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Purification and Characterization of meta Cresol Purple for Spectrophotometric Seawater pH Measurements

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TABLE S1. mCP e_3/e_2 values at different temperatures and salinities

T (S = 35)	e_3/e_2	S (T = 298.15 K)	e_3/e_2
278.21	0.05164	20	0.05518
278.21	0.05168	20	0.05516
278.21	0.05174	20	0.05513
278.21	0.05175	20	0.05512
283.24	0.05275	25	0.05584
283.24	0.05275	25	0.0559
283.24	0.05277	25	0.0559
283.24	0.05283	25	0.05587
283.24	0.05294	30	0.0563
288.24	0.05422	30	0.05632
288.24	0.05423	30	0.05636
288.24	0.05423	30	0.05633
288.25	0.05427	30	0.05631
293.48	0.05554	30	0.05631
293.47	0.05555	30	0.05633
293.48	0.05556	30	0.05628
293.48	0.0556	30	0.0563
293.48	0.05566	35	0.05684
293.48	0.05566	35	0.05686
298.23	0.05684	35	0.05688
298.23	0.05685	35	0.05689
298.23	0.05687	35	0.05687
298.23	0.05688	40	0.05737
303.31	0.05806	40	0.0573
303.33	0.05808	40	0.05738
303.34	0.05818	40	0.05734
303.31	0.05822	40	0.05736
308.39	0.05948	40	0.05729
308.32	0.05949		
308.32	0.05949		
308.29	0.05951		
308.37	0.05959		

TABLE S2. mCP K_1 at different temperatures in 0.7 m NaCl

T	K_1
279.45	0.0211±0.0002
288.75	0.0246±0.0002
298.15	0.0299±0.0001
307.95	0.0384±0.0015

TABLE S3. mCP $_{578}A/_{434}A$ and e_1 as a function of temperature at pH 4.5

T	$_{578}A/_{434}A$	e_1
279.20	0.00570	0.00485
281.21	0.00580	0.00494
288.14	0.00610	0.00525
288.24	0.00605	0.00526
288.84	0.00610	0.00529
297.88	0.00645	0.00569
298.18	0.00650	0.00571
298.18	0.00652	0.00571
307.85	0.00700	0.00614
307.89	0.00700	0.00615
308.12	0.00702	0.00616

TABLE S4. Comparison of two assessments of pH (total hydrogen concentration scale) in 0.04 mol (kg-H_2O)$^{-1}$ Tris buffer in synthetic seawater. Residual = expected pH (eq 6) minus pH as determined by mCP absorbance ratio *R* (eq 18).

S	*T*	*R*	pH_T(TRIS) (eq 6)	pH_T(mCP) (eq 18)	Residual
20	278.11	4.6082	8.7180	8.7177	0.00029
20	278.11	4.6079	8.7180	8.7177	0.00028
20	288.17	3.1142	8.3818	8.3819	-0.00010
20	288.17	3.1147	8.3817	8.3819	-0.00022
20	288.20	3.1107	8.3807	8.3809	-0.00018
20	288.23	3.1078	8.3799	8.3801	-0.00023
20	288.27	3.1034	8.3786	8.3789	-0.00029
20	298.12	2.1213	8.0701	8.0700	0.00002
20	298.16	2.1178	8.0690	8.0688	0.00016
20	298.19	2.1156	8.0680	8.0679	0.00008
20	298.21	2.1140	8.0674	8.0673	0.00009
20	298.25	2.1109	8.0662	8.0661	0.00005
20	298.25	2.1104	8.0661	8.0660	0.00013
20	307.77	1.4762	7.7835	7.7834	0.00012
20	307.80	1.4743	7.7827	7.7824	0.00023
20	307.89	1.4697	7.7799	7.7799	0.00001
20	307.91	1.4690	7.7794	7.7794	-0.00001
20	308.00	1.4637	7.7767	7.7767	0.00007
20	308.06	1.4607	7.7751	7.7750	0.00008
20	308.07	1.4594	7.7747	7.7745	0.00023
30	278.17	4.9437	8.7399	8.7396	0.00027
30	278.17	4.9436	8.7399	8.7396	0.00028

