

**PS07.03.08 STRUCTURAL CHARACTERIZATION OF  $(\text{CO})_6\text{Fe}_2\{\mu\text{SC}(\text{PH})=\text{C}(\text{H})\text{Se}\}$  &  $(\text{CO})_6\text{Fe}_2\{\mu\text{-SC}(\text{H})=\text{C}(\text{Ph})\text{Te}\}$ .** S. Narasinga Rao, Y.S. Chen, \*Elizabeth J. Holt, +Manuel-Soriano, ++Shubhangi Umbarkar and Pradeep Mathur, Department of Physics, University of Central Oklahoma, Edmond, OK, +Dept. of BioPhysical Science, UNAM, Mexico City Mexico, ++Dept. of Chemistry, Indian Institute of Technology, Bombay, India, \*Oklahoma State University, Stillwater, OK

When acetylene gas was bubbled through methanol solutions containing the mixed chalcogenide compounds  $(\text{CO})_6\text{Fe}_2(\mu\text{-EE}')$  ( $\text{E}=\text{E}'$ ;  $\text{E}, \text{E}'$ : S, Se, Te), the acetylene adducts,  $(\text{CO})_6\text{Fe}_2\{\mu\text{EC}(\text{H})=\text{C}(\text{H})\text{E}1\}$ , were obtained. Crystallographic analysis of the phenyl acetylene adducts  $(\text{CO})_6\text{Fe}_2\{\mu\text{-S}(\text{Ph})=\text{C}(\text{H})\text{Se}\}$  (I) and  $(\text{CO})_6\text{Fe}_2\{\mu\text{-SCCH}=\text{C}(\text{Ph})\text{Te}\}$  (II) were carried out. (I) crystallized in the space group  $\text{P2}_1/\text{c}$  where  $a=17.974(2)\text{ \AA}$ ,  $b=6.822(10)\text{ \AA}$ ,  $c=14.008(4)\text{ \AA}$ ,  $\beta=97.07(10)^\circ$ ,  $V=1704.4(4)\text{ \AA}^3$ ,  $Z=4$  and refined to  $R=0.053$ ; (II) crystallized in  $\text{P1}$  with  $a=7.494(9)\text{ \AA}$ ,  $b=10.5901(18)\text{ \AA}$ ,  $c=12.1323(8)\text{ \AA}$ ,  $\alpha=105.533(7)^\circ$ ,  $\beta=102.25(7)^\circ$ ,  $\gamma=106.553(15)^\circ$ ,  $V=876.6(2)\text{ \AA}^3$ ,  $Z=2$  and refined to an  $R$  of 0.054.

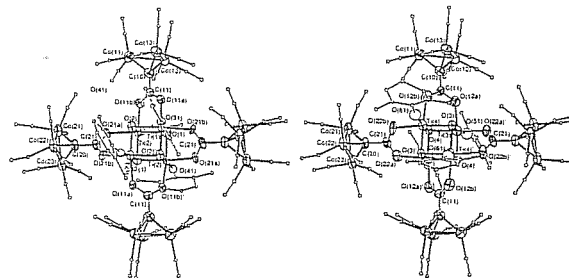
The structure consists of a  $\text{Fe}_2\text{S Se}$  butterfly core and the phenyl acetylene molecule is attached to the wing-tip S and Se atoms of the butterfly, such that the CH group is bonded to Se atom and the C Ph group to the S atom. Each Fe atom has three terminally bonded carbonyl groups. The three CO groups,  $\mu_3\text{-S}$  ligand,  $\mu_3\text{-Se}$  ligand and Fe-Fe bond define a distorted octahedral geometry around each Fe atom. The C-C distances indicate a reduction of acetylene triple bond to an olefinic bond. The average Se-Fe-S angle is consistent with the opening of  $\text{Fe}_2\text{SSe}$  and  $\text{Fe}_2\text{Se}_2$  butterfly cores to accommodate the phenylacetylene molecule.

**PS07.03.09 THE INVESTIGATION OF CLUSTERS DECAY IN COMPLICATED METAL MELTS: Ni-Cr-Mo-W-Nb-C I.** I. Panchenko, N. M. Kohegura, Institute of Foundry Problems, Ukrainian National Academy of Sciences, Kiev, Ukraine.

