Parahydrogen-induced polarization (PHIP) is an inexpensive method for bulk production of hyperpolarized gases and liquids. PHIP is based on the conversion of singlet-state spin order inherent in parahydrogen (p-H₂) into NMR-observable spin order by chemical hydrogenation reaction.

The intense hyperpolarized signals amplified by over 10,000 times relative to ordinary NMR can be achieved by the PHIP method. Maximum signal enhancement is achieved only if p-H₂ is added to the substrate in a pairwise fashion. Unfortunately, the pairwise selectivity is found to be limited to only a few percent universally over supported metal catalysts.

The stereoselectivity of the reaction that occurred is limited to only a few percent universally over supported metal catalysts. Hydrogenation on Pt/TiO₂ intermediates associated with hydrogenation on Pt/TiO₂ addition to propyne was measured as a function of reaction conditions. We hypothesize the reaction scheme presented below. The systematic variation of reaction conditions is used to test proposed reaction mechanism and kinetics.

Reactions were performed at pressure between 0.15 and 0.95 bar partial pressure of hydrogen at low field. Spectra obtained using normal hydrogen (n-H₂) were subtracted from spectra obtained using p-H₂ and baseline corrections were applied. As the hydrogen pressure is increased, the stereoselectivity decreased linearly. The spectra in black are simulated using SpinDynamica and blue spectra represent the experimental data. An expansion of the propene CH₂ region of the ALTADENA spectra recorded at the pressures indicated is shown right.

For hydrogenation in low field (ALTADENA condition), sharing of p-H₂ singlet order through the strong J coupling network complicates the stereoselectivity determination, and fitting to density matrix simulations is required. For reaction in high field (PASADENA condition), stereoselectivity can be determined directly from the spectrum. Therefore, a special high-field hydrogenation reactor that fits inside the bore of the superconducting NMR magnet was built.

Experimental spectra were fit to a linear combination of experimental and simulation confirmed results display a stereoselective distinction of pairwise hydrogenation addition is revealed under identical reaction conditions, thereby validating the density-matrix simulation methodology for stereoselectivity determination.