

# Intermolecular Interactions of CTAB and Potential Oxidation Inhibitors: Physico-chemical Controlled Approach for Food/Pharmaceutical

## Function

Varun Bhardwaj <sup>a</sup>, Kundan Sharma <sup>b</sup>, S. Chauhan <sup>c</sup>, Poonam Sharma <sup>a,\*</sup>

<sup>a</sup>*Department of Biotechnology, Bioinformatics and Pharmacy, Jaypee University of Information Technology, Waknaghat, Solan, 173234 Himachal Pradesh, India.*

<sup>b</sup>*Department of Applied Chemistry, Amity Institute of Applied Sciences, Amity University, Noida 201313, India.*

<sup>c</sup>*Department of Chemistry, Himachal Pradesh University, Summer hill, Shimla 173005 Himachal Pradesh, India.*

**ST1** Density,  $\rho$  ( $\text{kg}\cdot\text{m}^{-3}$ ), ultrasonic velocity,  $u$  ( $\text{m}\cdot\text{s}^{-1}$ ) and Isentropic Compressibility,  $\kappa_s$  ( $\text{TPa}^{-1}$ ) of CTAB (0.2–1.8)  $\text{mmol}\cdot\text{kg}^{-1}$  in water-ethanol compositions (v/v %) of 0.03  $\text{mol}\cdot\text{kg}^{-1}$  BHA over different temperatures ranging from (298.15 to 308.15) K.

$10^3\cdot[\text{CTAB}]$ $\text{mol}\cdot\text{kg}^{-1}$	100% v/v Ethanol			70% v/v Ethanol			30% v/v Ethanol		
	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K
$\rho/\text{kg}\cdot\text{m}^{-3}$									
0.0	792.834	787.242	775.189	846.883	835.142	822.195	888.165	878.283	869.232
0.2	781.841	776.522	764.291	839.832	828.914	816.732	882.670	873.384	864.442
0.4	780.271	775.885	764.192	838.615	827.889	816.003	881.193	872.142	863.438
0.6	781.152	776.171	764.182	838.884	827.992	816.005	881.024	872.003	863.399
0.8	782.529	777.318	765.608	839.788	828.878	817.154	882.663	873.332	864.392
1.0	782.317	777.343	765.542	839.715	828.804	817.096	882.616	873.312	864.316
1.2	782.263	777.310	765.471	839.656	828.735	817.004	882.574	873.256	864.278
1.4	782.165	777.262	765.401	839.601	828.697	816.985	882.492	873.184	864.224
1.6	782.002	777.182	765.337	839.534	828.622	816.889	882.403	873.102	864.169
1.8	781.994	777.095	765.283	839.473	828.584	816.815	882.378	873.047	864.116
$u/\text{m}\cdot\text{s}^{-1}$									
0.0	1162.32	1149.66	1120.11	1295.25	1281.45	1268.77	1528.14	1516.68	1501.18
0.2	1155.88	1138.55	1114.17	1291.14	1276.38	1261.28	1523.44	1510.73	1494.62
0.4	1156.11	1138.72	1114.84	1291.32	1276.51	1261.35	1523.58	1510.88	1494.84
0.6	1156.37	1138.97	1114.99	1291.45	1276.79	1261.44	1523.76	1510.96	1494.99
0.8	1156.72	1139.19	1115.23	1291.66	1276.94	1261.65	1523.97	1511.14	1495.16
1.0	1156.92	1139.36	1115.56	1291.79	1277.33	1261.79	1524.16	1511.25	1495.37
1.2	1157.34	1139.78	1115.85	1291.88	1277.58	1261.93	1524.45	1511.39	1495.52
1.4	1157.63	1140.02	1116.11	1291.97	1277.62	1262.09	1524.69	1511.54	1495.77
1.6	1157.84	1140.18	1116.35	1292.06	1277.73	1262.24	1524.84	1511.68	1495.88
1.8	1158.08	1140.32	1116.62	1292.15	1277.81	1262.38	1524.92	1511.77	1495.91
$10^{-10}\cdot\kappa_s \text{ TPa}^{-1}$									
0.2	9.573	9.934	1.054*	7.143	7.405	7.697	4.881	5.017	5.178
0.4	9.589	9.940	1.052	7.151	7.413	7.703	4.889	5.023	5.183
0.6	9.574	9.932	1.052	7.147	7.409	7.701	4.889	5.023	5.182
0.8	9.551	9.910	1.050	7.137	7.399	7.688	4.878	5.014	5.175
1.0	9.550	9.910	1.049	7.136	7.395	7.687	4.877	5.014	5.174
1.2	9.544	9.903	1.049	7.136	7.393	7.686	4.876	5.013	5.173
1.4	9.540	9.899	1.048	7.135	7.393	7.684	4.874	5.013	5.172
1.6	9.539	9.898	1.048	7.135	7.392	7.683	4.874	5.012	5.171
1.8	9.535	9.896	1.048	7.135	7.391	7.682	4.874	5.012	5.172

