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Erratum

Inorganica Chimica Acta, 40 (1980) pp. X165 and X172

The abstract **Influence of the Solvent on the Anionic Reactivity of Quaternary Onium Salts in Nucleophilic Aliphatic Substitutions. Leaving Group Effects**

A. MAIA, D. LANDINI and F. MONTANARI (Milan, Italy) page X 165.

The second part of this abstract – The specific solvation of the anion .... the leaving group by the solvent., plus three references – has unfortunately been printed on page X172 under the title **Dipolar Effects in Electrolytes** by S. Ciccariello (Padua, Italy), D. Gazzillo and C. Dejak (Venice, Italy), the abstract of this title being omitted altogether. We apologise for this mistake and publish the missing abstract hereafter.

Dipolar Effects in Electrolytes

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Today, in describing the statistical mechanical behaviour of dilute electrolyte primitive models such mathematical accuracy has been reached as to make unavoidable further research into more accurate models [1]. In fact, the previous choice of ion interactions is unsatisfactory mainly because the granular structure of the solvent, as well as ions' polarizability, have been completely overlooked [2]. These effects could be accounted for by describing the ions as suitable electrical charge distributions, which, as a first approximation, can be assumed to be independent of the relative ion distance. So, one is led to depict the ions of any electrolytic solutions as hard spheres with a suitable superposition of fixed electrical multipoles.

In order to make the relevant mathematical expressions tractable from a computering point of view, we have been led to make the further assumption that, when no dipoles can be present, multipole effects can still be described, at least on a heuristic level, by a single electric dipole moment.

The main mathematical implications of this model have been analyzed in ref. [3], where it has been shown that through a suitable regularization of the interaction at the origin, it is possible, by parallelling Mayer's procedure, to explicitly evaluate both the chain-potential and the ring approximation to the free-energy.

By considering the regularizing function $\exp(-\alpha r)/r$ as a 'fictitious function' [4], we have recently accomplished the evaluation of the leading contributors to the two-point prototype graphs and we are now performing parameter determination through the best-fit of experimental data.

Our preliminary results indicate that:

i) a suitable choice of the parameter α allows a considerable improvement in the fit for all considered salts;

ii) for the alkaline nitrates the presence of an electric dipole moment seems unavoidable;

iii) for the caesium halides, the dipoles' presence precludes the idea that ionic radii turn out to be smaller than crystallographic ones.

References

1 See, *e.g.* C. W. Outhwaite – Specialist periodical reports 'Statistical Mechanics' vol. 2 – The Chemical Society, London, 1975.
2 H. L. Friedman and B. Larsen, *J. Chem. Phys. 70*, 92 (1979).
3 S. Ciccariello, D. Gazzillo and C. Dejak, *Molec. Phys. 36*, 429 (1978).
4 S. Ciccariello, D. Gazzillo and C. Dejak, *Molec. Phys. 39*, 597 (1980).