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Supporting information for

Theoretical studies on the derivatives of tris([1,2,4]triazolo)[4,3-a:4',3'-c:4'',3''-e][1,3,5]triazine as high energetic compounds

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Table S1 The bond order for TTT and its derivatives with NBO.

	TTT	R=NO_2	R=NH_2	R=$NHNO_2$	R=N_3
N1–N2	1.206	1.214	1.154	1.206	1.179
N2=C3	1.683	1.661	1.570	1.622	1.581
C3–N4	1.090	1.076	1.056	1.067	1.069
N4–C5	1.098	1.091	1.064	1.095	1.073
C5=N1	1.609	1.610	1.647	1.608	1.638
C4–N6	1.014	1.008	1.011	1.011	1.007
C3–R	0.909	0.882	1.165	1.044	1.091
R (N-N)				0.949	1.376

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Table S2. The detonation velocity (*D*, in km/s) and pressure (*P*, in GPa) of the title compounds, TNT, HMX and CL-20.

Compound	*D*		*P*	
	ρ	ρ'	ρ	ρ'
TTT	8.15	7.66	20.51	20.07
1	10.55	9.27	38.57	36.82
2	9.34	8.08	22.78	21.65
3	9.40	9.02	34.78	34.27
4	8.60	8.71	29.22	29.34
TNT[a]	6.95		19.00	
HMX[a]	9.10		39.30	
CL-20[a]	9.38		44.10	

[a] Experimental values from *Cent. Eur. J. Energ. Mater.*, 2011, 8, 209-220.

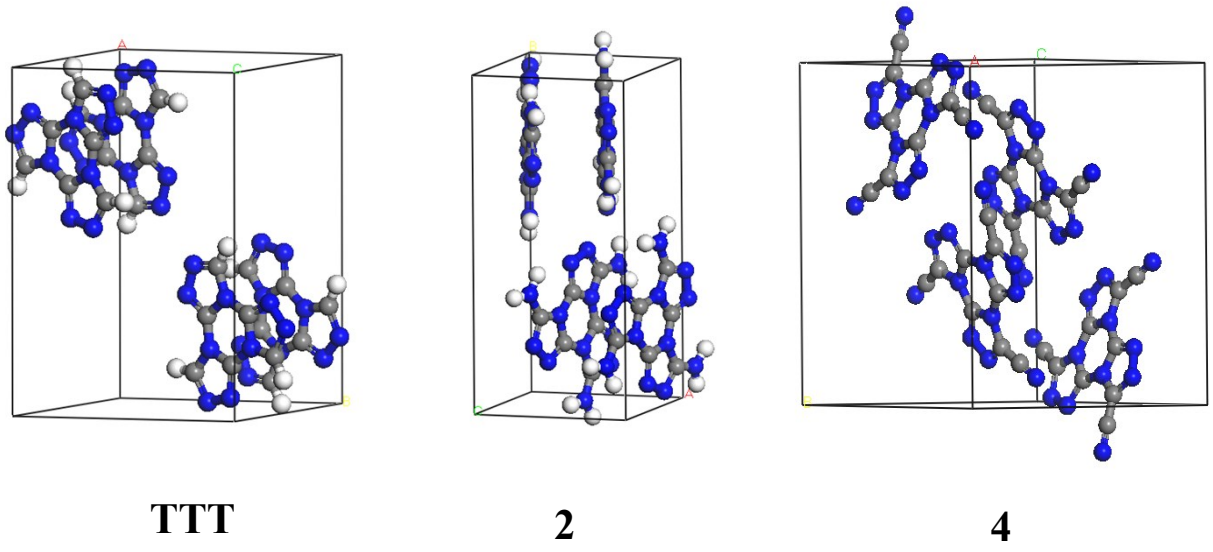

Fig.S1 The predicted cell structures of compound TTT, 2 and 4.

Listing XYZ coordinates of TTT and its derivatives in Å

TTT

C	1.21347700	0.68937300	0.00000000
N	0.00000000	1.35800500	0.00000000
N	1.17606700	-0.67900200	0.00000000
C	-0.00972400	-1.39558800	0.00000000
N	-1.17606700	-0.67900200	0.00000000
C	-1.20375300	0.70621500	0.00000000
C	-0.35986100	2.68643300	0.00000000
N	-1.65044300	2.79183200	0.00000000
N	-2.19846900	1.52447800	0.00000000
C	-2.14658900	-1.65486500	0.00000000
N	-1.59257600	-2.82524200	0.00000000
N	-0.22100200	-2.66616900	0.00000000
C	2.50644900	-1.03156800	0.00000000
N	3.24301900	0.03340900	0.00000000
N	2.41947100	1.14169100	0.00000000
H	2.83775900	-2.05516800	0.00000000
H	-3.19870700	-1.42998700	0.00000000
H	0.36094800	3.48515500	0.00000000

