

Supporting Information is available in PDF-format at:

<https://ipo.lukasiewicz.gov.pl/wydawnictwa/cejem-woluminy/vol-19-nr-1/>



Supporting Information is available under the Creative Commons Attribution-NonCommercial-NoDerivs 3.0 license CC BY-NC-ND 3.0.

Supporting Information

Please note:

- 1) The publisher is not responsible for the content of the section Supporting Information.
- 2) Any queries should be directed to the corresponding Author mentioned below.

Research paper

Assessment of the Thermal Decomposition Temperature of High-Energy Heterocyclic Aromatic Compounds in Order to Increase Their Safety during Storage, Handling, and Application

Mohammad Hossein Keshavarz^{*}, Sajjad Mousavi, Masoumeh Drikvand

Faculty of Applied Sciences, Malek-Ashtar University of Technology, Iran

** E-mail: mhkeshavarz@mut-es.ac.ir*

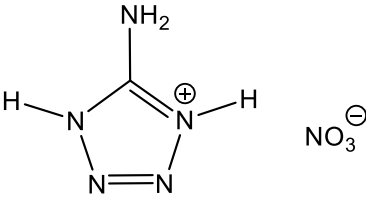
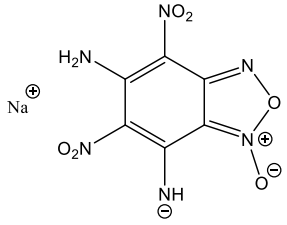
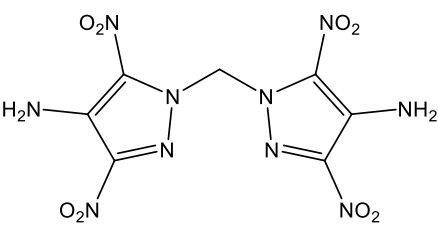
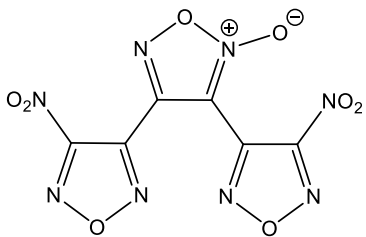
Table S1. The estimated outputs of Equations 1 and 5 for the training set of heterocyclic aromatic compounds and some of their salts. pp. 2-25

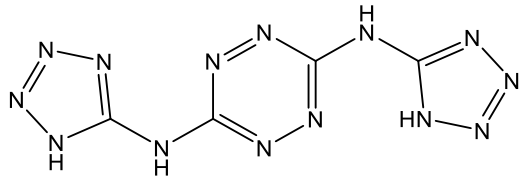
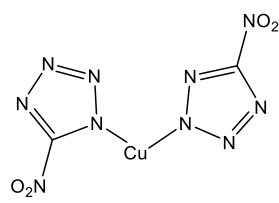
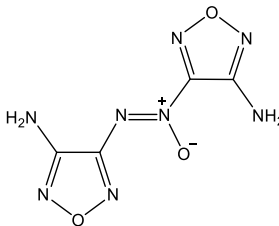
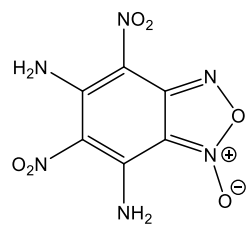
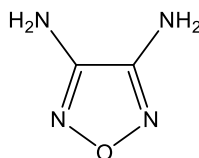
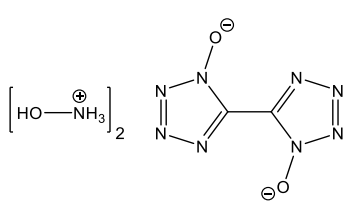
Table S2. The estimated outputs of Equations 1 and 5 for the test set of heterocyclic aromatic compounds and some of their salts. pp. 26-35

Table S3. Index, in alphabetical order, of compounds used in Tables S1 and S2. pp. 36-42

Table S1. The estimated outputs of Equations 1 and 5 for the training set of heterocyclic aromatic compounds and some of their salts

Note: The predicted results of the model by Zohari et al. [18] for azole compounds are given here. The molecular structures of different types of heterocyclic aromatic compounds and some of their salts are also added to this table.

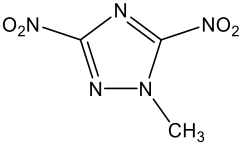
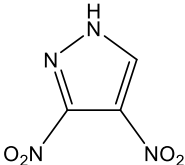
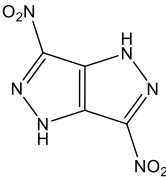
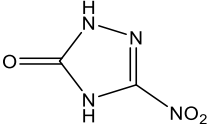
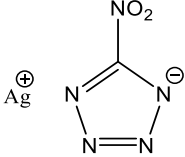
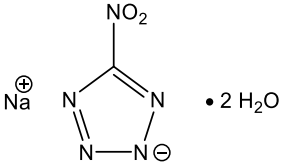
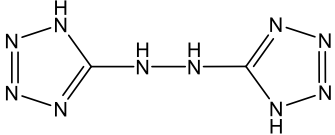
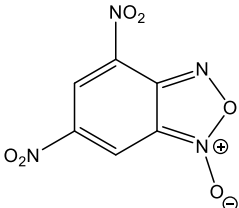
No.	Name and Structure	[4, 18]	Eq. 1	%Dev	Eq. 5	%Dev	[18]	%Dev
1	5-Aminotetrazolium nitrate 	466.00	468.00	0.43	462.00	-0.86	-	-
2	5,7-Diamino-4,6-dinitrobenzofuroxan dihydrate, sodium salt 	542.00	533.00	-1.66	530.00	-2.21	-	-
3	Bis(3,5-dinitro-4-aminopyrazolyl)methane 	583.00	540.00	-7.38	580.00	-0.51	273.66	-12.70
4	Bis(nitrofuranzono)furoxan 	521.00	476.00	-8.64	514.00	-1.34	-	-

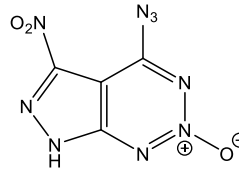
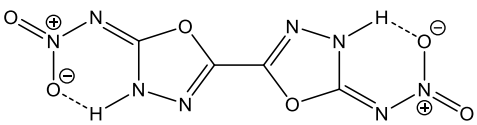
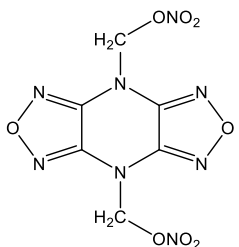
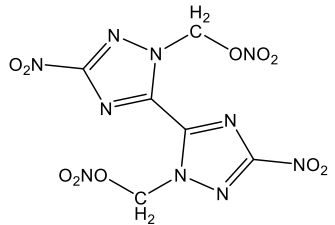
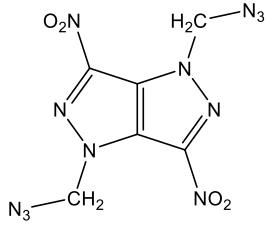
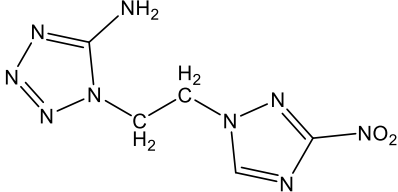
5	3,6-Bis(1 <i>H</i> -1,2,3,4-tetrazol-5-yl-amino)- <i>s</i> -tetrazine 	594.00							
6	Copper(I) 5-nitrotetrazolate 	576.00	574.00	-0.35	571.00	-0.87	-	-	
7	3,3'-Diamino-4,4'-azoxyfuran 	522.00	480.00	-8.05	519.00	-0.57	-	-	
8	5,7-Diamino-4,6-dinitrobenzofuroxan 	563.00	545.00	-3.20	542.00	-3.73	-	-	
9	3,4-Diaminofurazan 	518.00	541.00	4.44	538.00	3.86	277.01	-8.64	
10	Dihydroxylammonium 5,5'-bitetrazole-1,1'-dioxide 	494.00	485.00	-1.82	480.00	-2.83	-	-	

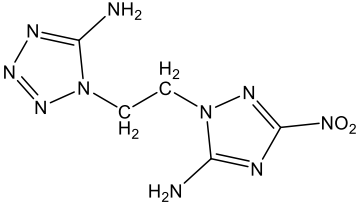
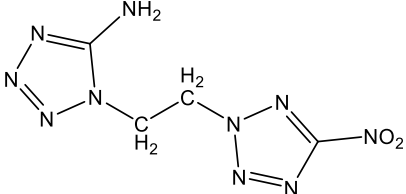
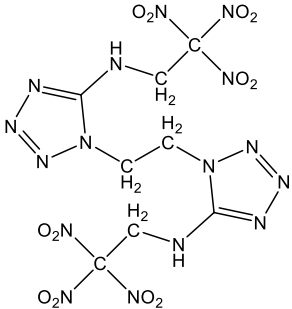
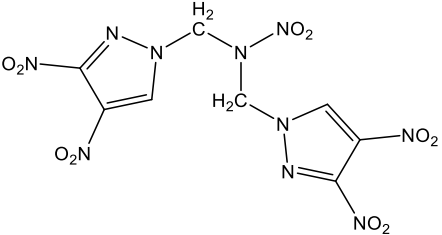
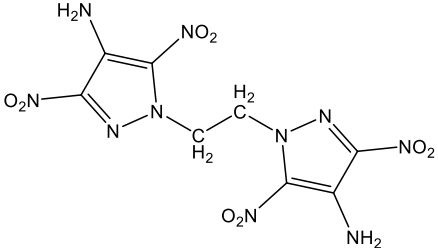
Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

11	Dinitromethyltriazole 	534.00	474.00	-11.24	530.00	-0.75	273.9	-10.10
12	3(5),4-Dinitropyrazole 	549.00	518.00	-5.65	558.00	1.64	274.79	-6.70
13	3,6-Dinitropyrazolo[4,3-c]pyrazole 	606.00	557.00	-8.09	616.00	1.65	274.8	-9.56
14	3-Nitro-1,2,4-triazole-5-one 	537.00	518.00	-3.54	545.00	1.49	274.64	-13.62
15	Silver nitrotetrazolate 	527.00	532.00	0.95	528.00	0.19	-	-
16	Sodium 5-nitrotetrazolate dihydrate 	473.00	470.00	-0.63	464.00	-1.90	-	-
17	5,5'-Bis(1H-tetrazolyl)hydrazine 	481.00	513.00	6.65	509.00	5.82	278.97	-3.21
18	4,6-Dinitrobenzofuroxan 	518.00	554.00	6.95	551.00	6.37	-	-

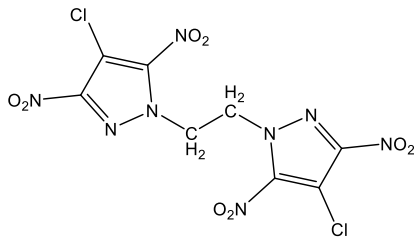
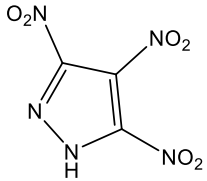
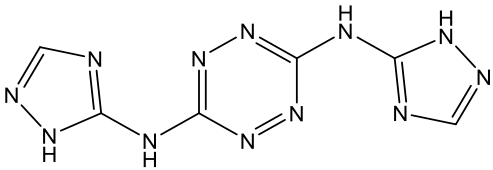
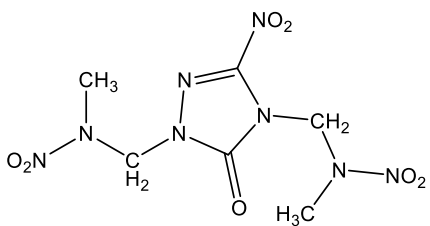
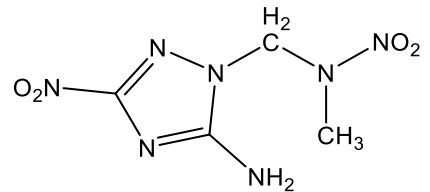
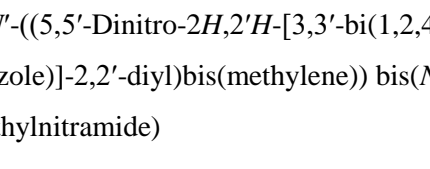
19	6-Nitro-7-azido-pyrazol[3,4-d][1,2,3]triazine-2-oxide 	433.00	462.00	6.70	435.00	0.46	273.61	26.56
20	[2,2'-Bi(1,3,4-oxadiazole)]-5,5'-dinitramide 	484.00	467.00	-3.51	470.00	-2.89	-	-
21	Bis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine-4,8-diylbis(methylene) dinitrate 	469.00	399.00	-14.93	462.00	-1.49	274.64	1.60
22	(5,5'-Dinitro-2 <i>H</i> ,2' <i>H</i> -[3,3'-bi(1,2,4-triazole)]-2,2'-diyl)bis(methylene) dinitrate 	449.00	407.00	-9.35	440.00	-2.00	275.15	-0.89
23	1,4-Bis(azidomethyl)-3,6-dinitro-1,4-dihydropyrazolo[4,3-c]pyrazole 	469.00	434.00	-7.46	468.00	-0.21	273.36	-0.12
24	1-(2-(3-Nitro-1 <i>H</i> -1,2,4-triazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine 	528.00	500.00	-5.30	539.00	2.08	275.23	-1.79

