Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

SUPPLEMENTARY INFORMATION

A Molecular Dynamics study of structure, stability and fragmentation patterns of Sodium bis(2-ethylhexyl)sulfosuccinate positively charged aggregates *in vacuo*

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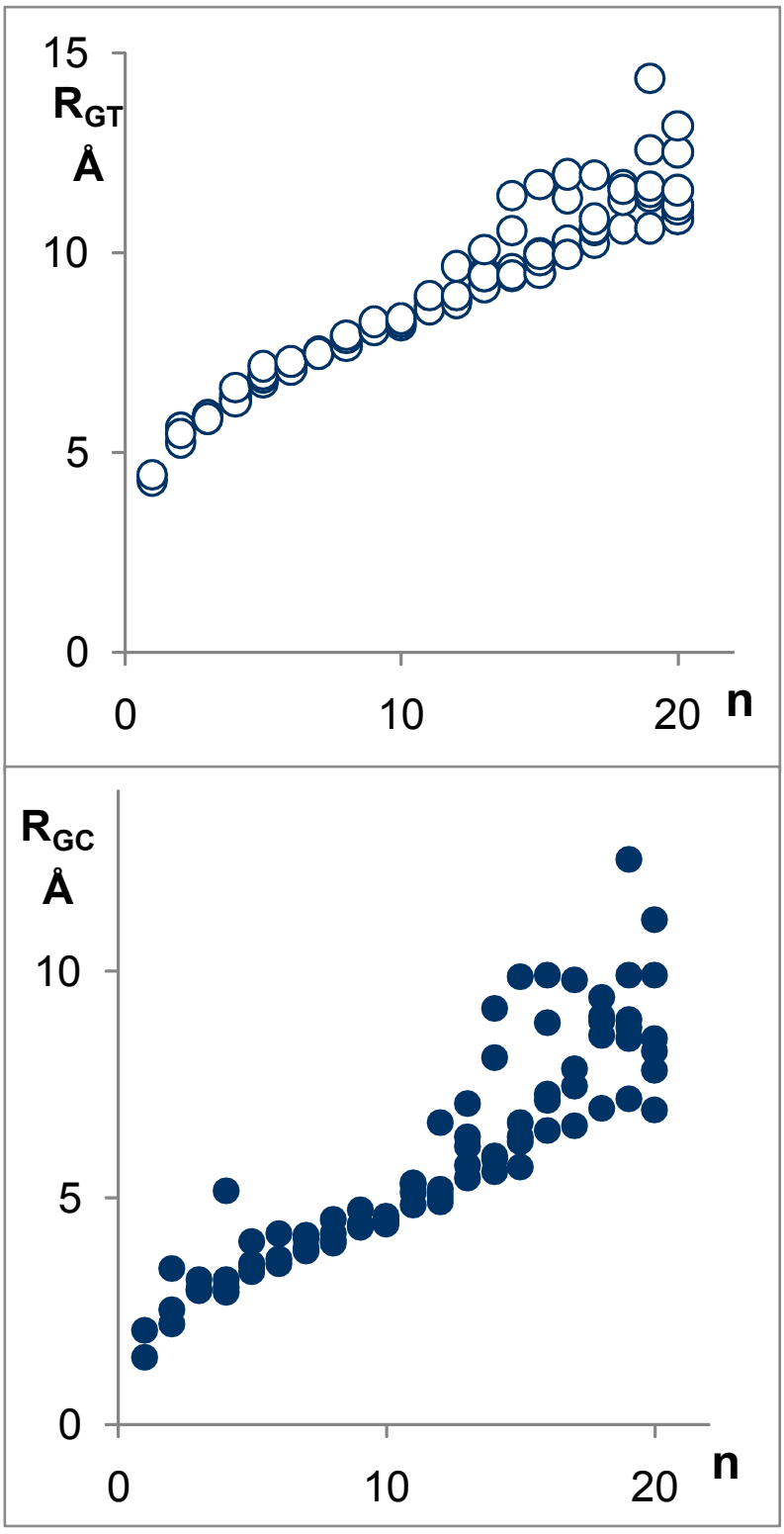

Figure SI-1 gyration radius (Å) calculated for all atoms, R_{GT}, and for the core atoms, R_{GC}, for n=1-20 for all possible charge values (n_c= 0-$n_{c,max}$).

