

C2/c space group, two pairs of oxygen atoms in the vicinity of a single hydrogen bond are related by a center of symmetry. The result is a rather diffusely located proton, distributed over four oxygen atoms in the high symmetry space group, whereas it is localized to the vicinity of two oxygen atoms in the low symmetry space group. The consequences of such a "distributed" proton are evident in the rather long O-O distances. The influence of this local hydrogen-bonding geometry on phase transitions is discussed.

**PS11.05.06 PHASE TRANSITION BETWEEN MICROEMULSION AND LAMELLAR PHASE IN AMPHIPHILIC SYSTEMS.** S. K. Ghosh, J. Matsuba, S. Komura\*, H. Seto\*, T. Takeda\*, M. Hikosaka\*, Graduate School of Biosphere Science, \*Faculty of Integrated Arts and Sciences, Hiroshima University, Higashi-Hiroshima 739, Japan

Amphiphiles are intriguing materials that exist in various forms in water-amphiphile binary systems or in water-oil-amphiphile ternary systems. Phase diagram of ternary system involving non-ionic amphiphile "C<sub>12</sub>E<sub>5</sub>/n-octane/water" has been presented by Kahlweit [1]. At equal volume fraction of octane and water with more than 15% volume fraction of amphiphile there are two microemulsion phases that are intervened by a lamellar phase with rising temperature. In order to study the first order phase transition between the microemulsion and lamellar phases we have measured small-angle X-ray scattering intensity from this system extensively. We observed a respective single peak from each of the two microemulsion phases and the lamellar phase. In the temperature ranges between the lamellar and the two microemulsion phases, we also observed a coexistence of two peaks.

These two peaks show a very systematic gradual change with respect to the peak positions  $q_l$  and  $q_m$  ( $l$  and  $m$  refer to the lamellar and the microemulsion phases, respectively) and the peak intensities  $I_l$  and  $I_m$ , as follows. As the temperature is increased from the lower microemulsion phase up to the lamellar phase,  $I_m$  decreased and disappeared, while  $I_l$  appeared and increased. Simultaneously both  $q_l$  and  $q_m$  decreased. As the temperature is further increased from the lamellar phase up to the upper microemulsion phase, a similar but opposite systematic change was observed. These behaviors are qualitatively in agreement with what is expected from the *lever rule* in the phase diagram.

We have explained the transitions between the lamellar and microemulsion phases on rising temperature, as a result of the change of spontaneous curvature of the interface film made of amphiphile and subsequent change of *bending elastic energy* within the interfacial model of Andelman et al [2].

1. M. Kahlweit et al., *J. Colloid and Interface Science*, **118** (1987) 436  
2. D. Andelman et al., *J. Chem. Phys.* **87** (1987) 7229

**PS11.05.07 X-RAY STUDIES OF MAGNETICALLY INTERESTING COMPOUNDS IN THE TEMPERATURE RANGE 10-300K.** A. E. Goeta, R. C. B. Copley, C. W. Lehmann, J. A. K. Howard, University of Durham, Durham Chemical Crystallography Group, UK

We present here an application of low temperature crystallography to the study of structure/property relationships. Two systems previously reported to show magnetic phase transitions at approximately 36K and 23K have been investigated using the Fddd high intensity cryogenic diffractometer at Durham, UK.

(i) [*p*-CNSSN·C<sub>6</sub>F<sub>4</sub>CN]<sub>2</sub>. The β-phase of this compound is the first purely organic material to exhibit spontaneous magnetisation above liquid helium temperatures. The compound crystallises in the orthorhombic space group Fdd2 and keeps the same symmetry from room temperature down to 10K. The observed magnetic behaviour has been explained in terms of a phase

transition, at the unprecedentedly high temperature of 36K, from a one-dimensional antiferromagnetic state to a weak ferromagnetic state. The fact that the structure remains in a non-centrosymmetric space group is a very positive finding since it is in accordance with the weak ferromagnetic signal postulated to result from the Dzyaloshinsky-Moriya interaction.

