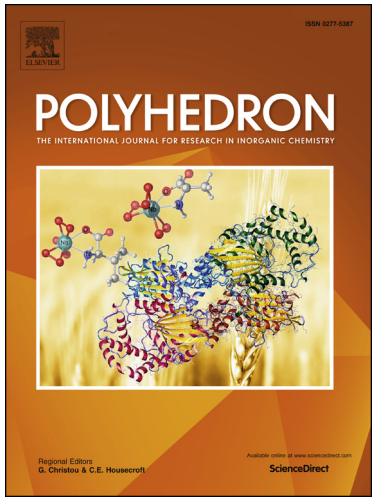

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Structural and spectroscopic studies of Au(III) chloride compounds with 7,8-benzoquinoline

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Au(III) chloride compounds with 7,8-benzoquinoline (bqn) – $[Au(bqn)Cl_3]$ and $[Au(bqn^*)Cl_2]$ (bqn* being deprotonated, at the C(10) carbon, monoanionic form of bqn) were studied by ^1H-^{13}C, ^1H-^{15}N HMQC and HMBC-NMR. ^1H, ^{13}C and ^{15}N coordination shifts were discussed in relation to the molecular structures, revealing characteristic variability patterns. Analogous NMR measurements were performed for the new $(bqnH^+)_2(AuCl_4^-)Cl^-$ salt, studied also by single crystal X-ray diffraction. All compounds exhibited fluorescence.

Keywords: Au(III) complexes, Au(III) organometallics, 7,8-benzoquinoline, ^{15}N NMR, X-ray

1. Introduction

7,8-benzoquinoline (*i.e.* benzo[h]quinoline, bqn, Scheme 1 left top) is an aza aromatic compound consisting of a pyridine ring fused with two benzene rings in a way analogous to phenanthrene or 1,10-phenanthroline. This molecule is similar to 2-phenylpyridine (Scheme 1 left bottom), which is the simplest example of a class of 2-arylpyridines, *i.e.* pyridine derivatives substituted in the 2 position by various aryl groups (*e.g.* 2-benzylpyridine *etc.*). These heterocycles, being well-known organic ligands, are further denoted here as L^{2Arpy}; for the purpose of this paper, the presently studied bqn species, although formally not being a 2-arylpyridine, will be classified to this group as well (however, one must keep in mind another numbering scheme of the ring system). The reason for such a joint classification is the similarity in the transition metal coordination modes, revealed by both types of heterocycles.

Like 2-arylpyridines, bqn in able to coordinate transition metal ions in two ways. It can act as either monodentate N(1)-donor neutral ligand (simply bqn) or the N(1),C(10)-chelating monovalent anion, deprotonated at the C(10) atom (denoted as bqn*). In consequence, during its reaction with $AuCl_4^-$ anions, it simultaneously forms two different Au(III) chloride species: $[Au(bqn)Cl_3]$ (Scheme 1 middle), being a classic complex (as it contains a typical Au-N(1) coordination bond), and $[Au(bqn^*)Cl_2]$ (Scheme 1 right), which can be regarded as either coordination or organometallic compound (as it contains both Au-N(1) and Au-C(10) bonds). These compounds are analogous to many $[Au(L^{2Arpy})Cl_3]$ and $[Au(L^{2Arpy^*})Cl_2]$ molecules (containing N(1)-monodentately bonded neutral L^{2Arpy} ligands or