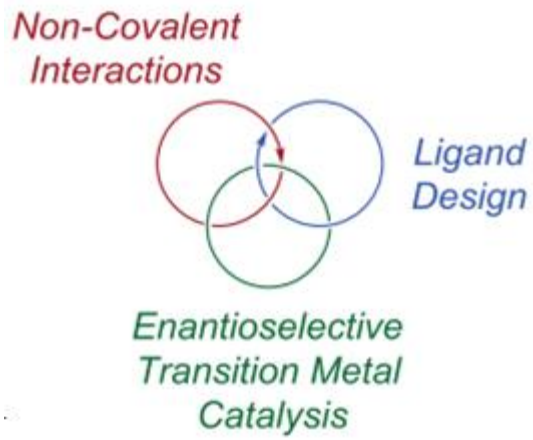
Enantioselective Transition Metal Catalysis Featuring Attractive Noncovalent Interactions between Ligand and Substrate



BaoLe Qu

Jun. 13, 2023

Outline

- Introduction: Noncovalent Interactions
- NCIs-Assisted Ferrocenyl Phosphine Ligands
- NCIs-Assisted Cinchona-Derived Ligands
- NCIs-Assisted Chiral-at-Iridium Octahedral Complex
- My Comments & Idea

Outline

- **Introduction: Noncovalent Interactions**
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Introduction: Noncovalent Interactions

非共价相互作用：是指分子间或单个的分子内部凭借一种分散变化的电磁力来维系一定的空间结构的一种作用。与共价键的不同之处在于它不涉及电子共享。主要分为四种类别：**静电相互作用(electrostatic interactions)**、**范德华力(Van der Waals interactions)**、**π共轭效应(π-effects)**、**以及疏水效应(Hydrophobic effects)**。

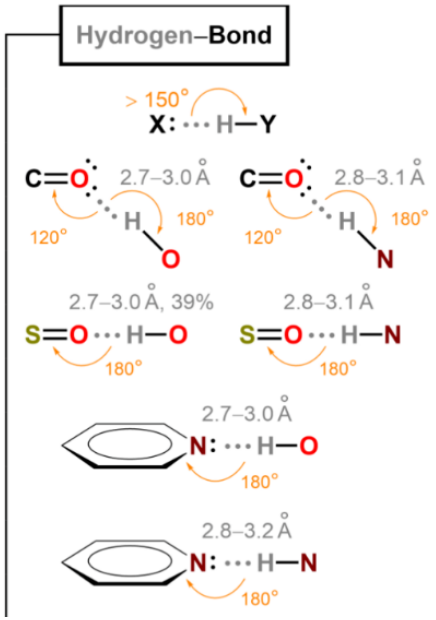
➢ **静电相互作用(electrostatic interactions)**

（1）离子相互作用：涉及具有相反符号的电荷的离子或分子的吸引力。

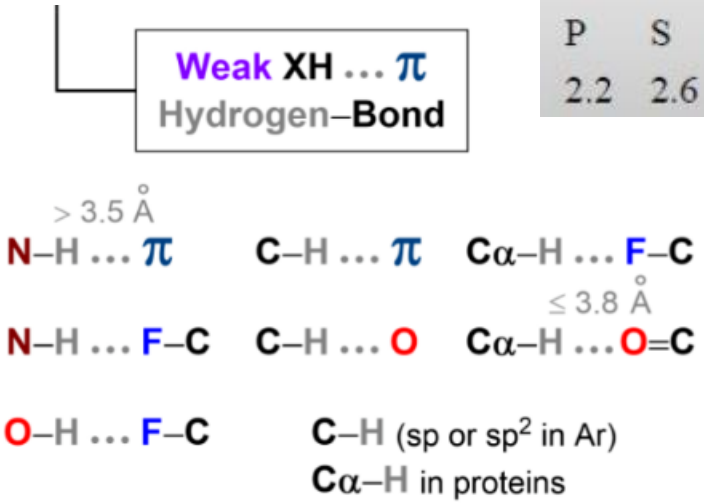
Introduction: Noncovalent Interactions

➢ **静电相互作用(electrostatic interactions)**

（2）氢键：氢键(H-bond)是一种特定类型的相互作用，它涉及部分正的氢原子与高度负电的、部分负的氧、氮或氟原子之间的偶极-偶极吸引力。只有电负性强的原子才能形成氢键，且氢键强度与成键原子的电负性呈正相关。通过实验发现，氟形成的氢键很强，氧形成的氢键较弱，氮形成的氢键更弱。氯的电负性虽与氮的电负性相等，但生成氢键的能力却极小；这是由于氯（与氮相比）的体积较大，使得静电作用力弱于氮。



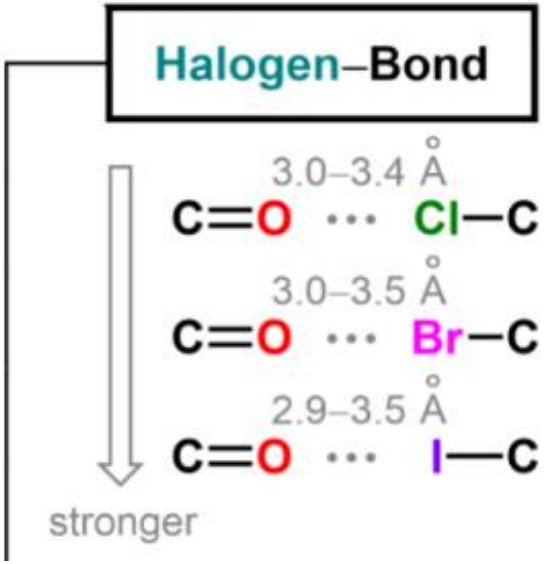
N	O	F
3.0	3.4	4.0
P	S	Cl
2.2	2.6	3.1



Introduction: Noncovalent Interactions

➢ 静电相互作用(electrostatic interactions)

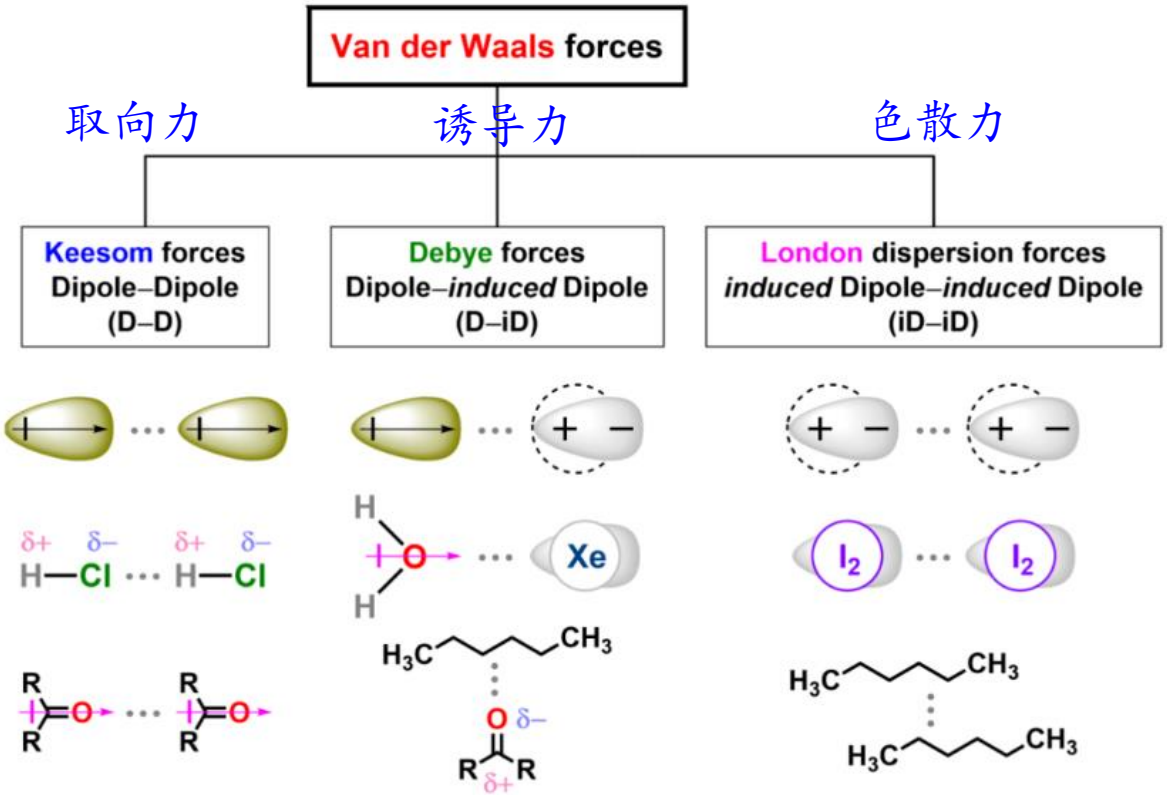
（3）卤键：一种新型的非共价相互作用力，是含卤素的化合物与路易斯碱形成的非共价键。具体地说，是卤原子连在大电负性原子上，电子向成键方向明显转移，从而导致成键方向的背面，卤原子电子密度下降，形成局部正电区域与另一分子的负电密集区域的静电相互吸引。与氢键相比，卤素原子代替部分带正电的氢作为亲电体。



