Electronic Supplementary Information

Design and Computational Insight on Two Novel CL-20 Analogues, BNMTNIW and BNIMTNIW: High Performance Energetic Materials

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Table S1. Calculated Total Energy (E_0), Zero-point Energy (ZPE), values of Thermal Correction (H_T) and Enthalpy of Formation ($\Delta H_f°$ (g)) of the compounds using B3LYP/6-31+G**//MP2/6-311++G** level of theory (Isodesmic)

Compounds	E_0 [Hartree/Particle]	ZPE[Hartree/Particle]	H_T[Hartree/Particle]	$\Delta H_f°$ (g) kJ/mol
BNMTNIW, **1**	-1865.8611257	0.277524	0.027101	731.52
BNIMTNIW, **2**	-2015.9359751	0.285933	0.028927	605.56
HNIW(CL-20)	-1787.4213305	0.219373	0.023319	764.70
CH_4	-40.3796224	0.044793	0.003812	-74.60[a]
NH_3	-56.43462	0.034377	0.003818	-45.9[a]
CH_3NO_2	-244.4784821	0.049840	0.005298	-74.30[a]
CH_3ONO_2	-319.509055	0.054251	0.005933	-137.28[b]
CH_3-NH-CH_3	-134.7787236	0.092336	0.005347	-19.54[b]
CH_3-CH_3	-79.5716305	0.07461	0.004428	-84.00[b]
NH_2-NO_2	-260.4931748	0.039257	0.004652	-6.11[b]
CH_3-CH_2-CH_3	-118.7673365	0.10328	0.005485	-103.80[b]
CH_3-NH_2	-95.5938424	0.064026	0.004375	-23.00[a]

[a] Data are from Ref. [D. R. Lide ed., CRC Handbook of Chemistry and Physics, 88th Edition (Internet Version **2008**), CRC Press/Taylor and Francis, Boca Raton, FL.]. [b]Obtained at G2 level.

The oxygen balance for $C_aH_bN_cO_d$ was calculated by using equation 1.

$$OB^{CO2}(\%) = -1600(2a-0.5b-d)/MW \quad (1)$$

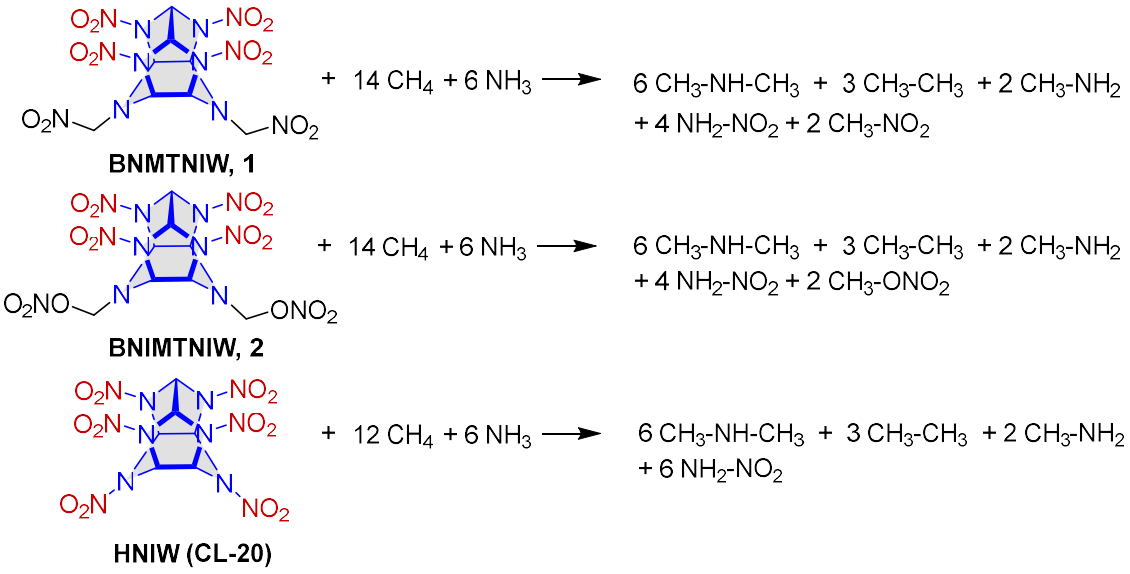


Figure S1. Isodesmic reactions for BNMTNIW, **1** and BNIMTNIW, **2** and HNIW (CL-20).

The gas phase enthalpies of formation $\Delta H_f°$(g) were predicted according to the isodesmic equation as shown in Figure S1.

For compound 1

$\Delta H_f°(g)_{BNMTNIW} = 6\Delta H_f°(g)_{CH3\text{-}NH\text{-}CH3} + 3\Delta H_f°(g)_{CH3\text{-}CH3} + 2\Delta H_f°(g)_{CH3\text{-}NH2} + 4\Delta H_f°(g)_{NH2\text{-}NO2}$

$2\Delta H_f°(g)_{CH3NO2} - 14\Delta H_f°(g)_{CH4} - 6\Delta H_f°(g)_{NH3}$ (2)

For compound 2

$\Delta H_f°(g)_{BNIMTNIW} = 6\Delta H_f°(g)_{CH3\text{-}NH\text{-}CH3} + 3\Delta H_f°(g)_{CH3\text{-}CH3} + 2\Delta H_f°(g)_{CH3\text{-}NH2} + 4\Delta H_f°(g)_{NH2\text{-}NO2}$

$2\Delta H_f°(g)_{CH3ONO2} - 14\Delta H_f°(g)_{CH4} - 6\Delta H_f°(g)_{NH3}$ (3)

Table S2. Gas phase enthalpies of formation $\Delta H_f°(g)$ of the title compounds at different level of theory[a]

Method	Compounds	E_0 [Hartree/Particle]	ZPE[Hartree/Particle]	$\Delta H_f°$ (g) kJ/mol
A	HNIW(CL-20)	-1791.465605	0.218974	517.61
A	RDX	-897.516473	0.141466	161.32
A	HMX	-1196.696388	0.190270	194.73
A	BNMTNIW, **1**	-1870.097564	0.276808	368.55
B	BNMTNIW, **1**	-1870.046386	0.277589	527.21
A	BNIMTNIW, **2**	-2020.497774	0.285121	247.35
B	BNIMTNIW, **2**	-2020.444159	0.285985	412.42

[a]Calculated using Gaussian 03 program[1] (atomization method). A= B3LYP/6-311++G (d,p). B = B3LYP/6-311G (d,p).

Subsequently, their solid phase enthalpies of formation $\Delta H_f°$ (s) were calculated by using equations 4-5.[2-4]

$\Delta H_f°$ (s) = $\Delta H_f°$ (g) - ΔH_{sub} (4)

Where, $\Delta Hf°(s)$ is solid phase enthalpy of formation, $\Delta Hf°(g)$ is enthalpy of formation in gas phase and ΔH_{sub} is represent the enthalpy of sublimation.

$\Delta H_{sub} = a(SA)^2 + b\sqrt{(\sigma^2_{tot}\upsilon)} + c$ (5)

Where, *a*, *b* and *c* are fitting parameters, SA is the surface area of the 0.001 electron bohr^{-3} isosurface of the electrostatic potential of the molecules, σ^2_{tot} is the measure of variability of electronic potential on the surface, and υ is the degree of balance between the positive and negative charges on the isosurface.

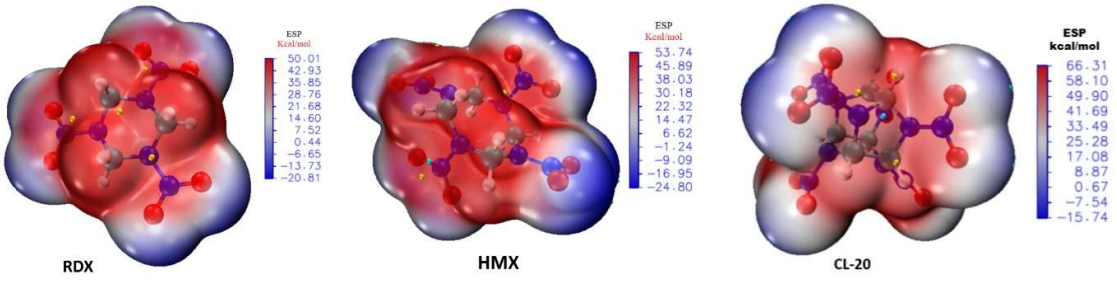


Figure S2. Computed electrostatic potential (ESP) maps of (a) RDX, (b) HMX and (c) HNIW (CL-20). Color ranges in kcal/mol: Red, more positive; Blue, more negative and Greyer, in between positive and negative.

