

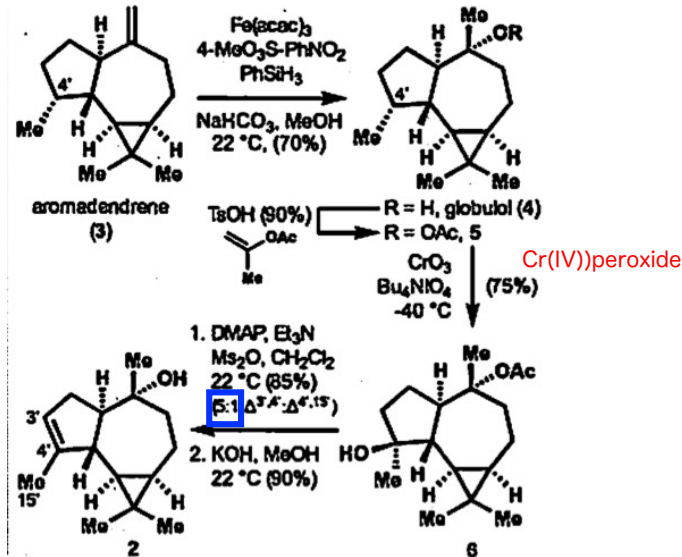
Iron-Catalyzed Hydrobenzylation: Stereoselective Synthesis of (-)-Eugenol C

Xu-cheng Gan, Simona Kotesova, Alberto Castanedo, Samantha A. Green, Søren Lau Borch Møller, and Ryan A. Shenvi*

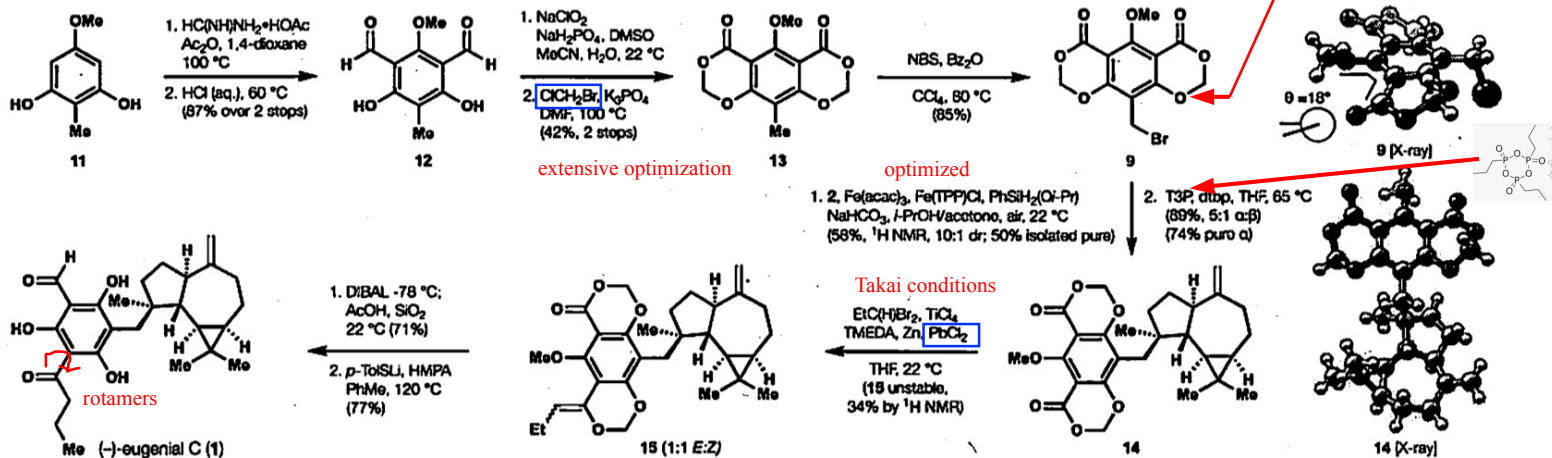
Cite this: J. Am. Chem. Soc. 2023, 145, 29, 15714–15720

"hydrofunctionalization" "MHAT/SH2 steps"

