Synthesis and Properties of 3,4,5-Trinitropyrazole-1-ol and Its Energetic Salts

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Part A: Computational Data

S-1 - Scheme 1s. Isodesmic reactions for 3,4,5-trinitropyrazole and 3,4,5-trinitropyrazolate anion.

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 3,4,5-trinitropyrazole-1-ol, 3,4,5-trinitropyrazole, 3,4,5-trinitropyrazole-1-olate, and 3,4,5-trinitropyrazolate.

Part B: Crystallographic Figures

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Part C: Crystallographic Data

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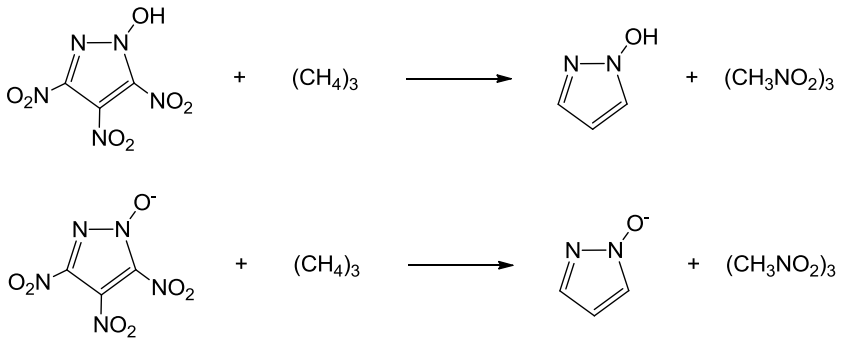

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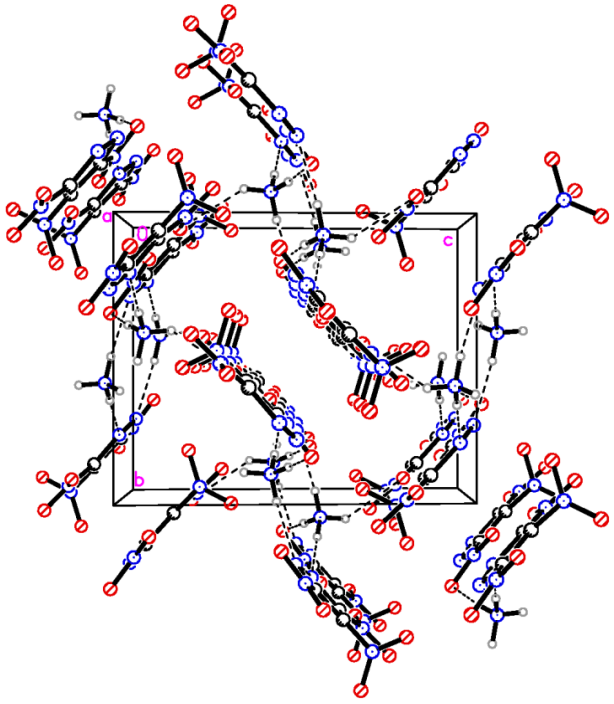
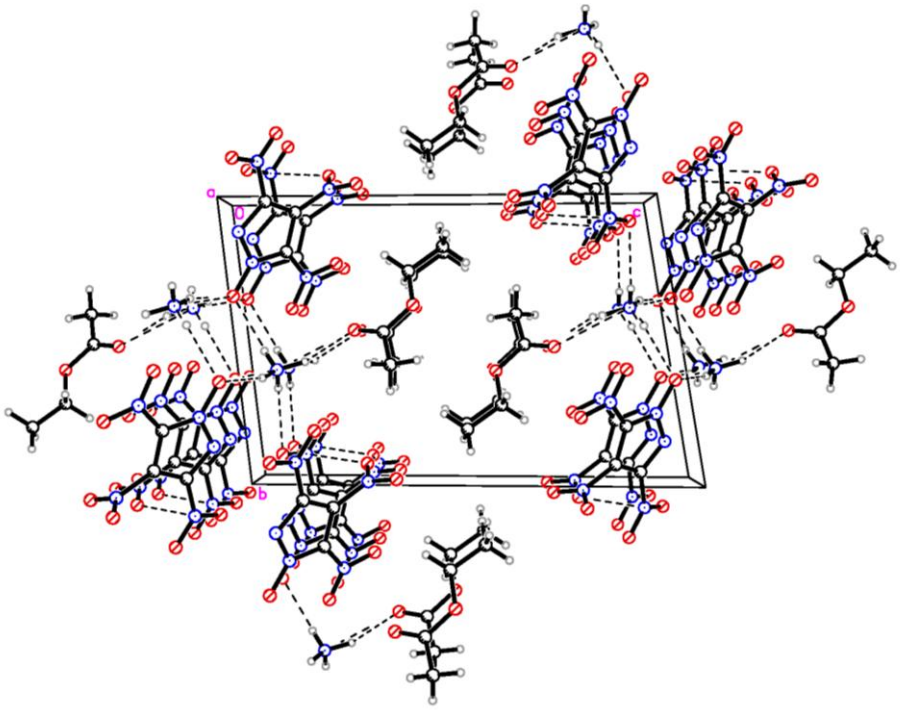
Name	E_0 [Hartree/Particle]	ZPE [Hartree/Particle]	H_T [Hartree/Particle]	HoF [kJ/mol]
CH_3NO_2	-244.478482	0.049842	0.055138	-81.0 (gas phase)[a]
CH_4	-40.3796220	0.044793	0.048605	-74.6 (gas phase) [a]
pyrazole-ol	-300.641835	0.074160	0.080285	167.6 (gas phase) [b]
pyrazole	-225.6230236	0.071265	0.075955	179.4 (gas phae)[a]
pyrazole-olate	-300.083167	0.061064	0.066396	70.43 (gas phase) [b]
pyrazolate	-225.0498361	0.056611	0.061165	124.2 (gas phae) [b]
3,4,5-trinitropyrazole-1-ol	-912.912525	0.081229	0.094636	203.5 (gas phase) 118.5 (solid phase)
3,4,5-trinitropyrazole	-837.9002801	0.078107	0.090481	218.6 (gas phase) 133.6 (solid phase)
3,4,5-trinitropyrazole-1-olate	-912.429959	0.068552	0.081650	-91.21 (gas phase)
3,4,5-trinitropyrazolate	-837.414305	0.064524	0.076672	-63.1 (gas phase)

