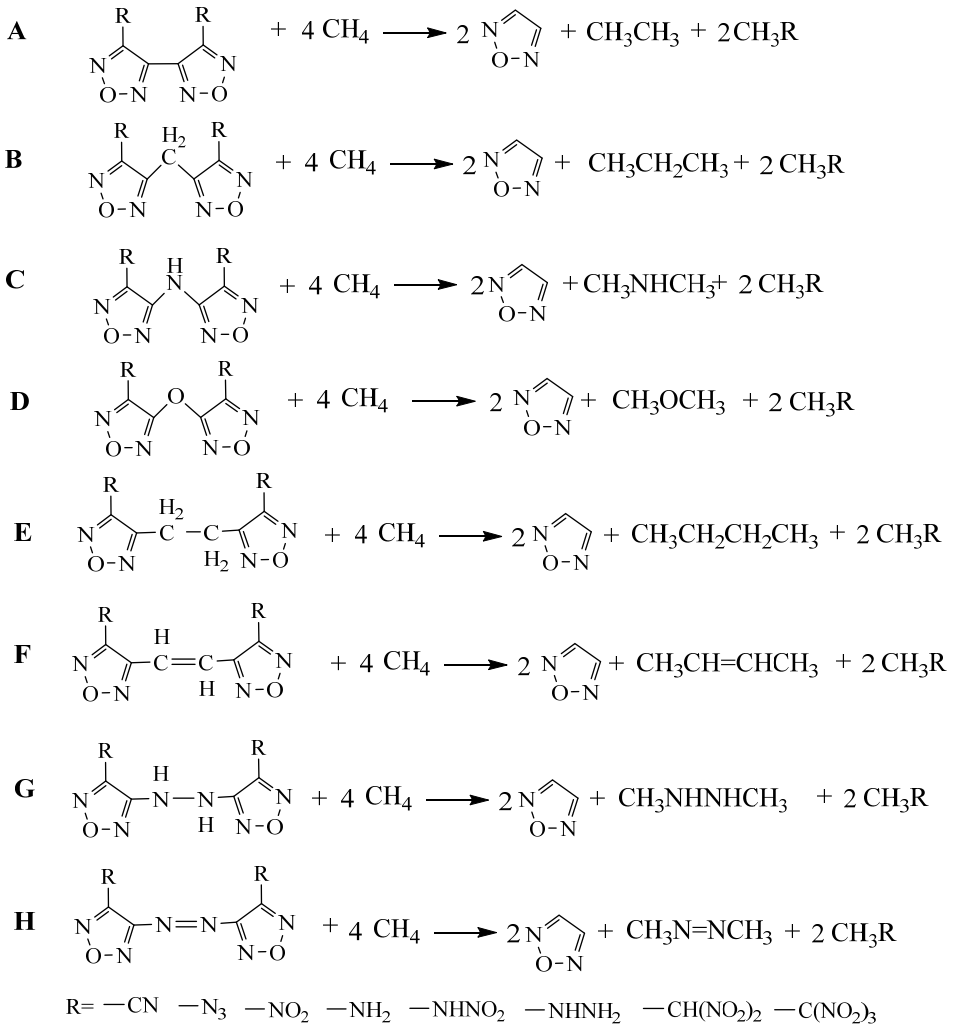
Supporting Information

1. Computational methods

Gaussian 03 program [1] was employed to calculate the frontier molecular orbitals, heats of formation, energetic properties and bond dissociation energies of the compounds. All the calculations were carried out by density functional theory (DFT) method at B3LYP/6-311G(*d*,*p*) level on. Gas-phase heats of formation ($\Delta H_{f,gas}$) of were predicted by the following isodesmic reactions (Scheme 1) combined with (equations 1 and 2)[2-4].



