Central European Journal of Energetic Materials
ISSN 1733-7178; e-ISSN 2353-1843

Cent. Eur. J. Energ. Mater. 2020, *17*(4): 492-505; DOI 10.22211/cejem/131687
Article is available in PDF-format, in colour, at:
http://www.wydawnictwa.ipo.waw.pl/cejem/Vol-17-Number4-2020/CEJEM_01163.pdf

Research paper

Estimation of the Detonation Pressure of Co-crystal Explosives through a Novel, Simple and Reliable Model

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Abstract: The detonation properties of energetic co-crystals have a substantial role in the design of new co-crystals and it is necessary to know about them. In this study, a linear relationship is proposed between the detonation pressure of energetic co-crystals and their molecular structures *via* a quantitative structure property relationship (QSPR) method. This model assumes that the detonation pressure of an energetic co-crystal is a function of n_N, M_w, n_C/n_H and n_O/n_H. The new model was obtained based on the calculated detonation pressures of 39 co-crystals as a training set. The R^2 or determination coefficient of the acquired model was 0.9409. This novel correlation provided a proper assessment for a further 12 energetic co-crystals as a test set. Additionally, the root mean square and average absolute deviation of this newly presented correlation were found to be 2.249 and 1.716 GPa, respectively. As a consequence, the proposed correlation can also be utilized to design new energetic co-crystals.

Keywords: energetic co-crystals, detonation pressure, QSPR approach, MLR method

Nomenclature:

AA	Anthranilic acid
ABA	Aminobenzoic acid
Ant	Anthracene
ANTA	5-Amino-3-nitro-1,2,4-triazole

3-AT	3-Amino-1,2,4-triazole
4-AT	4-Amino-1,2,4-triazole
BL	*γ*-Butyrolactone
1-BN	1-Bromonaphthalene
9-BN	9-Bromonaphthalene
BPYDL	4,4-Bipyridyl
BPYDN	4,4-Bipyridine
BTF	Benzotrifuroxane
CL-20	2,4,6,8,10,12-Hexanitrohexaazaisowurtzitane
DAT	3,4-Diaminotoluene
DBZ	Dibenzothiophene
DMB	1,4-Dimethoxybenzene
DMDBT	4,6-Dimethyldibenzothiophene
DMF	*N*,*N*-Dimethylformamide
DNB	1,3-Dinitrobenzene
DNBT	5,5'-Dinitro-3,3'-bi-1,2,4-triazole
DNDAP	2,4-Dinitro-2,4-diazapentane
DNPP	3,6-Dinitropyrazo[4,3-]pyrazole
DOX	1,4-Dioxane
DPYETA	1,2-Di(4-pyridyl)ethane
DPYETE	1,2-Di(4-pyridyl)ethene
EDNA	Ethylenedinitramine
FA	4-Fluoroaniline
HMPA	Hexamethylphosphoramide
HMX	1,3,5,7-Tetranitro-1,3,5,7-tetrazocane
MATNB	1-Methylamino-2,4,6-trinitrobenzene
NAP	Naphthalene
NNAP	Nitronaphthalene
NTO	3-Nitro-1,2,4-triazol-5-one
PA	Phenothiazine
PDA	1,2-Phenylenediamine
PDAP	4-(Phenyldiazenyl)pyridine
PDCA	1,4-Piperazinedicarboxaldehyde
Per	Perylene
Phe	Phenanthrene
PNox	2-Picoline-N-oxide
P_y	2-Pyrrolidone
PYDOXD	Pyrazine-1,4-dioxide
T_2	Thieno[3,2-b]thiophene

TATB	Triaminotrinitrobenzene
TNA	1-Amino-2,4,6-trinitrobenzene
TNAZ	1,3,3-Trinitroazetidine
TNB	1,3,5-Trinitrobenzene
TNT	2,4,6-Trinitrotoluene
TNTZ	5,6,7,8-Tetrahydrotetrazolo[1,5-b][1,2,4]-triazine
TT	Tetrathiafuvalene

1 Introduction

Energetic co-crystals are a new category in the field of energetic compounds. A co-crystal consists of two different components with a single crystalline homogenous phase that is formed *via* non-covalent interactions, such as hydrogen bonds, π-π stacking or halogen bonds, so that the properties of a co-crystal, such as morphology, thermal behaviour, sensitivity and detonation performance, are commonly different from its pure components [1-3].