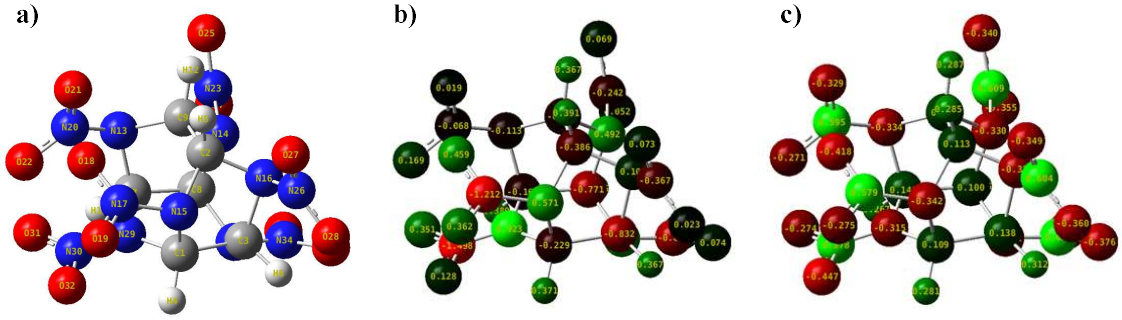


Figure S3: (a) HNIW (CL-20) optimized structure with atom numbering (b) Mulliken charges and (c) NBO charges

Impact sensitivity

The impact sensitivity (h_{50}) of the title compounds were predicted by using equation 6.[5]

$$h_{50\,[cm]} = \alpha\sigma^2_{+} + \beta\upsilon + \gamma \quad (6)$$

Where, the coefficients α, β, γ are -0.0064, 241.42 and -3.43, respectively. The σ^2_{+} is the measure of variability of the positive surface potentials and υ is the degree of balance between the positive and negative charges on the isosurface.

Then their corresponding impact energies were calculated by using 2.5 kg hammer weight.

Table S3. Total surface area (SA), σ^2_{tot}, σ^2_{+}, balance of charges, impact sensitivity ($h_{50[cm]}$) and impact energy [$h_{50[J]}$].

#	SA[a] Å^2	σ^2_{tot}[b] (kcal/mol)^2	σ^2_{+}[c] (kcal/mol)^2	υ[d]	h_{50}[e] [cm]	h_{50}[f] [J]
HNIW(CL-20)	324.62	239.42	224.49	0.05844748	9.25	2.27
RDX	209.49	214.34	182.25	0.12731604	26.14	6.41
HMX	251.50	246.97	207.61	0.13397103	27.58	6.76
1	357.83	288.47	256.36	0.09892218	18.81	4.61
2	375.20	248.91	218.68	0.10670471	20.93	5.13

[a]SA = Total surface area. [b]Overall variance (σ^2_{tot}). [c]Positive variance (σ^2_{+}). [d]Balance of charges (υ). [e]h_{50} [cm] = Height from where 50% probability of the dropped materials resulted in an explosion. [f]h_{50} [J] = Predicted impact sensitivities using 2.5 kg weight of a drop-hammer.

The standard enthalpies of combustion $\Delta H_{f(combust)}$ for the title compounds was calculated by following equation

$$\Delta H_{f(combust)} = \Sigma\Delta H_{f\,(products)} - \Sigma\Delta H_{f\,(reactants)} \quad (6)$$

RDX = $C_3H_6N_6O_6$ (s) + 1.5 O_2 (g) ⟶ $3CO_2$ (g) + $3H_2O$ (g) + $3N_2$ (g)

HMX = $C_4H_8N_8O_8$ (s) + 2 O_2 (g) ⟶ $4CO_2$ (g) + $4H_2O$ (g) + $4N_2$ (g)

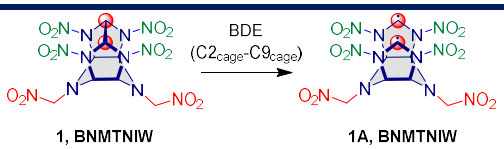
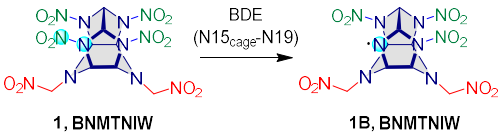
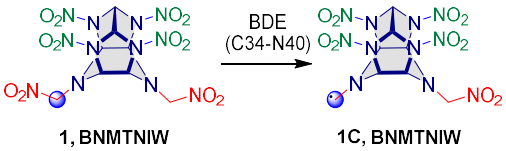
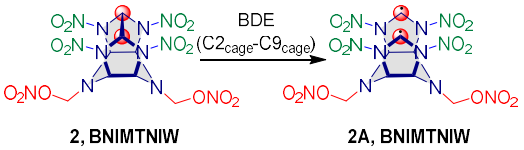
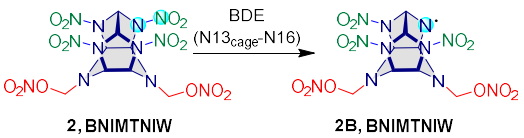
HNIW(CL-20) = $C_6H_6N_{12}O_{12}$ (s) + 1.5 O_2 (g) ⟶ $6CO_2$ (g) + $3H_2O$ (g) + $6N_2$ (g)

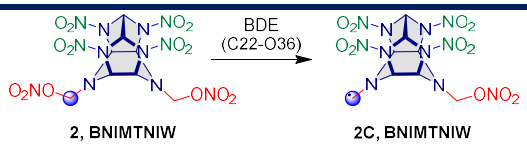
BNMTNIW = $C_8H_{10}N_{12}O_{12}$ (s) + 4.5 O_2 (g) ⟶ $8CO_2$ (g) + $5H_2O$ (g) + $6N_2$ (g)

BNIMTNIW = $C_8H_{10}N_{12}O_{14}$ (s) + 3.5 O_2 (g) ⟶ $8CO_2$ (g) + $5H_2O$ (g) + $6N_2$ (g)

The standard enthalpy of formation for CO_2 ($\Delta H_{f\,(CO2)}$ = -393.51 kJmol^{-1}); H_2O ($\Delta H_{f\,(H2O)}$ = -243.015 kJmol^{-1}).

Table S4. Plausible decomposition pathways and corresponding bond associated properties[a]

#	Plausible Decomposition Pathways	BL[b]	BL[b]	BO[c]	BO[c]	$\Delta H_f°(g)$[d]	BDE[e]
1A	 1, BNMTNIW 1A, BNMTNIW	1.6034	---	0.9543	---	645.52	276.96
1B	 1, BNMTNIW 1B, BNMTNIW	---	1.3857	---	0.9531	507.23	142.67
1C	 1, BNMTNIW 1C, BNMTNIW	---	1.5677	---	0.8829	565.87	201.30
2A	 2, BNIMTNIW 2A, BNIMTNIW	1.5968	---	0.9634	---	508.99	261.65
2B	 2, BNIMTNIW 2B, BNIMTNIW	---	1.4435	---	0.9755	378.93	135.55

2C	 2, BNIMTNIW 2C, BNIMTNIW	---	1.4949	---	0.6822	502.11	288.43

[a]Method: B3LYP/6-311++G (d,p). [b]Bond length (LB) in Å. [c]Wiberg bond order (BO).

[d]Enthalpy of formation $\Delta H_f°$(g) in kJ/mol, [e]Bond dissociation energy (BDE) in kJ/mol.

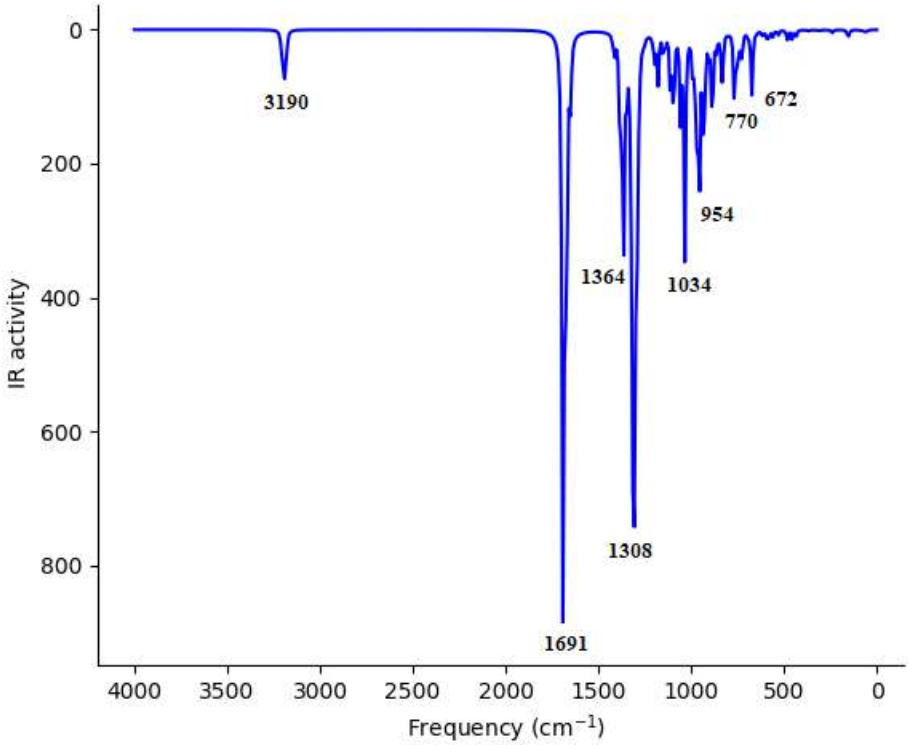


Figure S4. Computed IR spectrum for HNIW (CL-20)

