Electronic Supplementary Material (ESI) for RSC Advances.

Design on functionalized bridged 1,2,4-triazole N-Oxides as high energy density materials and their comprehensive correlations

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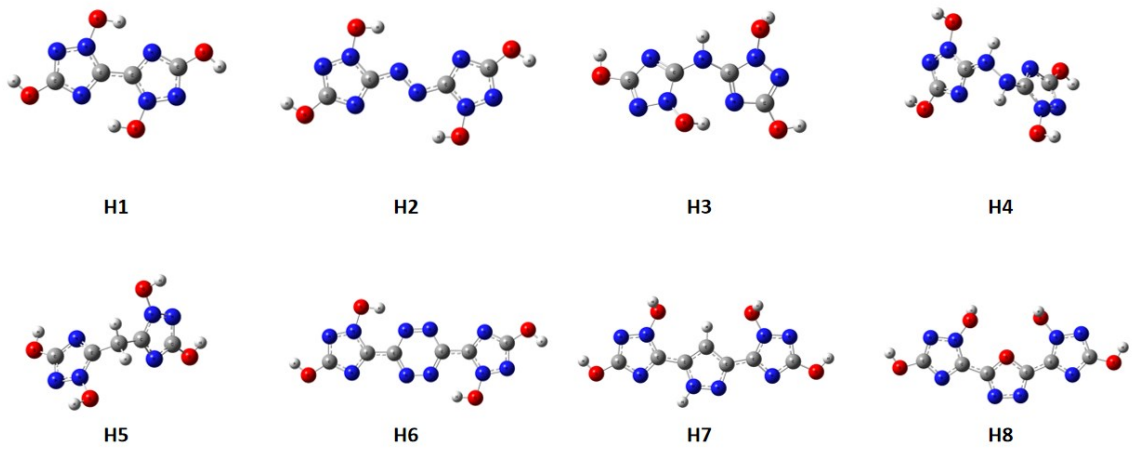
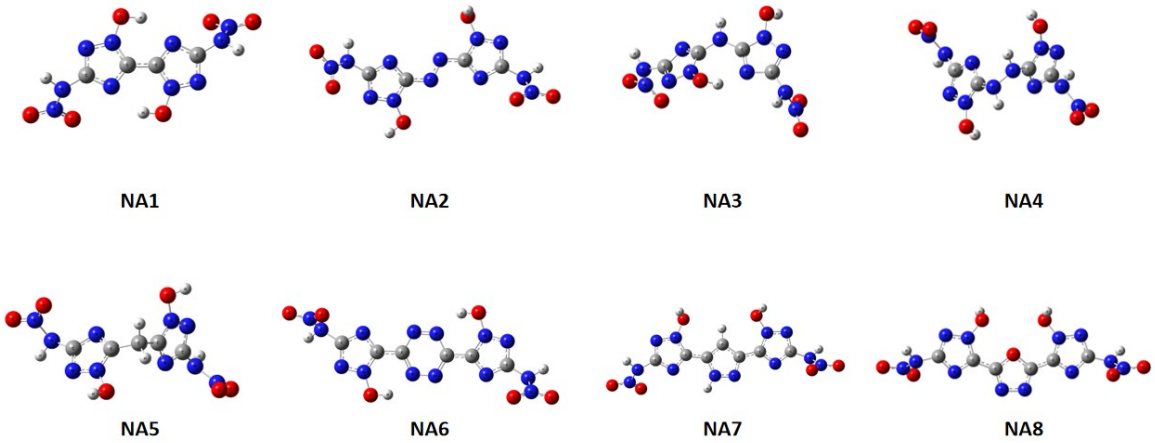


Figure S1 Optimized geometry of **H** series



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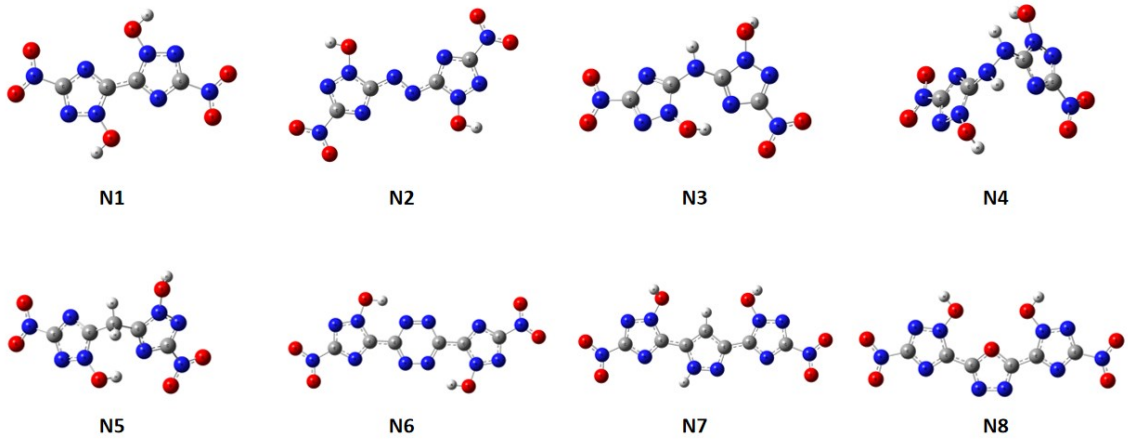

