Supplementary Material for

Application of Machine Learning in Developing Quantitative Structure-Property Relationship for Thermal Decomposition Temperature of Nitrogen-Rich Energetic Ionic Salts

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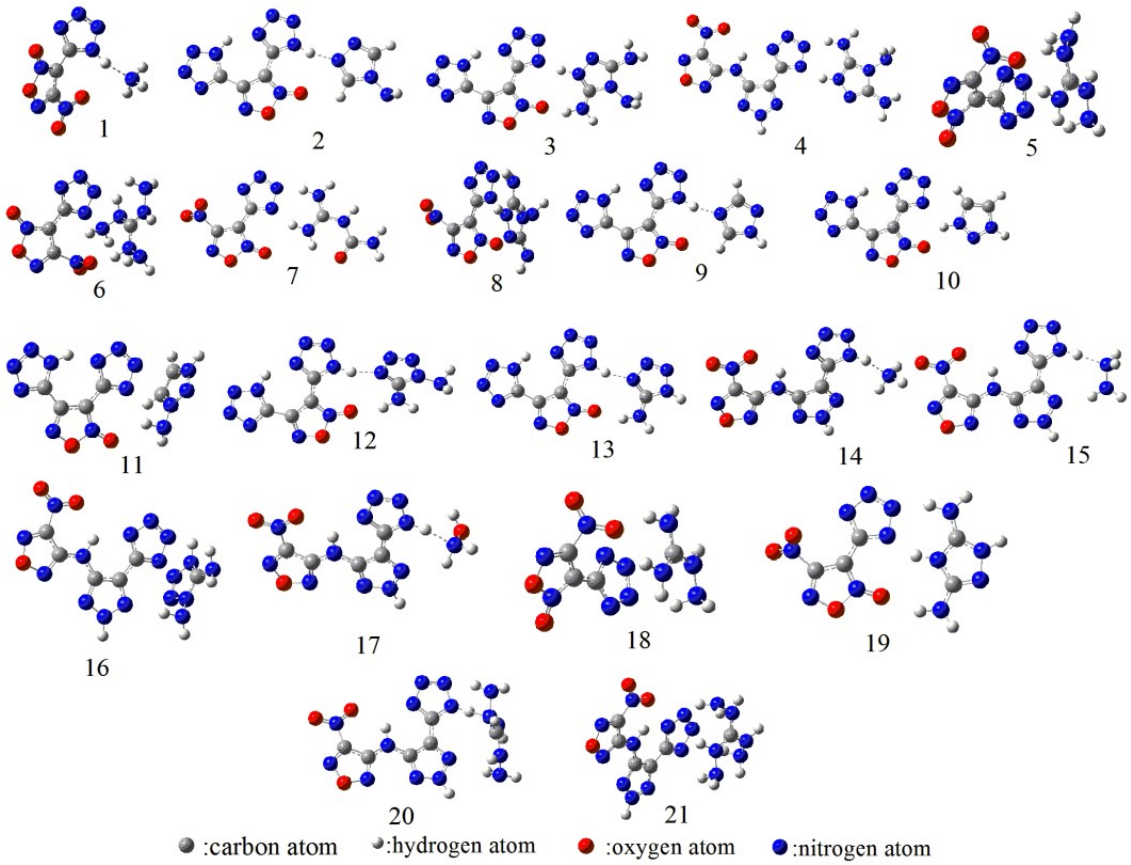

Figure S1. Optimized geometries of 21 nitrogen-rich energetic ionic salts at the M06-2X/6-311++G(3df,3pd) level of theory with the number referenced to Table 1.

Table S1. The values of *RMSE* and R^2 with different sets of descriptors.

Number of descriptors	7	8	9	10	11	12	13
RMSE	32.41	64.42	30.39	39.03	27.76	16.89	15.72
R^2	61.77%	50.89%	58.39%	14.08%	68.38%	92.34%	96.31%

Table S2. The correlation coefficients between each descriptor and T_d.

Descriptors	μ	E_{HOMO}	E_{LUMO}	ΔE	*OB*	$\Lambda_{NICS(0)F}$	$\Lambda_{NICS(1)Z}$	$\Delta V_{(0.003)}$	σ_+^2	I_a	A_a	α	*WBO*
R	0.52	0.06	0.61	0.45	0.67	0.66	0.62	0.59	0.26	0.09	0.6	0.54	0.72

Table S3. The values of quantum chemical parameters expressed in different ways for 21 nitrogen-rich energetic salts at the level of M06-2X/6-311++G(3df,3pd) in the QSPR model. The number of energetic salts is referenced to Table 1.

	$\Lambda_{NICS(0)F}$	$\Lambda_{NICS(1)F}$	$\Lambda_{NICS(0)Z}$	$\Lambda_{NICS(1)Z}$	σ_{tot}^2/ (kcal mol^{-1})^2	σ_+^2/ (kcal mol^{-1})^2	σ_-^2/ (kcal mol^{-1})^2	I_v/ev	I_a/ev	A_v/ev	A_a/ev
1	-13.33	-7.23	-12.02	-13.35	345.84	221.08	124.75	9.94	8.98	1.92	2.63
2	-10.95	-7.02	-12.06	-13.23	444.20	293.53	150.67	9.80	8.88	1.26	1.78
3	-11.26	-7.18	-11.69	-13.92	713.04	495.31	217.74	9.12	8.45	0.82	1.82
4	-12.32	-9.67	-11.27	-13.22	645.91	489.94	155.98	8.03	7.68	0.78	1.86
5	-13.34	-6.84	-12.44	-14.73	363.42	234.41	129.02	9.08	8.48	2.70	2.70
6	-13.78	-6.66	-11.80	-14.31	519.51	259.24	260.26	8.77	8.24	1.70	2.67
7	-13.70	-7.06	-11.83	-14.16	778.45	614.82	163.62	8.86	8.30	0.70	1.46
8	-13.81	-7.29	-11.08	-14.05	595.55	415.25	180.30	9.05	8.35	0.85	1.93
9	-11.11	-7.02	-11.97	-13.15	359.98	240.87	119.12	10.02	9.17	1.44	1.95
10	-11.38	-7.05	-11.19	-13.88	848.41	651.07	197.34	9.12	8.55	0.96	1.68
11	-11.29	-7.15	-12.15	-14.48	854.47	656.95	197.52	8.91	8.41	0.95	1.78
12	-11.10	-7.15	-12.00	-13.23	373.09	254.36	118.73	9.97	9.41	1.52	2.14
13	-11.18	-7.15	-11.90	-13.17	462.83	350.53	112.30	10.10	9.23	1.59	2.21
14	-12.13	-9.85	-11.53	-12.63	337.99	237.42	100.57	9.01	8.70	1.24	1.83
15	-12.13	-9.83	-11.43	-12.64	351.00	253.29	97.71	9.01	8.74	1.24	1.84
16	-12.26	-9.68	-10.74	-13.75	613.64	436.67	176.98	8.28	7.81	1.56	2.98
17	-12.10	-9.82	-11.28	-12.48	349.80	264.09	85.72	9.11	8.75	1.31	1.89
18	-13.33	-6.81	-12.58	-14.96	483.25	338.45	144.80	9.04	8.47	1.69	2.66

