**Empirical estimation of the molecular weights of gold complexes in solution by pulsed-field gradient NMR**

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Over the past 18 years, gold catalysis has opened new perspectives in organic chemistry and has played a key role in the synthesis of complex molecules from simple precursors. However, despite its growing importance, many mechanistic questions on gold catalysis remain unanswered, concerning, e.g., the role of counter-ions on the reactivity.[[1](#_ENREF_1)] Also, the choice of ligands, counterion, solvent and other experimental parameters remain a tedious task. Pulsed-field gradient (PFG) NMR and its implementation DOSY (for diffusion-ordered NMR spectroscopy) could bring us new information in this context[[2](#_ENREF_2)]. The ability of DOSY to investigate interaction between reagents, to study molecular assemblies, as well as to characterize intermediate, makes it a powerful technique to get a better understanding of the mechanism of gold catalyzed processes[[3](#_ENREF_3)].

While classic DOSY methods require several minutes of acquisition and are unsuitable for a reaction with a time-dependent composition, we have shown that the acquisition of DOSY NMR spectra can be accelerated significantly. [[4](#_ENREF_4)]This improvement opens up prospects for the monitoring of fast gold catalysed reactions and helps us to characterize intermediate species as well as to measure their diffusion coefficients.

For the interpretation of resulting diffusion coefficients, several strategies were developed to relate molecular weight and diffusion coefficients[[5](#_ENREF_5)]. In this work, we show that a simple empirical approach makes possible to derive estimates of molecular weights for gold complexes from their translational diffusion coefficients measured with DOSY. This approach is based on external calibration curves (ECC), modified to take into account the molecular density of gold catalysts.[[6](#_ENREF_7)]

The estimated molecular weight in turn provides information on the interactions, of gold(I) complexes with their counterion and substrate as illustrated here (scheme 1), and has the potential to provide key information to rationalize the reactivity of reagents in gold catalysed reaction.

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