\*  $\kappa_s \text{ TPa}^{-1}\cdot 10^{-9}$ . Standard uncertainties in  $\rho$ ,  $u$  and  $\kappa_s$  are  $\pm 2\cdot 10^{-3} \text{ kg}\cdot\text{m}^{-3}$ ,  $\pm 0.3 \text{ m}\cdot\text{s}^{-1}$  and  $\pm 0.02\cdot 10^{-10} \text{ TPa}^{-1}$ . For temperature measurements (T/K), it comes out to be  $\pm 0.02 \text{ K}$

**ST2**,  $\rho$  ( $\text{kg}\cdot\text{m}^{-3}$ ), ultrasonic velocity,  $u$  ( $\text{m}\cdot\text{s}^{-1}$ ) and Isentropic Compressibility,  $\kappa_s$  ( $\text{TPa}^{-1}$ ) of CTAB (0.2–1.8)  $\text{mmol}\cdot\text{kg}^{-1}$  in water-1-propanol compositions (v/v %) of 0.03  $\text{mol}\cdot\text{kg}^{-1}$  BHA over different temperatures ranging from (298.15 to 308.15) K.

$10^3\cdot[\text{CTAB}]$ $\text{mol}\cdot\text{kg}^{-1}$	100% v/v <b>1-propanol</b>			70% v/v <b>1-propanol</b>			30% v/v <b>1-propanol</b>		
	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K
<b><math>\rho/\text{kg}\cdot\text{m}^{-3}</math></b>									
0.0	831.943	828.849	820.442	856.664	847.192	836.838	889.838	875.719	868.424
0.2	810.024	806.543	798.786	848.223	839.348	829.744	880.323	866.948	858.778
0.4	808.915	805.455	797.834	847.938	839.124	829.712	879.857	866.933	858.723
0.6	807.564	804.684	796.459	847.893	839.094	829.675	879.548	866.675	858.699
0.8	810.876	806.588	798.658	847.812	839.573	829.616	880.304	866.649	858.747
1.0	810.816	806.504	798.586	847.238	839.515	829.688	880.275	866.592	858.683
1.2	810.776	806.449	798.512	847.189	839.456	829.594	880.237	866.535	858.624
1.4	810.558	806.398	798.442	847.095	839.398	829.535	880.183	866.489	858.598
1.6	810.495	806.315	798.388	846.993	839.332	829.489	880.116	866.435	858.556
1.8	810.435	806.264	798.311	846.924	839.284	829.444	880.078	866.408	858.525
<b><math>u/\text{m}\cdot\text{s}^{-1}</math></b>									
0.0	1228.82	1219.54	1198.39	1364.94	1355.33	1346.78	1574.84	1559.36	1542.04
0.2	1221.76	1214.34	1193.43	1361.48	1348.39	1339.39	1569.84	1552.43	1543.03
0.4	1221.84	1214.55	1193.54	1361.59	1348.48	1339.43	1569.97	1552.58	1543.28
0.6	1221.98	1214.68	1193.65	1361.84	1348.62	1339.68	1570.06	1552.69	1543.37
0.8	1222.12	1214.82	1193.78	1361.96	1348.85	1339.74	1570.28	1552.75	1543.48
1.0	1222.31	1215.04	1193.92	1362.15	1348.91	1339.87	1570.44	1552.84	1543.65
1.2	1222.42	1215.22	1194.09	1362.39	1349.06	1340.03	1570.68	1552.96	1543.78
1.4	1222.55	1215.39	1194.21	1362.54	1349.08	1340.16	1570.74	1553.12	1543.87
1.6	1222.56	1215.44	1194.35	1362.66	1349.17	1340.32	1570.81	1552.28	1543.98
1.8	1222.69	1215.45	1194.38	1362.69	1349.26	1340.34	1570.83	1552.35	1544.04
<b><math>10^{-10}\cdot\kappa_s \text{TPa}^{-1}</math></b>									
0.2	8.270	8.408	8.790	6.360	6.553	6.718	4.609	4.786	4.891
0.4	8.281	8.416	8.799	6.361	6.554	6.718	4.611	4.785	4.889
0.6	8.293	8.422	8.812	6.359	6.553	6.716	4.612	4.786	4.889
0.8	8.257	8.401	8.786	6.359	6.547	6.716	4.607	4.786	4.888
1.0	8.255	8.398	8.785	6.361	6.546	6.714	4.606	4.786	4.887
1.2	8.254	8.396	8.783	6.359	6.545	6.713	4.605	4.785	4.887
1.4	8.254	8.395	8.782	6.359	6.546	6.712	4.605	4.784	4.886
1.6	8.255	8.395	8.781	6.358	6.545	6.711	4.605	4.790	4.886
1.8	8.254	8.395	8.781	6.359	6.545	6.711	4.605	4.790	4.886