Introduction: Noncovalent Interactions

范德华力（Van der Waals interactions）

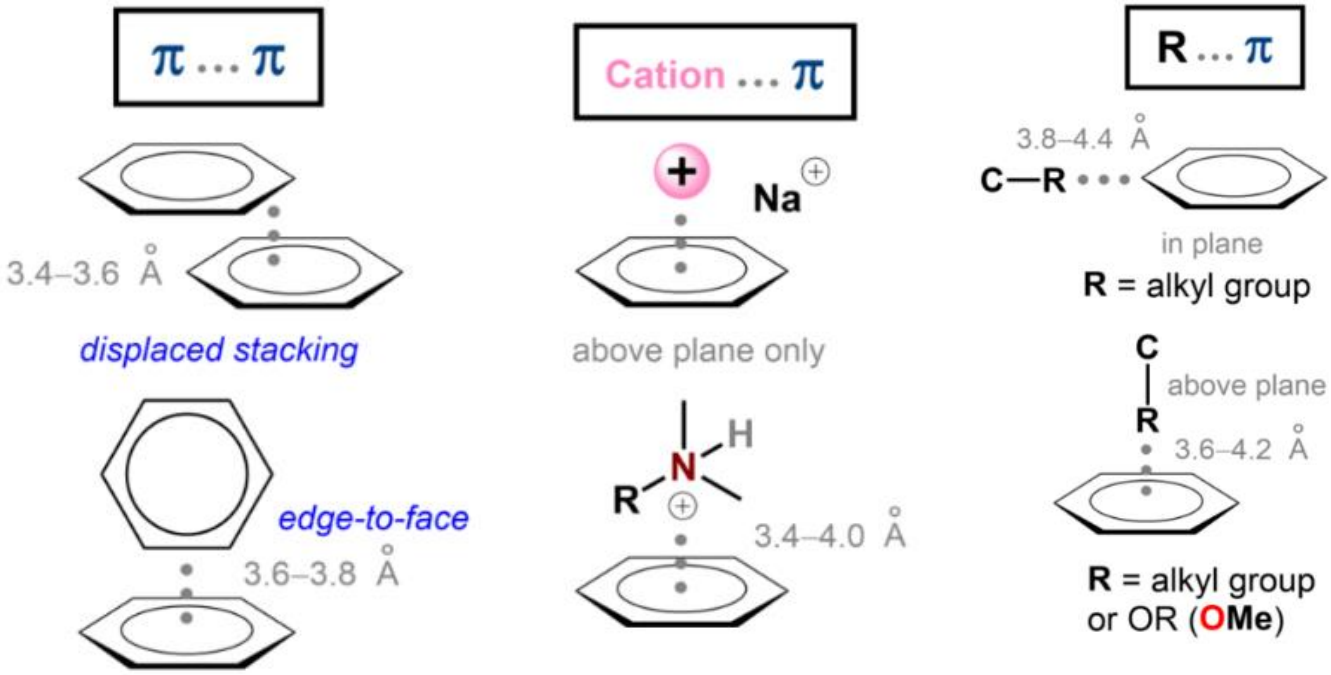
范德华力指分子间作用力即存在于中性分子或原子之间的一种弱碱性的电性吸引力。某物质的范德华力越大，则它的熔点、沸点就越高。对于组成和结构相似的物质，范德华力一般随着相对分子质量的增大而增强。



Introduction: Noncovalent Interactions

π 共轭效应 (π-effects)

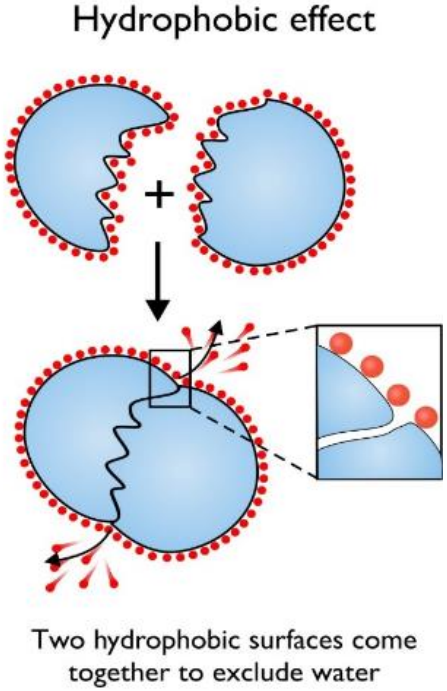
π-效应可以分为许多类别，包括π-π相互作用、阳离子-π和阴离子-π相互作用以及极性-π相互作用。通常，π效应与共轭分子（如苯）的π系统的相互作用有关。



Introduction: Noncovalent Interactions

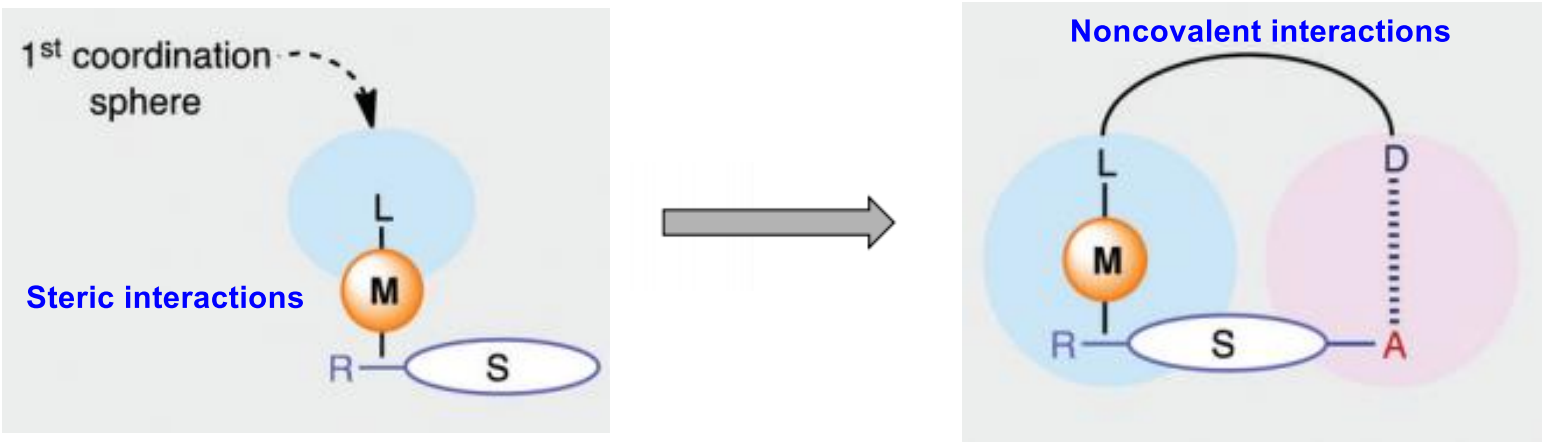
疏水效应（Hydrophobic effects）

当疏水性的溶质丢进水中，水本来的氢键网络会被破坏以腾出空间给疏水性的溶质，在疏水性溶质的周围水分子会形成一个类似牢笼的结构。当疏水性溶质聚集时，这个聚集的整体与水的接触表面比溶质完全均匀分散在溶液中的接触表面要小，有序化的水分子降到最少，自由的水分子达到更多，同时熵也增大，这就是疏水效应。



Introduction: Noncovalent Interactions

Noncovalent interactions in metal complex catalysis



Distance dependencies of the representative noncovalent interactions

noncovalent interactions	energy dependence on distance
steric repulsion	$1/r^{12}$
hydrogen bond	complicated, $\sim 1/r^{2}$
ion pair	$1/r$

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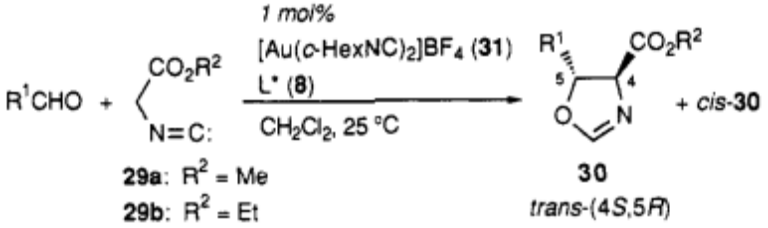
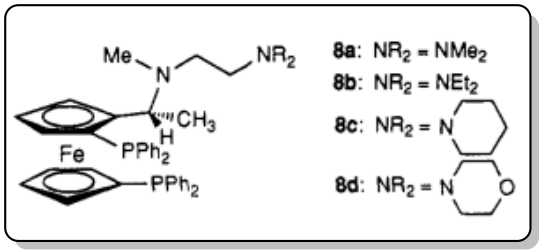
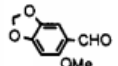
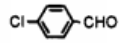
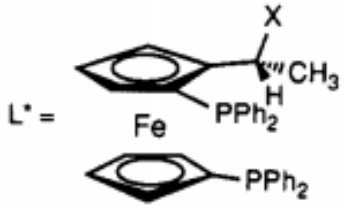
NCIs-Assisted Ferrocenyl Phosphine Ligands

- **Early reports**
  - **Gold-catalyzed asymmetric aldol reaction**





entry	aldehyde	L*	ratio of trans/cis	% ee of *trans*-30
1	PhCHO	8a	90/10	91
2	PhCHO	8b	89/11	93
3	PhCHO	8c	94/6	95
4	PhCHO	8d	95/5	95
5		8d	95/5	96
6		8d	92/8	92
7		8d	96/4	95
8		8d	94/6	94
9		8d	83/17	86
10	MeCHO	8a	78/22	37
11	MeCHO	8b	84/16	72
12	MeCHO	8d	89/11	89
13	*i*-BuCHO	8d	96/4	87
14	*i*-PrCHO	8a	99/1	94
15	*t*-BuCHO	8d	100/0	97
16	(*E*)-*n*-PrCH=CHCHO	8d	87/13	92