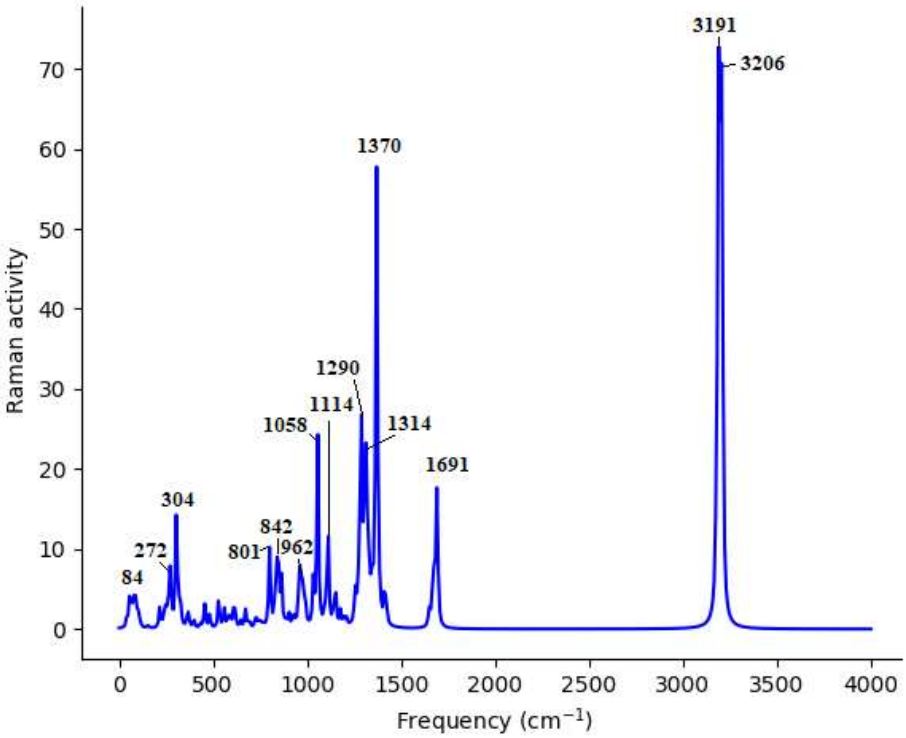


Figure S5. Computed Raman spectrum for HNIW (CL-20)

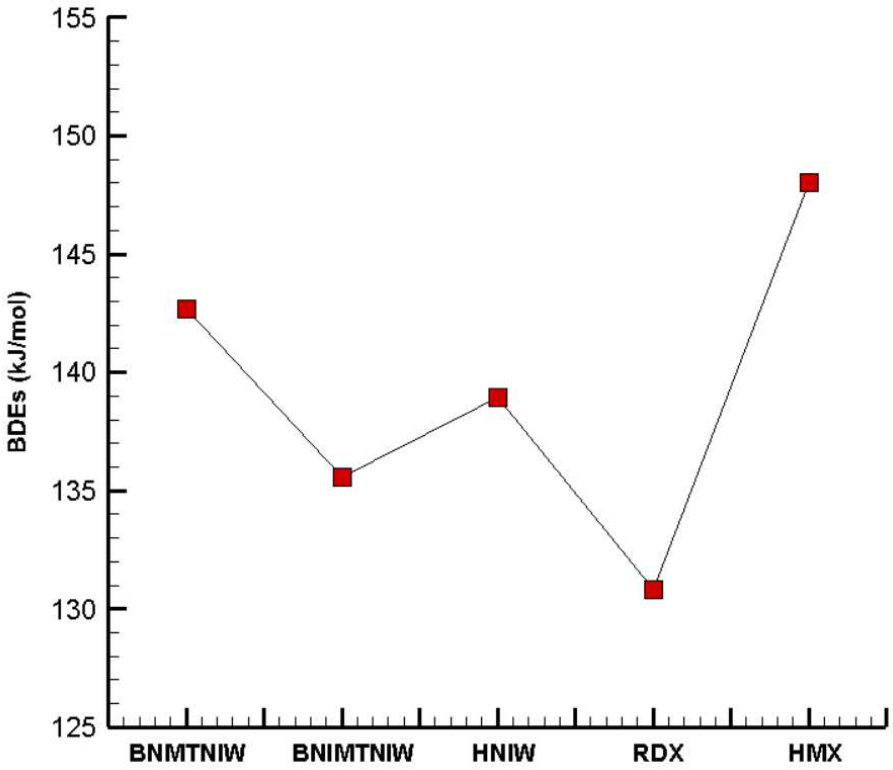


Figure S6. Comparison of bond dissociation energies (BDEs) of (-N-NO_2) bond.

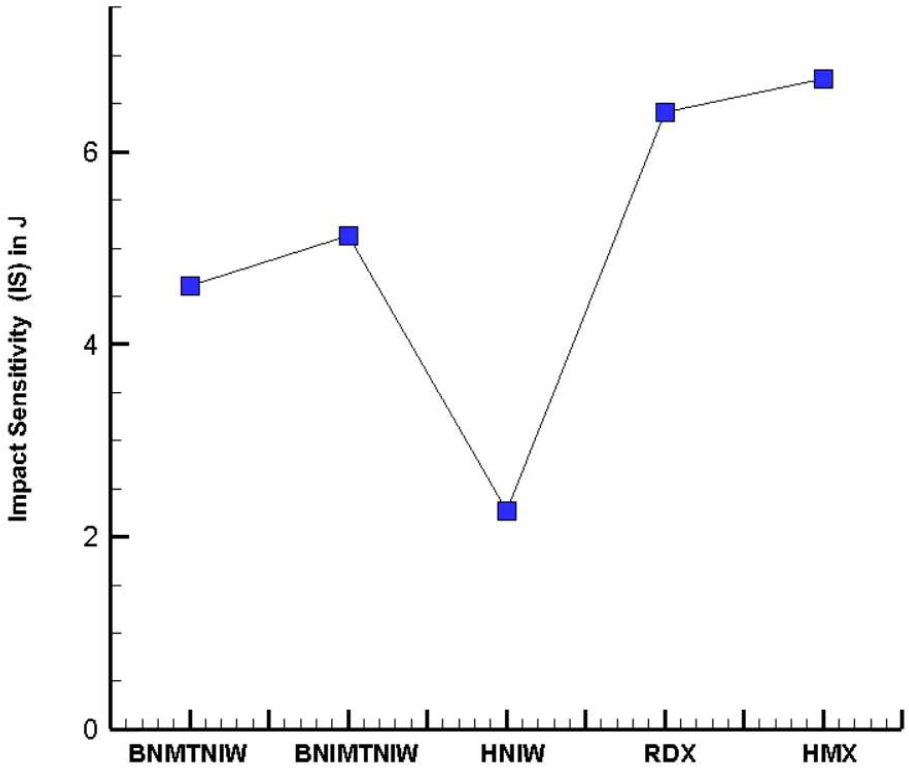
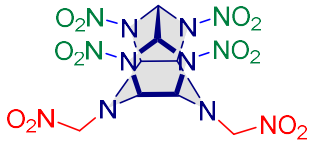


Figure S7. Comparison of impact sensitivities (IS) of the title compounds.

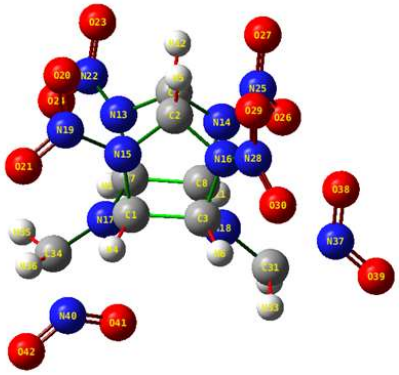
Table S5. Cartesian coordinates (in Å) for optimized structure of **BNMTNIW**, **1** obtained using the B3LYP/6-311++G(d,p) level of theory



1, BNMTNIW

MF = $C_8H_{10}N_{12}O_{12}$
MW = 466.24

≡



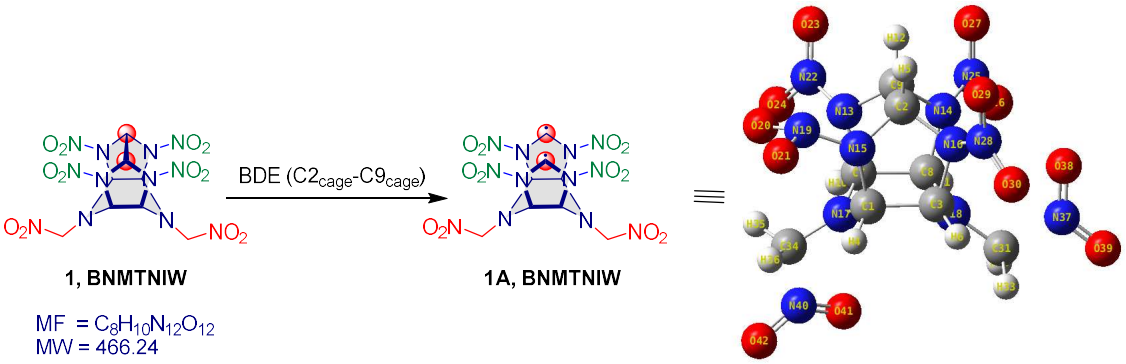
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-4.135091	0.374433	-1.845399
2	C	-2.158328	1.758166	-1.773883
3	C	-3.336372	0.131014	-0.492605
4	H	-5.196919	0.513028	-1.659607
5	H	-1.806462	2.783415	-1.773667
6	H	-3.992811	0.187884	0.370359