\*  $\kappa_s \text{TPa}^{-1}\cdot 10^{-9}$ . Standard uncertainties in  $\rho$ ,  $u$  and  $\kappa_s$  are  $\pm 3\cdot 10^{-3} \text{kg}\cdot\text{m}^{-3}$ ,  $\pm 0.4 \text{m}\cdot\text{s}^{-1}$  and  $\pm 0.15\cdot 10^{-10} \text{TPa}^{-1}$ . For temperature measurements (T/K), it comes out to be  $\pm 0.01 \text{K}$

**ST3** Density,  $\rho$  ( $\text{kg}\cdot\text{m}^{-3}$ ), ultrasonic velocity,  $u$  ( $\text{m}\cdot\text{s}^{-1}$ ) and Isentropic Compressibility,  $\kappa_s$  ( $\text{TPa}^{-1}$ ) of CTAB (0.2–1.8)  $\text{mmol}\cdot\text{kg}^{-1}$  in water-ethanol compositions (% v/v) of 0.02  $\text{mol}\cdot\text{kg}^{-1}$  BHT over different temperatures ranging from (298.15 to 308.15) K.

$10^3\cdot[\text{CTAB}]$ $\text{mol}\cdot\text{kg}^{-1}$	100% v/v Ethanol			70% v/v Ethanol			30% v/v Ethanol		
	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K
<b><math>\rho/\text{kg}\cdot\text{m}^{-3}</math></b>									
0.0	803.872	797.322	787.436	859.242	848.847	839.659	902.594	892.748	882.073
0.2	789.644	782.943	773.495	847.844	837.728	829.744	892.183	882.848	871.848
0.4	788.345	781.323	772.748	846.263	836.985	828.893	891.747	881.999	870.993
0.6	788.013	780.044	772.003	846.145	836.294	828.381	891.043	881.384	870.283
0.8	788.003	780.928	771.937	847.858	836.193	828.316	891.994	881.371	870.225
1.0	788.038	780.902	771.911	847.713	836.187	828.274	891.916	881.354	870.184
1.2	788.002	780.884	771.891	847.685	836.132	828.222	891.894	881.312	870.121
1.4	787.994	780.845	771.874	847.627	836.096	828.184	891.843	881.274	870.094
1.6	787.952	780.843	771.818	847.583	836.001	828.113	891.804	881.233	870.023
1.8	787.915	780.815	771.794	847.517	835.986	828.082	891.799	881.195	870.007
<b><math>u/\text{m}\cdot\text{s}^{-1}</math></b>									
0.0	1184.14	1168.38	1154.24	1326.39	1299.29	1284.92	1557.38	1543.45	1529.74
0.2	1171.23	1164.22	1152.43	1310.35	1294.43	1272.14	1548.84	1538.85	1518.84
