RSC Advances

PAPER

View Article Online
View Journal | View Issue

Cite this: *RSC Adv.*, 2017, 7, 21585

Computational assessment of nitrogen-rich peracids: a family of peroxide-based energetic materials†

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Received 22nd February 2017
Accepted 3rd April 2017

DOI: 10.1039/c7ra02201h

rsc.li/rsc-advances

Nitrogen-rich 5- and 6-membered compounds substituted with nitro and peracid groups were designed and investigated using density functional theory (DFT). The calculated energetic properties of peracid compounds were compared with those of some classical explosives such as TNT and RDX. The computed results show that most of the designed peracids possess large positive heats of formation (HOF) and much higher densities (1.79–1.89 g cm^{-3}). The predicted detonation properties impart performance superior to that of TNT and comparable to that of RDX. The relatively better oxygen balance results in higher heat of detonation and more gaseous combustion products. Based on the predicted energetic properties of the designed compounds, the present study emphasizes the potential of the peracid group in developing new energetic materials.

Introduction

The search and development of energetic materials with tunable properties is an unalterable goal for researchers working in this field as these materials belong to the class of hazardous materials. The importance of energetic materials in the civil and military field has led to significant growth in environmentally friendly compounds in recent years.[1–9] Furthermore, designing a new compound and estimating its energetic properties is a typical practice before synthesis to reduce the cost and associated hazardous effects.[10–13] Covalent peroxides (O–O) are classified as peracid (RC(O)OOH), perester (RC(O)OOR′), perether (ROOR′), and peracetal (ROOR′OOR) compounds.[14] TATP (triacetone triperoxide) and HMTD (hexamethylene triperoxide diamine) are known compounds of peroxide explosives containing three –O–O– linkages per molecule (see Fig. S1 in the ESI†). They are highly sensitive and brisant in nature, and their blast strength has been reported to be 88% and 60% that of TNT and RDX, respectively. In this study, we focused on the design of peracid (RC(O)OOH) group-containing explosives, which have not been widely explored. In recent studies, Klapötke *et al.*[15,16] have reported peroxide-containing explosives with reasonable sensitivity and performance and suggested the incorporation of peroxide-containing functional groups to improve the oxygen balance. Since peracid group has more oxygen atoms, it is expected that this would help in the rapid self-decomposition of a compound. In this study, we selected nitrogen-rich backbones that have been reported in the literature[1,17–22] and introduced the peracid group along with the nitro group. Herein, nitrogen-rich peracids have been described as promising energetic materials and potential propellants. Theoretical methods and correlations were used to investigate their electronic structure, heat of formation (HOF), density, performance properties, and sensitivity. We believe that our theoretical studies of peracid compounds will aid further investigations in the incorporation of peracid functionalities in energetic materials.

Results and discussion

Fig. 1 lists the molecular structures of the designed nitrogen-rich peracid compounds. For each of these, we optimized the structures and computed the surface properties at the B3PW91/6-31G (d,p) level using the Gaussian 09 (ref. 23) and Multiwfn program.[24] All of the optimized peracid structures were characterized to be true local energy minima on their potential energy surfaces without imaginary frequencies. The computational methodology used for the calculation of energetic properties is similar to that reported in our earlier studies[25–29] and has been illustrated in the ESI.† The nitro compounds **P4**, **P6**, **P10**, **P13**, **P16**, **P19**, **P25**, and **P28** have been reported in the literature[30–39] and their energetic properties were compared with those of the designed peracid analogues.

