

TABLE 2. Continuous Self-Consistent UV–Vis Spectrophotometric Basicity Scale of Neutral Bases in THF Solution^a

No	Compound	$pK_{ip}(\text{THF})^c$	$pK_a(\text{THF})^c$
1	2-Cl-C ₆ H ₄ P ₄ (pyrr)	25.6	26.6
2	EtP ₂ (dma)	24.9	25.3
3	4-MeO-C ₆ H ₄ P ₃ (pyrr)	24.8	25.7
4	PhP ₃ (pyrr)	24.1	25.0
5	4-MeO-C ₆ H ₄ P ₃ (dma)	23.5	24.0
6	PhP ₃ (dma)	23.0	23.5
7	4-CF ₃ -C ₆ H ₄ P ₃ (pyrr)	22.3	23.1
8	EtP ₁ (pyrr)	21.7	21.7
9	TBD	21.7	21.0
10	4-CF ₃ -C ₆ H ₄ P ₃ (dma)	21.2	21.7
11	2-Cl-C ₆ H ₄ P ₃ (pyrr) ₆ NEt ₂	21.1	22.0
12	4-MeOC ₆ H ₄ P ₂ (pyrr)	20.8	21.5
13	HP ₁ (pyrr)	20.8	20.8
14	MeP ₁ (dma)	20.7	20.7
15	2-Cl-C ₆ H ₄ P ₃ (dma) ₆ NEt ₂	20.3	20.8
16	PhP ₂ (pyrr)	20.2	20.9
17	<i>t</i> -ButP ₁ (pyrr)	20.2	20.2
18	HP ₁ (dma)	19.7	19.7
19	PhP ₂ (dma)	19.4	19.8
20	2,5-Cl ₂ -C ₆ H ₃ P ₃ (pyrr) ₆ NEt ₂	19.3	20.2
21	<i>t</i> -ButP ₁ (dma)	18.9	18.9
22	MTBD	18.6	17.9
23	DBU	18.0	16.8
24	4-Me ₂ N-C ₆ H ₄ P ₁ (pyrr)	17.3	17.3
25	TMG	17.0	15.5
26	2-Cl-C ₆ H ₄ P ₂ (pyrr)	16.8	17.5
27	4-MeO-C ₆ H ₄ P ₁ (pyrr)	16.8	16.8
28	PhP ₁ (pyrr)	16.0	16.0
29	PhP ₁ (dma) ₂ Me	15.4	15.5
30	PhTMG	15.0 ^b	14.0 ^b
31	4-CF ₃ -C ₆ H ₄ P ₁ (pyrr)	14.6 ^b	14.6 ^b

^aThe numbers on the arrows are the direct experimental ΔpK_{ip} values (uncorrected for ion pairing) obtained from UV–vis spectrophotometric titration of neutral bases with methanesulfonic acid. ^b Value from ref 1. ^c Absolute $pK_{ip}(\text{THF})$ and $pK_a(\text{THF})$ estimated values for conjugate acids of the respective bases. TMG denotes *N,N,N,N*-tetramethylguanidine.

TABLE 3. Results of the Gas-Phase Basicity Measurements^a

No	Base	GB ^c
27	4-MeO-C ₆ H ₄ P ₁ (pyrr)	255.2
21	t-BuP ₁ (dma)	253.2
14	MeP ₁ (dma)	252.2
28	PhP ₁ (pyrr)	252.0
32	1-NaphtP ₁ (pyrr)	251.1
33	2-Cl-C ₆ H ₄ P ₁ (pyrr)	251.1
18	HP ₁ (dma)	250.0
34	2,5-Cl ₂ -C ₆ H ₃ P ₁ (pyrr)	248.4
35	ITBD	248.2 ^b
22	MTBD	246.2 ^b

^a The numbers on the arrows are the direct experimental $\Delta\Delta G_b$ (kcal/mol) values obtained from FT-ICR measurements. ^b Values from ref 12. ^c Estimated absolute GB (kcal/mol) values for bases.

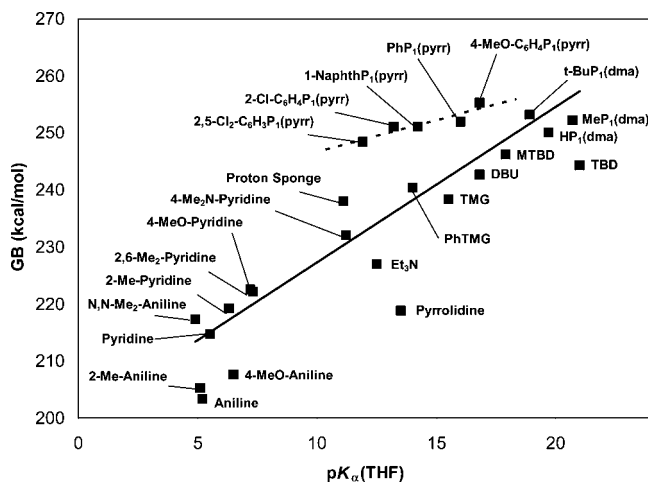


FIGURE 1. Comparison of the basicity data in THF (pK_a values) and in the gas phase (GB). The solid line corresponds to overall correlation (all available data included) and the dotted line corresponds to the series of aryl-P₁(pyrr) phosphazenes.