

Stojković, G., Dimitrieska-Stojković, E., & Popovski, E., Determination of protonation constants and structural correlations for some tertiary formamides and acetamides in sulfuric acid with UV spectroscopy. *Macedonian Journal of Chemistry and Chemical Engineering*, 34(2), 255-265, 2015.

Supplement-Table 1. Protonation parameters for FA

λ /nm	c(H ₂ SO ₄) /mol dm ⁻³	YMCM (H _A)		EAM		BOM	
		pK _{BH} ⁺	m'	pK _{BH} ⁺	m*	pK _{BH} ⁺	ϕ
196	0.1–15.0	-1.54	0.76	-1.47	0.35	-1.49	0.64
197	0.1–15.0	-1.18	0.60	-1.49	0.35	-1.48	0.65
198	0.1–15.0	-0.99	0.56	-1.31	0.32	-1.33	0.67
199	0.1–15.0	-1.10	0.57	-1.47	0.36	-1.47	0.63
201	0.1–15.0	-1.15	0.61	-1.43	0.36	-1.43	0.64
average pK_{BH}⁺		-1.19	0.62	-1.43	0.35	-1.44	0.65
confidence interval		0.26	0.10	0.09	0.02	0.08	0.02

Supplement-Table 2. Protonation parameters for DMFA

λ /nm	c(H ₂ SO ₄) /mol dm ⁻³	YMCM (H _A)		EAM		BOM	
		pK _{BH} ⁺	m'	pK _{BH} ⁺	m*	pK _{BH} ⁺	ϕ
197	0.0–15.0	-0.79	0.50	-1.05	0.24	-1.04	0.77
199	0.5–15.0	-1.02	0.61	-1.22	0.30	-1.22	0.71
200	0.5–15.0	-1.02	0.62	-1.21	0.31	-1.21	0.7
203	0.5–15.0	-0.95	0.62	-1.08	0.29	-1.07	0.72
199	0.0–15.0 [#]	-0.86	0.58	-1.21	0.29	-1.22	0.70
average pK_{BH}⁺		-0.93	0.59	-1.15	0.29	-1.15	0.72
confidence interval		0.13	0.06	0.10	0.03	0.11	0.04

[#] all 34 spectra

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Supplement-Table 3. Protonation parameters for DEFA

λ /nm	$c(\text{H}_2\text{SO}_4)^{\#}$ /mol dm ⁻³	YMCM (H_A)		EAM		BOM	
		$\text{p}K_{\text{BH}^+}$	m'	$\text{p}K_{\text{BH}^+}$	m^*	$\text{p}K_{\text{BH}^+}$	ϕ
200	0.0–15.0	-0.80	0.60	-0.90	0.20	-0.82	0.82
210	0.0–15.0	-0.77	0.70	-0.76	0.25	-0.77	0.72
200	0.0—9.5	-0.81	0.60	-0.90	0.21	-0.82	0.80
202	0.0—9.5	-0.80	0.65	-0.83	0.25	-0.81	0.75
203	0.0—9.5	-0.86	0.70	-0.80	0.24	-0.79	0.76
average $\text{p}K_{\text{BH}^+}$		-0.81	0.65	-0.84	0.23	-0.80	0.77
confidence interval		0.04	0.06	0.08	0.03	0.03	0.05

[#]- concentration increment is 0.1 (between 0.0 and 1.0 mol dm⁻³)

Supplement-Table 4. Protonation parameters for DiPFA

λ /nm	$c(\text{H}_2\text{SO}_4)^{\#}$ /mol dm ⁻³	YMCM (H_A)		EAM [§]		BOM	
		$\text{p}K_{\text{BH}^+}$	m'	$\text{p}K_{\text{BH}^+}$	m^*	$\text{p}K_{\text{BH}^+}$	ϕ
207	0.0–15.0	-0.35	0.76	-0.35	0.36	-0.31	0.68
206	0.0—7.0	-0.35	0.77	-0.29	0.31	-0.33	0.60
208	0.0—7.0	-0.34	0.78	-0.31	0.35	-0.36	0.61
215	0.0—5.5	-0.31	0.84	-0.30	0.44	-0.30	0.60
217	0.0—5.5	-0.31	0.85	-0.29	0.44	-0.28	0.60
average $\text{p}K_{\text{BH}^+}$		-0.33	0.80	-0.31	0.38	-0.32	0.62
confidence interval		0.03	0.05	0.03	0.07	0.04	0.04

[#] concentration increment is 0.1 (between 0.0 and 1.0 mol dm⁻³)

[§] 0.90 < r < 0.95

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Supplement-Table 5. Protonation parameters for DiBFA

λ /nm	c(H ₂ SO ₄) /mol dm ⁻³	YMCM (H _A)		EAM [#]		BOM	
		pK _{BH} ⁺	m'	pK _{BH} ⁺	m*	pK _{BH} ⁺	ϕ
213	0.5–15.0	-1.19	0.74	-1.30	0.39	-1.15	0.71
218	0.9–15.0	-1.11	0.79	-1.17	0.42	-1.13	0.62
210	0.9–15.0	-1.05	0.70	-1.15	0.35	-1.13	0.67
208	0.9–15.0	-1.00	0.69	-1.09	0.21	-1.08	0.74
210	0.9–9.0	-1.03	0.70	-1.13	0.34	-1.15	0.67
average pK_{BH}⁺		-1.08	0.72	-1.17	0.34	-1.13	0.68
confidence interval		0.09	0.05	0.10	0.10	0.04	0.06

