Cobalt-Catalyzed Hyperpolarization of Olefins via Signal Amplification by Reversible Exchange

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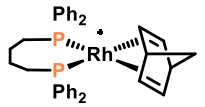
Development of 1st-row Transition Metal Catalysts

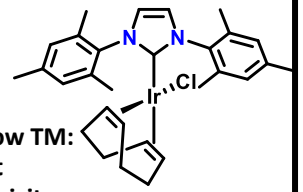
Iron	Cobalt	Nickel
26	27	28
Fe	Co	Ni
55.845	55.933	58.963
Ruthenium	Rhodium	Palladium
44	45	46
Ru	Rh	Pd
101.07	102.91	106.42
Osmium	Iridium	Platinum
76	77	78
Os	Ir	Pt
190.23	192.22	195.08

Benchmark Catalysts:

ALTADENA/PASADENA

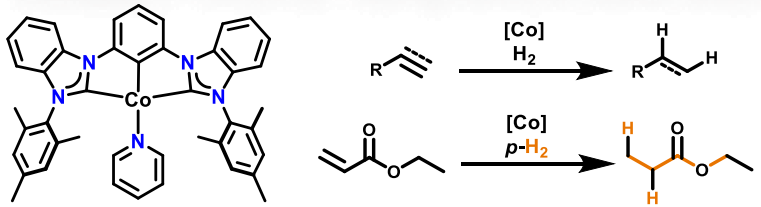


SABRE



Drawbacks to 2nd/3rd row TM:
- Environmental Impact
- Cost
- Potential Toxicity

Previously: (^{Mes}CCC)Co-py – Hydrogenation/ALTADENA catalyst

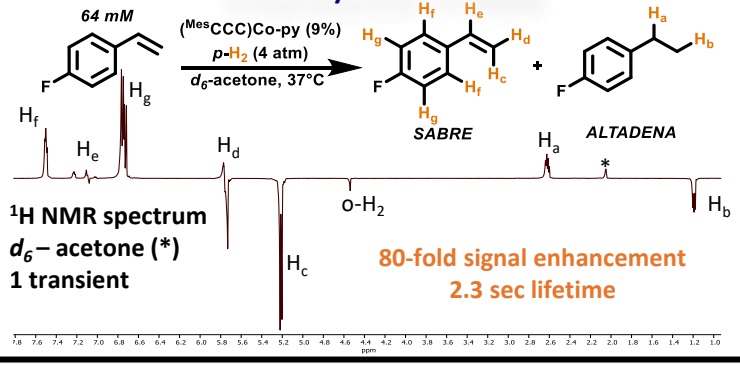


(^{Mes}CCC)Co-py

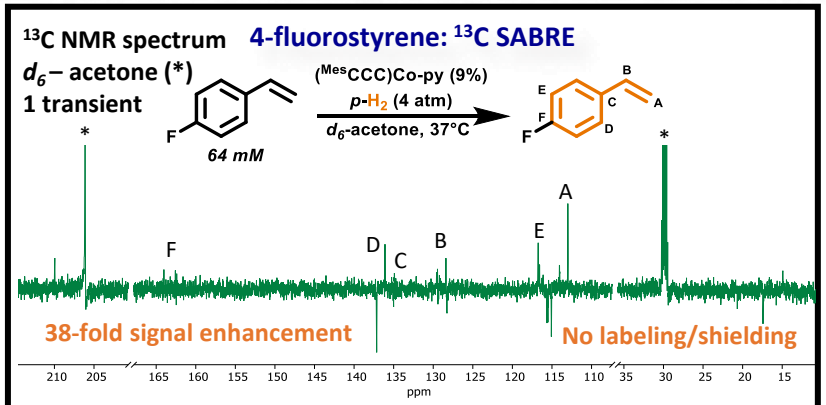
http://pubs.acs.org/doi/abs/10.1021/jacs.6b07066
http://pubs.acs.org/doi/abs/10.1021/jacs.6b08128
https://pubs.acs.org/doi/10.1021/jacs.8b08614

Goal: Establish (^{Mes}CCC)Co-py as a SABRE catalyst.