The practical use of energetic materials requires an efficient balance between safety and high detonation performance, therefore the limitations and problems in the use of energetic materials must be resolved before they can become more practical in many fields. In order to improve the properties and performance of these materials some modifications, such as coating with polymers and recrystallizing from mixtures, have been recently performed [4-6]. Co-crystallization, as a new technique, is a good approach for obtaining explosives with excellent inclusive performance.

In recent years several efforts have been made to improve the performance and safety properties of common energetic compounds, such as TNT, HMX, CL-20, TATB and so on, through co-crystalization [7-16]. For example the safety of CL-20 and the detonation properties of TNT were modified through co-crystallization in a 1:1 molar ratio [7]. The sensitivities of HMX [11] and CL-20 [15] were also optimized *via* the co-crystals HMX/TATB and CL-20/TATB, respectively. The synthesis of a CL-20/HMX co-crystal, in a 2:1 molar ratio, demonstrated that the sensitivity of CL-20 could be decreased to nearly that of HMX and the detonation performance of HMX was enhanced [16].

Detonation pressure is one of the important parameters to describe the properties of an explosive. According to the Kamlet-Jacob equation, the detonation pressure is directly proportional to the velocity and density [17]. There is a relation between the structure and the properties of a compound. Therefore, a substantial point in understanding the performance of a molecule

is an assessment of its molecular structure. Because synthesizing new compounds is both time consuming and costly, the quantitative structure property relationship (QSPR) method is proposed to efficiently anticipate the physiochemical properties of a component [18]. There are many reports concerning the prediction of density, detonation properties and also the decomposition temperature of energetic compounds through the QSPR approach. For instance, the detonation performance of CHNOFCl and aluminized explosives has been predicted by a model based on the chemical structures of various compounds [19]. Furthermore, an empirical method has been proposed for predicting the detonation pressure of CHNOFCl explosives [20]. However there are few reports concerning the prediction of the properties of energetic co-crystals, because the energetic co-crystal research area is new compared to other energetic materials. The artificial neural network method has been applied to derive correlations for predicting the densities and decomposition temperatures of energetic co-crystals [21, 22]. Furthermore, the multiple linear regression method has been used to obtain new models for evaluating the detonation velocities and densities of energetic co-crystals [23, 24].

Our aim in the present study was the perception and development of a new model based on the relation between the molecular structures of selected compounds and their detonation pressures *via* the multiple linear regression method (MLR). We have also compared the computed detonation pressures of some energetic co-crystals based on this new model with those derived on the basis of the Rothstein-Petersen equation [25]. We hope that the correlation demonstrated in this work provides helpful information for the design of new energetic co-crystal with relatively ideal properties.

2 Results and Discussion

2.1 Model building

The relationship between the detonation pressure of energetic co-crystals and their molecular structures was evaluated by the MLR method. In order to derive the best model to obtain a correlation between the detonation pressures and molecular structures of energetic co-crystals, several molecular descriptors were chosen. This means that a molecular descriptor can convert a molecular structure to numerical values. The chemical structure of the compounds was obtained by using Version 16 of Chemdraw. For calculating the molecular descriptor, Dragon software [26] was applied and more than 488 descriptors, such as topology, elemental composition, functional group count, *etc.* were

selected [27, 28]. A reliable correlation was then achieved by using the most substantial and relevant descriptors on the detonation pressures of a training set. The determination coefficient thus defined was used to evaluate the reliability of the model and cross-validation was used to estimate its predictive ability. Ultimately, the model was tested for some energetic co-crystals as a test set [29, 30].

