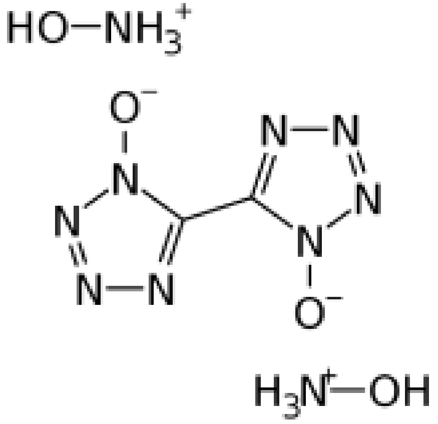
Energetic Polynitrogen Heterocycles: Synthesis and Performance

Leonid L. Fershtat, Alexander A. Larin, Daniil A. Chaplygin, Dmitry M. Bystrov, Nikita V. Muravyev

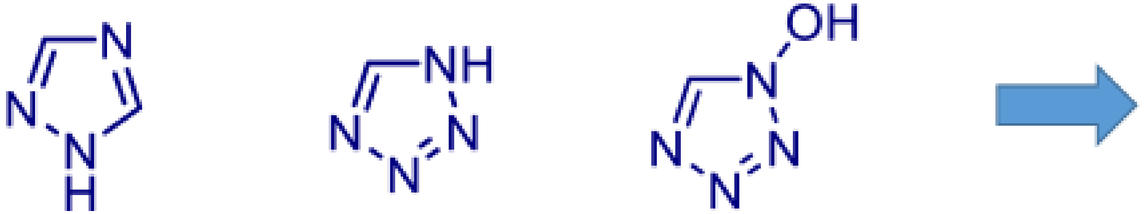
N. D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences

X International Voevodsky Conference "Physics and Chemistry of Elementary Chemical Processes" (VVV-2022)
Novosibirsk 05.09-09.09.2022

Energetic polynitrogen heterocycles

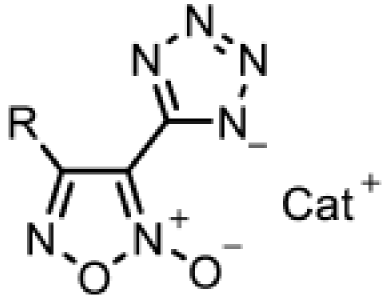


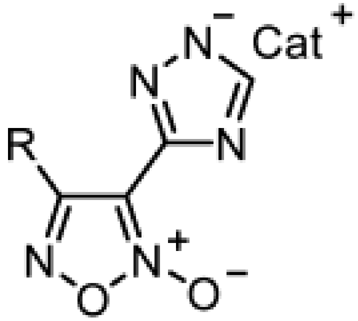
TKX-50
ρ = 1.92 g cm^{-3}
D = 9.7 km s^{-1}
P = 42.5 GPa

