Supporting Information

Molecular design of N-NO_2 substituted cycloalkanes derivatives $C_m(N\text{-}NO_2)_m$ for energetic materials with high detonation performance and low impact sensitivity

Yan-Yan Guo,[a] Wei-Jie Chi,[a] Ze-Sheng Li,*[,a,b] and Quan-Song Li*[,a,b]

[a] Beijing Key Laboratory of Photoelectronic/Electrophotonic Conversion Materials, Key Laboratory of Cluster Science of Ministry of Education, Beijing Key Laboratory for Chemical Power Source and Green Catalysis, School of Chemistry, Beijing Institute of Technology, Beijing 100081, China

[b] The Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin 150080, China.

Table S1 The coordinates of C3

atom	X	Y	Z
C	-0.82459800	0.16662700	-0.00006200
C	0.55672200	0.63107100	0.00005500
C	0.26826000	-0.79738300	-0.00001100
N	1.32169700	1.64625300	0.00006500
N	0.76503300	-1.96741000	0.00003800
N	-2.08628700	0.32119600	-0.00012700
N	-2.48294700	1.73734500	-0.00005200
O	-2.66399500	2.21489500	1.09793500
O	-2.66400700	2.21496600	-1.09800500
N	-0.26355900	-3.01844300	-0.00008100
O	-0.58704700	-3.41381300	1.09785700
O	-0.58662300	-3.41395000	-1.09809200
N	2.74644100	1.28101200	0.00014100
O	3.25056200	1.19873700	-1.09779800
O	3.25049100	1.19897000	1.09813100

Table S2 The coordinates of C4

atom	X	Y	Z
C	-0.16976900	-1.05136700	-0.00025000
C	-1.05134000	0.16968300	0.00003600
C	0.16970300	1.05124600	0.00038200
C	1.05126600	-0.16977400	-0.00014900
N	0.26511100	2.31691400	0.00071100
N	-2.31699400	0.26506500	-0.00021100
N	-0.26486000	-2.31702000	-0.00031600
N	2.31689600	-0.26495100	-0.00024300
N	1.64485400	2.81526000	0.00040000
O	2.10561400	3.03149600	1.09868800
O	2.10442500	3.03305300	-1.09811200
N	-2.81525400	1.64507700	-0.00018300
O	-3.03208600	2.10527100	1.09819100
O	-3.03234600	2.10496900	-1.09865600
N	2.81550800	-1.64496600	-0.00053400
O	3.03217000	-2.10494300	-1.09903500
O	3.03298200	-2.10514500	1.09772200
N	-1.64532300	-2.81534200	0.00031800
O	-2.10433100	-3.03296700	1.09902300
O	-2.10626900	-3.03160600	-1.09778400

Table S3 The coordinates of C5

atom	X	Y	Z
C	0.32868600	1.22879400	0.00009200
C	1.27004400	0.06723200	-0.00018100
C	0.45619100	-1.18698000	0.00006200
C	-0.98825400	-0.80052000	0.00020700
C	-1.06687000	0.69257300	0.00046000
N	2.53107100	0.26395400	-0.00054800
N	1.03273900	-2.32554700	0.00002600
N	-1.89273300	-1.70083200	0.00032000
N	-2.20257200	1.27480300	0.00005400
N	0.53174000	2.48881000	0.00060800
N	3.39649500	-0.90896400	-0.00076100
O	3.74472500	-1.27834500	-1.09928500
O	3.74448900	-1.27885200	1.09769900
N	1.91447500	2.94875700	0.00067900
O	2.37374400	3.16528800	1.09921100
O	2.37377800	3.16538400	-1.09782800
N	-2.21370100	2.73183800	-0.00046200
O	-2.27811700	3.23593700	1.09788200
O	-2.27836700	3.23527300	-1.09909200
N	-3.28235300	-1.26104700	-0.00010500
O	-3.78157800	-1.16669200	1.09827700
O	-3.78107300	-1.16705700	-1.09876400
N	0.18506500	-3.51076100	0.00044300
O	-0.05848200	-3.95617200	1.09910700
O	-0.05916200	-3.95647300	-1.09791200