19	-13.89	-7.20	-11.93	-14.19	524.87	369.49	155.38	9.16	7.77	0.99	2.23
20	-12.21	-9.75	-11.45	-12.68	341.81	249.80	92.00	9.06	7.95	2.44	2.44
21	-12.18	-9.62	-11.62	-14.14	424.11	320.33	103.77	8.45	7.84	2.91	2.91

$\Lambda_{NICS(0)F}$: index of aromaticity calculated at central of the furazan (furoxan)

$\Lambda_{NICS(1)F}$: index of aromaticity calculated at 1.0 Å out of the furazan (furoxan)

$\Lambda_{NICS(0)FZ}$: index of aromaticity calculated at central of the tetrazole

$\Lambda_{NICS(1)Z}$: index of aromaticity calculated at 1.0 Å out of the tetrazole

σ_{tot}^2/(kcal mol^{-1})^2: total ESP variance

σ_+^2/(kcal mol^{-1})^2: positive ESP variance

σ_-^2/(kcal mol^{-1})^2: negative ESP variance

I_v/ev: vertical ionization potential

I_a/ev: adiabatic ionization potential

A_v/ev: vertical electron affinity

A_a/ev: adiabatic electron affinity

Table S4. Quantum chemical parameters and *OB* of six new theoretically designed nitrogen-rich energetic salts at the level of M06-2X/6-311++G(3df,3pd) for the QSPR model. The number of energetic salts is referenced to Table 4.

Number	μ/ Debye	E_{HOMO}/ ev	E_{LUMO}/ ev	ΔE	*OB*	$\Lambda_{NICS(0)F}$	$\Lambda_{NICS(1)Z}$	$\Delta V_{(0.003)}$/ Å^3	σ_+^2/ (kcal mol^{-1})^2	I_a/ ev	A_a/ ev	α/ Bohr^3	*WBO*
1	11.56	-8.15	-2.01	-6.14	-67.1	-12.33	-12.17	83.31	300.55	8.52	1.75	195.79	0.69
2	19.24	-7.44	-1.63	-5.81	-63.2	-11.34	-13.26	89.87	585.11	7.72	1.77	219.66	0.62
3	7.85	-8.29	-2.11	-6.18	-54.8	-11.26	-12.34	84.34	342.62	8.41	1.86	201.1	0.67
4	12.83	-8.67	-1.59	-7.08	-64.9	-11.47	-14.05	70.54	332.99	8.65	2.01	173.11	0.67
5	13.41	-8.55	-1.46	-7.08	-64.3	-11.33	-14.06	74.35	309.47	8.59	1.97	181.8	0.68
6	11.77	-8.63	-1.47	-7.16	-63.8	-11.33	-14.21	74.35	243.46	8.57	1.55	185.43	0.70

μ/Debye: dipole moment

E_{HOMO}/ev: energy of the highest occupied molecular orbital

E_{LUMO}/ev: energy of the lowest unoccupied molecular orbital

ΔE: energy gap between HOMO and LUMO

OB: oxygen balance

$\Lambda_{NICS(0)F}$: index of aromaticity calculated at central of the furazan (furoxan)

$\Lambda_{NICS(1)Z}$: index of aromaticity calculated at 1.0 Å out of the tetrazole

$\Delta V_{(0.003)}$/Å^3: available free space per molecule in the unit cell

σ_+^2/(kcal mol^{-1})^2: positive ESP variance

I_a/ev: adiabatic ionization potential

A_a/ev: adiabatic electron affinity

α/Bohr^3: polarizability

WBO: wiberg bond order of the weakest chemical bond

Matrix A (17×13)

-4.3929	0.0635	-0.4276	0.4894	10.4118	-0.9329	-1.0459	-8.0535	-127.1806	-0.0006	0.5059	-17.7200	0.0947
0.2871	0.3835	-0.3576	0.7394	10.0118	-1.3729	-0.6259	-4.2035	-102.3506	-0.2406	0.4759	-8.4300	0.0947
5.4071	0.2635	0.5724	-0.3006	9.7118	-1.2929	-0.4759	-0.7435	253.2294	-0.1806	-0.7341	-8.0800	-0.0153
-0.4629	0.0835	0.3924	-0.3206	6.3118	-1.4029	-0.3659	-1.1235	53.6594	-0.1306	-0.2641	-3.4300	0.0147
-1.9529	-0.9365	-0.0376	-0.9006	-13.8882	1.2971	0.5341	-1.9935	-120.7206	0.6894	-0.2441	-7.1900	-0.0553
7.6871	-0.0365	0.2024	-0.2406	-13.8882	1.0271	-0.1959	-3.3635	289.4794	0.0694	-0.5141	-4.7300	-0.0653
6.2771	0.1735	0.3124	-0.1406	-13.0882	1.1171	-0.7959	-0.6335	295.3594	-0.0706	-0.4141	0.7100	-0.0053
0.2871	-0.8165	-0.0976	-0.7106	0.2118	1.3071	0.4541	3.8965	-107.2306	0.9294	-0.0541	9.6100	-0.0553
-0.4629	-0.9965	-0.1776	-0.8206	0.1118	1.2271	0.5141	-0.0735	-11.0606	0.7494	0.0159	-0.7500	-0.0453
-1.1529	0.1035	-0.0676	0.1694	-1.8882	0.2771	1.0541	-3.8235	-124.1706	0.2194	-0.3641	-12.3200	-0.0153
-0.9429	0.1035	-0.0676	0.1694	-1.6882	0.2771	1.0441	0.3465	-108.3006	0.2594	-0.3541	-3.2900	-0.0153
2.0571	0.8135	0.2624	0.5594	0.1118	0.1471	-0.0659	10.6965	75.0794	-0.6706	0.7859	31.6000	0.0247
-2.8529	0.0035	-0.1376	0.1394	6.5118	0.3071	1.2041	-1.3535	-97.5006	0.2694	-0.3041	-8.2600	0.0047
-3.5129	0.1135	-0.4376	0.5494	10.9118	-0.9229	-1.2759	-11.0235	-23.1406	-0.0106	0.4659	-26.3400	0.1047
-0.7929	0.0235	0.2924	-0.2706	6.5118	-1.4829	-0.5059	-3.4635	7.8994	-0.7106	0.0359	-9.1100	-0.0753
-1.9429	0.0235	-0.1276	0.1494	-8.3882	0.1971	1.0041	11.7165	-111.7906	-0.5306	0.2459	29.9700	-0.0153
-3.5329	0.6335	-0.0976	0.7394	-7.9882	0.2271	-0.4559	13.1965	-41.2606	-0.6406	0.7159	37.7600	0.0247

