Supporting Information for,

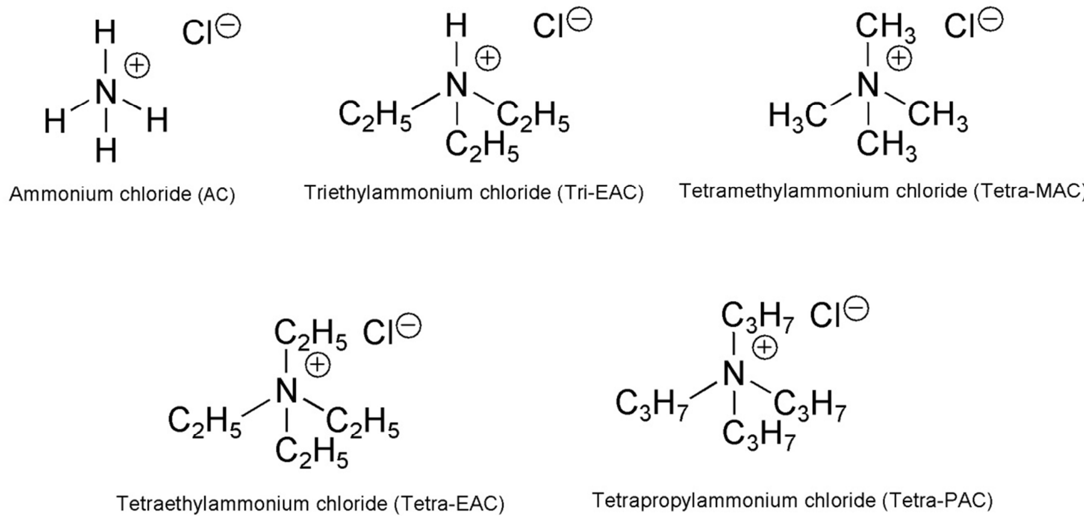
Decisive Role of Hydrophobicity on the Effect of Alkylammonium Chlorides on Protein Stability: A Terahertz Spectroscopic Finding

Debasish Das Mahanta, Nirnay Samanta, Rajib Kumar Mitra*

Chemical, Biological and Macromolecular Sciences

S. N. Bose National Centre for Basic Sciences
Block-JD, Sector-III, Salt Lake, Kolkata, 700106, India
Phone: 91-33-23355706, Fax: +91-33-23353477

* Corresponding author.
E-mail: rajib@bose.res.in (RKM)



Scheme S1. Chemical structures of the alkylammonium chloride salts.

