J. Chem. Sci. (2018) 130:104
https://doi.org/10.1007/s12039-018-1508-2
© Indian Academy of Sciences

REGULAR ARTICLE

Computational assessment of energetic salts containing 7*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazole

AYUSHI NIRWAN and VIKAS DASHARATH GHULE*
Department of Chemistry, National Institute of Technology, Kurukshetra, Kurukshetra, Haryana 136 119, India
E-mail: gvd@nitkkr.ac.in

MS received 8 January 2018; revised 29 May 2018; accepted 1 June 2018; published online 24 July 2018

Abstract. The computational design of energetic salts based on 3,6,7-triamino-7*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazol-2-ium (cation A) and 3,7-diamino-7*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazol-2-ium (cation B) is described. Selective energetic anions have been combined with these cations to tune the performance parameters. All the designed salts (A1–11 and B1–11) exhibited reasonable densities ranging from 1.54 to 1.85 g/cm^3, and positive heats of formation between 301 kJ/mol and 854 kJ/mol. The detonation properties for the A1–11 and B1–11 salts were computed using Kamlet–Jacobs method, and the corresponding values were found in the ranges of 6.12 km/s to 8.79 km/s and 15.12 GPa to 34.84 GPa. Admirable energetic performance and reasonable sensitivity indicate A4 and B4 as promising energetic salts.

Keywords. Triazole; energetic salts; detonation; power index; gurney energy.

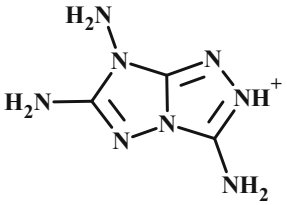
1. Introduction

High energy materials (HEMs) store a large amount of readily deliverable chemical energy in their molecular structures. HEMs include explosives, propellants, and pyrotechnics and play an important role in both military and civilian applications. HEMs with high heat of formation (HOF), enriched density, improved oxygen balance, superior detonation properties, and reduced sensitivity are always desirable. Thus, the heterocyclic rings substituted with explosophoric groups (–NO_2, –N_3, –$NHNO_2$, –ONO_2, etc.) received considerable interest in recent years for the purpose of development of the potential HEMs.[1–8] In general, heterocyclic compounds possess a higher oxygen balance, HOF and density than their carbocyclic analogues and are important energetic parameters for increasing the performance of HEMs. Heterocyclic compounds on decomposition release a large amount of environmentally friendly products. However, enhancement of detonation performance frequently results in decreased molecular stability and hence, more efforts are required to balance between the various energetic properties. In recent studies, the formation of energetic salts by combining nitrogen-rich heterocycles is a widely emerging area in HEMs.[8] Energetic salts with different combinations of cations and anions allow manipulating the energetic properties and also enhancing the hydrogen bonding interactions which confine enhanced density and stability. Moreover, it also provides the understanding about the influence of molecular structure on energetic properties. In pursuit of energetic salts with superior detonation properties and lower sensitivity, we are intrigued by the nitrogen-rich fused heterocycles. Recently, a variety of nitro (–NO_2) and nitrile (–CN) groups substituted anions were synthesized and combined with nitrogen-rich cations, exhibiting favorable energetic performance.[8] Cations A and B (Figure 1) were foreseen as significant precursors for energetic salts.[9–16] One of the driving forces for selecting these cations is their high nitrogen content that on decomposition produces large amounts of nitrogen gas and also helps to retain a good oxygen balance. Furthermore, the presence of amino groups in the cation can lead to a strong hydrogen bonding and will provide stability to structurally vibrant anions. Additionally, the judicious use of small anions contributes to produce salts with high density. In our effort to reduce experimental

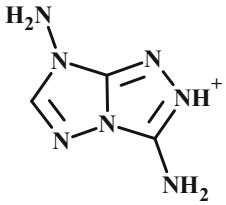
*For correspondence

Electronic supplementary material: The online version of this article (https://doi.org/10.1007/s12039-018-1508-2) contains supplementary material, which is available to authorized users.

