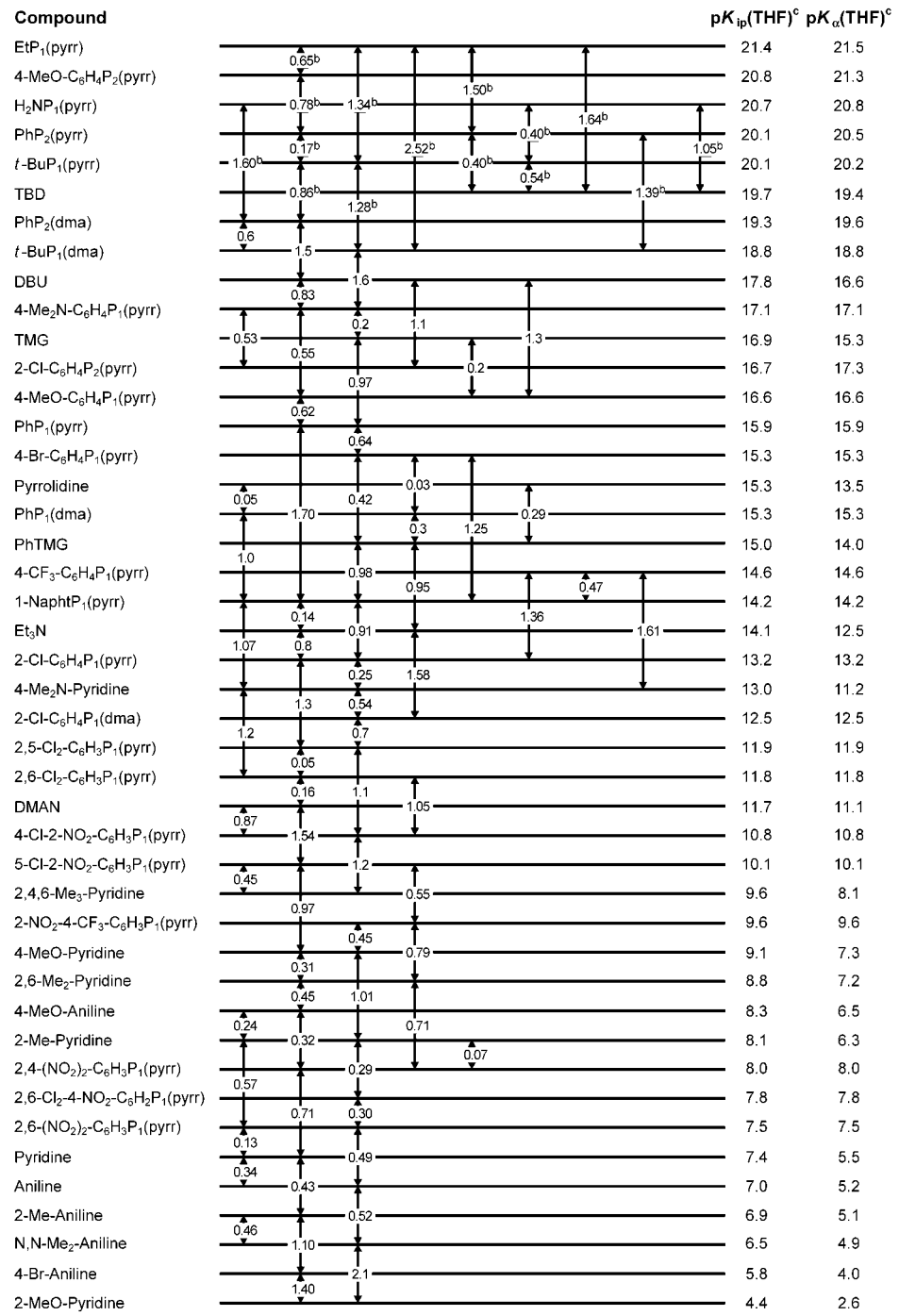
Table 2. Continuous Self-consistent Basicity Scale of Neutral Bases in THF Solution[a]



[a] The numbers on the arrows are the direct experimental ΔpK_{ip} values (uncorrected for ion pairing) obtained from UV−Vis spectrophotometric measurements if not indicated otherwise. [b] NMR measurements. [c] Absolute pK_{ip}(THF) and pK_{α}(THF) estimated values for conjugate acids of the respective bases.

Table 4. Basicity Data of the Bases in AN, H_2O, and the Gas Phase

base	pK_a values in AN[a]	GB (kcal/mol)[b]	pK_a values in H_2O[c]
EtP_1(pyrr)	28.89[d]		
t-BuP_1(pyrr)	28.35[d]		
PhP_2(dma)	26.28		
TBD	25.96[e]	244.3	
t-BuP_1(dma)	26.88[d]		
2-Cl-$C_6H_4P_2$(pyrr)	25.24		
4-Me_2N-$C_6H_4P_1$(pyrr)	23.71		
DBU	24.16	239.6	
4-MeO-$C_6H_4P_1$(pyrr)	22.95		
PhP_1(pyrr)	22.17		
4-Br-$C_6H_4P_1$(pyrr)	21.05		
TMG	23.3[f]	238.4	13.6
PhP_1(dma)	21.07		
4-CF_3-$C_6H_4P_1$(pyrr)	19.93		
1-NaphtP_1(pyrr)	20.42		
PhTMG	20.63	236.9	12.18[g]
pyrrolidine	19.34	218.8	11.1
2-Cl-$C_6H_4P_1$(pyrr)	19.97		
2-Cl-$C_6H_4P_1$(dma)	18.87		
Et_3N	18.63	227	10.7
2,5-Cl_2-$C_6H_3P_1$(pyrr)	18.32		
2,6-Cl_2-$C_6H_3P_1$(pyrr)	18.36		
DMAP	17.75	232.1	9.53
DMAN	18.42	238.0	12.1[h]
4-Cl-2-NO_2-$C_6H_3P_1$(pyrr)	17.48		
5-Cl-2-NO_2-$C_6H_3P_1$(pyrr)	17.07		
2-NO_2-4-CF_3-$C_6H_3P_1$(pyrr)	16.33		
2,4,6-Me_3-pyridine	14.78		
2,4-$(NO_2)_2$-$C_6H_3P_1$(pyrr)	14.68		
2,6-Cl_2-4-NO_2-$C_6H_2P_1$(pyrr)	14.25		
2,6-$(NO_2)_2$-$C_6H_3P_1$(pyrr)	13.91		
4-MeO-pyridine	14.04	222.2	6.5
2,6-Me_2-pyridine	13.92	222.5	6.70
4-MeO-aniline	11.66	207.6	5.3
2-Me-pyridine	13.11	219.2	5.94
pyridine	12.33[i]	214.7	5.25
aniline	10.42	203.3	4.6
2-Me-aniline			4.4
N,*N*-Me_2-aniline	11.23	217.3	5.1
4-Br-aniline	9.25		3.9
2-MeO-pyridine			3.1

[a] Slightly revised pK_a values of conjugate acids of corresponding bases obtained in previous work (ref 14) or in this work if not noted otherwise. [b] Gas-phase basicities from ref 25. [c] pK_a values of conjugate acids of corresponding bases from refs 24 or 23 if not noted otherwise. [d] Reference 17. [e] Reference 26. [f] Reference 27. [g] Reference 28. [h] Reference 29. [i] Anchor of AN scale; value taken from ref 22.