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Detonation Performance of Oxygen-rich Trinitromethyl-substituted Pyrazoles: an *in-silico* Investigation

Neeraj Naithani*, Benny Kattikkanal George

Analytical and Spectroscopy Division, Analytical Spectroscopy and Ceramic Group, Propellants Polymers Chemicals and Materials Entity, Vikram Sarabhai Space Centre, Thiruvananthapuram-695022, Kerala, India

**E-mails: neeraj_naithani@vssc.gov.in, neerajnaithani@gmail.com*

Table S1. Optimized energies of various possible configurations at RHF/6-31G(d,p) level

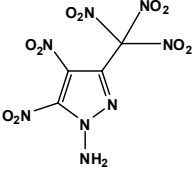
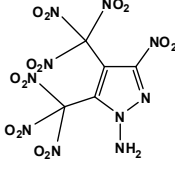
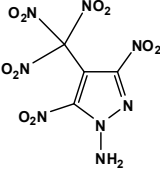
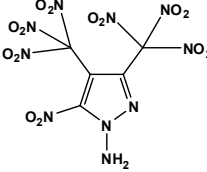
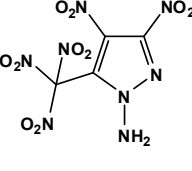
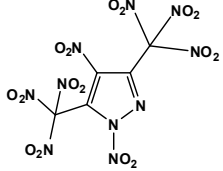
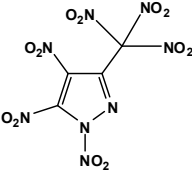
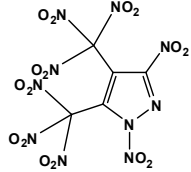
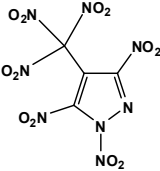
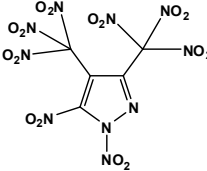
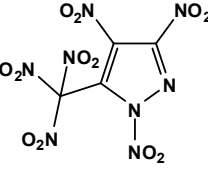
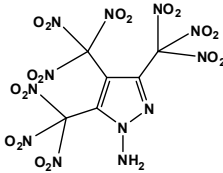
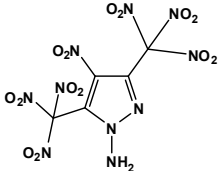
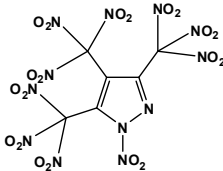
Designation	Compound	Zero point corrected energy (Hartree)	Designation	Compound	Zero point corrected energy (Hartree)
N01		-1335.921974	N08		-1781.781900
N02		-1335.917471	N09		-1781.786305
N03		-1335.915537	N10		-1930.203428
N04		-1484.335334	N11		-1930.180785
N05		-1484.329410	N12		-1930.196797
N06		-1484.321699	N13		-2227.644560
N07		-1781.797143	N14		-2376.037617

Table S2. Significant bond lengths of the molecules obtained from the optimized geometry at B3LYP/6-31G(d,p) level

Bond	N01	N04	Bond	N07	N10	Bond	N13	N14
N1-N3	1.3895	1.4979	N1-N3	1.3909	1.5340	N1-N3	1.3880	1.5705
C3-N4	1.4623	1.4716	C3-C4	1.4906	1.4935	C3-C4	1.5008	1.5086
C2-N5	1.4338	1.4390	C4-N4	1.5583	1.5469	C4-N4	1.5933	1.5769
C1-C4	1.4904	1.4929	C4-N5	1.5641	1.5831	C4-N5	1.5507	1.5525
C4-N6	1.5512	1.5536	C4-N6	1.5666	1.5596	C4-N6	1.5613	1.5860
C4-N7	1.5584	1.5568	C2-N7	1.4317	1.4388	C2-C6	1.4973	1.5040
C4-N8	1.5477	1.5449	C1-C5	1.4911	1.4927	C6-N10	1.6065	1.5454
			C5-N8	1.5521	1.5543	C6-N11	1.5399	1.6009
			C5-N9	1.5479	1.5470	C6-N12	1.5433	1.5421
			C5-N10	1.5579	1.5563	C1-C5	1.5080	1.5055
						C5-N7	1.5961	1.5777
						C5-N8	1.5465	1.5681
						C5-N9	1.5459	1.5323

Table S3. Energy, zero point correction (ZPE), thermal correction to energies (ET) and enthalpies (HT) of the optimized structures using B3LYP/6-31G(d,p)

Molecule	Energy (Hartree)	ZPE (Hartree)	(ET) (Hartree)	(HT) (Hartree)
N01	-1343.244965	0.126667	0.146195	0.147139
N04	-1492.3621715	0.110800	0.131630	0.132575
N07	-1791.5146648	0.158572	0.184384	0.185328
N10	-1940.6253325	0.142487	0.169647	0.170591
N13	-2239.7481494	0.190024	0.221930	0.222874
N14	-2388.8548143	0.173637	0.207027	0.207971
RDX	-897.4172154	0.142947	0.155461	0.156405

Received: July 25, 2017

First published online: December 17, 2018