Table S4 The coordinates of C6

atom	X	Y	Z
C	0.58821000	1.38668500	-0.05552200
C	-0.84175300	1.08935300	-0.41166400
C	-1.38188700	-0.15252400	0.27053100
C	-0.58822700	-1.38694400	-0.05538900
C	0.84189400	-1.08970900	-0.41125200
C	1.38191600	0.15239000	0.27064800
N	1.40263200	-1.80035900	-1.30882800
N	-0.96157700	-2.60564500	-0.07671900
N	-2.30200400	-0.23808200	1.14825600
N	-1.40240100	1.79953300	-1.30965700
N	0.96138300	2.60544600	-0.07683200
N	2.30203600	0.23821900	1.14838800
N	2.77326600	-1.39549400	-1.65238900
O	3.59447500	-2.26787800	-1.49468900
O	2.89841300	-0.27996500	-2.12480500
N	-2.36467900	-2.87709100	0.23141100
O	-3.13695100	-2.72122200	-0.68913000
O	-2.54517600	-3.33419100	1.33651400
N	-2.97241200	1.02912000	1.48368300
O	-4.16599500	1.01177400	1.30340800
O	-2.26436200	1.89164900	1.96953200
N	-2.77269000	1.39479500	-1.65289600
O	-2.89770100	0.28003000	-2.12717600
O	-3.59428100	2.26652800	-1.49313100
N	2.36391100	2.87757800	0.23110700
O	3.13614900	2.72279500	-0.68970200
O	2.54446000	3.33424700	1.33642700
N	2.97254600	-1.02876800	1.48405800
O	4.16593600	-1.01187700	1.30228300
O	2.26490800	-1.89067400	1.97157100

Table S5 The coordinates of C7

atom	X	Y	Z
C	-1.31654600	0.84874900	-0.24192600
C	-0.34600900	1.546800000	0.67977200
C	0.94067100	0.76909000	0.82877900
C	-1.55523500	-0.57445700	0.21327700
C	1.34991900	-0.09144800	-0.36546300
C	-0.77692900	-1.59048500	-0.58750200
C	0.72700200	-1.46875300	-0.53682200
N	-2.21072500	-0.74152600	1.29093300
N	-1.74022900	1.17382300	-1.39627300
N	-0.50363800	2.58693000	1.39478800
N	1.52376500	0.83511500	1.96093800
N	2.15307300	0.23254900	-1.30157100
N	1.36484300	-2.56180900	-0.69709400
N	-1.24971100	-2.47238600	-1.37816900
N	-2.26836900	-2.14009500	1.77152500
O	-3.38610900	-2.55422500	1.94938500
O	-1.19114500	-2.65955200	2.00617000
N	-1.33445500	2.49688700	-1.87289200
O	-2.11223200	3.39645600	-1.64752500
O	-0.30983100	2.49193300	-2.52298900
N	-1.83317000	3.22538600	1.29159300
O	-1.78115100	4.42472200	1.17623400
O	-2.80118000	2.49476100	1.41256300
N	2.76664900	0.08037700	2.09800700
O	3.71608000	0.51277700	1.47094400
O	2.70935800	-0.82421700	2.89625600
N	2.79406500	1.56520500	-1.14940000
O	2.09257600	2.47801200	-0.74380900
O	3.94089100	1.58113100	-1.51015100
N	2.82300500	-2.48003900	-0.72569700
O	3.36638400	-2.25822300	0.33808500
O	3.29999300	-2.74918800	-1.80217700
N	-2.71123400	-2.56385600	-1.40888500
O	-3.14341200	-3.60137100	-0.95962900
O	-3.29451100	-1.64462800	-1.94902200

Table S6 The coordinates of C8

atom	X	Y	Z
C	1.43139000	0.33127900	-0.24596000
C	1.24167700	-1.13017800	-0.57197900
C	0.48269900	0.96562200	0.76091700
C	0.60581200	-2.02178400	0.47182400
C	-0.89233100	1.28846400	0.23415700
C	-0.75037800	-1.62825600	0.98928100
C	-1.55361400	0.23557500	-0.62857700
C	-1.76110900	-1.12755500	-0.02789000
N	1.52505100	-1.73118000	-1.66288500
N	2.33265700	0.94676200	-0.90539500
N	0.68594300	1.218600000	1.99383600
N	-1.56845600	2.35156100	0.41508800
N	-1.93176400	0.39122300	-1.83776000
N	-2.68744200	-1.96954500	-0.27147400
N	-0.96571500	-1.77920300	2.23835500
N	1.07528100	-3.11780700	0.92391400
N	2.49294900	2.37714100	-0.62801000
O	2.96376100	2.65329000	0.45927700
O	2.21446500	3.09019600	-1.55988600
N	2.09664000	-0.96801600	-2.77470900
O	1.28439700	-0.38737900	-3.46117300
O	3.28265000	-1.13334600	-2.92741100
N	2.39097100	-3.51316700	0.41218600
O	2.36295200	-4.49373300	-0.29448000
O	3.33774300	-2.87970400	0.83165700
N	-2.30600300	-1.37742100	2.66860400
O	-2.94895400	-2.25691700	3.18568100
O	-2.57509700	-0.19426500	2.52953500
N	-3.73379000	-1.58569100	-1.23183200
O	-3.64757200	-2.14927400	-2.29674700
O	-4.59605600	-0.85828600	-0.79170300
N	-1.69395000	1.72227800	-2.41394900
O	-0.52794500	2.03078600	-2.56581200
O	-2.70317000	2.29837700	-2.73577200
N	-0.92295600	3.41114000	1.20983300
O	-0.00988300	3.98999100	0.65709700
O	-1.45972800	3.62281700	2.26831400
N	2.02845500	0.84783100	2.49898900
O	2.45960800	-0.24038100	2.14828300
O	2.49408400	1.65150900	3.26137000