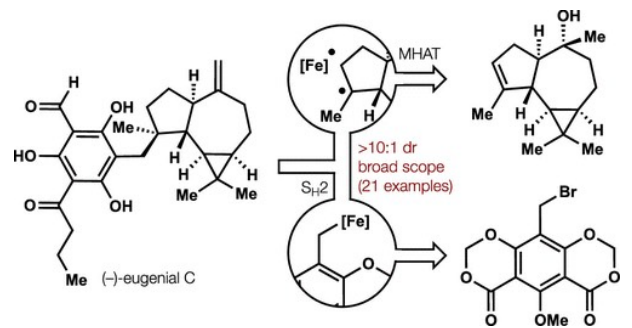
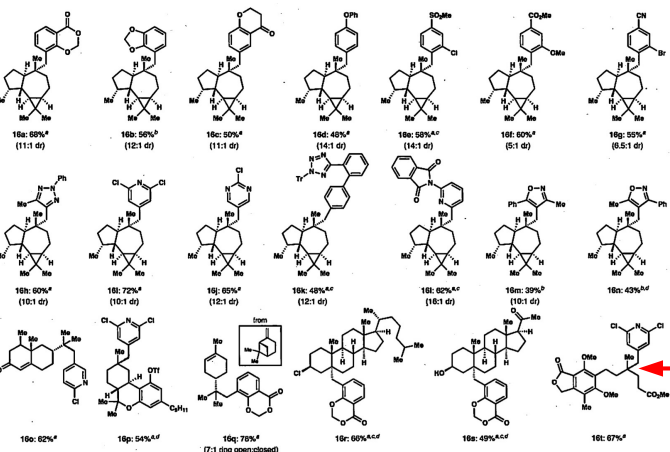
from 3.2Kg of fruit Eucalyptus globulus, 4(13.2g), 3(29.3g) isolated



Scheme 3. 10-Step Synthesis of (-)-Eugenol C via MHAT/SH₂ Hydrobenzylation

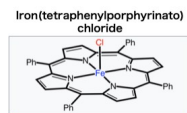
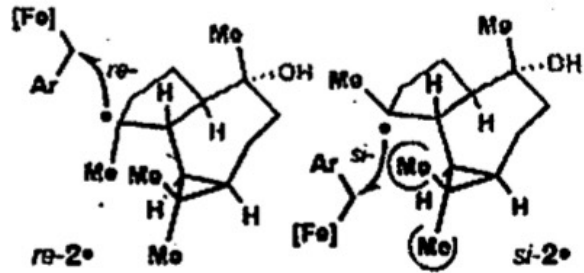


"hydrobenzylation"



SH₂ > radical heterodimerization, reductive elimination

can S_H2 favor C4' re-face approach due to geminal dimethyl repulsion?



limited steric clash
limited chelation

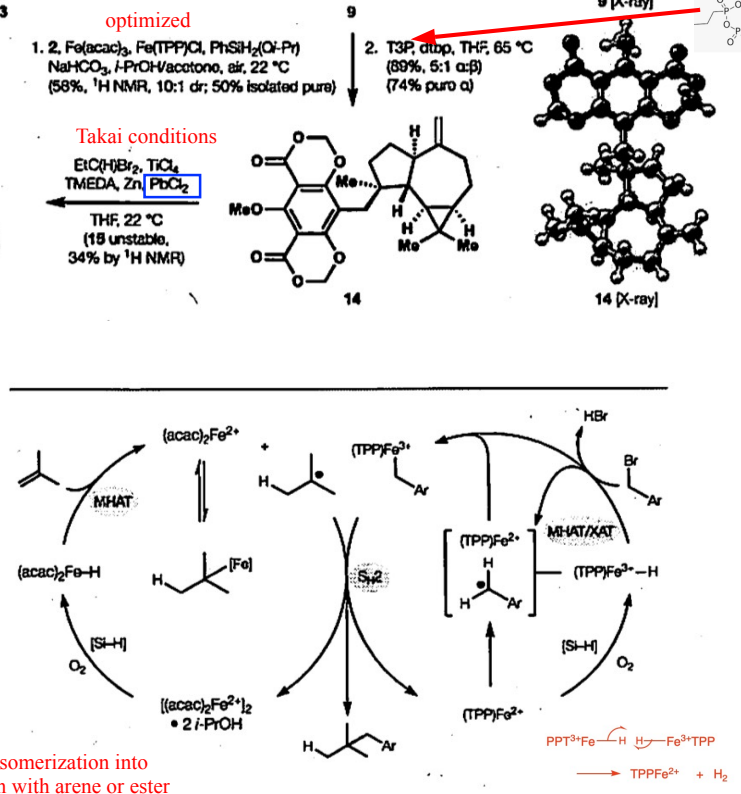


Figure 2. Proposed intersection of catalytic cycles. See the text for competing hypotheses.

more likely than persistent radical (PRE)-driven heterodimerization

SH₂: bimolecular homolytic substitution

exceeded 10:1 dr

efficient with electron-poor and rich arenes

*5 mol % Fe(acac)₃ and 5 mol % Fe(PP)/Cl. ^b10 mol % Fe(acac)₃ and 10 mol % Fe(PP)/Cl. See Supporting Information for solvent deviations.

^cOne diastereomer observed.