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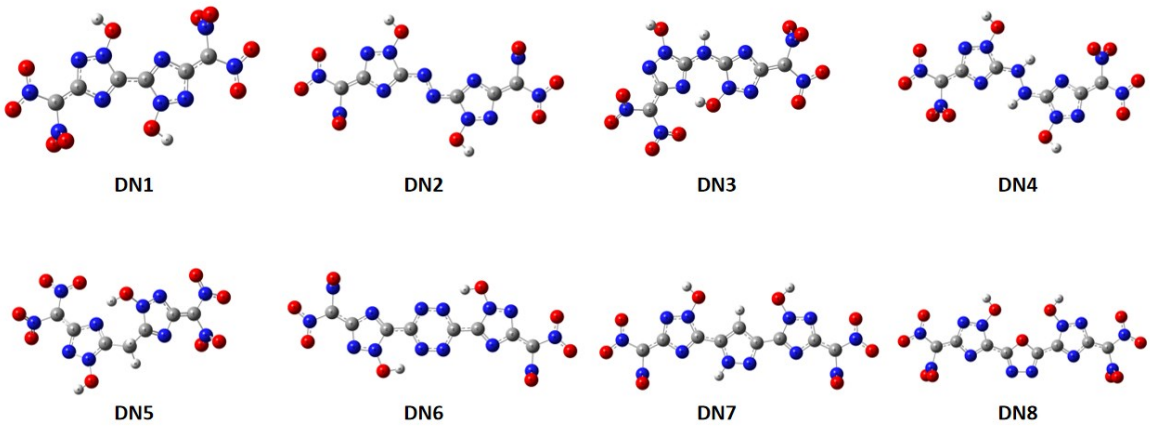