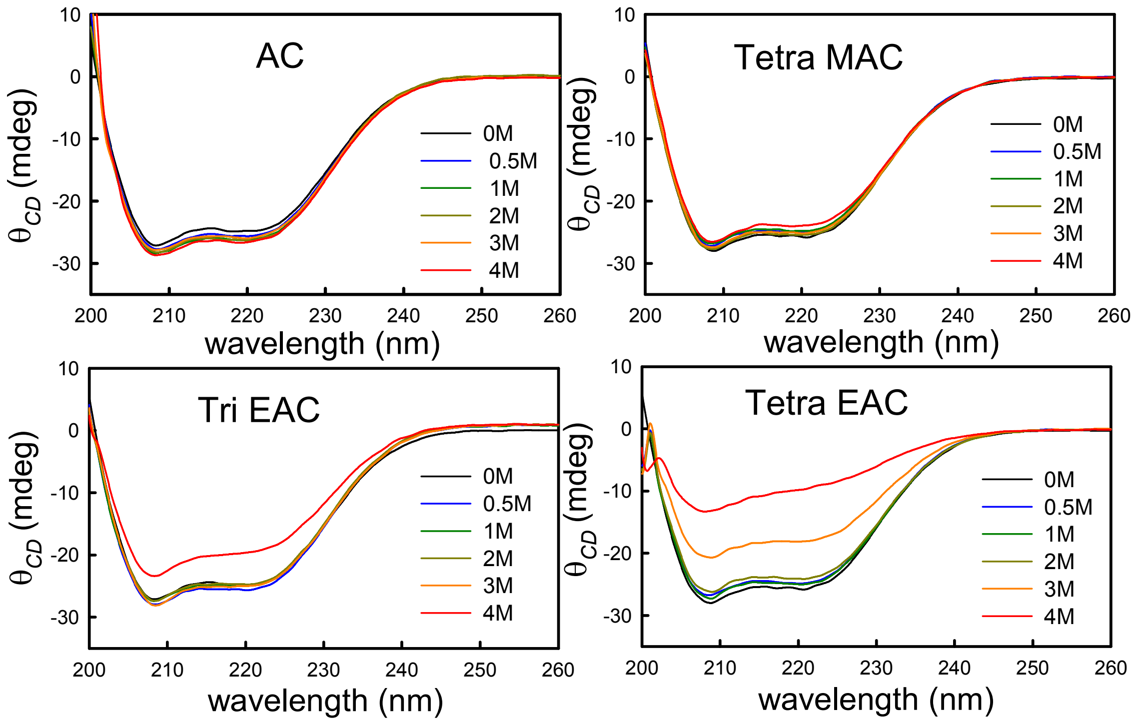


Figure S1. CD spectra of BSA protein at different concentrations of the various salts.

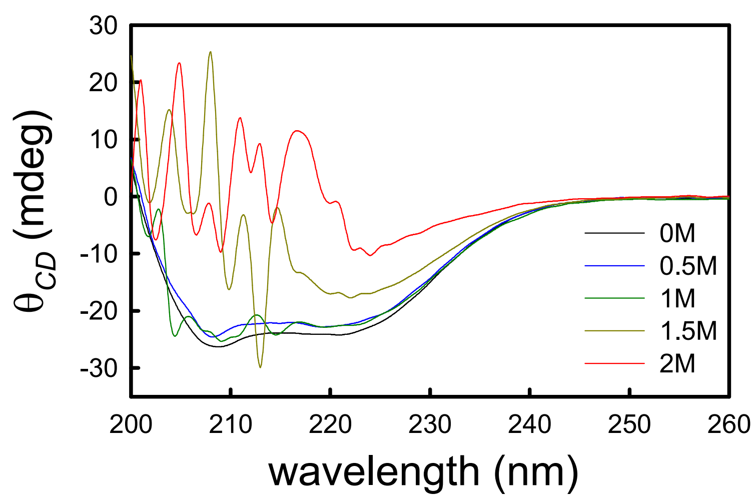


Figure S2. CD spectra of BSA in presence of tetra-PAC.

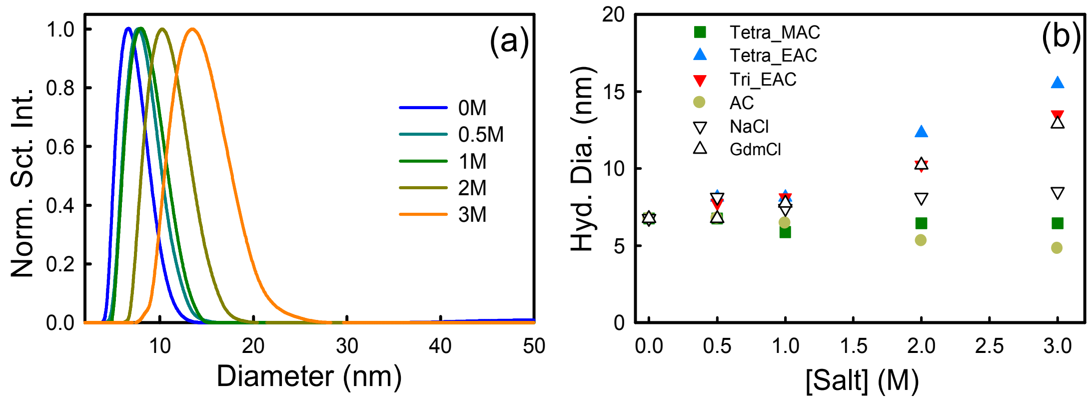


Figure S3. (a) Representative scattering profile of BSA in presence of Tri-EAC at different concentrations. (b) The hydrodynamic diameter of BSA in various salt solutions with increasing salt concentrations.