Selected cations



A



B

Selected anions

NO_3^-	N_3^-	$N(NO_2)_2^-$	$C(NO_2)_3^-$	$N(CN)_2^-$	$C(NO_2)_2(CN)^-$
1	**2**	**3**	**4**	**5**	**6**
$C(NO_2)(CN)_2^-$	$CH(NO_2)(CN)^-$	$C(NO_2)(CN)(NO)^-$	$CH(NO_2)_2^-$	$C(CN)_3^-$	
7	**8**	**9**	**10**	**11**	

Figure 1. Molecular structures of selected cations and anions for energetic salts.

hazards, we have combined various energetic anions with nitrogen-rich cations (A and B) in a single molecule which result in new HEMs possessing a set of useful energetic properties. In the energetic salts, anions 1–11 have been identified by experimentalists as suitable ions because of their small size and excellent detonation properties.[17–20] Though the syntheses of cations and anions have been reported in the literature (Tables S1 and S2 in Supplementary Information), so far structurally similar combination of energetic salts is not established.

2. Computational

All quantum chemical computations were performed using the Gaussian 09 program[21] and the surface properties were measured using Multiwfn program.[22] The density functional theory (DFT), especially the B3PW91/6-31G(d,p) method which is proved to be a reliable and efficient tool for structure optimization and energy prediction, has been used in the present work.[23–27] The computational methods and equations used in prediction of energetic properties are similar to our previous studies[25–30] and have been summarized in the Supplementary Information.

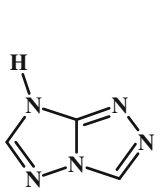
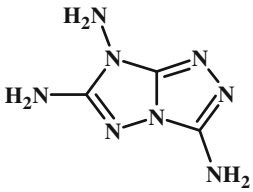
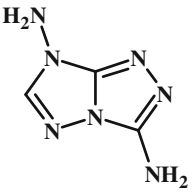
3. Results and Discussion

In the present work, the Gaussian-3 (G3) method has been used for the estimation of gas phase HOF (HOF_{Gas}) which is reported to achieve accuracy comparable with that of the experimental results.[31,32] To assess the reliability of the G3 method, HOF_{Gas} have been also calculated using G4[33] and G4(MP2)[34] composite methods for different nitrogen-rich cations and the obtained results are compared with the reported values (see Table S3). A comparison between the computed HOF_{Gas} using G3, G4, G4(MP2) methods and reported values showed the good agreement and reveals the accuracy of G3 method. The molecular structures of selected cations and anions are shown in Figure 1.

3.1 *Heat of formation*

HOF of an energetic material is related to the molecular composition and imperative for evaluating the energetic performance. HOF indicates the energy content of the HEMs and frequently governs its practical utility. The HOF values increase noticeably with the replacement of the CH groups by nitrogen atoms in the backbone due to their high-energy N–N and C–N bonds (Tables S4 and S5). The higher positive HOF values always lead to better detonation properties. The predicted HOF_{Solid} for basic skeleton (7*H*-[1,2,4]triazolo[4,3-*b*][1,2,4]triazole) of selected cations and neutral analogs of cation A and B are 360, 456, and 482 kJ/mol (Table 1). These high positive HOF_{Solid} values originate from the N–N and C–N bonds that exist in the backbone. The HOF_{Gas} for cations and anions were calculated by the G3 method, and the HOF_{Solid} for salts were obtained using Jenkins approach.[35] The details are given

Table 1. Effect of $-NH_2$ group on the nitrogen content (NC) and the HOF of the neutral analogs of cations.

			
NC (%)	64.2	72.7	70.5
HOF_{Gas} (kJ/mol)	466[a]	580[b]	583[b]
HOF_{Sub} (kJ/mol)	106	124	101
HOF_{Solid} (kJ/mol)	360	456	482

[a]Predicted using the G3 method. [b]Predicted using isodesmic reaction approach (given in Supplementary Information).