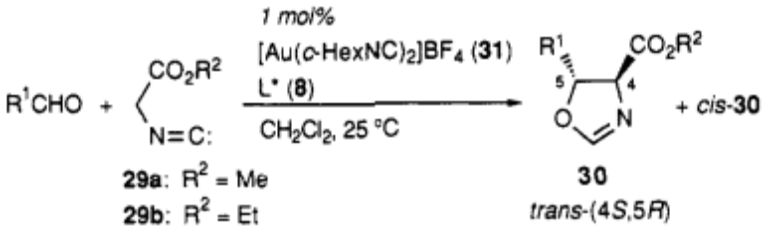


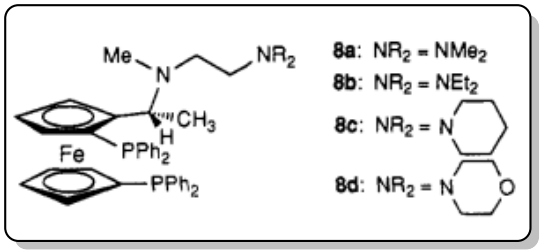
L*	X in L*	ratio of trans/cis	% ee of *trans*-30
32a	$NMe(CH_2)_3NMe_2$	89/11	23
32b	$NMe(CH_2)_3NEt_2$	86/14	26
5a	$NMeCH_2CH_2OH$	69/31	37
5h	NMe_2	68/32	racemic
5j	OMe	86/14	racemic

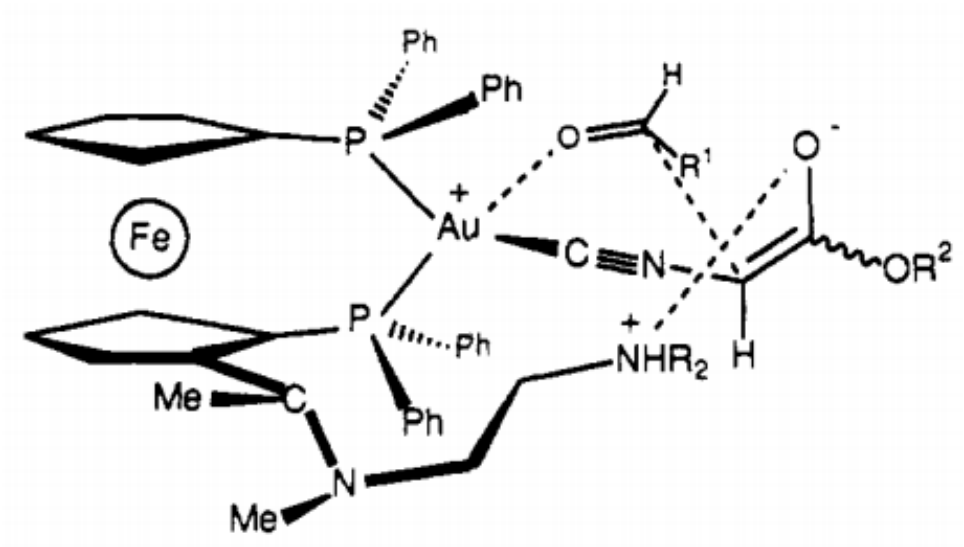
Ito, Y.; Sawamura, M.; Hayashi, T. *J. Am. Chem. Soc.* **1986**, *108,* 6405

NCIs-Assisted Ferrocenyl Phosphine Ligands

- **Early reports**
  - **Gold-catalyzed asymmetric aldol reaction**





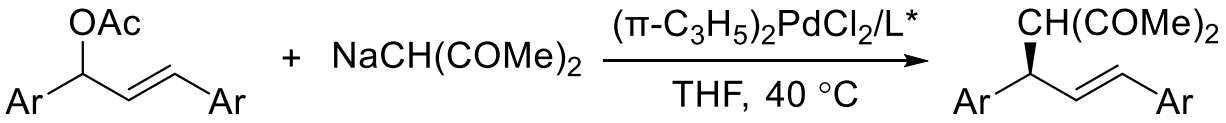


Ito, Y.; Sawamura, M.; Hayashi, T. *J. Am. Chem. Soc.* **1986**, *108,* 6405

NCIs-Assisted Ferrocenyl Phosphine Ligands

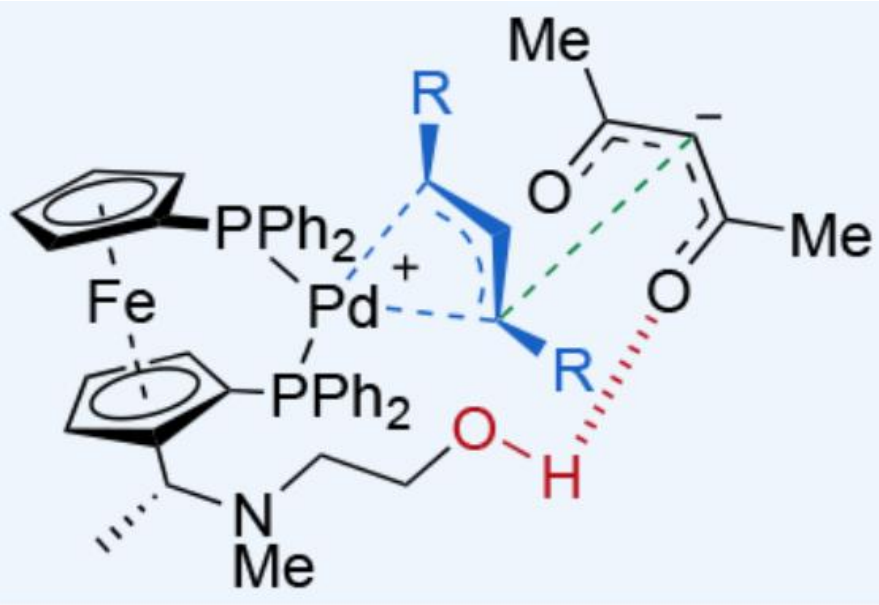
Early reports

Palladium-catalyzed allylic alkylation



Ar = Ph
Ar = 1-naph

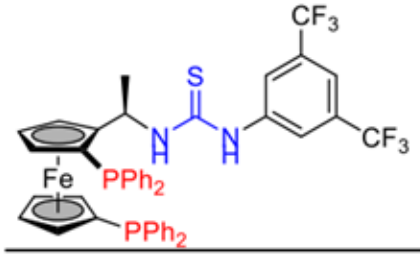
up to 97% yield
90% ee



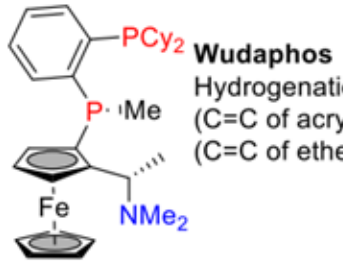
Hayashi, T. *Tetrahedron Lett.* **1986**, *27,* 191

NCIs-Assisted Ferrocenyl Phosphine Ligands

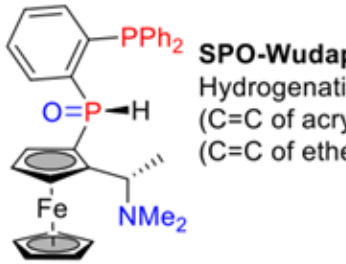
- **Zhang group's work**



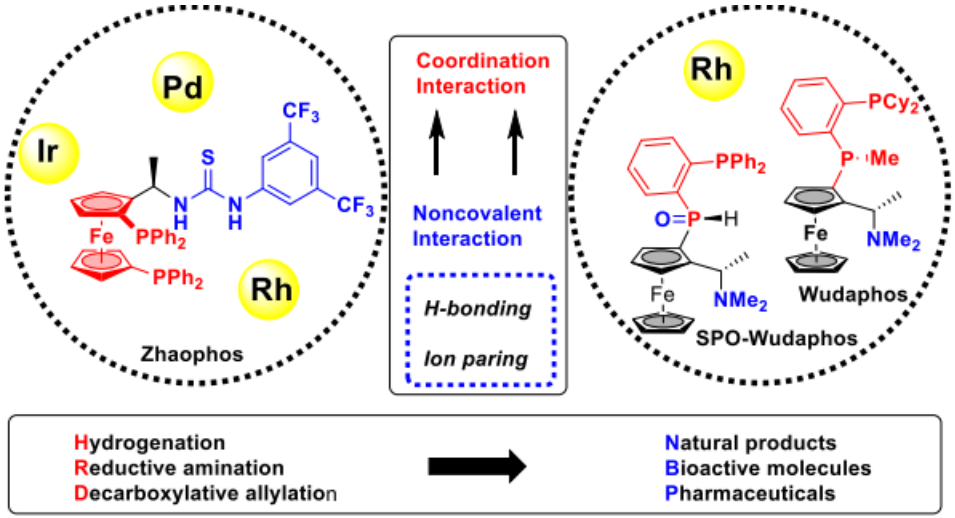
Zhaophos
Hydrogenation
(C=C of neutral substrates)
(C=N of ionic substrates)
(Carbocations)
Reductive amination
Decarboxylative allylation



Wudaphos
Hydrogenation
(C=C of acrylic acids)
(C=C of ethenylsulfonates)