Scheme 1 The designed isodesmic reactions for each series of compounds

$$\Delta H_{298\mathrm{K}} = \sum \Delta H_{\mathrm{f,p}} - \sum \Delta H_{\mathrm{f,R}} \quad (1)$$

$$\Delta H_{298\mathrm{K}} = \Delta E_{298\mathrm{K}} + \Delta(PV) = \Delta E_0 + \Delta \mathrm{ZPE} + \Delta H_{\mathrm{T}} + \Delta nRT \quad (2)$$

$\Delta H_{f,p}$ and $\Delta H_{f,R}$ were presented as heats of formation of the products and reactants; ΔE_0 were energy changes between products and reactants; ΔZPE were difference between the zero-point energy (ZPE) of products and reactants; ΔH_T were thermal correction from 0 to298 *K*; *n* was the number of the energetic groups; Δ(*PV*) equals to Δ*nRT*.

Atomization reactions ($C_aH_bN_c \rightarrow aC(g)+bH(g)+cN(g)$) were employed to calculated the $\Delta H_{f,gas}$ of these unknown compounds (CH_3NF_2, CH_3NHNO_2, CH_3N_3, $CH_3NHNHCH_3$, $CH_3N{=}NCH_3$) at CBS-Q level.[5] Also, HOFs of compounds $CH_3CH(NO_2)_2$ and $CH_3C(NO_2)_3$ were calculated via isodesmic reactions:

$$CH_3CH(NO_2)_2 + 2CH_4 \rightarrow CH_3CH_3 + 2CH_3NO_2$$

$$CH_3C(NO_2)_3 + 3CH_4 \rightarrow CH_3CH_3 + 3CH_3NO_2$$

The related parameters were summarized in Table 1.

Table 1. Calculated total energies (E_0), zero-point energies (ZPE), thermal corrections (H_T) and heats of formation (HOFs) of the reference compounds

Compound.	E_0 (a.u.)[a]	ZPE (kJ mol^{-1})[a]	H_T (kJ mol^{-1})[a]	$\Delta H_{f,gas}$ (kJ mol^{-1})
NH_3	-56.576035	90.1	10.0	-45.9[b]
CH_4	-40.533748	117.0	10.0	-74.6[b]
CH_3NHNH_2	-151.217035	213.0	14.3	94.5[b]
CH_3NF_2	-294.298331	122.8	13.6	-98.4[c]
CH_3NH_2	-95.888444	167.6	11.4	-23.5[b]
CH_3NHNO_2	-300.434462	176.5	16.0	-8.5[c]
CH_3NO_2	-245.081687	130.6	13.9	-81.0[b]
CH_3CN	-132.793330	118.7	11.9	74.0[b]
CH_3N_3	-204.148401	131.7	14.2	289.9[c]
CH_3CH_3	-79.856261	195.3	11.6	84.0[b]
$CH_3CH_2CH_3$	-119.180686	270.4	14.4	-104.7[b]

CH_3NHCH_3	-135.695161	254.5	14.9	-19.0[b]
CH_3OCH_3	-155.071921	208.2	13.8	-184.1[b]
$CH_3CH_2CH_2CH_3$	-158.504982	345.1	17.7	-125.6[b]
$CH_3CH=CHCH_3$	-157.273161	282.0	16.9	-10.7[b]
$CH_3NHNHCH_3$	-190.535853	286.9	17.1	109.3[c]
$CH_3N=NCH_3$	-189.328011	220.6	16.0	160.5[c]
$CH_3CH(NO_2)_2$	-488.950712	212.3	22.8	81.8[d]
$CH_3C(NO_2)_3$	-693.479196	215.6	29.3	105.1[d]
	-262.112125	119.6	11.6	197.4[c]

a, calculated at B3LYP/ 6-311G (d,p) level; b, obtained from http://webbook.nist.gov; c, calculated values were calculated at the CBS-Q level; d, obtained by isodesmic reaction.

Solid-phase HOFs ($\Delta H_{f,solid}$) were calculated according to Hess's law since most of the energetic materials were in condensed phase (equation 3).[6]

$$\Delta H_{\text{f,solid}} = \Delta H_{\text{f,gas}} - \Delta H_{\text{sub}} \quad (3)$$

Where, ΔH_{sub} is the heat of sublimation. ΔH_{sub} is the sublimation enthalpy and can be calculated by the following empirical expression (equation 4).[7]

$$\Delta H_{\text{sub}} = aA^2 + b(\nu\sigma_{tot}^2)^{0.5} + c \quad (4)$$

where, a, b and c were coefficients according to the reference;[8] A was the surface area of the 0.001 e bohr^{-3} isosurface of electronic density of the molecule; ν was the degree of balance between positive and negative potential on the isosurface; σ_{tot}^2 was the measure of variability of the electrostatic potential on the molecular surface.