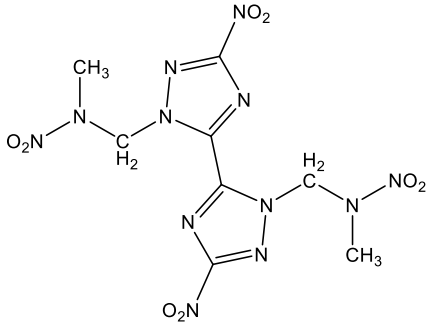
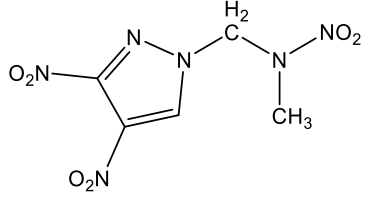
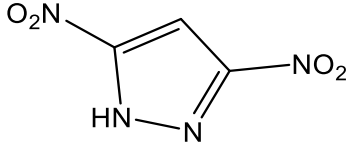
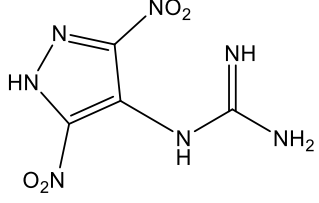
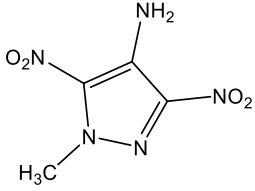
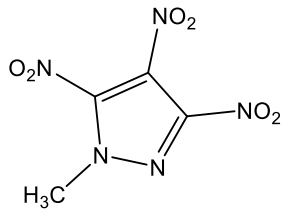
25	<p>1-(2-(5-Amino-3-nitro-1<i>H</i>-1,2,4-triazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p> 	550.00	504.00	-8.36	543.00	-1.27	274.42	-8.74
26	<p>1-(2-(5-Nitro-2<i>H</i>-tetrazol-2-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p> 	507.00	468.00	-7.69	506.00	-0.20	273.35	-3.15
27	<p>1,1'-(Ethane-1,2-diyl)bis(<i>N</i>-(2,2,2-trinitroethyl)-1<i>H</i>-tetrazol-5-amine)</p> 	456.00	402.00	-11.84	456.00	0.00	273.15	-2.26
28	<p><i>N,N</i>-Bis((3,4-dinitro-1<i>H</i>-pyrazol-1-yl)methyl) nitramide</p> 	534.00	506.00	-5.24	533.00	-0.19	273.34	-4.74
29	<p>1,1'-(Ethane-1,2-diyl)bis(3,5-dinitro-1<i>H</i>-pyrazol-4-amine)</p> 	584.00	551.00	-5.65	591.00	1.20	274.35	-5.04

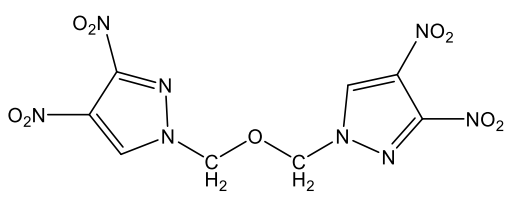
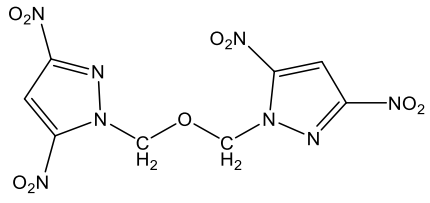
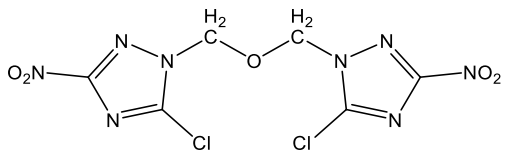
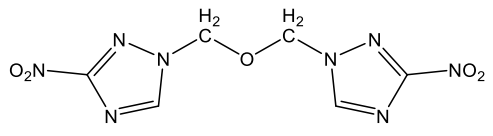
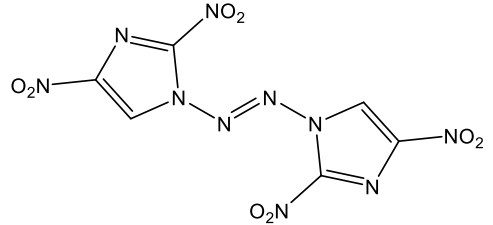
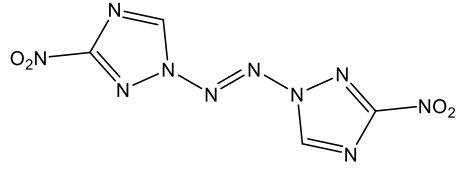
Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

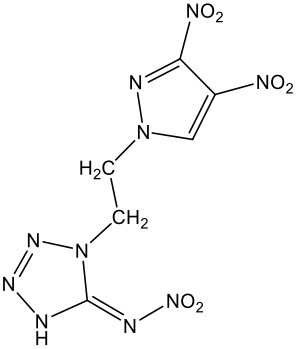
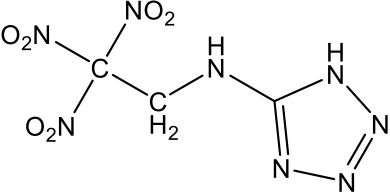
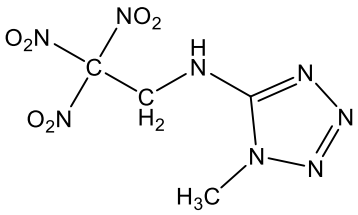
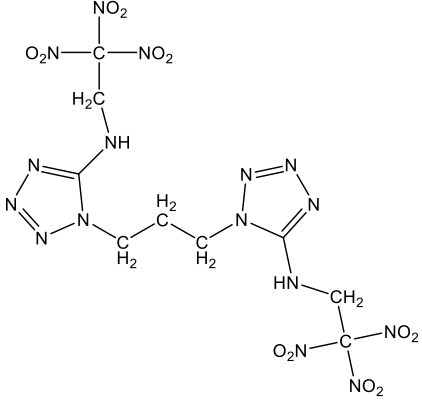
Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

30	<p>1,2-Bis(4-chloro-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)ethane</p> 	592.00	565.00	-4.56	563.00	-4.90	278.05	-0.33
31	<p>3,4,5-Trinitro-1<i>H</i>-pyrazole</p> 	531.00	478.00	-9.98	535.00	0.75	273.9	0.10
32	<p><i>N</i>³,<i>N</i>⁶-Bis(1<i>H</i>-1,2,4-triazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine</p> 	623.00	605.00	-2.89	603.00	-3.21	276.36	0.20
33	<p><i>N,N'</i>-((3-Nitro-5-oxo-1<i>H</i>-1,2,4-triazole-1,4(5<i>H</i>)-diyl)bis(methylene))bis(<i>N</i>-methylnitramide)</p> 	484.00	441.00	-8.88	496.00	2.48	275.63	0.25
34	<p><i>N</i>-((5-Amino-3-nitro-1<i>H</i>-1,2,4-triazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	497.00	468.00	-5.84	506.00	1.81	274.96	0.96
35	<p><i>N,N'</i>-((5,5'-Dinitro-2<i>H</i>,2'<i>H</i>-[3,3'-bi(1,2,4-triazole)]-2,2'-diyl)bis(methylene)) bis(<i>N</i>-methylnitramide)</p> 	501.00	460.00	-8.18	498.00	-0.60	273.75	-3.41

								
36	<p><i>N</i>-((3,4-Dinitro-1<i>H</i>-pyrazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	507.00	480.00	-5.33	506.00	-0.20	273.35	-7.62
37	<p>3,5-Dinitro-1<i>H</i>-pyrazole</p> 	568.00	518.00	-8.80	577.00	1.58	274.73	-1.07
38	<p>1-(3,5-Dinitro-1<i>H</i>-pyrazol-4-yl)guanidine</p> 	581.00	563.00	-3.10	591.00	1.72	274.87	1.10
39	<p>1-Methyl-3,5-dinitro-1<i>H</i>-pyrazol-4-amine</p> 	543.00	509.00	-6.26	549.00	1.10	274.25	-1.33
40	<p>1-Methyl-3,4,5-trinitro-1<i>H</i>-pyrazole</p> 	558.00	489.00	-12.37	547.00	-1.97	275.12	-2.89

41	1,1'-(Oxybis(methylene))bis(3,4-dinitro-1 <i>H</i> -pyrazole) 	571.00	534.00	-6.48	574.00	0.53	273.68	0.73
42	1,1'-(Oxybis(methylene))bis(3,5-dinitro-1 <i>H</i> -pyrazole) 	572.00	534.00	-6.64	574.00	0.35	273.5	0.55
43	1,1'-(Oxybis(methylene))bis(5-chloro-3-nitro-1 <i>H</i> -1,2,4-triazole) 	553.00	525.00	-5.06	552.00	-0.18	273.33	-4.43
44	1,1'-(Oxybis(methylene))bis(3-nitro-1 <i>H</i> -1,2,4-triazole) 	593.00	503.00	-15.18	560.00	-5.56	278.71	-3.15
45	1,2-Bis(2,4-dinitro-1 <i>H</i> -imidazol-1-yl)diazene 	531.00	502.00	-5.46	528.00	-0.56	273.71	-1.24
46	1,2-Bis(3-nitro-1 <i>H</i> -1,2,4-triazol-1-yl)diazene 	520.00	470.00	-9.62	508.00	-2.31	275.46	-2.46

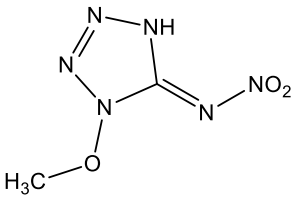
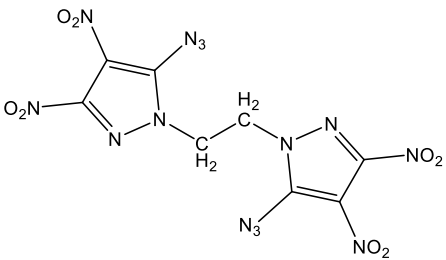
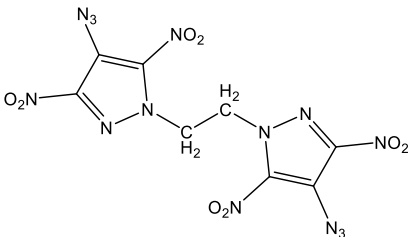
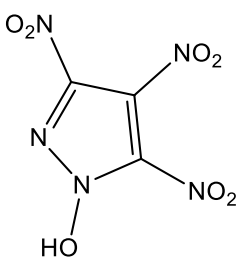
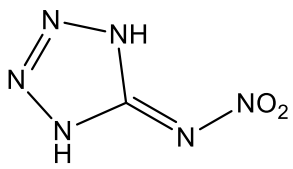
47	<p>2,3'-Dimethyl-5,5'-dinitro-2<i>H</i>,3'<i>H</i>-4,4'-bi(1,2,3-triazole)</p>	548.00	511.00	-6.75	551.00	0.55	273.7	-2.15
48	<p>5-Azido-1<i>H</i>-tetrazole</p>	438.00	384.00	-12.33	448.00	2.28	275.43	-5.87
49	<p>5-Imino-1-(2<i>H</i>-tetrazol-5-yl)-1<i>H</i>-1,2,4-triazole-3,4(5<i>H</i>)-diamine</p>	597.00	574.00	-3.85	572.00	-4.19	277.34	-1.05
50	<p><i>N,N</i>-Bis((5-chloro-3,4-dinitro-1<i>H</i>-pyrazol-1-yl)methyl)nitramide</p>	627.00	578.00	-7.81	619.00	-1.28	274.43	-0.30
51	<p>2,4-Dinitro-1<i>H</i>-imidazole-1,5-diamine</p>	463.00	502.00	8.42	466.00	0.65	273.8	-2.48
52	<p>1-(2-(4-Chloro-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p>	494.00	527.00	6.68	523.00	5.87	279.02	5.39