Table 2. Effect of $-NO_2$ and –CN group on the HOF of anions.

Anion	**$N(NO_2)_2^-$**		**$N(CN)_2^-$**	
	3		**5**	
HOF_{Gas} (kJ/mol)	−121		115	
Anion	**$CH(NO_2)_2^-$**		**$CH(NO_2)(CN)^-$**	
	10		**8**	
HOF_{Gas} (kJ/mol)	−216		−62	
Anion	**$C(NO_2)_3^-$**	**$C(NO_2)_2(CN)^-$**	**$C(NO_2)(CN)_2^-$**	**$C(CN)_3^-$**
	4	**6**	**7**	**11**
HOF_{Gas} (kJ/mol)	−219	−112	21	193

in the Supplementary Information (SI). The HOF_{Gas} of cations A and B are predicted using G3 method (1112 kJ/mol and 1143 kJ/mol, respectively), and isodesmic reactions (1103 kJ/mol and 1146 kJ/mol, respectively) and values are found to be comparable. The HOF_{Gas} of anions are predicted using the G3 method and found comparable with the reported results. In the case of anions, replacement of $-NO_2$ group with –CN were found to be favorable in increasing the HOF_{Gas} values and can be observed in Table 2. The HOFs of A1–11 salts range from 301 kJ/mol to 830 kJ/mol while for B1–11 it is found between 323 kJ/mol and 854 kJ/mol (Table 3). Compared with A1–11 salts, B1–11 salts possess slightly higher HOF (∼20 kJ/mol) due to higher HOF_{Gas} of cation B (1143 kJ/mol) than cation A (1112 kJ/mol). Among the designed salts, A2, A11, B2 and B11 show the HOFs above 800 kJ/mol due to high energy contribution from the corresponding cations and anions.

3.2 *Density and oxygen balance*

Density and oxygen balance (OB) are important indexes for finding the detonation performance of energetic materials as explosives. Performance of HEMs is mainly dependent on the density as the detonation parameters are roughly proportional to it.[36] In the present study, densities were predicted by using a Politzer approach[37] and range from 1.54g/cm^3 to 1.85g/cm^3 (Table 3). Salts A4 (1.84g/cm^3) and B4 (1.85g/cm^3) are the densest of these compounds and superior to the commonly used RDX (1.80g/cm^3). Even though in anions, –CN group helps in improving HOF over $-NO_2$ group but shows a reverse trend in density and OB. Hence the –CN containing salts show lower density compared to its –CN analogs and can be observed in salts containing anion 3 and 5, anion 8 and 10, anion 4 and 6, and in anion 7 and 11. OB reveals the availability of oxygen in the molecular structure for combustion of carbon to CO_2 and hydrogen to H_2O and provides significant information on the gases present in combustion products. The positive or less negative OB values ensure higher exothermicity during combustion and detonation process. All the designed salts (A1–11 and B1–11) show negative oxygen balance in the range of −27% (B4) to −118% (B11) and represent oxygen deficiency (see Table 3). The three $-NO_2$ groups in A4 and B4 salts helps to achieve good oxygen balance in these salts. Overall, salts with similar anion in A and B series reveal minor deviation in density and OB values.

Table 3. Oxygen balance, HOF and density for designed salts.

Salt	OB (%)	HOF_{cation} (kJ/mol)	HOF_{anion} (kJ/mol)	HOF_{salt} (kJ/mol)	Density (g/cm^3)
A1	−47.9	1112	−309	301	1.69
A2	−77.2	1112	198	808	1.55
A3	−33.7	1112	−121	507	1.77
A4	−28.9	1112	−219	424	1.84
A5	−97.7	1112	115	739	1.56
A6	−53.3	1112	−112	528	1.75
A7	−81.5	1112	21	661	1.65
A8	−80.0	1112	−62	567	1.62
A9	−62.5	1112	−19	617	1.70
A10	−49.2	1112	−216	414	1.73
A11	−114.3	1112	193	830	1.55
B1	−47.5	1143	−309	323	1.69
B2	−79.1	1143	198	829	1.54
B3	−32.5	1143	−121	530	1.78
B4	−27.6	1143	−219	448	1.85
B5	−101.0	1143	115	762	1.55
B6	−53.3	1143	−112	552	1.75
B7	−83.2	1143	21	685	1.65
B8	−81.8	1143	−62	590	1.62
B9	−63.0	1143	−19	641	1.70
B10	−49.0	1143	−216	438	1.73
B11	−118.3	1143	193	854	1.54