0.4	1171.39	1164.34	1152.47	1310.64	1294.75	1272.47	1548.92	1538.98	1519.35
0.6	1171.54	1164.58	1152.64	1310.87	1294.81	1272.69	1549.26	1539.15	1519.44
0.8	1171.73	1164.74	1152.72	1310.98	1294.99	1272.83	1549.43	1539.32	1519.61
1.0	1171.94	1164.89	1152.88	1311.34	1295.12	1273.14	1549.64	1539.48	1519.74
1.2	1172.28	1165.03	1152.95	1311.49	1295.35	1273.32	1549.82	1539.64	1519.85
1.4	1172.43	1165.25	1153.05	1311.58	1295.54	1273.58	1549.98	1539.79	1519.97
1.6	1172.64	1165.48	1153.24	1311.74	1295.71	1273.93	1550.04	1539.85	1520.05
1.8	1172.88	1165.49	1153.28	1311.83	1295.79	1273.99	1550.11	1539.92	1520.16
<b><math>10^{-10}\cdot\kappa_s \text{ TPa}^{-1}</math></b>									
0.2	9.232	9.423	9.734	6.869	7.124	7.447	4.672	4.783	4.972
0.4	9.244	9.441	9.743	6.879	7.127	7.451	4.674	4.787	4.974
0.6	9.246	9.452	9.749	6.878	7.132	7.453	4.676	4.789	4.977
0.8	9.243	9.439	9.749	6.863	7.131	7.452	4.670	4.788	4.976
1.0	9.239	9.437	9.746	6.860	7.130	7.449	4.669	4.787	4.976
1.2	9.234	9.435	9.745	6.859	7.128	7.447	4.668	4.787	4.975
1.4	9.232	9.432	9.744	6.858	7.126	7.444	4.667	4.786	4.975
1.6	9.229	9.428	9.741	6.857	7.125	7.441	4.667	4.786	4.975
1.8	9.226	9.428	9.741	6.856	7.124	7.440	4.667	4.786	4.974

\*  $\kappa_s \text{ TPa}^{-1}\cdot 10^{-9}$ . Standard uncertainties in  $\rho$ ,  $u$  and  $\kappa_s$  are  $\pm 4\cdot 10^{-3} \text{ kg}\cdot\text{m}^{-3}$ ,  $\pm 0.5 \text{ m}\cdot\text{s}^{-1}$  and  $\pm 0.25\cdot 10^{-10} \text{ TPa}^{-1}$ . For temperature measurements (T/K), it comes out to be  $\pm 0.01 \text{ K}$

**ST4** Density,  $\rho$  ( $\text{kg}\cdot\text{m}^{-3}$ ), ultrasonic velocity,  $u$  ( $\text{m}\cdot\text{s}^{-1}$ ) and Isentropic Compressibility,  $\kappa_s$  ( $\text{TPa}^{-1}$ ) of CTAB (0.2–1.8)  $\text{mmol}\cdot\text{kg}^{-1}$  in water-1-propanol compositions (% v/v) of 0.02  $\text{mol}\cdot\text{kg}^{-1}$  BHT over different temperatures ranging from (298.15 to 308.15) K.