Figure S4 Optimized geometry of **DN** series

2. HOMO-LUMO orbitals and energy gap

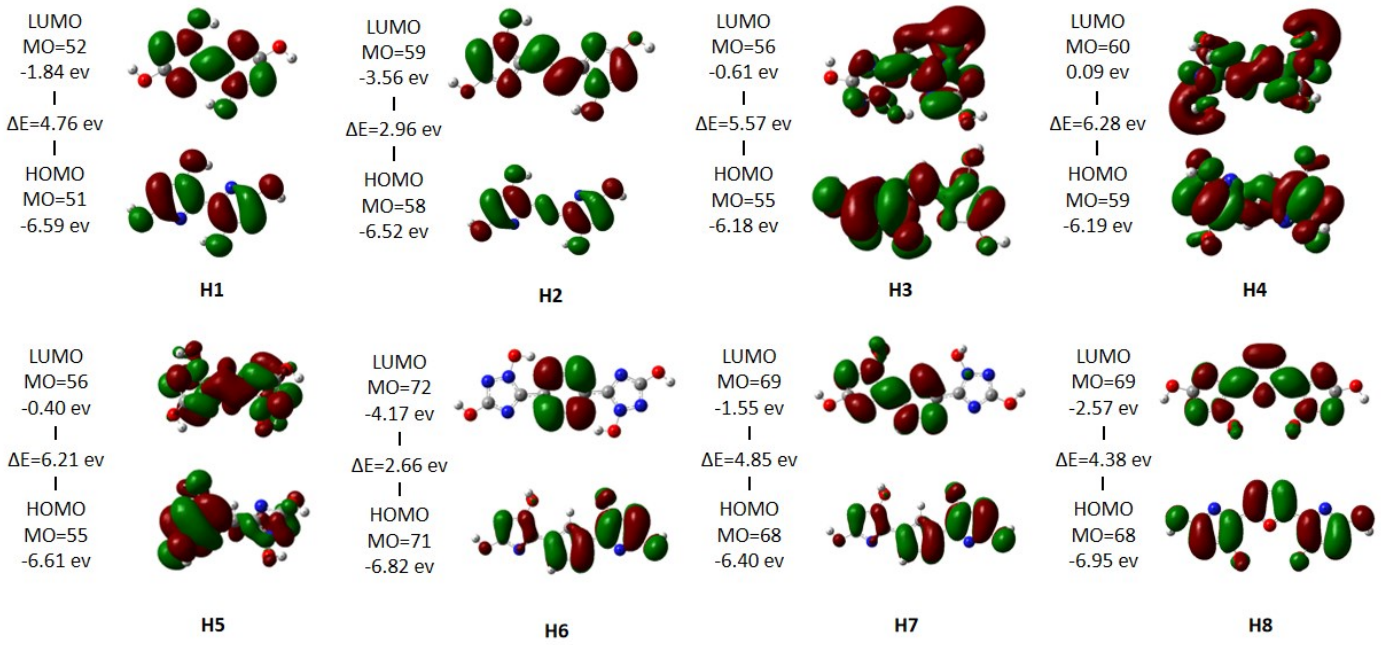

Figure S5 HOMO-LUMO energy and HOMO-LUMO gap of **H** series

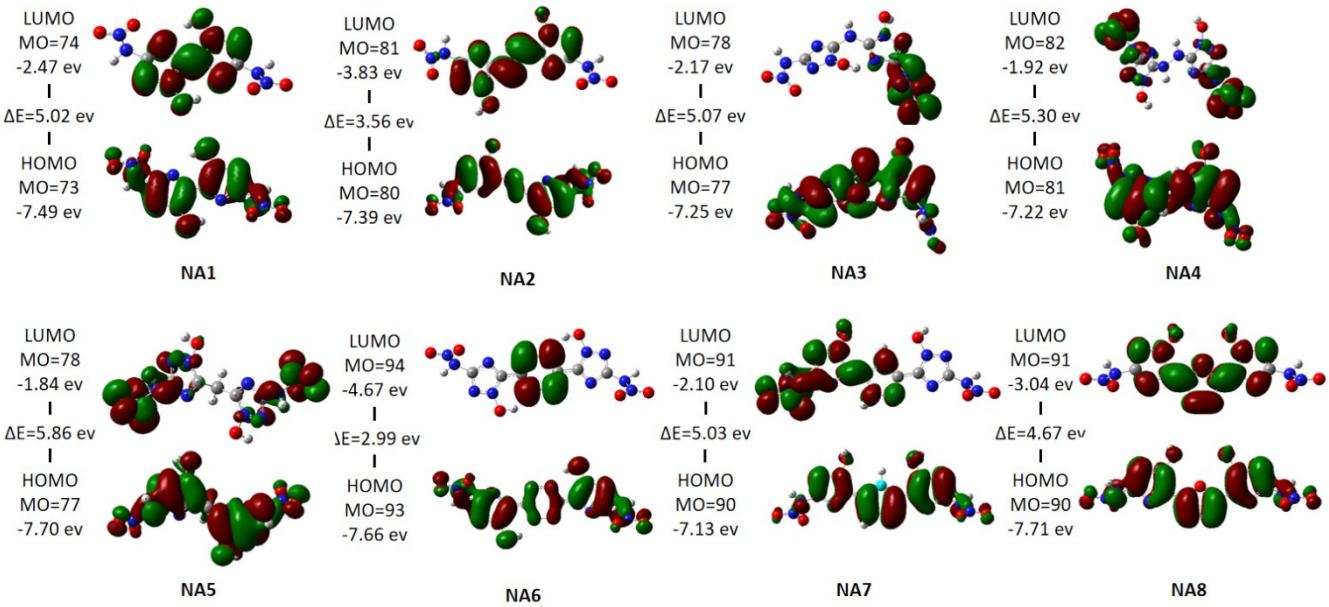

Figure S6 HOMO-LUMO energy and HOMO-LUMO gap of **NA** series

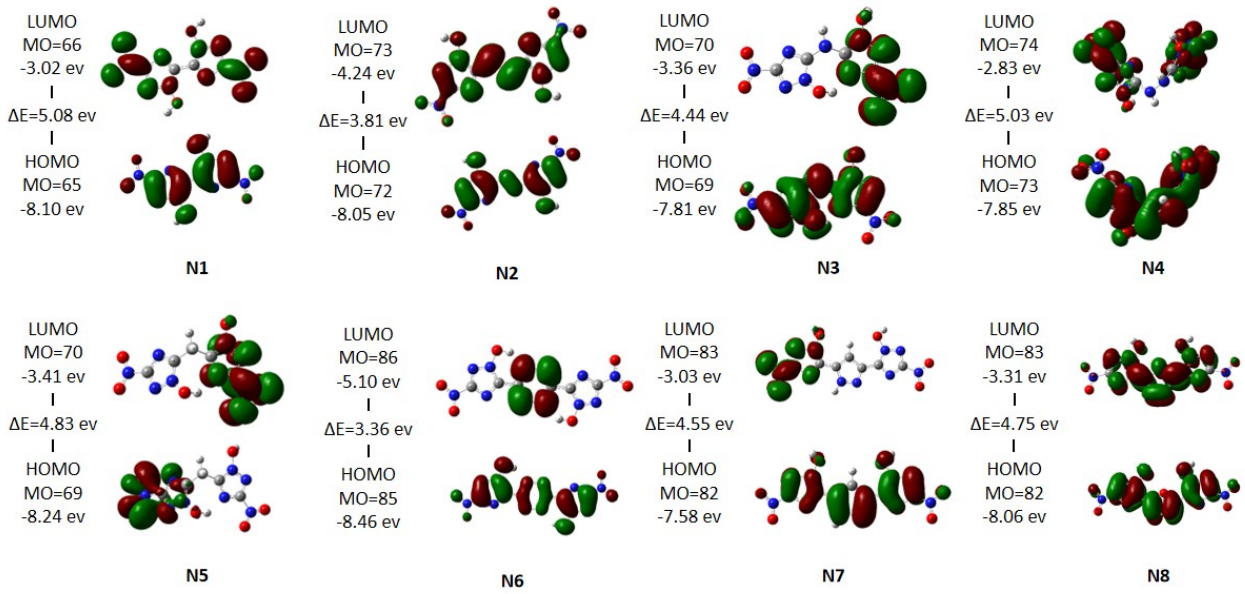