SPO-Wudaphos
Hydrogenation
(C=C of acrylic acids)
(C=C of ethenylphosphonic acids)

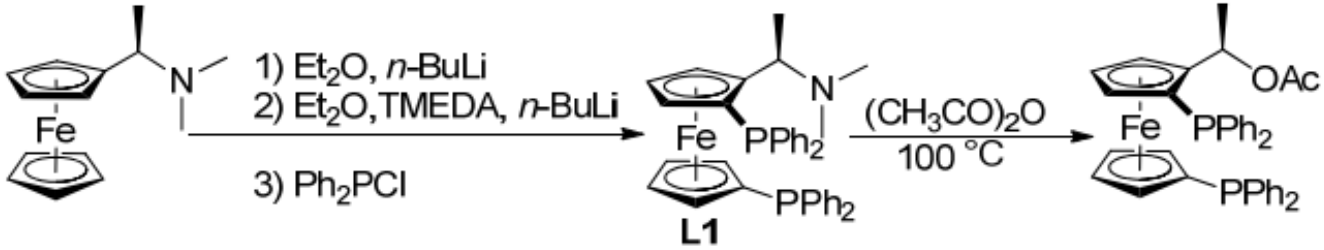


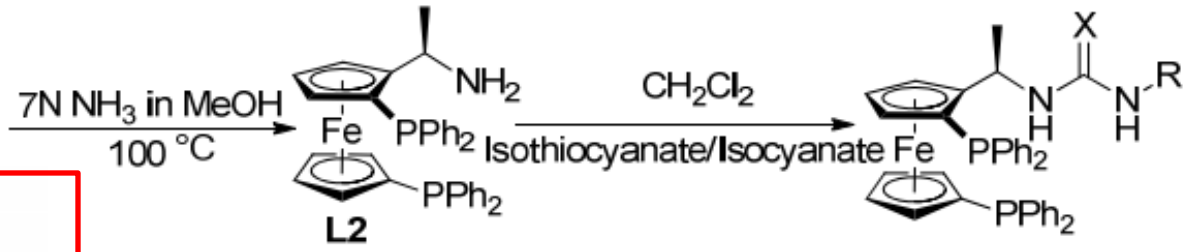
Zhang, X. et al *Acc. Chem. Res.* **2020**, *53,* 1905

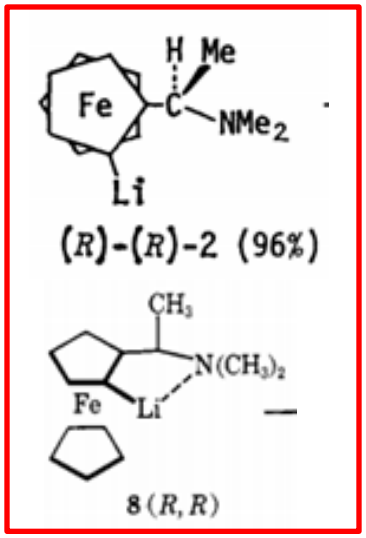
NCIs-Assisted Ferrocenyl Phosphine Ligands

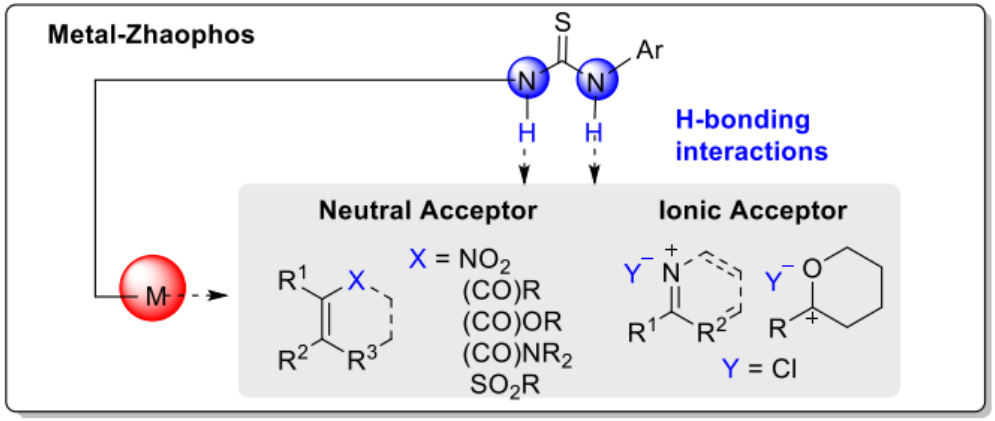
Zhaophos

Design and synthesis of Zhaophos





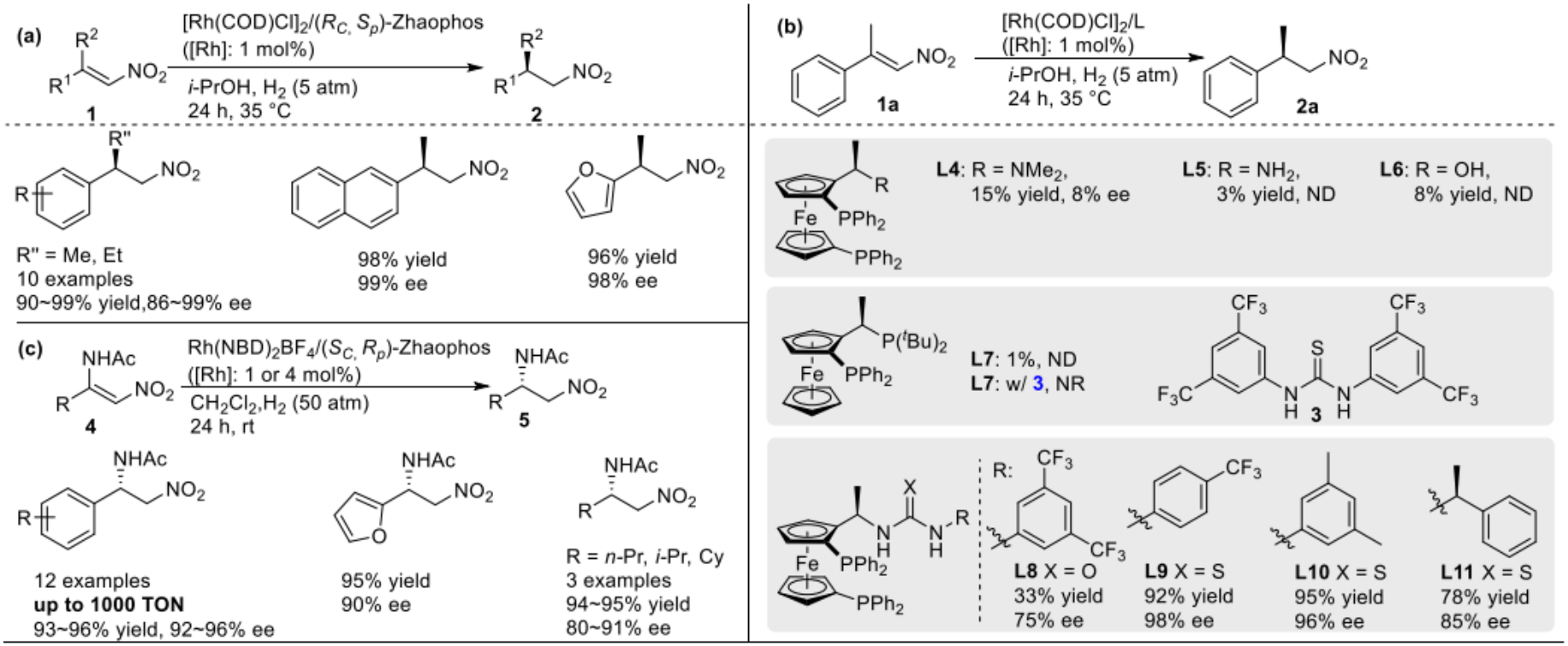




NCIs-Assisted Ferrocenyl Phosphine Ligands

Zhaophos

Asymmetric Hydrogenation of Neutral Substrates

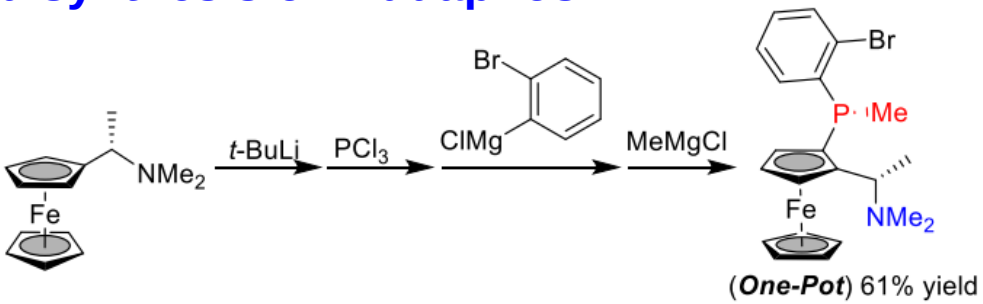


Zhang, X. et al *Org. Lett.* **2013**, *15,* 4014

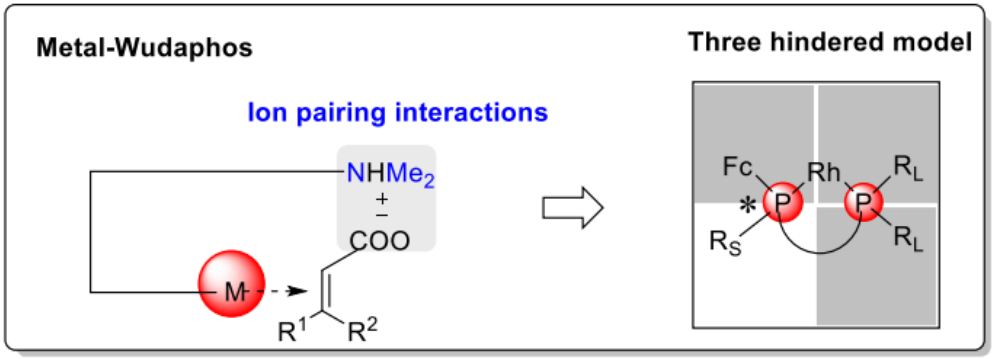
NCIs-Assisted Ferrocenyl Phosphine Ligands