Heat of formation

The heat of formation (HOF) is an important thermochemical property for an explosive, and it plays a significant role in the prediction of the heat of explosion, heat of combustion, and

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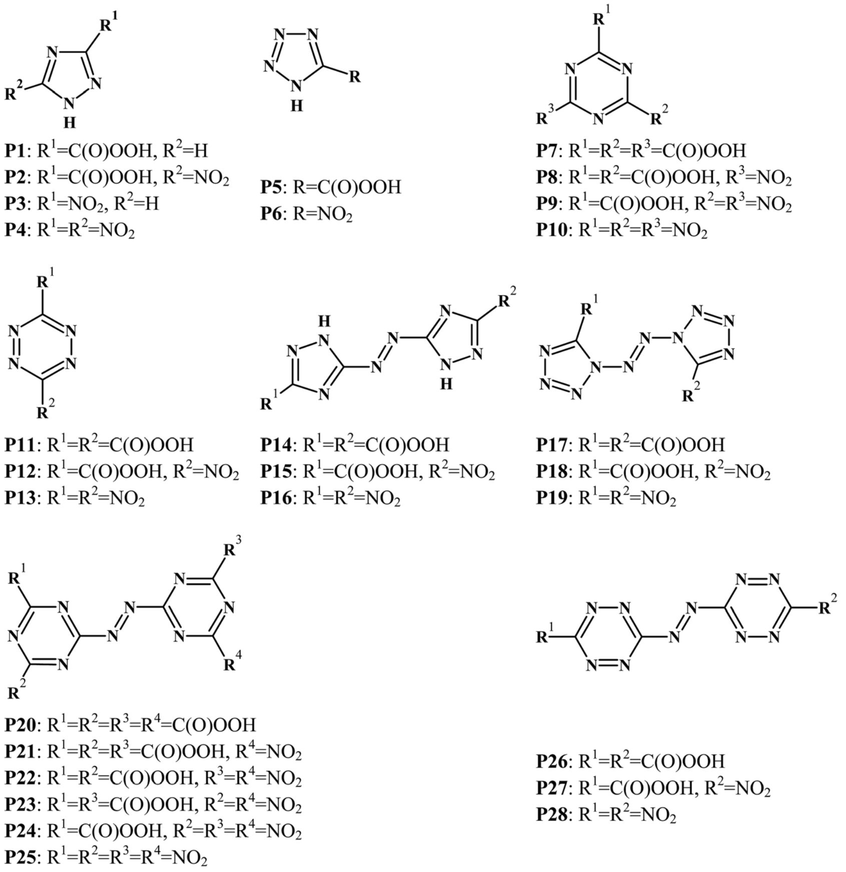
† Electronic supplementary information (ESI) available. See DOI: 10.1039/c7ra02201h



P1: R^1=C(O)OOH, R^2=H
P2: R^1=C(O)OOH, $R^2=NO_2$
P3: $R^1=NO_2$, R^2=H
P4: $R^1=R^2=NO_2$

P5: R=C(O)OOH
P6: $R=NO_2$

P7: $R^1=R^2=R^3$=C(O)OOH
P8: $R^1=R^2$=C(O)OOH, $R^3=NO_2$
P9: R^1=C(O)OOH, $R^2=R^3=NO_2$
P10: $R^1=R^2=R^3=NO_2$

P11: $R^1=R^2$=C(O)OOH
P12: R^1=C(O)OOH, $R^2=NO_2$
P13: $R^1=R^2=NO_2$

P14: $R^1=R^2$=C(O)OOH
P15: R^1=C(O)OOH, $R^2=NO_2$
P16: $R^1=R^2=NO_2$

P17: $R^1=R^2$=C(O)OOH
P18: R^1=C(O)OOH, $R^2=NO_2$
P19: $R^1=R^2=NO_2$

P20: $R^1=R^2=R^3=R^4$=C(O)OOH
P21: $R^1=R^2=R^3$=C(O)OOH, $R^4=NO_2$
P22: $R^1=R^2$=C(O)OOH, $R^3=R^4=NO_2$
P23: $R^1=R^3$=C(O)OOH, $R^2=R^4=NO_2$
P24: R^1=C(O)OOH, $R^2=R^3=R^4=NO_2$
P25: $R^1=R^2=R^3=R^4=NO_2$

