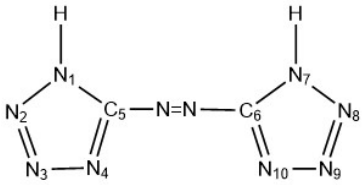
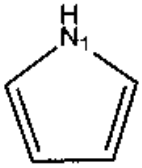
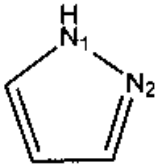
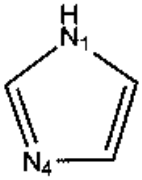
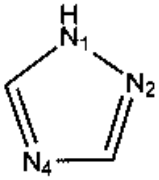
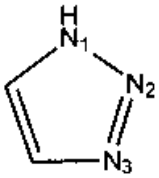
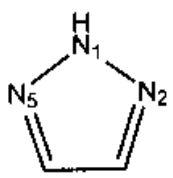
5		1-nitrotetrazole	N_1	409.04
			N_2	407.79
			N_3	407.29
			N_4	406.49
			N	413.88
6		2H-tetrazole	N_1	406.58
			N_2	408.50
			N_3	407.09
			N_4	406.07
7		2-aminotetrazole	N_1	406.20
			N_2	408.84
			N_3	406.74
			N_4	405.78
			N	407.26
8		2-methyltetrazole	N_1	406.04
			N_2	408.13
			N_3	406.53
			N_4	405.57
9		2-cyanotetrazole	N_1	407.28
			N_2	409.79
			N_3	407.80
			N_4	406.82
			N	406.12

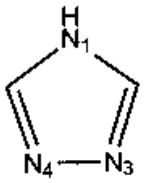
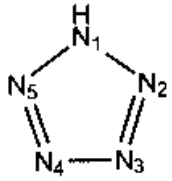
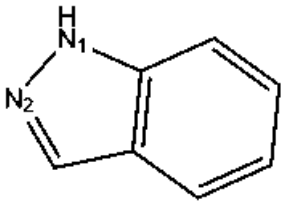
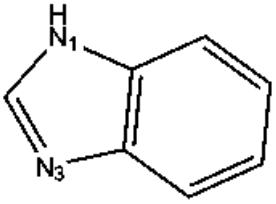
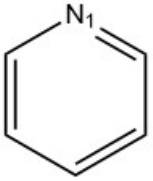
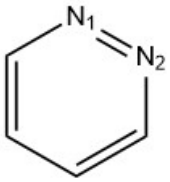
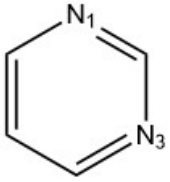
10		2-nitrotetrazole	N_1	407.23
			N_2	409.21
			N_3	407.74
			N_4	406.71
			N	413.60
11		5-amino-1H-tetrazole	N_1	407.34
			N_2	406.28
			N_3	406.06
			N_4	404.98
			N	406.56
12		5-methyl-1H-tetrazole	N_1	407.58
			N_2	406.55
			N_3	406.15
			N_4	405.27
13		5-cyano-1H-tetrazole	N_1	408.71
			N_2	407.58
			N_3	407.19
			N_4	406.45
			N	405.95
14		5-nitro-1H-tetrazole	N_1	408.94
			N_2	407.82
			N_3	407.40
			N_4	406.79
			N	412.88

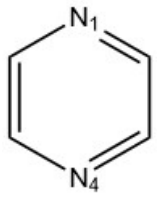
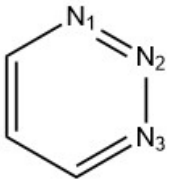
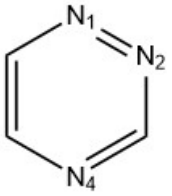
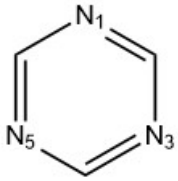
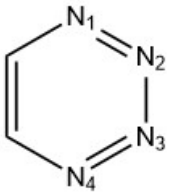
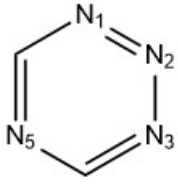
15		5-amino-2H-tetrazole	N_1	405.60
			N_2	407.88
			N_3	406.57
			N_4	405.27
			N	405.96
16		5-methyl-2H-tetrazole	N_1	406.03
			N_2	408.09
			N_3	406.72
			N_4	405.55
17		5-cyano-2H-tetrazole	N_1	407.18
			N_2	409.12
			N_3	407.73
			N_4	406.71
			N	405.58
18		5-nitro-2H-tetrazole	N_1	407.52
			N_2	409.36
			N_3	407.94
			N_4	407.02
			N	412.35
19		furazan	N_2	406.88
			N_5	406.88