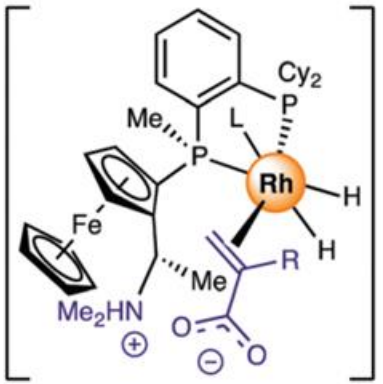
Wudaphos

Design and synthesis of Wudaphos



(*S_C for C-chirality; R_p for planar chirality; S_P for P-chirality)

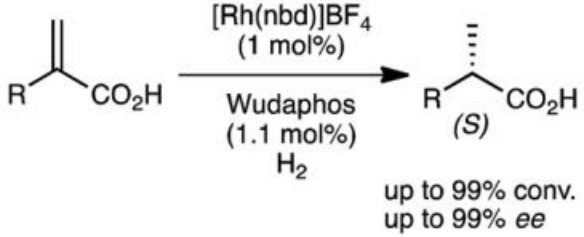


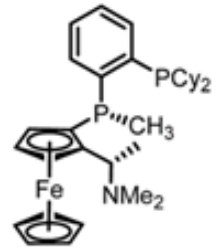


NCIs-Assisted Ferrocenyl Phosphine Ligands

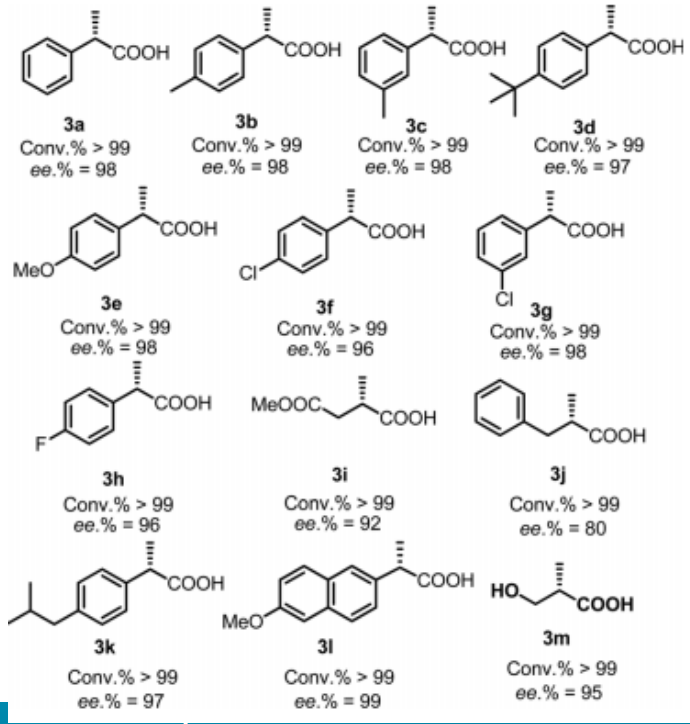
Wudaphos

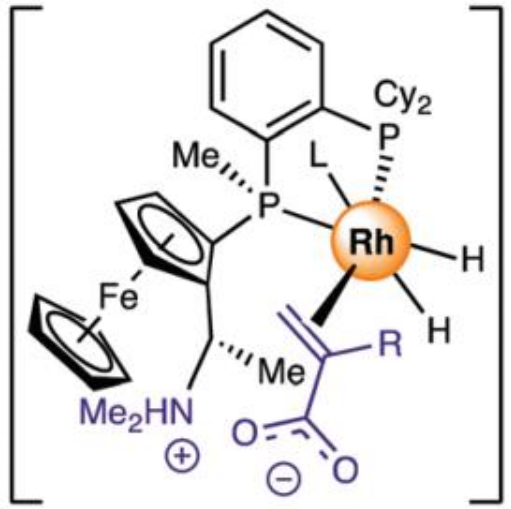
Asymmetric hydrogenation via noncovalent ion pair interaction





L2, *Wudaphos*



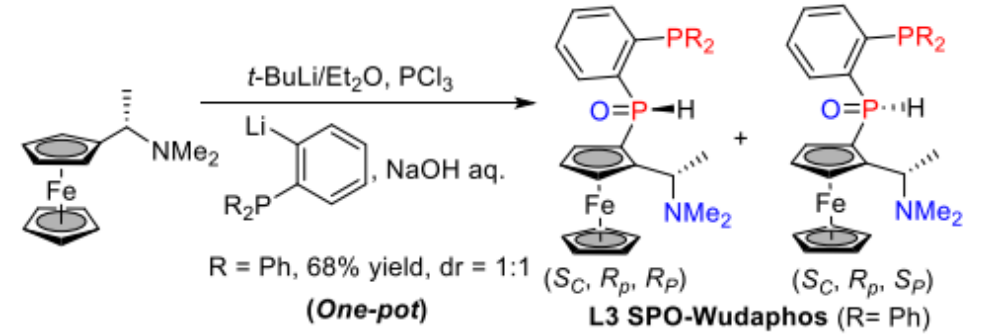


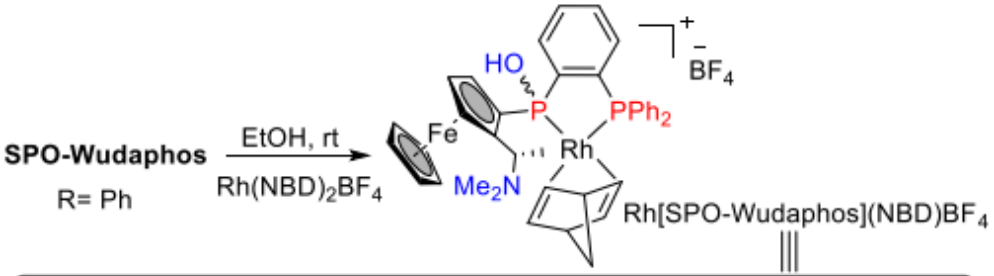
Zhang, X. et al *Chem. Sci.* **2016**, *7,* 6669

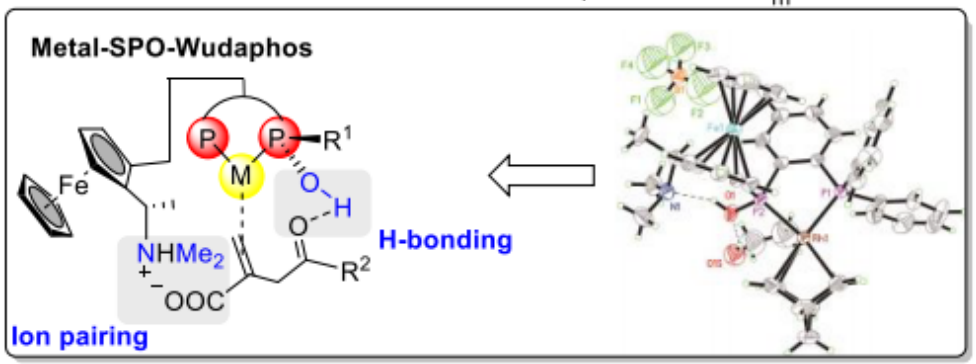
NCIs-Assisted Ferrocenyl Phosphine Ligands

SPO-Wudaphos

Design and synthesis of SPO-Wudaphos



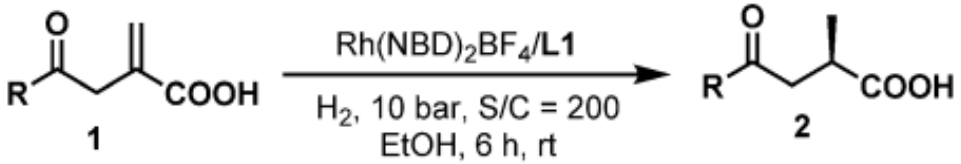




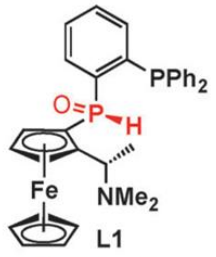
NCIs-Assisted Ferrocenyl Phosphine Ligands