Covariance matrix B (13×13)

12.2031	0.1767	0.7066	-0.5270	-10.5383	0.7264	-0.4293	0.4948	454.9328	-0.0668	-0.8415	2.0351	-0.0748
0.1767	0.2434	0.0281	0.2158	0.9014	-0.2628	-0.1394	0.7499	17.6036	-0.2030	0.0800	2.4150	0.0141
0.7066	0.0281	0.0858	-0.0576	-0.5038	-0.0223	-0.0117	0.4479	31.5236	-0.0403	-0.0706	0.9492	-0.0086
-0.5270	0.2158	-0.0576	0.2738	1.4025	-0.2394	-0.1278	0.3196	-13.8412	-0.1630	0.1512	1.5122	0.0226
-10.5383	0.9014	-0.5038	1.4025	77.7749	-7.0953	-2.2582	-25.2663	-307.9552	-0.5422	0.8816	-70.7511	0.2673
0.7264	-0.2628	-0.0223	-0.2394	-7.0953	1.0628	0.4221	2.1804	4.2723	0.2937	-0.1008	5.7312	-0.0298
-0.4293	-0.1394	-0.0117	-0.1278	-2.2582	0.4221	0.6268	1.8257	-49.2457	0.1566	-0.1226	3.2534	-0.0230
0.4948	0.7499	0.4479	0.3196	-25.2663	2.1804	1.8257	43.1965	-24.0923	-1.0674	0.8869	113.8630	-0.0925
454.9328	17.6036	31.5236	-13.8412	-307.9552	4.2723	-49.2457	-24.0923	21748.3009	-16.9717	-27.7790	16.6074	-1.8473
-0.0668	-0.2030	-0.0403	-0.1630	-0.5422	0.2937	0.1566	-1.0674	-16.9717	0.2408	-0.0976	-3.3332	-0.0080
-0.8415	0.0800	-0.0706	0.1512	0.8816	-0.1008	-0.1226	0.8869	-27.7790	-0.0976	0.2093	3.2514	0.0151
2.0351	2.4150	0.9492	1.5122	-70.7511	5.7312	3.2534	113.8630	16.6074	-3.3332	3.2514	309.9877	-0.1759
-0.0748	0.0141	-0.0086	0.0226	0.2673	-0.0298	-0.0230	-0.0925	-1.8473	-0.0080	0.0151	-0.1759	0.0031

Eigenvectors C (13×13)

0.02092	0.00775	-0.06726	0.85892	-0.48445	-0.10601	-0.06291	-0.06919	0.04859	0.01158	-0.00660	0.00396	0.00066
0.00081	0.00581	0.03217	-0.07113	-0.10423	-0.39199	0.43622	-0.12753	-0.30337	0.42414	0.12514	0.01099	0.57887
0.00145	0.00274	0.00354	0.04069	0.08212	-0.09530	-0.17020	0.14201	-0.26580	0.71311	0.14197	0.00168	-0.57795
-0.00064	0.00320	0.02882	-0.11120	-0.18657	-0.29518	0.60794	-0.27901	-0.02891	-0.28001	-0.02333	-0.10608	-0.57130
-0.01421	-0.24474	0.95968	0.09024	-0.00397	0.09383	0.02947	0.01652	-0.00144	0.01237	-0.02534	0.00306	0.00009
0.00020	0.02071	-0.09801	0.12349	0.06945	0.69938	0.48052	-0.16163	0.16468	0.34340	-0.27534	0.05361	0.00201
-0.00226	0.01166	-0.03689	0.25900	0.29509	-0.02053	0.41374	0.77792	-0.02339	-0.16102	0.20265	-0.00174	-0.00547
-0.00109	0.33512	0.08960	0.33261	0.71248	-0.24079	-0.00590	-0.39400	0.20867	0.00964	0.06628	-0.01096	0.00358
0.99967	-0.00400	0.01489	-0.01583	0.01138	0.00369	0.00291	0.00238	0.00010	-0.00204	0.00143	-0.00028	-0.00001
-0.00078	-0.00858	-0.03025	0.11235	0.07783	0.40740	-0.01555	-0.26058	-0.60941	-0.24464	0.54565	-0.13126	0.00418
-0.00128	0.00847	0.02411	-0.13102	-0.19647	0.07222	0.04908	-0.04294	0.61838	0.15283	0.72161	-0.08705	0.00731
0.00082	0.90937	0.22778	-0.10881	-0.26119	0.10623	-0.01059	0.14321	-0.08984	-0.01374	-0.03011	0.00423	-0.00130
-0.00009	-0.00067	0.00344	-0.01376	-0.01839	-0.00772	0.03807	-0.06229	-0.03248	-0.07445	0.14938	0.98019	-0.06619

The four-dimensional new matrix D (13×4)

