Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

for

Theoretical design of highly energetic poly-nitro cage compounds

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Table S1 Optimized coordinates of ONOP at B3LYP/6-31G (d, p) level.

Atom	X	Y	Z
C	-1.95058400	-0.66823100	-0.76275200
C	-0.89529300	-1.81867000	-0.80680200
C	0.65242800	-1.91574300	-0.81397300
C	1.80840400	-0.87978200	-0.79931200
C	1.94729700	0.67558600	-0.75638500
C	0.88154700	1.81513300	-0.78817400
C	-0.66509000	1.91472400	-0.75264800
C	-1.82859300	0.87171700	-0.76261400
C	-0.65483600	1.89242500	0.80211000
C	0.90622900	1.83644800	0.77503400
C	1.90605200	0.63825200	0.80761400
C	1.81857100	-0.90834700	0.75385000
C	0.64435500	-1.93662600	0.75098100
C	-0.89958300	-1.86098700	0.75744000
C	-1.90816700	-0.68661100	0.79361900
C	-1.82708300	0.87779900	0.79627600
N	-1.51814300	-3.01383700	-1.52747800
O	-0.86841800	-3.57541600	-2.39675600
O	-2.65047600	-3.31224700	-1.16165800
N	3.04236000	-1.44413000	-1.50238600

O	2.87833200	-2.24792100	-2.40681600
O	4.11666300	-1.01081600	-1.09938100
N	1.45934100	3.00837100	-1.56672500
O	0.73535300	3.56209800	-2.38290200
O	2.62149100	3.29803300	-1.32076500
N	-3.02634700	1.50696400	-1.46168300
O	-3.54932200	0.89391200	-2.37998400
O	-3.34969000	2.61392900	-1.04596100
N	-1.06510400	3.17657600	1.51939900
O	-1.86447700	3.09355100	2.43954300
O	-0.52042600	4.19834800	1.11681200
N	-3.19143900	-1.09437200	1.51186900
O	-3.11887100	-1.93377200	2.39587000
O	-4.20575900	-0.51382800	1.13968700
N	1.13151700	-3.22251500	1.42031000
O	2.23167300	-3.62032100	1.05066000
O	0.41427000	-3.75451300	2.25427300
N	3.15147900	1.05754000	1.60801200
O	3.61400100	0.25487900	2.40710800
O	3.57366700	2.18507300	1.39434600
H	2.87183900	1.01085300	-1.22344300
H	2.69621600	-1.32595500	1.24323300

H	-1.32228600	-2.72250100	1.27374900
H	-2.68541000	1.30883300	1.30861900
H	-0.96901100	2.83794800	-1.24281400
H	1.35147200	2.70759000	1.25292900
H	0.96766500	-2.80160500	-1.36487500
H	-2.87417700	-0.96777900	-1.25480800

Table S2 Optimized coordinates of ONOAP at B3LYP/6-31G (d, p) level.

Atom	X	Y	Z
C	0.70774800	1.76787700	0.72546600
C	1.76787700	-0.70774800	0.72546600
C	-0.70774800	-1.76787700	0.72546600
C	-1.76787700	0.70774800	0.72546600
C	-1.75053100	-0.74962400	-0.72546600
C	0.74962400	-1.75053100	-0.72546600
C	1.75053100	0.74962400	-0.72546600
C	-0.74962400	1.75053100	-0.72546600
N	1.19424800	2.97122300	1.53032400
O	1.08539700	2.79897100	2.73220100
O	1.62577800	3.92497500	0.91514800
N	2.97122300	-1.19424800	1.53032400
O	2.79897100	-1.08539700	2.73220100
O	3.92497500	-1.62577800	0.91514800
N	-1.19424800	-2.97122300	1.53032400
O	-1.08539700	-2.79897100	2.73220100
O	-1.62577800	-3.92497500	0.91514800
N	-2.97122300	1.19424800	1.53032400
O	-2.79897100	1.08539700	2.73220100
O	-3.92497500	1.62577800	0.91514800

N	-2.94543200	-1.25651100	-1.53032400
O	-2.74666300	-1.21168000	-2.73220100
O	-3.92497500	-1.62577800	-0.91514800
N	-1.25651100	2.94543200	-1.53032400
O	-1.21168000	2.74666300	-2.73220100
O	-1.62577800	3.92497500	-0.91514800
N	2.94543200	1.25651100	-1.53032400
O	3.92497500	1.62577800	-0.91514800
O	2.74666300	1.21168000	-2.73220100
N	1.25651100	-2.94543200	-1.53032400
O	1.21168000	-2.74666300	-2.73220100
O	1.62577800	-3.92497500	-0.91514800
N	-0.71935800	-1.79592100	-0.76100700
N	0.76124500	-1.77857100	0.76100700
N	-0.76124500	1.77857100	0.76100700
N	1.79592100	-0.71935800	-0.76100700
N	0.71935800	1.79592100	-0.76100700
N	-1.79592100	0.71935800	-0.76100700
N	-1.77857100	-0.76124500	0.76100700
N	1.77857100	0.76124500	0.76100700

Table S3 Optimized coordinates of TNOP at B3LYP/6-31G (d, p) level.