7	C	-2.563125	-1.031901	-3.015380
8	C	-1.786784	-1.301939	-1.654404
9	C	-1.124882	0.804771	-2.544597
10	H	-2.488592	-1.884875	-3.681911
11	H	-1.341651	-2.292622	-1.641842
12	H	-0.273219	1.366058	-2.913459
13	N	-1.846073	0.123368	-3.622231
14	N	-0.719524	-0.285956	-1.671093
15	N	-3.530704	1.655084	-2.288239
16	N	-2.371467	1.264065	-0.425668
17	N	-3.935386	-0.708492	-2.764168
18	N	-2.680604	-1.141833	-0.539100
19	N	-3.861629	2.186883	-3.524342
20	O	-3.074397	2.981900	-4.006377
21	O	-4.935362	1.833639	-3.991263
22	N	-1.151766	-0.099509	-4.845218
23	O	-0.245713	0.662109	-5.105236
24	O	-1.584142	-1.000640	-5.542602
25	N	0.629083	-0.671816	-1.609333
26	O	0.844648	-1.810674	-1.231627
27	O	1.449568	0.179510	-1.892157
28	N	-2.568572	2.231669	0.592740
29	O	-2.057067	3.319082	0.417545
30	O	-3.184131	1.857514	1.574235
31	C	-2.621973	-1.991237	0.584331
32	H	-2.401610	-3.019811	0.302304
33	H	-3.546644	-1.970431	1.159704
34	C	-4.980565	-1.240090	-3.543399
35	H	-4.682661	-1.475678	-4.566039
36	H	-5.856060	-0.596863	-3.567291
37	N	-1.522015	-1.651851	1.645488
38	O	-0.793838	-0.700361	1.444143
39	O	-1.501051	-2.398018	2.606790
40	N	-5.505055	-2.612470	-2.996561
41	O	-4.822907	-3.207947	-2.180413
42	O	-6.558621	-2.990451	-3.470990

E = -1870.097564 Hartree/particle; ZPE = 0.276808 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S6. Cartesian coordinates (in Å) for optimized structure of **BNMTNIW**, **1A** obtained using the B3LYP/6-311++G(d,p) level of theory

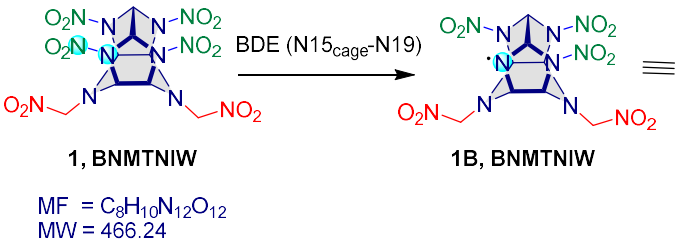


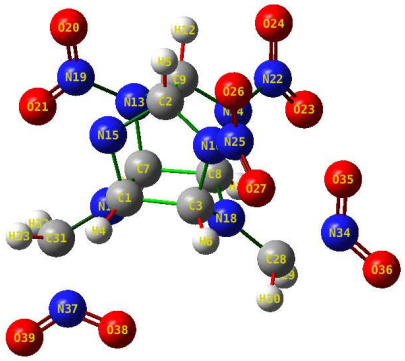
Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.62640388	0.09905176	-1.19632583
2	C	-2.07393534	1.59958997	-1.92981467
3	C	-2.57694263	0.28560700	-0.08639654
4	H	-4.59629222	-0.14750014	-0.81760593
5	H	-1.98375912	2.52622029	-2.45718973
6	H	-2.98320356	0.52423614	0.87428456
7	C	-2.01012785	-1.31708301	-2.53077214
8	C	-1.06815204	-1.24095903	-1.30240913
9	C	-0.95786477	0.70562507	-2.52932039
10	H	-2.13982850	-2.30066366	-2.93157986
13	H	-0.42201797	-2.09002024	-1.22175030
12	H	-0.25675223	1.41032399	-2.92522533
13	N	-1.39922732	-0.33217021	-3.49841925
14	N	-0.25388273	-0.13129664	-1.58811697
15	N	-3.54289443	1.28822707	-1.90477946
16	N	-1.82114238	1.57450313	-0.51293459
17	N	-3.31699424	-0.97677548	-2.07848182
18	N	-1.82342615	-1.03383973	-0.02122851
19	N	-4.11824496	1.16637034	-3.17526075
20	O	-3.43136612	0.78538988	-4.13166292
21	O	-5.31373363	1.43962956	-3.34196406
22	N	-2.26021334	0.10787615	-4.51087284
23	O	-2.15480264	1.25766358	-4.95644124
24	O	-3.12673564	-0.65291030	-4.96031344
25	N	0.87573242	-0.58432887	-2.28002114
26	O	1.33967365	-1.70630077	-2.04003919
27	O	1.41037095	0.13716251	-3.13164638
28	N	-2.45369263	2.69212678	0.04455762
29	O	-2.50340732	3.75467960	-0.58802733
30	O	-2.96315229	2.61755330	1.16996572
31	C	-2.76264063	-2.14126964	0.20762766
32	H	-2.22145904	-3.06282211	0.26019689
33	H	-3.46500685	-2.18559107	-0.59836073
34	C	-4.18263498	-0.84060852	-3.25874647
35	H	-3.58531675	-0.88015034	-4.14562152
36	H	-4.69769999	0.09634099	-3.21710935

37	N	-3.48041451	-1.92175131	1.47155502
38	O	-4.54535359	-1.29125214	1.47697025
39	O	-3.01977257	-2.36743681	2.53024628
40	N	-5.16127781	-1.93732876	-3.27779641
41	O	-4.89090545	-2.99797418	-3.85536355
42	O	-6.25557417	-1.80001739	-2.71626742

E = -1869.992074 Hartree/particle; ZPE = 0.272659 Hartree/particle
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S7. Cartesian coordinates (in Å) for optimized structure of **BNMTNIW**, **1B** obtained using the B3LYP/6-311++G(d,p) level of theory





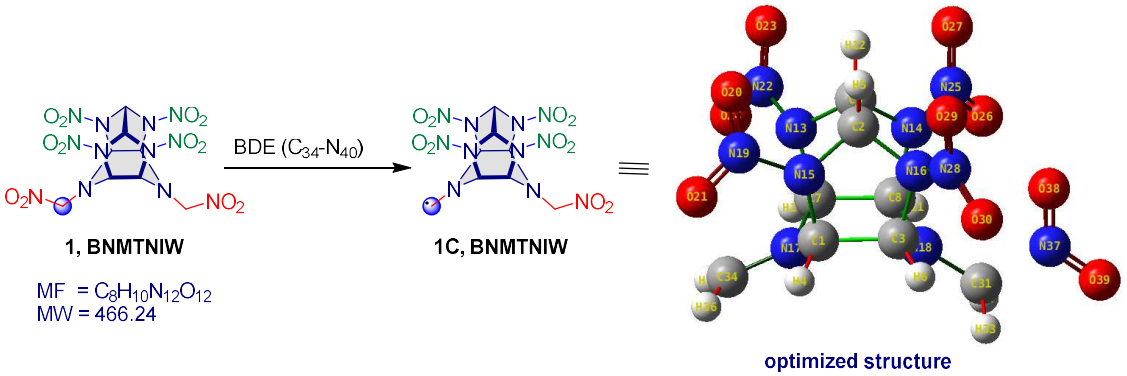
optimized structure

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.928646	0.426020	-1.988685
2	C	-2.017667	1.729274	-1.825089
3	C	-3.292142	0.158406	-0.571563
4	H	-4.998010	0.615561	-1.904054
5	H	-1.645117	2.750146	-1.814254
6	H	-4.020900	0.226872	0.230201
7	C	-2.336080	-1.101501	-3.006420
8	C	-1.668705	-1.316250	-1.580310
9	C	-0.907745	0.754856	-2.472546
10	H	-2.277564	-2.005277	-3.607308
11	H	-1.219094	-2.301399	-1.501602
12	H	-0.031957	1.314997	-2.777400
13	N	-1.442482	-0.063835	-3.569655
14	N	-0.583043	-0.297851	-1.531181
15	N	-3.261166	1.608332	-2.556037
16	N	-2.336890	1.278421	-0.466252
17	N	-3.706448	-0.691096	-2.881274
18	N	-2.639547	-1.125832	-0.544062
19	N	-1.722180	0.502314	-4.805416
20	O	-1.216070	1.583888	-5.038770
21	O	-2.414747	-0.168712	-5.558431
22	N	0.755528	-0.757660	-1.500418