Table 1 lists the calculated data of detonation pressures of co-crystals which were selected from various references. The study illustrated that in order to derive a reliable correlation for predicting the detonation pressure of an energetic co-crystal it is essential to consider a suitable combination of the compounds. Therefore, the equation can be represented as an appropriate correlation by using the multiple linear regression method [31].

$$P(\text{GPa}) = 20.093 - 8.554\frac{n_C}{n_H} + 12.210\frac{n_O}{n_H} + 0.826n_N \ - 0.017\,Mw \qquad (1)$$

where P is the detonation pressure of the compound in GPa, n_N is the number of nitrogen atoms, M_w is the molecular weight in g·mol^{-1} of the compound, n_C/n_H is ratio of the number of carbon to hydrogen atoms and n_O/n_H is ratio of the number of oxygen to hydrogen atoms. The correlation coefficient matrix of all variables of the suggested model is shown in Table 2. As can be seen in Table 2, the values of the coefficients confirm that the variables of Equation 1 are independent and do not overlap with each other.

Table 1. Comparison of the predicted detonation pressures of energetic cocrystals with those calculated by reliable methods as a training set

No.	Name	$P_{D\,(Predicted)}$[a] [GPa]	$P_{D\,(Calc.)}$[b] [GPa]	DEV	Ref.	$P_{D\,(Calc.)}$[c] [GPa]	DEV
1	CL-20:HMX	39.28	37.50	–1.78	[16]	43.41	–5.91
2	CL-20:TATB	40.86	41.30	0.44	[15]	41.95	–0.65
3	CL-20:DNB	30.62	36.48	5.86	[34]	34.03	2.45
4	CL-20:DMF	25.14	24.40	–0.74	[39]	28.07	–3.67
5	CL-20:BL	28.21	29.50	1.29		32.66	–3.16
6	CL-20:DO	18.04	18.20	0.16		18.34	–0.14
7	CL-20:HMPA	20.48	15.00	–5.48		12.27	2.73
8	DNBT:ANTA	30.38	30.38	0.00		38.35	–7.97
9	DNBT:DNPP	31.76	31.06	–0.70	[8]	36.75	–5.69
10	DNBT:3,4-DNP	34.25	31.44	–2.81		36.46	–5.02
11	DNPP:4-AT	23.47	25.60	2.13	[35]	26.92	–1.32

No.	Name	$P_{D\ (Predicted)}$[a] [GPa]	$P_{D\ (Calc.)}$[b] [GPa]	DEV	Ref.	$P_{D\ (Calc.)}$[c] [GPa]	DEV
12	EDNA:PYDOXD	22.78	27.73	4.95	[37]	22.70	5.03
13	EDNA:BPYDN	16.00	15.24	–0.76		7.62	7.62
14	EDNA:DPYETE	17.17	17.21	0.04		10.03	7.18
15	HMX:PDA	22.24	20.20	–2.04	[39]	21.64	–1.44
16	HMX:PDCA	22.93	20.60	–2.33		23.12	–2.52
17	HMX:PNox	18.94	17.40	–1.54		15.65	1.75
18	HMX:FA	21.47	21.40	–0.07		–	–
19	HMX:DNDAP	27.27	26.90	–0.37		32.02	–5.12
20	HMX:T_2	20.29	18.90	–1.39		–	–
21	HMX:P_y	23.81	21.80	-2.01		25.08	–3.28
22	HMX:DAT	21.44	19.80	–1.64		19.86	–0.06
23	TNT:TNB	21.98	22.00	0.02	[38]	19.99	2.01
24	TNT:1-BN	9.18	12.50	3.32	[39]	–	–
25	TNT:NAP	10.98	9.81	–1.17		4.92	4.89
26	TNT:9-BN	9.18	10.70	1.52		–	–
27	TNT:Per	5.14	7.73	2.59		2.26	5.47
28	TNT:TT	11.02	9.33	–1.69		–	–
29	TNT:DBZ	8.71	8.51	–0.20		–	–
30	TNT:ABA	15.36	12.80	–2.56		10.60	2.20
31	TNT:DMB	14.32	11.70	–2.62		6.89	4.81
32	TNT:DMDBT	8.84	7.95	–0.89		–	–
33	TNT:T_2	12.11	11.20	–0.91		–	–
34	TNT:PDA	15.60	12.40	–3.20		9.66	2.74
35	TNT:Phe	8.59	8.63	0.04		3.45	5.18
36	BTF:TNA	31.16	30.60	–0.56		28.65	1.95
37	BTF:MATNB	25.84	27.60	1.76	[40]	26.27	1.33
38	BTF:(TNB)	34.24	30.50	–3.74	[39]	27.40	3.10
39	BTF:TNT	26.44	27.70	1.26		25.50	2.20
RMSD [GPa]		2.249					
AAD [GPa]		1.716					

