

Supporting Material

Table S1. Pseudo-first-order Rate Constants (k_{obs}) for the Reactions of IQ^+ , T^+ , and Xn^+ by the NAD(P)H Models 1 [$\text{X} = \text{OCH}_3$ (a), CH_3 (b), H (c), Cl (d), Br (e)] in Buffered Aqueous Solutions

$[\text{S}] \times 10^3$ (M)	$k_{\text{obs}} \times 10^3 \text{ (s}^{-1}\text{)}$				
	a	b	c	d	e
$\text{IQ}^+{}^a$					
8.20	0.80	0.74	0.51	0.27	0.27
9.80	0.96	0.87	0.61	0.35	0.36
11.50	1.09	1.02	0.74	0.43	0.44
12.87	1.26	1.09	0.81	0.51	0.53
14.14	1.37	1.19	0.89	0.57	0.60
16.80	1.65	1.36	1.00	0.69	0.69
$\text{T}^+{}^b$					
1.00	8.01	1.54	0.91	0.37	0.34
1.50	11.0	2.51	1.52	0.57	0.51
2.00	13.8	3.57	2.00	0.78	0.69
2.50	17.2	4.47	2.54	0.97	0.90
3.00	19.9	6.01	3.60	1.27	1.12
3.50	23.2	6.74	4.00	1.45	1.33
$\text{Xn}^+{}^c$					
1.00	0.41	0.34	0.18	0.08	0.07
1.24	0.50	0.44	0.24	0.11	0.10
1.48	0.61	0.51	0.28	0.13	0.12
1.72	0.70	0.60	0.33	0.16	0.14
1.98	0.83	0.70	0.37	0.17	0.16
2.17	0.88	0.78	0.42	0.19	0.18

^a T = 323K, 30% acetonitrile-70% H_2O , 0.025M KH_2PO_4 -0.025M K_2HPO_4 buffer solution, pH = 6.90, I = 0.1, [1] = 0.05 M, $\lambda_{\text{max}} = 442\text{nm}$. ^b T = 298K, 30% acetonitrile-70% H_2O , 0.25M KH_2PO_4 -0.25M K_2HPO_4 buffer solution, pH = 7.56, I = 0.5, [1] = 0.05M, $\lambda_{\text{max}} = 357.0\text{nm}$. ^c T = 298K, 30% acetonitrile-70% H_2O , 0.025M KH_2PO_4 -0.025M K_2HPO_4 buffer solution, pH = 6.90, I = 0.1, [1] = 0.05M, $\lambda_{\text{max}} = 357.0\text{nm}$.