a=9.358(1), b=13.408(1), c=13.755(5) Å, space group: Pmcn, R=0.042 for 1590 reflections. Those of the second compound are: monoclinic, a=9.688(2), b=14.157(2), c=25.520(3), β=94.72(1)°, space group: $P2_1/n$, R=0.044 for 3297 reflections. Those of the third compound are: monoclinic, a=8.050(1), b=12.490(2), c=20.193(4), β=95.97(1), space group: $P2_1/c$, R=0.024 for 3542 reflections. [Work was supported by National Science Council, Taiwan, China].

PS-07.04.44 THE PREPARATION AND CRYSTAL STRUCTURE OF $(C_{10}H_{21}NH_3)_2SnCl_6$. By Wei Wang*, Yonghua Lin, Laiming Li and Shiquan Xi, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China.

The Bis(n-decylammonium) tetrahalometallates(II) are known to crystallize in a perovskite-type bidimensional structure. They are of much current interest from both magnetic and structural points of view (K. J. Schenk, G. Chapuis, J. Phys. Chem., 1988, 92, 7141). But very few studies have been performed on bis(n-alkylammonium) hexahalometallates(IV) with general formula $(n\text{-}C_nH_{2n+1}NH_3)_2MX_6$. Up to now, no structure of a long-chain bis(n-alkylammonium) hexahalometallates(IV) has been reported. We have prepared $(C_{10}H_{21}NH_3)_2SnCl_6$ (abbreviated as $C_{10}Sn$) and determined its crystal structure.

The colorless plate-shaped crystals of $C_{10}Sn$ were grown at room temperature from absolute alcohol solution containing decylammonium chloride and $SnCl_4$. Intensity data were collected using a Nicolet R3M/E diffractometer. The structure was solved by the Patterson method and final R=0.069 for 2148 unique reflections [$I>3\sigma(I)$]. At room temperature the crystal is monoclinic with a=11.960(4)Å, b=7.288(2)Å, c=35.602(17)Å, β=94.05(3)°, V=3095.30(2.02)Å^3 and belongs to the space group $P2_1/m$ with four molecules in the unit cell. The structure of $C_{10}Sn$ is characterized by a layer of almost regular $SnCl_6^{2-}$ octahedra sandwiched between two hydrocarbon layers. The NH_3^+ polar heads of the decylammonium cations are linked to the chloride atoms by three N-H...Cl hydrogen bonds. There are two types of inequivalent hydrocarbon chains which are packed together. One has a perfectly ordered all-trans conformation, and the other has an extended conformation with only a single gauche turn between the second and the third carbon atoms. The general arrangement of the alkyl chain of $C_{10}Sn$ is comparable to the bilayer structure of biological membranes.

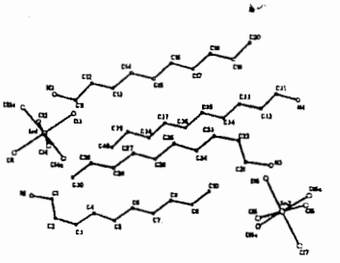

Fig. 1. Perspective view of $C_{10}Sn$.

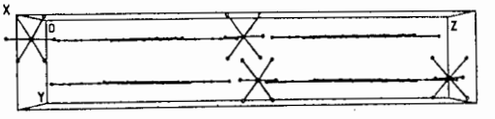

Fig. 2. Arrangement of $C_{10}Sn$ in unit cell.

PS-07.04.45 THE CRYSTAL AND MOLECULAR STRUCTURE OF [1,2-DIMETHYL-1,2-(DI-ISOBUTYL)ETHYL] BISCYCLOPENTADIENYL TITANIUM DICHORIDE. By Zu-tao Wang, Shou-shan Chen, Ru-ji Want and Xin-kan Yao, Cental Laboratory, Institute of Elemento-organic Chemistry, Nankai University, Tianjin 300071, China.

The study of chiral bridged bis cyclopentadienylmetal complexes has now become a very active field in organometallic chemistry. We report the structure determination of a new compound $C_{22}H_{32}Cl_2Ti$ by X-ray crystallography.

A sample was recrystallized from mixed solvent of dichloromethane and petroleum ether as red transparent crystals. Intensities were collected on a CAD4 diffractometer, $\omega-2\theta$ scan mode, Mok_α in the range of $2° < \theta < 25°$. 2008 independent reflections were measured, of wheeh 1344 were observed reflections with $I > 3\sigma(I)$. The intensities were corrected for Lp factors and absorption.

This compound crystallizes in the monoclinic system,space group C 2/c with unit cell parameters: a = 13.217(3), b = 9.496(2), c = 16.449 (8)Å, $\beta = 94.75(3)°$, $v = 2057.3Å^3$, Mr = 415.31, Z = 4, $Dx = 1.34g/cm^3$, $\mu = 6.76cm^{-1}$, F(000) = 880.

The structure was solved by direct method (MALTAN-82) and sequent difference Fourier syntheses. Full-matrix least-squares refinement with anisotropic thermal parameters for non-hydrogen atoms led to an R of 0.065 and an Rw of 0.070.

The molecule is shown in Figure 1. Its molecular structure possesses C_2 symmetry which belongs to the type of equivalent homotopic faces of cyclopentadienyl ligands (Ronald L. Halterman, Chem. Rev., 1992, 92, 965-994). There is half molecule in an asymmetric unit. the second half is generated by C_2 symmetry. the dihedral angle between two cyclopentadienyl planes is 53.35Å.