23	O	0.923800	-1.889990	-1.084641
24	O	1.612275	0.035791	-1.835656
25	N	-2.501870	2.233564	0.547057
26	O	-1.911685	3.288922	0.403923
27	O	-3.182854	1.898429	1.502591
28	C	-2.668505	-1.944311	0.602230
29	H	-2.436280	-2.982369	0.367324
30	H	-3.632699	-1.900261	1.106584
31	C	-4.706976	-1.144640	-3.760534
32	H	-4.302926	-1.626497	-4.646951
33	H	-5.403590	-0.365117	-4.068925
34	N	-1.644601	-1.589141	1.734219
35	O	-0.877049	-0.664528	1.557448
36	O	-1.714877	-2.302308	2.718696
37	N	-5.639763	-2.228126	-3.110937
38	O	-5.505208	-2.481084	-1.927244
39	O	-6.453648	-2.721271	-3.868230

E = -1664.915198 Hartree/particle; ZPE = 0.261587 Hartree/particle
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S8. Cartesian coordinates (in Å) for optimized structure of **BNMTNIW**, **1C** obtained using the B3LYP/6-311++G(d,p) level of theory

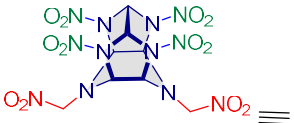


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-4.170241	0.264499	-1.839852
2	C	-2.224367	1.688760	-1.809704

3	C	-3.365988	0.071600	-0.484163
4	H	-5.236437	0.384394	-1.666330
5	H	-1.893249	2.720540	-1.835688
6	H	-4.023732	0.139472	0.377019
7	C	-2.569034	-1.142156	-2.965140
8	C	-1.783308	-1.357127	-1.607194
9	C	-1.175897	0.740294	-2.559428
10	H	-2.483986	-2.006725	-3.616669
11	H	-1.311357	-2.335175	-1.567782
12	H	-0.337659	1.309345	-2.946165
13	N	-1.882486	0.012061	-3.616461
14	N	-0.743138	-0.318651	-1.657938
15	N	-3.591330	1.546553	-2.307390
16	N	-2.419524	1.219890	-0.446801
17	N	-3.954360	-0.859979	-2.712265
18	N	-2.682560	-1.193167	-0.491225
19	N	-3.998542	2.160282	-3.481116
20	O	-3.203163	2.933510	-3.990610
21	O	-5.129243	1.905617	-3.858944
22	N	-1.145406	-0.252161	-4.812957
23	O	-0.277767	0.544131	-5.102040
24	O	-1.503973	-1.219459	-5.458526
25	N	0.609981	-0.655228	-1.546655
26	O	0.852174	-1.771360	-1.115710
27	O	1.411894	0.208188	-1.846656
28	N	-2.619234	2.199406	0.554228
29	O	-2.129862	3.293197	0.354456
30	O	-3.214934	1.832108	1.551928
31	C	-2.544694	-1.961936	0.683949
32	H	-2.275429	-2.993534	0.460368
33	H	-3.454128	-1.949505	1.283811
34	C	-4.899957	-1.193065	-3.686863
35	H	-4.676229	-2.032183	-4.326978
36	H	-5.899529	-0.807525	-3.573455
37	N	-1.439332	-1.512939	1.699729
38	O	-0.764324	-0.538672	1.437213
39	O	-1.362366	-2.209854	2.694969

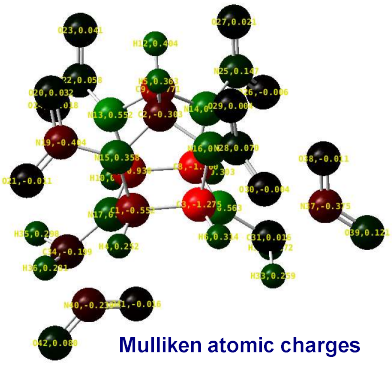
E = -1664.892860 Hartree/particle; ZPE = 0.259404 Hartree/particle
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S9. Mulliken atomic charges for optimized structure of **BNMTNIW**, **1** obtained using the B3LYP/6-311++G(d,p) level of theory

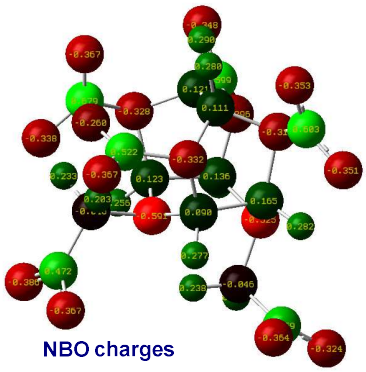


1, BNMTNIW

MF = $C_8H_{10}N_{12}O_{12}$
MW = 466.24



Mulliken atomic charges



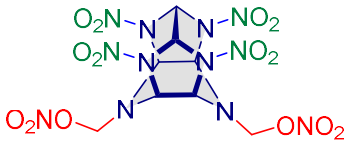
NBO charges

Center Number	Atomic Symbol	Mulliken Atomic Charges
1	C	-0.551891
2	C	-0.302566
3	C	-1.274929
4	H	0.251839
5	H	0.362872
6	H	0.314395
7	C	-0.930331
8	C	-1.100398
9	C	-0.770593
10	H	0.299896
11	H	0.303298
12	H	0.404485
13	N	0.551632
14	N	0.442146
15	N	0.358007
16	N	0.352505
17	N	0.309869
18	N	0.563317
19	N	-0.403851
20	O	0.031596
21	O	-0.010884
22	N	0.057770
23	O	0.040961
24	O	-0.018488
25	N	0.147411
26	O	-0.006138
27	O	0.021424
28	N	0.069675
29	O	0.003775
30	O	-0.003971
31	C	0.015875
32	H	0.272193
33	H	0.259258
34	C	-0.199242
35	H	0.297631

36	H	0.280593
37	N	-0.374644
38	O	-0.010554
39	O	0.120598
40	N	-0.239381
41	O	-0.015570
42	O	0.080411

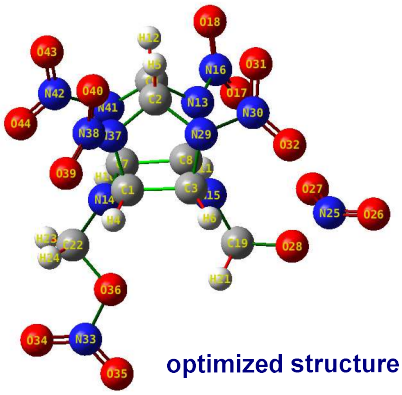
Sum of Mulliken charges= 0.00000

Table S10. Cartesian coordinates (in Å) for optimized structure of **BNIMTNIW**, **2** obtained using the B3LYP/6-311++G(d,p) level of theory



2, BNIMTNIW

MF = $C_8H_{10}N_{12}O_{14}$
MW = 498.24

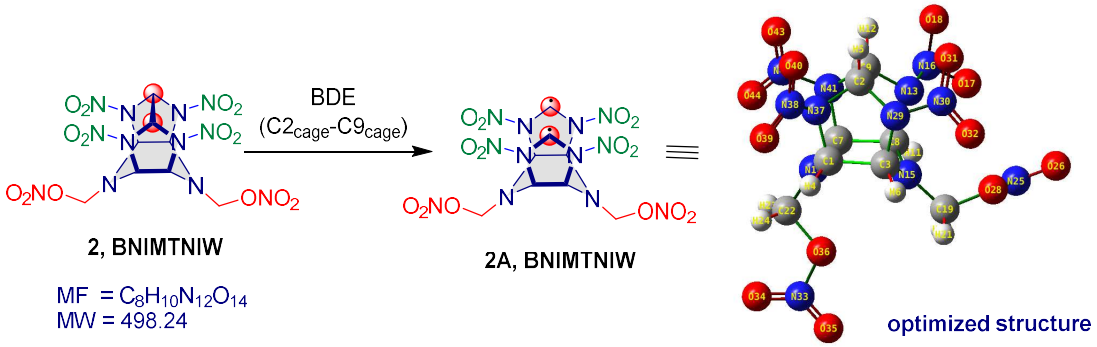


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.818457	0.552629	-1.907482
2	C	-1.781458	1.747003	-1.628291
3	C	-3.178565	0.135408	-0.512550
4	H	-4.866047	0.816714	-1.805834
5	H	-1.356078	2.740199	-1.547572
6	H	-3.914292	0.142786	0.287835
7	C	-2.311673	-0.967935	-3.056265
8	C	-1.638233	-1.335707	-1.663263
9	C	-0.780045	0.763014	-2.389087
10	H	-2.311130	-1.813108	-3.739536
11	H	-1.243834	-2.346539	-1.660140
12	H	0.125444	1.284878	-2.674676
13	N	-0.493890	-0.384113	-1.538041
14	N	-3.660486	-0.491574	-2.879271
15	N	-2.561709	-1.162372	-0.581918
16	N	0.821426	-0.951284	-1.716941
17	O	0.928875	-2.138644	-1.496003
18	O	1.701989	-0.172649	-2.012116
19	C	-3.141558	-2.280458	0.103725
20	H	-2.763941	-3.205276	-0.328261
21	H	-4.232017	-2.279489	0.056017
22	C	-4.758562	-1.119127	-3.490222
23	H	-4.486064	-1.564112	-4.445127
24	H	-5.599159	-0.438433	-3.615809

