

Electronic Supplementary Information

Stripping off Hydrogens in Imidazole Triggered by the Attachment of a Single Electron

Anita Ribar,^{a,b} Katharina Fink,^a Zhou Li,^{c,d} Sylwia Ptasińska,^{c,d} Ian Carmichael,^c
Linda Feketeová^{a,e*} and Stephan Denifl^{a*}

^aInstitut für Ionenphysik und Angewandte Physik and Center for Molecular Biosciences Innsbruck (CMBI), Leopold Franzens Universität Innsbruck, Technikerstrasse 25, A-6020 Austria

^bDepartment of Plasma Physics, Comenius University, Mlynská dolina F2, 84248 Bratislava, Slovakia

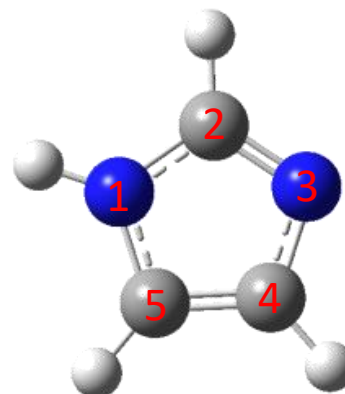
^cRadiation Laboratory, University of Notre Dame, Notre Dame, IN 46556, USA

^dDepartment of Physics, University of Notre Dame, Notre Dame, IN 46556, USA

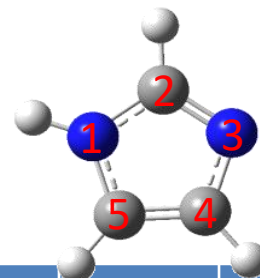
^eUniversité de Lyon, 69003 Lyon, France; CNRS/IN2P3, UMR5822, Institut de Physique Nucléaire de Lyon, 69622 Villeurbanne, France

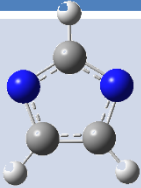
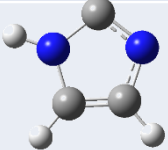
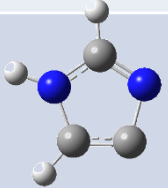
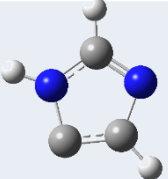
Reaction Enthalpies for DEA to Imidazole with Complete Basis Set Method (cbs-qb3)

Aug 2016



IMD-H⁻

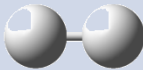


Anion	Byproduct	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)	EA (eV) at 25 C	EA (eV) at 75 C	EA (eV) at 160 C
IMD-H1- 	H 	1.54	1.55	1.56	2.653	2.65	2.66
IMD-H2- 		3.3	3.31	3.32	1.803	1.8	1.8
IMD-H4- 		3.94	3.95	3.97	1.186	1.18	1.18
IMD-H5- 		3.21	3.22	3.23	2.043	2.04	2.04

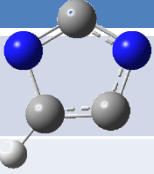
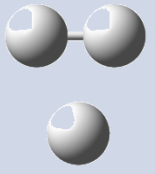
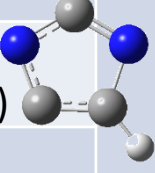
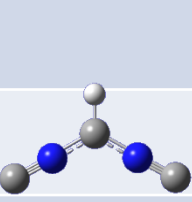
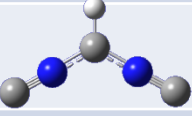
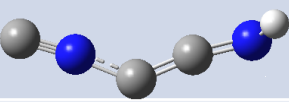
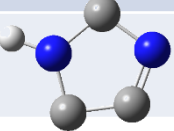
EA = Electron Affinity

IMD-2H⁻

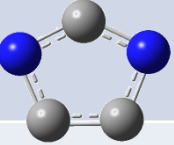
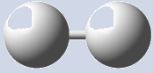
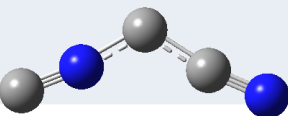
When byproducts are 2 atomic H, the ΔH is higher by 4.57eV