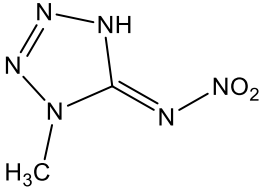
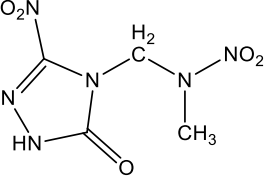
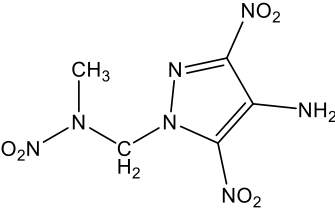
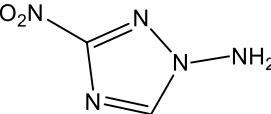
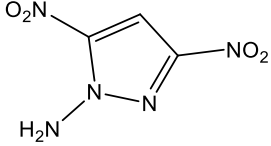
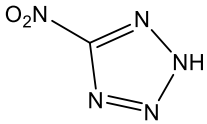
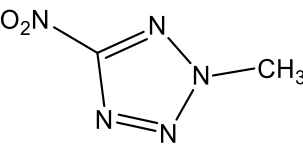
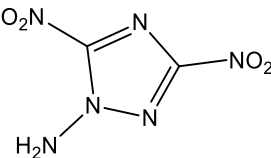
53	<p>(Z)-N-(1-(2-(3,4-Dinitro-1H-pyrazol-1-yl)ethyl)-1H-tetrazol-5(4H)-ylidene)nitramide</p> 	430.00	475.00	10.47	425.00	-1.16	274.31	3.30
54	<p>N-(2,2,2-Trinitroethyl)-1H-tetrazol-5-amine</p> 	423.00	465.00	9.93	427.00	0.95	274.1	-3.99
55	<p>1-Methyl-N-(2,2,2-trinitroethyl)-1H-tetrazol-5-amine</p> 	417.00	452.00	8.39	414.00	-0.72	273.87	3.29
56	<p>1,1'-(Propane-1,3-diyl)bis(N-(2,2,2-trinitroethyl)-1H-tetrazol-5-amine)</p> 	416.00	446.00	7.21	440.00	5.77	278.92	1.17

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

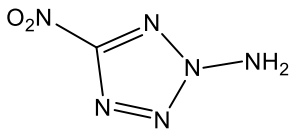
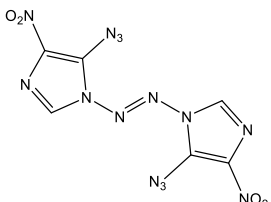
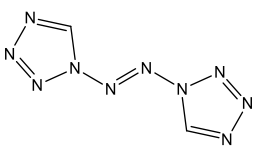
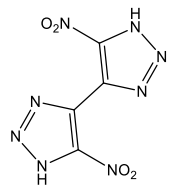
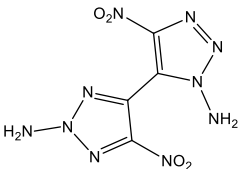
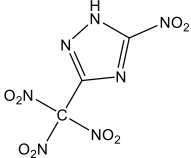
57	(<i>E</i>)- <i>N</i> -(1-Methoxy-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide 	389.00	400.00	2.83	401.00	3.08	276.23	4.11
58	1,2-Bis(5-azido-3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)ethane 	385.00	446.00	15.84	380.00	-1.30	274.45	2.58
59	1,2-Bis(4-azido-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)ethane 	408.00	446.00	9.31	406.00	-0.49	273.64	-3.20
60	3,4,5-Trinitro-1 <i>H</i> -pyrazol-1-ol 	419.00	470.00	12.17	420.00	0.24	273.39	1.22
61	<i>N</i> -(1 <i>H</i> -Tetrazol-5(4 <i>H</i>)-ylidene)nitramide 	395.00	422.00	6.84	423.00	7.09	280.24	1.65
62	(<i>E</i>)- <i>N</i> -(1-Methyl-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	398.00	409.00	2.76	410.00	3.02	276.17	0.88

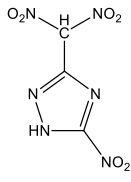
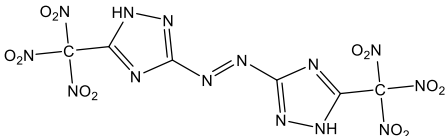
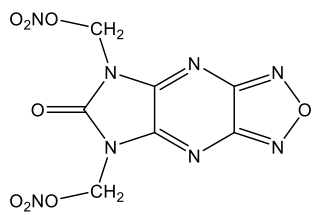
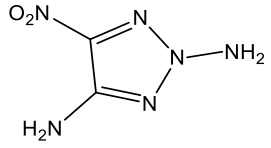
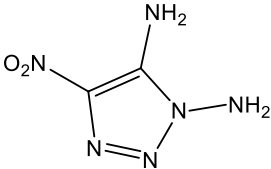
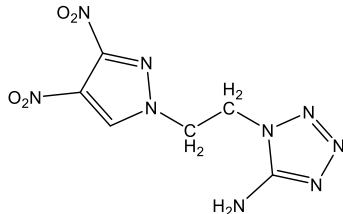
									
63	<i>N</i> -Methyl- <i>N</i> -((3-nitro-5-oxo-1 <i>H</i> -1,2,4-triazol-4(5 <i>H</i>)-yl)methyl)nitramide 	424.00	479.00	12.97	430.00	1.42	274.57	4.75	
64	<i>N</i> -((4-Amino-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)- <i>N</i> -methylnitramide 	438.00	484.00	10.50	435.00	-0.68	273.83	3.75	
65	1-Amino-3-nitro-1,2,4-triazole 	410.00	483.00	17.80	408.00	-0.49	273.64	-3.41	
66	1-Amino-3,5-dinitropyrazole 	385.00	382.00	-0.78	393.00	2.08	275.23	7.28	
67	5-Nitro-2 <i>H</i> -tetrazole 	403.00	471.00	16.87	421.00	4.47	277.62	-2.68	
68	2-Methyl-5-nitro-2 <i>H</i> -tetrazole 	423.00	458.00	8.27	408.00	-3.55	276.7	0.83	
69	3,5-Dinitro-1 <i>H</i> -1,2,4-triazol-1-amine 	438.00	467.00	6.62	429.00	-2.05	275.2	-4.90	

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

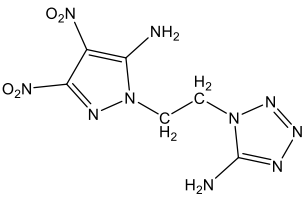
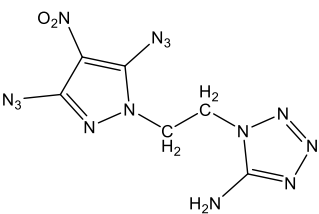
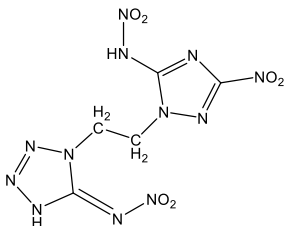
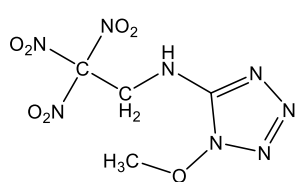
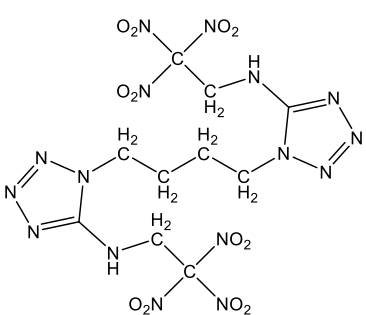
70	2-Amino-5-nitrotetrazole 	413.00	451.00	9.20	401.00	-2.91	276.06	0.95
71	1,2-Bis(5-azido-4-nitro-1 <i>H</i> -imidazol-1-yl)diazene 	427.00	498.00	16.63	425.00	-0.47	273.62	2.02
72	1,2-Di(1 <i>H</i> -tetrazol-1-yl)diazene 	353.00	439.00	24.36	363.00	2.83	275.98	2.39
73	5,5'-Dinitro-1 <i>H</i> ,1' <i>H</i> -4,4'-bi(1,2,3-triazole) 	428.00	421.00	-1.64	433.00	1.17	274.32	0.31
74	5,5'-Dinitro-2 <i>H</i> ,3' <i>H</i> -[4,4'-bi(1,2,3-triazole)]-2,3'-diamine 	464.00	497.00	7.11	461.00	-0.65	273.8	4.16
75	5-Nitro-3-(trinitromethyl)-1 <i>H</i> -1,2,4-triazole 	408.00	466.00	14.22	416.00	1.96	275.11	3.61

76	3-(Dinitromethyl)-5-nitro-1 <i>H</i> -1,2,4-triazole 	360.00	345.00	-4.17	358.00	-0.56	273.71	6.93
77	(<i>E</i>)-1,2-Bis(5-(trinitromethyl)-1 <i>H</i> -1,2,4-triazol-3-yl)diazene 	423.00	477.00	12.77	427.00	0.95	274.1	-6.45
78	(6-Oxo-5 <i>H</i> -imidazo[4,5- <i>b</i>][1,2,5]oxadiazolo[3,4- <i>e</i>]pyrazine-5,7(6 <i>H</i>)-diyl)bis(methylene) dinitrate 	463.00	455.00	-1.73	458.00	-1.08	274.23	2.53
79	5-Nitro-2 <i>H</i> -1,2,3-triazole-2,4-diamine 	485.00	462.00	-4.74	487.00	0.41	273.56	0.37
80	4-Nitro-1 <i>H</i> -1,2,3-triazole-1,5-diamine 	467.00	487.00	4.28	482.00	3.21	276.36	4.28
81	1-(2-(3,4-Dinitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine 	505.00	515.00	1.98	511.00	1.19	274.34	2.73

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

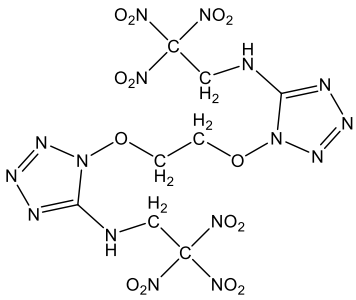
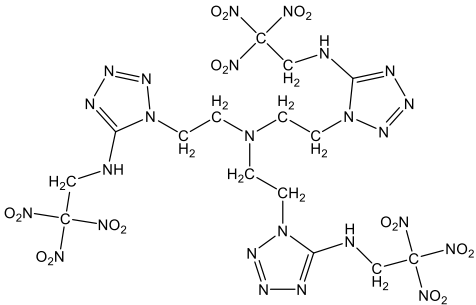
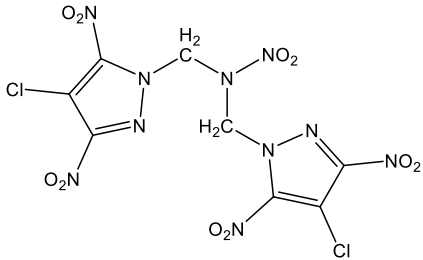
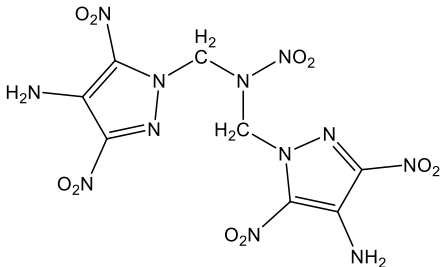
Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

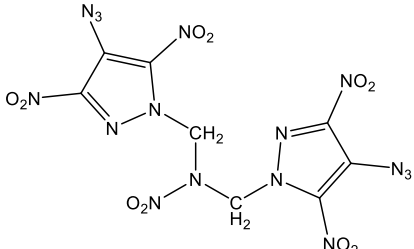
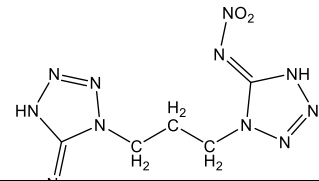
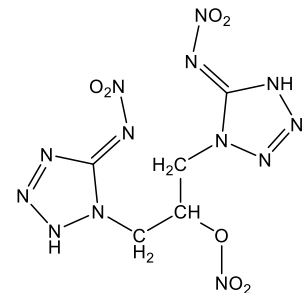
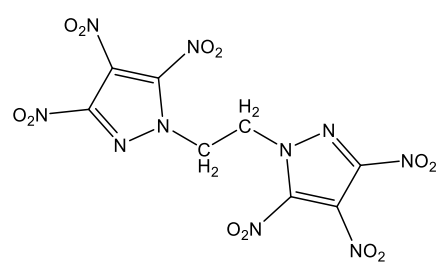
82	<p>1-(2-(5-Amino-3,4-dinitro-1<i>H</i>-pyrazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p> 	512.00	519.00	1.37	515.00	0.59	273.74	-1.65
83	<p>1-(2-(3,5-Diazido-4-nitro-1<i>H</i>-pyrazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p> 	400.00	434.00	8.50	394.00	-1.50	274.65	5.99
84	<p>(<i>Z</i>)-<i>N</i>-(1-(2-(3-Nitro-5-(nitroamino)-1<i>H</i>-1,2,4-triazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5(4<i>H</i>)-ylidene)nitramide</p> 	369.00	370.00	0.27	369.00	0.00	273.15	-6.18
85	<p>1-Methoxy-<i>N</i>-(2,2,2-trinitroethyl)-1<i>H</i>-tetrazol-5-amine</p> 	421.00	443.00	5.23	436.00	3.56	276.71	-1.53
86	<p>1,1'-(Butane-1,4-diyl)bis(<i>N</i>-(2,2,2-trinitroethyl)-1<i>H</i>-tetrazol-5-amine)</p> 	439.00	457.00	4.10	451.00	2.73	275.88	-3.12