3.3 *Performance properties*

Detonation velocity (D), pressure (P), heat of detonation (Q), Power Index (PI), Gurney energy ($\sqrt{2E}$), the heat of combustion (ΔH_c), and isochoric flame temperature (T_v) are the main parameters in assessing the performance and efficiency of detonating explosive. The predicted performance properties are listed in Table 4. The D and P values represent the potential and effectiveness of HEMs and these are a function of molecular structure, which controls density, oxygen balance and HOF. The Q values were determined using Kamlet–Jacobs method[36] by the HOF difference among products and explosives according to exothermic reactions. Q expresses the chemical energy in the detonation reaction which is available for mechanical work. All the designed salts, except A5, A7, A8 and A11, reveal Q values higher than TNT (1043 cal/g) and RDX (1138 cal/g), while B3 and B4 exhibit the highest Q values (>1400 cal/g). The calculated values of D range from 6.08 km/s to 8.79 km/s while the values of P were observed between 14.86 GPa and 34.84 GPa. Upon comparing the D and P values of A4 and B4 with RDX (D = 8.60 km/s and P = 33.9 GPa), it appears that these are slightly better due to their superior densities (Figure 2). Furthermore, most of the designed salts reveal better performance than that of TNT (D = 6.94 km/s and P = 22.0 GPa).

The power index (PI) relative to picric acid is obtained *via* the method suggested by Akhavan[38] In general, the higher values of Q and gas volume in combustion confirm the greater power index. The predicted results of PI reveal that salts B2 (165%) and B3 (165%) are close to RDX (169%) while most of the other salts are better than picric acid (100%) and TNT (116%). Gurney velocity is a useful property of detonating explosive representing the energy output and calculated using the Kamlet–Finger (K–F) method[39] and Hardesty–Kennedy (H–K) method.[40] $\sqrt{2E}$ obtained from both these methods resulted in comparable values. The $\sqrt{2E}$ values of A1–11 salts lie in the range 2.22 km/s to 2.83 km/s, while for B1-11 salts they are found in the range 2.21 km/s to 2.85 km/s. $\sqrt{2E}$ of A4 (2.83 km/s) and B4 (2.85 km/s) are close to RDX (2.93 km/s) while most of other salts perform better than TNT (2.37 km/s) (Figure 2). The heat of combustion (ΔH_c) is predicted for the designed salts to take an account of the maximum heat released during combustion, ensuring the complete oxidation of C and H present in the molecular framework to CO_2 and H_2O, respectively.[41] The combustion products of salts are summarized in Supplementary Information (Table S12). All the designed salts resulted in high ΔH_c values than RDX (2255 cal/g) due to the presence of more C and H atoms in their molecular framework. The maximum temperature of the gaseous combustion products raised after explosion is important to represent the power

Table 4. Calculated performance parameters for salts of cations A and B.

