spectra we will discus the electric structure, distortion of polyhedra related to ferroelectricity and thermal vibration.

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Keywords: ferroelectric, XANES, phase transition

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Temperature dependence of pre-edge feature in Ti K-edge XANES spectra for $ATiO_3$, A_2TiO_4 (A=Mg, Ca, Fe, Sr and Ba) and TiO_2 compounds

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X-ray absorption near edge structure (XANES) provides important information on the electronic structure and local symmetry around X-ray absorption atom. There are three distinct pre-edge peaks correspond to electronic transitions in Ti K-edge XANES spectra. The composition, structure and temperature dependence of XANES spectra on three peaks was investigated. We measured Ti K-edge XANES spectra of various titanates, $MgTiO_3$, $CaTiO_3$, $SrTiO_3$, $BaTiO_3$, Mg_2TiO_4, Fe_2TiO_4, TiO_2 rutile and anatase, in the temperature range from 20K to 800K. Ti atoms are placed in TiO_6 octahedral and TiO_4 tetrahedral sites in crystal structures. The measurements of Ti k-edge XANES spectra were carried out in transmission mode at beam line BL-7C and BL-9A of the Photon Factory in KEK, Tsukuba. High temperature X-ray absorption measurements were made under a helium atmosphere. XANES spectra of all sample on each peaks is increasing as the temperature increases except for tetragonal $BaTiO_3$ and tetragonal $SrTiO_3$ phases. TiO_2 rutile and anatase have largely different rate of rising pre-egde absorption to the temperature. The XANES spectra in the high temperature region were strongly affected by the harmonic thermal vibration of the atoms. There is an interesting relation between electronic transition and local distortion of coordination environment coming from the harmonic thermal vibration. We will discuss harmonic and anharmonic thermal vibration models by XAFS method.

Keywords: XANES, pre-edge peak, titanate

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A gold(III) complex of the neuroepileptic drug gabapentin

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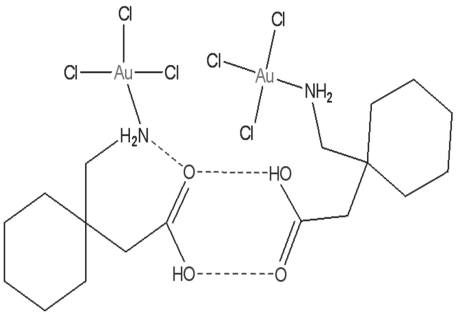
Gabapentin, a neuro-epileptic drug, has been the subject of interest lately as new polymorphs, [1] salts and hydrates have been reported, as well as the high pressure crystallisation of a novel heptahydrate [2]. The first complexes with transition metal complexes, Cu(II) and Zn(II) were reported recently by Braga and co-workers [3]. Since gold is known to have pharmaceutical applications [4] we were interested to see if we could prepare a Au(III)-Gp complex.



Auric acid was reacted with gabapentin in an aqueous solution. Two distinct types of crystals precipitated from this solution: pale yellow needle shaped crystals (**I**) and dark yellow blocks (**II**, not shown here). Their structures were determined by single crystal structure analysis. The MeOD solution ^1H and ^{15}N-NMR were then recorded to confirm that the gold remains coordinated to the nitrogen of the amino group in solution (**I**).

The crystal structure of (**I**) clearly shows the Au-N coordination (Au-N bond 2.043(2) Å) in the hydrogen bonded dimer. The cyclohexane is disordered over two positions, both having a chair conformation. The ^1H -NMR shows peaks at δ = 2.45, 2.88 ppm for the free gabapentin $–CH_2$- groups ($–CH_2$-COOH and -CH_2-$NH3^+$ respectively). On dissolving (**I**) in MeOD four peaks are apparent in the ^1H-NMR; at 2.45, 2.51, 3.05 and 3.12 ppm. Our current interpretation of this is that (**I**) exists as two different isomers in solution and that on crystallisation these persist in the solid state.

In conclusion, auric acid reacts with gabapentin in aqueous solution to form a Au(III)-gabapentin complex in which the Au(III) is coordinated to the amino nitrogen [5]. It appears that in this reaction an intermediate complex has been trapped given that Au(III) is known to oxidise amino acids.

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Crystal structure of Zn complex with chelidamic acid and acridine

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4-Hydroxypyridine-2,6-dicarboxylic acid as carboxylate derivative has drawn extensive attention in coordination chemistry. This ligand could potentially provide various coordination motifs to form both discrete and consecutive metal complexes under appropriate synthesis condition [1,2]. We prepared new mononuclear complex of Zn(II) containing 4-hydroxypyridine-2,6-dicarboxylic