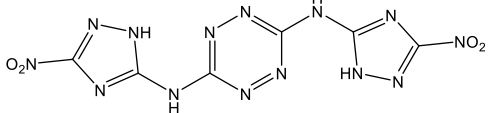
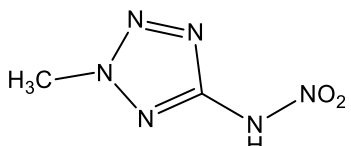
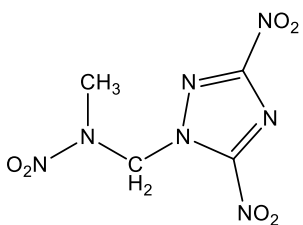
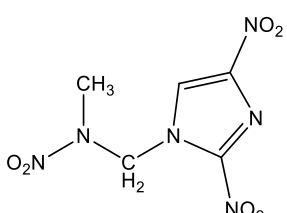
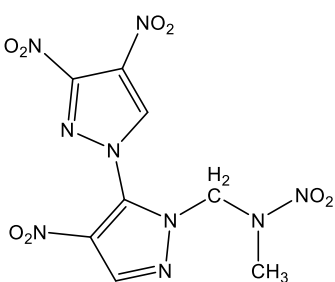
Central European Journal of Energetic Materials

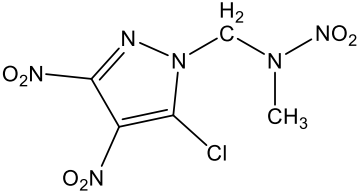
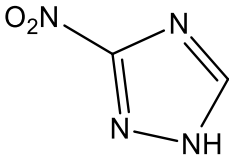
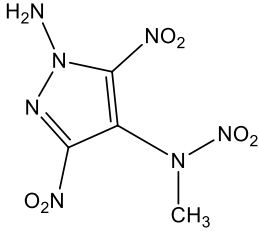
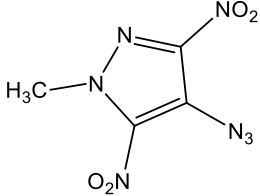
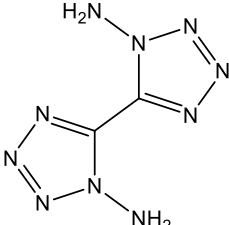
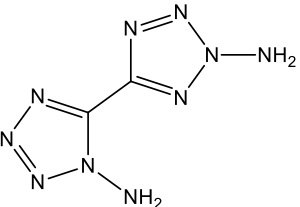
ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

87	<p>1,1'-(Ethane-1,2-diylbis(oxy))bis(<i>N</i>-(2,2,2-trinitroethyl)-1<i>H</i>-tetrazol-5-amine)</p> 	420.00	418.00	-0.48	410.00	-2.38	275.53	-5.30
88	<p>1-(2-(Bis(2-(5-((2,2,2-trinitroethyl)amino)-1<i>H</i>-tetrazol-1-yl)ethyl)amino)ethyl)-<i>N</i>-(2,2,2-trinitroethyl)-1<i>H</i>-tetrazol-5-amine</p> 	414.00	431.00	4.11	424.00	2.42	275.57	2.81
89	<p><i>N,N</i>-Bis((4-chloro-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)methyl)nitramide</p> 	525.00	528.00	0.57	525.00	0.00	273.15	-1.37
90	<p><i>N,N</i>-Bis((4-amino-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)methyl)nitramide</p> 	505.00	514.00	1.78	510.00	0.99	274.14	-4.11

91	<p><i>N,N</i>-Bis((4-azido-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)methyl)nitramide</p> 	439.00	409.00	-6.83	412.00	-6.15	279.3	-0.37
92	<p><i>N</i>-((<i>E</i>)-1-(3-((<i>Z</i>)-5-(Nitroimino)-4,5-dihydro-1<i>H</i>-tetrazol-1-yl)propyl)-1,4-dihydro-5<i>H</i>-tetrazol-5-ylidene)nitramide</p> 	446.00	413.00	-7.40	414.00	-7.17	280.32	5.01
93	<p>1-((<i>Z</i>)-5-(Nitroimino)-2,5-dihydro-1<i>H</i>-tetrazol-1-yl)-3-((<i>E</i>)-5-(nitroimino)-4,5-dihydro-1<i>H</i>-tetrazol-1-yl)propan-2-yl nitrate</p> 	412.00	386.00	-6.31	387.00	-6.07	279.22	6.49
94	<p>1,2-Bis(3,4,5-trinitro-1<i>H</i>-pyrazol-1-yl)ethane</p> 	523.00	511.00	-2.29	507.00	-3.06	276.21	-2.07

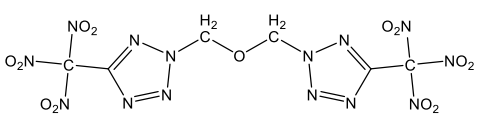
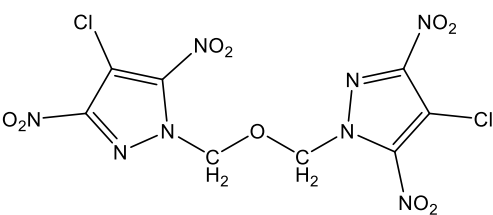
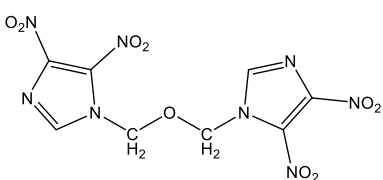
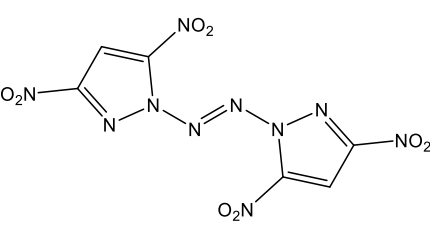
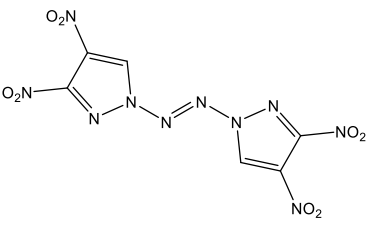
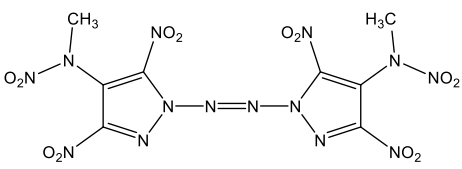
95	<p><i>N</i>³,<i>N</i>⁶-Bis(3-nitro-1<i>H</i>-1,2,4-triazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine</p> 	575.00	573.00	-0.35	570.00	-0.87	274.02	0.79
96	<p><i>N</i>-(2-Methyl-2<i>H</i>-tetrazol-5-yl)nitramide</p> 	395.00	385.00	-2.53	385.00	-2.53	275.68	-5.45
97	<p><i>N</i>-((3,5-Dinitro-1<i>H</i>-1,2,4-triazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	438.00	448.00	2.28	442.00	0.91	274.06	1.96
98	<p><i>N</i>-((2,4-Dinitro-1<i>H</i>-imidazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	456.00	480.00	5.26	475.00	4.17	277.32	2.71
99	<p><i>N</i>-Methyl-<i>N</i>-((3,4,4'-trinitro-2'<i>H</i>-[1,3'-bipyrazol]-2'-yl)methyl)nitramide</p> 	537.00	522.00	-2.79	518.00	-3.54	276.69	-3.30

100	<p><i>N</i>-((5-Chloro-3,4-dinitro-1<i>H</i>-pyrazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	487.00	516.00	5.95	511.00	4.93	278.08	-2.39
101	<p>3-Nitro-1<i>H</i>-1,2,4-triazole</p> 	491.00	503.00	2.44	498.00	1.43	274.58	0.69
102	<p><i>N</i>-(1-Amino-3,5-dinitro-1<i>H</i>-pyrazol-4-yl)-<i>N</i>-methylnitramide</p> 	449.00	473.00	5.35	467.00	4.01	277.16	-0.54
103	<p>4-Azido-1-methyl-3,5-dinitro-1<i>H</i>-pyrazole</p> 	434.00	426.00	-1.84	429.00	-1.15	274.3	-7.89
104	<p>1<i>H</i>,1'<i>H</i>-[5,5'-Bitetrazole]-1,1'-diamine</p> 	458.00	466.00	1.75	460.00	0.44	273.59	1.54
105	<p>1<i>H</i>,2'<i>H</i>-[5,5'-Bitetrazole]-1,2'-diamine</p> 	448.00	466.00	4.02	460.00	2.68	275.83	3.81

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

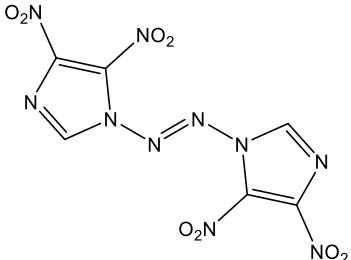
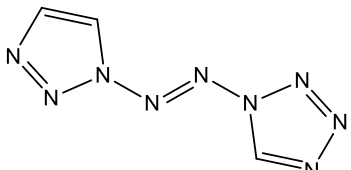
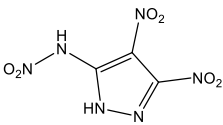
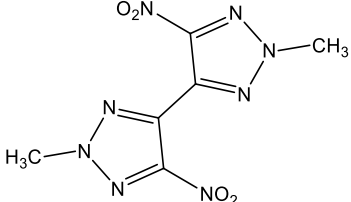
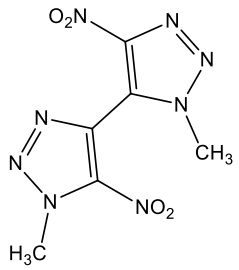
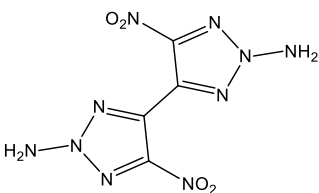
Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

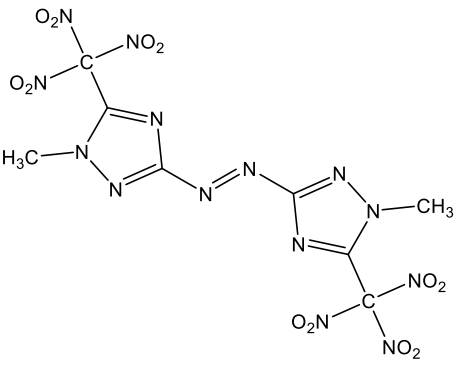
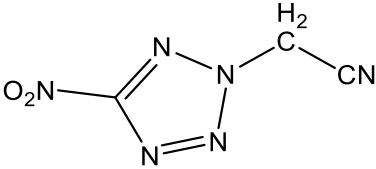
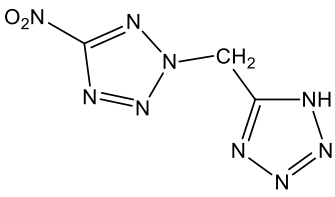
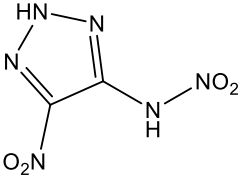
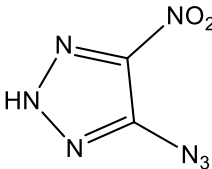
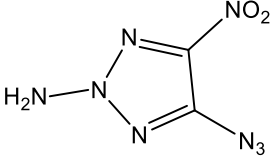
106	<p>2,2'-(Oxybis(methylene))bis(5-(trinitromethyl)-2H-tetrazole)</p> 	403.00	397.00	-1.49	389.00	-3.47	276.62	-0.64
107	<p>1,1'-(Oxybis(methylene))bis(4-chloro-3,5-dinitro-1H-pyrazole)</p> 	557.00	556.00	-0.18	554.00	-0.54	273.69	-4.65
108	<p>1,1'-(Oxybis(methylene))bis(4,5-dinitro-1H-imidazole)</p> 	543.00	534.00	-1.66	531.00	-2.21	275.36	-3.97
109	<p>1,2-Bis(3,5-dinitro-1H-pyrazol-1-yl)diazene</p> 	513.00	502.00	-2.14	497.00	-3.12	276.27	2.23
110	<p>1,2-Bis(3,4-dinitro-1H-pyrazol-1-yl)diazene</p> 	496.00	502.00	1.21	497.00	0.20	273.35	5.73
111	<p><i>N,N'</i>-(1,1'-(Diazene-1,2-diyl)bis(3,5-dinitro-1H-pyrazole-4,1-diyl))bis(<i>N</i>-methylnitramide)</p> 	468.00	450.00	-3.85	444.00	-5.13	278.28	2.74

