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Derivatives of 5-Nitro-1,2,3-2H-triazole – High Performance Energetic Materials

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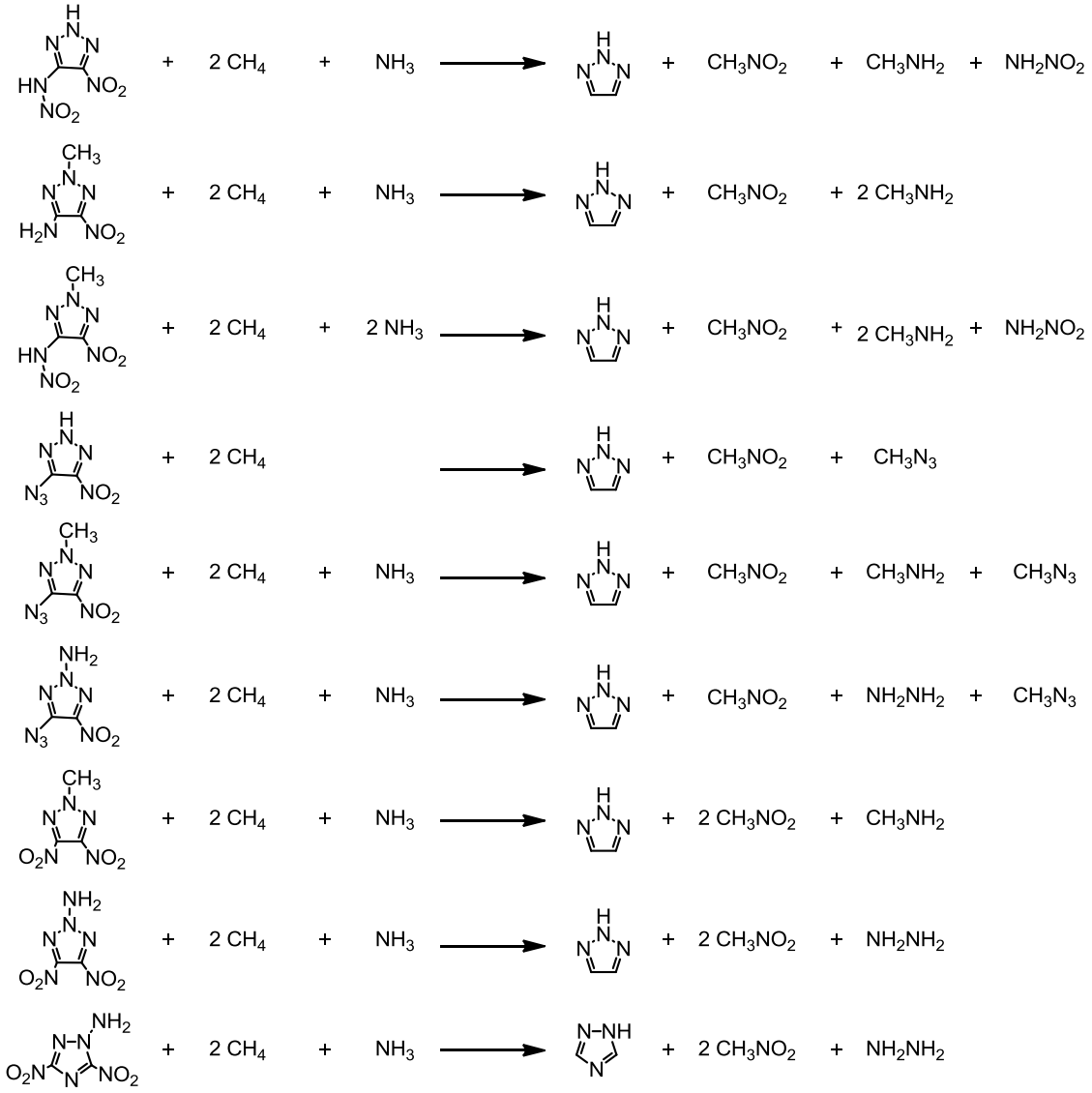
Computational Data

S-1 - Scheme 1s. Isodesmic reactions for the derivatives of 5-nitro-1,2,3-2H-triazole and 3,5-dinitro-1,2,4-1H-triazole.

S-2 - Table 1s. Calculated (MP2/6-311++G** // B3LYP/6-31+G**) total energy (E_0), zero-point energy (ZPE), values of thermal correction (H_T), and heats of formation (HoF) of the derivatives of 5-nitro-1,2,3-2H-triazole and 3,5-dinitro-1,2,4-1H-triazole.



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Name	E_0 [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	HoF [kJ/mol]
NH_2NO_2	-260.4931748	0.039257	0.043909	-6.1[a]
CH_3NH_2	-95.59384	0.06403	0.06840	-23.5[b]
CH_3NO_2	-244.478482	0.049842	0.055138	-81.0 [b]
CH_3N_3	-203.60768	0.05025	0.05567	296.5[a]
NH_2NH_2	-111.5836915	0.05331	0.057521	95.4[b]
NH_3	-56.4154647	0.034384	0.038203	-45.9[b]
CH_4	-40.3796220	0.044793	0.048605	-74.6 [b]
1,2,3-2H-triazole	-241.63672	0.05903	0.06358	267.6[a]
12,4-1H-triazole	-241.6632438	0.059886	0.064393	192.7[b]
4-nitramino-5-nitro-1,2,3-2H-triazole	-705.0431379	0.09203	0.07823	302.4
2-methyl-4-amino-5-nitro-1,2,3-2H-triazole	-540.1730305	0.106545	0.116537	208.2
2-methyl-4-nitramino-5-nitro-1,2,3-2H-triazole	-744.2420841	0.108862	0.121272	268.5
4-azido-5-nitro-1,2,3-2H-triazole	-608.9727498	0.065215	0.07471	602.4
2-methyl-4-azido-5-nitro-1,2,3-2H-triazole	-648.1716397	0.092575	0.103906	568.6
2-amino-4-azido-5-nitro-1,2,3-2H-triazole	-664.1671349	0.081087	0.092307	670.8
2-methyl-4,5-dinitro-1,2,3-2H-triazole	-689.0234399	0.091674	0.103094	240.2
2-amino-4,5-dinitro-1,2,3-2H-triazole	-705.0185478	0.080331	0.091534	343.6
2-amino-3,5-dinitro-1,2,4-1H-triazole	-705.0372789	0.080597	0.091386	286.7

[a] Data from NIST Chemistry WebBook. [b] Data calculated with the G2 method by using the Gaussian 03 program.