One of informed characteristics of the melt's structure is its density. The density is responded on the change of melt structure which is connected with the clusters quantity and their size. In the study of complicated metal melts (Ni-Cr-Mo-W-Nb-C) cluster decay and the changes in the melt density was observed. This procedure was done to show a non-reversible clusters decay of these elements after the thermal effect. This phenomenon was discovered by the means of gamma-absorbing technique of the density measurement. The measurement was performed continuously in the temperature interval of 293-2093 K. There was the temperature hysteresis of melt density after such thermal treatment. The density of cooling melts was lower than one of the heating melts if compare at the same temperature point. This hysteresis of the density took place due to the Mo-, W-, Nb- and Cr-clusters decay and their turning to the solution. This phenomenon was a threshold process. It was necessary to transfer the melt up to higher energy level to the refractory element clusters be decayed. This crossing transition achieved after the fixed temperature - homogenising temperature. It is concluded that gamma-absorbing technique of the density measurement is a possible mean of study non-reversible cluster decays after different melt treatments. In addition, laser or electron beam treatment of melts changed the energy state of melt too and could be studied using this method.

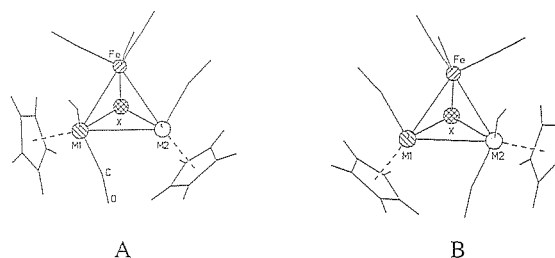
**PS07.03.10 HIGHLY DISORDERED CLUSTER COMPOUND  $\text{Ti}_4\text{O}_4(\text{Me}_2\text{PhO})_4[(\text{CO})_9\text{Co}_3\text{CCO}_2]_4$ .** Maoyu Shang, Xinjian Lei, Thomas P. Fehlner, Dept. of Chem. & Biochem., University of Notre Dame, Notre Dame, IN 46556.

The reaction of the cluster substituted carboxylic acid  $(\text{CO})_9\text{Co}_3\text{CCO}_2\text{H}$  with  $\text{Ti}(\text{OR})_4$  produces a series of new compounds,  $\text{Ti}_4(\mu\text{-O})_4(\text{OR})_4[\mu\text{-O}_2\text{CCC}(\text{CO})_9]_4$ , with a cube-like core  $\text{Ti}_4\text{O}_4$ . When  $\text{R} = \text{Me}_2\text{Ph-}$ , the structure is unusually disordered, but solved and refined satisfactorily with the help of SHELXL-93. The cube-like core has a  $90^\circ$  rotational disorder so that each apex is occupied by 50% Ti and 50% O, however,  $\text{Me}_2\text{PhO-}$  is dislocated to a position other than the  $90^\circ$  rotation. Except for the rotation of the  $\text{-CO}_2^-$  part,  $(\text{CO})_9\text{Co}_3\text{CCO}_2^-$  remains intact.



**PS07.03.11 UNEXPECTED CHIRALITY IN THE NOVEL MIXED-METAL CLUSTER COMPOUNDS  $\text{M}_2\text{Fe}(3\text{-X})(\text{CO})_7(5\text{-C}_5\text{H}_5)_2$  ( $\text{M}=\text{Mo}, \text{W}$ ,  $\text{X}=\text{Se}, \text{Te}$ ).** A.V.Virovets, S.N.Konchenko, N.V.Podberezskaya, S.V.Tkachev, E0104 Institute of Inorganic Chemistry SB RAS, Novosibirsk, Russia

Single crystals of four new mixed-metal clusters were investigated by X-ray structural analysis ( $\text{X}=\text{Se}$ ,  $\text{M}_2=\text{Mo}_2$ ,  $\text{W}_2$  and  $\text{MoW}$ ;  $\text{X}=\text{Te}$ ,  $\text{M}_2=\text{Mo}_2$ ). It has been found that in the solid state cluster molecule contains two non-equivalent M-Fe bonds (even if  $\text{M}_1=\text{M}_2$ ) due to the different arrangement of two Cp ligands: the  $\text{M}_1$  atoms have Cp ligand in *cis*- position with respect to the  $\text{M}_1\text{-Fe}$  bond in contrast to the  $\text{M}_2$  which have *trans*- Cp. In molybdenum clusters the difference in the lengths of Mo-Fe bonds is higher when  $\text{X}=\text{Te}$  than in  $\text{X}=\text{Se}$  case (0.133 and 0.025  $\text{\AA}$  respectively). Such an asymmetrical ligand arrangement makes molecules to be chiral. All crystals are centrosymmetrical and, therefore, they are racemic mixtures of chiral isomers A and B:



The NMR investigations show that fast AB ligand exchange process takes place in the solution. More interesting case is  $\text{M}_1=\text{Mo}$ ,  $\text{M}_2=\text{W}$ , when chirality of ligand arrangement adds to the chirality of tetrahedral cluster core resulting in four different diastereomers present in one single crystal (with crystallographic Mo/W disorder).