0.02092	0.00775	-0.06726	0.85892
0.00081	0.00581	0.03217	-0.07113
0.00145	0.00274	0.00354	0.04069
-0.00064	0.00320	0.02882	-0.11120
-0.01421	-0.24474	0.95968	0.09024
0.00020	0.02071	-0.09801	0.12349
-0.00226	0.01166	-0.03689	0.25900
-0.00109	0.33512	0.08960	0.33261
0.99967	-0.00400	0.01489	-0.01583
-0.00078	-0.00858	-0.03025	0.11235
-0.00128	0.00847	0.02411	-0.13102
0.00082	0.90937	0.22778	-0.10881
-0.00009	-0.00067	0.00344	-0.01376

Matrix E (17×4)

235.1789	175.4298	3.5912	-1.0244
260.1072	185.2034	5.7752	2.8195
615.6822	185.3635	10.7518	3.0514
416.1057	191.0504	5.9469	0.1959
242.0330	193.0197	-17.2427	0.7501
652.3076	193.2288	-11.2313	1.4288
658.1479	198.8592	-8.7673	0.3174
255.3721	206.7837	0.7018	3.8144
351.4921	195.6657	-0.6237	1.4435
238.4275	184.8219	-7.0077	2.3011
254.2966	194.3198	-4.1638	2.6533
437.6738	228.3739	9.1115	1.4971
264.9339	187.1676	2.6983	1.6042
339.1930	166.0618	3.3416	-1.9853
370.3489	185.2363	4.0129	0.3399
250.8966	230.0309	-1.9395	1.2255
321.3724	237.2126	1.6109	-2.1327

Matrix F(4×4)

221.6063	129.3751	6.8117	0.9851
294.7612	204.0157	-13.1142	3.9755
496.6123	225.0615	-3.6404	5.9945
491.1942	252.4864	4.7390	4.7025

Training set (17×13)

6.81	-8.37	-2.46	-5.91	-44.4	-13.34	-14.73	65.55	234.41	8.48	2.70	158.41	0.77
11.49	-8.05	-2.39	-5.66	-44.8	-13.78	-14.31	69.40	259.24	8.24	2.67	167.70	0.77
16.61	-8.17	-1.46	-6.70	-45.1	-13.70	-14.16	72.86	614.82	8.30	1.46	168.05	0.66
10.74	-8.35	-1.64	-6.72	-48.5	-13.81	-14.05	72.48	415.25	8.35	1.93	172.70	0.69
9.25	-9.37	-2.07	-7.30	-68.7	-11.11	-13.15	71.61	240.87	9.17	1.95	168.94	0.62
18.89	-8.47	-1.83	-6.64	-68.7	-11.38	-13.88	70.24	651.07	8.55	1.68	171.40	0.61
17.48	-8.26	-1.72	-6.54	-67.9	-11.29	-14.48	72.97	656.95	8.41	1.78	176.84	0.67
11.49	-9.25	-2.13	-7.11	-54.6	-11.10	-13.23	77.50	254.36	9.41	2.14	185.74	0.62
10.74	-9.43	-2.21	-7.22	-54.7	-11.18	-13.17	73.53	350.53	9.23	2.21	175.38	0.63
10.05	-8.33	-2.10	-6.23	-56.7	-12.13	-12.63	69.78	237.42	8.70	1.83	163.81	0.66
10.26	-8.33	-2.10	-6.23	-56.5	-12.13	-12.64	73.95	253.29	8.74	1.84	172.84	0.66
13.26	-7.62	-1.77	-5.84	-54.7	-12.26	-13.75	84.30	436.67	7.81	2.98	207.73	0.70
8.35	-8.43	-2.17	-6.26	-48.3	-12.10	-12.48	72.25	264.09	8.75	1.89	167.87	0.68
7.69	-8.32	-2.47	-5.85	-43.9	-13.33	-14.96	62.58	338.45	8.47	2.66	149.79	0.78
10.41	-8.41	-1.74	-6.67	-48.3	-13.89	-14.19	70.14	369.49	7.77	2.23	167.02	0.60
9.26	-8.41	-2.16	-6.25	-63.2	-12.21	-12.68	85.32	249.80	7.95	2.44	206.10	0.66
7.67	-7.80	-2.13	-5.66	-62.8	-12.18	-14.14	86.80	320.33	7.84	2.91	213.89	0.70

Testing set (4×13)

6.25	-9.16	-2.77	-6.39	-29.6	-13.33	-13.35	53.04	221.08	8.98	2.63	116.30	0.64
13.62	-9.16	-1.88	-7.28	-67.9	-10.95	-13.23	75.94	293.53	8.88	1.78	179.84	0.62
20.37	-8.49	-1.46	-7.03	-66.6	-11.26	-13.92	82.04	495.31	8.45	1.82	201.92	0.56
18.36	-7.38	-1.61	-5.77	-65.4	-12.32	-13.22	92.30	489.94	7.68	1.86	228.61	0.61

Latent

21762.47
371.19
55.51
2.83
1.34
0.54
0.21
0.08
0.02
0.02
0.01
0.00
0.00

Table S5. Geometry of No.1. Units are in angstrom.

Atom	X	Y	Z
O	-2.729	0.993	0.457
O	-1.327	2.719	0.649
O	-1.892	-2.702	-0.689
O	0.169	-2.100	-0.493
N	-2.664	-0.306	0.146
N	-1.435	1.560	0.387
N	1.862	0.114	0.137
N	2.959	0.771	-0.213
N	2.589	1.889	-0.727
N	1.254	1.993	-0.729
N	-1.028	-1.906	-0.464
C	-1.426	-0.549	-0.104
C	-0.591	0.587	0.029
C	0.813	0.877	-0.191
N	2.626	-2.376	1.163
H	1.966	-0.840	0.558
H	2.192	-3.130	0.643
H	2.539	-2.595	2.148
H	3.616	-2.382	0.941

Table S6. Geometry of No.2. Units are in angstrom.

