Fundamental Knowledge in Gold Chemistry: A Sound Basis for Multidisciplinary Development

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For many centuries gold alchemy and chemistry were solely orientated towards the 'production' and recovery of gold metal from its natural sources. Only the second half of the 20th century has seen a rapid development focusing on a growing number of advanced technologies ranging from electrical engineering and electronics to pharmacology, dentistry and medicine. In the course of only a few decades, gold chemistry has thus quickly caught up with platinum chemistry, where applications other than in the jewellery and monetary world have had much longer traditions, mainly in catalysis.

Progress in gold chemistry was possible through a multidisciplinary approach to the subject which allowed a deeper understanding of the special position held by gold amongst the metals in the Periodic Table. A number of modern physical and analytical methods have become efficient routine techniques of investigation which help to elucidate complex structures on the molecular and supramolecular level, in bulk materials and in the intermediate area of nanocomposites. Theoretical physics and chemistry have become of great value in understanding relations between the structure and the intriguing properties of gold and its compounds, and predicting compositions with novel functionality.

Examples taken from several areas of research will serve as an introduction to the rich programme of the scientific sessions of this meeting, and reflect the state of the art in all its details.

Gold, Relativity and Nanosized Systems

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Relativistic effects have a major influence on the properties of gold and its compounds. For the latest published summaries, see (1,2). Also the aurophilic attraction between Au(I) ions is enhanced by relativistic effects (3). Its dispersion nature has been confirmed using local-orbital techniques (4). An overview of the computational chemistry of gold will be presented.

Ab initio quantum chemistry and isoelectronic thinking can be used to predict new inorganic species. Our latest proposals approach nanotechnology: the closed-shell icosahedral WAu_{12} (5) has very short W-Au bonds of about 270 pm and a large HOMO-LUMO gap. It was synthesized in the gas phase (6) shortly after our proposal. WAu_{12} has very strong bonding due to a perfect 18-electron rule, relativistic effects and the metallophilic attraction. Extensions are being studied. It could be covered with ligands (Xe, thiolate etc.), extended to nanotubes and nanostructures and extended to isoelectronic ions ($TaAu_{12}^-$, $ReAu_{12}^+$). The strong modification of the gold electronic structure might be catalytically interesting. The degenerate h_g HOMO and LUMO could give high densities-of-states in a possible doped superconductor.

A large series of 'polyicosahedral' bulk compounds, containing coupled icosahedra has been synthesized by B.K. Teo (7). They turn out to have the same electron count as WAu_{12}.

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