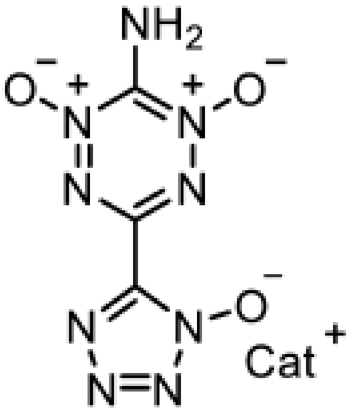


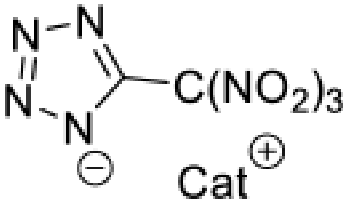
energetic salts

Content

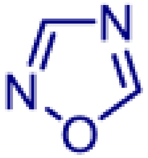






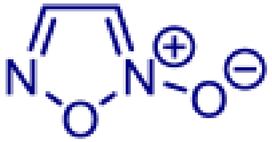


Enthalpies of formation for different azoles

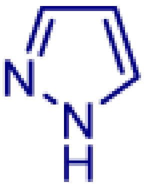


100.6 kJ mol^{-1}

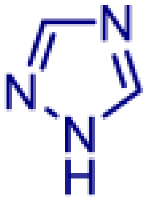
216.9 kJ mol^{-1}



226.0 kJ mol^{-1}

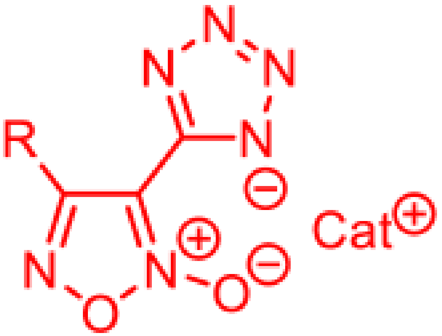


160.4 kJ mol^{-1}



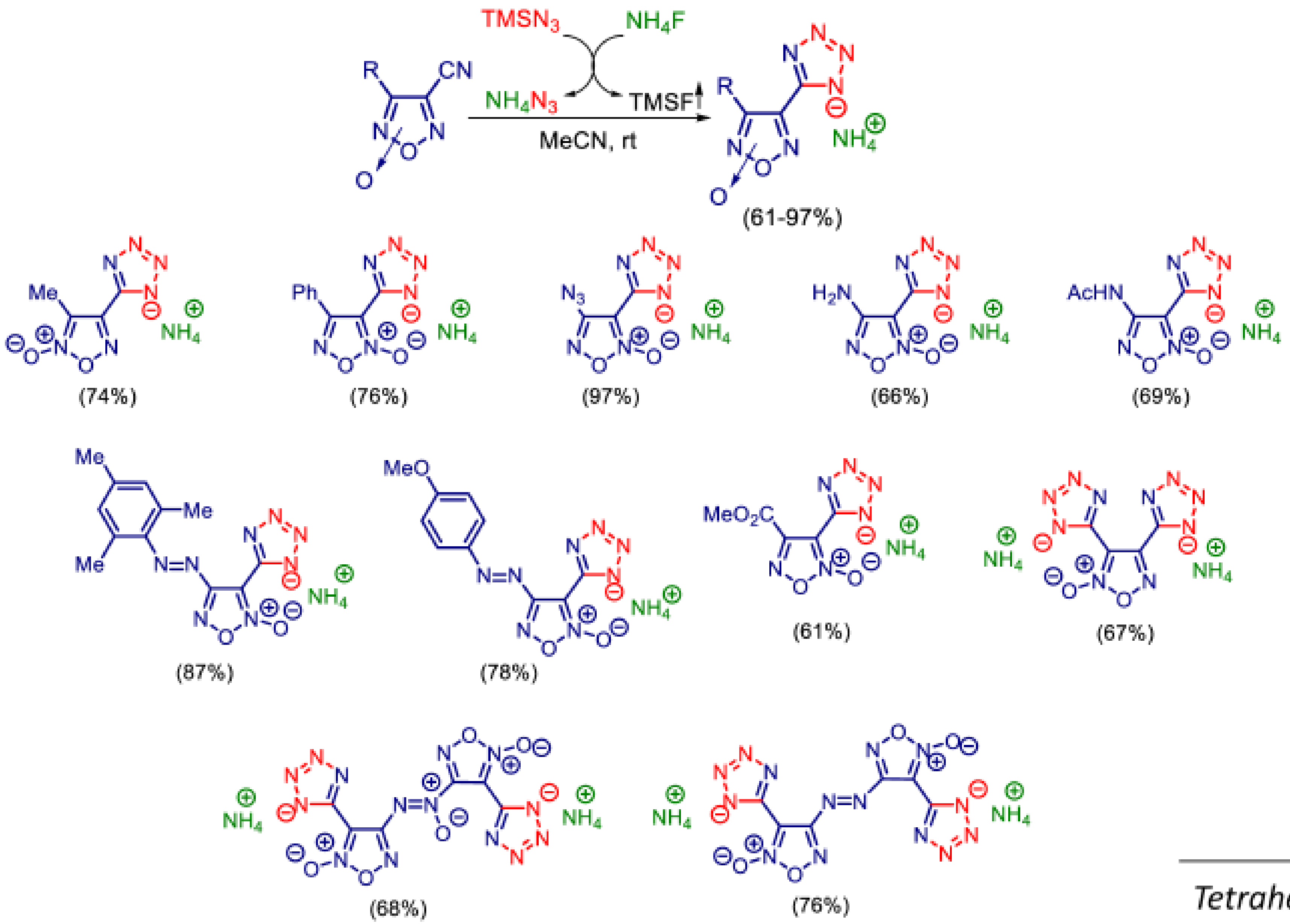
182.7 kJ mol^{-1}

333.3 kJ mol^{-1}



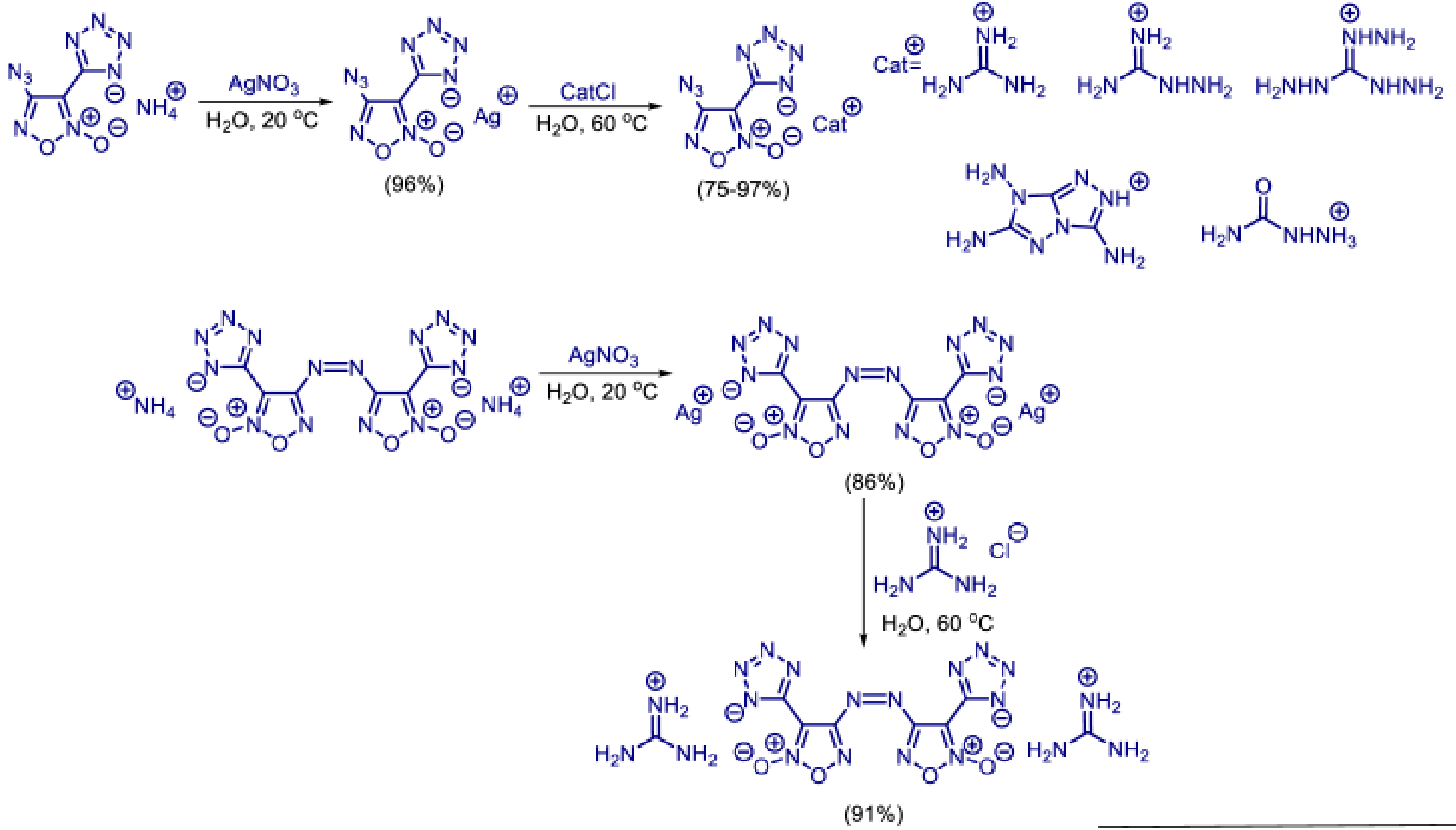
- **High ΔH_f^o**
- **High nitrogen content**

Assembly of tetrazolylfuroxan core



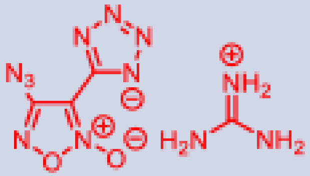
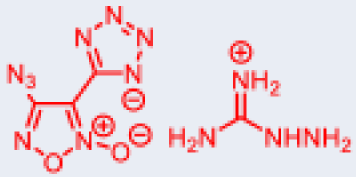
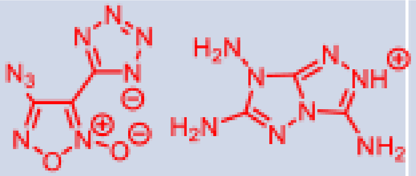
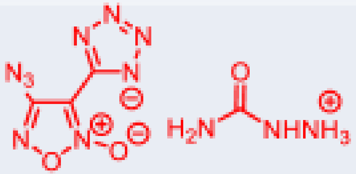
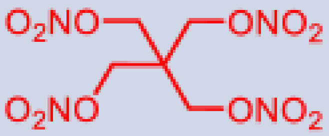
Tetrahedron, **2015**, *71*, 6764