Atom	X	Y	Z

O	3.762	0.658	0.491
O	2.714	2.627	0.255
O	2.099	-2.842	-0.651
O	0.473	-2.064	0.523
N	3.463	-0.644	0.374
N	2.603	1.435	0.212
N	-0.376	0.202	-1.374
N	-1.551	0.796	-1.484
N	-1.595	1.839	-0.686
N	-0.450	1.964	-0.029
N	1.548	-1.973	-0.047
C	2.216	-0.680	0.062
C	1.613	0.589	-0.054
C	0.278	0.948	-0.482
N	-1.889	-0.393	1.348
H	-1.938	0.586	1.593
H	-0.963	-0.799	1.358
N	-3.876	-0.193	0.189
N	-2.468	-1.975	-0.227
H	-2.973	-2.148	-1.081
H	-1.500	-2.270	-0.245
H	-4.404	-0.464	-0.626
C	-2.723	-0.827	0.411
N	-4.150	1.092	0.645

H	-4.291	1.095	1.646
H	-3.420	1.737	0.332

Table S7. Geometry of No.3. Units are in angstrom.

Atom	X	Y	Z
O	3.978	-0.588	-0.365
O	3.002	-2.560	0.069
O	2.165	2.952	0.304
O	0.574	1.967	-0.756
N	3.625	0.704	-0.404
N	2.844	-1.377	-0.027
N	-0.230	-0.118	1.341
N	-1.381	-0.755	1.481
N	-1.358	-1.872	0.793
N	-0.188	-2.008	0.185
N	1.649	1.992	-0.183
C	2.369	0.724	-0.128
C	1.814	-0.549	0.117
C	0.483	-0.919	0.547
N	-1.664	0.085	-1.575
H	-1.628	-0.887	-1.843
H	-0.768	0.552	-1.514
N	-3.686	-0.294	-0.513
N	-2.434	1.576	0.009

H	-1.468	1.882	0.078
H	-4.271	-0.022	0.264
C	-2.587	0.429	-0.680
N	-3.824	-1.598	-0.974
H	-3.869	-1.624	-1.984
H	-3.078	-2.177	-0.587
N	-3.215	1.681	1.170
H	-3.391	2.657	1.357
H	-2.712	1.240	1.940

Table S8. Geometry of No.4. Units are in angstrom.

Atom	X	Y	Z
O	4.138	-0.688	0.070
O	4.155	1.556	0.023
O	0.378	-1.943	-1.261
O	0.371	-2.273	0.864
N	3.222	-1.675	0.040
N	3.476	0.570	-0.003

N	-0.157	0.888	0.106
N	-0.864	2.007	-0.033
N	-0.076	3.002	-0.337
N	1.176	2.582	-0.409
N	0.848	-1.837	-0.158
C	2.092	-1.076	-0.053
C	2.172	0.328	-0.086
C	1.094	1.286	-0.134
N	-2.646	0.263	1.410
H	-2.619	1.274	1.419
N	-3.458	0.408	-0.750
N	-2.473	-1.546	-0.031
H	-1.733	-1.931	0.545
H	-3.543	-0.039	-1.650
C	-2.828	-0.273	0.194
N	-3.796	1.755	-0.658
H	-4.506	1.892	0.051
H	-2.948	2.289	-0.462
N	-2.656	-2.051	-1.323
H	-3.139	-2.938	-1.262
H	-1.748	-2.189	-1.753
N	-1.779	-0.305	2.343
H	-0.855	-0.422	1.933
H	-2.160	-1.167	2.708

Table S9. Geometry of No.5. Units are in angstrom.

Atom	X	Y	Z
O	2.426	-2.602	0.085
O	0.291	-1.926	0.133
O	5.489	0.015	0.625
O	4.514	0.899	-1.089
N	3.647	-2.038	0.035
N	1.456	-1.591	0.079
N	1.968	2.010	0.303
N	0.976	2.882	0.302
N	-0.147	2.259	0.074
N	0.069	0.961	-0.079
N	4.589	0.136	-0.163
C	3.448	-0.769	-0.008
C	2.078	-0.422	0.019
C	1.383	0.839	0.065
O	-4.587	-1.821	-0.138
N	-2.870	1.987	-0.031
N	-2.381	-0.257	-0.099
N	-4.601	0.469	-0.016
N	-6.567	-0.733	0.013
C	-3.245	0.716	-0.050
C	-5.208	-0.794	-0.043
H	-1.854	2.262	0.002

H	-3.558	2.709	0.082
H	-1.361	-0.012	-0.110
H	-2.720	-1.208	-0.138
H	-5.198	1.277	-0.082
H	-7.044	0.068	0.387
H	-7.030	-1.623	0.103

Table S10. Geometry of No.6. Units are in angstrom.

Atom	X	Y	Z
O	1.886	2.511	-0.149
O	-0.173	1.733	-0.562
O	5.129	0.063	-0.090
O	3.893	-0.884	1.409
N	3.106	2.012	0.120
N	0.985	1.452	-0.299
N	1.727	-2.105	-0.462
N	0.803	-3.040	-0.589
N	-0.382	-2.500	-0.472
N	-0.275	-1.194	-0.259
N	4.104	-0.112	0.512
C	2.967	0.734	0.144
C	1.640	0.317	-0.116
C	1.037	-0.984	-0.262
C	-3.236	1.313	0.198

C	-3.190	-0.869	0.480
N	-2.956	0.112	-0.420
H	-3.884	-0.650	2.440
N	-3.644	-0.244	1.553
N	-3.675	1.129	1.405
N	-2.456	0.006	-1.705
H	-1.498	-0.337	-1.616
H	-3.028	-0.647	-2.229
N	-3.105	2.480	-0.469
N	-3.064	-2.180	0.245
H	-3.312	-2.776	1.021
H	-2.174	-2.481	-0.207
H	-3.054	3.290	0.129
H	-2.394	2.451	-1.189

Table S11. Geometry of No.7. Units are in angstrom.

Atom	X	Y	Z
O	-2.096	-2.500	-0.056
O	0.053	-1.879	-0.167
O	-5.051	0.255	-0.644
O	-4.124	1.003	1.161
N	-3.303	-1.905	0.013
N	-1.111	-1.516	-0.086
N	-1.556	2.098	-0.252

N	-0.552	2.955	-0.293
N	0.576	2.311	-0.171
N	0.350	1.012	-0.048
N	-4.187	0.298	0.190
C	-3.073	-0.641	0.032
C	-1.694	-0.332	-0.031
C	-0.975	0.912	-0.099
C	3.489	-1.306	0.035
C	3.659	0.868	0.059
N	2.766	-0.134	-0.016
H	5.751	0.735	0.214
N	4.853	0.292	0.147
N	4.766	-1.089	0.139
N	2.900	-2.516	-0.070
N	3.359	2.160	0.046
H	4.088	2.846	0.099
H	2.365	2.452	-0.050
H	3.464	-3.308	0.185
H	1.906	-2.578	0.085
H	1.720	0.059	-0.045

Table S12. Geometry of No.8. Units are in angstrom.