P26: $R^1=R^2$=C(O)OOH
P27: R^1=C(O)OOH, $R^2=NO_2$
P28: $R^1=R^2=NO_2$

Fig. 1 Molecular structures of the peracid compounds.

other performance parameters. In the present study, HOF_{gas} was predicted using an isodesmic reaction approach with single point energies calculated at the B3PW91/6-31G(d,p) level. Detailed information of the designed isodesmic reactions, carried out to obtain HOF_{gas} of peracid derivatives, has been provided in the ESI (Fig. S2†). HOF_{solid} for all the peracid derivatives were obtained by subtracting the heat of sublimation (HOF_{sub}) from HOF_{gas}, according to the Politzer approach. Table 1 summarizes the calculated oxygen balance, nitrogen content, HOF_{gas}, HOF_{sub}, and HOF_{solid} of the peracid derivatives. It was observed that the calculated HOF_{gas} of **P6**, **P13**, **P19**, and **P25** are close to the reported values, indicating that our calculated results are reliable. Compared with other nitrogen-rich peracid derivatives, **P27** has an extremely high HOF_{solid} of 867 kJ mol^{-1}, may stem from the rich N–N and C–N bonds of the s-tetrazine ring and azo bond in the compound. All the peracid substituted derivatives possess lower HOF_{solid} when compared to the corresponding nitro derivatives, indicating that the peracid groups decrease the HOF. We observed that the peracid group was unfavourable for increasing the HOF, resulting in the negative values. All the designed peracid derivatives possess negative HOF_{solid} except for **P12**, **P15**, **P17**, **P18**, **P24**, **P26**, and **P27**. Among **P14–15** and **P17–18**, HOF_{solid} of the compounds **P17–18** were greater, owing to higher energy contribution from the tetrazole rings. This may be due to difference in the HOFs of triazine and tetrazine peracid derivatives.

Density and oxygen balance

Density is an essential physical parameter to calculate the detonation performance of an energetic material.[40–43] A higher density value also ensures the packing of more material per unit volume, thereby results in a greater explosion. The densities of the peracid derivatives were predicted using the Politzer *et al.*[44] approach (Table 1) and was found in the range of 1.79–1.88 g cm^{-3}, which were much higher than those of TNT (1.65 g cm^{-3}) and comparable to those of RDX (1.80 g cm^{-3}). Note that replacement of peracid group by nitro does not show a significant change in the density. However, nitro group has a slight advantage over peracid functionality in terms of improved density. The hydrogen atoms in peracid groups and N–H of the azole rings may help in building strong inter- and intra-molecular hydrogen bond network, thereby contributing in improving the density at the same time. It was observed that densities of triazine peracid derivatives (**P7–9** and **P20–24**) were higher than those of tetrazine peracid derivatives (**P11–12** and **P26–27**). This could be attributed to the substitution of peracid and nitro groups in triazine derivatives. Along with density, oxygen balance (OB) is also an essential parameter that indicates the index of oxygen in a compound required to convert all the carbon and hydrogen atoms into CO_2 and H_2O, respectively, releasing most of the energy. The designed peracids have a nitrogen-rich backbone,

Table 1 Calculated oxygen balance (OB, %), nitrogen content (NC, %), density (ρ, g cm^{-3}), heat of formation in gas phase (HOF$_{gas}$, kJ mol^{-1}) and solid phase (HOF$_{solid}$, kJ mol^{-1}), and heat of sublimation (HOF$_{sub}$, kJ mol^{-1}) of the peracid compounds[a]