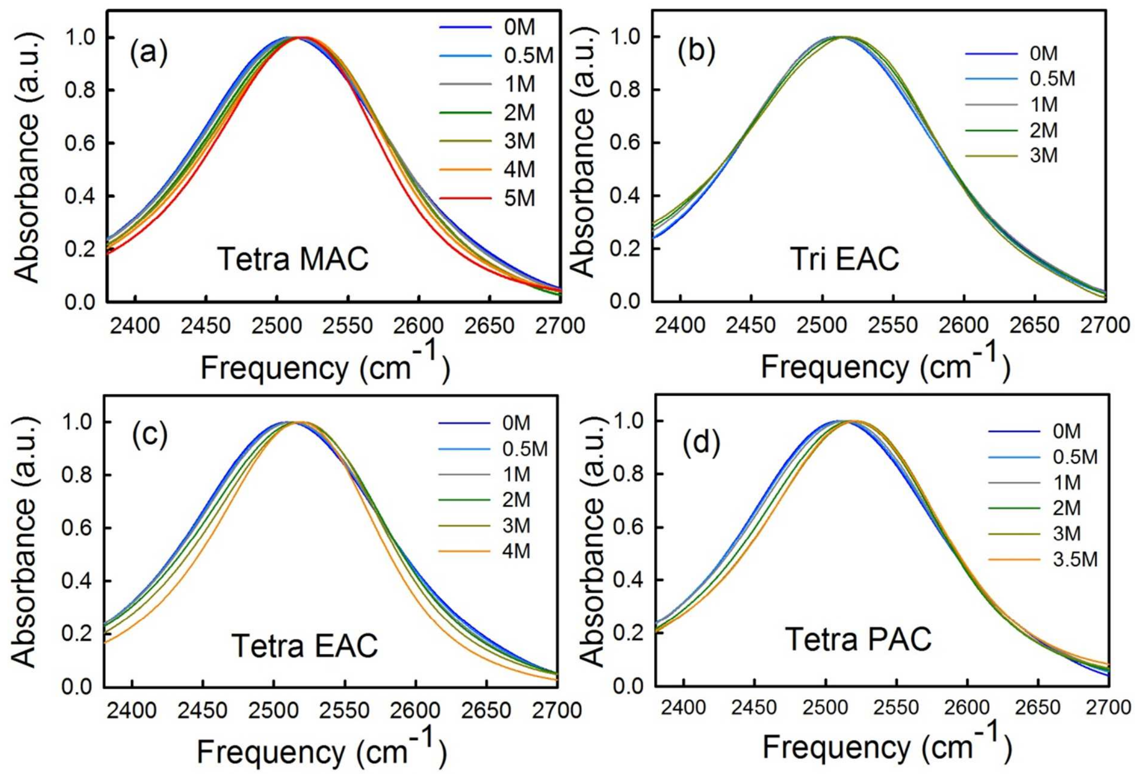


Figure S4. Normalized FTIR absorption spectra of HOD (4% D_2O in water) in presence of different salts.