30	278.17	4.9441	8.7399	8.7396	0.00022
30	278.17	4.9493	8.7399	8.7403	-0.00038
30	278.18	4.9426	8.7398	8.7394	0.00032
30	288.12	3.3913	8.4033	8.4026	0.00073
30	288.12	3.3907	8.4033	8.4025	0.00083
30	288.13	3.3932	8.4028	8.4027	0.00009
30	288.14	3.3944	8.4027	8.4028	-0.00016
30	288.23	3.3877	8.3998	8.4007	-0.00090
30	288.23	3.3840	8.3997	8.4001	-0.00039
30	288.25	3.3826	8.3991	8.3996	-0.00051
30	288.26	3.3836	8.3988	8.3996	-0.00083
30	298.17	2.3260	8.0832	8.0834	-0.00016
30	298.18	2.3265	8.0831	8.0834	-0.00033
30	298.18	2.3259	8.0829	8.0832	-0.00030
30	298.20	2.3241	8.0824	8.0826	-0.00025
30	298.20	2.3233	8.0823	8.0824	-0.00008
30	298.20	2.3235	8.0823	8.0825	-0.00016
30	298.20	2.3244	8.0823	8.0827	-0.00040
30	308.07	1.6139	7.7836	7.7839	-0.00033
30	308.07	1.6141	7.7836	7.7840	-0.00040
30	308.08	1.6142	7.7834	7.7839	-0.00052
30	308.09	1.6128	7.7831	7.7834	-0.00029
30	308.09	1.6130	7.7831	7.7834	-0.00037
30	308.12	1.6093	7.7822	7.7820	0.00025
30	308.13	1.6117	7.7821	7.7826	-0.00056
30	308.14	1.6109	7.7816	7.7822	-0.00057
35	278.22	5.0751	8.7518	8.7518	0.00000
35	278.22	5.0800	8.7518	8.7524	-0.00056

35	278.23	5.0814	8.7518	8.7526	-0.00074
35	278.23	5.0759	8.7517	8.7519	-0.00016
35	278.23	5.0816	8.7516	8.7525	-0.00087
35	278.23	5.0772	8.7516	8.7520	-0.00037
35	278.23	5.0774	8.7516	8.7520	-0.00039
35	278.41	5.0387	8.7455	8.7452	0.00026
35	278.41	5.0404	8.7455	8.7454	0.00007
35	278.41	5.0402	8.7455	8.7454	0.00009
35	278.41	5.0382	8.7455	8.7451	0.00032
35	278.41	5.0426	8.7455	8.7456	-0.00018
35	278.41	5.0448	8.7455	8.7459	-0.00044
35	278.41	5.0430	8.7454	8.7457	-0.00025
35	278.42	5.0402	8.7451	8.7452	-0.00013
35	288.16	3.4962	8.4137	8.4128	0.00092
35	288.16	3.4958	8.4137	8.4127	0.00096
35	288.17	3.4961	8.4136	8.4127	0.00086
35	288.17	3.4943	8.4135	8.4124	0.00109
35	298.16	2.4076	8.0931	8.0922	0.00092
35	298.17	2.4075	8.0931	8.0922	0.00090
35	298.17	2.4078	8.0931	8.0922	0.00084
35	308.11	1.6729	7.7895	7.7892	0.00036
35	308.13	1.6713	7.7889	7.7885	0.00045
35	308.14	1.6710	7.7887	7.7883	0.00045
35	308.14	1.6708	7.7886	7.7882	0.00045
35	308.15	1.6705	7.7886	7.7881	0.00047
40	278.11	5.2013	8.7707	8.7698	0.00089
40	278.11	5.2049	8.7706	8.7701	0.00044
40	278.11	5.2079	8.7706	8.7705	0.00010

40	278.11	5.2018	8.7705	8.7698	0.00076
40	278.12	5.2085	8.7704	8.7705	-0.00008
40	278.12	5.2092	8.7704	8.7706	-0.00015
40	288.67	3.5331	8.4101	8.4108	-0.00070
40	288.67	3.5332	8.4101	8.4108	-0.00073
40	288.67	3.5331	8.4100	8.4107	-0.00075
40	288.67	3.5326	8.4100	8.4107	-0.00068
40	298.16	2.4864	8.1045	8.1049	-0.00033
40	298.23	2.4797	8.1023	8.1026	-0.00032
40	298.24	2.4793	8.1021	8.1024	-0.00034
40	298.24	2.4780	8.1018	8.1020	-0.00024
40	298.25	2.4775	8.1017	8.1019	-0.00019
40	308.44	1.7063	7.7886	7.7882	0.00036
40	308.44	1.7078	7.7886	7.7887	-0.00006
40	308.44	1.7083	7.7886	7.7888	-0.00022
40	308.44	1.7068	7.7885	7.7883	0.00016
40	308.45	1.7064	7.7883	7.7881	0.00016
40	308.50	1.7060	7.7869	7.7875	-0.00052

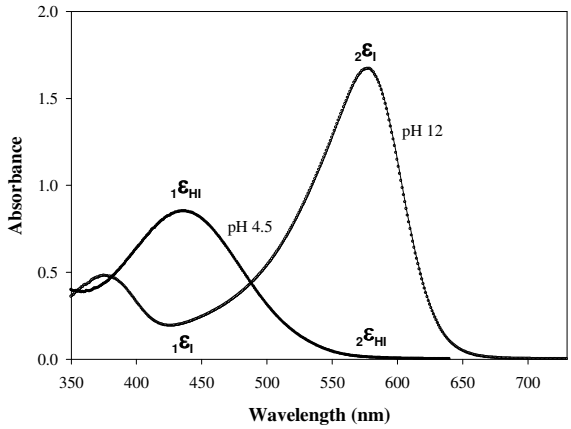

FIGURE S1. Spectra of mCP at pH =4.5 and pH =12.