Figure S7 HOMO-LUMO energy and HOMO-LUMO gap of **N** series

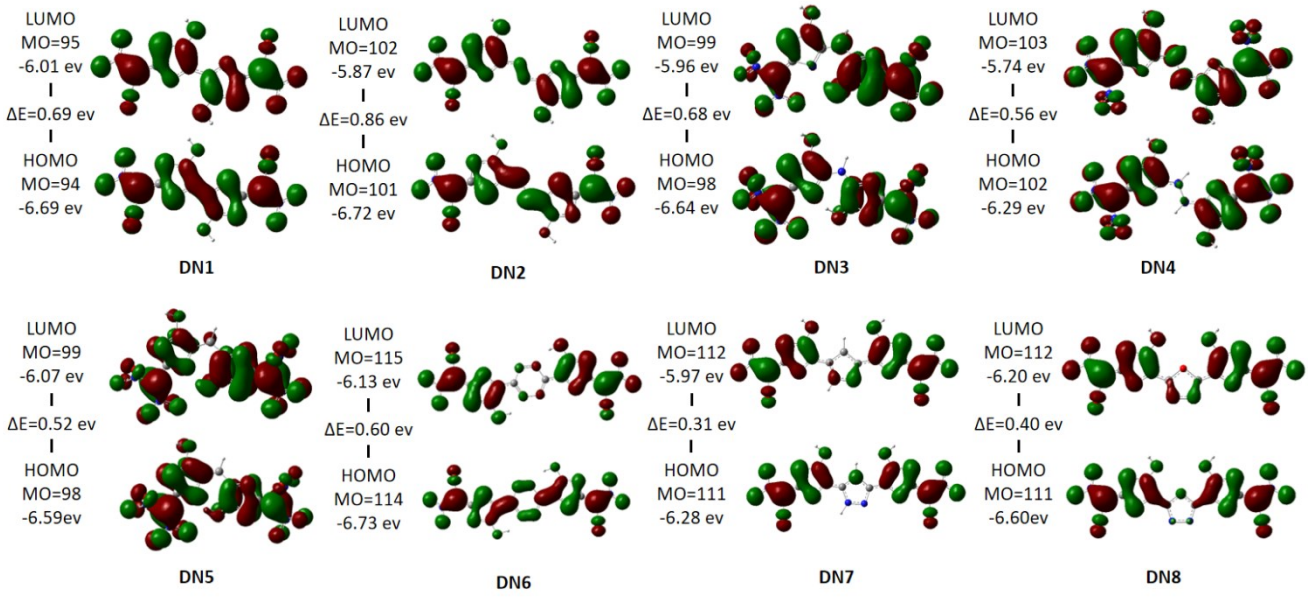

Figure S8 HOMO-LUMO energy and HOMO-LUMO gap of **DN** series

3. Molecular electrostatic potential (ESP)

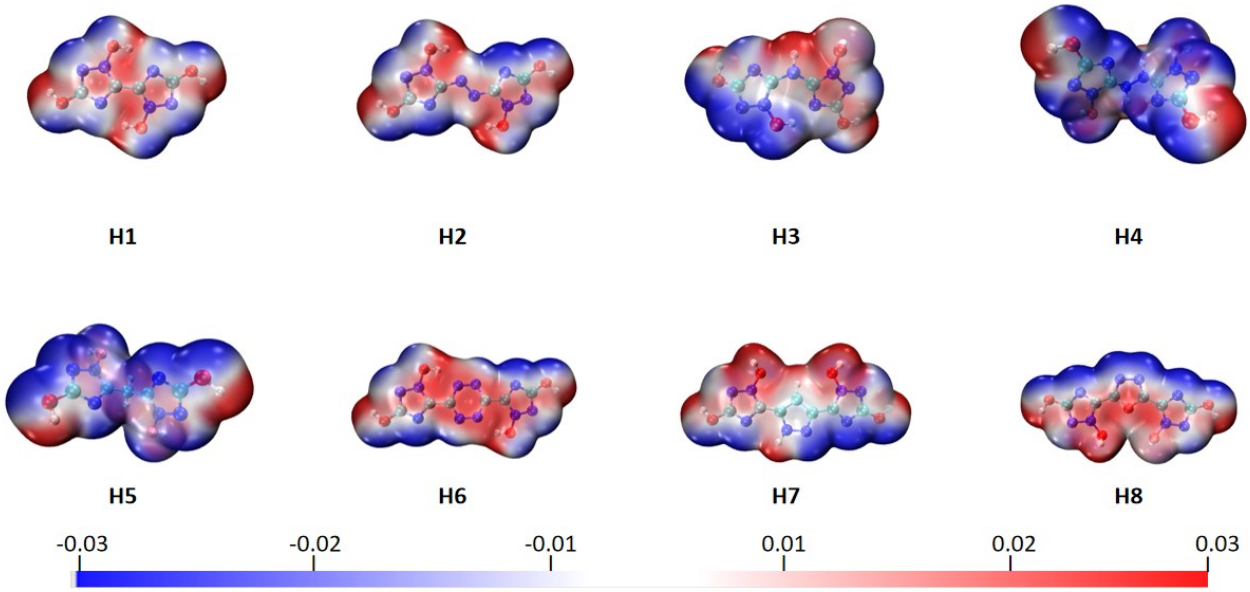

Figure S9 Molecular electrostatic potential of -OH**(H)** series ranging from -0.03 a.u.(blue) to 0.03 a.u.(red), isosurface=0.001