Modification of energetic tetrazolylfuroxan salts



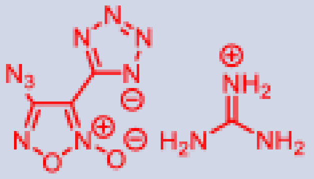
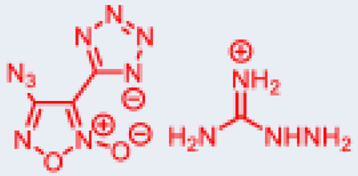
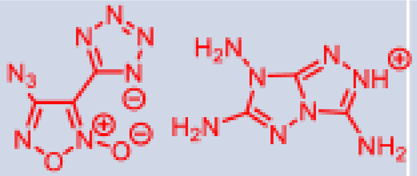
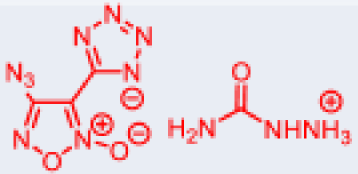
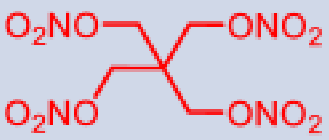
Chem. Eur. J., **2019**, *25*, 4225

Physicochemical parameters and detonation performance (secondary explosives)

	T_d [°C]	ρ [g cm^{-3}]	Ω_{CO} [%]	Ω_{CO2} [%]	N [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1} (kJ g^{-1})]	D [km s^{-1}]	P [GPa]	IS [J]	FS [N]
	166	1.59	-31.5	-56.7	66.1	818 (3.2)	7.54	23.4	29	240
	129	1.56	-32.7	-56.5	67.6	926 (3.4)	7.60	23.4	17	>360
	115	1.67	-34.4	-61.9	68.1	1363 (3.9)	7.76	25.5	5.4	251
	139	1.70	-23.7	-47.4	62.2	857 (3.2)	8.07	27.9	5.0	116
	165	1.78	15.2	-10.1	17.7	-561 (-1.8)	8.40	31.9	3.3	70

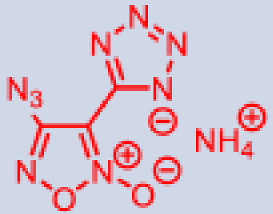
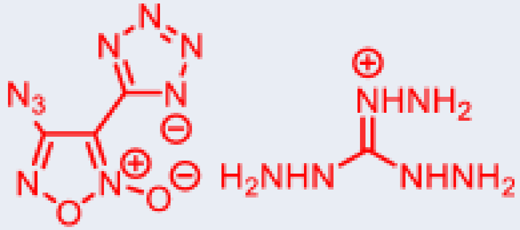
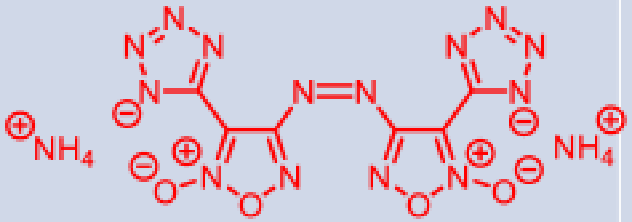
Chem. Eur. J., **2019**, *25*, 4225

Physicochemical parameters and detonation performance (secondary explosives)

	T_d [°C]	ρ [g cm^{-3}]	Ω_{CO} [%]	Ω_{CO2} [%]	N [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1} (kJ g^{-1})]	D [km s^{-1}]	P [GPa]	IS [J]	FS [N]
	166	1.59	-31.5	-56.7	66.1	818 (3.2)	7.54	23.4	29	240
	129	1.56	-32.7	-56.5	67.6	926 (3.4)	7.60	23.4	17	>360
	115	1.67	-34.4	-61.9	68.1	1363 (3.9)	7.76	25.5	5.4	251
	139	1.70	-23.7	-47.4	62.2	857 (3.2)	8.07	27.9	5.0	116
	165	1.78	+15.2	-10.1	17.7	-561 (-1.8)	8.40	31.9	3.3	70

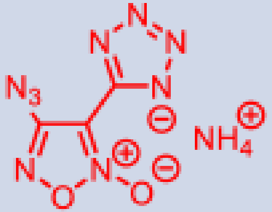
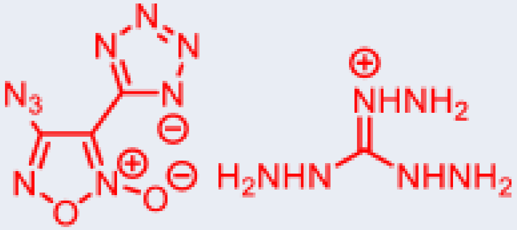
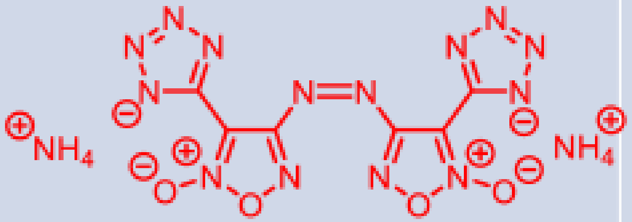
Chem. Eur. J., **2019**, *25*, 4225

Physicochemical parameters and detonation performance (primary explosives)

	T_d [°C]	ρ [g cm^{-3}]	Ω_{CO} [%]	N [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1} (kJ g^{-1})]	D [km s^{-1}]	P [GPa]	IS [J]	FS [N]
	168	1.71	-22.6	66.0	857 (4.0)	8.26	29.3	2.2	49
	133	1.57	-34.7	70.2	1141 (3.8)	7.90	25.4	2.7	43
	173	1.69	-26.1	60.8	1104 (3.0)	7.68	24.6	1.5	129
$Pb(N_3)_2$	315	4.80	-11.0	28.9	450 (1.6)	5.88	33.4	~2	0.3-0.5