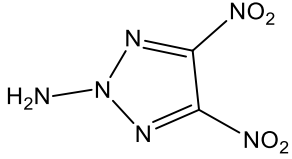
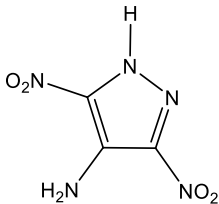
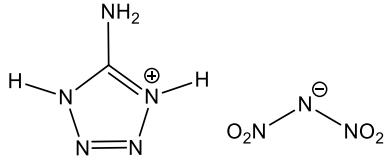
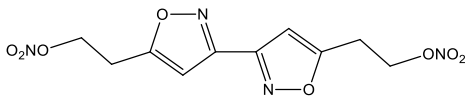
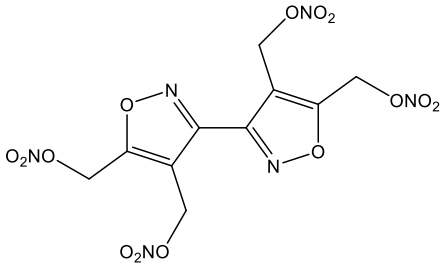
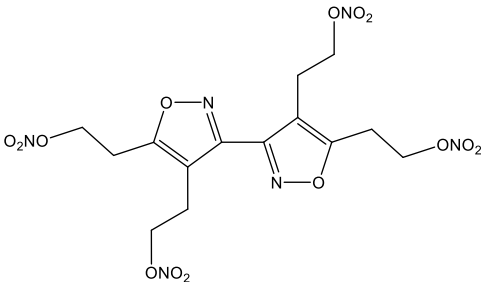
Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

112	<p>1,2-Bis(4,5-dinitro-1<i>H</i>-imidazol-1-yl)diazene</p> 	505.00	502.00	-0.59	497.00	-1.58	274.73	3.85
113	<p>1-((1<i>H</i>-1,2,3-Triazol-1-yl)diazenyl)-1<i>H</i>-tetrazole</p> 	467.00	471.00	0.86	465.00	-0.43	273.58	0.13
114	<p><i>N</i>-(3,4-Dinitro-1<i>H</i>-pyrazol-5-yl)nitramide</p> 	408.00	429.00	5.15	431.00	5.64	278.79	-4.75
115	<p>2,2'-Dimethyl-5,5'-dinitro-2<i>H</i>,2'<i>H</i>-4,4'-bi(1,2,3-triazole)</p> 	500.00	511.00	2.20	507.00	1.40	274.55	0.90
116	<p>1,3'-Dimethyl-5,5'-dinitro-1<i>H</i>,3'<i>H</i>-4,4'-bi(1,2,3-triazole)</p> 	510.00	511.00	0.20	507.00	-0.59	273.74	-1.08
117	<p>5,5'-Dinitro-2<i>H</i>,2'<i>H</i>-[4,4'-bi(1,2,3-triazole)]-2,2'-diamine</p> 	508.00	497.00	-2.17	493.00	-2.95	276.1	-4.86

118	(E)-1,2-Bis(1-methyl-5-(trinitromethyl)-1H-1,2,4-triazol-3-yl)diazene 	438.00	450.00	2.74	444.00	1.37	274.52	-4.70
119	2-(5-Nitro-2H-tetrazol-2-yl)acetonitrile 	483.00	493.00	2.07	488.00	1.04	274.19	4.88
120	5-((5-Nitro-2H-tetrazol-2-yl)methyl)-1H-tetrazole 	487.00	477.00	-2.05	472.00	-3.08	276.23	1.01
121	N-(5-Nitro-2H-1,2,3-triazol-4-yl)nitramide 	403.00	413.00	2.48	415.00	2.98	276.13	1.86
122	4-Azido-5-nitro-2H-1,2,3-triazole 	422.00	423.00	0.24	426.00	0.95	274.1	1.06
123	4-Azido-5-nitro-2H-1,2,3-triazol-2-amine 	414.00	379.00	-8.45	411.00	-0.72	273.87	-3.08

124	4,5-Dinitro-2 <i>H</i> -1,2,3-triazol-2-amine 	463.00	467.00	0.86	461.00	-0.43	273.58	1.56
125	4-Amino-3,5-dinitro-1 <i>H</i> -pyrazole 	452.00	522.00	15.49	449.00	-0.66	273.81	17.74
126	5-Aminotetrazolium dinitramide 	390.00	386.00	-1.03	386.00	-1.03	-	-
127	[3,3'-Biisoxazole]-5,5'-diylbis(ethane-2,1-diyl)dinitrate 	474.00	548.00	15.61	485.00	2.32	-	-
128	Biisoxazoletetrakis(methyl)nitrate 	467.00	499.00	6.85	472.00	1.07	-	-
129	[3,3'-Biisoxazole]-4,4',5,5'-tetrayltetrakis(ethane-2,1-diyl)tetranitrate 	461.00	543.00	17.79	480.00	4.12	-	-

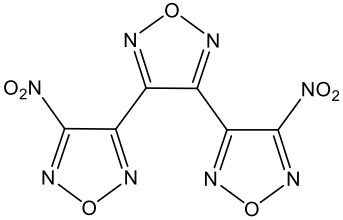
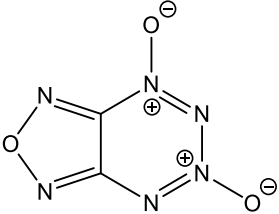
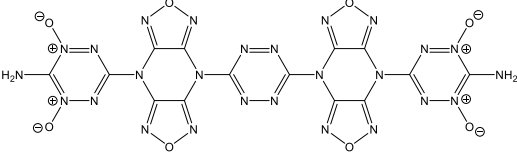
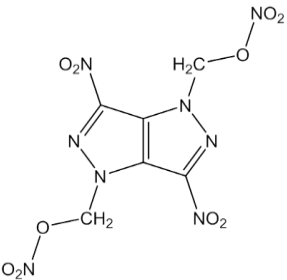
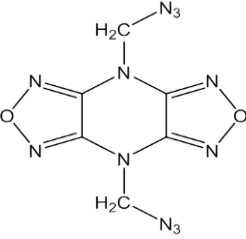
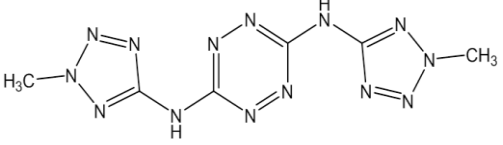
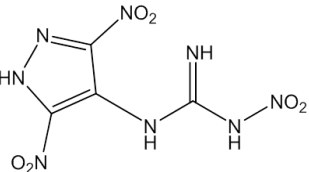
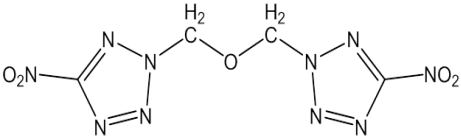
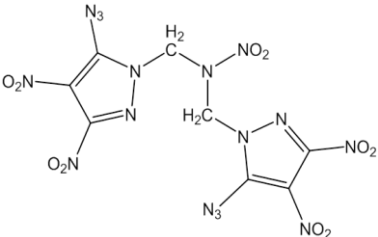
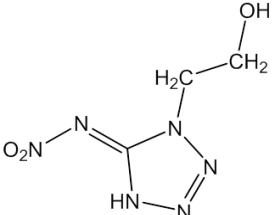
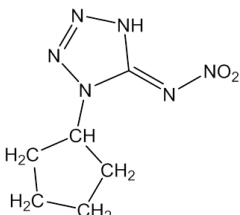
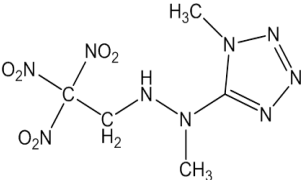
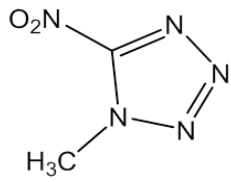
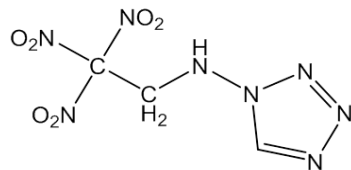
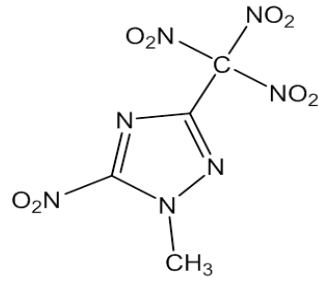
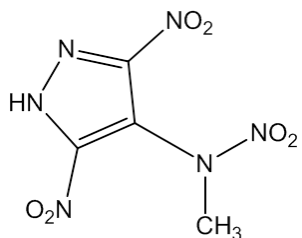
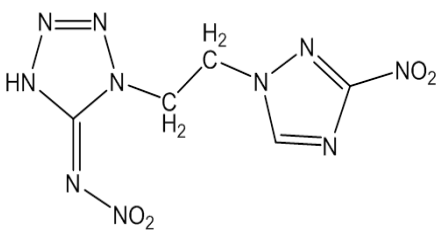
130	<p>3,4-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole</p> 	460.00	484.00	5.22	479.00	4.13	–	–
131	<p>Furazano-1,2,3,4-tetrazine-1,3-dioxide</p> 	408.00	451.00	10.54	400.00	-1.96	275.11	19.26
132	<p>6,6'-{1,2,4,5-Tetrazine-3,6-diylbis[(4<i>H</i>,8<i>H</i>-bis[1,2,5]oxadiazolo[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine-8,4-diyl)]}bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)</p> 	499.00	552.00	10.62	480.00	-3.81	276.96	16.18

Table S2. The estimated outputs of Equations 1 and 5 for the test set of heterocyclic aromatic compounds and some of their salts

Note: The predicted results of the model by Zohari et al. [18] for azole compounds are given here. The molecular structures of different types of heterocyclic aromatic compounds and some of their salts are also added to this table.

No.	Structure	Exp. [4, 18]	Eq. 1	%Dev	Eq. 5	%Dev	[18]	%Dev
1	(3,6-Dinitropyrazolo[4,3-c]pyrazole-1,4-diyl)bis(methylene) dinitrate 	479.00	426.29	-11.00	490.47	2.39	482.22	0.67
2	4,8-Bis(azidomethyl)-4,8-dihydrobis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine 	461.00	406.14	-11.90	439.82	-4.59	456.15	-1.05
3	<i>N</i> ³ , <i>N</i> ⁶ -Bis(2-methyl-2 <i>H</i> -tetrazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine 	579.00	515.13	-11.03	573.07	-1.02	591.60	2.18
4	1-(3,5-Dinitro-1 <i>H</i> -pyrazol-4-yl)-3-nitroguanidine 	506.00	469.13	-7.29	503.21	-0.55	505.82	-0.04

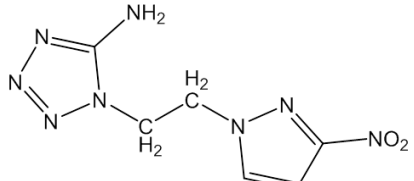
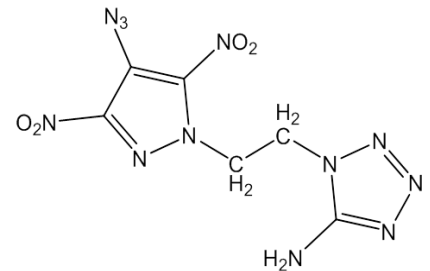
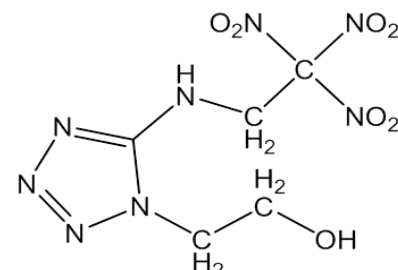
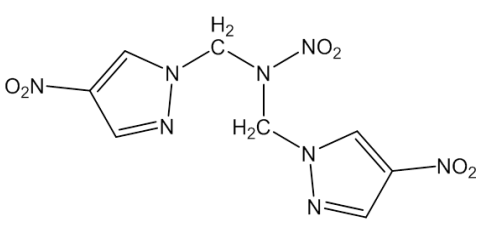
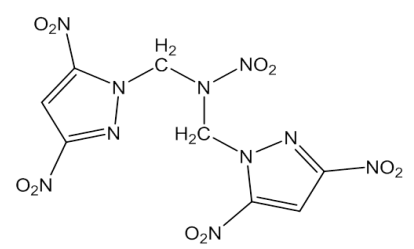
5	<p>2,2'-(Oxybis(methylene))bis(5-nitro-2H-tetrazole)</p> 	476.00	439.33	-7.70	432.69	-9.10	467.93	-1.70
6	<p><i>N,N</i>-Bis((5-azido-3,4-dinitro-1H-pyrazol-1-yl)methyl)nitramide</p> 	442.00	471.04	6.57	465.45	5.31	437.38	-1.05
7	<p>(<i>E</i>)-<i>N</i>-(1-(2-Hydroxyethyl)-1H-tetrazol-5(4H)-ylidene)nitramide</p> 	431.00	463.78	7.61	457.91	6.24	434.39	0.79
8	<p>(<i>E</i>)-<i>N</i>-(1-Cyclopentyl-1H-tetrazol-5(4H)-ylidene)nitramide</p> 	397.00	450.90	13.58	453.43	14.21	403.77	1.71
9	<p>1-Methyl-5-(1-methyl-2-(2,2,2-trinitroethyl)hydrazinyl)-1H-tetrazole</p> 	355.50	441.99	24.33	403.93	13.62	367.42	3.35