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
IMD-H _{1,2} ⁻		1.85	1.86	1.87
IMD-H _{1,4} ⁻		1.9	1.92	1.93
IMD-H _{1,5} ⁻		1.91	1.92	1.93
IMD-H _{2,4} ⁻		3.55	3.57	3.59
		1.753	1.77	1.79
IMD-H _{2,5} ⁻		3.49	3.51	3.53
IMD-H _{4,5} ⁻		3.59	3.6	3.62

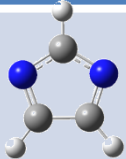
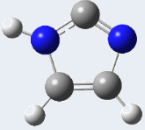
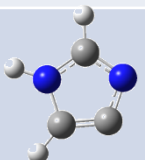
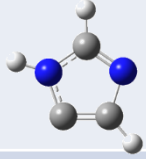
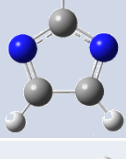
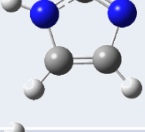
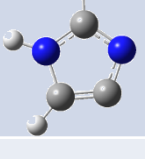
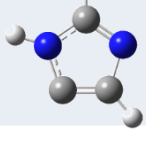
IMD-3H⁻

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
IMD-H _{1,2,4} ⁻ 	H ₂ , H 	6.77	6.8	6.83
IMD-H _{1,2,5} ⁻ (EA < 0, not stable) 		6.77	6.8	6.83
		3.625	3.65	3.69
		4.997	5.02	5.06
		4.936	4.96	5
IMD-H _{2,4,5} ⁻ 		8.14	8.16	8.2

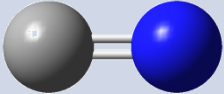
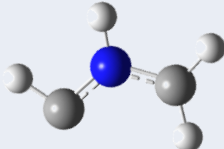
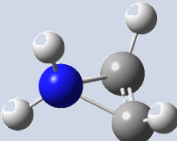
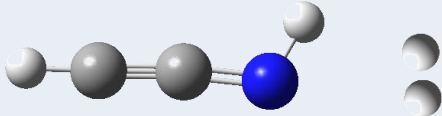
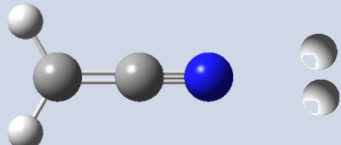
IMD-4H⁻

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
IMD-H _{1,2,4,5} ⁻ 	2 x H ₂ 	6.77	6.79	6.83
		2.957	2.99	3.03

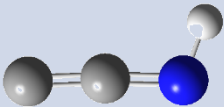
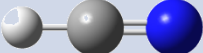
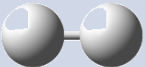
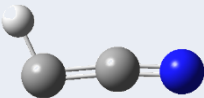
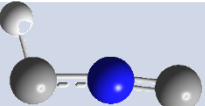
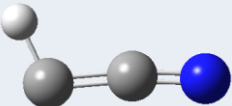
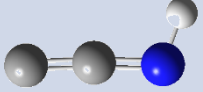
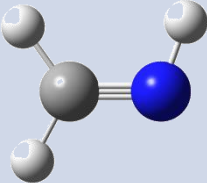
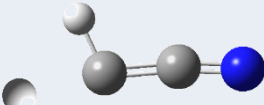
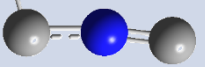
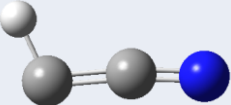
H⁻

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
H⁻ 	IMD-H ₁ 	3.65	3.66	3.68
	IMD-H ₂ 	4.56	4.57	4.58
	IMD-H ₄ 	4.59	4.6	4.61
	IMD-H ₅ 	4.71	4.72	4.74
	IMD-H ₁ ⁺ 	13.36	13.37	13.38
	IMD-H ₂ ⁺ 	13.61	13.62	13.64
	IMD-H ₄ ⁺ 	13.48	13.49	13.50
	IMD-H ₅ ⁺ 	13.64	13.65	13.66