Salt	D (km/s)	P (GPa)	Q (cal/g)	Explosive Power ($kJdm^3/g^2$)	Power Index (%)	Gurney Energy (km/s)		ΔH_c (cal/g)	T_V (°C)
						K–F method	H–K method		
A1	7.78	25.90	1156	3904	145	2.64	2.63	2718	3003
A2	7.16	20.73	1173	4196	155	2.49	2.5	3608	3065
A3	8.44	31.32	1329	4253	157	2.82	2.78	2448	3918
A4	8.68	33.93	1381	4214	156	2.87	2.83	2338	4201
A5	6.48	17.03	970	3045	113	2.25	2.32	3992	2560
A6	7.87	27.03	1236	3743	138	2.64	2.64	3249	3592
A7	7.01	20.62	1094	2008	74	2.39	2.44	3614	3043
A8	7.12	21.06	1137	3673	136	2.44	2.47	3645	2971
A9	7.60	24.76	1214	3739	138	2.57	2.58	3172	3445
A10	8.03	27.92	1271	4119	153	2.70	2.69	2864	3510
A11	6.12	15.12	965	2786	103	2.12	2.22	4457	2578
B1	7.87	26.45	1241	4027	149	2.67	2.65	2778	3483
B2	7.20	20.85	1268	4483	166	2.50	2.51	3748	3345
B3	8.56	32.30	1411	4482	166	2.86	2.81	2483	4225
B4	8.79	34.84	1453	4379	162	2.90	2.85	2363	4485
B5	6.47	16.91	1041	3212	119	2.25	2.31	4145	2802
B6	7.92	27.36	1306	3835	142	2.66	2.65	2978	3844
B7	7.03	20.76	1161	3346	124	2.40	2.44	3718	3258
B8	7.16	21.28	1213	3797	141	2.45	2.48	3763	3192
B9	7.65	25.05	1286	3793	140	2.59	2.59	3249	3693
B10	8.09	28.40	1349	4248	157	2.73	2.70	2924	3772
B11	6.08	14.86	1029	2889	107	2.11	2.21	4626	2740