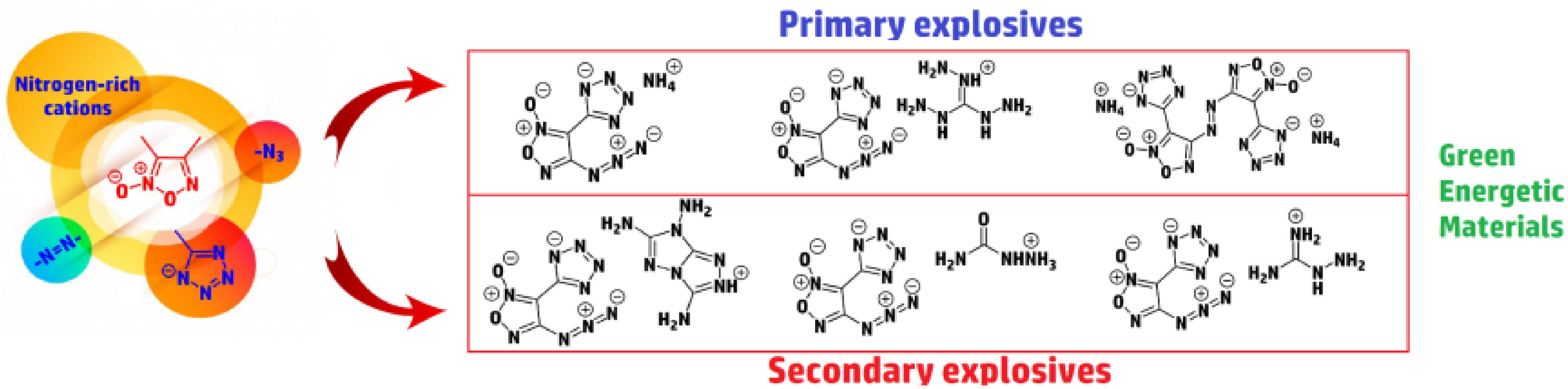
Chem. Eur. J., **2019**, *25*, 4225

Physicochemical parameters and detonation performance (primary explosives)

	T_d [°C]	ρ [g cm^{-3}]	Ω_{CO} [%]	N [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1} (kJ g^{-1})]	D [km s^{-1}]	P [GPa]	IS [J]	FS [N]
	168	1.71	-22.6	66.0	857 (4.0)	8.26	29.3	2.2	49
	133	1.57	-34.7	70.2	1141 (3.8)	7.90	25.4	2.7	43
	173	1.69	-26.1	60.8	1104 (3.0)	7.68	24.6	1.5	129
$Pb(N_3)_2$	315	4.80	-11.0	28.9	450 (1.6)	5.88	33.4	~2	0.3-0.5

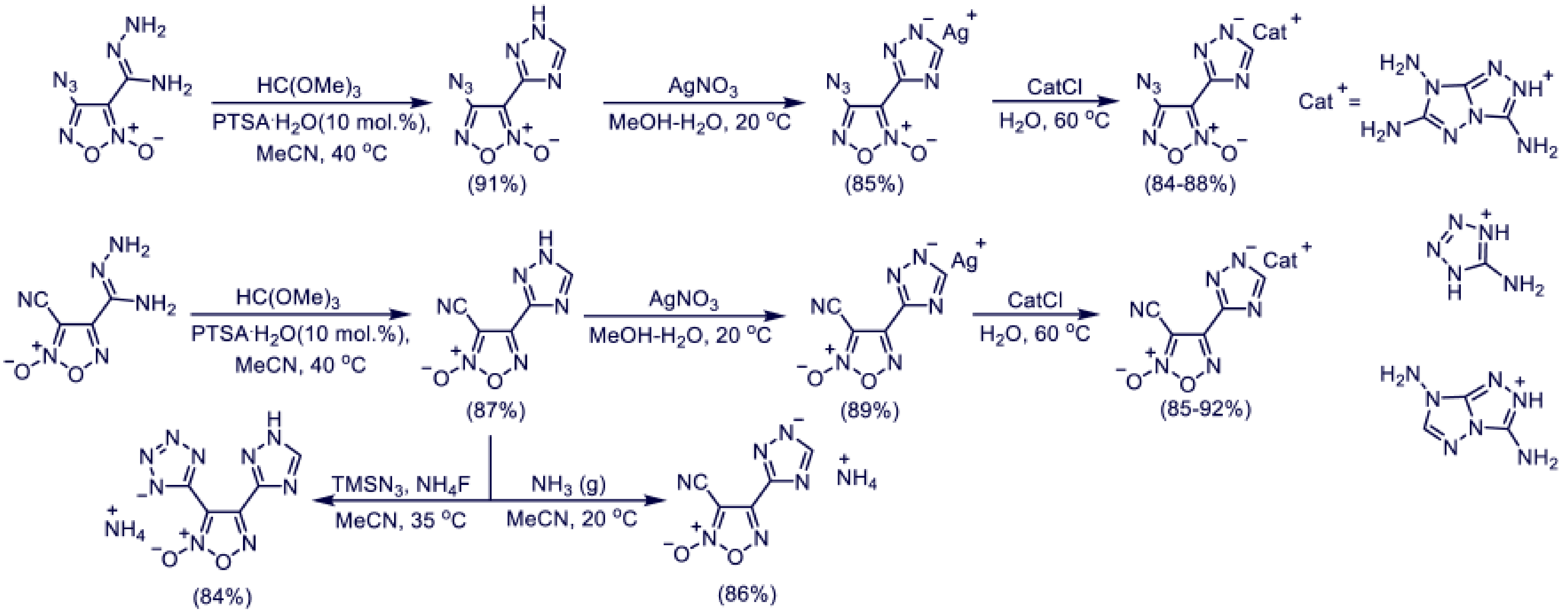
Chem. Eur. J., **2019**, *25*, 4225

Influence of the cation



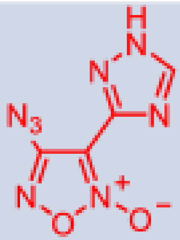
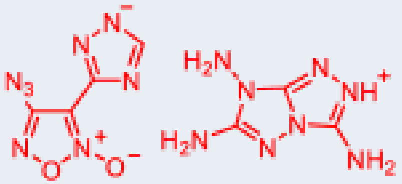
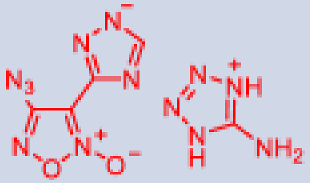
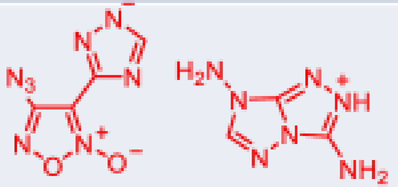
Chem. Eur. J., **2019**, 25, 4225

Energetic (1,2,4-triazolyl)furoxan salts

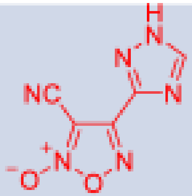
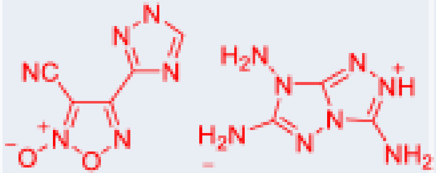
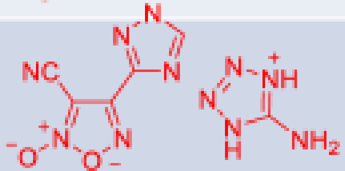
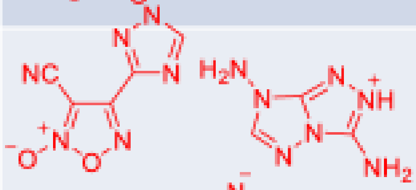
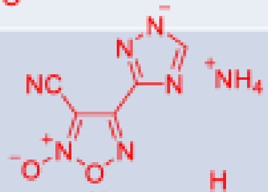
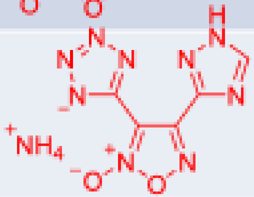