Atom	X	Y	Z
O	-0.761	-2.681	0.000
O	1.230	-1.667	0.000
N	-3.559	0.999	-0.000
N	-4.861	1.247	-0.000
N	-5.455	0.107	-0.000
N	-4.570	-0.900	-0.000
N	-0.946	1.952	0.000
N	-0.062	2.957	0.000
N	1.134	2.499	0.000
N	1.058	1.171	0.000
N	-2.063	-2.322	-0.000
N	0.017	-1.548	0.000
C	-3.388	-0.329	-0.000
C	-2.108	-1.024	0.000
C	-0.780	-0.494	0.000
C	-0.236	0.841	0.000
H	-2.835	1.725	-0.000
C	4.121	-1.037	0.000
C	4.684	0.991	-0.000
N	3.599	0.170	0.000

H	1.961	0.616	0.000
H	3.580	-1.967	0.000
H	6.145	-1.661	-0.000
H	4.612	2.065	-0.000
N	5.831	0.359	-0.000
N	5.452	-0.931	-0.000

Table S13. Geometry of No.9. Units are in angstrom.

Atom	X	Y	Z
O	-0.818	-2.725	-0.000
O	1.217	-1.818	-0.000
N	-3.445	1.061	0.000
N	-4.731	1.378	0.000
N	-5.388	0.271	0.000
N	-4.560	-0.782	0.000
N	-0.867	1.929	-0.000
N	0.050	2.884	-0.000
N	1.233	2.344	-0.000
N	1.130	1.018	-0.000
N	-2.102	-2.322	-0.000
N	-0.003	-1.617	-0.000
C	-3.349	-0.274	0.000
C	-2.100	-1.024	-0.000
C	-0.755	-0.534	-0.000

C	-0.177	0.789	-0.000
H	-2.660	1.739	0.000
N	4.404	-1.216	0.000
H	2.482	-0.539	-0.000
H	3.358	1.829	-0.000
H	6.390	-1.081	0.000
N	5.528	-0.555	0.000
N	3.498	-0.296	-0.000
C	5.355	0.788	0.000
C	4.000	0.959	-0.000
H	6.172	1.483	0.000

Table S14. Geometry of No.10. Units are in angstrom.

Atom	X	Y	Z
O	-1.680	-2.852	-0.102
O	0.521	-2.513	-0.005
N	-3.220	1.488	0.043
N	-4.377	2.133	0.026
N	-5.299	1.238	-0.054
N	-4.775	0.006	-0.091
N	-0.517	1.647	0.124
N	0.608	2.343	0.176
N	1.619	1.525	0.180
N	1.191	0.266	0.130

N	-2.810	-2.121	-0.112
N	-0.594	-2.002	-0.020
C	-3.474	0.177	-0.030
C	-2.463	-0.873	-0.039
C	-1.037	-0.757	0.021
C	-0.132	0.370	0.096
H	-2.282	1.931	0.094
N	4.328	0.303	0.971
H	3.429	-0.614	-1.972
H	5.036	2.141	0.725
N	4.684	1.324	0.247
N	3.838	-0.535	0.116
C	4.425	1.169	-1.068
C	3.859	-0.065	-1.156
H	4.617	1.930	-1.800
N	3.270	-1.701	0.597
H	3.505	-2.451	-0.043
H	2.253	-1.541	0.567

Table S15. Geometry of No.11. Units are in angstrom.

Atom	X	Y	Z
O	-0.880	-2.623	-0.000
O	1.027	-1.461	-0.000
N	-3.958	0.827	-0.000
N	-5.276	0.969	0.000

N	-5.775	-0.216	0.000
N	-4.812	-1.147	0.000
N	-1.434	1.976	-0.000
N	-0.642	3.055	-0.000
N	0.590	2.706	-0.000
N	0.634	1.376	-0.000
N	-2.205	-2.364	0.000
N	-0.191	-1.433	-0.000
C	-3.680	-0.482	0.000
C	-2.348	-1.073	0.000
C	-1.064	-0.442	-0.000
C	-0.628	0.933	-0.000
H	-3.291	1.607	-0.000
N	4.175	1.434	0.000
N	3.220	0.455	-0.000
N	5.153	-0.516	0.000
N	6.095	-1.541	-0.000
C	5.327	0.838	0.000
H	6.294	1.311	0.000
C	3.814	-0.704	-0.000
H	3.349	-1.673	-0.000
H	6.674	-1.466	-0.827
H	6.674	-1.466	0.827
H	1.579	0.890	-0.000

Table S16. Geometry of No.12. Units are in angstrom.

Atom	X	Y	Z
O	-1.518	-2.636	0.376
O	0.477	-1.649	0.199
N	-4.325	0.990	-0.115
N	-5.624	1.241	-0.107
N	-6.218	0.121	0.118
N	-5.335	-0.875	0.261
N	-1.798	1.933	-0.349
N	-0.955	2.946	-0.506
N	0.263	2.520	-0.392
N	0.257	1.213	-0.153
N	-2.817	-2.285	0.355
N	-0.750	-1.507	0.202
C	-4.154	-0.316	0.113
C	-2.869	-1.000	0.179
C	-1.543	-0.464	0.077
C	-1.030	0.871	-0.131
H	-3.572	1.688	-0.269
N	3.607	1.254	0.710
N	2.735	0.366	0.117
N	4.704	-0.418	-0.202
N	5.694	-1.324	-0.534
C	4.779	0.762	0.521

C	3.381	-0.633	-0.435
H	6.303	-0.939	-1.247
H	6.231	-1.557	0.293
H	1.664	0.616	0.046
N	5.977	1.207	1.030
N	2.911	-1.660	-1.149
H	6.699	1.348	0.335
H	5.846	2.042	1.585
H	3.555	-2.423	-1.287
H	1.932	-1.886	-0.998

Table S17. Geometry of No.13. Units are in angstrom.