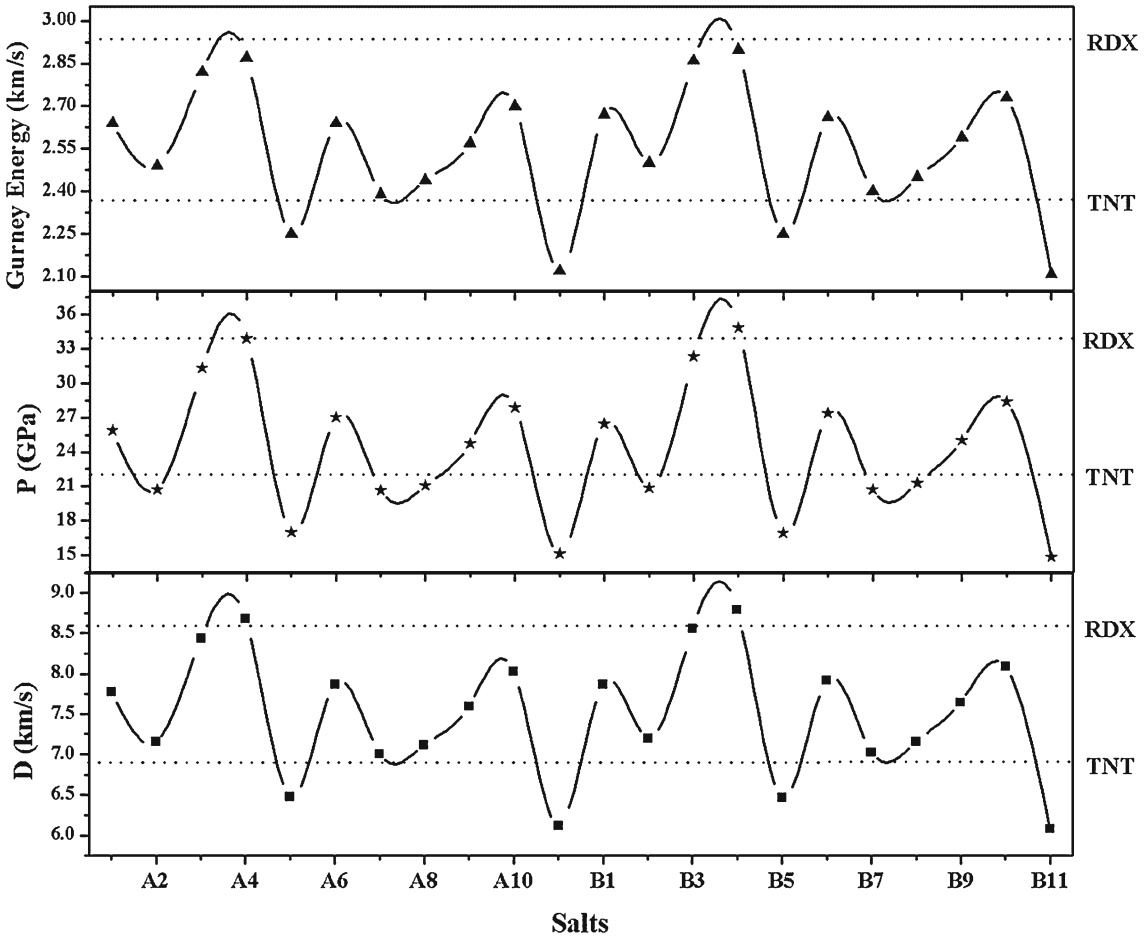


Figure 2. Comparison of performance parameters of designed salts with TNT and RDX.

of explosives.[41] In general, the maximum value of T_V denotes the higher power of that explosive. Among the designed salts, B4 displays higher flame temperature than other designed salts and RDX (4331 °C), while A3, A4, B3, B6, B9, B10 are better than that of TNT (3603 °C).

4. Conclusions

A series of energetic salts containing nitrogen-rich cations and small energetic anions have been proposed by using density functional theory. All the salts possess positive HOF range from 301 to 854 kJ/mol. Salts A1, A3, A6, A9, A10, B1, B3, B6, B9 and B10 show superior performance compared to that of TNT, while the values for A4 and B4 are better than those of RDX. Overall, salts A4 and B4 display superior performance and efforts can be made to develop these as potential HEMs.

Supplementary Information (SI)

The computational details are given in the Supplementary Information. Table S1 and S2 list the reported synthetic routes for the preparation of cations and anions. Computed HOF_{Gas} for different nitrogen-rich cations using G3, G4 and G4(MP2) methods are summarized in Table S3. Table S4–S12 presents various molecular and energetic properties calculated for designed salts. Supplementary Information is available at www.ias.ac.in/chemsci.

Acknowledgements

Authors are thankful to Young Scientists scheme in DST-SERB, Government of India (No. SB/FT/CS-110/2014) for providing financial support.

References

1. Zhang J, Dharavath S, Mitchell L A, Parrish D A and Shreeve J M 2016 Energetic salts based on 3,5-bis(dinitromethyl)-1,2,4-triazole monoanion and dianion: controllable preparation, characterization, and high performance *J. Am. Chem. Soc.* **138** 7500
2. Yin P, Zhang Q and Shreeve J M 2016 Dancing with energetic nitrogen atoms: versatile N-functionalization strategies for N-heterocyclic frameworks in high energy density materials *Acc. Chem. Res.* **49** 4