25	N	-1.591121	-2.636965	1.935166
26	O	-1.429556	-2.538336	3.111522
27	O	-0.836008	-2.997976	1.065641
28	O	-2.925423	-2.272729	1.527924
29	N	-2.215823	1.237598	-0.324253
30	N	-1.325519	1.233935	0.748628
31	O	-0.312317	1.898343	0.606849
32	O	-1.671007	0.606238	1.731354
33	N	-6.296616	-2.981413	-3.028009
34	O	-6.768463	-2.674062	-4.096458
35	O	-6.612630	-3.849451	-2.265263
36	O	-5.188087	-2.214769	-2.568404
37	N	-3.056179	1.761093	-2.331692
38	N	-3.771759	2.999840	-2.330836
39	O	-4.972427	2.917409	-2.512064
40	O	-3.113301	4.010128	-2.215860
41	N	-1.395032	0.079629	-3.536065
42	N	-1.682567	0.774870	-4.703794
43	O	-1.156282	1.867029	-4.830358
44	O	-2.402884	0.202029	-5.505875

E = -2020.497774 Hartree/particle; ZPE = 0.285121 Hartree/particle.
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S11. Cartesian coordinates (in Å) for optimized structure of **BNIMTNIW**, **2A** obtained using the B3LYP/6-311++G(d,p) level of theory

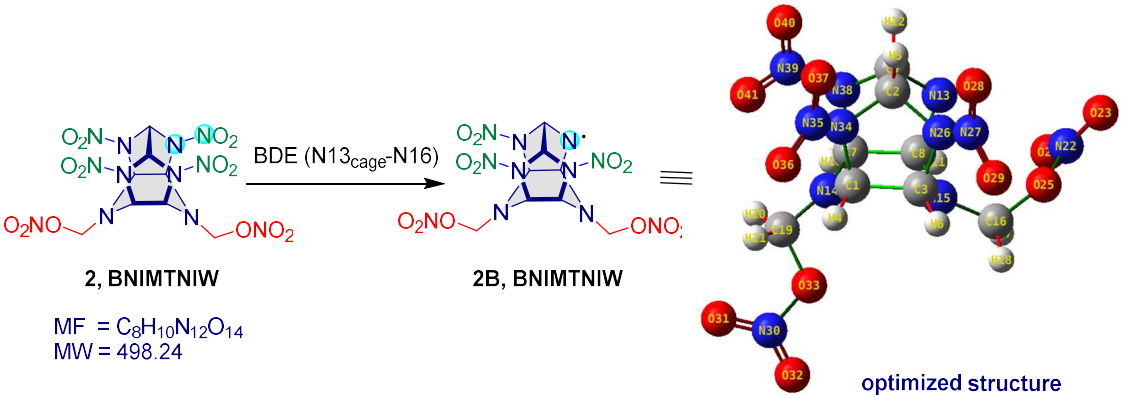


Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.75083551	-0.02595024	-1.22986563
2	C	-2.20302538	1.49381656	-1.93270166
3	C	-2.69911699	0.13747807	-0.11846956
4	H	-4.71935148	-0.28296182	-0.85460323
5	H	-2.11620150	2.43235165	-2.43917330
6	H	-3.10361584	0.35354058	0.84827636
7	C	-2.13504736	-1.40820896	-2.59991018
8	C	-1.19031607	-1.35816733	-1.37230998
9	C	-1.08665324	0.61596235	-2.55502118
10	H	-2.26392844	-2.38268708	-3.02261821
11	H	-0.54239434	-2.20758590	-1.31243096

12	H	-0.38796051	1.33095170	-2.93649031
13	N	-0.37878918	-0.24068417	-1.63467873
14	N	-3.44147902	-1.08077775	-2.13697838
15	N	-1.94300227	-1.18165912	-0.08499053
16	N	0.75005292	-0.67567353	-2.33930615
17	O	1.21672221	-1.80187812	-2.12591262
18	O	1.28128005	0.06600049	-3.17559031
19	C	-2.87960540	-2.29580457	0.12081159
20	H	-2.33657864	-3.21726995	0.15120053
21	H	-3.58376755	-2.32316748	-0.68436352
22	C	-4.31013681	-0.91944399	-3.31184222
23	H	-3.71482609	-0.93763931	-4.20075959
24	H	-4.82685347	0.01532310	-3.24769905
25	N	-2.68036373	-2.07679389	2.37987567
26	O	-2.92556743	-1.41118578	3.39402298
27	O	-1.62070106	-2.71075300	2.29702245
28	O	-3.57537356	-2.11157289	1.35647552
29	N	-1.94634635	1.43707227	-0.51737050
30	N	-0.60534212	1.48237267	-0.11780135
31	O	0.22176235	2.10483477	-0.79610281
32	O	-0.24699884	0.89995619	0.91371930
33	N	-6.06385075	-1.83819019	-4.43941754
34	O	-5.62829725	-1.29124696	-5.46059335
35	O	-7.23073135	-2.24930581	-4.40736523
36	O	-5.26019458	-1.98745134	-3.35246866
37	N	-3.67122097	1.17903319	-1.91105863
38	N	-4.33637423	2.19678957	-1.21698150
39	O	-5.34382242	1.93344828	-0.54813677
40	O	-3.91692147	3.35982750	-1.27226197
41	N	-1.52811557	-0.40054804	-3.54645195
42	N	-2.22458818	-0.00986694	-4.48459809
43	O	-2.44890678	1.16460776	-4.57792100
44	O	-2.64507912	-0.82264345	-5.25983386

E = -2020.398120 Hartree/particle; ZPE = 0.281786 Hartree/particle
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

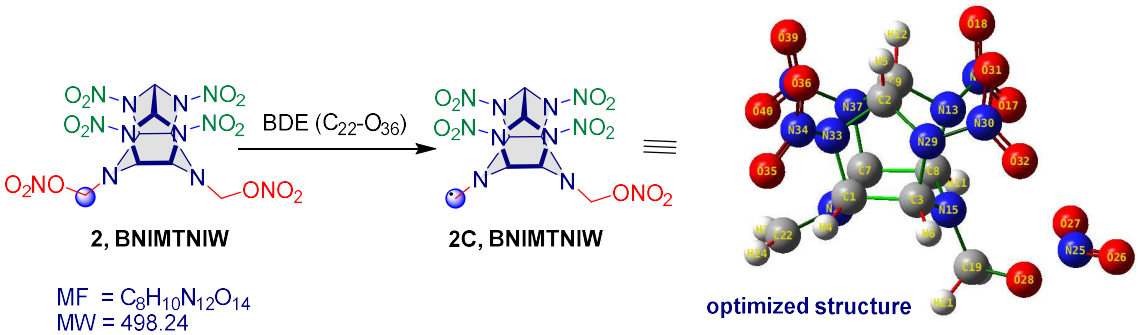
Table S12. Cartesian coordinates (in Å) for optimized structure of **BNIMTNIW**, **2B** obtained using the B3LYP/6-311++G(d,p) level of theory



Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.829683	0.420060	-1.865123
2	C	-1.710245	1.395972	-1.381676
3	C	-3.332613	-0.062599	-0.437436
4	H	-4.848407	0.792519	-1.820898
5	H	-1.185187	2.334291	-1.244099
6	H	-4.109105	0.056276	0.313099
7	C	-2.425940	-1.242349	-2.920750
8	C	-1.893013	-1.684630	-1.508053
9	C	-0.771300	0.282825	-2.061878
10	H	-2.456419	-2.066307	-3.628280
11	H	-1.622554	-2.739104	-1.487309
12	H	0.209559	0.705863	-2.262877
13	N	-0.691396	-0.881205	-1.204483
14	N	-3.719653	-0.620433	-2.841821
15	N	-2.916891	-1.441619	-0.499681
16	C	-2.879359	-2.189064	0.718494
17	H	-2.734662	-3.245351	0.503295
18	H	-3.810166	-2.036435	1.264297
19	C	-4.781974	-0.969296	-3.696004
20	H	-4.420671	-1.376137	-4.638021
21	H	-5.450110	-0.129476	-3.882177
22	N	-0.594330	-2.392627	1.580602
23	O	0.215007	-1.894904	2.300441
24	O	-0.496166	-3.329838	0.826387
25	O	-1.882398	-1.755706	1.685083
26	N	-2.214791	0.857164	-0.117139
27	N	-2.353400	1.744533	0.977231
28	O	-1.580052	2.681181	1.013113
29	O	-3.192187	1.448919	1.810100
30	N	-6.687854	-2.500450	-3.711087
31	O	-6.893102	-2.011534	-4.798569
32	O	-7.300297	-3.346277	-3.122660
33	O	-5.560218	-2.028179	-2.992950
34	N	-2.915100	1.546759	-2.193591
35	N	-3.470537	2.845279	-2.343320
36	O	-4.653214	2.888101	-2.635567
37	O	-2.706999	3.780215	-2.228010
38	N	-1.352964	-0.293872	-3.277977
39	N	-1.415623	0.426548	-4.456098
40	O	-0.733083	1.436364	-4.518755
41	O	-2.123422	-0.039677	-5.337719