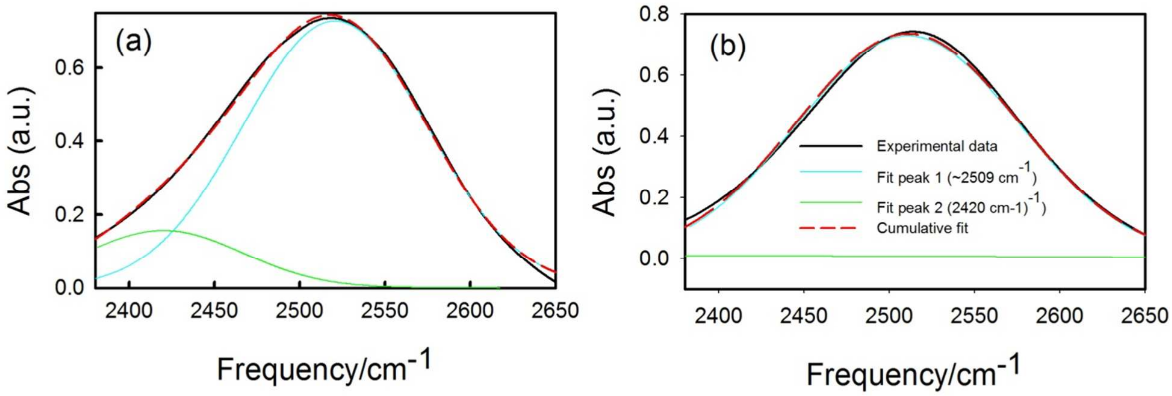


Figure S5. Representative deconvoluted FTIR absorption spectrum for (a) Tetra EAC and (b) NaCl.

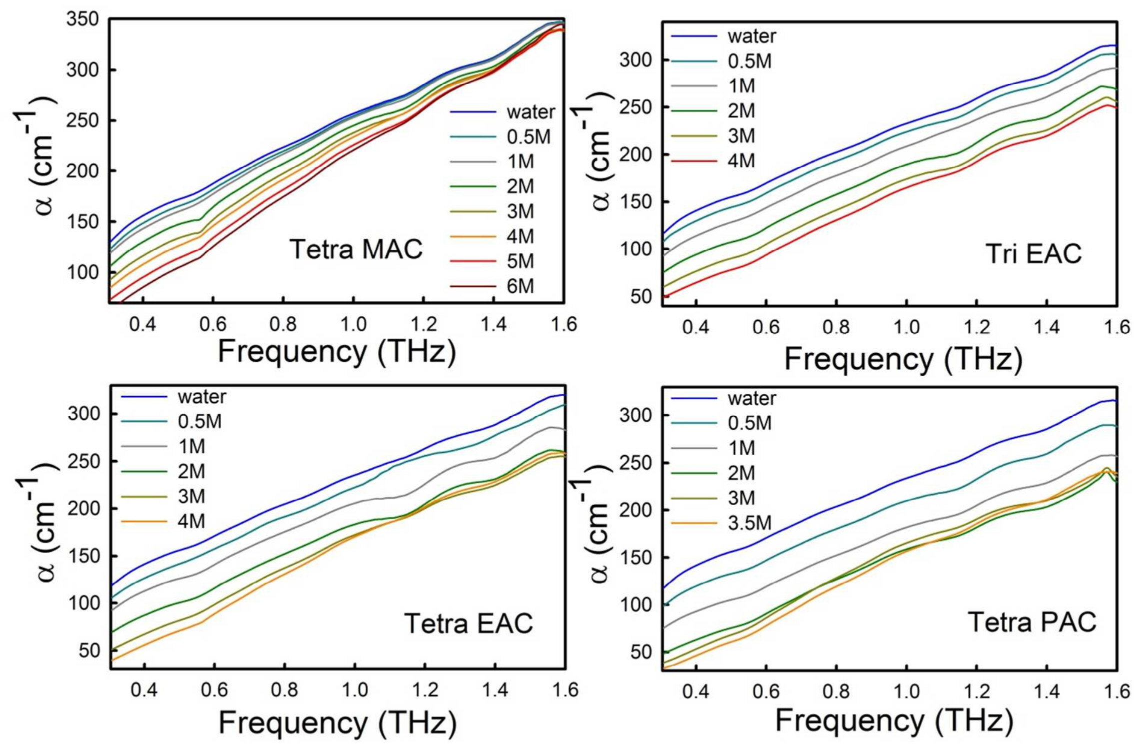


Figure S6. Absorption ($\alpha(\nu)$) profiles in the THz regime of the aqueous solutions of different alkylammonium chloride salts.

