Table VII. 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_3CH_2OH	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_3OH	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_3NH_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

[a] See footnotes in Table I and V for method description.
[b] Deviation from experiment $P(A)_{calc.} - P(A)_{exp.}$
[c] Experimental data from ref. 34.
[d] 348.96(3.8) for DZ6D$^{(+)}$ basis set)
[e] 343.42(−1.8) for DZ6D$^{(+)}$ basis set)
[f] Experimental data from ref. 41.