10	<p>1-Methyl-5-nitro-1<i>H</i>-tetrazole</p> 	428.00	458.06	7.02	452.04	5.62	459.43	7.34
11	<p><i>N</i>-(2,2,2-Trinitroethyl)-1<i>H</i>-tetrazol-1-amine</p> 	389.00	440.57	13.26	402.47	3.46	406.13	4.40
12	<p>1-Methyl-5-nitro-3-(trinitromethyl)-1<i>H</i>-1,2,4-triazole</p> 	426.00	452.82	6.30	446.63	4.84	446.98	4.92
13	<p><i>N</i>-(3,5-Dinitro-1<i>H</i>-pyrazol-4-yl)-<i>N</i>-methylnitramide</p> 	431.00	492.90	14.36	418.79	-2.83	465.35	7.97
14	<p>(<i>Z</i>)-<i>N</i>-(1-(2-(3-Nitro-1<i>H</i>-1,2,4-triazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5(4<i>H</i>)-ylidene)nitramide</p> 	454.00	483.21	6.43	477.99	5.28	439.43	-3.21

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

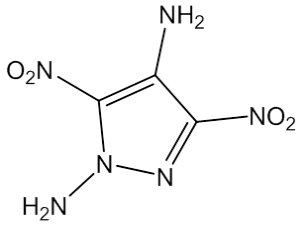
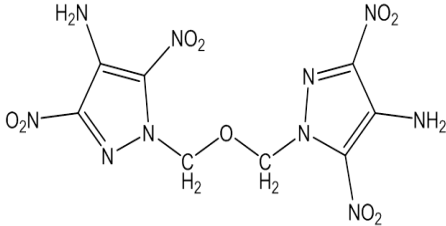
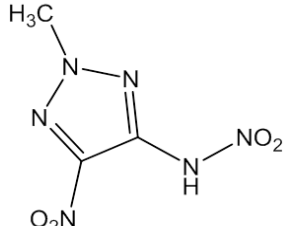
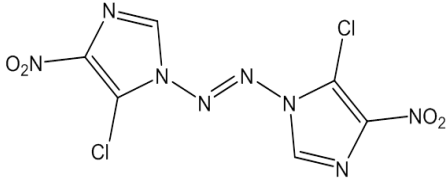
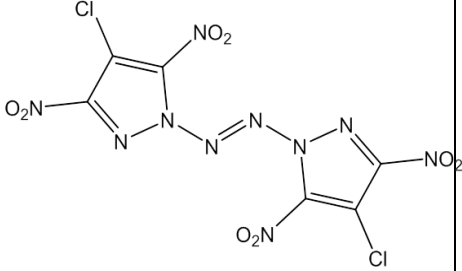
Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

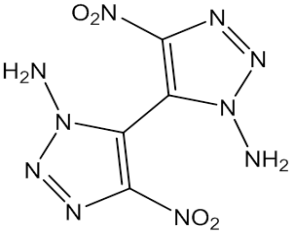
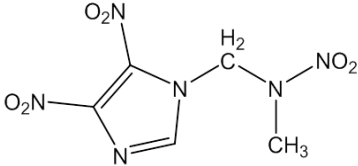
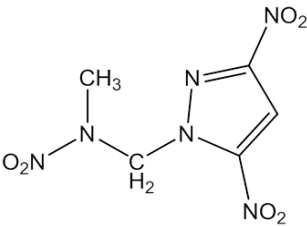
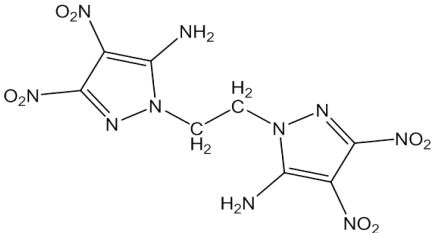
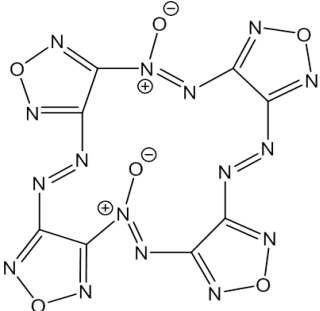
15	<p>1-(2-(3-Nitro-1<i>H</i>-pyrazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p> 	527.00	531.42	0.84	527.80	0.15	539.49	2.37
16	<p>1-(2-(4-Azido-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)ethyl)-1<i>H</i>-tetrazol-5-amine</p> 	432.00	436.02	0.93	439.51	1.74	464.47	7.52
17	<p>2-(5-((2,2,2-Trinitroethyl)amino)-1<i>H</i>-tetrazol-1-yl)ethanol</p> 	419.00	453.88	8.32	416.22	-0.66	427.20	1.96
18	<p><i>N,N</i>-Bis((4-nitro-1<i>H</i>-pyrazol-1-yl)methyl)nitramide</p> 	535.00	538.17	0.59	534.83	-0.03	529.89	-0.96
19	<p><i>N,N</i>-Bis((3,5-dinitro-1<i>H</i>-pyrazol-1-yl)methyl)nitramide</p> 	523.00	515.77	-1.38	511.67	-2.17	508.68	-2.74

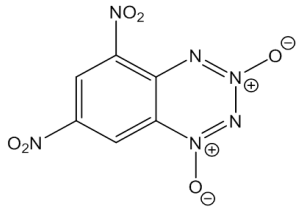
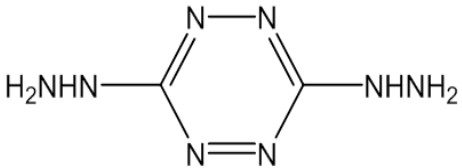
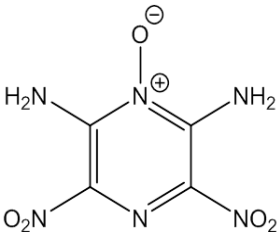
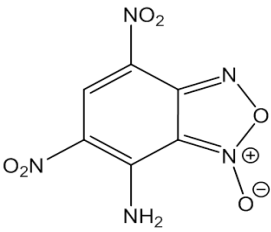
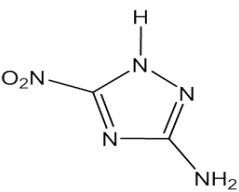
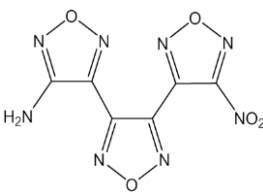
Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

20	<p>3,5-Dinitro-1<i>H</i>-pyrazole-1,4-diamine</p> 	514.00	502.38	-2.26	497.75	-3.16	505.41	-1.67
21	<p>1,1'-(Oxybis(methylene))bis(3,5-dinitro-1<i>H</i>-pyrazol-4-amine)</p> 	503.00	542.05	7.76	538.75	7.11	495.26	-1.54
22	<p><i>N</i>-(2-Methyl-5-nitro-2<i>H</i>-1,2,3-triazol-4-yl)nitramide</p> 	385.00	400.29	3.97	401.13	4.19	391.98	1.81
23	<p>1,2-Bis(5-chloro-4-nitro-1<i>H</i>-imidazol-1-yl)diazene</p> 	544.00	555.80	2.17	553.04	1.66	571.54	5.06
24	<p>1,2-Bis(4-chloro-3,5-dinitro-1<i>H</i>-pyrazol-1-yl)diazene</p> 	524.00	523.83	-0.03	520.01	-0.76	535.95	2.28

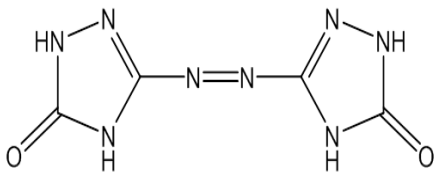
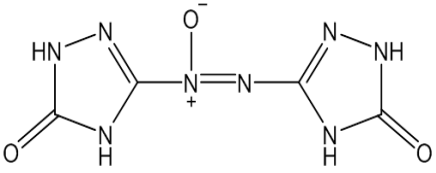
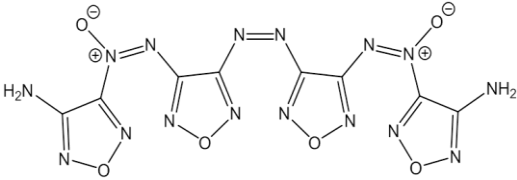
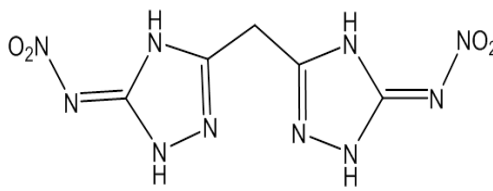
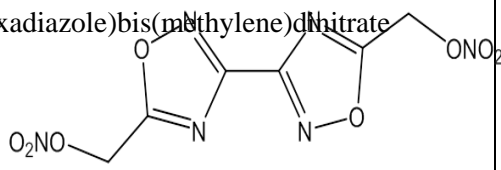
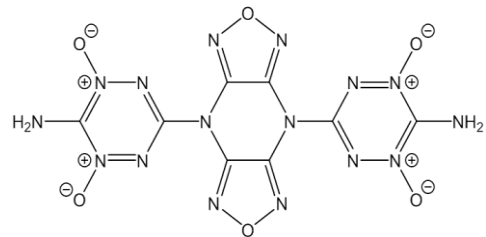
25	<p>5,5'-Dinitro-3<i>H</i>,3'<i>H</i>-[4,4'-bi(1,2,3-triazole)]-3,3'-diamine</p> 	471.00	497.36	5.60	492.56	4.58	483.30	2.61
26	<p><i>N</i>-((4,5-Dinitro-1<i>H</i>-imidazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	463.00	479.84	3.64	474.55	2.49	468.38	1.16
27	<p><i>N</i>-((3,5-Dinitro-1<i>H</i>-pyrazol-1-yl)methyl)-<i>N</i>-methylnitramide</p> 	483.00	479.84	-0.65	474.55	-1.75	468.38	-3.03
28	<p>1,1'-(Ethane-1,2-diyl)bis(3,4-dinitro-1<i>H</i>-pyrazol-5-amine)</p> 	529.00	550.81	4.12	547.80	3.55	554.59	4.84
29	<p>3,4:7,8:11,12:15,16-Tetrafurazano-1,2,5,6,9,10,13,14-octaazacyclohexadeca-1,3,5,7,9,11,13,15-octane-1,10-dioxide</p> 	485.15	460.54	-5.07	454.76	-6.26	-	-

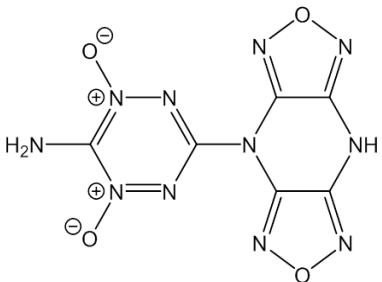
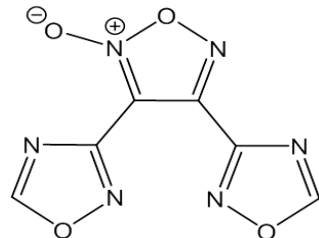
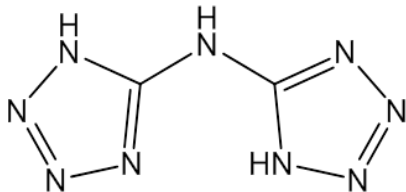
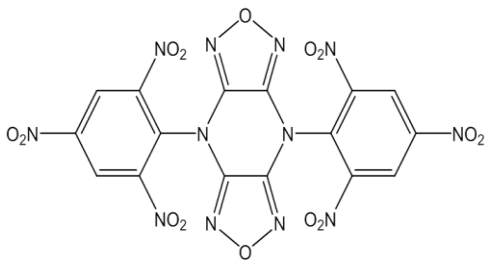
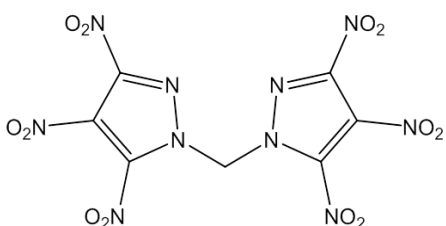
30	<p>5,7-Dinitrobenzo-1,2,3,4-tetrazine-1,3-dioxide</p> 	484.95	557.40	14.94	510.66	5.30	589.07	21.47
31	<p>1,4-Dihydrazino tetrazine</p> 	433.15	461.82	6.62	455.84	5.24	447.92	3.41
32	<p>2,6-Diamino-3,5-dinitropyrazine-1-oxide</p> 	572.25	576.10	0.67	573.84	0.28	487.82	-14.75
33	<p>7-Amino-4,6-dinitrobenzofuroxan</p> 	547.15	558.03	1.99	555.35	1.50	-	-
34	<p>3-Amino-5-nitro-1,2,4-triazole</p> 	500.15	506.78	1.33	502.30	0.43	461.93	-7.64
35	<p>3-(4-Amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole</p> 	507.15	504.27	-0.57	499.87	-1.44	-	-