SPO-Wudaphos

Asymmetric hydrogenation

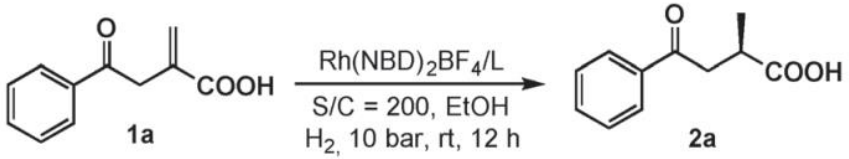


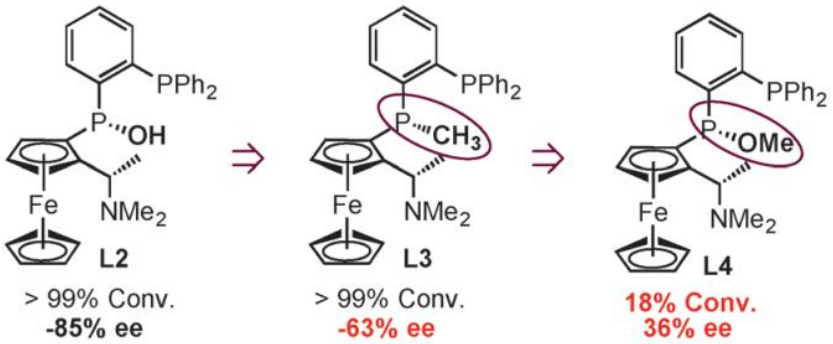
up to >99% Conv.
>99% ee



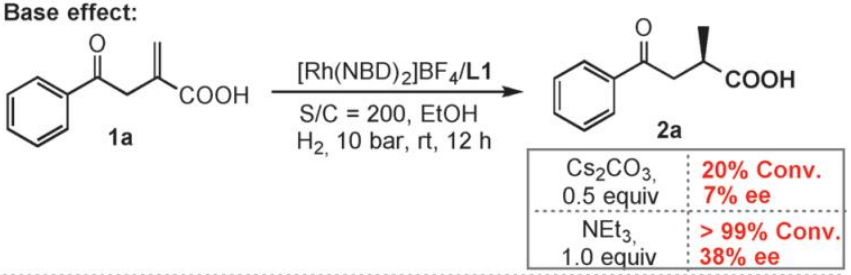
SPO-Wudaphos
(S_C, R_{FC}, R_P)

a) Results using ligands without the hydroxy group:

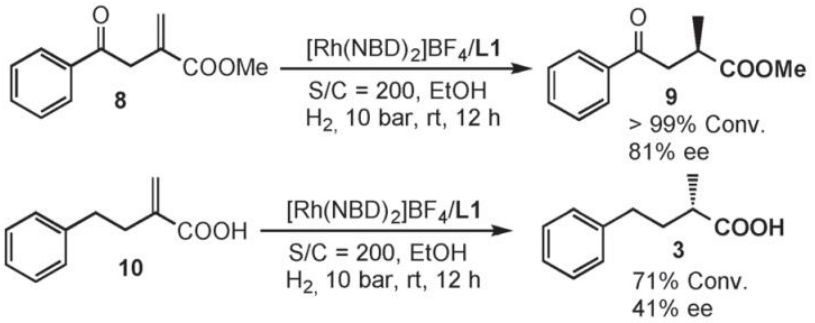




b) Base effect:



c) Substrate effect:

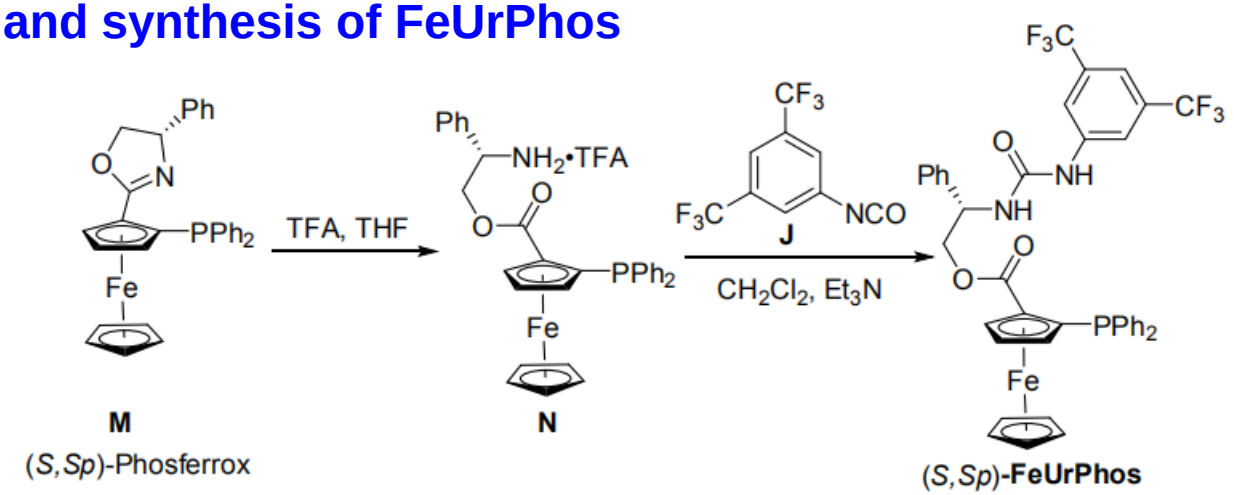


Zhang, X. et al *Angew. Chem. Int. Ed.* **2017**, *56,* 6808

NCIs-Assisted Ferrocenyl Phosphine Ligands

FeUrPhos

Design and synthesis of FeUrPhos

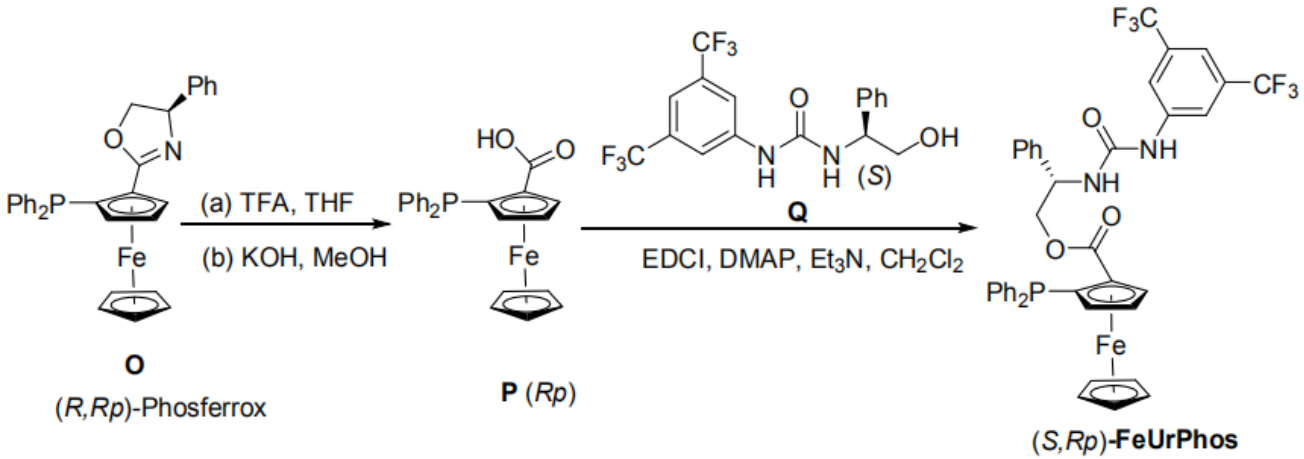


M

(*S,Sp*)-Phosferrox

N

(*S,Sp*)-**FeUrPhos**



O

(*R,Rp*)-Phosferrox

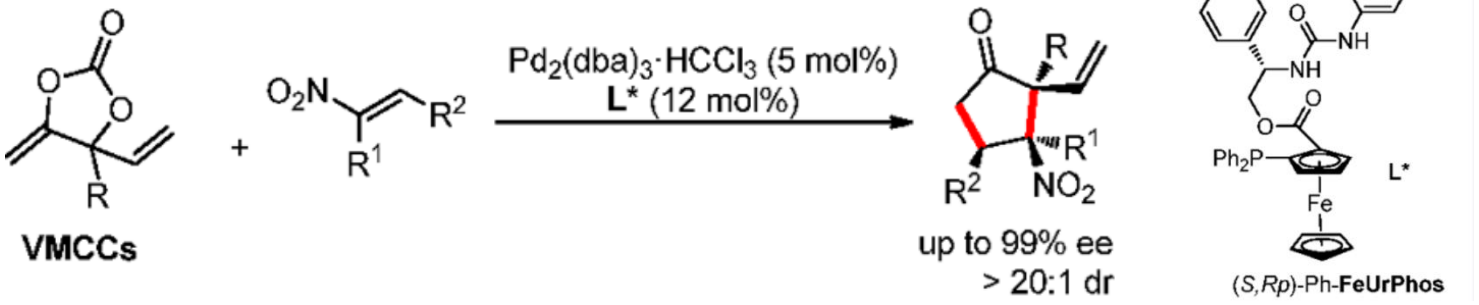
P (*Rp*)