Table S7 The formula and the quantity of decomposition products of the designed compounds

compd.	formula	Quantity of decomposition products (mol)					
		N_2	H_2O	CO	CO_2	O_2	n totle
C3	$C_3N_6O_6$	3	0	0	3	0	6
C4	$C_4N_8O_8$	4	0	0	4	0	8
C5	$C_5N_{10}O_{10}$	5	0	0	5	0	10
C6	$C_6N_{12}O_{12}$	6	0	0	6	0	12
C7	$C_7N_{14}O_{14}$	7	0	0	7	0	14
C8	$C_8N_{16}O_{16}$	8	0	0	8	0	16

Table S8 The oxygen balance (OB_{100}) and the net charge of the nitro group (Q_{NO2}) of the designed compounds

Compd.	OB_{100}	Q_{NO2}
C3	2.78	-0.0708
C4	2.78	-0.0597
C5	2.78	-0.0411
C6	2.78	-0.0538
C7	2.78	-0.0261
C8	2.78	-0.0264

Table S9 Calculated the heats of formation (HOF_{solid}), detonation performance (D and P), power index, *BDE* and h_{50} of C3 and C6 at the MP2/ 6-31G(d,p) level.

Compd.	HOF_{gas} (kJ mol^{-1})	HOF_{solid} (kJ mol^{-1})	D (km s^{-1})	P (GPa)	power index %	*BDE* (kJ mol^{-1})		h_{50} (cm)
						N-NO_2	C-C (ring)	
C3	782.09	698.62	9.66	42.73	112.80	168.07	177.13	117
C6	1078.12	923.31	9.17	37.87	98.59	178.08	249.15	85

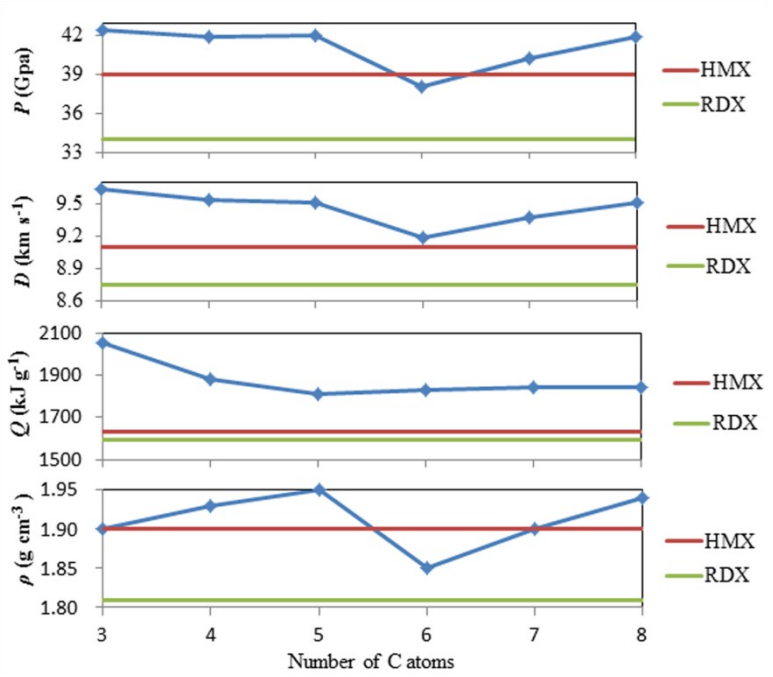

Figure S1 Crystal densities (ρ), heats of detonation (Q), detonation velocities (D) and detonation pressure (P) versus the number of C atoms for all designed compounds, HMX and RDX.