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

36	<p>Azotriazolone</p> 	575.15	581.07	1.03	578.99	0.67	533.73	-7.20
37	<p>Azoxytriazolone</p> 	540.15	572.32	5.96	569.94	5.51	515.24	-4.61
38	<p>Bis[4-aminofurazanyl-3-azoxy]azofurazan</p> 	500.15	465.45	-6.94	459.75	-8.08	-	-
39	<p>5,5'-Dinitrimino-3,3'-methylene-1H-1,2,4-triazole</p> 	515.15	502.65	-2.43	506.74	-1.63	499.52	-3.03
40	<p>Bis(1,2,4-oxadiazole)bis(methylene)dinitrate</p> 	456.55	462.92	1.40	466.18	2.11	-	-
41	<p>6,6'-(4H,8H-Bis[1,2,5]oxadiazolo[3,4-b:3',4'-e]pyrazine-4,8-diyl)bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)</p> 	501.15	510.39	1.84	506.11	0.99	545.56	8.86

42	<p>6-(4<i>H</i>,8<i>H</i>-Bis[1,2,5]oxadiazolo[3,4-<i>b</i>:3',4'-3]pyrazine-4-yl)-2,4-dioxo-1,2,4,5-tetrazin-3-amine oxolan-2-one</p> 	503.15	519.82	3.31	515.86	2.53	559.53	11.21
43	<p>Bis(1,2,4-oxadiazolyl) furoxan</p> 	500.15	507.51	1.47	503.26	0.62	–	–
44	<p>5,5'-Bis(1<i>H</i>-tetrazolyl)amine</p> 	523.15	509.61	-2.59	505.18	-3.43	484.21	-7.44
45	<p>4,8-Bis(2,4,6-trinitrophenyl)-4<i>H</i>,8<i>H</i>-bis([1,2,5]oxadiazolo)[3,4-<i>b</i>:3',4'-<i>e</i>]pyrazine</p> 	688.15	694.98	0.99	696.94	1.28	–	–
46	<p>Bis(3,4,5-trinitropyrazolyl)methane</p> 	478.15	499.84	4.54	495.21	3.57	513.39	7.37

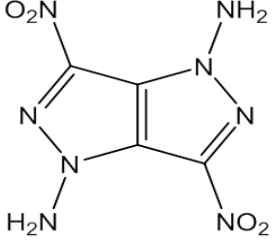
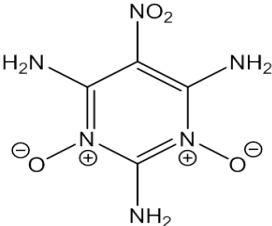
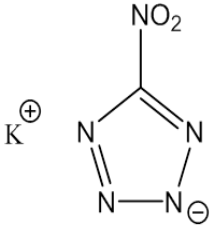
47	1,4-Diamino-3,6-dinitropyrazolo[4,3-c]pyrazole 	503.15	516.47	2.65	512.31	1.82	497.51	-1.12
48	5-Nitro-2,4,6-triaminopyrimidine-1,3-dioxide 	541.40	538.04	-0.62	534.56	-1.26	467.19	-13.71
49	Potassium 5-nitrotetrazolate 	468.15	458.12	-2.14	452.10	-3.43	-	-

Table S3. Index, in alphabetical order, of compounds used in Tables S1 and S2

Name	Table:No. of row
1-(2-(5-Amino-3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:82
<i>N</i> -((4-Amino-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)- <i>N</i> -methylnitramide	S1:64
<i>N</i> -(1-Amino-3,5-dinitro-1 <i>H</i> -pyrazol-4-yl)- <i>N</i> -methylnitramide	S1:102
4-Amino-3,5-dinitro-1 <i>H</i> -pyrazole	S1:125
7-Amino-4,6-dinitrobenzofuroxan	S2:33
1-Amino-3,5-dinitropyrazole	S1:66
2-Amino-5-nitrotetrazole	S1:70
1-(2-(5-Amino-3-nitro-1 <i>H</i> -1,2,4-triazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:25
<i>N</i> -((5-Amino-3-nitro-1 <i>H</i> -1,2,4-triazol-1-yl)methyl)- <i>N</i> -methylnitramide	S1:34
1-Amino-3-nitro-1,2,4-triazole	S1:65
3-Amino-5-nitro-1,2,4-triazole	S2:34
3-(4-Amino-1,2,5-oxadiazol-3-yl)-4-(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole	S2:35
5-Aminotetrazolium dinitramide	S1:126
5-Aminotetrazolium nitrate	S1:1
4-Azido-1-methyl-3,5-dinitro-1 <i>H</i> -pyrazole	S1:103
1-(2-(4-Azido-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S2:16
4-Azido-5-nitro-2 <i>H</i> -1,2,3-triazole	S1:122
4-Azido-5-nitro-2 <i>H</i> -1,2,3-triazol-2-amine	S1:123
5-Azido-1 <i>H</i> -tetrazole	S1:48
Azotriazolone	S2:36
Azoxytriazolone	S2:37
[2,2'-Bi(1,3,4-oxadiazole)]-5,5'-dinitramide	S1:20
[3,3'-Biisoxazole]-5,5'-diylbis(ethane-2,1-diyl)dinitrate	S1:127
[3,3'-Biisoxazole]-4,4',5,5'-tetrayltetrakis(ethane-2,1-diyl)tetranitrate	S1:129
Biisoxazoletetrakis(methyl)nitrate	S1:128
<i>N,N</i> -Bis((4-amino-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S1:90
Bis[4-aminofurazanyl-3-azoxy]azofurazan	S2:38
<i>N,N</i> -Bis((4-azido-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S1:91

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

1,2-Bis(5-azido-3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)ethane	S1:58
1,2-Bis(4-azido-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)ethane	S1:59
<i>N,N</i> -Bis((5-azido-3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S2:6
1,2-Bis(5-azido-4-nitro-1 <i>H</i> -imidazol-1-yl)diazene	S1:71
4,8-Bis(azidomethyl)-4,8-dihydrobis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine	S2:2
1,4-Bis(azidomethyl)-3,6-dinitro-1,4-dihydropyrazolo[4,3-c]pyrazole	S1:23
1,2-Bis(4-chloro-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)diazene	S2:24
1,2-Bis(4-chloro-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)ethane	S1:30
<i>N,N</i> -Bis((4-chloro-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S1:89
<i>N,N</i> -Bis((5-chloro-3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S1:50
1,2-Bis(5-chloro-4-nitro-1 <i>H</i> -imidazol-1-yl)diazene	S2:23
Bis(3,5-dinitro-4-aminopyrazolyl)methane	S1:3
1,2-Bis(2,4-dinitro-1 <i>H</i> -imidazol-1-yl)diazene	S1:45
1,2-Bis(4,5-dinitro-1 <i>H</i> -imidazol-1-yl)diazene	S1:112
1,2-Bis(3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)diazene	S1:110
1,2-Bis(3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)diazene	S1:109
<i>N,N</i> -Bis((3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl) nitramide	S1:28
<i>N</i> ³ , <i>N</i> ⁶ -Bis(2-methyl-2 <i>H</i> -tetrazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine	S2:3
(<i>E</i>)-1,2-Bis(1-methyl-5-(trinitromethyl)-1 <i>H</i> -1,2,4-triazol-3-yl)diazene	S1:118
<i>N,N</i> -Bis((3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S2:19
3,4-Bis(4-nitro-1,2,5-oxadiazol-3-yl)-1,2,5-oxadiazole	S1:130
<i>N,N</i> -Bis((4-nitro-1 <i>H</i> -pyrazol-1-yl)methyl)nitramide	S2:18
1,2-Bis(3-nitro-1 <i>H</i> -1,2,4-triazol-1-yl)diazene	S1:46
<i>N</i> ³ , <i>N</i> ⁶ -Bis(3-nitro-1 <i>H</i> -1,2,4-triazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine	S1:95
Bis(nitrofuranzano)furoxan	S1:4
Bis(1,2,4-oxadiazole)bis(methylene)dinitrate	S2:40
6,6'-(4 <i>H</i> ,8 <i>H</i> -Bis[1,2,5]oxadiazolo[3,4-b:3',4'-e]pyrazine-4,8-diyl)bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)	S2:41
6-(4 <i>H</i> ,8 <i>H</i> -Bis[1,2,5]oxadiazolo[3,4-b:3',4'-3]pyrazine-4-yl)-2,4-dioxo-1,2,4,5-tetrazin-3-amine oxolan-2-one	S2:42
Bis([1,2,5]oxadiazolo)[3,4-b:3',4'-e]pyrazine-4,8-diylbis(methylene) dinitrate	S1:21
Bis(1,2,4-oxadiazolyl) furoxan	S2:43

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

3,6-Bis(1 <i>H</i> -1,2,3,4-tetrazol-5-yl-amino)- <i>s</i> -tetrazine	S1:5
5,5'-Bis(1 <i>H</i> -tetrazolyl)amine	S2:44
5,5'-Bis(1 <i>H</i> -tetrazolyl)hydrazine	S1:17
<i>N</i> ³ , <i>N</i> ⁶ -Bis(1 <i>H</i> -1,2,4-triazol-5-yl)-1,2,4,5-tetrazine-3,6-diamine	S1:32
1,2-Bis(3,4,5-trinitro-1 <i>H</i> -pyrazol-1-yl)ethane	S1:94
1-(2-(Bis(2-(5-((2,2,2-trinitroethyl)amino)-1 <i>H</i> -tetrazol-1-yl)ethyl)amino)ethyl)- <i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine	S1:88
(<i>E</i>)-1,2-Bis(5-(trinitromethyl)-1 <i>H</i> -1,2,4-triazol-3-yl)diazene	S1:77
4,8-Bis(2,4,6-trinitrophenyl)-4 <i>H</i> ,8 <i>H</i> -bis([1,2,5]oxadiazolo)[3,4- <i>b</i> :3',4'- <i>e</i>]pyrazine	S2:45
Bis(3,4,5-trinitropyrazolyl)methane	S2:46
1 <i>H</i> ,1' <i>H</i> -[5,5'-Bitetrazole]-1,1'-diamine	S1:104
1 <i>H</i> ,2' <i>H</i> -[5,5'-Bitetrazole]-1,2'-diamine	S1:105
1,1'-(Butane-1,4-diyl)bis(<i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine)	S1:86
<i>N</i> -((5-Chloro-3,4-dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)- <i>N</i> -methylnitramide	S1:100
1-(2-(4-Chloro-3,5-dinitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:52
Copper(I) 5-nitrotetrazolate	S1:6
(<i>E</i>)- <i>N</i> -(1-Cyclopentyl-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S2:8
3,3'-Diamino-4,4'-azoxyfuran	S1:7
5,7-Diamino-4,6-dinitrobenzofuroxan	S1:8
5,7-Diamino-4,6-dinitrobenzofuroxan dihydrate, sodium salt	S1:2
2,6-Diamino-3,5-dinitropyrazine-1-oxide	S2:32
1,4-Diamino-3,6-dinitropyrazolo[4,3- <i>c</i>]pyrazole	S2:47
3,4-Diaminofuran	S1:9
<i>N,N'</i> -(1,1'-(Diazene-1,2-diyl)bis(3,5-dinitro-1 <i>H</i> -pyrazole-4,1-diyl))bis(<i>N</i> -methylnitramide)	S1:111
1-(2-(3,5-Diazido-4-nitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:83
1,4-Dihydrazino tetrazine	S2:31
Dihydroxylammonium 5,5'-bitetrazole-1,1'-dioxide	S1:10
1,3'-Dimethyl-5,5'-dinitro-1 <i>H</i> ,3' <i>H</i> -4,4'-bi(1,2,3-triazole)	S1:116
2,2'-Dimethyl-5,5'-dinitro-2 <i>H</i> ,2' <i>H</i> -4,4'-bi(1,2,3-triazole)	S1:115
2,3'-Dimethyl-5,5'-dinitro-2 <i>H</i> ,3' <i>H</i> -4,4'-bi(1,2,3-triazole)	S1:47