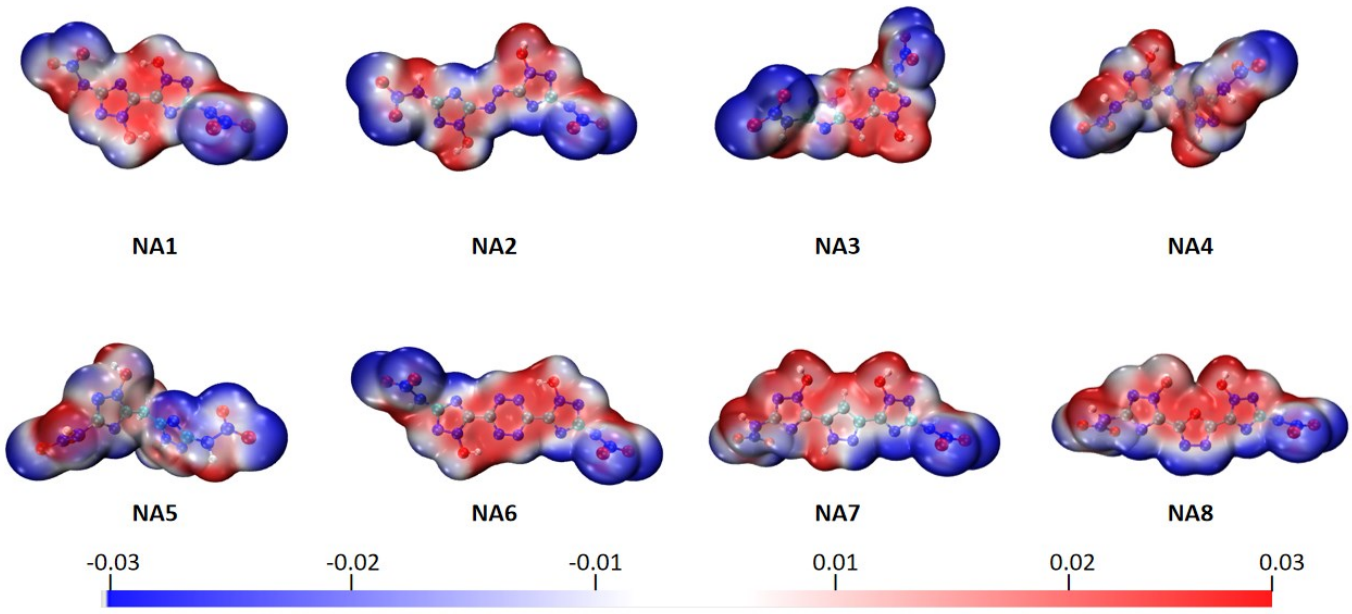

Figure S10 Molecular electrostatic potential of $-NHNO_2$**(NA)** series ranging from -0.03 a.u.(blue) to 0.03 a.u.(red), isosurface=0.001

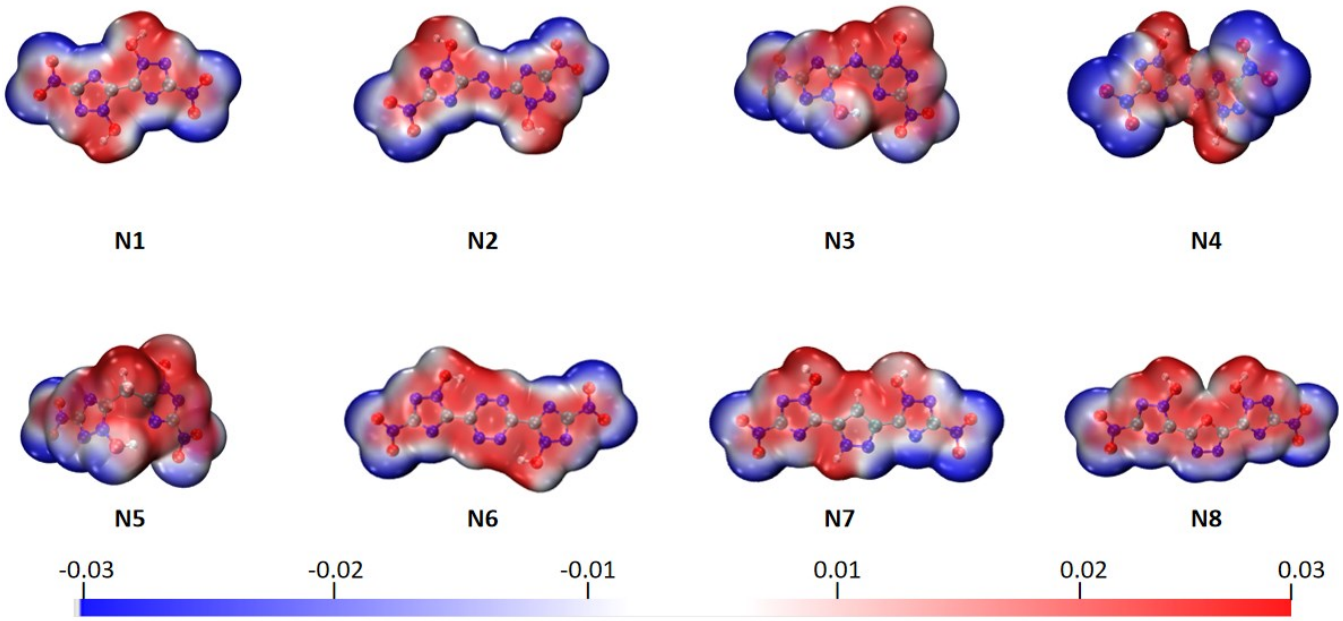

Figure S11 Molecular electrostatic potential of $-NO_2$**(N)** series ranging from -0.03 a.u.(blue) to 0.03 a.u.(red), isosurface=0.001