3. Zhang Q and Shreeve J M 2014 Energetic ionic liquids as explosives and propellant fuels: a new journey of ionic liquid chemistry *Chem. Rev.* **114** 10527
4. Klapötke T M and Stierstorfer J 2009 The CN_7^- anion *J. Am. Chem. Soc*. **131** 1122
5. Klapötke T M and Piercey D G 2011 1,1′-Azobis(tetrazole): a highly energetic nitrogen-rich compound with a N10 chain *Inorg. Chem.* **50** 2732
6. Haiges R and Christe K O 2013 Energetic high-nitrogen compounds: 5-(trinitromethyl)-2H-tetrazole and -tetrazolates, preparation, characterization, and conversion into 5-(dinitromethyl)tetrazoles *Inorg. Chem.* **52** 7249
7. Kommu N, Balaraju M, Ghule V D and Sahoo A K 2017 Synthetic manifestation of nitro substituted tetrazole-N-(hetero)aryl derivatives and energetic studies *J. Mater. Chem. A* **5** 7366
8. Gao Hand Shreeve J M 2011 Azole-based energetic salts *Chem. Rev.* **111** 7377
9. Yin P, Zhang J, Parrish D A and Shreeve J M 2015 Energetic fused triazoles – a promising C–N fused heterocyclic cation *J. Mater. Chem. A* **3** 8606
10. Klapötke T M, Schmid P C, Schnell S and Stierstorfer J 2015 3,6,7-Triamino-[1,2,4]triazolo[4,3-b][1,2,4]triazole: a non-toxic, high-performance energetic building block with excellent stability *Chem. Eur. J.* **21** 9219
11. Klapötke T M, Leroux M, Schmid P C and Stierstorfer J 2016 Energetic materials based on 5,5′-diamino-4,4′-dinitramino-3,3′-bi-1,2,4-triazole *Chem. Asian J.* **11** 844
12. Klapötke T M, Schmid P C, Stierstorfer J and Szimhardt N 2016 Synthesis and characterization of tetrahedral zinc(II) complexes with 3, 6,7-triamino-7*H*-[1, 2,4]triazolo[4, 3-*b*][1, 2,4]triazole as nitrogen-rich ligand *Z. Anorg. Allg. Chem.* **642** 383
13. Yin P, Zhang J, Mitchell L A, Parrish D A and Shreeve J M 2016 3,6-Dinitropyrazolo[4,3-c]pyrazole-based multipurpose energetic materials through versatile N-functionalization strategies *Angew. Chem. Int. Ed.* **55** 12895
14. Yin P, He C and Shreeve J M 2016 Fully C/N-polynitro-functionalized 2,2′-biimidazole derivatives as nitrogen- and oxygen-rich energetic salts *Chem. Eur. J.* **22** 2108
15. Tang Y, He C and Shreeve J M 2017 A furazan-fused pyrazole N-oxide via unusual cyclization *J. Mater. Chem. A* **5** 4314
16. Dharavath S, Zhang J, Imler G H, Parrish D A and Shreeve J M 2017 5-(Dinitromethyl)-3-(trinitromethyl)-1,2,4-triazole and its derivatives: a new application of oxidative nitration towards gem-trinitro-based energetic materials *J. Mater. Chem. A* **5** 4785
17. Göbel M and Klapötke T M 2007 Potassium-, ammonium-, hydrazinium-, guanidinium, aminoguanidinium-, diaminoguanidinium-, triaminoguanidinium- and melaminiumnitroformate – synthesis, characterization and energetic properties *Z. Anorg. Allg. Chem.* **633** 1006
18. Östmark H, Bemm U, Bergman H and Langlet A 2002 N-guanylurea-dinitramide: a new energetic material with low sensitivity for propellants and explosives applications *Thermochim. Acta* **384** 253
19. Tyrkov A G and Yurtaeva E A 2014 Novel transformation of ethyl cyano(dinitro)acetate in the reactions with diazomethane and diazoethane *Russ. J. Org. Chem.* **50** 902
20. Haiges R and Christe K O 2015 5-(Fluorodinitromethyl)-2H-tetrazole and its tetrazolates – preparation and characterization of new high energy compounds *Dalton Trans.* **44** 10166
21. Frisch M J, Trucks G W, Schlegel H B, Scuseria G E, Robb M A, Cheeseman J R, Scalmani G, Barone V, Petersson G A, Nakatsuji H, Li X, Caricato M, Marenich A, Bloino J, Janesko B G, Gomperts R, Mennucci B, Hratchian H P, Ortiz J V, Izmaylov A F, Sonnenberg J L, Williams-Young D, Ding F, Lipparini F, Egidi F, Goings J, Peng B, Petrone A, Henderson T, Ranasinghe D, Zakrzewski V G, Gao J, Rega N, Zheng G, Liang W, Hada M, Ehara M, Toyota K, Fukuda R, Hasegawa J, Ishida M, Nakajima T, Honda Y, Kitao O, Nakai H, Vreven T, Throssell K, Montgomery Jr J A, Peralta J E, Ogliaro F, Bearpark M, Heyd J J, Brothers E, Kudin K N, Staroverov V N, Keith T, Kobayashi R, Normand J, Raghavachari K, Rendell A, Burant J C, Iyengar S S, Tomasi J, Cossi M, Millam J M, Klene M, Adamo C, Cammi R, Ochterski J W, Martin R L, Morokuma K, Farkas O, Foresman J B and Fox D J 2013 Gaussian 09, Revision E.01, Gaussian, Inc, Wallingford
22. Lu T and Chen F 2012 Multiwfn: A multifunctional wavefunction analyser *J. Comput. Chem.* **33** 580
23. Srinivas D, Ghule V D, Muralidharan K and Jenkins H D B 2013 Tetraanionic nitrogen-rich tetrazole-based energetic salts *Chem. Asian J.* **8** 1023
24. Ghule V D 2013 Computational screening of nitrogen-rich energetic salts based on substituted triazine *J. Phys. Chem. C* **117** 16840
25. Srinivas D, Ghule V D and Muralidharan K 2014 Energetic salts prepared from phenolate derivatives *New J. Chem.* **38** 3699
26. Srinivas D, Ghule V D and Muralidharan K 2014 Synthesis of nitrogen-rich imidazole, 1,2,4-triazole and tetrazole-based compounds *RSC Adv.* **4** 7041
27. Jadhav P M, Radhakrishnan S, Ghule V D and Pandey R K 2015 Energetic salts from nitroformate ion *J. Mol. Model.* **21** 134
28. Ghule V D, Deswal S, Devi A and Tittal R K 2016 Computer-aided design of energetic tris(tetrazolyl)amine derivatives and salts *Ind. Eng. Chem. Res.* **55** 875
29. Devi A and Ghule V D 2016 Hydroxide derivatives of tetrazole: computational design approach for high-energy materials *Can. J. Chem.* **94** 738
30. Parbat P, Devi A and Ghule V D 2017 Computational assessment of nitrogen-rich peracids: a family of peroxide-based energetic materials *RSC Adv.* **7** 21585
31. Curtiss L A and Raghavachari K 1998 Gaussian-3 (G3) theory for molecules containing first and second-row atoms *J. Chem. Phys.* **109** 7764
32. Curtiss L A and Raghavachari K 2002 Gaussian-3 and related methods for accurate thermochemistry *Theor. Chem. Acc.* **108** 61

