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)Py][L] or [RhCl(IPr)L], (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.


**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. As the bonding parameters of this interaction are very predictable haloogen bonding can be exploited to create some intriguing solid state structures using both halogen containing hydrocarbons (aliphatic or aromatic) and dihalogen species (e.g. 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 reaction mechanisms which include crystallization of the complexes from solutions as well as solid state complexation.


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

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### Crystal Structure of PrAgAlGe$_{13}$

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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$_{120}$Ag$_{238}$Al$_{14}$Ge$_{41}$ 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$_{13}$ (87.32%), Ag,Ge (9.26%) and Ge (3.42%). Automatic indexation of the peaks of the phase PrAgAlGe$_{13}$ resulted in an I-centered tetragonal unit-cell with the parameters a = 0.423(1) and c = 2.489(1) nm. The crystal structure of the quaternary compound was solved in the space group I4/mmm. It was established that its crystal structure belongs to a new type. For the refined composition PrAg$_{30}$Al$_{14}$Ge$_{41}$ (Pearson symbol r32-8.70, space group I4/mmm) the unit-cell parameters are: a = 0.42332(2) nm, c = 2.4902(1) nm. The final values of the reliability factors (R1 = 0.1066, R2 = 0.1690, Rfn = 0.1449, Rwp = 0.0763) were obtained for the following distribution of atoms: Pr 4e 0 0 0 1.04281(9) (B$_{mn}$ = 0.43(3)·10$^{-2}$ nm$^2$), 0.446(6)Ag + 0.554(6)Al 4d 1/2 0 1/4 (B$_{mn}$ = 0.68(4)·10$^{-2}$ nm$^2$), Ge 1e 0 0 0 0.1441(5), occ. 0.354(8), (B$_{mn}$ = 0.84(4)·10$^{-2}$ nm$^2$), 0.500(9)Ag + 0.500(9)Al 4e 0 0 0.3150(2) (B$_{mn}$ = 0.70(4)·10$^{-2}$ nm$^2$), Ge 16r 1/2 0.063(2) 0.0474(2), occ. 0.455(2), (B$_{mn}$ = 1.64(4)·10$^{-2}$ nm$^2$).

The crystal structure of PrAgAlGe$_{13}$ is a quaternary substitution derivative of the closely-related types ScNiSi$_2$ [2] and UNi$_3$Si$_2$ [3] with splitting of one small-size atom site. The structure types ScNi$_3$Si$_2$ and UNi$_3$Si$_2$ differ by the distribution of the small-size atoms. In ScNi$_3$Si$_2$, the small-size atoms are distributed in an orderly manner, whereas in UNi(Ni,Si)$_3$Si$_2$ both 4e 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$_{13}$ splitting of the 8g site takes place; the new 16n site is occupied by Ge atoms. Moreover, another kind of small-size atom distribution is observed. The crystal structure of PrAgAlGe$_{13}$ (like the ScNi$_3$Si$_2$ and UNi$_3$Si$_2$ structures) is an intergrowth of structural segments of the simple type BaAl$_3$ (or its ordered ternary variant CeAl$_3$(Ga$_2$)), which are separated along the crystallographic [001] axis by segments of the α-Po type.


**Keywords:** alloy, X-ray powder diffraction, crystal structure

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### Synthesis and crystal structure of mer-[Co(C$_2$H$_4$O$_2$)(H$_2$N)$_2$H](H$_2$O)$_2$]

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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