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

5,5'-Dinitrimino-3,3'-methylene-1 <i>H</i> -1,2,4-triazole	S2:39
5,5'-Dinitro-1 <i>H</i> ,1' <i>H</i> -4,4'-bi(1,2,3-triazole)	S1:73
5,5'-Dinitro-2 <i>H</i> ,2' <i>H</i> -[4,4'-bi(1,2,3-triazole)]-2,2'-diamine	S1:117
5,5'-Dinitro-2 <i>H</i> ,3' <i>H</i> -[4,4'-bi(1,2,3-triazole)]-2,3'-diamine	S1:74
5,5'-Dinitro-3 <i>H</i> ,3' <i>H</i> -[4,4'-bi(1,2,3-triazole)]-3,3'-diamine	S2:25
<i>N,N'</i> -((5,5'-Dinitro-2 <i>H</i> ,2' <i>H</i> -[3,3'-bi(1,2,4-triazole)]-2,2'-diyl)bis(methylene)) bis(<i>N</i> -methylnitramide)	S1:35
(5,5'-Dinitro-2 <i>H</i> ,2' <i>H</i> -[3,3'-bi(1,2,4-triazole)]-2,2'-diyl)bis(methylene) dinitrate	S1:22
<i>N</i> -((2,4-Dinitro-1 <i>H</i> -imidazol-1-yl)methyl)- <i>N</i> -methylnitramide	S1:98
<i>N</i> -((3,5-Dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)- <i>N</i> -methylnitramide	S2:27
<i>N</i> -((4,5-Dinitro-1 <i>H</i> -imidazol-1-yl)methyl)- <i>N</i> -methylnitramide	S2:26
2,4-Dinitro-1 <i>H</i> -imidazole-1,5-diamine	S1:51
1-(3,5-Dinitro-1 <i>H</i> -pyrazol-4-yl)-3-nitroguanidine	S2:4
3,5-Dinitro-1 <i>H</i> -pyrazole-1,4-diamine	S2:20
3,5-Dinitro-1 <i>H</i> -1,2,4-triazol-1-amine	S1:69
4,5-Dinitro-2 <i>H</i> -1,2,3-triazol-2-amine	S1:124
<i>N</i> -((3,5-Dinitro-1 <i>H</i> -1,2,4-triazol-1-yl)methyl)- <i>N</i> -methylnitramide	S1:97
4,6-Dinitrobenzofuroxan	S1:18
5,7-Dinitrobenzo-1,2,3,4-tetrazine-1,3-dioxide	S2:30
Dinitromethyltriazole	S1:11
3(5),4-Dinitropyrazole	S1:12
3,6-Dinitropyrazolo[4,3- <i>c</i>]pyrazole	S1:13
(3,6-Dinitropyrazolo[4,3- <i>c</i>]pyrazole-1,4-diyl)bis(methylene) dinitrate	S2:1
1-(2-(3,4-Dinitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:81
(<i>Z</i>)- <i>N</i> -(1-(2-(3,4-Dinitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S1:53
1-(3,5-Dinitro-1 <i>H</i> -pyrazol-4-yl)guanidine	S1:38
<i>N</i> -((3,4-Dinitro-1 <i>H</i> -pyrazol-1-yl)methyl)- <i>N</i> -methylnitramide	S1:36
<i>N</i> -(3,5-Dinitro-1 <i>H</i> -pyrazol-4-yl)- <i>N</i> -methylnitramide	S2:13

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

<i>N</i> -(3,4-Dinitro-1 <i>H</i> -pyrazol-5-yl)nitramide	S1:114
3,5-Dinitro-1 <i>H</i> -pyrazole	S1:37
3-(Dinitromethyl)-5-nitro-1 <i>H</i> -1,2,4-triazole	S1:76
1,2-Di(1 <i>H</i> -tetrazol-1-yl)diazene	S1:72
1,1'-(Ethane-1,2-diyl)bis(3,5-dinitro-1 <i>H</i> -pyrazol-4-amine)	S1:29
1,1'-(Ethane-1,2-diyl)bis(3,4-dinitro-1 <i>H</i> -pyrazol-5-amine)	S2:28
1,1'-(Ethane-1,2-diyl)bis(<i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine)	S1:27
1,1'-(Ethane-1,2-diyl)bis(oxy))bis(<i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine)	S1:87
Furazano-1,2,3,4-tetrazine-1,3-dioxide	S1:131
(<i>E</i>)- <i>N</i> -(1-(2-Hydroxyethyl)-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S2:7
5-Imino-1-(2 <i>H</i> -tetrazol-5-yl)-1 <i>H</i> -1,2,4-triazole-3,4(5 <i>H</i>)-diamine	S1:49
(<i>E</i>)- <i>N</i> -(1-Methoxy-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S1:57
1-Methoxy- <i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine	S1:85
1-Methyl-3,5-dinitro-1 <i>H</i> -pyrazol-4-amine	S1:39
1-Methyl-5-(1-methyl-2-(2,2,2-trinitroethyl)hydrazinyl)-1 <i>H</i> -tetrazole	S2:9
<i>N</i> -Methyl- <i>N</i> -((3-nitro-5-oxo-1 <i>H</i> -1,2,4-triazol-4(5 <i>H</i>)-yl)methyl)nitramide	S1:63
1-Methyl-5-nitro-1 <i>H</i> -tetrazole	S2:10
2-Methyl-5-nitro-2 <i>H</i> -tetrazole	S1:68
<i>N</i> -(2-Methyl-5-nitro-2 <i>H</i> -1,2,3-triazol-4-yl)nitramide	S2:22
1-Methyl-5-nitro-3-(trinitromethyl)-1 <i>H</i> -1,2,4-triazole	S2:12
<i>N</i> -(2-Methyl-2 <i>H</i> -tetrazol-5-yl)nitramide	S1:96
(<i>E</i>)- <i>N</i> -(1-Methyl-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S1:62
<i>N</i> -Methyl- <i>N</i> -((3,4,4'-trinitro-2' <i>H</i> -[1,3'-bipyrazol]-2'-yl)methyl)nitramide	S1:99
1-Methyl-3,4,5-trinitro-1 <i>H</i> -pyrazole	S1:40
1-Methyl- <i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine	S1:55
6-Nitro-7-azido-pyrazol[3,4- <i>d</i>][1,2,3]triazine-2-oxide	S1:19
(<i>Z</i>)- <i>N</i> -(1-(2-(3-Nitro-5-(nitroamino)-1 <i>H</i> -1,2,4-triazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S1:84
<i>N,N'</i> -((3-Nitro-5-oxo-1 <i>H</i> -1,2,4-triazole-1,4(5 <i>H</i>)-diyl)bis(methylene))bis(<i>N</i> -methylnitramide)	S1:33
1-(2-(3-Nitro-1 <i>H</i> -pyrazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S2:15

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, 19(1): 39-62.

2-(5-Nitro-2 <i>H</i> -tetrazol-2-yl)acetonitrile	S1:119
1-(2-(5-Nitro-2 <i>H</i> -tetrazol-2-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:26
5-((5-Nitro-2 <i>H</i> -tetrazol-2-yl)methyl)-1 <i>H</i> -tetrazole	S1:120
5-Nitro-2 <i>H</i> -tetrazole	S1:67
5-Nitro-2,4,6-triaminopyrimidine-1,3-dioxide	S2:48
1-(2-(3-Nitro-1 <i>H</i> -1,2,4-triazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5-amine	S1:24
(<i>Z</i>)- <i>N</i> -(1-(2-(3-Nitro-1 <i>H</i> -1,2,4-triazol-1-yl)ethyl)-1 <i>H</i> -tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S2:14
<i>N</i> -(5-Nitro-2 <i>H</i> -1,2,3-triazol-4-yl)nitramide	S1:121
3-Nitro-1 <i>H</i> -1,2,4-triazole	S1:101
4-Nitro-1 <i>H</i> -1,2,3-triazole-1,5-diamine	S1:80
5-Nitro-2 <i>H</i> -1,2,3-triazole-2,4-diamine	S1:79
3-Nitro-1,2,4-triazole-5-one	S1:14
5-Nitro-3-(trinitromethyl)-1 <i>H</i> -1,2,4-triazole	S1:75
1-((<i>Z</i>)-5-(Nitroimino)-2,5-dihydro-1 <i>H</i> -tetrazol-1-yl)-3-((<i>E</i>)-5-(nitroimino)-4,5-dihydro-1 <i>H</i> -tetrazol-1-yl)propan-2-yl nitrate	S1:93
<i>N</i> -((<i>E</i>)-1-(3-((<i>Z</i>)-5-(Nitroimino)-4,5-dihydro-1 <i>H</i> -tetrazol-1-yl)propyl)-1,4-dihydro-5 <i>H</i> -tetrazol-5-ylidene)nitramide	S1:92
(6-Oxo-5 <i>H</i> -imidazo[4,5- <i>b</i>][1,2,5]oxadiazolo[3,4- <i>e</i>]pyrazine-5,7(6 <i>H</i>)-diyl)bis(methylene) dinitrate	S1:78
1,1'-(Oxybis(methylene))bis(4-chloro-3,5-dinitro-1 <i>H</i> -pyrazole)	S1:107
1,1'-(Oxybis(methylene))bis(5-chloro-3-nitro-1 <i>H</i> -1,2,4-triazole)	S1:43
1,1'-(Oxybis(methylene))bis(4,5-dinitro-1 <i>H</i> -imidazole)	S1:108
1,1'-(Oxybis(methylene))bis(3,5-dinitro-1 <i>H</i> -pyrazol-4-amine)	S2:21
1,1'-(Oxybis(methylene))bis(3,4-dinitro-1 <i>H</i> -pyrazole)	S1:41
1,1'-(Oxybis(methylene))bis(3,5-dinitro-1 <i>H</i> -pyrazole)	S1:42
2,2'-(Oxybis(methylene))bis(5-nitro-2 <i>H</i> -tetrazole)	S2:5
1,1'-(Oxybis(methylene))bis(3-nitro-1 <i>H</i> -1,2,4-triazole)	S1:44
2,2'-(Oxybis(methylene))bis(5-(trinitromethyl)-2 <i>H</i> -tetrazole)	S1:106
Potassium 5-nitrotetrazolate	S2:49
1,1'-(Propane-1,3-diyl)bis(<i>N</i> -(2,2,2-trinitroethyl)-1 <i>H</i> -tetrazol-5-amine)	S1:56
Silver nitrotetrazolate	S1:15
Sodium 5-nitrotetrazolate dihydrate	S1:16
3,4:7,8:11,12:15,16-Tetrafurazano-1,2,5,6,9,10,13,14-octaazacyclohexadeca-1,3,5,7,9,11,13,15-octane-1,10-dioxide	S2:29

Central European Journal of Energetic Materials

ISSN 1733-7178; e-ISSN 2353-1843

Supporting Information (SI) for *Cent. Eur. J. Energ. Mater.* **2022**, *19*(1): 39-62.

6,6'-{1,2,4,5-Tetrazine-3,6-diylbis[(4 <i>H</i> ,8 <i>H</i> -bis[1,2,5]oxadiazolo[3,4- <i>b</i> :3',4'- <i>e</i>]pyrazine-8,4-diyl)]}bis(2,4-dioxo-1,2,4,5-tetrazin-3-amine)	S1:132
<i>N</i> -(1 <i>H</i> -Tetrazol-5(4 <i>H</i>)-ylidene)nitramide	S1:61
1-((1 <i>H</i> -1,2,3-Triazol-1-yl)diazenyl)-1 <i>H</i> -tetrazole	S1:113
3,4,5-Trinitro-1 <i>H</i> -pyrazol-1-ol	S1:60
3,4,5-Trinitro-1 <i>H</i> -pyrazole	S1:31
<i>N</i> -(2,2,2-Trinitroethyl)-1 <i>H</i> -tetrazol-1-amine	S2:11
<i>N</i> -(2,2,2-Trinitroethyl)-1 <i>H</i> -tetrazol-5-amine	S1:54
2-(5-((2,2,2-Trinitroethyl)amino)-1 <i>H</i> -tetrazol-1-yl)ethanol	S2:17

References

Note: Reference numbers are given according to the enumeration in the main part of this paper.

[4] Klapötke, T.M. *Energetic Materials Encyclopedia*. 2nd ed., Walter de Gruyter GmbH, Berlin/Boston, **2021**; ISBN 978-3-11-067245-9.

[18] Zohari, N.; Abrishami, F.; Zeynali, V. Prediction of Decomposition Temperature of Azole-based Energetic Compounds in Order to Assess of Their Thermal Stability. *J. Therm. Anal. Calorim.* **2020**, *141*: 1453-1463.

Received: August 11, 2021

First published online: March 29, 2022