

Supplementary Material (ESI) for New Journal of Chemistry
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Supporting Information

Structure and Synthesis of Energetic Salts of N,N'-dinitrourea (DNU)

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S2 Table 1 G3 enthalpy ($H_{298}(G3)$), experimental & calculated heats of formation of energetic salts.

S3 Table 2 G3MP2 enthalpy ($H_{298}(G3MP2)$), experimental & calculated heats of formation of energetic salts.

Table 1 G3 enthalpy ($H_{298}(\text{G3})$), experimental & calculated heats of formation of

Species	$H_{298}(\text{G3})^a$	$\Delta H_f^{\text{Exp.}}^b$ (KJ/mol)	$\Delta H_f^{\text{calcd.}}^c$ (KJ/mol)	energ etic salts.
CH4	-40.45381	-74.87		
C2H6	-79.71891	-83.80		
CH2=CH2	-78.50342	52.47		
CH2=NH	-94.55099		89.87	
CH3NH2	-95.75573	-23.01		
CH3NH3	-96.09702	609.10		
CH3(+) ^(1P)	-39.42678	1101.79		
NH3	-56.50321	-45.94		
HN=NH (cis)	-110.56042		228.28	
H2NNH2	-111.77104	95.35		
tetrazole	-258.09848	334.50		
imidazole	-226.05312	132.90		
1,2,3-triazole	-242.06394		271.75	
1,2,4-triazole	-242.09155		192.88	
1,2,4-triazolium (+)	-242.42750	836.80		
4-amino-1,2,4-triazole	-297.36005		329.62	
1-methyl-4-amino-1,2,4-triazolium (+)	-336.98644		907.30	
4-amino-1,2,4-triazolium (+)	-297.70886		937.80	
3-amino-1,2,4-triazolium (+)	-297.76331		799.41	
3,5-diamino-1,2,4-triazolium (+)	-353.09837		763.99	
NH ₃ CH ₂ CH ₂ NH ₃ (2+)	-190.87608		1622.76	
guanidine	-205.22077		19.96	
guanidinium (+)	-205.59560		563.74	
aminoguanidinium (+)	-260.88051		660.18	

^a G3 enthalpy calculated using Gaussian 03, unit in Hartree, ^b from NIST webbook, webbook.nist.gov. ^c calculated value using atomization or isodesmic reactions.

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Table 2 G3MP2 enthalpy ($H_{298}(\text{G3MP2})$), experimental & calculated heats of formation of energetic salts.

Species	$H_{298}(\text{G3MP2})^a$	$\Delta H_f^{\text{Exp. } b}$ (KJ/mol)	$\Delta H_f^{\text{iso. } c}$ (KJ/mol)
CH ₄	-40.41828	-74.87	
NH ₃	-56.45954	-45.94	
NH ₂ (-)	-55.824397	111.78	
NH ₂ NH ₂	-111.695401	95.35	
CH ₃ NH ₂	-95.681770	-22.5	
HNO ₂	-205.477367	-76.73	
NH ₂ (CO)NH ₂	-224.963117	-235.50	
Urea(-)	-224.386855	-251.58	
Dinitrourea (DNU)	-633.455494		24.88
DNU(-)	-632.965488		-198.46
DNU(2-)	-632.302877		31.38
1,2,4-triazolium(+)	-242.234752	836.78	
3,4,5-triamino-1,2,4-triazolium(+)	-408.075774		877.55

^a G3 enthalpy calculated using Gaussian 03, unit in Hartree, ^b from NIST webbook, webbook.nist.gov. ^c calculated value using atomization or isodesmic reactions.