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



S-3 - Figure 1s. Ball and stick packing diagram of ammonium 3,4,5-trinitropyrazolate viewed down the a axis. Dashed lines indicate strong hydrogen bonding.



S-4 - Figure 2s. Ball and stick packing diagram of ammonium 3,4,5-trinitropyrazole-olate viewed down the a axis. Dashed lines indicate strong hydrogen bonding.

S-5 - Table 2s. Hydrogen bond data for ammonium 3,4,5-trinitropyrazolate [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(1S)-H(1SA)...N(2)	0.91(2)	2.07(2)	2.9733(18)	171.4(18)
N(1S)-H(1SB)...N(1)#1	0.921(19)	1.99(2)	2.9137(17)	177.4(16)
N(1S)-H(1SC)...O(7)#2	0.93(2)	2.20(2)	3.0951(17)	162.2(18)
N(1S)-H(1SD)...O(14)#3	0.85(2)	2.52(2)	3.2511(18)	143.8(18)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y,-z+1 #2 -x+2,-y,-z+1 #3 x+1/2,-y+1/2,z-1/2

S-6 - Table 3s. Hydrogen bond data for ammonium 3,4,5-trinitropyrazole-olate [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(22)-H(22A)...O(16)	0.96(3)	1.95(3)	2.875(2)	162(2)
N(22)-H(22B)...O(6)	0.93(3)	2.01(3)	2.910(2)	163(2)
N(22)-H(22C)...O(6)#1	0.86(3)	2.10(3)	2.891(2)	153(2)

Symmetry transformations used to generate equivalent atoms:
#1 -x+1,-y+1,-z+2

S-7 - Table 4s. Hydrogen bond data for triazolium 3,4,5-trinitropyrazole-olate [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N(17)-H(17)...O(6)#1	0.88	2.04	2.886(2)	161.6
N(19)-H(19)...O(6)#2	0.88	1.90	2.666(2)	145.1

Symmetry transformations used to generate equivalent atoms:
#1 -x-5/2,-y-2,z-1/2 #2 x+1/2,-y-3/2,-z-1