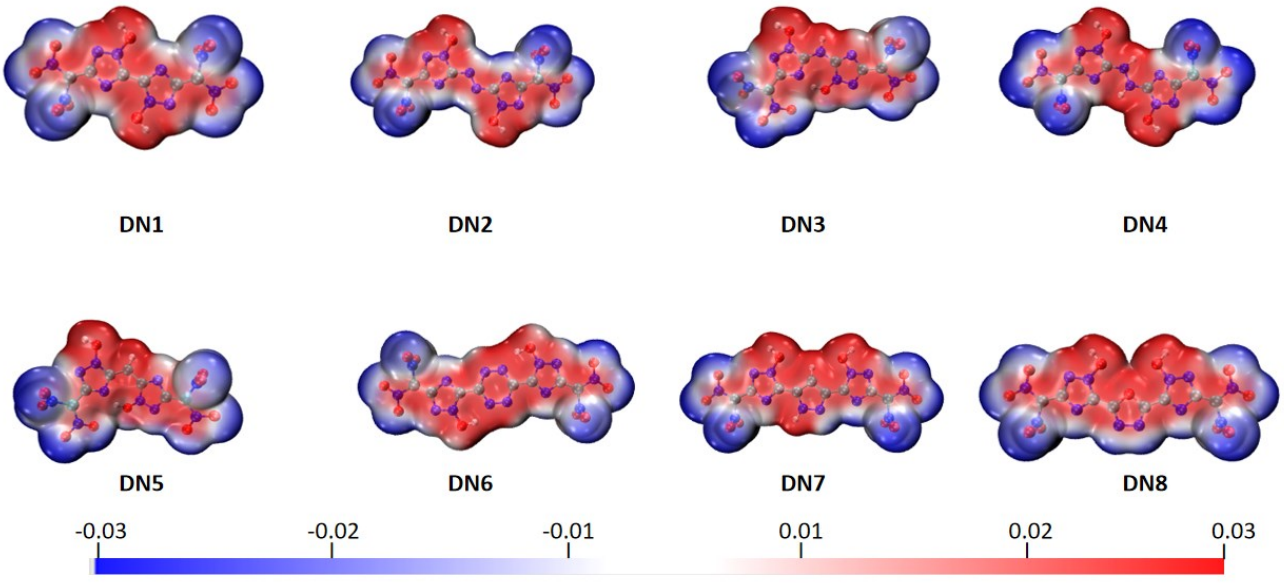

Figure S12 Molecular electrostatic potential of $-C(NO_2)_2$ **(DN)** series ranging from -0.03 a.u.(blue) to 0.03 a.u.(red), isosurface=0.001

4. Thermodynamic parameters

Table. S1 40 substituted 1,2,4-triazole-N-oxides, their sum of electronic and zero-point energy E_0, thermal correction from 0K to 298K H_T, gas-phase heat of formation under 0K HOF(g,0K), gas-phase heat of formation under 298K HOF(g,298K), condensed-phase heat of formation under 298K HOF(c,298K), compared with HMX and RDX.

