SSbN and O=SSbN (1/2,1/3,2/3) in the complexes I-III are: 84.0, 84.0, 84.0°(II) and 79.4, 80.4, 163.1°(III).

The angles Se-Se-Se, Se-Sb-Se and O-Se-Se-O of chelate metalloccycles I-III are 87.1, 87.1, 87.1° (I); 87.3, 84.3 and 87.2° (II) and 86.5, 86.5 and 75.4°(III). The breach of five membered metalloccycles through the lines Se-Se, N-Se, S-N and O-Se, N angles are 20.1, 20.1, 20.1°(I); 29.6, 11.2, 28.2°(II); 0.3, 2.2 and 9.8°(III). Crystal data I - a = b = c= 11.2710(10) Å, α=β=γ=99.32(2°), Z = 2, sp.gr. R3. The present research was made possible in part of Grants LBC000 and LJ100 from the International Science Foundation.

PS07.00.34 STRUCTURAL AND SPECTROSCOPIC STUDIES IN THE \( [\text{M(CNH}_{2}\text{N}_{3}\text{S}_{2}] \) \( \text{M= Cu(II), Ni(II)} \) COMPOUNDS. J. L. Pizarro, J. GarciaTojal, L. Lezama, M. I. Arriortua, Depts. de Mineralogia-Petrologia y Quimica Inorgánica, Universidad del Pais Vasco, Apdo 644, 48080 Bilbao, Spain.

The \( [\text{M(CNH}_{2}\text{N}_{3}\text{S}_{2}] \) \( \text{M= Cu(II), Ni(II)} \) compounds, where M= Cu(II), Ni(II), crystallize in the P2₁/c monoclinic space group, with a= 7.541(1), b= 7.243(1), c= 16.179(5) Å, α= β= 90.00(3), γ= 117.90(5), Z = 2. R= 0.024, wR= 0.043, for the copper(II) compound, and a= 7.476(1), b= 7.298(1), c= 15.862(5) Å, α= β= 101.32(2), γ= 92°, Z = 2. R= 0.032, wR= 0.049, for the nickel(II) complex. The structure of both compounds consists of discrete monomeric molecules with four coordinate square planar copper(II) and nickel(II) ions (see Figure). The metal ion is joined to two thiophene-2-carbaldehyde thiosuccinocarbazone ligand by the azomethinic nitrogen and the sulphur atom of the thioamide group. IR, reflectance and EPR spectra together with the antitumor activity will be discussed.

PS07.00.35 A LONG C-C BOND IN A TROUBLESOME STRUCTURE. Douglas Powell, Department of Chemistry, University of Wisconsin, 1101 University Ave, Madison, WI 53706 USA; Xiang Ouyang, Zhao Hanhua, and Kim R. Dunbar, Department of Chemistry, Michigan State University, East Lansing, MI 48824 USA.

The synthesis of \( \text{Mn(TCNQ)}_2 \) was undertaken as part of a study of the electronic and magnetic properties of compounds with metal-based radicals bonded to organic ligands. In the crystal structure there are two independent Mn sites each on a crystallographic 2-fold axis. Both Mn sites are bonded in an octahedral arrangement to two TCNQ groups, two CH₂OH groups, and two 1/2TCNQ₂^- groups. The \( \text{TCNQ}^- \) moieties are dimers of TCNQ anions joined by a long (1.654(5) Å) σ bond. This type of dimer formation has been seen in other structures. The packing of the \( \text{Cl}^- \) ions, formed by the \( \text{Cl}^- \) ions, is shown to increase in the trigonal loops of the layer in structure I. The one-layer stacking explains a strong quasiperiodicity (c2) in this structure. In vacancies of the trigonal loops there are F^- ions; the common faces of triangular prisms, formed by complex cations, are occupied by F^- ions and outer-sphere H₂O molecules.

Activation of the H₃ ligands in the \( \text{d}^0 \) octahedral series \( [\text{trans-M(H)}(\text{H})_{2}(\text{dippe})_3]\), \( \text{M}\) = Fe, Ru, Os, by single-crystal neutron diffraction. J. Ricci1, A. Albinati1, J. Fortin1,2, W. Klooster1, T. Kociet1, F. Malby4, R. Morris3, A. Petroff1, Dept. of Chem., Brookhaven Nat. Lab., Upton, NY 11973 USA, and Univ. Toronto, Toronto, Ontario M5S 1A1 Canada; and Inst. of Phys. Chem., Univ. Milan, I-20131 Milan, Italy.

The synthesis of \( \text{Mn(TCNQ)}_2 \) was undertaken as part of a study of the electronic and magnetic properties of compounds with metal-based radicals bonded to organic ligands. In the crystal structure there are two independent Mn sites each on a crystallographic 2-fold axis. Both Mn sites are bonded in an octahedral arrangement to two TCNQ groups, two CH₂OH groups, and two 1/2TCNQ₂^- groups. The \( \text{TCNQ}^- \) moieties are dimers of TCNQ anions joined by a long (1.654(5) Å) σ bond. This type of dimer formation has been seen in other structures. The packing of the \( \text{Cl}^- \) ions, formed by the \( \text{Cl}^- \) ions, is shown to increase in the trigonal loops of the layer in structure I. The one-layer stacking explains a strong quasiperiodicity (c2) in this structure. In vacancies of the trigonal loops there are F^- ions; the common faces of triangular prisms, formed by complex cations, are occupied by F^- ions and outer-sphere H₂O molecules.

The synthesis of two novel Rh(III) compounds - \( [\text{Rh(H}_2\text{O})_6]\text{Cl}^- \) - containing halogen ions, have been determined. In these complexes, a radically different functional role of the F- and Cl- ions is due to their size and a composition of outer-sphere components. The octahedral environment of Rh in \( \text{I} \) is provided by six \( \text{H}_2\text{O} \) molecules which have displaced the F^- ions into the outer sphere involving the additional four \( \text{H}_2\text{O} \). In \( \text{II} \), the Rh-octahedra, formed by the Cl- ions, are combined into dimers via a common face. The packing of the \( [\text{Rh(H}_2\text{O})_6]\text{Cl}^- \) ions formed pseudoheaxagonal layers with Rh-Rh distances equal to 1010, 121110 and 1211-101 in the trigonal loops of the layer in structure I. The one-layer stacking explains a strong quasiperiodicity (c2) in this structure. In vacancies of the trigonal loops there are F^- ions; the common faces of triangular prisms, formed by complex cations, are occupied by F^- ions and outer-sphere H₂O molecules.

In \( \text{II} \), Rh atoms of dimeric units (on the \( z \)) 0.35, 0.5 and 0.85 levels) in combination with C atoms of the cations (situated on the axes 3) form regular hexagonal nets of the 1/6v3 dimension. The one-layer packing (with a pseudoquartic c4) is formed without regard for atomic sorts.

Crystal data: (SYNTHEX P2₁/m, MoKα, 64 beam scan) for \( \text{I} \): a = 11.910(2), b = 6.877(1), c = 13.590(3) Å, \( \beta = 90.00(3) \), \( V \) = 1113.1(3) Å³, space group C2/c, \( Z \) = 8, \( \alpha = 62.0(2) \) cm⁻¹, \( \beta = 91.9(3) \) cm⁻¹ for \( \text{II} \): a = 20.705(4), b = 9.804(3), c = 15.862(5) Å, space group C2/c, \( Z \) = 2, \( \alpha = 62.0(2) \) cm⁻¹, \( \beta = 91.9(3) \) cm⁻¹.