Kamlet-Jacobs equations (equation 5 and 6) were employed to calculated the detonation velocities (D) and detonation pressures (P) of the designed compounds.[9]

$$D = 1.01(N\overline{M}^{0.5}Q^{0.5})^{0.5}(1+1.3\rho) \quad (5)$$

$$P = 1.558\rho^2 N\overline{M}^{0.5}Q^{0.5} \quad (6)$$

where, N was the mole of detonation gases per-gram explosive (mol g^{-1}), $\overline{M}$ was average molecular weight of these gases (g mol^{-1}), Q was heat of detonation (cal g^{-1})

and ρ was the density. Also, accurate densities can be obtained by an improved equation (equation 7) proposed by Politzer et al.[10]

$$\rho = \beta_1\left(\frac{M}{V}\right) + \beta_2(\nu\sigma_{tot}^2) + \beta_3 \quad (7)$$

Where, β_1, β_2, and β_3 were coefficients, M was the molecular mass (g mol^{-1}), V was the volume of a molecule (m^3 mol^{-1}).

Finally, bond dissociation energies (BDEs) of the designed compounds were also predicted according to equation (8) and (9).

$$BDE_0(A–B)=E_0(A\cdot)+E_0(B\cdot)–E_0(A–B) \quad (8)$$

$$BDE(A–B)_{ZPE} = BDE_0(A–B) + \Delta E_{ZPE} \quad (9)$$

where $E_0(A\cdot)$, $E_0(B\cdot)$ and E_0(A–B) were the energy of A·, B· and A–B; ΔE_{ZPE} was the difference between the *ZPE*s of the products and the reactants.

2. Data of $\Delta E_{LUMO–HOMO}$, HOFs, detonation properties and BDEs

Table 2 Calculated HOMO and LUMO energies (eV) and energy gaps ($\Delta E_{LUMO–HOMO}$) of the designed compounds

Compd.	**A[a]**	**A1**	**A2**	**A3**	**A4**	**A5**	**A6**	**A7**	**A8**
HOMO	-8.58	-9.44	-7.85	-9.29	-6.83	-8.47	-6.84	-9.29	-9.70
LUMO	-2.59	-3.52	-2.81	-3.67	-2.23	-3.41	-2.35	-3.63	-4.18
$\Delta E_{HOMO-LUMO}$	5.99	5.92	5.04	5.62	4.60	5.06	4.49	5.66	5.52
Compd.	**B[a]**	**B1**	**B2**	**B3**	**B4**	**B5**	**B6**	**B7**	**B8**
HOMO	-8.86	-9.39	-7.78	-9.32	-6.85	-8.62	-6.89	-9.34	-9.77
LUMO	-2.11	-3.13	-2.35	-3.86	-1.36	-3.14	-1.70	-3.60	-4.26
$\Delta E_{HOMO-LUMO}$	6.75	6.26	5.43	5.46	5.49	5.48	5.19	5.74	5.51
Compd.	**C[a]**	**C1**	**C2**	**C3**	**C4**	**C5**	**C6**	**C7**	**C8**
HOMO	-7.27	-8.16	-7.26	-8.34	-6.65	-7.51	-6.26	-8.22	-8.47
LUMO	-2.04	-2.92	-2.29	-4.05	-1.69	-3.00	-1.18	-3.77	-4.44
$\Delta E_{HOMO-LUMO}$	5.23	5.24	4.97	4.29	4.96	4.51	5.08	4.45	4.03
Compd.	**D[a]**	**D1**	**D2**	**D3**	**D4**	**D5**	**D6**	**D7**	**D8**
HOMO	-8.21	-9.12	-7.83	-9.35	-7.11	-8.44	-6.85	-8.94	-9.43
LUMO	-2.32	-3.07	-2.41	-4.01	-1.80	-2.80	-1.24	-3.32	-4.19
$\Delta E_{HOMO-LUMO}$	5.89	6.05	5.42	5.34	5.31	5.64	5.61	5.62	5.24
Compd.	**E[a]**	**E1**	**E2**	**E3**	**E4**	**E5**	**E6**	**E7**	**E8**
HOMO	-8.66	-9.27	-7.68	-9.21	-7.04	-8.54	-6.84	-9.35	-9.67