E = -1815.318111 Hartree/particle; ZPE = 0.269774 Hartree/particle
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

Table S13. Cartesian coordinates (in Å) for optimized structure of **BNIMTNIW**, **2C** obtained using the B3LYP/6-311++G(d,p) level of theory



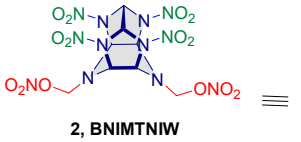
MF = $C_8H_{10}N_{12}O_{14}$
MW = 498.24

Center Number	Atomic Symbol	Coordinates (Angstroms) X	Y	Z
1	C	-3.905937	0.259024	-1.578160
2	C	-1.968645	1.632857	-1.705719
3	C	-3.060670	0.051337	-0.258019
4	H	-4.951389	0.457958	-1.365302
5	H	-1.627805	2.658682	-1.778109
6	H	-3.684113	0.089002	0.632121
7	C	-2.436461	-1.249237	-2.776556
8	C	-1.560235	-1.413979	-1.461528
9	C	-0.986483	0.652839	-2.491324
10	H	-2.448883	-2.153309	-3.379680
11	H	-1.081678	-2.387289	-1.419239
12	H	-0.171647	1.207220	-2.941188
13	N	-0.500154	-0.372978	-1.576715
14	N	-3.792432	-0.898289	-2.422557
15	N	-2.333073	-1.193662	-0.272943
16	N	0.828250	-0.853492	-1.856569
17	O	1.068712	-1.994277	-1.519883
18	O	1.595531	-0.052214	-2.345227
19	C	-2.809570	-2.294981	0.510667
20	H	-2.390598	-3.223298	0.125516
21	H	-3.900304	-2.368217	0.530451
22	C	-4.859304	-1.247532	-3.256691
23	H	-4.656423	-1.848248	-4.126802
24	H	-5.798756	-0.738388	-3.115510
25	N	-1.135443	-2.402237	2.261971
26	O	-0.907528	-2.162988	3.406364
27	O	-0.419386	-2.817501	1.385754
28	O	-2.519551	-2.162180	1.913703
29	N	-2.186960	1.235055	-0.310628
30	N	-1.180326	1.418985	0.633931
31	O	-0.254433	2.139166	0.298303
32	O	-1.348781	0.880156	1.711714
33	N	-3.318047	1.473809	-2.231036
34	N	-4.132086	2.653931	-2.236101
35	O	-5.334119	2.467685	-2.236559
36	O	-3.553950	3.717182	-2.304028
37	N	-1.672334	-0.190130	-3.472302

38	N	-2.065978	0.322700	-4.698729
39	O	-1.659260	1.440034	-4.974708
40	O	-2.739141	-0.412749	-5.401510

E = -1740.094171 Hartree/particle; ZPE = 0.263456 Hartree/particle
Number of imaginary frequencies at the B3LYP/6-311++G(d,p) level = 0

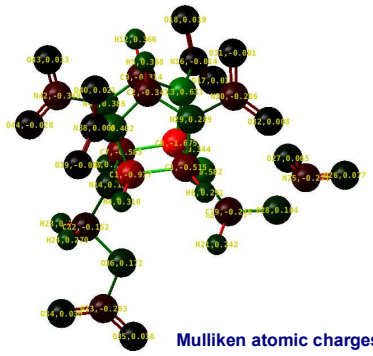
Table S14. Mulliken atomic charges for optimized structure of **BNMTNIW**, **2** obtained using the B3LYP/6-311++G(d,p) level of theory



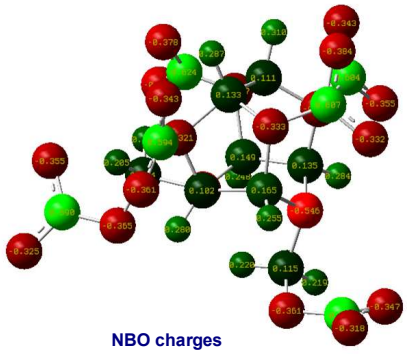
2, BNIMTNIW

MF = $C_8H_{10}N_{12}O_{14}$
MW = 498.24

≡



Mulliken atomic charges



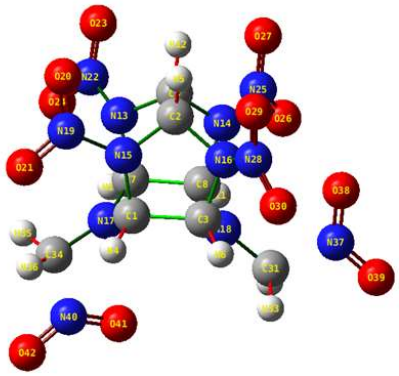
NBO charges

Center Number	Atomic Symbol	Mulliken Atomic Charges
1	C	-0.976717
2	C	-0.346525
3	C	-0.514584
4	H	0.310365
5	H	0.368072
6	H	0.290795
7	C	-0.582629
8	C	-1.674598
9	C	-0.313984
10	H	0.247941
11	H	0.343848
12	H	0.366412
13	N	0.631282
14	N	0.135211
15	N	0.582271
16	N	-0.013568
17	O	0.012272
18	O	0.018824
19	C	-0.245616
20	H	0.207202
21	H	0.241702
22	C	-0.152468
23	H	0.269544
24	H	0.270488
25	N	-0.271191
26	O	0.076969
27	O	0.064771

28	O	0.183991
29	N	0.289277
30	N	-0.286322
31	O	-0.000848
32	O	0.008343
33	N	-0.202737
34	O	0.030096
35	O	0.015877
36	O	0.172335
37	N	0.401610
38	N	0.007813
39	O	-0.007439
40	O	0.020513
41	N	0.385639
42	N	-0.349113
43	O	0.012887
44	O	-0.028012

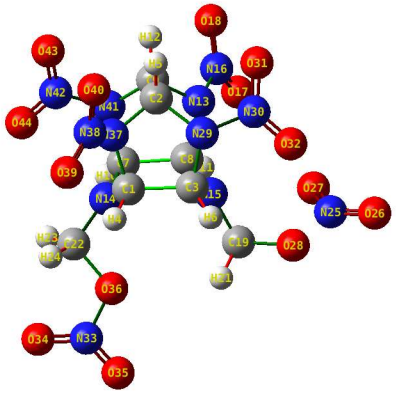
Sum of Mulliken charges= 0.00000

Table S15. Comparison of selected bond lengths for optimized structure of **BNMTNIW**, **1** and **BNIMTNIW**, **2** obtained using the B3LYP/6-311++G(d,p) level of theory



1, BNMTNIW

optimized structure



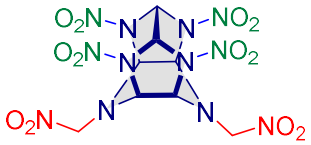
2, BNIMTNIW

optimized structure

Atom	Atom	Bond Lengths (Å) **BNMTNIW, 1**	Atom	Atom	Bond Lengths (Å) **BNIMTNIW, 2**
C1	C3	1.5897	C1	C3	1.5904
C1	H4	1.0868	C1	H4	1.0851
C1	N15	1.4837	C1	N14	1.4352
C1	N17	1.4341	C1	N37	1.4904
C2	H5	1.0839	C2	H5	1.0835
C2	**C9**	**1.6034**	**C2**	**C9**	**1.5968**
C2	N15	1.4692	C2	N29	1.4658
C2	N16	1.4516	C2	N37	1.4560
C3	H6	1.0858	C3	H6	1.0872
C3	N16	1.4897	C3	N15	1.4386
C3	N18	1.4326	C3	N29	1.4755