Atom	X	Y	Z
O	1.118	-2.607	-0.183
O	-0.806	-1.473	-0.099
N	4.157	0.870	0.061
N	5.474	1.024	0.055
N	5.984	-0.151	-0.060
N	5.029	-1.088	-0.131
N	1.614	1.981	0.173
N	0.810	3.048	0.257
N	-0.418	2.687	0.207
N	-0.446	1.363	0.087
N	2.438	-2.332	-0.172

N	0.417	-1.431	-0.098
C	3.892	-0.437	-0.054
C	2.567	-1.043	-0.086
C	1.274	-0.431	-0.036
C	0.820	0.935	0.068
H	3.485	1.640	0.139
N	-3.855	1.482	-0.575
N	-3.057	0.516	-0.053
N	-5.096	-0.131	-0.079
N	-6.228	-0.905	0.055
C	-3.848	-0.494	0.253
H	-6.868	-0.450	0.697
H	-6.675	-0.993	-0.850
H	-1.383	0.876	0.029
N	-3.538	-1.663	0.846
H	-4.245	-2.380	0.796
H	-2.576	-1.958	0.761
N	-5.066	1.121	-0.599

Table S18. Geometry of No.14. Units are in angstrom.

Atom	X	Y	Z
O	-0.902	-2.629	0.199
O	1.066	-1.571	0.131
N	-3.798	0.968	-0.063

N	-5.107	1.175	-0.073
N	-5.665	0.020	0.024
N	-4.750	-0.955	0.098
N	-1.211	1.976	-0.149
N	-0.364	3.010	-0.229
N	0.848	2.600	-0.183
N	0.822	1.275	-0.070
N	-2.211	-2.301	0.177
N	-0.155	-1.481	0.119
C	-3.587	-0.350	0.043
C	-2.287	-1.008	0.088
C	-0.971	-0.448	0.049
C	-0.462	0.898	-0.050
H	-3.096	1.712	-0.125
N	4.242	1.294	0.532
N	3.419	0.333	0.046
N	5.445	-0.350	0.041
C	4.184	-0.694	-0.260
H	1.733	0.749	-0.017
N	3.797	-1.859	-0.837
H	4.384	-2.661	-0.681
H	2.807	-2.047	-0.753
N	5.445	0.910	0.539
H	6.308	-0.853	-0.074

Table S19. Geometry of No.15. Units are in angstrom.

Atom	X	Y	Z
O	3.819	-1.859	0.000
O	2.214	2.141	-0.000
O	4.371	2.086	0.000
N	4.264	-0.613	0.000
N	2.452	-1.932	0.000
N	0.749	-0.275	-0.000
N	-0.339	-2.415	-0.000
N	-1.624	-2.730	-0.000
N	-2.476	-1.736	-0.000
N	-1.343	1.745	-0.000
N	-2.136	2.831	-0.000
N	-3.370	2.492	0.000
N	-3.412	1.158	0.000
N	3.288	1.573	0.000
C	3.210	0.127	0.000
C	2.039	-0.695	-0.000
C	-0.355	-1.095	-0.000
C	-1.699	-0.661	-0.000

C	-2.155	0.710	-0.000
H	-1.924	-3.690	-0.000
H	0.573	0.728	-0.000
H	-6.158	-0.722	-0.816
H	-6.158	-0.722	0.817
H	-4.959	-1.486	0.000
H	-4.303	0.616	0.000
N	-5.561	-0.668	0.000

Table S20. Geometry of No.16. Units are in angstrom.

Atom	X	Y	Z
O	-4.060	-1.965	-0.009
O	-2.614	2.095	-0.058
O	-4.766	1.954	-0.128
N	-4.553	-0.738	-0.052
N	-2.692	-1.983	0.032
N	-1.056	-0.260	0.038
N	0.115	-2.356	0.099
N	1.411	-2.620	0.129
N	2.222	-1.592	0.127
N	0.961	1.839	0.040
N	1.712	2.954	0.040
N	2.957	2.661	0.074
N	3.050	1.329	0.098

N	-3.664	1.484	-0.079
C	-3.529	0.043	-0.041
C	-2.328	-0.732	0.013
C	0.079	-1.037	0.074
C	1.405	-0.550	0.091
C	1.812	0.835	0.076
H	1.748	-3.568	0.152
H	-0.919	0.748	0.018
H	5.889	-0.220	1.071
H	6.219	0.600	-0.311
H	3.981	0.851	0.135
N	5.539	0.004	0.144
N	5.350	-1.153	-0.669
H	6.057	-1.855	-0.482
H	4.441	-1.540	-0.445

Table S21. Geometry of No.17. Units are in angstrom.

Atom	X	Y	Z
O	5.307	1.601	-0.166
O	3.370	-2.247	-0.045
O	5.520	-2.373	-0.190
N	5.640	0.322	-0.189
N	3.952	1.794	-0.078
N	2.116	0.294	0.039

N	1.215	2.527	0.095
N	-0.035	2.946	0.193
N	-0.962	2.014	0.274
N	-0.125	-1.561	0.263
N	-1.014	-2.543	0.333
N	-2.212	-2.039	0.390
N	-2.147	-0.704	0.356
N	4.484	-1.770	-0.119
C	4.527	-0.324	-0.119
C	3.432	0.596	-0.046
C	1.091	1.213	0.114
C	-0.276	0.880	0.225
C	-0.853	-0.445	0.279
H	-0.257	3.926	0.199
H	1.840	-0.687	0.072
C	-4.649	-0.575	0.224
N	-4.571	0.713	-0.117
H	-4.527	-2.199	-1.096
N	-4.451	0.818	-1.471
N	-4.530	-0.330	-1.959
N	-4.693	-1.214	-0.942
N	-4.747	-1.082	1.450
H	-4.224	-1.951	1.542
H	-4.495	-0.400	2.157

N	-4.164	1.680	0.772
H	-4.676	2.534	0.593
H	-3.153	1.816	0.651

Table S22. Geometry of No.18. Units are in angstrom.