[a] These data are predicted by our new model.

[b] These data were calculated by reliable computational methods, such as the Kamlet-Jacobs Equation, Explo5 software, *etc.*

[c] These data were calculated on the basis of the Rothstein-Petersen equation [25].

Table 2. The correlation coefficient matrix of the variables in Equation 1

Variable	$\frac{n_C}{n_H}$	$\frac{n_O}{n_H}$	n_N	M_w
$\frac{n_C}{n_H}$	1	–	–	–
$\frac{n_O}{n_H}$	0.818	1	–	–
n_N	–0.180	0.300	1	–
M_w	–0.132	0.218	0.886	1

Table 3. Standardized coefficients and some statistical parameters of Equation 1

Variable	Coefficient	Standard Error	t stat	*P*-value	Lower 95%	Upper 95%
Intercept	20.093	1.422	14.124	8.7E–16	17.202	22.984
$\frac{n_C}{n_H}$	–8.554	1.600	–5.346	6.09E–06	–11.806	–5.303
$\frac{n_O}{n_H}$	12.210	1.465	8.331	1E–09	9.232	15.189
n_N	0.826	0.156	5.287	7.27E–06	0.509	1.144
M_w	–0.017	0.003	–4.718	3.97E–05	–0.025	–0.010

2.2 Reliability and model validation

The value of R^2 or the coefficient of determination of Equation 1 was 0.9409. As may be seen in Table 1, the deviation of the detonation pressures calculated by the suggested equation from data calculated by reliable methods, was used to evaluate the reliability of this new method. As shown in Table 1, the predicted detonation pressures for the energetic co-crystals have root mean square deviations (RMSD) and average absolute deviations (AAD) of 2.249 and 1.716 GPa, respectively.

Table 3 lists the statistical parameters of Equation 1 that can be allowed when comparing the relative weights of the variables in the model. The standard error is a statistical term that can show the accuracy of the assessed coefficient and can specify the precision over repeated measurements. Furthermore, the values of *t* demonstrate the good precision of the model. The *P*-value can determine the significance of an observed effect or variation. A *P*-value less than 0.05 may prove that the observed effect due to a variation is not random and that the effect is highly significant or important. Therefore appropriate values of the statistical parameters and a relatively good R^2 value of 0.9409, confirm that

the assessment results from the new model are in good agreement with data that were calculated by several other reliable methods.

In order to investigate the predictive ability of the suggested correlation, a cross-validation method by a QSPR approach was used. Leave-one-out cross validation (Q^2_{LOO}) was utilized for checking the internal validation. Moreover, the (leave-20%-out) or (leave-many-out) cross validation (Q^2_{LMO}) was carried out as another internal validation method to confirm the new model [30]. Table 4 includes a further 12 energetic co-crystals which were utilized as a test set for checking the predictive ability of the derived equation through external validation [30]. As may be seen in Table 4, this represents a fairly good result that verifies the predictive power of the new correlation [30].

