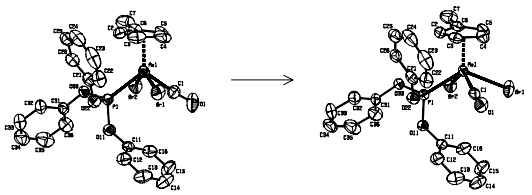
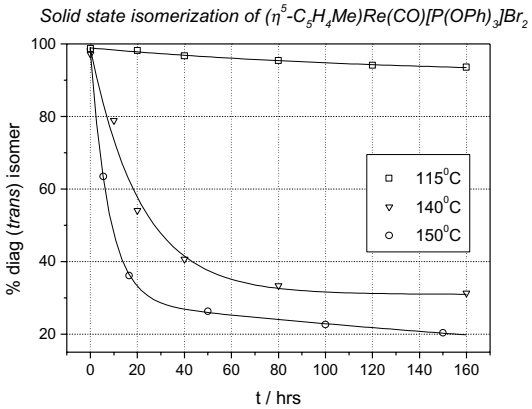
s9'.m1.p22.la **The single-to-single crystal isomerization reaction of $(\eta^5\text{-}C_5H_4Me)Re(CO)[P(OPh)_3]Br_2$.** R.S. Bogadi and D.C. Levendis *Centre for Molecular Design, Department of Chemistry, University of the Witwatersrand PO Wits 2050, Johannesburg, South Africa*
Keywords: molecular interactions, organic materials, molecular solids.

Solid state diag-to-lat (*trans-to-cis*) thermal isomerization reaction studies of $(\eta^5\text{-}C_5H_4R)Re(CO)LBr_2$ (R = Me, tBu, $SiMe_3$; L = CO, $CNC_6H_3Me_2$, $P(OMe)_3$, $P(OPh)_3$) were reported recently (Cheng, Coville et al). Single crystals of complexes such as $(\eta^5\text{-}C_5H_4Me)Re(CO)_2Br_2$, which change space group on heating, disintegrate during the diag-to-lat isomerization process. However, we have demonstrated by X-ray diffraction that crystals of the title compound remain single after thermal diag-to-lat isomerization. Furthermore, the crystal symmetry is retained (space group $P2_1/c$), at least on average, as the reaction proceeds, with small changes in the unit cell parameters.



diag-$(\eta^5$-$C_5H_4Me)Re(CO)[P(OPh)_3]Br_2$ *lat-$(\eta^5$-$C_5H_4Me)Re(CO)[P(OPh)_3]Br_2$*

In this work, a single crystal of diag-$(\eta^5\text{-}C_5H_4Me)Re(CO)[P(OPh)_3]Br_2$ was heated for various times at the same temperature. This was then repeated at different temperatures. Complete data sets (at least 20) were collected on a Bruker SMART CCD diffractometer and solved using variable site occupancies linked to the carbonyl and bromine positions. The reactions were monitored as a function of the relative site occupancy of the diagonal isomer with respect to time as shown below.



s9'.m2.p6.la **Structural systematics for structure prediction.** M.B. Hursthouse and S. Ward, *Department of Chemistry, University of Southampton, Southampton, UK, and Terry L Threlfall, Department of Chemistry, University of York, York, UK.*
Keywords: molecular interactions, ab initio structure prediction, crystal packing.

Structure prediction is particularly difficult when the target molecule possesses a number of functional groups which can participate in strong intermolecular interactions. By their very nature, most pharmaceuticals fall into this class. As part of our general study on polymorphism of pharmaceuticals and related topics, we have been investigating a number of sulphonamide compounds. Well-known examples such as sulfanilamide, sulfathiazole and sulfapyridine have been extensively studied by many authors, but much still remains to be learnt. In an attempt to gain some insight into the way in which different functional groups link into structure generating patterns, we have made a study of series of closely related compounds which have a common core, in this case some sulfonamides of general form R–SO_2-NH-R', in which functional groups on R or R' fragments are systematically changed. It was hoped that the results would provide useful examples for structure prediction studies.

In our first project we have looked at systems where R is a clean or substituted phenyl group and R' is a clean or substituted pyridyl or pyrazyl group. The substitutions have been made either to add in functional groups or to modify the properties of functional groups already present. Sixteen compounds were synthesized and the structures of fifteen have been elucidated. The patterns that have emerged are quite bewildering. Of the fifteen structures determined, eleven have two crystallographically independent molecules in the asymmetric unit. All structures have H-bonding interactions. Those with independent molecules A and B have variously A-A, B-B or A-B links. Some longstanding principles of crystal engineering are tested.

Details of the structures and some assessments of the structural systematics will be given.