MS27-O5 **Crystallographic and kinetic investigation of nitrosyl, cyanide and acetonitrile complexes of Rh(I)/(III)** T.J. Muller, H.G. Visser and A. Roodt *Department of Chemistry, University of the Free State, Nelson Mandela Avenue, Bloemfontein, 9300, South Africa*
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The reactivity of Rh(I) is well known and has been studied intensely in the last couple of decades while little is known about the reactivity of Rh(III) phosphine complexes. The complexes studied were those of the general form $[Rh(PX_3)_2(NO)(Cl)_2]$, $[Rh(PX_3)_2(CO)(CN)]$ and $[Rh(PX_3)_2(Cl)_3(CH_3CN)]$, where PX_3= arylThe steric and electronic parameters of the phosphine ligand may be tuned by varyingsubstituents on the phosphorous(III) coordinating atom.One aim of this study was to investigate the affinity of the rhodium metal centre for the phosphine by tuning the electronic and steric properties thereof. The solution state behaviour of these complexes were investigated by following the formation and reactivity of different monodentateentering ligands. The different complexes were successfully characterised by IR, NMR and X-Ray crystallography. IR data of the NO, CO and CN stretching frequencies of the different complexes allowed a comparison of the electronic properties of the different phosphine ligands. The first-order coupling constants from the NMR data also correlate well with the Rh-P bond length from the crystal structures [1]. The difference in electronic and steric properties of the different phosphine ligandswere further correlated with the NO bond angle and the Cl-Rh-Cl bond angles. The reactivity of Rh(III) complexes were also evaluated with respect to differences in steric and electronic properties. This presentation thus deals with an overall correlation of the complexes' spectroscopic, solid state and kinetic reactivities, which will be discussed in detail.

[1] Roodt, A., Visser, H.G. & Brink, A. (2011) *Crystallography Reviews*. **17**, 4, 241-280.

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MS29-O1 **Statitistics package R for prototyping in Macromolecular Crystallography** Garib N Murshudov, *MRC Laboratory of Molecular Biology, Hills Road, Cambridge, UK, CB2 0QH*
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Most problems of Macromolecular Crystallography (MX) and Structural Bioinformatics (SB) by their nature are statistical ones. Therefore their solution require statistical approaches. The field of statistics is very large and often it is not clear what approaches or methods may work for particular scientific problems. It would be impossible to rewrite and implement all available statistical methods to solve problems in MX and SB. Fortunately there are many high level statistical packages that have already implementation of most of the required techniques. These include S, SAS, S-Plus, MatLab, SPSS, PSPP, GenStat, R (http://www.dmoz.org/Science/Math/Statistics/Software/). Many standard mathematical packages like Maple, Mathematica also offer tools for statistical data analysis. The package R is a comprehensive statistical package that is distributed freely to all (under GPL license). It offers ideal platform for teaching, scientific research as well as for methods' prototyping. We have used R to prototype methods for MX and SB statistical analysis such as 1) testing probability distribution assumptions for structure factors, 2) simulations of random variables with known distributions to analyse behaviour of crystallographic reliability index – R-factor (Murshudov, 2011), 3) procrustes analysis for conformation independent protein structure alignment and comparison (Nicholls et al, 2011), 4) analysis and classification of short polypeptide fragments, 5) Modelling of B value distributions as inverse gamma.

R also offers an excellent platform for researchers who want to use programming as a part of their research. Easy scripting language as well as large class of already available statistical functions allow immediately to get results. R's visualisation tools are very helpful for visual analysis of data, results and therefore irreplaceable in intuition building.

[1] R Development Core team. "R: A Language and Environment for Statistical Computing", http://www.R-project.org/, 2011
[2] Murshudov GN "Some statistical properties of the crystallographic reliability index Rfactor: Effect of twinning." *Applied and Computational Mathematics* , 2011:10;250-261
[3] Nicholls RA, Long F and Murshudov GN "Low Resolution Refinement Tools in REFMAC5" *Acta Cryst* 2012:D68;404-417