33. Curtiss L A, Redfern P C and Raghavachari K 2007 Gaussian-4 theory *J. Chem. Phys.* **126** 084108
34. Curtiss L A, Redfern P C and Raghavachari K 2007 Gaussian-4 theory using reduced order perturbation theory *J. Chem. Phys.* **127** 124105
35. Jenkins H D B, Tudela D and Glasser L 2002 Lattice potential energy estimation for complex ionic salts from density measurements *Inorg. Chem.* **41** 2364
36. Kamlet M J and Jacobs S J 1968 Chemistry of detonations. I. a simple method for calculating detonation properties of C–H–N–O explosives *J. Chem. Phys.* **48** 23
37. Politzer P, Martinez J, Murray J S and Concha M C 2010 An electrostatic correction for improved crystal density predictions of energetic ionic compounds *Mol. Phys.* **108** 1391
38. Akhavan J 2004 *The Chemistry of Explosives* 2nd edn. (UK: RSC Paperbacks)
39. Kamlet M J and Finger M 1979 An alternative method for calculating gurney velocities *Combust. Flame* **34** 213
40. Hardesty D R and Kennedy J E 1977 Thermochemical estimation of explosive energy output *Combust. Flame* **28** 45
41. Venugopalan S 2015 *Demystifying explosives: concepts in high energy materials* (Amsterdam: Elsevier Inc.)