

s12.m34.p7 **On the Microscopic Structure of Some Aqueous Electrolyte Solutions.** Ildikó Harsányi and László Pusztai, *Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, P.O. Box 49., H-1525, Hungary. E-mail: i_harsanyi@hotmail.com*

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The Reverse Monte Carlo (RMC) method of structural modeling [1] has been applied for the study of aqueous LiCl and HCl solutions. For both solutions, one neutron and one X-ray total structure factors have been considered as experimental input for RMC. LiCl solutions where the LiCl:water ratio was 1:3, 1:8, 1:16 were selected from a detailed study of the material [2]. The case of pure water, which served as a reference system, has also been studied. Considering contributions of the different partial pair correlation functions (ppcf) to the total structure factors (tsf), this study was focused on the changes of the hydrogen bonded network of water molecules. (Ion-ion correlations, which would be of considerable interest, have too small contributions.) For this purpose, geometrical constraints, mostly on the O..H atom pairs, have been introduced for maximizing the number of hydrogen-bonded water molecules. It was found that the highest possible number of hydrogen bonds decreases dramatically as the salt concentration increases. In relation to this, the O-H...O (hydrogen bond) angle becomes less straight with increasing LiCl concentration. The geometry of water molecules, represented by the H-O-H bond angle, also becomes distorted. As for the hydration of ions, a neat hydration shell of Li ions (with a coordination number of two) was detected at the lowest concentration, which shell becomes less distinct as concentration increases.

For hydrochloric acid solutions, concentrations with HCl:water ratios of 1:3, 1:9, 1:30 were selected from an earlier diffraction study [3]. Based on the (water-)H/D-O partial pair correlation functions it may be suggested that at very high acid concentrations H(D)Cl acts as a 'structure maker'. Concerning the hydration shell of the chloride ions, a straight O-H(D)...Cl hydrogen bond angle was found at each concentration. The change of the H(D)-O-H(D) cosine distribution function with concentration is consistent with a change of the molecular structure of water: the bond angle becomes smaller with the increasing number of ions. Concerning the coordination of protons, it is demonstrated that the concentration of H(D)₃O⁺ species must be much less than it has been assumed previously.

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s12.m34.p8 **Structural Polymorphism in Calcium Aluminate (CaAl₂O₄:Eu²⁺) Persistent Luminescence Materials.** Jorma Hölsä^a, Mika Lastusaari^a, Hannu Mutka^b, Janne Niittykoski^{ac}, Clemens Ritter^b and Mika Tukka^a, ^aUniversity of Turku, Department of Chemistry, FI-20014 Turku, Finland, ^bInstitute Laue Langevin, BP 156, FR-38042 Grenoble Cedex 9, France, and ^cGraduate School of Materials Research, Turku, Finland. E-mail: miklas@utu.fi

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Alkaline earth aluminates, MA₂O₄, doped with divalent europium are promising persistent luminescence materials with a wide range of commercial applications including luminous paints. CaAl₂O₄ has two polymorphs with different luminescence properties. The crystal structure of only one of the polymorphs has been solved, so far. The solid state reaction of monoclinic CaAl₂O₄ must be carried out at high temperatures (around 1300 °C) since impurities such as M₃Al₂O₆ are formed at lower temperatures. On the other hand, a successful preparation of CaAl₂O₄ powders at a much lower temperature (900 °C) has been reported using a sol-gel synthesis [1]. A metastable CaAl₂O₄:Eu²⁺ form was obtained with the sol-gel method at 850 °C. This form possessed a structure different from monoclinic and was probably stabilized by impurities. Other products or starting materials were then not observed. The structure of metastable CaAl₂O₄:Eu²⁺ was determined as hexagonal with the space group P6₃ (Z = 6), in contrast to earlier data [1] suggesting an orthorhombic structure. The calculated lattice parameters were a = 8.74 and c = 8.08 Å [2]. The detailed structure of this metastable phase was not, however, solved in detail, since the X-ray derived structure suggested possible disorder in the oxygen position around one of the Ca²⁺ sites. Due to the higher neutron scattering power of oxygen in comparison with Ca and Al, a neutron powder diffraction study was carried out. The results obtained from the neutron data for the hexagonal polymorph will be discussed and compared to those of the monoclinic one.

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