C7	C8	1.5899	C7	C8	1.5904
C7	H10	1.0851	C7	H10	1.0868
C7	N13	1.4890	C7	N14	1.4414
C7	N17	1.4321	C7	N41	1.4724
C8	H11	1.0862	C8	H11	1.0851
C8	N14	1.4736	C8	H13	1.4936
C8	N18	1.4382	C8	N15	1.4325
C9	H12	1.0846	C9	H12	1.0834
C9	N13	1.4648	C9	N13	1.4567
C9	N14	1.4550	C9	N41	1.4700
N13	N22	1.4239	**N13**	**N16**	**1.4435**
N14	N25	1.4041	N14	C22	1.4046
N15	**N19**	**1.3857**	N15	C19	1.4340
N16	N28	1.4185	N16	O17	1.2125
N17	C34	1.4079	N16	O18	1.2119
N18	C31	1.4096	C19	H20	1.0883
N19	O20	1.2183	C19	H21	1.0915
N19	O21	1.2230	C19	O28	1.4405
N22	O23	1.2119	C22	H23	1.0882
N22	O24	1.2187	C22	H24	1.0889
N25	O26	1.2191	**C22**	**O36**	**1.4949**
N25	O27	1.2157	N25	O26	1.1915
N28	O29	1.2144	N25	O27	1.2069
N28	O30	1.2175	N25	O28	1.4418
C31	H32	1.0891	N29	N30	1.3942
C31	H33	1.0893	N30	N31	1.2199
C31	N37	1.5656	N30	O32	1.2162
C34	H35	1.0909	N33	O34	1.2078
C34	H36	1.0866	N33	O35	1.1980
C34	**N40**	**1.5677**	N33	O36	1.4240
N37	O38	1.2150	N37	N38	1.4306
N37	O39	1.2171	N38	O39	1.2171
N40	O41	1.2190	N38	O40	1.2114
N40	O42	1.2157	N41	N42	1.3891
----	----	----	N42	O43	1.2180
----	----	----	N42	O44	1.2208

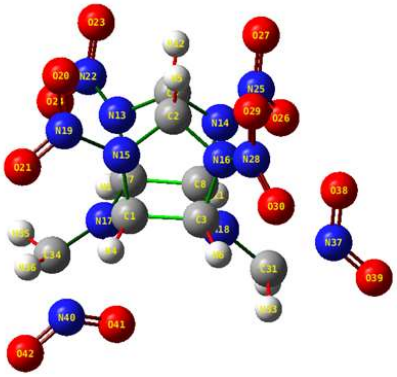
Table S16. Comparison of selected bond angles for optimized structure of **BNMTNIW**, **1** obtained using the B3LYP/6-311++G(d,p) level of theory



1, BNMTNIW

MF = $C_8H_{10}N_{12}O_{12}$
MW = 466.24

≡



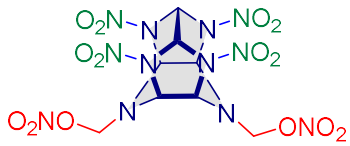
optimized structure

Atom	Atom	Atom	Bond Angle (°) **BNMTNIW, 1**
C3	C1	H4	111.40
C3	C1	N15	100.45
C3	C1	N17	111.07
H4	C1	N15	109.81
H4	C1	N17	109.99
N15	C1	N17	113.82
H5	C2	C9	110.69
H5	C2	N15	111.69
H5	C2	N16	111.68
C9	C2	N15	113.08
C9	C2	N16	109.79
N15	C2	N16	99.44
C1	C3	H6	111.38
C1	C3	N16	104.31
C1	C3	N18	109.78
H6	C3	N16	108.42
H6	C3	N18	110.43
N16	C3	N18	112.38
C8	C7	H10	111.02
C8	C7	N13	104.21
C8	C7	N17	110.86
H10	C7	N13	109.05
H10	C7	N17	110.55
N13	C7	N17	110.96
C7	C8	H11	111.40
C7	C8	N14	103.11
C7	C8	N18	109.96
H11	C8	N14	109.40
H11	C8	N18	110.32
N14	C8	N18	112.46
C2	C9	H12	111.21
C2	C9	N13	108.23
C2	C9	N14	109.68
H12	C9	N13	112.15
H12	C9	N14	111.92

N13	C9	N14	103.30
C7	N13	C9	107.35
C7	N13	N22	117.61
C9	N13	N22	117.68
C8	N14	C9	108.77
C8	N14	N25	120.37
C9	N14	N25	120.00
C1	N15	C2	109.66
C1	N15	N19	120.01
C2	N15	N19	120.56
C2	N16	C3	108.19
C2	N16	N28	117.06
C3	N16	N28	117.45
C1	N17	C7	114.60
C1	N17	C34	122.43
C7	N17	C34	121.93
C3	N18	C8	114.11
C3	N18	C31	121.90
C8	N18	C31	121.67
N15	N19	O20	116.68
N15	N19	O21	116.06
N15	N19	H36	80.69
O20	N19	O21	127.21
O20	N19	H36	154.39
O21	N19	H36	41.33
N19	O20	N22	83.27
N19	O20	O23	101.30
N19	O20	O24	76.85
O23	O20	O24	28.74
N13	N22	O20	54.96
N13	N22	O23	116.77
N13	N22	O24	115.73
O23	N22	O24	127.38
O20	O24	H35	73.46
N22	O24	H35	105.76
N14	N25	O26	116.12
N14	N25	O27	116.46
O26	N25	O27	127.37
N16	N28	O29	116.66
N16	N28	O30	116.06
O29	N28	O30	127.19
N18	C31	H32	111.78
N18	C31	H33	111.97
N18	C31	N37	116.03
H32	C31	H33	109.06
H32	C31	N37	103.77
H33	C31	N37	103.55
N17	C34	H35	113.43
N17	C34	H36	112.75
N17	C34	N40	112.69

H35	C34	H36	109.10
H35	C34	N40	103.25
H36	C34	N40	104.85
O24	H35	C34	120.35
N19	H36	C34	90.67
C31	N37	O38	118.59
C31	N37	O39	114.49
O38	N37	O39	126.92
C34	N40	O41	118.29
C34	N40	O42	115.21
O41	N40	O42	126.46

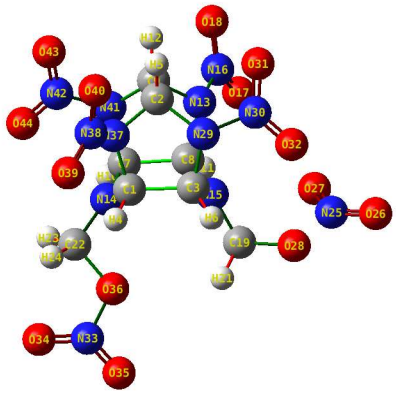
Table S17. Comparison of selected bond angles for optimized structure of **BNIMTNIW**, **2** obtained using the B3LYP/6-311++G(d,p) level of theory



2, BNIMTNIW

MF = $C_8H_{10}N_{12}O_{14}$
MW = 498.24

≡



optimized structure

Atom	Atom	Atom	Bond Angle (°) **BNIMTNIW, 2**
C3	C1	N14	111.0233
C3	C1	N37	104.8665
H4	C1	N14	110.2894
H4	C1	N37	108.8497
N14	C1	N37	109.9325
H5	C2	C9	110.7414
H5	C2	N29	111.631
H5	C2	N37	111.7683
C9	C2	N29	113.2996
C9	C2	N37	108.9559
N29	C2	N37	100.0038
C1	C3	H6	111.818
C1	C3	N15	111.5238
C1	C3	N29	100.2818
H6	C3	N15	109.3778
H6	C3	N29	110.0312
N15	C3	N29	113.5935
C8	C7	H10	111.7542
C8	C7	N14	111.4156

C8	C7	N41	100.7392
H10	C7	N14	109.5529
H10	C7	N41	110.3718
N14	C7	N41	112.7969
C7	C8	H11	111.8311
C7	C8	H13	104.5096
C7	C8	N15	111.1135
H11	C8	N13	108.3495
H11	C8	N15	110.1737
H13	C8	N15	110.7037
C2	C9	H12	110.6648
C2	C9	N13	109.2744
C2	C9	N41	113.3199
H12	C9	N13	111.662
H12	C9	N41	111.5869
N13	C9	N41	99.9007
C8	N13	C9	107.5917
C8	N13	N16	115.9388
C9	N13	N16	114.5816
C1	N14	C7	115.2528
C1	N14	C22	122.246
C7	N14	C22	122.0397
C3	N15	C8	114.959
C3	N15	C19	120.4593
C8	N15	C19	121.8184
N13	N16	O17	116.2906
N13	N16	O18	116.091
O17	N16	O18	127.5272
N15	C19	H20	109.4182
N15	C19	H21	112.4807
N15	C19	28	114.0699
H20	C19	O21	109.2711
H20	C19	O28	110.1771
H21	C19	O28	101.1339
N14	C22	H23	111.6314
N14	C22	H24	111.9858
N14	C22	O36	106.4914
H23	C22	H24	110.3488
H23	C22	O36	108.2623
H24	C22	O36	107.9072
O26	N25	O27	130.6348
O26	N25	O28	112.5467
O27	N25	O28	116.8127
C19	O28	N25	114.629
C2	N29	C3	109.8409
C2	N29	N30	119.7545
C3	N29	N30	120.8577
N29	N30	N31	116.0735
N29	N30	O32	116.2169
N31	N30	O32	127.6589

O34	N33	O35	130.1351
O34	N33	O36	116.9136
O35	N33	O36	112.9513
C22	O36	N33	114.7862
C1	N37	C2	107.6032
C1	N37	N38	116.4931
C2	N37	N38	116.4887
N37	N38	O39	115.768
N37	N38	O40	116.7647
O39	N38	O40	127.3623
C7	N41	C9	109.692
C7	N41	N42	120.0772
C9	N41	N42	120.6535
N41	N42	O43	116.5099
N41	N42	O44	116.0778
O43	N42	O44	127.3706

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