LUMO	-1.68	-2.94	-2.12	-3.71	-1.17	-2.63	-0.98	-3.50	-4.13
$\Delta E_{\text{HOMO-LUMO}}$	6.98	6.33	5.56	5.50	5.87	5.91	5.86	5.85	5.54
Compd.	**F[a]**	**F1**	**F2**	**F3**	**F4**	**F5**	**F6**	**F7**	**F8**
HOMO	-7.47	-8.30	-7.30	-8.33	-6.80	-7.69	-6.40	-8.41	-8.50
LUMO	-2.91	-3.72	-3.02	-3.87	-2.65	-3.15	-2.20	-3.81	-4.15
$\Delta E_{\text{HOMO-LUMO}}$	4.56	4.58	4.28	4.46	4.15	4.54	4.20	4.60	4.35
Compd.	**G[a]**	**G1**	**G2**	**G3**	**G4**	**G5**	**G6**	**G7**	**G8**
HOMO	-6.98	-8.16	-7.16	-8.24	-6.40	-7.37	-6.21	-7.75	-7.61
LUMO	-1.66	-2.99	-2.15	-3.85	-1.24	-2.79	-0.84	-3.45	-4.22
$\Delta E_{\text{HOMO-LUMO}}$	5.32	5.17	5.01	4.39	5.16	4.58	5.37	4.30	3.39
Compd.	**H[a]**	**H1**	**H2**	**H3**	**H4**	**H5**	**H6**	**H7**	**H8**
HOMO	-7.79	-8.62	-7.78	-8.65	-7.06	-8.75	-6.88	-8.91	-8.92
LUMO	-3.99	-4.83	-4.04	-4.54	-3.71	-4.65	-2.94	-5.02	-4.93
$\Delta E_{\text{HOMO-LUMO}}$	3.80	3.79	3.74	4.11	3.35	4.10	3.94	3.89	3.99

[a]A-H stand for the unsubstituted compounds.

Table 3. Calculated total energy (E_0), thermal correction (H_T), zero point energy (ZPE), molecular properties and heat of formation (ΔH_f) of the designed compounds

Compd.	E_0(a.u)	ZPE (kJ mol^{-1})	H_T (kJ mol^{-1})	$\Delta H_{f,gas}$ (kJ mol^{-1})	A (Å^2)	v	σ^2_{tot} (kcal mol^{-1})^2	ΔH_{sub} (kJ mol^{-1})	$\Delta H_{f,solid}$ (kJ mol^{-1})
A1	-707.523968	180.1	30.0	934.4	195.2	0.198	174.9	95.6	838.8
A2	-850.266702	204.7	34.7	1279.3	212.5	0.211	99.0	94.5	1184.8
A3	-932.078535	199.3	32.5	676.4	203.6	0.113	151.3	87.3	589.1
A4	-633.791677	274.0	26.1	529.1	173.5	0.202	202.7	90.3	438.8
A5	-1042.825431	288.2	41.1	714.4	230.3	0.179	175.1	110.4	604.0
A6	-744.453624	367.7	35.8	759.4	205.0	0.229	118.7	95.4	664.0
A7	-1419.837630	362.0	54.9	950.7	282.6	0.092	198.1	131.2	819.5