Front. Chem., **2022**, *doi: 10.3389/fchem.2022.1012605*

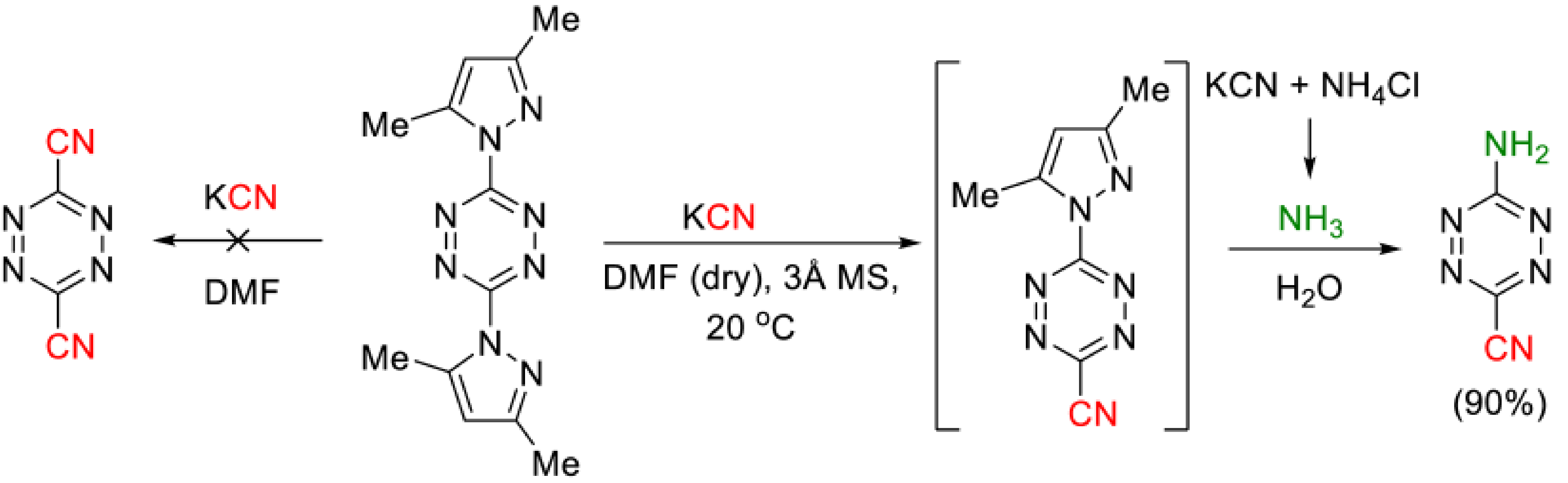
Physicochemical parameters and detonation performance

	T_d [°C]	ρ [g cm^{-3}]	N [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1} (kJ g^{-1})]	D [km s^{-1}]	P [GPa]	IS [J]	FS [N]
	154	1.70	57.7	623 (3.2)	8.0	29	4	270
	155	1.68	64.4	1044 (3.0)	7.9	27	8	> 360
	150	1.80	65.2	896 (3.2)	8.4	32	9	> 360
	152	1.68	63.1	1095 (3.3)	7.9	28	5	260

Physicochemical parameters and detonation performance

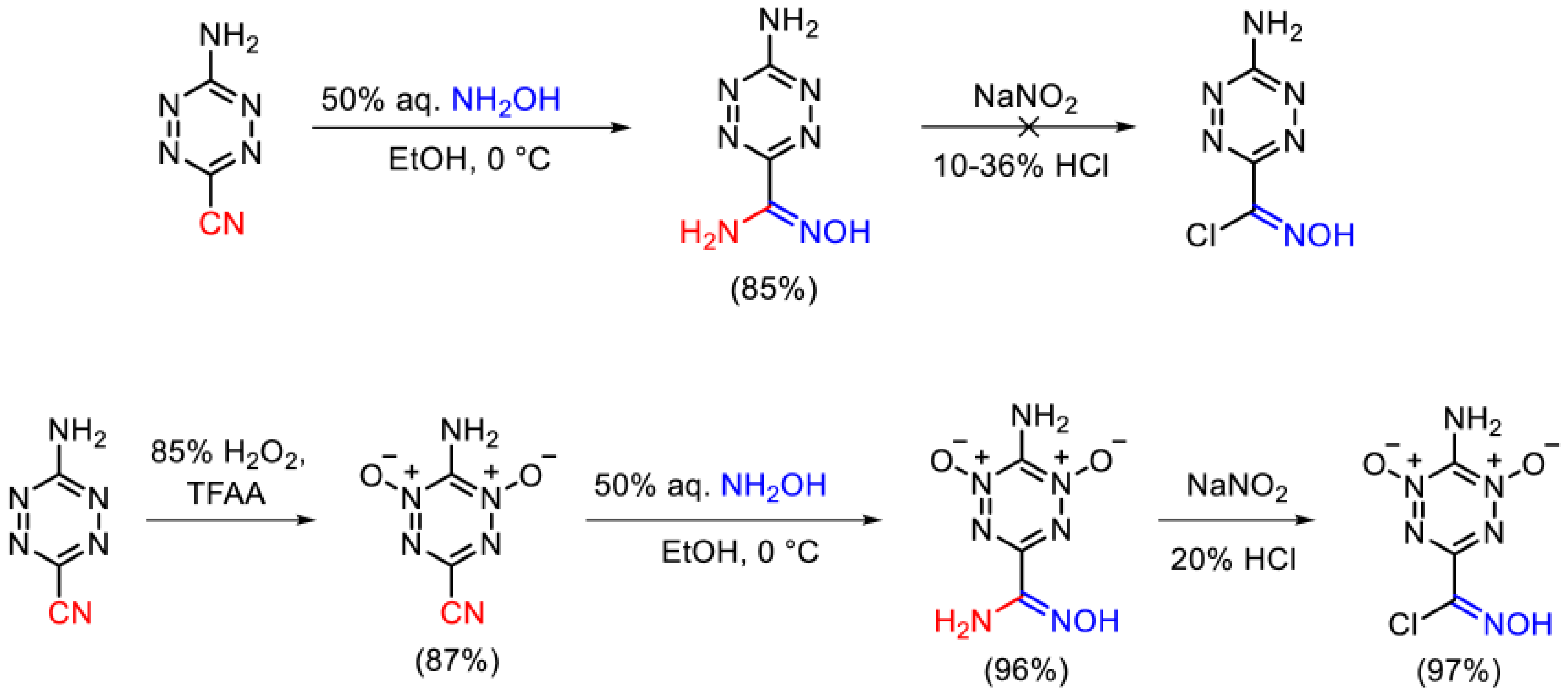
	T_d [°C]	ρ [g cm^{-3}]	N [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1} (kJ g^{-1})]	D [km s^{-1}]	P [GPa]	IS [J]	FS [N]
	229	1.55	47.2	453 (2.5)	7.0	22	19	220
	153	1.68	59.0	834 (2.5)	7.5	25	14	290
	172	1.76	58.6	703 (2.7)	7.9	29	21	250
	154	1.66	57.4	887 (2.8)	7.5	26	22	350
	232	1.61	50.3	344 (1.8)	7.2	23	11	260
	217	1.64	58.8	467 (2.0)	7.5	24	12	>360