No.	Formula	E_0 (a.u.) 6-311G(d,p)	H_T (a.u.)	$HOF_{(g,0K)}$ (kJ/mol)	$HOF_{(g,298K)}$ (kJ/mol)	$HOF_{(c,298K)}$ (kJ/mol)
H1	$C_4H_4N_6O_4$	-784.186546	0.012266	114.00	81.67	-10.85
H2	$C_4H_4N_8O_4$	-893.63995	0.014198	382.43	346.47	231.81
H3	$C_4H_5N_7O_4$	-839.534881	0.0137	150.64	113.50	-13.34
H4	$C_4H_6N_8O_4$	-894.844054	0.015413	290.01	248.80	121.70
H5	$C_5H_6N_6O_4$	-823.47276	0.014428	138.98	102.83	-19.28
H6	$C_6H_4N_{10}O_4$	-1079.344129	0.016442	658.64	617.79	483.13
H7	$C_7H_6N_8O_4$	-1009.193377	0.017011	372.07	331.92	178.32
H8	$C_6H_4N_8O_4$	-1045.103403	0.016888	302.90	267.57	114.59
N1	$C_4H_2N_8O_6$	-1042.76136	0.016269	562.13	531.36	411.08
N2	$C_4H_2N_{10}O_6$	-1152.22184	0.01802	812.00	777.13	637.67
N3	$C_4H_3N_9O_6$	-1098.126597	0.016645	554.44	516.08	382.73
N4	$C_4H_4N_{10}O_6$	-1153.441191	0.017357	679.58	634.53	491.82
N5	$C_5H_4N_8O_6$	-1082.075687	0.016749	513.36	474.37	337.71
N6	$C_6H_2N_{12}O_6$	-1337.930249	0.019493	1077.11	1035.32	879.05
N7	$C_7H_4N_{10}O_6$	-1267.786886	0.020321	771.16	730.75	566.41
N8	$C_6H_2N_{10}O_7$	-1303.691041	0.020098	717.39	681.54	524.52
NA1	$C_4H_4N_{10}O_6$	-1153.467918	0.017677	609.47	565.26	439.04
NA2	$C_4H_4N_{12}O_6$	-1262.915519	0.020509	893.13	847.66	687.56
NA3	$C_4H_5N_{11}O_6$	-1208.816801	0.019002	644.68	595.38	445.89
NA4	$C_4H_6N_{12}O_6$	-1264.130669	0.019748	771.73	715.82	556.03
NA5	$C_5H_6N_{10}O_6$	-1192.756957	0.019741	627.04	578.76	420.07
NA6	$C_6H_4N_{14}O_6$	-1448.624693	0.021842	1156.23	1103.48	927.41
NA7	$C_7H_6N_{12}O_6$	-1378.476562	0.022494	862.79	810.95	619.67
NA8	$C_6H_4N_{12}O_7$	-1414.383975	0.022322	800.47	753.32	568.33
DN1	$C_6H_2N_{10}O_{10}$	-1529.131261	0.02381	974.33	935.18	766.37
DN2	$C_6H_2N_{12}O_{10}$	-1638.598307	0.025372	1206.98	1163.24	973.13
DN3	$C_6H_3N_{11}O_{10}$	-1584.50177	0.024527	952.81	906.98	723.89
DN4	$C_6H_4N_{12}O_{10}$	-1639.80613	0.027181	1104.80	1057.37	858.16
DN5	$C_7H_4N_{10}O_{10}$	-1568.442715	0.024683	933.10	886.76	702.92
DN6	$C_8H_2N_{14}O_{10}$	-1824.298284	0.027391	1494.20	1444.98	1229.32
DN7	$C_9H_4N_{12}O_{10}$	-1754.14919	0.02805	1203.29	1155.00	935.98
DN8	$C_8H_2N_{12}O_{11}$	-1790.052601	0.027729	1151.47	1107.48	895.90
TN1	$C_4H_2N_8O_6$	-1939.48026	0.029936	775.80	726.66	539.40
TN2	$C_4H_2N_{10}O_6$	-2048.940483	0.031612	1026.35	972.91	755.12

TN3	$C_4H_3N_9O_6$	-1994.845461	0.030242	768.21	711.30	507.69
TN4	$C_4H_4N_{10}O_6$	-2050.163156	0.031347	885.22	822.64	608.92
TN5	$C_5H_4N_8O_6$	-1978.795106	0.030288	725.68	667.97	457.31
TN6	$C_6H_2N_{12}O_6$	-2234.64977	0.033061	1289.16	1228.74	986.40
TN7	$C_7H_4N_{10}O_6$	-2164.50662	0.03365	982.65	922.98	670.35
TN8	$C_6H_2N_{10}O_7$	-2200.411179	0.033772	927.82	873.61	624.83
RDX	$C_3H_6N_6O_6$	---	---	---	192.00	79.00[1]
HMX	$C_4H_8N_8O_8$	---	---	---	---	102.41[1]

5. Detonation parameters

Table. S2 40 substituted 1,2,4-triazole derivatives, their predicted values of density $\boldsymbol{\rho}$, oxygen balance *OB*, detonation energy *Q*, detonation velocity *D*, detonation pressure *P*, and ΔV_{Truazl}, compared with **HMX** and **RDX**.

No.	ρ (g/cm^3)	OB (%)	Q (cal/g)	D (km/s)	P (GPa)	ΔV_{Truazl} (cm^3)
H1	1.76	-48.00	1035.24	7.45	24.22	265.28
H2	1.78	-42.11	1162.47	7.82	26.92	305.27
H3	1.90	-48.37	985.29	7.87	28.40	253.49
H4	1.80	-48.70	1084.77	7.83	27.19	281.56
H5	1.75	-67.29	1008.43	7.23	22.78	227.61
H6	1.82	-57.14	1161.11	7.67	26.23	266.64
H7	1.86	-78.20	988.83	7.27	23.87	189.19
H8	1.95	-53.73	1059.90	7.88	28.90	252.44
N1	1.88	-18.60	1515.62	8.79	35.17	442.25
N2	1.88	-16.78	1556.51	8.92	36.15	453.21
N3	1.91	-20.51	1427.25	8.84	35.92	417.16
N4	1.87	-22.21	1462.09	8.81	35.23	425.28
N5	1.86	-35.28	1412.71	8.46	32.42	388.18
N6	1.88	-33.12	1487.60	8.55	33.26	396.55
N7	1.86	-49.36	1354.56	8.11	29.69	337.01
N8	1.90	-29.44	1426.78	8.51	33.15	392.41
NA1	1.81	-22.22	1418.83	8.54	32.37	413.53
NA2	1.85	-20.25	1481.08	8.81	34.94	430.44
NA3	1.85	-23.76	1371.76	8.67	33.90	399.79
NA4	1.82	-25.16	1406.77	8.65	33.44	408.18
NA5	1.81	-37.09	1373.71	8.35	30.97	377.72
NA6	1.83	-34.78	1427.56	8.43	31.89	381.36
NA7	1.86	-49.72	1306.68	8.18	30.25	327.15
NA8	1.90	-31.46	1366.71	8.55	33.50	376.24
DN1	1.89	-12.83	1775.90	9.17	38.45	524.77
DN2	1.87	-11.94	1775.13	9.15	38.02	523.66
DN3	1.95	-14.40	1695.17	9.32	40.36	501.65
DN4	1.90	-15.84	1724.99	9.22	38.92	508.29
DN5	1.89	-24.74	1700.50	8.97	36.69	485.52

