recent years these ligands have been studied for their capacity as conductors and in optical applications.^{0} Our objective is to use these previously reported ligands as well as novel ligands and coordinate them to various transition metals in order to prepare unique metal-organic frameworks (MOFs). Coordination of the ligand 1,4-bis(4'-pyridyl)butadiyne, with $CuNO_3$ has been shown to form square-grid architectures with the inclusion of methylene chloride solvent. This supramolecular material and other related examples have been investigated for their gas sorption abilities.

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MS13 P19

A gating mechanism accounts for gas transport through calixarene crystals. Charl G. Marais, Jan A. Gertenbach, Leonard J Barbour and Catharine Esterhuysen. *Department of Chemistry, University of Stellenbosch, South Africa.* E-mail: charl@sun.ac.za

Keywords: calixarene, gate-opening, storage

Porous solids have attracted considerable attention owing to their unusual physico-chemical properties [1] and are of particular economic interest with regard to their potential applications in gas storage [2], separation and sensing [3]. Commercially, alternative safe storage mechanisms for acetylene, a highly reactive and dangerous gas, should be investigated as it plays a crucial part as a starting material in several chemical products and electronic materials [1,4]. Since it is important to purify acetylene for the manufacture of these materials, it is necessary to devise systems to separate acetylene from gas mixtures that also contain carbon dioxide and other impurities.

An investigation of gas transport and storage mechanisms in *t*-butylcalix[4/8/9]arenes using standard crystallographic and computational molecular force field techniques was conducted with a view to gaining greater insight into solid-gas interactions and solid-state dynamics. Furthermore, X-ray structural studies have also been undertaken in order to identify the active site within the guest-accessible voids.

Results from computational calculations were used to predict a mechanism for gas transport and storage. These findings are correlated with the crystallographic and sorption data. The investigation suggests that a gating mechanism is the driving force for gas transport and sequestration in the calixarene crystals.

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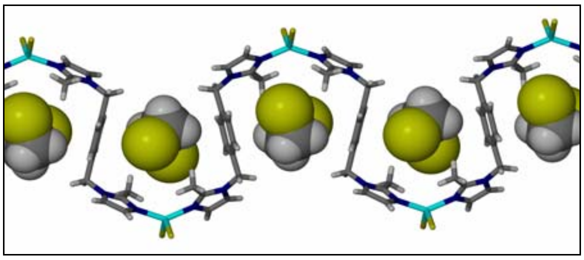
MS13 P20

Porosity studies of wave-like, one-dimensional coordination polymers. Storm Potts, Liliana Dobrzańska, Martin W. Bredenkamp and Leonard J Barbour. *Department of Chemistry, University of Stellenbosch, South Africa.* E-mail: storm@sun.ac.za

Keywords: porous materials, coordination compounds, gas-solid interactions

The formation of porous crystalline materials is a central theme of our research efforts. Our approach is to design and prepare solvent-templated host-guest systems consisting of simple coordination compounds grown from common solvents. In general, the solvent molecules can be removed as single-crystal to single-crystal processes to afford porous or seemingly nonporous systems that are still permeable to various gases.

A range of such compounds have been characterised by X-ray diffraction methods with supporting data obtained using thermogravimetry, sorption isotherms and modeling studies. Although we are primarily interested in forming discrete dinuclear complexes, we have also obtained interesting new results using wave-like one-dimensional coordination polymeric systems. These are obtained from the crystallization of $CuCl_2$:**L** from 1,2-dichloroethane. We find that that the polymeric waves stack one over the other to form guest-accessible pockets of approximately 143Å^3. We will present X-ray structural data as well as the results of gas sorption studies.



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MS13 P21

Crystal Structures and Properties of $[M(NH_3)_5Cl]_2[Re_6S_8(CN)_6]\cdot 3H_2O$ Kirill Yusenko[a], Elena Shusharina[b], Iraida Baidina[a], Sergey Gromilov[a] [a]*Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia.* [b]*Faculty of Natural Science, Novosibirsk State University, Russia.* E-mail: yusenko@che.nsk.su

Keywords: clusters in coordination complexes, platinum group, rhenium

Using an inert $[M(NH_3)_5Cl]^{2+}$ (M = Rh, Ir, Ru) cations upon crystallisation of the salt with the $[Re_6S_8(CN)_6]^{4-}$ anion makes possible the preparation of compounds with the island crystal structures containing the isolated cations and large cyanide anions. The compounds $[M(NH_3)_5Cl]_2[Re_6S_8(CN)_6]\cdot 3H_2O$ (M = Rh (1); Ir (2); Ru (3)) have been synthesized by crystallization from aqueous solutions. The compounds are isostructural. They crystallize in the triclinic space group P-1 with the cell parameters for 1: a = 10.7574(7), b = 13.9423(9), c = 14.7975(9) Å, α = 92.031(2) Å, β = 110.137(2), γ = 109.976(2)°, V = 1928.7(2) Å^3.