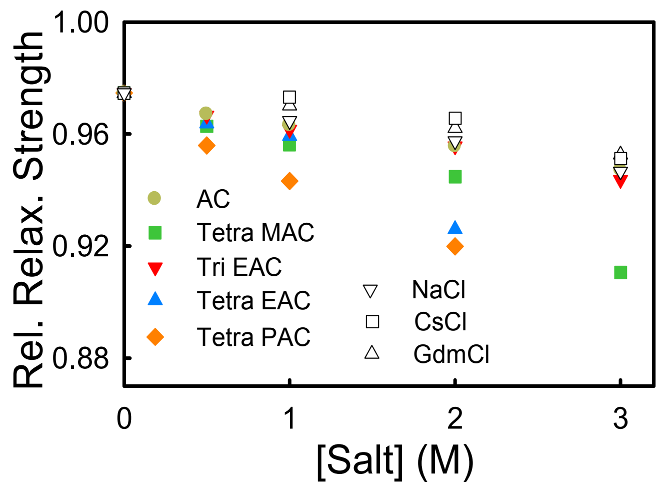


Figure S7. Cooperative relaxation strength ($\frac{S_1}{S_1+S_2+S_3}$) in presence of different salts as a function of concentration.

Table S1. Multiple Debye fitting parameters of THz DR study in various salt solutions. The time constant τ_3 has been fixed constant at 0.06 ps.

Concentration (M)	ε_s	S_1	S_2	S_3	τ_1 (ps)	τ_2 (ps)
AC						
0	77	74.3	0.45	1.36	8.93±0.1	0.26±0.05
0.5	69	64.9	0.61	1.59	7.59±0.1	0.22±0.04
1	62	57.8	0.71	1.50	6.72±0.08	0.21±0.03
2	57	52.6	0.89	1.54	5.66±0.06	0.19±0.03
3	53	48.3	1.06	1.64	5.07±0.05	0.19±0.03
4	48	43.2	1.16	1.16	4.37±0.04	0.18±0.03
5	40	35.1	1.26	1.77	3.41±0.03	0.17±0.02
MAC						
1	67	64.1	0.83	1.11	9.87±0.1	0.31±0.03
2	60	56.8	1.25	1.17	14.8±0.6	0.27±0.03
3	57	53.7	1.25	1.16	14.9±0.6	0.27±0.03
4	48	44.6	1.42	1.21	17.3±0.9	0.25±0.03
5	40	36.5	1.53	1.35	22.9±2.7	0.27±0.03
6	30	26.3	1.66	1.40	25.5±1.9	0.25±0.03
Tri-EAC						
1	70.2	67.3	0.66	1.34	9.61±0.1	0.29±0.06
2	66	63.1	0.77	1.26	10.8±0.1	0.27±0.03
3	62	58.9	0.94	1.23	13.2±0.2	0.26±0.03
4	52	48.9	1.00	1.14	14.7±0.3	0.26±0.02
6	42	38.9	1.04	1.27	25.0±2	0.25±0.04
Tetra-EAC						
0.25	71	68.1	0.75	1.43	9.47±0.2	0.38±0.06
0.5	63.5	60.5	0.81	1.40	9.09±0.2	0.35±0.04
1	54.2	51.3	0.87	1.18	10.0±0.2	0.28±0.03

1.5	46	42.8	1.11	1.29	11.2±0.3	0.30±0.03
2	38	34.7	1.23	1.34	14.6±1	0.33±0.04
3	30	26.7	1.26	1.35	22.3±3	0.34±0.04
Tetra-PAC						
0.5	68.9	65.4	0.59	1.439	10.9±0.1	0.29±0.06
1	63.8	60.2	1.01	1.28	15.6±0.3	0.23±0.04
2	48	44.5	1.38	0.87	36.6±2	0.19±0.04