

Table III. Proton affinities in kcal/mol

Molecule	RHF/6d ^a	MP2/6d	RHF/5d	MP2/5d	DMol	DG/L	DG/N)	DN/L	DN/N	Ex
CH ₃ CH ₂ OH	190.56(2.3 ^b)	187.54(-0.8)	190.56(2.3)	187.59(-0.7)	176.72(-11.6)	180.28(-8.0)	185.07(-3.2)	179.99(-8.3)	185.35(-3.0)	188
HCOO ⁻	353.88(8.7) ^d	351.72(6.5) ^e	354.03(8.8)	351.81(6.6)	334.75(-10.5)	340.46(-4.7)	345.75(0.5)	340.10(-5.1)	345.67(0.5)	345
HCOOH	182.99(4.2)	176.94(-1.9)	183.04(4.2)	176.95(-1.9)	167.29(-11.5)	172.16(-6.6)	176.83(-2.0)	172.57(-6.2)	176.76(-2.0)	178
CH ₃ OH	185.34(3.4)	182.74(0.8)	185.33(3.4)	182.78(0.9)	170.07(-11.8)	174.61(-7.3)	178.98(-2.9)	174.32(-7.6)	179.24(-2.7)	181
CH ₃ NH ₂	219.27(5.2)	218.54(4.4)	219.21(5.1)	218.59(4.5)	205.25(-8.8)	209.69(-4.4)	214.57(0.5)	209.42(-4.7)	214.37(0.3)	214

^aSee footnotes *a-h* in Table I for method description.

^bDeviation from experiment $P(A)_{calc.} - P(A)_{exp.}$

^cExperimental data from ref [Lias].

^d348.96(3.8) for DZ6D⁽⁺⁾ basis set)

^e343.42(-1.8) for DZ6D⁽⁺⁾ basis set)

^fExperimental data from ref [BARTMESS].