Compd	OB (%)	NC (%)	ρ (g cm^{-3})	HOF$_{gas}$ (kJ mol^{-1})	HOF$_{sub}$ (kJ mol^{-1})	HOF$_{solid}$ (kJ mol^{-1})
P1	−56	33	1.79	−80	99	−179
P2	−18	32	1.85	−71	97	−168
P3	−42	49	1.80	192	92	100
P4	−05	44	1.87	204	88	116
P5	−25	43	1.82	58	90	−32
P6	−07	61	1.85	338 (363)[32]	74	264
P7	−28	16	1.85	−534	144	−678
P8	−20	23	1.86	−270	126	−396
P9	−10	30	1.88	−4	108	−112
P10	00	39	1.89	265	92	173
P11	−24	28	1.83	−11	103	−114
P12	−13	37	1.84	260	86	174
P13	00	49	1.85	534 (533)[34]	70	464
P14	−45	39	1.81	144	180	−36
P15	−39	47	1.83	394	166	228
P16	−31	55	1.84	645	150	495
P17	−17	49	1.83	642	157	485
P18	−09	57	1.84	934	140	794
P19	00	66	1.85	1229 (1186)[37]	123	1106
P20	−37	26	1.80	−289	303	−592
P21	−33	30	1.81	−28	283	−311
P22	−28	35	1.82	239	261	−22
P23	−28	35	1.82	237	260	−23
P24	−23	40	1.83	506	239	267
P25	−17	46	1.84	774 (770)[38]	217	557
P26	−36	45	1.80	762	184	578
P27	−30	52	1.81	1032	165	867
P28	−23	60	1.83	1304	147	1157

[a] The parenthesis values indicate the reported HOF$_{gas}$.

which is beneficial to achieve better OB. Among the designed compounds, **P10**, **P13**, and **P19** possess neutral oxygen balance, indicating that oxygen is sufficient for their complete combustion. Moreover, other compounds such as **P2**, **P4**, **P6**, **P8**, **P9**, **P12**, **P17**, **P18**, and **P25** have good OB, better than those of RDX (−21.6%) and HMX (−21.6%). The deceased C–H group in the backbone of the tetrazole peracid derivatives (**P5**, **P17**, and **P18**) helped to achieve better OB than that of the corresponding triazole derivatives (**P1**, **P14**, and **P15**). The high densities and OB were apparently ascribed to the high nitrogen content, and peracid and nitro groups in these compounds.

Performance parameters

Detonation velocity (D), pressure (P), heat of detonation (Q), explosive power (EP), power index (PI), brisance, Gurney velocity $\left(\sqrt{2E}\right)$, and heat of combustion (ΔH_c) are important measures of the performance of detonating explosives. All these performance parameters have been listed in Table 2. Fig. 2 and 3 compare the energetic properties of the peracid compounds with those of TNT and RDX. The designed peracids have detonation velocities ranging from 7.14 (**P1**) to 8.96 km s^{-1} (**P18**) and pressures were found in the range from 22.53 (**P1**) to 36.06 GPa (**P18**), which were higher than those of TNT ($D = 6.94$ km s^{-1} and $P = 22.0$ GPa). The compounds **P12** and **P18** have D and P comparable with RDX ($D = 8.60$ km s^{-1} and $P = 33.92$ GPa). Among these, **P18** has the highest D and P of 8.96 km s^{-1} and 36.06 GPa, respectively. It can be seen from Table 2 that all peracids show Q values higher than 1100 cal g^{-1}, except for **P1**, **P7**, **P14**, and **P20**. The Q values of these compounds are comparable or higher than those of the common explosives TNT (1043 cal g^{-1}) and RDX (1138 cal g^{-1}). Power index (PI) is an important parameter to represent the strength of the explosives, and it depends on the volume of the gas liberated during the explosion and the heat of detonation. In peracid derivatives, **P18** (170%) surpassed the power index of RDX (169%) due to more volume of gaseous explosion products, whereas **P2**, **P9**, **P11**, **P12**, **P17**, **P26**, and **P27** were found to be more powerful than TNT (116%). Most of the designed peracids have negative OB, eventually reducing the gaseous explosion products and performance. Detonation performance is also linked with brisance, and superior brisance indicates effectiveness of an explosion in the fragmentation of shells and casings.[45] The estimated brisance values relative to that of TNT (∼100) for peracid derivatives were found in the range from 96 to 142. Compared to TNT, designed compounds exhibited higher brisance values (except for **P1**), whereas those of **P18** and **P24** were comparable with that of RDX (140). Gurney[46] has derived a series of equations to