(ii) [(T<sup>5</sup>-Cp\*)Cr(T<sup>5</sup>-P<sub>3</sub>)Cr(T<sup>5</sup>-Cp\*)](SbF<sub>6</sub>) A previous SQUID investigation on this triple-decker compound showed it to undergo a spin crossover at approximately 23K. The diffraction study carried out clearly shows a sharp and non-destructive structural phase change at 21K and initial analysis of the full and extensive data suggests that the Cr-Cr separation has shortened from 3.1Å at room temperature to 2.7Å at 12K. This is a first and is seen as clear and exciting experimental evidence for the spin pairing of the chromium atoms.

**PS11.05.08 THALLIUM (I) ORTHOFLUORBERILLATE** González-Silgo, C.<sup>a</sup>, Ruiz-Pérez, C., Martínez-Sarrión, M. L.<sup>b</sup>, Mestres L., Solans, X.<sup>c</sup> <sup>a</sup>Dpto. Física Fundamental y Experimental, Universidad de La Laguna, Spain, <sup>b</sup>Dpto. Química Inorgánica, <sup>c</sup>Depto. Cristallografía, Mineralogía y Deposits Minerals Universitat de Barcelona, Spain.

(NH<sub>4</sub>)<sub>2</sub>BeF<sub>4</sub> and Tl<sub>2</sub>BeF<sub>4</sub>, with similar ion radii from Rb<sup>+</sup>, are isostructural in Pnam space group. The first shows undergoes two phase transition at lower temperature and crystal structure of Tl<sub>2</sub>BeF<sub>4</sub> isn't reported, but it isn't known phase transition. Otherwise, Thallium oxisalts, some of them show structural instabilities, has been lately studied and may be inferred two types of cation with 11 and 9 surrounding O atoms and the importance of the shortest bonds. The structural determination is important to access the role of the atoms placed in large cavities like a particular result of the general rule pointed out I.D. Brown (1992). Tl<sub>2</sub>BeF<sub>4</sub> was obtained via reaction BeF<sub>2</sub>+H<sub>2</sub>F<sub>2</sub>+Tl<sub>2</sub>CO<sub>3</sub>=Tl<sub>2</sub>BeF<sub>4</sub>+CO<sub>2</sub>+H<sub>2</sub>O. Mixed crystal were obtaining mixing aqueous solution of (NH<sub>4</sub>)<sub>2</sub>BeF<sub>4</sub> and Tl<sub>2</sub>BeF<sub>4</sub> thermostating at 30C. We have determined the structure of Tl<sub>2</sub>BeF<sub>4</sub> and Tl<sub>1.84</sub>(NH<sub>4</sub>)<sub>0.16</sub>BeF<sub>4</sub>: orthorhombic, Pnam, Z=4, a=7.679(2), 7.689(2), b=10.383(3), 10.398(3), and c=5.871(2), 5.886(2). We have found differences between the crystals at room temperature: 1<sup>st</sup>) In Tl<sub>2</sub>BeF<sub>4</sub>, a BeF<sub>4</sub> group deformation mainly along b direction and one Be-F bond is near to parallel a axis. 2<sup>nd</sup>) The arrangement of 11-coordinated cation is similar in both compounds, but the linkage of 9-coordinated cation indicates this (NH<sub>4</sub>)<sup>+</sup> ion plays the most important role in (NH<sub>4</sub>)<sub>2</sub>BeF<sub>4</sub> phase transition. 3<sup>rd</sup>) Bond-Valence model predicts structural instabilities in (NH<sub>4</sub>)<sub>2</sub>BeF<sub>4</sub> while Tl<sub>2</sub>BeF<sub>4</sub> is more stable.

Brown, I. D., *Acta Cryst.*, **B48** (1992), 553.  
Fàbry, J., Prez-Mato, J. M., *Phase Transitions*, **49** (1994), 193  
Fàbry, J., Breczewski, T. *Acta Cryst.*, **C49** (1993), 1724.  
González-Silgo, C., Ruiz-Pérez, C., Solans, X., Martínez-Sarrión, M.L., Mestres, L., Rodríguez, A., Bocanegra, E. To appear in *Ferroelectrics* (1996).  
Martínez-Sarrión, M.L., Mestres, L., Rodríguez, A., Solans, X., *Ferroelectrics*, **141** (1993), 37.  
Onodera, A., Shiozaki Y., *J. Phys. Soc. Japan* **46** (1979), 1.