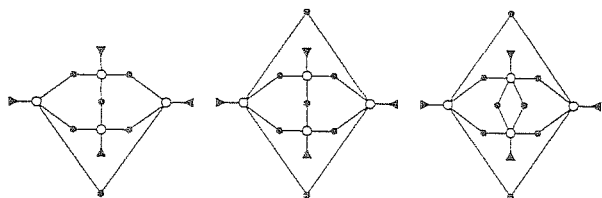


of the retrieved structures can be classified and divided into ten subgroups.

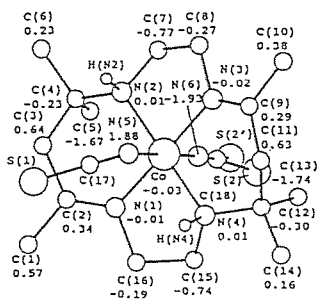
Figure Comparison of the metal and oxo-oxygen atom core fragment of the three structures I, II and III, respectively.



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PS07.00.10 CRYSTAL STRUCTURE OF TRANS-DIISOTHIOCYANATO(5,7,7,12,14,14-HEXAMETHYL-1,4,8,11-TETRAAZACYCLOTETRADECA-4,11-DIENE) COBALT(III) THIOCYANATE. B. H. Chen¹, T. H. Lu², W. T. Huang¹, H. H. Yao¹, J. M. Lo¹, and C. S. Chung³ ¹Department of Nuclear Science, ²Department of Physics, and ³Department of Chemistry, National Tsing Hua University, Hsinchu, Taiwan 300, ROC

Transition-metal complexes of macrocyclic ligand containing asymmetric centers have been studied extensively, because of their particular stereochemistry. The crystal structure of trans-dichloro(c-meso-3,5,7,7,10,12,14,14-octamethyl-1,4,8,11-tetraazacyclopentadeca-4,11-diene) cobalt(III) perchlorate have been reported previously (Lu et al., *J. Chin. Chem. Soc.*, 1992, 39, 343-345). Here we report crystal structure of the title complex. Orthorhombic, $P2_12_12_1$, $a=12.169(2)$, $b=13.576(1)$, $c=14.929(1)\text{\AA}$, $R=0.051$, $wR=0.055$ for 2804 observed reflections. The Co(III) ion is six coordinated in a distorted octahedral geometry with the four N atoms of the two isothiocyanato group axial. The quadridentate macrocyclic ligand is in planar conformation with the two five-membered rings in gauche form and the two six-membered ring in twist form. The complex has the RR or SS configuration for the two chiral amine N centers. The intermolecular hydrogen bonds among the two NH groups and the unbonded thiocyanate ion help to stabilize the crystal structure.



PS07.00.11 TO BEND OR NOT TO BEND—STRUCTURAL STUDIES OF OXO-BRIDGED BINUCLEAR TITANIUM COMPLEXES. Michael Y. Chiang, Bella M. Chen, Hui-Wen Feng, Department of Chemistry, National Sun Yat-Sen University, Kaohsiung, Taiwan, Republic of China

Oxo-bridged binuclear transition metal complexes often display a wide MOM angle much larger than the HOH angle of 104.5° found in water. In extreme case it reaches the 180° limit becoming linear. Although most people agree the geometry may be governed by steric reasons, no one can be sure of that. We have examined three crystal structures of the same complex, μ -oxo-bis[chlorobis(2,4-pentanedionato)titanium(IV)], and found both linear and bent Ti-O-Ti moieties. The bent geometry was found in the crystal structure done by Watenpaugh et al. involving the aforementioned Ti complex with cocrystallized chloroform (1). However we have found two structures of the same complex, with and without cocrystallized acetonitrile, both displaying linear Ti-O-Ti framework. Detailed structural comparison among the three crystal structures as well as other related group IVB complexes will be presented.

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PS07.00.12 STRUCTURAL SYSTEMATICS OF TRANSITION METAL TRIPHOSPHORUS MACROCYCLES. Simon J. Coles and Michael B. Hursthouse Department of Chemistry University of Wales, Cardiff, P.O. Box 912, Cardiff, Cf1 3Tb, U.K.

A number of transition metal triphosphacyclododecane complexes have been structurally characterised by X-ray crystallography, enabling a systematic structural study, the results of which have been incorporated into the development of extended force field parameter sets for transition metal complexes.

Data for the air-sensitive crystals of these complexes were collected on the FAST TV Area detector, equipped with an Oxford Cryosystems low temperature device, using the oil drop mounting method. Structures were solved using the SHELX suite of programs to give experimental parameters.

A force field parameter set for the complex $[\text{Cr}(\text{CO})_3\{\text{cyclo}(\text{HPC}_3\text{H}_6)_3\}]$ was derived, using the classical approach, giving force constants for stretch and bend parameters and energy barriers for torsional and nonbonded interaction parameters. This extended force field parameter set is applied to the molecular modelling of structures determined by X-ray diffraction, in order to determine the accuracy of the derived parameters, and then used to model uncharacterised structures. Molecular mechanics calculations were performed using the software packages HyperChem and Cerius², which have also been used to perform semi-empirical calculations upon these systems.