Table 2 Calculated detonation velocity (D, km s^{-1}), detonation pressure (P, GPa), chemical energy of detonation (Q, cal g^{-1}), explosive power (EP, kJ dm^3 g^{-2}), power index (PI, %), heat of combustion (ΔH_c, cal g^{-1}), brisance, and Gurney velocity ($\sqrt{2E}$, km s^{-1}) of peracid compounds

								$\sqrt{2E}$ (km s^{-1})	
Compd	D (km s^{-1})	P (GPa)	Q (cal g^{-1})	EP (kJ dm^3 g^{-2})	PI (%)	ΔH_c (cal g^{-1})	Brisance	K–F method[a]	H–K method[b]
P1	7.14	22.53	886	2111	78	2639	96	2.38	2.44
P2	8.15	29.97	1181	3304	122	1777	107	2.69	2.69
P3	7.84	27.28	1129	3118	115	2451	102	2.61	2.62
P4	8.76	34.78	1391	3910	145	1569	113	2.88	2.84
P5	8.02	28.72	1108	2846	105	1905	105	2.66	2.66
P6	8.90	35.72	1413	4315	160	1659	111	2.94	2.88
P7	7.66	26.45	1061	2279	84	1928	104	2.53	2.56
P8	8.02	29.06	1186	2850	106	1799	110	2.64	2.65
P9	8.44	32.40	1332	3403	126	1658	116	2.77	2.76
P10	8.87	35.89	1497	3900	144	1497	122	2.91	2.86
P11	8.16	29.80	1315	3274	121	2061	107	2.70	2.69
P12	8.63	33.49	1508	4039	150	1912	113	2.85	2.81
P13	9.17	37.90	1738	4737	175	1738	119	3.02	2.95
P14	7.52	25.12	1038	2466	91	2431	119	2.50	2.54
P15	7.85	27.60	1136	2870	106	2326	125	2.60	2.62
P16	8.18	30.07	1248	3344	124	2215	131	2.70	2.70
P17	8.57	32.91	1428	3971	147	1956	136	2.84	2.80
P18	8.96	36.06	1587	4586	170	1866	142	2.96	2.90
P19	9.38	39.63	1767	5178	192	1768	148	3.09	3.00
P20	7.38	24.17	1037	1940	72	2181	124	2.46	2.50
P21	7.60	25.70	1110	2331	86	2114	130	2.52	2.56
P22	7.83	27.40	1194	2740	101	2047	136	2.60	2.61
P23	7.83	27.40	1194	2737	101	2046	136	2.60	2.61
P24	8.08	29.25	1285	3144	116	1974	142	2.67	2.68
P25	8.34	31.27	1383	3541	131	1895	148	2.76	2.74
P26	8.08	28.98	1390	3513	130	2483	131	2.69	2.68
P27	8.39	31.33	1517	4007	148	2410	137	2.79	2.76
P28	8.76	34.35	1659	4563	169	2331	143	2.90	2.85

[a] Kamlet–Finger method [ref. 47]. [b] Hardesty–Kennedy method [ref. 48].