A8	-1828.871097	365.9	69.0	1057.4	317.8	0.076	80.1	142.3	915.1
B1	-746.857127	255.1	33.6	723.4	217.2	0.163	192.5	103.8	619.6
B2	-889.589149	279.4	38.4	1096.3	227.8	0.163	190.3	108.9	987.4
B3	-971.424374	275.7	37.6	435.1	219.4	0.144	155.9	98.9	336.2
B4	-673.103963	351.2	32.4	377.9	197.4	0.199	250.4	104.7	273.2
B5	-1082.155342	365.7	43.4	513.1	249.9	0.165	223.4	124.1	389.0
B6	-783.763873	442.7	38.3	607.5	224.3	0.250	202.3	117.8	489.7
B7	-1459.172744	437.2	58.5	734.8	298.1	0.089	150.1	137.0	597.8
B8	-1868.201178	440.8	72.8	854.6	333.6	0.067	119.2	156.3	698.3
C1	-762.825067	221.4	34.1	2226.3	213.6	0.122	215.9	98.9	2127.4
C2	-905.638624	249.5	38.1	2388.0	232.0	0.199	129.0	107.6	2280.4
C3	-987.461750	245.5	37.0	1758.0	214.4	0.127	176.5	96.5	1661.5
C4	-689.150512	324.3	30.4	1678.6	189.9	0.175	275.6	100.7	1577.9
C5	-1098.192957	335.3	43.1	1835.5	240.9	0.115	211.6	111.3	1724.2
C6	-799.806462	415.1	36.7	1918.4	216.9	0.224	266.8	118.4	1800.0
C7	-1475.207905	406.8	57.8	2063.2	288.1	0.095	193.4	134.8	1928.4
C8	-1884.241465	411.5	71.8	2170.4	330.2	0.077	144.3	157.3	2013.1
D1	-782.672946	187.6	33.6	837.3	213.0	0.185	119.1	95.5	741.8
D2	-925.487852	216.0	37.4	995.7	230.4	0.222	87.3	102.2	893.5
D3	-1007.302416	211.2	36.9	387.9	213.7	0.141	145.1	94.7	293.2
D4	-709.001384	289.3	30.3	281.1	187.2	0.184	225.6	96.1	185.0
D5	-1118.039653	301.5	42.6	449.7	238.2	0.137	220.6	113.8	335.9

D6	-819.651969	379.7	37.0	534.9	216.8	0.213	235.3	113.8	421.1
D7	-1494.998318	374.4	41.4	810.7	285.4	0.119	215.4	138.4	672.3
D8	-1904.088957	376.0	72.3	781.8	332.2	0.065	98.5	153.2	628.6
E1	-786.188013	329.6	37.4	685.5	239.1	0.204	156.9	115.4	570.1
E2	-928.931862	354.2	42.2	1027.6	259.6	0.248	85.2	119.5	908.1
E3	-1010.753196	349.7	41.5	402.2	241.8	0.168	147.7	112.2	290.0
E4	-712.435411	426.9	35.5	339.0	219.2	0.216	214.4	113.1	225.9
E5	-1121.486507	440.6	47.1	474.8	271.1	0.131	166.7	126.8	348.0
E6	-823.093973	518.5	41.6	572.5	246.8	0.228	254.0	133.1	439.4
E7	-1498.491914	510.5	62.7	726.8	331.2	0.073	257.2	164.9	561.9
E8	-1907.534256	515.4	76.7	811.1	363.8	0.070	112.7	179.7	631.4
F1	-784.957264	268.5	36.0	799.0	233.7	0.222	129.8	110.5	688.5
F2	-927.703032	293.0	40.8	1136.0	254.4	0.246	76.5	114.7	1021.3
F3	-1009.520742	288.3	40.5	520.3	237.5	0.178	125.8	108.1	412.2
F4	-711.207065	365.5	34.3	446.1	214.4	0.177	252.5	110.0	336.1
F5	-1120.254607	379.1	46.0	591.2	214.4	0.177	252.5	110.0	481.2
F6	-821.866135	457.8	40.2	678.7	242.0	0.218	251.6	129.0	549.7
F7	-1497.258880	448.4	62.0	846.0	328.2	0.071	251.5	162.0	684.0
F8	-1906.300490	453.3	75.7	932.0	361.6	0.073	98.0	177.0	755.0
G1	-818.232494	268.7	36.9	882.1	229.6	0.120	256.7	109.7	772.4
G2	-960.975337	293.7	41.5	1227.0	250.6	0.219	166.8	124.4	1102.6
G3	-1042.806078	289.7	40.3	576.9	231.8	0.133	158.5	104.2	472.7