Atom	X	Y	Z
O	-6.204	1.353	0.009
O	-3.919	-2.303	0.016
O	-6.052	-2.622	0.018
N	-6.418	0.048	0.014
N	-4.870	1.672	0.005
N	-2.900	0.345	0.003
N	-2.211	2.647	-0.012
N	-1.000	3.183	-0.023
N	0.015	2.354	-0.027
N	-0.527	-1.268	0.002
N	0.404	-2.209	-0.000
N	1.570	-1.645	-0.018
N	1.449	-0.316	-0.029
N	-5.073	-1.927	0.016
C	-5.247	-0.491	0.012
C	-4.239	0.527	0.006
C	-1.955	1.352	-0.008
C	-0.555	1.159	-0.017

C	0.139	-0.112	-0.016
H	-0.872	4.180	-0.028
H	-2.536	-0.607	0.007
C	4.718	-0.850	-0.005
C	6.083	0.879	0.032
N	4.052	0.284	-0.017
H	2.987	0.336	-0.031
N	4.896	1.379	-0.004
N	6.039	-0.506	0.039
N	4.236	-2.083	-0.084
N	7.270	1.536	0.136
H	8.067	1.039	-0.230
H	7.224	2.513	-0.109
H	4.824	-2.852	0.188
H	3.178	-2.160	-0.048
N	7.145	-1.330	-0.019
H	7.243	-1.864	0.836
H	7.088	-1.943	-0.824

Table S23. Geometry of No.19. Units are in angstrom.

Atom	X	Y	Z
O	-4.033	-1.959	-0.126
O	-2.578	2.097	-0.074
O	-4.723	1.963	-0.272

N	-4.522	-0.731	-0.193
N	-2.670	-1.980	-0.009
N	-1.034	-0.259	0.095
N	0.131	-2.355	0.225
N	1.424	-2.619	0.319
N	2.235	-1.594	0.346
N	0.996	1.845	0.181
N	1.760	2.953	0.177
N	3.001	2.650	0.238
N	3.077	1.316	0.286
N	-3.627	1.490	-0.160
C	-3.498	0.049	-0.120
C	-2.303	-0.729	-0.002
C	0.097	-1.035	0.189
C	1.421	-0.550	0.265
C	1.833	0.833	0.248
H	1.760	-3.567	0.357
H	-0.899	0.750	0.085
H	6.136	-0.592	0.461
H	3.975	0.798	0.327
H	4.665	-1.322	0.386
N	5.203	-0.520	0.067
O	5.357	-0.720	-1.325
H	5.063	0.101	-1.727

Table S24. Geometry of No.20. Units are in angstrom.

Atom	X	Y	Z
O	-4.563	-2.209	0.397
O	-3.559	1.967	0.048
O	-5.653	1.623	0.437
N	-5.172	-1.037	0.459
N	-3.221	-2.096	0.150
N	-1.796	-0.225	-0.185
N	-0.440	-2.199	-0.360
N	0.858	-2.340	-0.577
N	1.549	-1.239	-0.730
N	-0.007	2.064	-0.559
N	0.641	3.241	-0.608
N	1.902	3.060	-0.730
N	2.110	1.741	-0.769
N	-4.526	1.260	0.249
C	-4.249	-0.161	0.256
C	-2.993	-0.816	0.056
C	-0.606	-0.889	-0.371
C	0.647	-0.278	-0.602
C	0.923	1.138	-0.655
H	1.293	-3.248	-0.619
H	-1.766	0.791	-0.234
C	4.239	-0.355	0.513

N	3.864	0.293	1.667
N	4.276	-1.730	0.649
N	4.506	0.314	-0.548
H	4.026	-0.222	2.519
H	3.702	-2.090	1.397
H	4.751	-0.290	-1.323
H	3.069	1.329	-0.803
N	4.216	-2.546	-0.485
H	5.150	-2.690	-0.848
H	3.631	-2.108	-1.191
N	4.139	1.660	1.824
H	4.943	1.902	1.251
H	3.352	2.195	1.478

Table S25. Geometry of No.21. Units are in angstrom.

Atom	X	Y	Z
O	5.210	-0.427	-0.664
O	2.039	2.266	0.462
O	3.940	3.247	0.191
N	5.041	0.864	-0.436
N	4.069	-1.157	-0.456
N	1.876	-0.548	0.227
N	1.787	-2.883	-0.340
N	0.782	-3.743	-0.280

N	-0.359	-3.290	0.181
N	-0.697	0.220	1.192
N	-1.804	0.808	1.638
N	-2.771	-0.064	1.680
N	-2.335	-1.256	1.273
N	3.230	2.281	0.215
C	3.807	0.990	-0.084
C	3.165	-0.290	-0.087
C	1.246	-1.772	0.121
C	-0.105	-2.019	0.457
C	-1.052	-1.054	0.987
H	0.900	-4.704	-0.553
H	1.302	0.212	0.588
C	-3.547	1.178	-0.723
N	-4.833	0.823	-0.602
N	-3.220	2.444	-0.423
N	-2.614	0.372	-1.221
H	-5.472	1.573	-0.386
H	-3.804	2.908	0.256
H	-1.666	0.539	-0.893
N	-1.933	2.966	-0.498
H	-1.601	2.967	-1.453
H	-1.310	2.469	0.137
N	-5.270	-0.428	-0.135

H	-5.147	-1.104	-0.876
H	-4.690	-0.693	0.660
N	-2.949	-0.895	-1.710
H	-2.417	-1.054	-2.555
H	-2.698	-1.590	-1.008

Calculation script: 2-4.gjf

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%nproc=8

M062X/6-311++g(3df,3pd) opt(tight) freq=noraman

Title Card Required

0 1

8	0	-2.948213	-0.627463	-0.207363
8	0	-2.781007	1.634452	-0.339422
8	0	0.134607	-2.960799	1.001893
8	0	1.116850	-1.901761	-0.632747
7	0	-2.103521	-1.684578	-0.026614
7	0	-2.161986	0.583320	-0.201027
7	0	1.467349	0.974473	0.244721
7	0	2.044841	2.186429	0.354877
7	0	1.118239	3.126745	0.268757
7	0	-0.091548	2.561614	0.097584

7	0	0.207111	-2.077665	0.161390
6	0	-0.914970	-1.163344	0.057570
6	0	-0.883642	0.247516	-0.040578
6	0	0.164619	1.245009	0.086790
7	0	3.832238	-0.984843	-0.500940
1	0	3.192099	-0.449590	-0.175248
1	0	3.603088	-1.729265	-0.933645
1	0	4.341738	-1.268010	0.172983
1	0	4.300070	-0.482108	-1.056918