Table 4. Comparison of the predicted detonation pressures of energetic cocrystals with those calculated by reliable methods as a test set

No	Name	$P_{D\ (Predicted)}$[a] [GPa]	$P_{D\ (Calc.)}$[b] [GPa]	DEV	Ref.	$P_{D\ (Calc.)}$[c] [GPa]	DEV
1	CL-20:DNDAP	36.21	37.50	1.29	[12]	40.82	–3.32
2	CL-20:BTF	42.75	34.05	–8.70	[14]	39.11	–5.06
3	CL-20:TNT	31.04	32.30	1.26	[39]	33.80	–1.50
4	BTF:TNAZ	38.18	35.80	–2.38		33.58	2.22
5	DNPP:3-AT	23.47	23.90	0.43	[35]	27.18	–3.28
6	NTO:TNTZ	23.01	23.50	0.49	[36]	28.59	–5.09
7	EDNA:DPYETE	15.15	13.70	–1.45	[37]	4.36	9.34
8	EDNA:BPYDN	14.97	14.32	–0.65		5.93	8.39
9	EDNA:PDAP	13.05	13.75	0.70		4.44	9.31
10	TNT:AA	15.36	12.90	–2.46	[7]	10.70	2.20
11	TNT:Ant	8.59	8.17	–0.42	[39]	3.51	4.66
12	TNT:PA	9.77	9.05	–0.72		–	–
RMSD [GPa]		2.810					
AAD [GPa]		1.746					

[a] These data were predicted by our new model.
[b] These data were calculated by reliable computational methods, such as the Kamlet-Jacobs Equation, Explo5 software, *etc.*
[c] These data were calculated on the basis of the Rothstein-Petersen equation [25].

In order to evaluate the value of Q^2 of the internal validation and to better indicate the power of predictability, Roy *et al.* proposed two statistical parameters, and, which are defined by Equations 2-5 [32]:

$$\overline{r_m^2} = \frac{(r_m^2 + r_m'^2)}{2} \tag{2}$$

$$\Delta r_m^2 = |r_m^2 - r_m'^2| \tag{3}$$

$$r_m^2 = r^2 \times \left(1 - \sqrt{(r^2 - r_0^2)}\right) \tag{4}$$

$$r_m'^2 = r^2 \times \left(1 - \sqrt{(r^2 - r_0'^2)}\right) \tag{5}$$

where r^2 and r_0^2 are the squared correlation coefficients between the cross-validation predicted results and the calculated data, with and without intercept, respectively. The parameter $r_0'^2$ has the same meaning as r_0^2 but uses reversed axes.

Roy *et al.* demonstrated that for a model with a good power of predictability, the value of Δr_m^2 should be less than 0.2, and $\overline{r_m^2}$ should be more than 0.5. As demonstrated in Table 5, the values of Δr_m^2 and $\overline{r_m^2}$ were 0.000 and 0.899, respectively. The reliability and validation results of this regression model are summarised in Table 5. As may be seen in this table, there is little difference between Q^2_{LOO}, Q^2_{LMO}, Q^2_{EXT} and R^2 values of Equation 1, consequently the obtained correlation has good predictive power and the model is acceptable.

Table 5. Validation test results for the regression model obtained

Property	R^2	Q^2_{EXT}	Q^2_{LOO}	Q^2_{LMO}	*RMSD* [GPa]	*AAD* [GPa]	$\overline{r_m^2}$	Δr_m^2
Equation 1	0.9409	0.9679	0.9411	0.9406	2.493	1.716	0.899	0.000

The predicted values of the detonation pressures of the studied co-crystals, were also compared with the values obtained based on the Rothstein-Petersen equation, which is defined by Equations 6-8 [15, 25].

$$D = \frac{F - 0.26}{0.55} \tag{6}$$

$$F = 100 \times \frac{n_O + n_N - \left(\frac{n_H}{2n_O}\right) + \left(\frac{\alpha}{3}\right) - \left(\frac{n_\beta}{1.75}\right) - \left(\frac{n_\gamma}{2.5}\right) - \left(\frac{n_\delta}{4}\right) - \left(\frac{n_\varepsilon}{5}\right)}{Mw} - G \tag{7}$$

$$P = \rho_0 D^2 (1 - 0.713 \rho_0^{0.07}) \tag{8}$$

where D, P and ρ_0 are detonation velocity, detonation pressure and density of a compound, respectively. G is 0.4 for liquid explosives and zero for solid

explosives. The value of α is one for aromatic compounds and zero for other cases. The number of oxygen atoms in excess of those already available to form CO_2 and H_2O is shown by n_β. The number of oxygen atoms doubly and singly bonded directly to carbon are illustrated by n_γ and n_δ, respectively. Finally the number of nitrato groups, existing either in a nitrate ester configuration or as a nitric acid salt, is shown by n_ε. As can be seen from Tables 1 and 4, the new model is simple, reliable and user-friendly in comparison to previous methods.