G4	-744.475826	367.0	32.1	544.4	210.8	0.193	244.7	109.5	434.9
G5	-1153.534702	381.5	45.6	662.4	258.6	0.126	198.2	121.7	540.7
G6	-855.145071	460.0	40.0	753.0	234.5	0.232	257.3	127.2	625.8
G7	-1530.526163	448.5	60.4	947.4	329.7	0.045	383.3	162.6	784.8
G8	-1939.578857	454.7	73.2	1004.6	359.4	0.062	118.6	175.5	829.1
H1	-816.982887	202.7	33.3	1040.7	227.2	0.205	157.7	109.4	931.3
H2	-959.729786	227.1	38.1	1374.6	247.6	0.247	92.0	113.9	1260.7
H3	-1041.539893	222.8	39.7	781.2	234.1	0.130	150.4	104.2	677.0
H4	-743.248622	300.0	33.6	648.3	206.5	0.187	212.3	103.6	544.7
H5	-1152.213329	323.0	40.3	1015.3	256.2	0.162	224.8	127.5	887.8
H6	-853.894844	391.3	39.8	914.0	236.9	0.214	247.7	125.4	788.6
H7	-1529.293439	383.9	61.1	1067.4	324.3	0.085	190.0	157.7	909.7
H8	-1938.331638	388.5	74.8	1162.0	357.8	0.072	95.0	173.6	988.4

Table 4. Predicted densities (ρ), heats of detonation (Q), detonation velocities (D) and detonation pressures (P) of the designed compounds

Compound	OB	ρ (g cm^{-3})	Q (cal g^{-1})	D (km s^{-1})	P (GPa)
A1	-85.11	1.64	1566.6	6.90	20.0
A2	-43.64	1.74	1714.6	8.24	29.5
A3	-14.04	1.88	1855.0	9.07	37.5
A4	-76.19	1.63	1312.3	7.24	21.9
A5	-18.60	1.85	1694.9	8.95	36.1
A6	-72.73	1.60	1385.3	7.68	24.3
A7	-13.87	1.89	1956.3	9.33	39.7
A8	7.34	2.02	1795.9	9.71	44.7
B1	-102.97	1.57	1252.0	6.25	15.9

B2	-61.54	1.67	1456.5	7.57	24.2
B3	-33.06	1.80	1542.5	8.28	30.4
B4	-96.70	1.53	993.9	6.54	17.1
B5	-35.29	1.77	1458.4	8.23	29.8
B6	-90.57	1.53	1097.4	7.05	19.9
B7	-26.67	1.83	1762.9	8.79	34.6
B8	-3.56	1.95	1857.8	9.54	42.3
C1	-82.76	1.61	2994.5	8.24	28.1
C2	-44.26	1.72	2742.4	9.31	37.4
C3	-16.46	1.87	2817.4	10.1	46.7
C4	-74.32	1.61	2692.5	8.87	32.6
C5	-20.51	1.83	2602.2	9.96	44.5
C6	-71.36	1.60	2562.4	9.14	34.4
C7	-15.51	1.87	2624.1	10.0	45.6
C8	5.32	2.00	2382.1	10.4	51.1
D1	-70.59	1.66	1560.6	7.15	21.6
D2	-33.90	1.76	1502.6	8.14	29.0
D3	-6.56	1.92	1636.2	9.01	37.4
D4	-60.87	1.67	1124.1	7.23	22.1
D5	-11.68	1.86	1533.7	8.83	35.3
D6	-44.14	1.64	1280.6	7.55	23.9
D7	-8.84	1.93	1902.6	9.46	41.4
D8	10.62	2.01	1580.8	9.38	41.6
E1	-118.52	1.51	1166.0	5.89	13.8
E2	-77.42	1.60	1341.3	7.08	20.7
E3	-50.00	1.73	1457.1	7.83	26.5
E4	-114.29	1.48	865.3	6.21	15.1
E5	-50.35	1.70	1390.4	7.80	26.1
E6	-106.19	1.49	976.2	6.73	17.8
E7	-38.50	1.77	1702.9	8.43	31.2
E8	-13.79	1.90	1790.5	9.20	38.8
F1	-112.15	1.55	1258.8	6.03	14.7
F2	-71.54	1.63	1418.4	7.21	21.7