Synthesis of 3-amino-6-cyanotetrazine



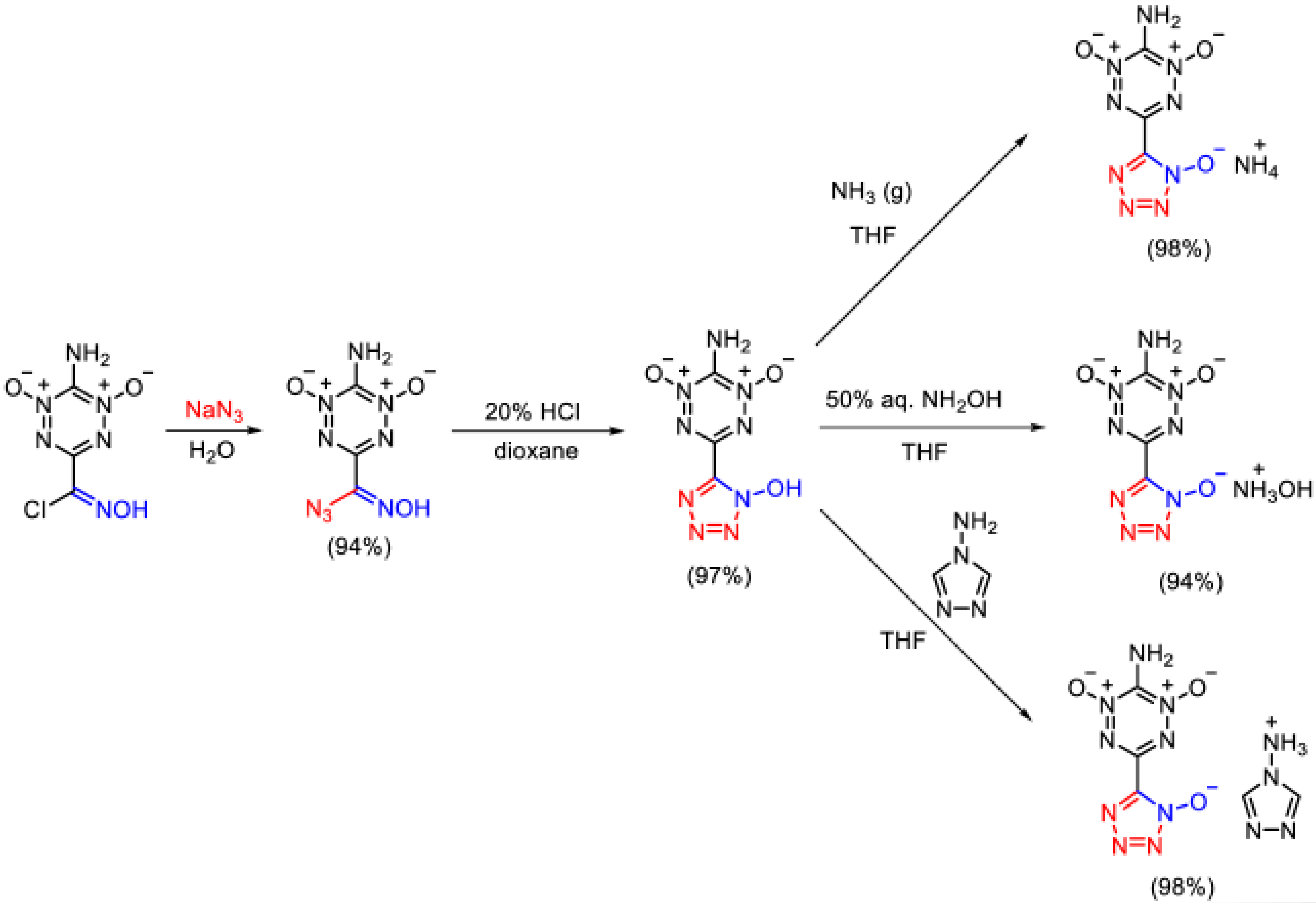
Molecules, **2022**, *accepted*

Preparation of (chloroximino)tetrazines



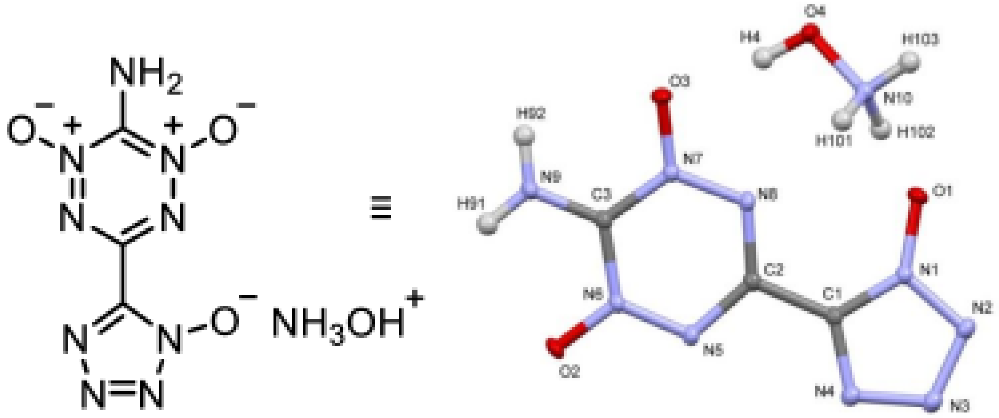
Molecules, **2022**, *accepted*

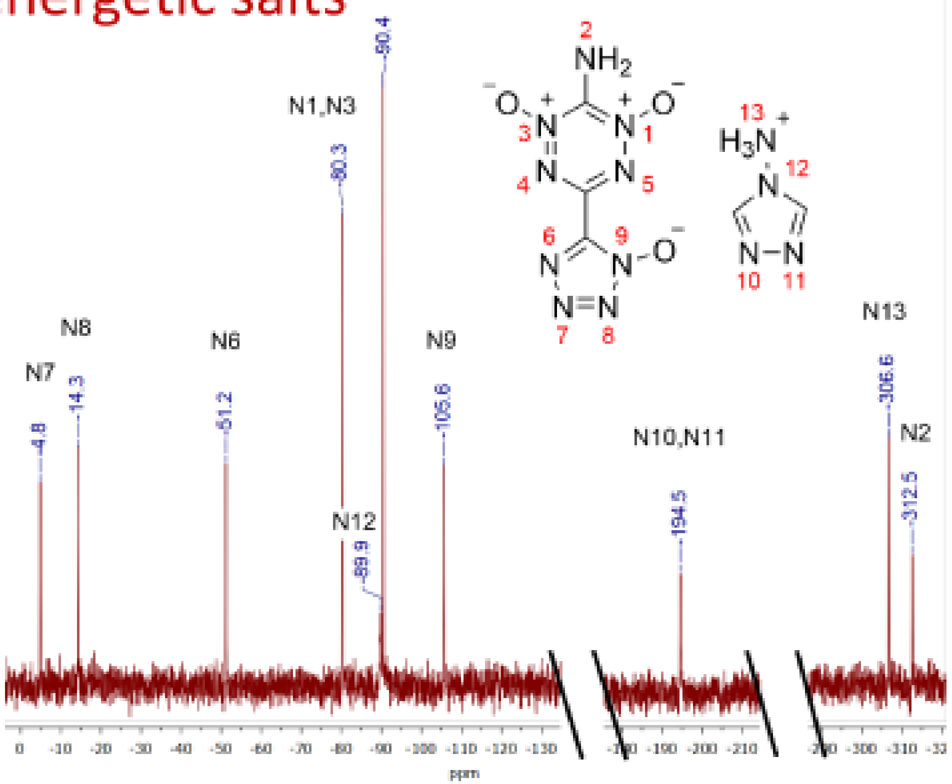
Assembly of tetrazinedioxide-hydroxytetrazole energetic salts



Molecules, **2022**, *accepted*

Physicochemical properties of energetic salts

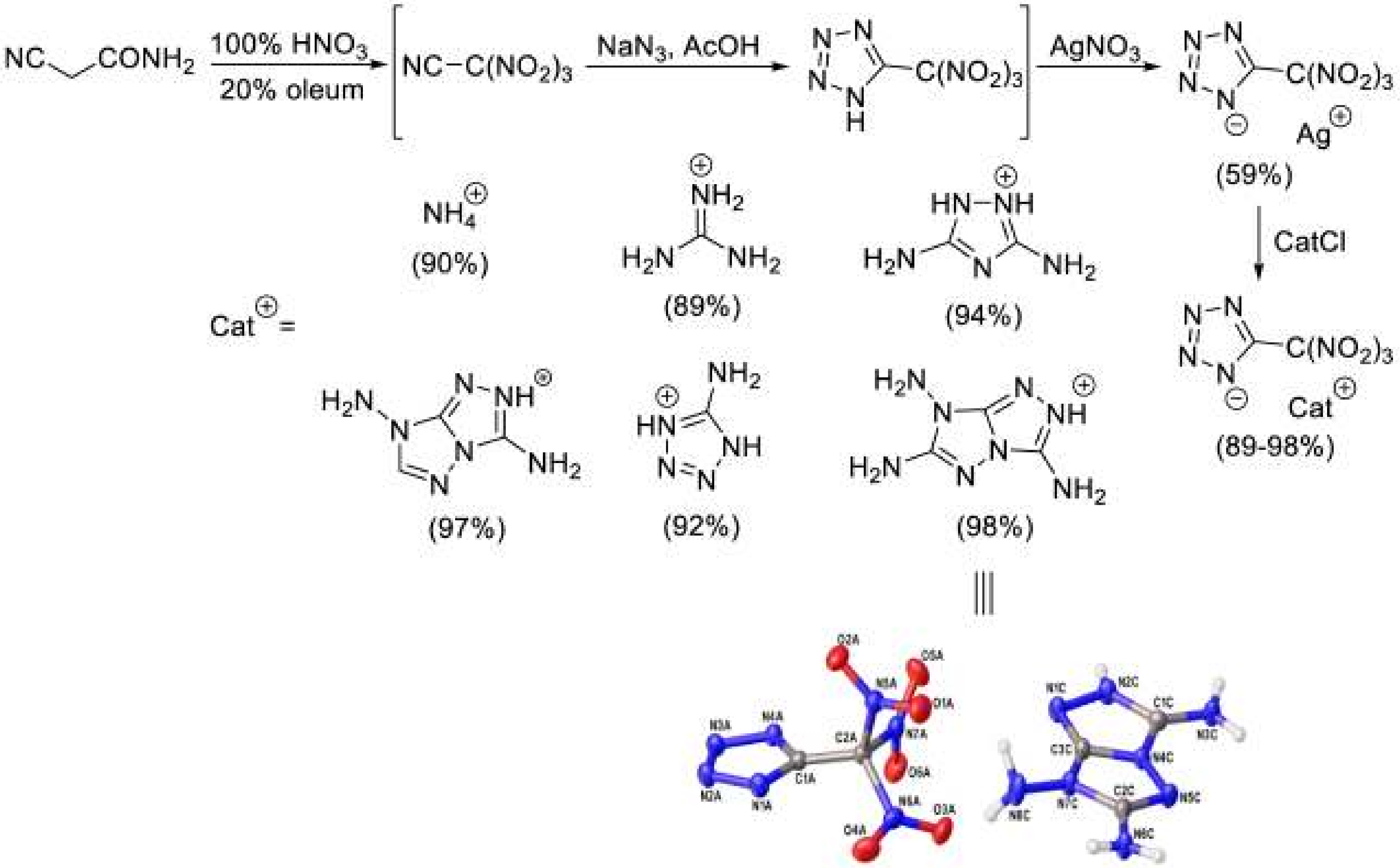




	T_d	ρ, g cm^{-3}	[N], %	[N+O], %	Ω_{CO}, %	$\Delta H_f°$, kJ mol^{-1}	D, km s^{-1}	P, GPa	IS, J	FS, N
NH_4^+ →	212	1.75	60.9	81.7	-20.9	416.5	8.5	31	9	265
NH_3OH^+ →	195	1.78	56.9	82.9	-13.0	413.1	8.8	33	10	190
 →	206	1.77	61.3	77.4	-29.6	779.2	8.5	32	15	260
RDX	204	1.81	37.8	81.1	0	68.0	8.8	34	10	130

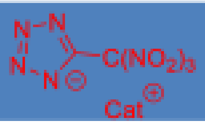
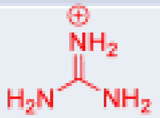
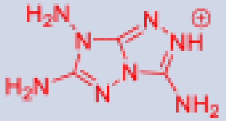
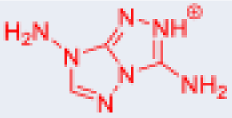
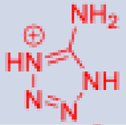
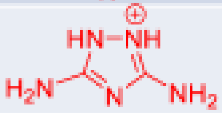
Molecules, **2022**, *accepted*