1

N	3.54881200	1.46757000	0.06018500
O	4.26212000	2.16900300	-0.60118300
O	3.86101800	0.62118000	0.86130600
N	-3.04535900	2.33957600	0.06018500
O	-2.46846700	3.03315000	0.86130600
O	-4.00947100	2.60660300	-0.60118300
C	0.00000000	1.40074700	0.00073100
N	-1.18329500	0.67414300	0.06412100
N	1.17547200	0.68769200	0.06412100
C	1.21308300	-0.70037400	0.00073100
N	0.00782300	-1.36183500	0.06412100
C	-1.21308300	-0.70037400	0.00073100
C	-2.51489700	0.98513300	-0.08080400
N	-3.23816000	-0.06989100	-0.20067200
N	-2.40751200	-1.16039400	-0.15228300
C	0.40429800	-2.67053100	-0.08080400
N	1.67960700	-2.76938300	-0.20067200
N	2.20868700	-1.50476900	-0.15228300
C	2.11059900	1.68539800	-0.08080400
N	1.55855300	2.83927400	-0.20067200
N	0.19882500	2.66516300	-0.15228300
N	-0.50345300	-3.80714600	0.06018500
O	-1.39255200	-3.65433000	0.86130600
O	-0.25264900	-4.77560600	-0.60118300

2

C	1.29663400	0.53182500	-0.04365600
N	0.17659000	1.34497500	-0.06945000
N	1.07648700	-0.82541800	-0.06945000
C	-0.18774300	-1.38883100	-0.04365600
N	-1.25307700	-0.51955600	-0.06945000
C	-1.10889100	0.85700600	-0.04365600
C	0.00000000	2.71013300	0.00355400
N	-1.26953400	2.99385100	0.06331600
N	-1.97922200	1.79444300	0.03196600
C	-2.34704400	-1.35506600	0.00355400
N	-1.95798400	-2.59637400	0.06331600
N	-0.56442200	-2.61127800	0.03196600
C	2.34704400	-1.35506600	0.00355400
N	3.22751700	-0.39747700	0.06331600
N	2.54364500	0.81683500	0.03196600
N	1.05994700	3.55588100	-0.05285200
N	2.54951000	-2.69588100	-0.05285200
N	-3.60945700	-0.86000000	-0.05285200
H	1.96217700	3.17024100	0.18715900
H	0.87186500	4.49878300	0.24259600
H	1.76442100	-3.28441600	0.18715900
H	3.46012700	-3.00444900	0.24259600
H	-3.72659800	0.11417500	0.18715900
H	-4.33199300	-1.49433400	0.24259600

3

C	-1.21558400	0.69174600	-0.48597200
N	0.00000000	1.35578600	-0.46447400
N	-1.17414500	-0.67789300	-0.46447400
C	0.00872200	-1.39860000	-0.48597200
N	1.17414500	-0.67789300	-0.46447400
C	1.20686100	0.70685400	-0.48597200
C	0.36828100	2.68138000	-0.48624500
N	1.65777300	2.78888200	-0.53443900
N	2.20091500	1.52562000	-0.54499500
C	2.13800300	-1.65963000	-0.48624500
N	1.58635600	-2.83011400	-0.53443900
N	0.22076800	-2.66885900	-0.54499500
C	-2.50628300	-1.02175000	-0.48624500
N	-3.24412900	0.04123300	-0.53443900
N	-2.42168400	1.14323900	-0.54499500
N	-0.55254700	3.71468800	-0.54898100
N	-2.94074000	-2.33586300	-0.54898100
N	3.49328700	-1.37882400	-0.54898100
H	-0.22575000	4.57633800	-0.96811100
N	-1.26523300	4.00308700	0.63655100
H	-3.85035000	-2.48367400	-0.96811100
N	-2.83415800	-3.09726700	0.63655100
H	4.07610000	-2.09266400	-0.96811100
N	4.09939100	-0.90581900	0.63655100
O	-1.78580700	5.08214400	0.65949500
O	-1.29798000	3.13485600	1.46497700
O	5.29416900	-0.99451800	0.65949500
O	3.36385500	-0.44334500	1.46497700
O	-2.06587600	-2.69151200	1.46497700
O	-3.50836300	-4.08762600	0.65949500

4

N	2.88114300	-2.34979900	0.00000000
N	0.59441400	3.67004200	0.00000000
C	1.22040900	0.69803400	0.00000000
N	0.00000000	1.36012600	0.00000000
N	1.17790400	-0.68006300	0.00000000
C	-0.00568900	-1.40592200	0.00000000
N	-1.17790400	-0.68006300	0.00000000
C	-1.21472000	0.70788800	0.00000000
C	-0.37039800	2.68446400	0.00000000
N	-1.66310700	2.79593800	0.00000000
N	-2.20615500	1.52466200	0.00000000
C	-2.13961500	-1.66300600	0.00000000
N	-1.58979900	-2.83826200	0.00000000
N	-0.21731900	-2.67291800	0.00000000
C	2.51001300	-1.02145800	0.00000000
N	3.25290700	0.04232500	0.00000000
N	2.42347400	1.14825500	0.00000000
N	-3.47555700	-1.32024300	0.00000000
N	-4.23407400	-2.30783900	0.00000000
N	0.11839000	4.82073500	0.00000000
N	4.11568400	-2.51289600	0.00000000
N	5.19190500	-2.78253300	0.00000000
N	-5.00569700	-3.10505600	0.00000000
N	-0.18620900	5.88758800	0.00000000