^s 0.90 < r < 0.95

Supplement-Table 6. Protonation parameters for DBFA

λ /nm	c(H ₂ SO ₄) /mol dm ⁻³	YMCM (H _A)		EAM		BOM	
		pK _{BH} ⁺	m'	pK _{BH} ⁺	m*	pK _{BH} ⁺	ϕ
210	0.0–8.5	-0.70	0.80	-0.76	0.42	-0.80	0.55
215	0.0–8.5	-0.67	0.55	-0.75	0.48	-0.77	0.57
220	0.0–8.5	-0.67	0.55	-0.75	0.48	-0.75	0.52
210	0.4–8.5	-0.63	0.72	-0.85	0.46	-0.85	0.54
207	0.0–15.0	-0.69	0.72	-0.77	0.35	-0.81	0.61
average pK_{BH}⁺		-0.67	0.67	-0.78	0.44	-0.80	0.56
confidence interval		0.03	0.14	0.05	0.07	0.05	0.04

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Supplement-Table 7. Protonation parameters for AA

λ /nm	$c(\text{H}_2\text{SO}_4)$ /mol dm ⁻³	YMCM (H_A) [#]		EAM [#]		BOM [§]	
		pK_{BH^+}	m'	pK_{BH^+}	m^*	pK_{BH^+}	ϕ
196	0.0–15.0	-0.51	0.53	-	-	-0.41	0.94
196	0.1–15.0	-0.29	0.45	-	-	-0.56	0.87
196–198 [§]	0.0–15.0	-0.80	0.67	-0.75	0.28	-0.61	0.85
196–201 [§]	0.0–15.0	-0.29	0.41	-0.61	0.18	-0.60	0.87
198–201 [§]	0.0–15.0	-0.35	0.61	-	-	-0.65	0.86
calculated from reconstructed spectra using one characteristic vector							
195	0.0–15.0	-0.42	0.47	-0.7	0.19	-0.61	0.87
195	0.1–15.0	-0.20	0.37	-0.61	0.18	-0.53	0.87
199	0.1–15.0	-0.26	0.41	-0.61	0.18	-0.53	0.87
195–199 [§]	0.1–15.0	-0.42	0.47	-0.59	0.13	-0.59	0.87
average pK_{BH^+}		-0.39	0.49	-0.65	0.19	-0.57	0.87
confidence interval		0.14	0.08	0.07	0.05	0.05	0.02

[#] $r < 0.90$ [§] $0.97 < r < 0.99$ [§] - difference between absorbance at two wavelenght

Supplement-Table 8. Protonation parameters for DMAA

λ /nm	$c(\text{H}_2\text{SO}_4)$ [#] /mol dm ⁻³	YMCM (H_A)		EAM		BOM	
		pK_{BH^+}	m'	pK_{BH^+}	m^*	pK_{BH^+}	ϕ
200	0.0–15.0	-0.26	0.29	-	-	-0.33	1.04
205	0.0–15.0	-0.21	0.34	-	-	-0.23	1.03
200	0.0–9.0	-0.30	0.54	-0.32 [§]	0.15	-0.29	0.87
205	0.0–9.0	-0.28	0.72	-0.28	0.29	-0.26	0.72
calculated from reconstructed spectra using two characteristics vectors							
200	0.0–9.0	-0.36	0.52	-	-	-0.35	0.93
205	0.0–9.0	-0.29	0.48	-	-	-0.28	0.96
average pK_{BH^+}		-0.28	0.48	-0.30	-	-0.29	0.93
confidence interval		0.05	0.16	-	-	0.05	0.12

[#] - concentration increment is 0.1 (between 0.0 and 1.0 mol dm⁻³)

[§] $r < 0.90$

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Supplement-Table 9. Protonation parameters for DEAA

λ /nm	c(H ₂ SO ₄) /mol dm ⁻³	YMCM (H_A)		EAM		BOM	
		p <i>K</i> _{BH⁺}	<i>m</i> '	p <i>K</i> _{BH⁺}	<i>m</i> *	p <i>K</i> _{BH⁺}	ϕ
203	0.1–14.0	-0.32	0.46	-	-	-0.33	0.95
203	0.1–9.0	-0.34	0.91	-	-	-0.32	0.95
203	0.1–7.0	-0.37	0.64	-	-	-0.29	0.90
226	0.1–7.0	-0.31	0.92	-0.35	0.51	-0.33	0.52
227	0.1–4.5	-0.38	0.82	-0.35	0.28	-0.31	0.78
average p<i>K</i>_{BH⁺}		-0.34	0.75	-0.35	-	-0.32	0.82
confidence interval		0.04	0.24	-	-	0.02	0.23

Supplement-Table 10. Protonation parameters for DiPAA

λ /nm	c(H ₂ SO ₄) /mol dm ⁻³	YMCM (H_A)		EAM		BOM	
		p <i>K</i> _{BH⁺}	<i>m</i> '	p <i>K</i> _{BH⁺}	<i>m</i> *	p <i>K</i> _{BH⁺}	ϕ
208	0.0–10.0	0.29	1.07	-	-	0.23	0.98
215	0.0–8.0	0.35	0.97	0.37	0.64	0.39	0.41
218	0.0–3.5	0.41	1.06	0.39	0.93	0.42	0.18
x_i /UV [#]	0.0–3.0	0.36	1.07	0.33	0.97	-	-
x_i /rec ^{\$}	0.0–3.0	0.34	1.18	0.42	2.34	0.43	-1.34
average p<i>K</i>_{BH⁺}		0.35	1.07	0.38	-	0.36	-
confidence interval		0.05	0.09	0.06	-	0.15	-

[#] x_{BH^+}/x_B calculated from experimental UV spectra

^{\$} x_{BH^+}/x_B calculated from reconstructed UV spectra