Experimental measurement of [LAuCO]⁺ dissociation energy to probe ligand electronic effect

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Homogenous gold(I) catalyzed reactions are known to achieve a perfect control of chemio-, regio- and stereoselectivity in a very broad range of chemical reactions.¹² To control this selectivity, the choice of the ligand bound to the gold center is a key parameter.³ Predicting the ligand electronic and/or steric influence is thus of most importance to access a very fine tuning of the reaction pathway. Well known experimental approaches developed to evaluate these effects (such as Tolman Electronic Parameter) fail nevertheless mostly in the case of Gold(I) complexes. Recently, several theoretical works succeeded in the interpretation of this particular behavior and could evidence the ability of gold to transmit electronic effects.⁴ To strengthen these findings, experimental indication of the capability of Gold to transmit electronic effect from a ligand to another one was highly desirable. In this context, a mass-spectrometry (MS)–based work was undertaken to determine experimentally the M-CO bond dissociation energies of 16 [L-Au-CO]⁺ complexes bearing ligands widely used in gold catalysis. Coupled to DFT calculations, this approach enables first to observe well-defined ligand effects considering the LAu-CO bond strength. Quantitative interpretation of the LAu-CO bond is further also made possible via an energy decomposition analysis (EDA).

Figure 1. [L-Au-CO]⁺ formation and dissociation inside a tandem mass spectrometer.

References

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