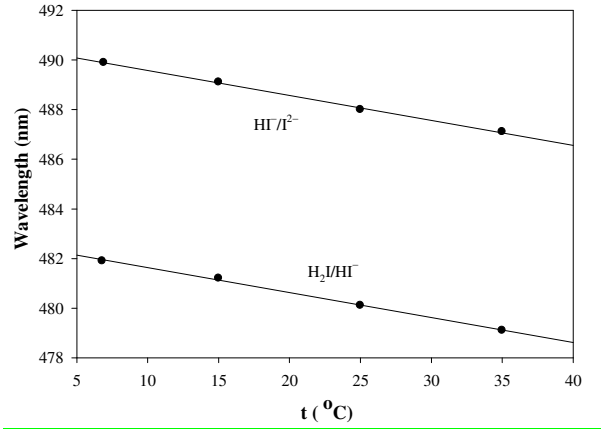

FIGURE S2. Isosbestic point wavelengths of H_2I/HI^- and HI^-/I^{2-} as a function of temperature.

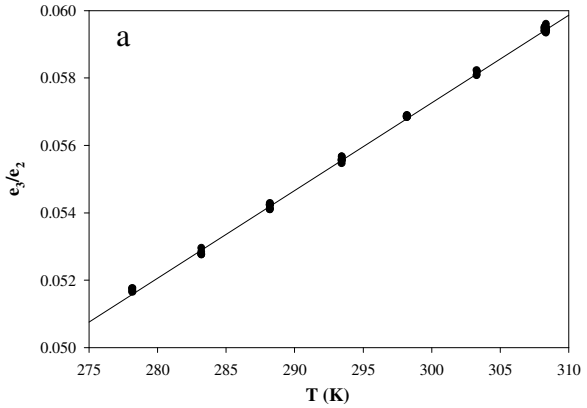

FIGURE S3a. mCP e_3/e_2 as a function of temperature at pH 12 in modified synthetic seawater.

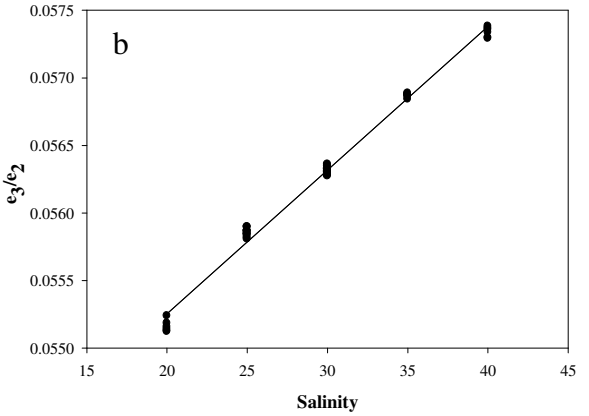

FIGURE S3b. mCP e_3/e_2 as a function of salinity (298.15 K) at pH 12 in modified synthetic seawater.

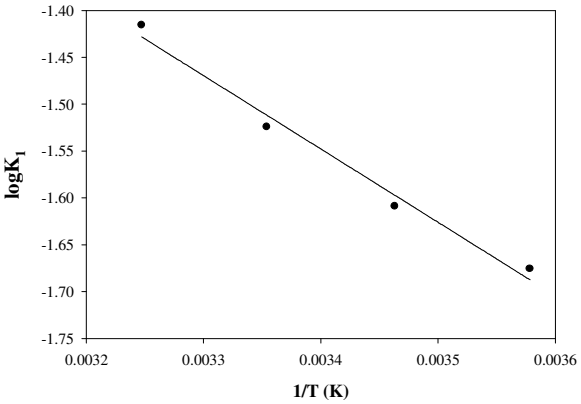

FIGURE S4. mCP K_1 as a function of temperature in 0.7 m NaCl.

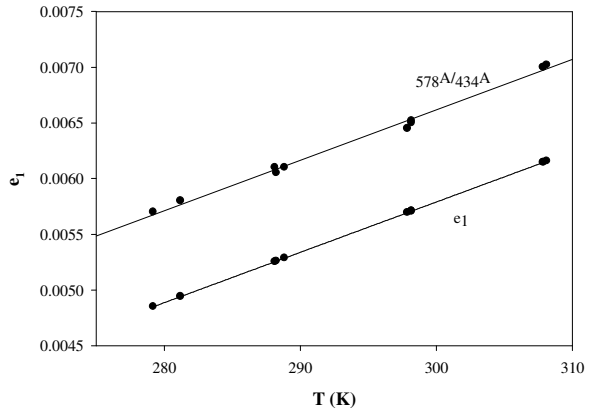

FIGURE S5. mCP A_{578}/A_{434} and e_1 as a function of temperature in a strongly buffered solution of 0.7 m NaCl at pH 4.5.