20		3-amino-1,2,5-oxadiazole	N_2	405.75
			N_5	406.45
			N	406.28
21		3-methyl-1,2,5-oxadiazole	N_2	406.28
			N_5	406.54
22		3-cyano-1,2,5-oxadiazole	N_2	407.46
			N_5	407.51
			N	405.81
23		3-nitro-1,2,5-oxadiazole	N_2	407.84
			N_5	407.67
			N	412.67
24		1,2,4,5-tetrazine	N_1	406.85
			N_2	406.85
			N_4	406.85
			N_5	406.85
25		3-amino-1,2,4,5-tetrazine	N_1	406.20
			N_2	405.75
			N	406.24
26		3-methyl-1,2,4,5-tetrazine	N_1	406.48
			N_2	406.29

27		3-cyano-1,2,4,5-tetrazine	N_1	407.36
			N_2	407.29
			N	405.85
28		3-nitro-1,2,4,5-tetrazine	N_1	407.50
			N_2	407.53
			N	411.87
29		5,5’-bistetrazole	N_1	408.18
			N_2	407.12
			N_3	406.82
			N_4	405.97
30		5,5’-ethylbistetrazole	N_1	407.70
			N_2	406.68
			N_3	406.31
			N_4	405.43
31		5,5’-vinylbistetrazole	N_1	407.75
			N_2	406.65
			N_3	406.40
			N_4	405.39
32		5,5’-hydrazinebistetrazole	N_1	407.63
			N_2	406.66
			N_3	406.42
			N_4	405.38
			N	407.21

33		5,5’-azobistetrazole	N_1	408.03
			N_2	406.89
			N_3	406.59
			N_4	405.71
			N	406.92
34		pyrrole	N_1	406.00
35		pyrazole	N_1	406.79
			N_2	405.00
36		imidazole	N_1	406.54
			N_4	404.15
37		1,2,4-triazole	N_1	407.38
			N_2	405.63
			N_4	404.80
38		1,2,3-triazole	N_1	407.38
			N_2	406.20
			N_3	405.80
39		1,2,5-triazole	N_1	407.79
			N_2	405.81
			N_5	405.81

40		1,3,4-triazole	N_1	407.17
			N_3	405.08
			N_4	405.08
41		pentazole	N_1	409.32
			N_2	408.01
			N_3	407.36
42		1H-indazole	N_1	406.26
			N_2	404.84
43		benzimidazole	N_1	406.12
			N_3	403.89
44		pyridine	N_1	404.43
45		pyridazine	N_1	405.38
			N_2	405.38
46		pyrimidine	N_1	404.90
			N_3	404.90

47		pyrazine	N_1	405.14
			N_4	405.14
48		1,2,3-triazine	N_1	405.90
			N_2	406.61
			N_3	405.90
49		1,2,4-triazine	N_1	406.17
			N_2	405.09
			N_4	405.90
50		1,3,5-triazine	N_1	405.43
			N_3	405.43
			N_5	405.43
51		1,2,3,4-tetrazine	N_1	406.71
			N_2	407.14
			N_3	407.14
			N_4	406.71
52		1,2,3,5-tetrazine	N_1	406.35
			N_2	406.48
			N_3	407.50
			N_5	406.48

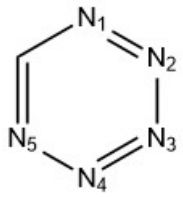
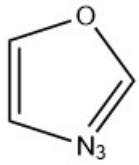
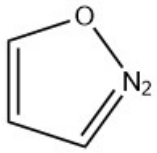
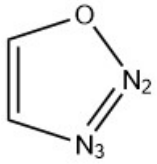
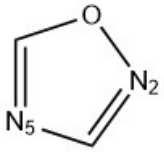
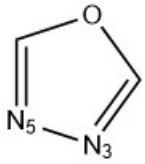
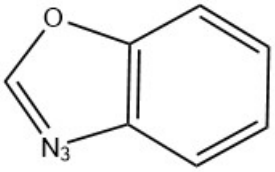
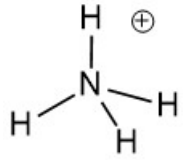
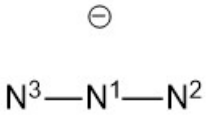
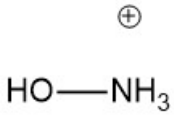
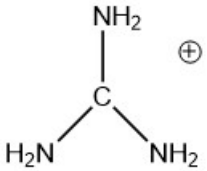
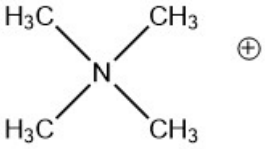
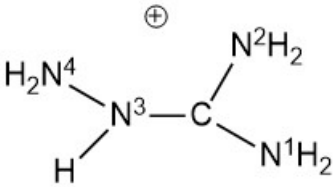
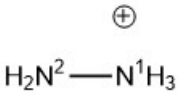
53		pentazine	N_1	407.48
			N_2	408.11
			N_3	407.72
			N_4	408.11
			N_5	407.48
54		oxazole	N_3	405.05
55		isoxazole	N_2	406.05
56		1,2,3-oxadiazole	N_2	407.44
			N_3	406.57
57		1,2,4-oxadiazole	N_2	406.75
			N_4	405.76
58		1,3,4-oxadiazole	N_3	406.01
			N_4	406.01
59		benzoxazole	N_3	404.71

