High-Field Electron Paramagnetic Resonance Studies of Titanium-Containing Catalysts

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Titanium is an "Earth abundant" transition metal, unlike precious metals such as palladium (Pd) and platinum (Pt). Partly for this reason, titanium containing-molecules are widely used as catalysts for the production of polymers such as polyethylene, polycarbonates and other "plastics". There is, however, always a need for improvement in these catalysts to make them more efficient, cheaper and safer. Oftentimes, the differences between a better functioning (i.e., higher activity) catalyst and a poorer (i.e., lower activity) one are related to very slight differences in the geometrical and electronic structure of the catalyst molecule.

Techniques such as X-ray crystallography can provide geometrical structures, while spectroscopic information is essential for gaining insights into the electronic structure and functionality of catalysts. One such technique is electron paramagnetic resonance (EPR), which can provide precise details about the role of unpaired electrons in chemical activity. However, the EPR spectra of many transition metals, e.g., titanium, often span a very wide magnetic field range (see Figure). This necessitates high-field measurements that can only be performed at the MagLab.

In this extensive investigation, a series of titanium-containing molecules was prepared by the group of Daniel Mindiola at U. Penn, a leading expert in this area. High-field EPR results from the MagLab show small but distinct differences among them which, when combined with electronic structure calculations, will guide further synthetic efforts aimed at making more catalytically useful molecules.

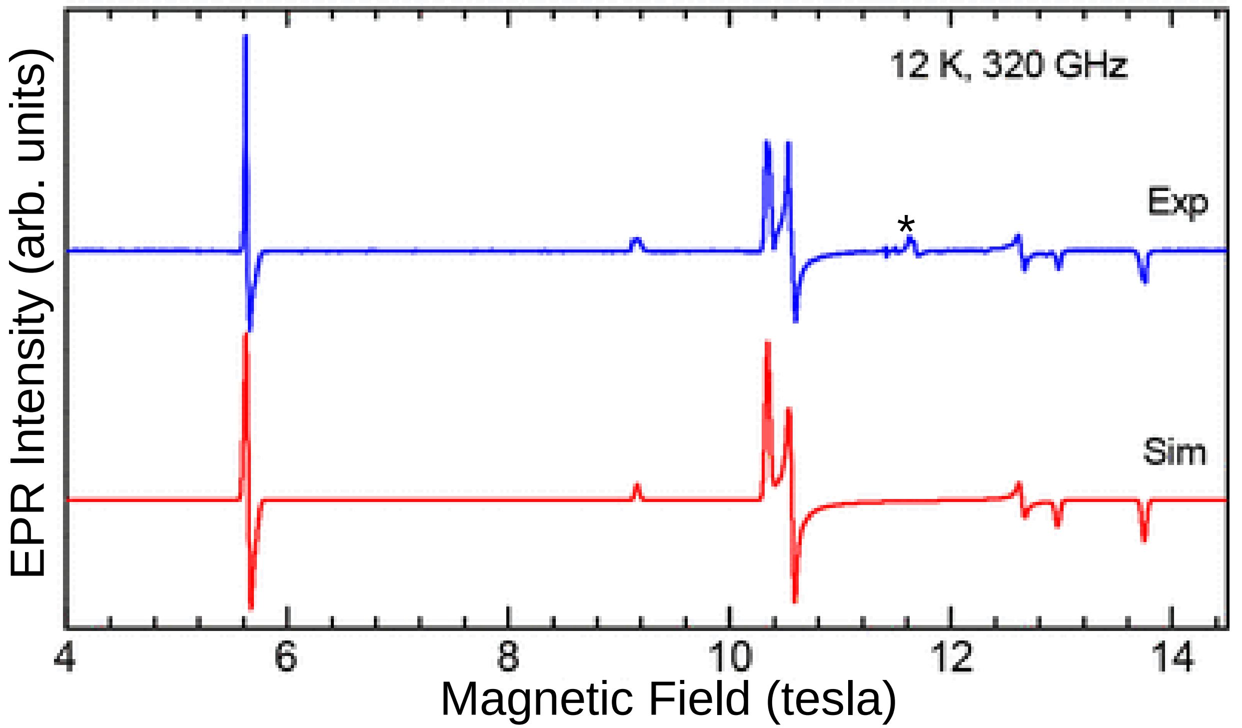

Figure. 1. *Example high-field EPR spectrum (Exp) spanning a wide magnetic field range (up to 15T) compared to commercial instruments, which are typically limited to below 1.2T. The corresponding simulation (Sim) is also shown, and the feature marked by an asterisk is due to a minor species.*

Facilities and instrumentation used: Electron Magnetic Resonance (EMR) Facility: 15/17 Tesla Superconducting Magnet System

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