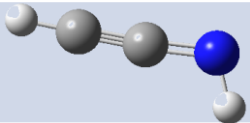
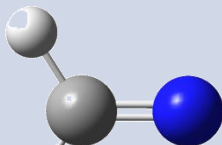
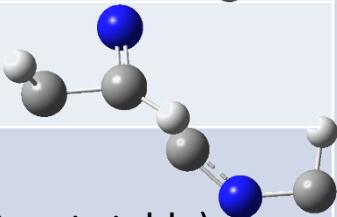
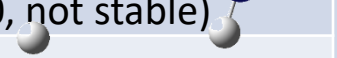
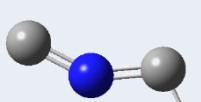
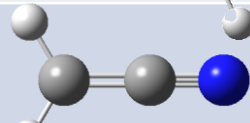
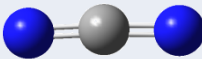
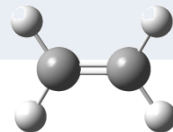
CN⁻

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
 CN ⁻	 CHCHNH ₂	3.62	3.63	3.64
	 CHNHCH ₂	3.65	3.66	3.67
	 CHNH ₂ CH	4.68	4.68	4.7
	 C ₂ H ₂ N, H ₂	3.42	3.44	3.47
	 CH ₂ CN, H ₂	2.012	2.03	2.06

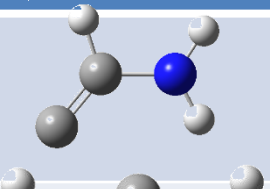
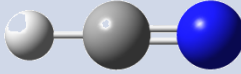
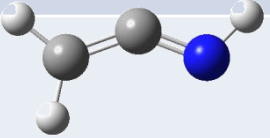
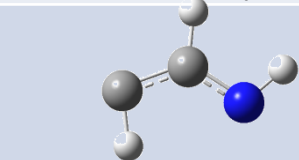
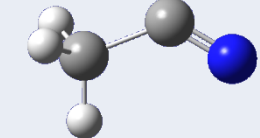
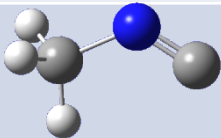
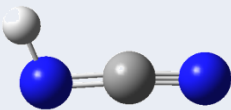
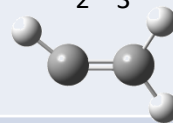
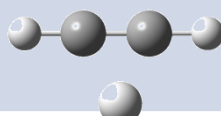
39 amu

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
C_2NH^- 	CHN, H_2  	4.05	4.07	4.1
HC_2N^- 		2.92	2.94	2.97
$HCNC^-$ 		4.12	4.15	4.18
HC_2N^- 		2.916	2.94	2.97
C_2NH^- 	H_2CNH 	3.688	3.7	3.71
HC_2N^- 		2.558	2.57	2.58
$HCNC^-$ 		3.765	3.77	3.78
HC_2N^- 		2.558	2.57	2.58

40 amu

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
HCCHN ⁻ 	CH ₂ N 	3.66	3.67	3.69
HCHCN ⁻ 		5.62	5.63	5.64
HCHNC ⁻ (AE < 0, not stable) 		7.46	7.47	7.48
HCNHC ⁻ 		6.47	6.49	6.5
H ₂ CCN ⁻ 		2.291	2.3	2.31
NCN ⁻ 	C ₂ H ₄ 	1.4	1.41	1.41

41 amu

Anion	Byproduct(s)	ΔH at 25 C (eV)	ΔH at 75 C (eV)	ΔH at 160 C (eV)
 CCHNH ₂ ⁻	 CHN	4.15	4.16	4.17
 CH ₂ CNH ⁻ (AE < 0, not stable)		2.76	2.77	2.78
 CHCHNH ⁻		3.44	3.45	3.46
 CH ₃ CN ⁻		2.613	2.63	2.64
 CH ₃ NC ⁻		2.841	2.85	2.87
 NCNH ⁻	 C ₂ H ₃	2.44	2.45	2.46
	 C ₂ H ₂ , H	3.46	3.37	3.20