account the effectiveness of an explosive that will accelerate/fragment the surrounding layer of metal or other material when detonated. Gurney velocity is a useful parameter to estimate the energy output of the detonating explosive. In the present study, we used the Kamlet–Finger method[47] to calculate Gurney velocity of designed peracid derivatives. To validate the consistency of Kamlet–Finger method, Gurney velocities were also calculated using the Hardesty–Kennedy method[48] (see Table 2). It was found that both these methods resulted in comparable values. From the computed $\sqrt{2E}$ values (in Table 2), **P18** (2.96 km s^{-1}) showed highest value among the peracids and RDX (2.93 km s^{-1}) due to the higher kinetic energy of its explosion products. All the other designed peracids possess better $\sqrt{2E}$ when compared to TNT (2.37 km s^{-1}), ranging from 2.38 to 2.96 km s^{-1}. Overall, the designed peracids have performance parameters between TNT and RDX. ΔH_c mainly depends on the composition of the molecule and are required to account the total combustion energy of explosives and decomposition products. The higher oxygen balance (OB) ensures the supply of oxygen during the explosion process and results in a large amount of gaseous combustion products. In the present study, ΔH_c is predicted to account the heat released during the combustion and has been summarized in Table 2. ΔH_c values were always higher than those of Q as oxygen was supplied to the explosive and complete conversion of C and H atoms to CO_2 and H_2O occurred, respectively. The detonation products of the designed peracids have been listed in Table S4.† Among the designed peracids, **P1**, **P14**, **P15**, **P26**, and **P27** possess superior ΔH_c when compared to RDX (2255 cal g^{-1}).

Sensitivity correlations

Along with higher detonation properties, the explosive candidate should be less sensitive towards external stimuli, concomitantly improving chances for practical application. Politzer *et al.*[49] have suggested that the heat of detonation (Q) can be used to assess the sensitivity of energetic materials and sensitivity of energetic material tend to increase as Q becomes higher. The predicted Q values have been listed in Table 2, and it can be seen that **P2**, **P8–9**, **P11–12**, **P17–18**, and **P22–27** have higher Q values in comparison to TNT (1044 cal g^{-1}) and RDX (1138 cal g^{-1}), indicating their sensitivity behavior. It was observed that replacement of peracid group with the nitro group increased the sensitivity of the resultant compounds. Therefore, adjusting the peracid and nitro groups in nitrogen-

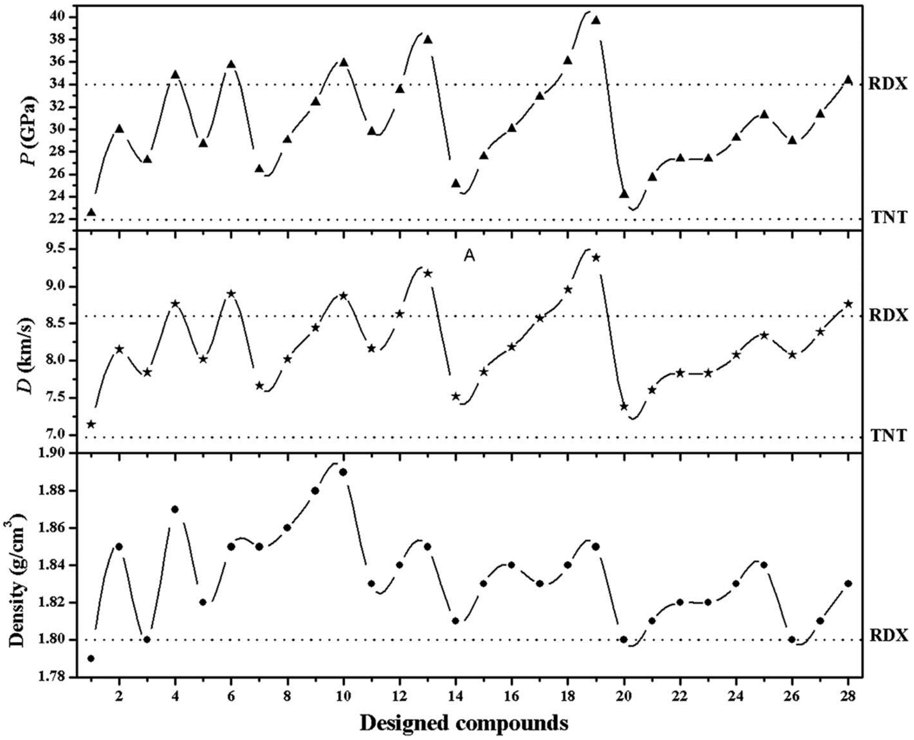


Fig. 2 Correlation between density, detonation velocity (*D*), and pressure (*P*) of the peracid compounds and their comparison with those of TNT and RDX.