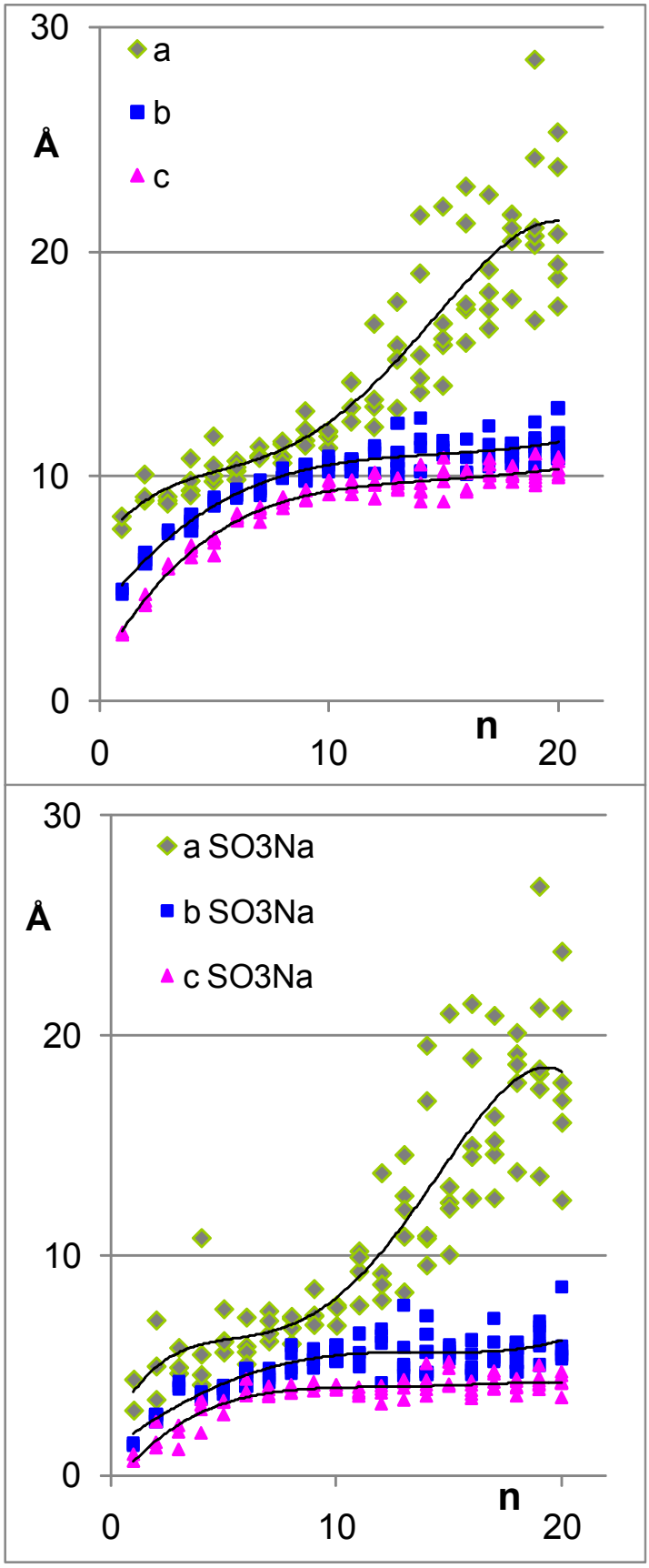

Figure SI-2 Lengths of the three semi-axes *a b c* (Å) of the equivalent ellipsoid, calculated from inertia moments as explained in the text, for all atoms (*top*) and for the core atoms (SO_3Na) (*bottom*) for all n and n_c values. Lines are added just as eye-guides.