Lin *et al.* [33] studied the structure and properties of several HMX/LLM-105 complexes as co-crystal explosives. The average predicted detonation pressure for seven HMX/LLM-105 complexes which were estimated by them was 35.99 GPa. The predicted detonation pressure for a HMX/LLM-105 co-crystal using the new model was 30.48 GPa. This result confirms the compatibility of the new method with the method based on Monte Carlo simulation.

Figure 1 displays the relation between the predicted detonation pressures of the studied energetic co-crystals with those calculated by reliable methods. From this figure, it is evident that the new predicted correlation shows a suitable linear fit to the reliable calculated data for both the training and test sets.

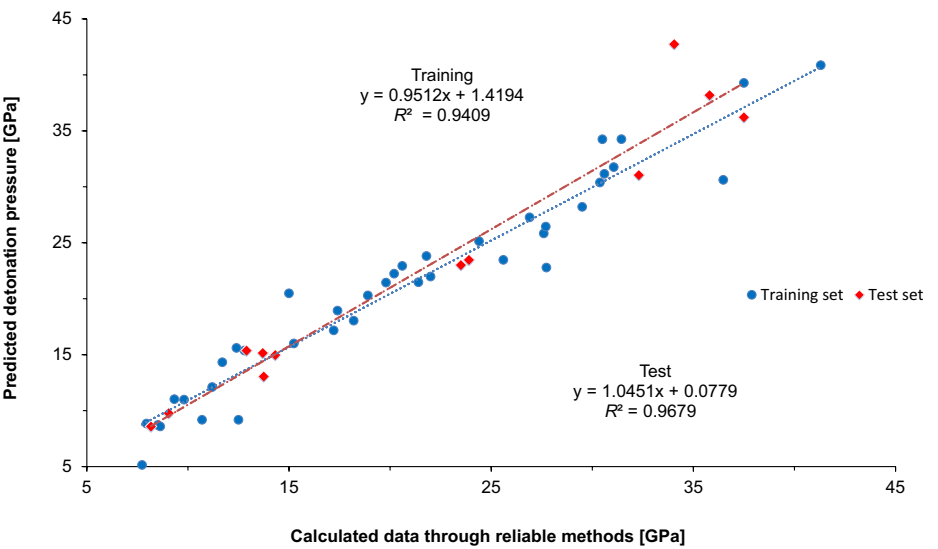

Figure 1. Predicted detonation pressure of energetic cocrystals *vs.* calculated data for both the training and the test sets

3 Conclusions

In this study, a new reliable correlation was developed for anticipating the detonation pressure of energetic co-crystals *via* the QSPR approach. In this work, it is shown that the detonation pressure of a co-crystal is a variable of the n_N, M_w, n_C/n_H and n_O/n_H values. Due to the appropriate statistical results ($R^2 = 0.9409$, $Q^2_{LOO} = 0.9411$, $Q^2_{LMO} = 0.9406$, $Q^2_{EXT} = 0.9679$), the new predicted correlation has an accurate performance and reliability for predicting the detonation pressure of new energetic co-crystals. The validity of the model was also studied via external and internal validation. However, there was little difference between the values of Q^2_{LOO}, Q^2_{LMO}, Q^2_{EXT} and R^2, and the best correlation between detonation pressure and molecular structure of energetic co-crystals was proposed through a multilinear regression (MLR) method. It is hoped that the new simple model will help chemists to design new energetic co-crystals with ideal performance.

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Received: September 4, 2020
Revised: December 15, 2020
First published online: December 28, 2020