

Abstract Submitted
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Parahydrogen Induced Polarization by Pairwise Replacement on Pt and Ir Nanoparticles CLIFFORD BOWERS, RONGHUI ZHOU, EVAN ZHAO, WEI CHENG, LUKE NEAL, HELENA WEAVER, Univ of Florida - Gainesville — Parahydrogen Induced Polarization (PHIP) is a robust and scalable method for production of bulk quantities of hyperpolarized fluids. The symmetrization order inherent in parahydrogen is transformed via symmetry breaking hydrogenation reaction into NMR-observable hyperpolarization. Spin polarization of order unity can be obtained. A key requirement of PHIP is pairwise hydrogenation by addition of H atoms originating from the same H₂ molecule. PHIP using supported metal catalysts is a promising recent development because it exploits the advantages over homogeneous and supported metal complexes. The present work demonstrates a new PHIP mechanism involving the pairwise replacement of parahydrogen into propene (the substrate) over TiO₂ supported Ir and Pt nanoparticle catalysts. Analysis of the stereoselectivity of the pairwise replacement process is facilitated by density matrix spectral simulations. The cis and trans dispositions of the symmetrization order give strikingly different PHIP spectra. The observed stereoselectivity of the pairwise replacement step, together with control experiments, rule out an alternative mechanism involving dehydrogenation of free propane over the catalyst.

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