

[s8b.m5.p4.la] Comparison of Solubility and Interactions of Aprotinin (BPTI) solutions in H₂O and D₂O. M. Budayova-Spano^{1*}, S. Lafont^{1#}, J.-P. Astier¹, C. Ebel² and S. Veessler¹. *1 Centre de Recherche sur les Mécanismes de la Croissance Cristalline CRMC2* - CNRS, Campus de Luminy, case 913, 13288 Marseille cedex 09, France. 2 IBS J.-P. Ebel CEA-CNRS / LBM, 41 rue Jules Horowitz, 38027 Grenoble cedex 1, France. *at present: IBS J.-P. Ebel CEA-CNRS / LCCP, 41 rue Jules Horowitz, 38027 Grenoble cedex 1, France. # at present: Hoechst Marion Roussel, Bat. Velluz, 102 route de Noisy, 93235 Romainville cedex, France.*

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Small-angle neutron scattering experiment are often performed with proteins solubilized in heavy water because of the large difference in neutrons scattering properties of protons and deuterons. In order to characterize the effect of D₂O on physico-chemical properties of protein solutions, we investigated the effect of D₂O on the phase diagram and the interactions in BPTI solutions. We measured the solubility in D₂O of BPTI solutions in the presence of NaCl (reverse solubility) and KSCN (direct solubility) and compared with the values measured by Lafont et al. [1] in H₂O in the same conditions. In both salts we found that BPTI solubility in D₂O is significantly lower than in H₂O. The curves representing the solubility of BPTI in KSCN are shifted by 7.2°C between light and heavy water, a shift obtained previously with lysozyme and representing the difference in the temperature of maximum density of both types of water [2-3]. In the case of BPTI in NaCl, we did not find this relation between the solubility in H₂O and D₂O. We found, by dynamic light scattering (DLS), that BPTI attractive intermolecular interactions in the presence of NaCl in D₂O are significantly stronger than in H₂O. We investigated the association of BPTI molecules in crystallization conditions in presence of NaCl in H₂O and D₂O by small-angle X-ray and neutrons scattering respectively.

In the presence of heavy water the transition monomer-multimer is observed at about 2 mg/ml of BPTI in 1M NaCl whereas in light water and in 1.4M NaCl solution this transition is observed at about 15 mg/ml.

These results clearly showed that BPTI in crystallization conditions is a multimer and confirm the importance of the isotopic nature of water in the crystallization of proteins. The replacement of H₂O by D₂O decreases the solubility and increases the attractive intermolecular interactions.

[1] S. Lafont et al., J. Crystal Growth 173 (1997) 132.

[2] G. Gripon et al., J. Crystal Growth 177 (1997) 238.

[3] G. Gripon et al., J. Crystal Growth 178 (1997) 575.

[s9.m1.p21.la] Crystal Architecture and Magnetic Properties of Four Transition-metal Adipato Coordination Polymers. E. Bakalbassis^a, M. Korabik^b, A. Michaelides^c, J. Mronziski^b, C. Raptopoulou^d, S. Skoulika^c, A. Terzis^d and D. Tsaousis^c. *a Laboratory of Applied Quantum Chemistry, Department of General and Inorganic Chemistry, Faculty of Chemistry, Aristotle University of Thessaloniki, P.O.B. 135, 540 06 Thessaloniki, Greece, b Faculty of Chemistry, University of Wrocław, 14F. Joliot-Curie street, 503 83 Wrocław, Poland, c Department of Chemistry, University of Ioannina, 451 10 Ioannina, Greece and d Institute of Material Science, NCSR Demokritos, 153 10 Aghia Paraskevi Attikis, Greece.*

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The controlled assembly of structural units in the solid state is essential for the rational synthesis of functional materials. Of particular interest is the combination of metal-ligand coordination with hydrogen bonding, which might utilize the hydrogen bonding capability of coordinated ligands. This combination could lead to the assembly of 3D solids, involving cooperative effects (magnetic, optic e.t.c.) transmitted in the three directions of space.

In the present study, we investigate the synthesis, crystal structure and magnetic properties of some coordination polymers based on M(II) centers (M(II)=Cd(II), Cu(II) and Ni(II)), adipate anions and water molecules, namely [Cd(ad)(H₂O)₂]_n (**1**), two copper complexes [Cu(ad)(H₂O)₂]_n (**2**) and [Cu₃(ad)₂(OH)₂(H₂O)₄]_n (**3**) and [Ni(ad)(H₂O)₄]_n (**4**). The single crystals were prepared by the silica gel method.

In the case of compounds **1,2** and **4** it was seen that the combination of the metal cation and the dicarboxylate ligand leads to the formation of infinite chains. The coordinated water molecules and the carboxylate oxygen atoms collaborate nicely to hydrogen-bond the chains into 3-D structures. In all cases the ligand occupies an inversion center. We examine how the local symmetry operators (symmetry of the ligand and symmetry of the metal center) combine to lead to the observed space group. The observations made are useful for the control of the space group symmetry in crystalline solids.

Variable temperature magnetic susceptibility measurements made on compounds **2, 3** and **4**, showed weak antiferromagnetic interaction for **2** and **3** and isolated Ni(II) ions for **4**. A possible interpretation of the magnetic behaviour, in correlation with structural data and the results of quantum chemical calculations is attempted. Hydrogen bonds play an important role in the interaction between magnetic centers.