F3	-44.09	1.77	1541.1	7.99	28.0
F4	-107.22	1.52	1009.9	6.33	16.0
F5	-45.07	1.73	1474.3	7.95	27.4
F6	-100.00	1.52	1102.6	6.83	18.6
F7	-34.41	1.79	1761.5	8.53	32.1
F8	-10.39	1.92	1838.9	9.29	39.7
G1	-80.73	1.61	1327.7	6.87	19.5
G2	-44.80	1.70	1473.4	7.98	27.3
G3	-18.60	1.84	1573.3	8.75	34.4
G4	-72.73	1.59	1108.8	7.23	21.5
G5	-22.22	1.81	1503.2	8.68	33.5
G6	-52.63	1.59	1163.0	7.60	23.7
G7	-17.02	1.84	1806.8	9.09	37.1
G8	3.43	1.97	1760.2	9.61	43.2
H1	-74.07	1.64	1465.9	7.04	20.7
H2	-38.71	1.73	1594.2	8.17	28.9
H3	-12.50	1.86	1734.2	8.95	36.2
H4	-47.06	1.63	1254.0	7.31	22.3
H5	-16.78	1.85	1766.1	9.11	37.4
H6	-63.72	1.61	1345.5	7.73	24.7
H7	-12.83	1.86	1867.5	9.18	38.1
H8	6.90	1.99	1725.3	9.55	42.9
RDX	-21.6	1.82	1590.7	8.75	34.0
HMX	-21.6	1.91	1633.9	9.10	39.0

Table 5. Bond dissociation energies (BDE, kJ mol^{-1}) for the weakest bonds of the designed compounds.

Compd.	ring-R		C-C/C=C(bridge)		C-N(bridge)		C-O(bridge)		N-N/N=N(bridge)		$NH-NH_2/NH-NO_2/C-NO_2$	
	BO	BDE	BO	BDE	BO	BDE	BO	BDE	BO	BDE	BO	BDE
A1	1.0766	543.6	1.0557	509.8	--	--	--	--	--	--	--	--
A2	1.0840	345.6	1.0601	515.5	--	--	--	--	--	--	--	--
A3	0.8856	231.6	1.0514	488.0	--	--	--	--	--	--	--	--
A4	1.1931	472.0	1.0756	548.1	--	--	--	--	--	--	--	--
A5	1.1025	417.4	1.0689	544.7	--	--	--	--	--	--	0.9808	117.4