Table S2. Simulated N1s ionic potentials in eV for 9 ions. IP was computed by the ΔKS method with the BP86 functional, based on geometry optimized at M06-2X/aug-cc-pVTZ level.

NO.	Structure	Name	Atom	IP
1		ammonium cation	N	416.74
2		azide anion	N^1	403.60
			N^2	397.83
3		hydroxyammonium cation	N	417.68
4		guanidinium cation	N	411.70
5		tetramethylammonium cation	N	413.23
6		aminoguanidinium cation	N^1	411.35
			N^2	411.04
			N^3	411.86
			N^4	411.25
7		hydrazinium cation	N^1	416.49
			N^2	413.35

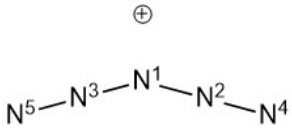
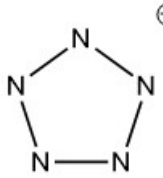
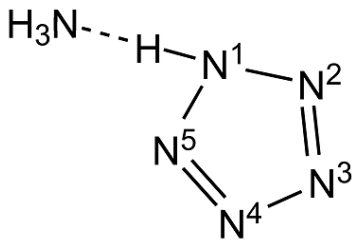
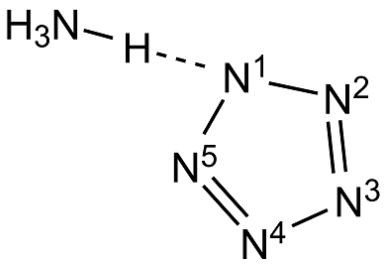
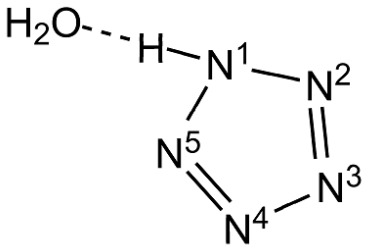
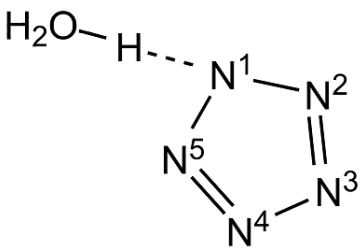
8		pentazenium cation	N^1	416.69
			N^2	418.19
			N^4	416.01
9		pentazolate anion	N	400.46

Table S3. Simulated N1s IPs (in eV) for a few dimer systems, each in neutral-neutral (optimized in gas phase) or cation-anion (taken from crystal structure) forms. Gas phase geometry was optimized at M06-2X/aug-cc-pVTZ level. Solid state geometry was directly extracted from crystal structures in ref. 62 without optimization. IP was computed by the ΔKS method with the BP86 functional.

No.	Structure	Name	Atom	IP
1		ammonia-pentazole dimer (gas geom.) $NH_3 \cdots HN_5$	N^1	407.79
			N^2	406.95
			N^3	406.42
			N	406.83
2		ammonium-pentazolate dimer (solid geom.) $[H_3N\text{-}H]^+ \cdots [N_5]^-$	N^1	404.55
			N^2	404.42
			N^3	404.17
			N^4	404.23
			N^5	404.34
			N	411.90
3		water-pentazolate dimer (gas geom.) $H_2O \cdots HN_5$	N^1	408.31
			N^2	407.25
			N^3	406.68
4		hydronium-pentazolate dimer (solid geom.) $[H_2O\text{-}H]^+ \cdots [N_5]^-$	N^1	405.44
			N^2	404.99
			N^3	404.85
			N^4	404.96
			N^5	405.06