Nitrogen-oxygen-rich salts of trinitromethyltetrazole



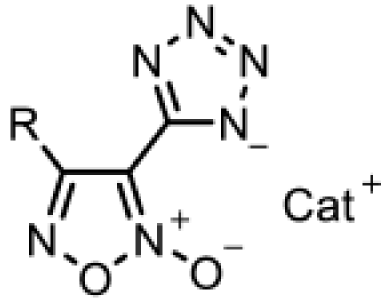
Dalton Trans., **2021**, 50, 13778-13785

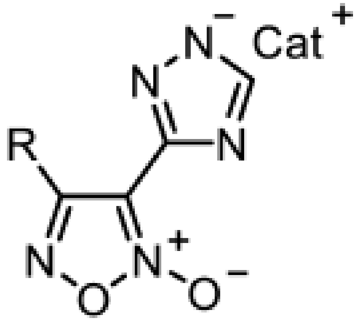
Nitrogen-oxygen-rich salts of trinitromethyltetrazole

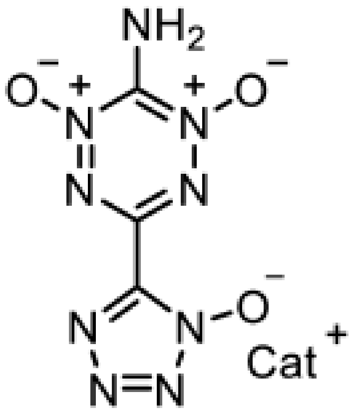
	T_d [°C]	ρ [g cm^{-3}]	Ω_{CO} [%]	N + O [%]	$\Delta H^0_{f,solid}$ [kJ mol^{-1}]	D [km s^{-1}]	P [GPa]	FS [N]
$NH_4^{\oplus}$	126	1.768	+13.6	88.1	188.2	9.1	36.2	6
	114	1.845	0	84.9	139.6	9.0	36.9	25
	136	1.728	-10.7	82.0	683.4	8.5	31.6	40
	118	1.648	-8.9	81.6	725.5	8.2	28.5	50
	112	1.816	+5.3	86.8	551.7	9.2	37.8	7
	124	1.698	-5.0	83.0	347.1	8.3	29.8	50
PETN	181	1.780	+15.2	78.5	-561.0	8.4	31.9	70
$Pb(N_3)_2$	315	4.800	-11.0	28.9	450.0	5.9	33.4	< 5

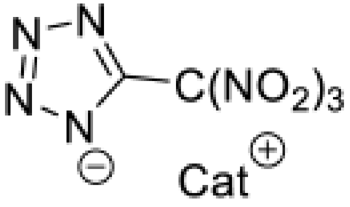
Dalton Trans., **2021**, 50, 13778-13785

Summary









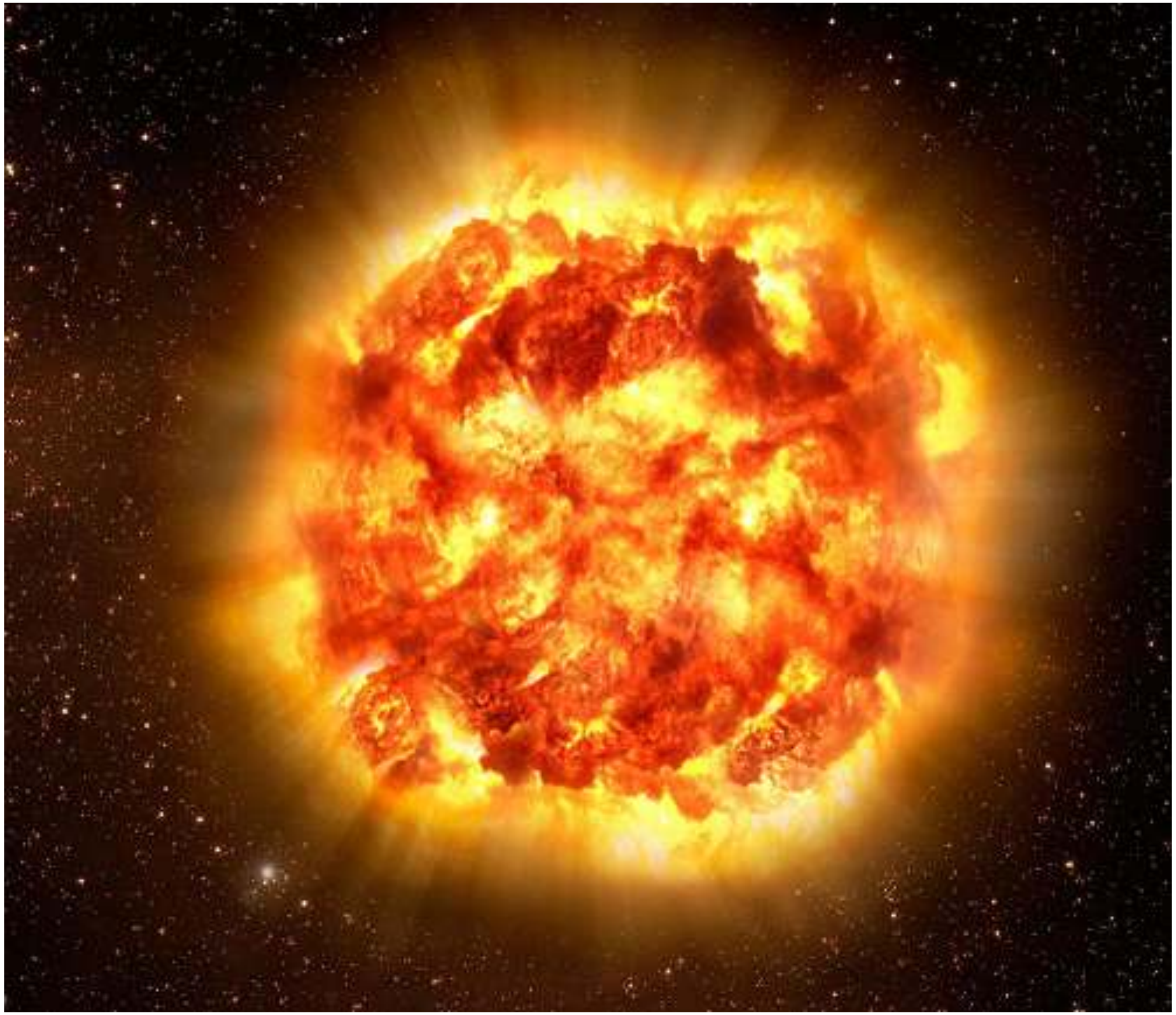
multipurpose heterocycle-based high-energy materials

THANK YOU FOR YOUR ATTENTION

РНФ

РФФИ

https://nc-lab.ru/



THANK YOU FOR YOUR ATTENTION