A6	1.1764	377.9	1.0750	543.8	--	--	--	--	--	--	1.0371	238.0
A7	1.0083	444.0	1.0508	529.8	--	--	--	--	--	--	0.8292	133.5
A8	1.0086	447.4	1.0485	501.4	--	--	--	--	--	--	0.8063	112.7
B1	1.0763	550.6	1.0118	381.2	--	--	--	--	--	--	--	--
B2	1.0819	344.8	1.0091	371.3	--	--	--	--	--	--	--	--
B3	0.9172	257.0	1.0104	391.8	--	--	--	--	--	--	--	--
B4	1.1243	450.1	1.0127	372.0	--	--	--	--	--	--	--	--
B5	1.0184	414.2	1.0120	380.5	--	--	--	--	--	--	0.9605	112.3
B6	1.1259	353.5	1.0022	397.3	--	--	--	--	--	--	1.0320	222.0
B7	1.0153	454.9	1.0081	388.1	--	--	--	--	--	--	0.8379	118.8
B8	1.0147	449.3	1.0069	375.2	--	--	--	--	--	--	0.8017	95.0
C1	1.0426	463.7	--	--	1.0527	385.2	--	--	--	--	--	--
C2	1.0789	363.9	--	--	1.0504	380.0	--	--	--	--	--	--
C3	0.9066	235.8	--	--	1.0611	397.6	--	--	--	--	--	--
C4	1.1127	451.9	--	--	1.0435	388.6	--	--	--	--	--	--
C5	1.0362	419.4	--	--	1.0621	382.7	--	--	--	--	0.9844	116.1
C6	1.0880	365.1	--	--	1.0581	374.9	--	--	--	--	0.0036	203.8
C7	1.0153	432.8	--	--	1.0397	387.6	--	--	--	--	0.8167	109.0
C8	1.0153	440.7	--	--	1.0686	390.3	--	--	--	--	0.7886	99.1
D1	1.0477	454.0	--	--	--	--	0.9444	314.1	--	--	--	--
D2	1.0906	355.5	--	--	--	--	0.9438	308.7	--	--	--	--
D3	0.9140	244.4	--	--	--	--	0.9567	320.9	--	--	--	--
D4	1.1496	456.6	--	--	--	--	0.9318	295.0	--	--	--	--
D5	1.0460	413.2	--	--	--	--	0.9550	309.2	--	--	0.9484	107.8
D6	1.1011	350.4	--	--	--	--	0.9483	296.0	--	--	1.0266	206.6
D7	1.0057	296.2	--	--	--	--	0.9686	164.7	--	--	0.8183	136.7
D8	1.0120	452.8	--	--	--	--	0.9476	314.3	--	--	0.8050	108.8
E1	1.0785	551.7	1.0119	249.5	--	--	--	--	--	--	--	--
E2	1.0799	361.8	1.0125	248.7	--	--	--	--	--	--	--	--
E3	0.9186	255.1	1.0072	253.3	--	--	--	--	--	--	--	--
E4	1.1312	449.4	1.0121	247.6	--	--	--	--	--	--	--	--
E5	1.0296	418.7	1.0098	257.5	--	--	--	--	--	--	0.9682	111.7
E6	1.0908	351.8	1.0102	249.1	--	--	--	--	--	--	1.0251	207.4
E7	1.0104	440.6	1.0100	255.8	--	--	--	--	--	--	0.8287	122.2
E8	1.0142	455.5	1.0069	257.2	--	--	--	--	--	--	0.8073	104.9
F1	1.0789	550.0	1.0928	500.6	--	--	--	--	--	--	--	--
F2	1.0859	362.7	1.0956	504.9	--	--	--	--	--	--	--	--
F3	0.9155	251.1	1.0884	501.0	--	--	--	--	--	--	--	--
F4	1.1369	450.8	1.0988	500.8	--	--	--	--	--	--	--	--
F5	1.0350	415.7	1.0885	496.0	--	--	--	--	--	--	0.9614	108.4
F6	1.1048	352.6	0.0086	499.9	--	--	--	--	--	--	1.0283	207.2
F7	1.0102	436.3	1.0880	496.5	--	--	--	--	--	--	0.8287	120.6

F8	1.0147	450.2	1.0840	232.7	--	--	--	--	--	--	0.8037	104.0
G1	1.0848	554.4	--	--	1.0996	346.3	--	--	1.0292	185.0	--	--
G2	1.0755	362.8	--	--	1.0872	340.8	--	--	1.0258	165.3	--	--
G3	0.9347	267.5	--	--	1.1348	360.2	--	--	0.0002	207.2	--	--
G4	1.1172	439.8	--	--	1.0973	329.4	--	--	1.0000	148.7	--	--
G5	1.0348	425.3	--	--	1.1061	346.0	--	--	1.0279	189.2	0.9978	102.8
G6	1.0991	358.0	--	--	1.0919	340.2	--	--	1.0232	160.8	1.0277	203.5
G7	1.0152	415.2	--	--	1.1159	321.0	--	--	1.0003	169.9	0.8413	69.5
G8	1.0224	453.2	--	--	1.1360	339.0	--	--	1.0000	195.0	0.7895	78.0
H1	1.0760	546.3	--	--	1.1016	275.6	--	--	1.7788	885.0	--	--
H2	1.1020	360.6	--	--	1.1105	277.3	--	--	1.7613	263.9	--	--
H3	0.9066	237.4	--	--	1.0766	264.9	--	--	1.8295	387.2	--	--
H4	1.1832	467.8	--	--	1.1312	295.4	--	--	1.7212	833.4	--	--
H5	1.0859	195.0	--	--	1.1178	79.5	--	--	1.7272	413.4	0.9975	155.1
H6	1.1192	354.1	--	--	1.0880	271.4	--	--	1.7973	473.7	1.0279	219.2
H7	1.0078	443.3	--	--	1.1015	284.8	--	--	1.7736	326.3	0.8293	121.0
H8	1.0109	454.8	--	--	1.0892	275.4	--	--	1.7932	308.8	0.8051	108.8

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