$10^3\cdot[\text{CTAB}]$ $\text{mol}\cdot\text{kg}^{-1}$	100% v/v <b>1-propanol</b>			70% v/v <b>1-propanol</b>			30% v/v <b>1-propanol</b>		
	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K	298.15K	303.15K	308.15K
<b><math>\rho/\text{kg}\cdot\text{m}^{-3}</math></b>									
0.0	858.588	847.257	834.954	887.969	869.658	855.359	926.268	906.709	887.958
0.2	825.658	815.365	803.265	865.748	848.254	833.265	901.965	884.328	866.768
0.4	824.748	814.354	802.369	865.455	848.176	833.658	900.258	883.195	865.847
0.6	823.198	813.582	801.472	865.158	848.119	833.614	900.005	882.759	864.995
0.8	825.554	815.654	803.546	864.996	848.075	833.547	901.856	884.584	865.688
1.0	825.494	815.598	803.502	864.935	848.006	833.468	901.782	884.507	865.824
1.2	825.422	815.542	803.476	864.886	847.984	833.405	901.716	884.468	865.775
1.4	825.381	815.488	803.434	864.812	847.967	833.364	901.649	884.408	865.711
1.6	825.313	815.426	803.384	864.759	847.914	833.318	901.601	884.356	865.666
1.8	825.276	815.395	803.335	864.711	847.863	833.286	901.579	884.297	865.613
<b><math>u/\text{m}\cdot\text{s}^{-1}</math></b>									
0.0	1245.26	1233.59	1210.65	1395.65	1386.26	1373.09	1598.35	1580.48	1571.85
0.2	1241.25	1228.35	1204.65	1386.98	1371.65	1359.65	1586.95	1570.26	1562.95
0.4	1241.31	1228.51	1204.86	1387.16	1371.83	1359.87	1587.06	1570.39	1563.14
0.6	1241.49	1228.62	1204.99	1387.36	1371.96	1360.15	1587.29	1570.47	1563.36
0.8	1241.68	1228.77	1205.16	1387.47	1372.19	1360.39	1587.48	1570.62	1563.58
1.0	1241.85	1228.94	1205.48	1387.59	1372.38	1360.52	1587.62	1570.77	1563.72
1.2	1242.01	1229.28	1205.64	1387.78	1372.49	1360.68	1587.83	1570.91	1563.8
1.4	1242.27	1229.37	1205.81	1387.86	1372.64	1360.83	1588.01	1571.09	1563.97
1.6	1242.33	1229.49	1206.03	1387.91	1372.77	1360.91	1588.28	1571.22	1564.08
1.8	1242.36	1229.51	1206.09	1387.98	1372.81	1360.99	1588.33	1571.34	1564.11
<b><math>10^{-10}\cdot\kappa_s\text{ TPa}^{-1}</math></b>									
0.2	7.861	8.128	8.579	6.004	6.266	6.491	4.402	4.586	4.722
0.4	7.869	8.136	8.585	6.004	6.264	6.486	4.410	4.591	4.726
0.6	7.882	8.143	8.593	6.005	6.264	6.484	4.410	4.593	4.730
0.8	7.857	8.120	8.568	6.005	6.262	6.482	4.399	4.582	4.725
1.0	7.855	8.118	8.564	6.004	6.261	6.482	4.399	4.582	4.723
1.2	7.854	8.114	8.562	6.003	6.260	6.480	4.398	4.581	4.723
1.4	7.851	8.114	8.560	6.003	6.259	6.479	4.398	4.580	4.722
1.6	7.851	8.113	8.558	6.003	6.258	6.479	4.396	4.580	4.722
1.8	7.851	8.113	8.557	6.002	6.258	6.478	4.396	4.580	4.722

\*  $\kappa_s$   $\text{TPa}^{-1}\cdot 10^{-9}$ . Standard uncertainties in  $\rho$ ,  $u$  and  $\kappa_s$  are  $\pm 5\cdot 10^{-3}\text{ kg}\cdot\text{m}^{-3}$ ,  $\pm 0.4\text{ m}\cdot\text{s}^{-1}$  and  $\pm 0.20\cdot 10^{-10}\text{ TPa}^{-1}$ . For temperature measurements (T/K), it comes out to be  $\pm 0.01\text{ K}$