Currently we are exploring the use of N-heterocyclic carbenes in the chemistry of rhodium complexes. Our idea is to increase the stability of potential rhodium catalysts by incorporating this sort of electron-rich ligands, whereas we try to direct selectivity by introducing bulky substituents exerting steric control over the interaction of substrates with catalysts [2].

We have chosen the 1,3-bis-(2,6-diisopropylphenyl)imidazol-2-carbene (IPr) ligand in the synthesis of a family of rhodium complexes of the types [RhCl(IPr)PyL] or $[RhCl(IPr)L]_2$ (Py = pyridine or substituted pyridines; L = ethylene, cyclo-octene, oxygen) (see figure). The additional presence in all these complexes of an unsaturated labile ligand L confers them a good suitability to be used as catalyst precursors in different processes [3]. In the present communication, we will discuss the structural features of these complexes trying to understand the relationships between these features with their chemical and catalytic behavior.

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Keywords: organometallic, carbene, rhodium complexes

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Molecular iodine trapped as alternating layers with amphiphilic salts

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Halogen bonding is a term used to describe a non-covalent interaction between a halogen atom acting as a Lewis acid and a Lewis base.[1] As the bonding parameters of this interaction are very predictable halogen bonding can be exploited to create some intriguing solid state structures using both halogen containing hydrocarbons (aliphatic or aromatic) and dihalogen species (eg. I_2).

We have investigated the insertion of molecular iodine (I_2) to amphiphilic salts where mono-alkylated DABCO (1,4-diazabicyclo[2.2.2]octane) moiety acts as the cationic species and the halogen bond acceptor. The solid state structures of the I_2···DABCO complexes will be presented in addition to the complexation reactions which include crystallization of the complexes from solutions as well as solid state complexation.

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Keywords: halogen bonding, x-ray diffraction, amphiphilic salts

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Crystal Structure of $PrAgAlGe_{3-x}$

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A systematic investigation of the Pr-Ag-Al-Ge system led to the discovery of a new quaternary compound.

An alloy of the nominal composition $Pr_{0.125}Ag_{0.250}Al_{0.250}Ge_{0.375}$ was synthesized by arc-melting of the constituent elements under argon atmosphere. For homogenization the sample was annealed in an evacuated silica tube at 873 K for 720 h and subsequently quenched into cold water. X-ray powder diffraction data were collected on a diffractometer PANalytical (Cu *Kα* radiation). The profile and structural parameters were refined using the WinCSD [1] program package.

X-ray phase analysis of the alloy indicated a three-phase sample. It contained: $PrAgAlGe_{3-x}$ (87.32%), Ag_3Ge (9.26%) and Ge (3.42%). Automatic indexation of the peaks of the phase $PrAgAlGe_{3-x}$ resulted in an *I*-centered tetragonal unit-cell with the parameters $a \approx 0.423(1)$ and $c \approx 2.489(1)$ nm. The crystal structure of the quaternary compound was solved in the space group *I*4/*mmm*. It was established that its crystal structure belongs to a new type. For the refined composition $PrAg_{0.94(1)}Al_{1.06(2)}Ge_{2.17(2)}$ (Pearson symbol *tI*32-8.70, space group *I*4/*mmm*) the unit-cell parameters are: $a = 0.42332(2)$, $c = 2.4902(1)$ nm. The final values of the reliability factors ($R_I = 0.1068$, $R_p = 0.1690$, $R_{wp} = 0.1449$, $R_{dbw} = 0.0763$) were obtained for the following distribution of atoms: Pr 4*e* 0 0 0.14281(9) ($B_{iso.} = 0.43(3)\cdot10^{-2}$ nm^2), 0.440(6)Ag + 0.560(6)Al 4*d* 1/2 0 1/4 ($B_{iso.} = 0.68(4)\cdot10^{-2}$ nm^2), Ge1 4*e* 0 0 0.4141(5), occ. 0.354(8), ($B_{iso.} = 0.84(4)\cdot10^{-2}$ nm^2), 0.500(9)Ag + 0.500(9)Al 4*e* 0 0 0.3150(2) ($B_{iso.} = 0.70(4)\cdot10^{-2}$ nm^2), Ge2 16*n* 1/2 0.063(2) 0.0474(2), occ. 0.455(2), ($B_{iso.} = 1.04(4)\cdot10^{-2}$ nm^2).

The crystal structure of $PrAgAlGe_{3-x}$ is a quaternary substitution derivative of the closely-related types $ScNi_2Si_3$ [2] and UNi_2Si_3 [3] with splitting of one small-size atom site. The structure types $ScNi_2Si_3$ and UNi_2Si_3 differ by the distribution of the small-size atoms. In $ScNi_2Si_3$ the small-size atoms are distributed in an orderly manner, whereas in $UNi(Ni,Si)_2Si_2$ both 4*e* sites are occupied by a statistical mixture of Ni and Si atoms in the ratio 1:1. In comparison with these prototypes, in the structure of $PrAgAlGe_{3-x}$ splitting of the 8*g* site takes place; the new 16*n* site is occupied by Ge atoms. Moreover, another kind of small-size atom distribution is observed. The crystal structure of $PrAgAlGe_{3-x}$ (like the $ScNi_2Si_3$ and UNi_2Si_3 structure types) is an intergrowth of structural segments of the simple type $BaAl_4$ (or its ordered ternary variant $CeAl_2Ga_2$), which are separated along the crystallographic [001] axis by segments of the α-Po type.

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Synthesis and crystal structure of *mer*-$[Co(C_8H_4O_4)(C_3H_4N_2)_3(H_2O)_2]\ H_2O$

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The design and synthesis of metal–organic frameworks (MOFs) have received attention in recent years due to their potential applications in diverse areas such as electrical conductivity, magnetism, host–guest chemistry, molecular separation, gas storage, sensors and catalysis [1][2].

Recently, great success has been achieved by the combination