

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* 2020, 17(1): 31-48.

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Research paper

Prediction of the Density of Energetic Co-crystals: a Way to Design High Performance Energetic Materials

Narges Zohari*, **Faezeh Ghiasvand Mohammadkhani**

Faculty of Chemistry and Chemical Engineering, Malek-ashtar University of Technology, Tehran, Iran

* E-mail: nargeszohari@gmail.com

Content

Table S1. Computed variables of Equation 1 for all of the investigated co-crystals

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Table S1. Computed variables of Equation 1 for all of the investigated co-crystals

No.	Name	<i>sp</i>	<i>OB</i>	<i>DU</i>	<i>n</i> _{AT}
1	CL-20:HMX	58.16	-13.64	23	100
2	CL-20:Trinitrotoluene (TNT)	34.75	-32.46	16	57
3	CL-20:Dinitrobenzene (DNB)	31.83	-34.30	15	52
4	CL-20:Benzotrifuroxane (BTF)	33.72	-20.86	19	54
5	CL-20:1,3,5-Triamino-2,4,6-trinitrobenzene (TATB)	78.48	-18.31	34	132
6	CL-20:7 <i>H</i> -tris-1,2,5-Oxadiazolo[3,4-b:3',4'-d:3'',4''-f] azepine	30.53	-55.71	13	50
7	CL-20:Benzoquinone	29.67	-43.93	14	48
8	CL-20:Naphthoquinone	34.43	-64.39	17	54
9	HMX:1,3-Dimethyl-2-imidazolidinone	26.19	-70.18	6	46
10	HMX:2,4-Dinitro-2,4-diazapentane	36.40	-40.99	7	66
11	HMX:N-Methylpyrrolidone	25.19	-70.82	6	44
12	HMX:N,N-Dimethylformamide (DMF)	22.42	-54.16	5	40
13	HMX:Pyridine-N-oxide	23.66	-63.38	8	40
14	TNT:Nitronaphtalene (NNAP)	27.71	-127.89	14	41
15	TNT:Trinitrobenzene (TNB)	25.25	-65.41	13	39
16	NNAP:Trinitrophenol	26.40	-111.36	14	39
17	1,3,3-Trinitroazetidine:Benzotrifuroxane (BTF)	22.23	-28.81	13	35

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Table S1. Continuation

No.	Name	<i>sp</i>	<i>OB</i>	<i>DU</i>	<i>n</i> _{AT}
18	Diacetonediperoxide (DADP):1,3,5-Tribromo-2,4,6-trinitrobenzene (TBTNB)	28.19	-53.51	8.5	40
19	DADP:1,3,5-Triiodo-2,4,6-trinitrobenzene(TITNB)	32.11	-43.30	8.5	40
20	3,4-Dinitro-1 <i>H</i> -Pyrazole:5,5'-Dinitro-2 <i>H</i> ,2 <i>H'</i> -3,3'-Bi-1,2,4-triazole	27.74	-32.45	16	44
21	Ammonium perchlorate:Benzo-18-Crown-6	33.07	-133.98	3.5	56
22	Ethylenedinitramine (EDNA):4,4-Bipyridyl	25.66	-154.05	10	40
23	EDNA:1,2-Di(4-pyridyl)ethane	28.18	-165.32	9	45
24	EDNA:1,2-Di-4-pyridylethene	24.15	-129.21	10	38
25	EDNA:Pyrazine-1,4-dioxide	16.28	-67.12	5	28
26	TNB:NNAP	25.94	-120.11	14	38
27	TNB:BTF	24.22	-46.43	16	36
28	TNB:TITNB	43.20	-33.04	20.5	54
29	5,5'-Dinitro-3,3'-bi-1,2,4-triazol (DNBT): 5-Amino-3-nitro-1,2,4-triazole (ANTA)	25.94	-39.64	14	42
30	DNBT:3,6-Dinitropyrazo[4,3-]pyrazole (DNPP)	21.91	-37.71	14	34
31	DNBT:3,4-Dinitropyrazole (3,4-DNP)	27.74	-32.45	16	44
32	DNPP:3-Amino-1,2,4-triazole (3-AT)	22.37	-74.25	11	36
33	BTF:TNT	25.99	-55.08	16	39

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No.	Name	<i>sp</i>	<i>OB</i>	<i>DU</i>	<i>n</i> _{AT}
34	BTF:1,3,3-Trinitroazetidine (TNAZ)	22.23	-28.81	13	35
35	BTF:1-Amino-2,4,6-trinitrobenzene (TNA)	25.23	-46.64	16	38
36	BTF:1-Methyl-amino-2,4,6-trinitrobenzene (MATNB)	26.99	-55.03	16	41
37	CL-20: <i>N,N</i> -Dimethylformamide (DMF)	34.72	-54.75	10	60
38	CL-20:γ-Butyrolactone (BL)	28.43	-36.62	11	48
39	CL-20:1,4-Dioxane	53.04	-87.01	10	92
40	CL-20:Hexamethylphosphoramide (HMPA)	72.96	-103.28	5.5	123
41	HMX:1,2-Phenylenediamine (PDA)	25.98	-79.14	8	44
42	HMX:1,4-Piperazinedicarboxaldehyde (PDCA)	27.65	-69.35	7	48
43	HMX:2-Picoline-N-oxide	35.16	-102.63	11	58
44	HMX:4-Fluoroaniline (FA)	24.91	-74.63	8.5	42
45	HMX:Thieno[3,2-b]thiophene (T2)	26.50	-65.99	9	40
46	HMX:2-Pyrrolidone (Py)	23.42	-60.84	6	41
47	HMX:3,4-Diaminotoluene (DAT)	27.74	-87.96	8	47
48	TNT:1-Bromonaphthalene (1-BN)	27.91	-125.28	13.5	39
49	TNT:Naphthalene (NAP)	26.56	-155.35	13	39

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No.	Name	<i>sp</i>	<i>OB</i>	<i>DU</i>	<i>n</i> _{AT}
50	TNT:9-Bromonaphthalene (9-BN)	27.91	-125.28	13.5	39
51	TNT:Anthracene (Ant)	31.32	-171.69	16	45
52	TNT:Perylene (Per)	38.08	-188.54	21	53
53	TNT:Tetrathiafulvalene (TT)	27.62	-90.84	11	35
54	TNT:Dibenzothiophene (DBZ)	30.20	-149.73	15	42
55	TNT:Aminobenzoic acid (ABA)	24.71	-114.19	11	38
56	TNT:Anthranilic acid (AA)	24.71	-114.19	11	38
57	TNT:1,4-Dimethoxybenzene (DMB)	26.23	-129.20	10	41
58	TNT:4,6-Dimethyldibenzothiophene (DMDBT)	33.73	-162.01	15	48
59	TNT:Phenothiazine (PA)	31.21	-146.33	15	44
60	TNT:Thieno[3,2-b]thiophene (T2)	24.33	-106.70	11	33
61	TNT:1,2-Phenylenediamine	23.81	-126.45	10	37
62	TNT:Phenanthrene (Phe)	31.32	-171.69	16	45

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