DN6	1.88	-24.67	1706.68	8.90	36.08	475.50
DN7	1.85	-36.36	1626.12	8.54	32.86	436.97
DN8	1.88	-21.72	1679.12	8.84	35.56	477.65
TN1	1.89	3.43	1611.63	9.28	39.35	543.25
TN2	1.89	3.24	1624.65	9.32	39.66	542.46
TN3	1.92	1.66	1605.69	9.39	40.60	525.41
TN4	1.91	0.00	1664.17	9.49	41.31	525.83
TN5	1.89	-6.67	1840.09	9.40	40.39	508.49
TN6	1.88	-8.79	1915.67	9.37	39.92	497.69
TN7	1.87	-18.05	2109.52	9.46	40.65	463.68
TN8	1.92	-5.99	1796.89	9.36	40.34	496.60
						465.00[2]
RDX	1.80	-21.62	1501	8.75	34.70	475.00[2]
						480.00[2]
HMX	1.90	-21.62	1498	9.10	39.30	450.00[2]

6. Sensitivity parameters

Table S3. 40 substituted 1,2,4-triazole derivatives, their predicted values of impact, electrostatic, and shock sensitivities(h_{50}, E_{ES}, $P9_{0\%}TMD$, $P_{95\%}TMD$, $P_{98\%}TMD$), compared with **TMBT**, **DNBF**.

No.	h_{50} (cm)	E_{ES}(J)	$P_{90\%TMD}$(MPa)	$P_{95\%TMD}$(MPa)	$P_{98\%TMD}$(MPa)
H1	47.61	13.72	2131.60	2692.20	2987.10
H2	29.62	13.72	2131.60	2692.20	2987.10
H3	51.10	16.01	2244.75	2816.15	3097.65
H4	54.34	18.30	2357.90	2940.10	3208.20
H5	128.30	17.57	2584.20	3188.00	3429.30
H6	37.19	12.26	2584.20	3188.00	3429.30
H7	122.40	16.11	3036.80	3683.80	3871.50
H8	43.73	11.15	2357.90	2940.10	3208.20
N1	92.37	9.07	4996.50	8532.70	11602.20
N2	59.30	9.07	4996.50	8532.70	11602.20
N3	94.17	10.59	5109.65	8656.65	11712.75
N4	95.81	12.12	5222.80	8780.60	11823.30
N5	194.75	11.39	5449.10	9028.50	12044.40
N6	64.35	7.60	5449.10	9028.50	12044.40
N7	175.23	9.92	5901.70	9524.30	12486.60
N8	75.02	7.89	5222.80	8780.60	11823.30
NA1	95.81	12.12	4591.40	8143.80	11407.10
NA2	63.95	12.12	4591.40	8143.80	11407.10
NA3	97.31	13.65	4704.55	8267.75	11517.65
NA4	98.70	15.17	4817.70	8391.70	11628.20
NA5	187.26	14.44	5044.00	8639.60	11849.30
NA6	68.20	10.65	5044.00	8639.60	11849.30
NA7	170.98	12.97	5496.60	9135.40	12291.50
NA8	78.64	10.50	4817.70	8391.70	11628.20

DN1	43.11	9.27	8087.70	14621.10	20438.40
DN2	33.17	9.27	8087.70	14621.10	20438.40
DN3	45.01	10.19	8200.85	14745.05	20548.95
DN4	46.83	11.11	8314.00	14869.00	20659.50
DN5	74.77	10.37	8540.30	15116.90	20880.60
DN6	37.68	7.81	8540.30	15116.90	20880.60
DN7	77.46	8.91	8992.90	15612.70	21322.80
DN8	41.58	8.37	8314.00	14869.00	20659.50
TN1	20.51	11.65	10726.30	20213.70	28832.40
TN2	17.28	11.65	10726.30	20213.70	28832.40
TN3	21.73	12.30	10839.45	20337.65	28942.95
TN4	22.95	12.96	10952.60	20461.60	29053.50
TN5	32.71	12.22	11178.90	20709.50	29274.60
TN6	20.44	10.18	11178.90	20709.50	29274.60
TN7	36.52	10.76	11631.50	21205.30	29716.80
TN8	21.88	10.82	10952.60	20461.60	29053.50
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DNBF	12.00	--	--	--	--

7. References

1. J. S. P. Politzer; Murray, *Central European Journal of Energetic Materials*, 2011, 209-220.
2. M. K. Kamalvand, M. H.; Jafari, M., *Propellants, Explosives, Pyrotechnics*, 2015, **40**, 551-557.