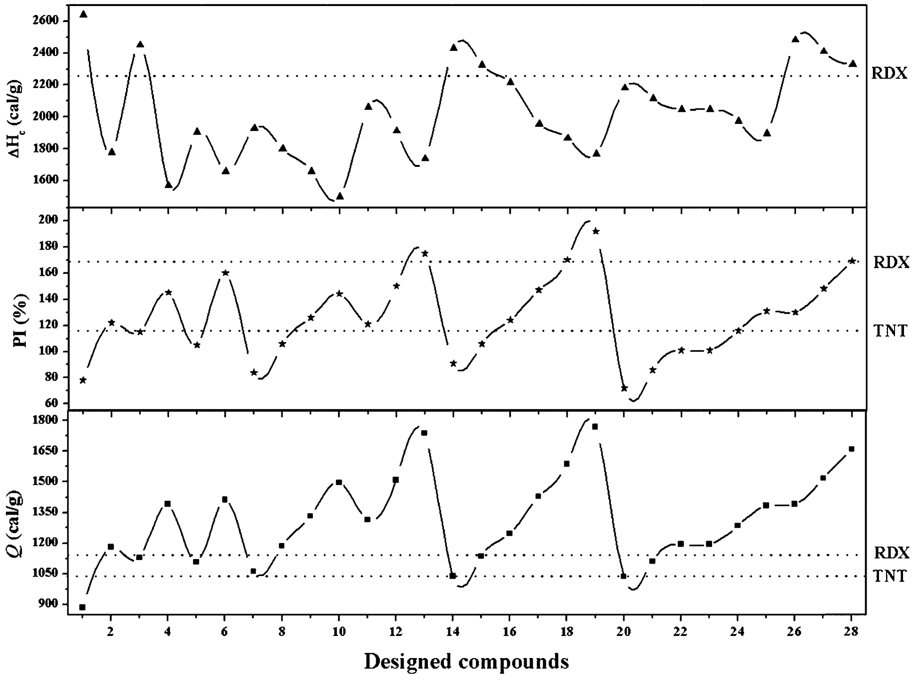


Fig. 3 The heat of detonation (*Q*), power index (PI), and the heat of explosion (ΔH_e) of the peracid compounds.

rich framework is an efficient way to reduce sensitivity without losing too much performance. However, further studies are required to understand the influence of π conjugated system on the stability of the framework.

Conclusions

In this study, 20 peracid-substituted nitrogen-rich compounds were designed, and their energetic properties were investigated using computational methods. Most of the peracid compounds showed comparable/higher density (in the range of 1.79–1.88 g cm^{-3}) than TNT and RDX. In addition, these compounds exhibited good energetic properties (detonation velocity 7.14–8.96 km s^{-1}, detonation pressure 22.5–36.0 GPa, power index 78–170%, brisance 96–142, and Gurney velocity 2.38–2.96 km s^{-1}) that surpassed those of TNT. Moreover, heat of detonation was used as the measure of sensitivity, and most of these compounds exhibited acceptable sensitive behavior. The good energetic properties imply the explosophoric nature of the peracid group and suggest its potential in designing new energetic materials.

Acknowledgements

This work was supported by the grant received from DST-SERB, Government of India (Young Scientists, No. SB/FT/CS-110/2014). Alka Devi would like to thank CSIR for research fellowship (No. 09/1050(0005) 2015-EMR-1).

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