Atom	X	Y	Z
C	-1.95058400	-0.66823100	-0.76275200
C	-0.89529300	-1.81867000	-0.80680200
C	0.65242800	-1.91574300	-0.81397300
C	1.94729700	0.67558600	-0.75638500
C	0.88154700	1.81513300	-0.78817400
C	-0.66509000	1.91472400	-0.75264800
C	0.90622900	1.83644800	0.77503400
C	1.90605200	0.63825200	0.80761400
C	1.81857100	-0.90834700	0.75385000
C	-0.89958300	-1.86098700	0.75744000
C	-1.90816700	-0.68661100	0.79361900
C	-1.82708300	0.87779900	0.79627600
N	-1.51814300	-3.01383700	-1.52747800
O	-0.86841800	-3.57541600	-2.39675600
O	-2.65047600	-3.31224700	-1.16165800
N	1.45934100	3.00837100	-1.56672500
O	0.73535300	3.56209800	-2.38290200
O	2.62149100	3.29803300	-1.32076500
N	-3.19143900	-1.09437200	1.51186900
O	-3.11887100	-1.93377200	2.39587000
O	-4.20575900	-0.51382800	1.13968700
N	3.15147900	1.05754000	1.60801200
O	3.61400100	0.25487900	2.40710800
O	3.57366700	2.18507300	1.39434600
H	2.87183900	1.01085300	-1.22344300
H	2.69621600	-1.32595500	1.24323300
H	-1.32228600	-2.72250100	1.27374900
H	-2.68541000	1.30883300	1.30861900
H	-0.96901100	2.83794800	-1.24281400
H	1.35147200	2.70759000	1.25292900
H	0.96766500	-2.80160500	-1.36487500
H	-2.87417700	-0.96777900	-1.25480800
C	-1.82859300	0.87171700	-0.76261400
H	-2.40188269	1.14151372	-1.62484869
C	1.80840400	-0.87978200	-0.79931200
H	2.36434729	-1.15078836	-1.67245724
C	0.64435500	-1.93662600	0.75098100
H	0.84244879	-2.55273693	1.60307617
C	-0.65483600	1.89242500	0.80211000
H	-0.86365011	2.47066353	1.67785932

Table S4 Optimized coordinates of TNOAP at B3LYP/6-31G (d, p) level.

Atom	X	Y	Z
C	0.70774800	1.76787700	0.72546600
C	-0.70774800	-1.76787700	0.72546600
C	-1.75053100	-0.74962400	-0.72546600
C	1.75053100	0.74962400	-0.72546600
N	1.19424800	2.97122300	1.53032400
O	1.08539700	2.79897100	2.73220100
O	1.62577800	3.92497500	0.91514800
N	-1.19424800	-2.97122300	1.53032400
O	-1.08539700	-2.79897100	2.73220100
O	-1.62577800	-3.92497500	0.91514800
N	-2.94543200	-1.25651100	-1.53032400
O	-2.74666300	-1.21168000	-2.73220100
O	-3.92497500	-1.62577800	-0.91514800
N	2.94543200	1.25651100	-1.53032400
O	3.92497500	1.62577800	-0.91514800
O	2.74666300	1.21168000	-2.73220100
N	-0.71935800	-1.79592100	-0.76100700
N	0.76124500	-1.77857100	0.76100700
N	-0.76124500	1.77857100	0.76100700
N	1.79592100	-0.71935800	-0.76100700
N	0.71935800	1.79592100	-0.76100700
N	-1.79592100	0.71935800	-0.76100700
N	-1.77857100	-0.76124500	0.76100700
N	1.77857100	0.76124500	0.76100700
C	0.74962400	-1.75053100	-0.72546600
H	0.99985674	-2.33355100	-1.58707569
C	-0.74962400	1.75053100	-0.72546600
H	-0.99985674	2.33355040	-1.58707609
C	-1.76787700	0.70774800	0.72546600
H	-2.35707598	0.94306334	1.58707569
C	1.76787700	-0.70774800	0.72546600
H	2.35707598	-0.94306416	1.58707546

Table S5 The identity and the quantity of the gas products of decomposition of the target compounds.

Compd	Formula	Quantity of decomposition products (mol)				
		N_2	H_2O	CO	C(s)	V(dm^3)
ONOP	$C_{16}H_8N_8O_{16}$	4	4	12	4	448.0
ONOAP	$C_8N_{16}O_{16}$	8	0	8	0	358.4
TNOP	$C_{16}H_{12}N_4O_8$	2	6	2	14	224.0
TNOAP	$C_8H_4N_{12}O_8$	6	2	6	2	313.6

Table S6 Corresponding parameters for the calculations of I_s for the designed compounds.

Compd	*n*	*N*	*M*	$C_{P,gases}$(J(mol*K)$^{-1}$)	T_c	ΔH_{comb} (kJmol^{-1})
ONOP	14.0	0.0246	568	559.96	17176.7	-9451.45
ONOAP	16.0	0.0278	576	532.08	13777.9	-7172.39
TNOP	9.0	0.0232	388	423.30	22680.0	-9474.28
TNOAP	11.0	0.0278	396	395.42	17597.5	-6840.59
HMX	10.0	0.0338	296	340.88	6166.5	-2000.00

Note: $C_{P,gases}$ (kJ (mol*k)$^{-1}$): H_2O, 33.33; CO_2, 37.65; N_2, 28.86; C, 8.53.

ΔH_f (kJ mol^{-1}): H_2O, -241.83; CO_2, -393.51; N_2,0; C, 0