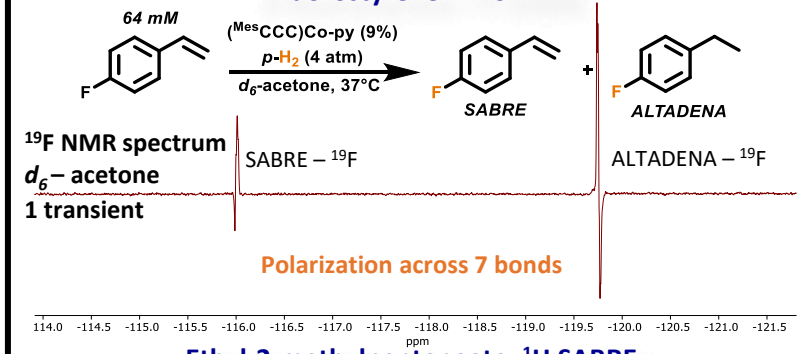
4-fluorostyrene: ^{1}H SABRE



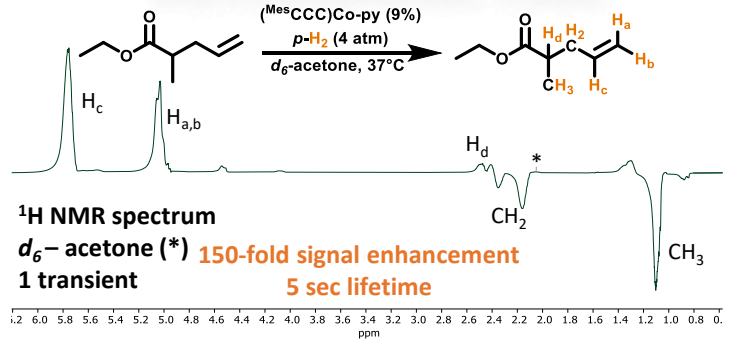
^{13}C NMR spectrum 4-fluorostyrene: ^{13}C SABRE



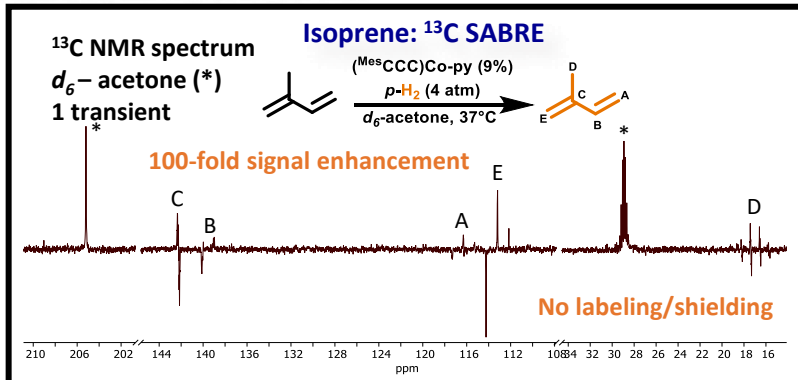
4-fluorostyrene: ^{19}F SABRE



Ethyl-2-methylpentenoate: ^{1}H SABRE



Isoprene: ^{13}C SABRE



Conclusions and Future Work

- Demonstrates first non-iridium and first-row TM SABRE catalyst
- Polarization observed in ^{1}H, ^{13}C, and ^{19}F nuclei
- Demonstrated SABRE of olefins for the first time
- Amenable to variety of olefins, with polarization observed across up to 7 bonds
- Up to 150-fold enhancement for ^{1}H and 100-fold for ^{13}C without shielding or labeling
- Future work: optimization of reaction conditions and application towards MRI contrast agents.

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