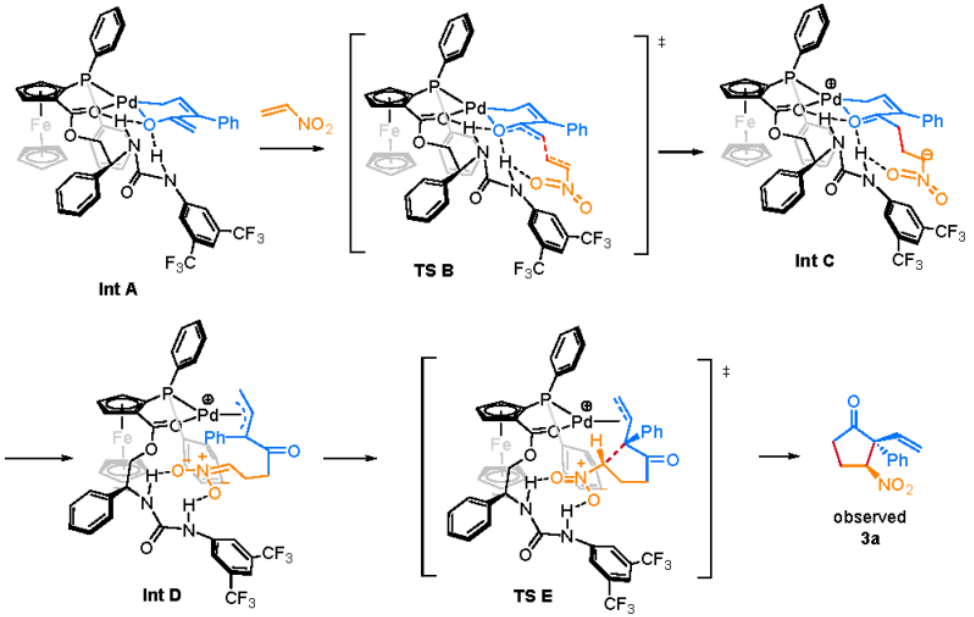
(*S,Rp*)-**FeUrPhos**

Zi, W. -W. et al *J. Am. Chem. Soc.* **2021**, *143,* 1038

NCIs-Assisted Ferrocenyl Phosphine Ligands

- **FeUrPhos**
  - **Asymmetric (3 + 2) annulation**





Zi, W. -W. et al *J. Am. Chem. Soc.* **2021**, *143,* 1038

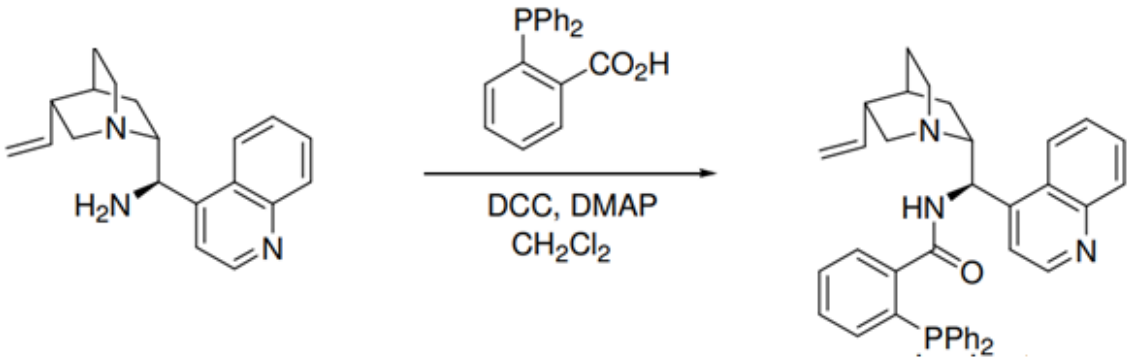
Outline

- Background
- NCIs-Assisted Ferrocenyl Phosphine Ligands
- **NCIs-Assisted Cinchona-Derived Ligands**
- NCIs-Assisted Chiral-at-Iridium Octahedral Complex
- My Comments & Idea

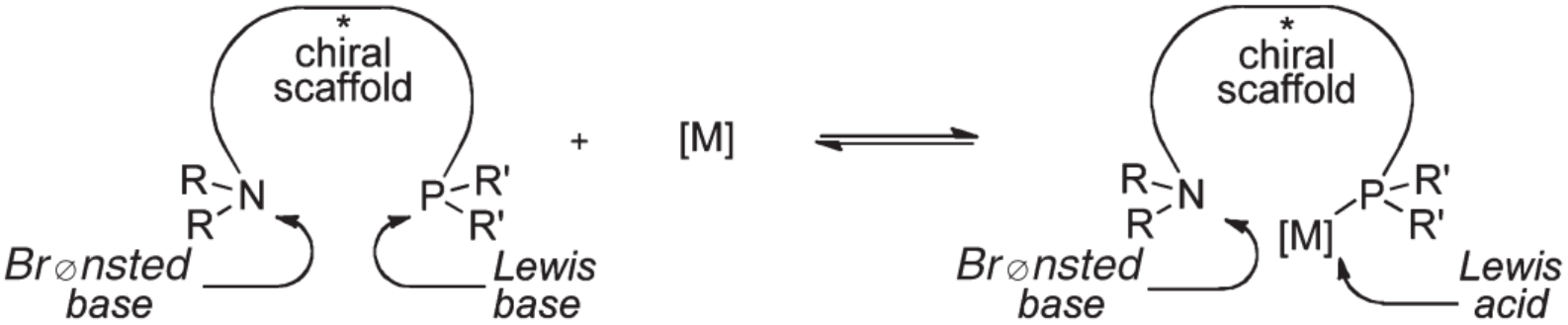
NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Amino Phosphine

Design and synthesis of Cinchona-Derived Amino Phosphine



83% yield

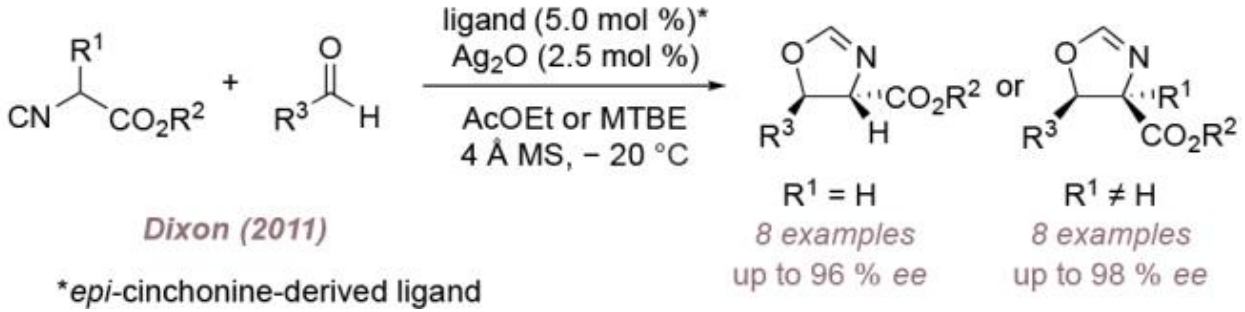


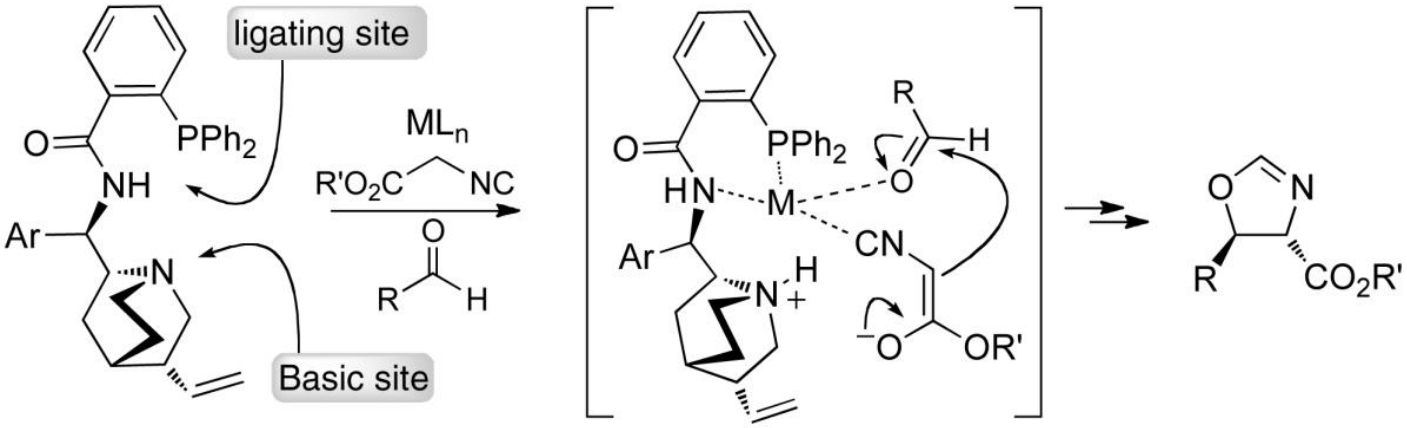
Dixon, D. J. et al *J. Am. Chem. Soc.* **2011**, *133,* 1710

NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Amino Phosphine

Asymmetric Aldol Reaction



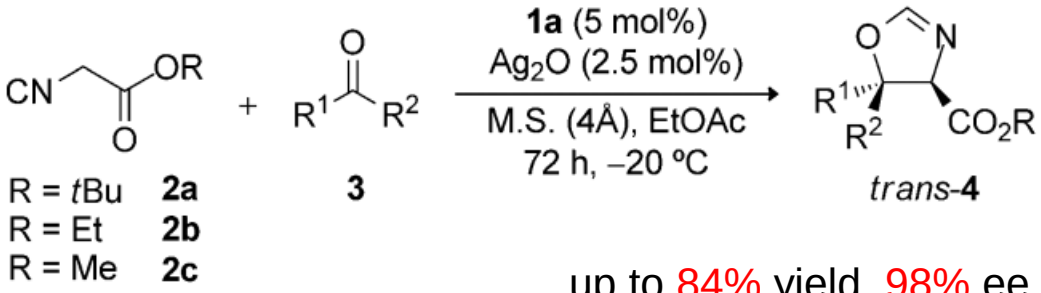


Dixon, D. J. et al *J. Am. Chem. Soc.* **2011**, *133,* 1710

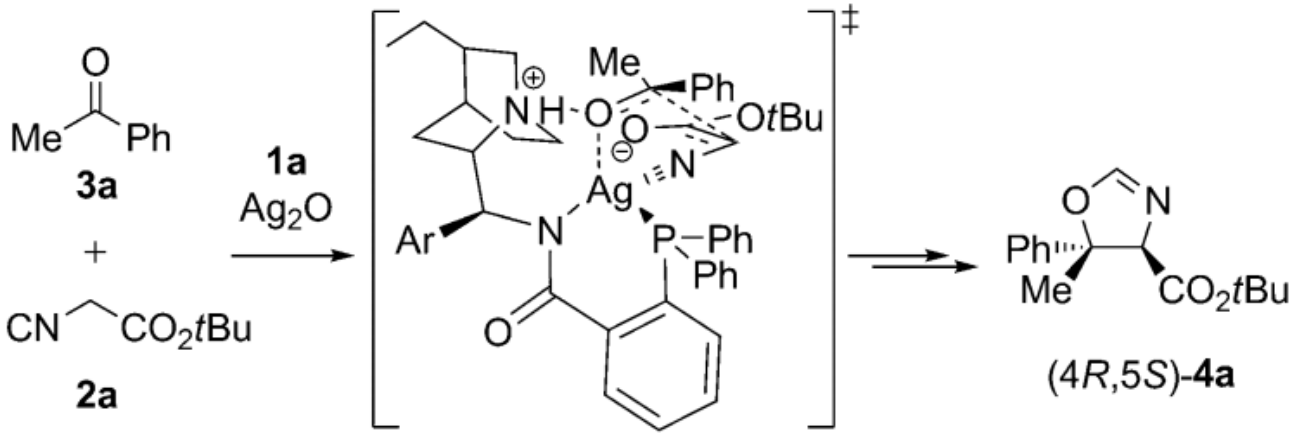
NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Amino Phosphine

Asymmetric Aldol Reaction



up to 84% yield, 98% ee, 96:4 d.r.

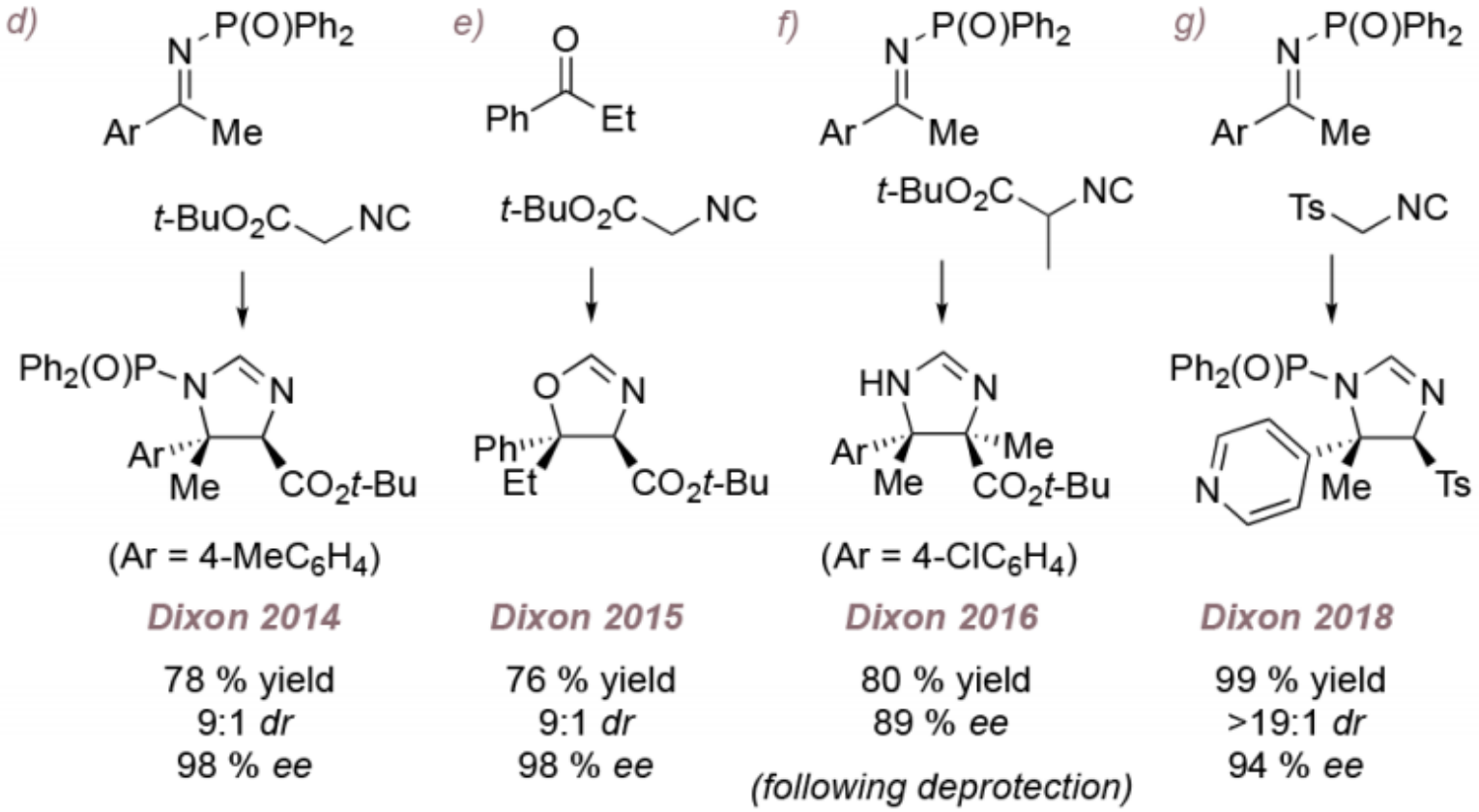


Dixon, D. J. et al *Angew. Chem. Int. Ed.* **2015**, *54,* 1

NCIs-Assisted Cinchona-Derived Ligands

- **Cinchona-Derived Amino Phosphine**
  - **Further applications**

further applications - representative examples



NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Amino Phosphine

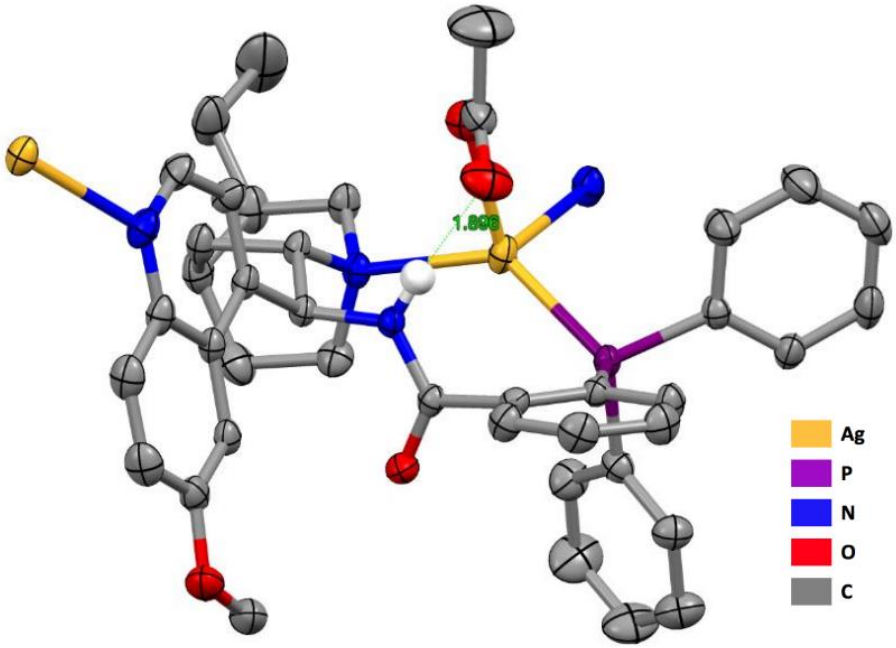


Figure S1. Crystal structure of complex **1a**·AgOAc with highlighted intramolecular H-bond.

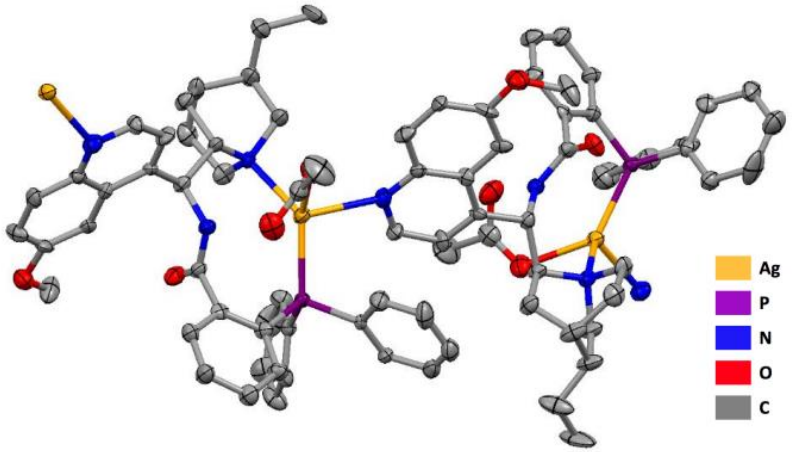
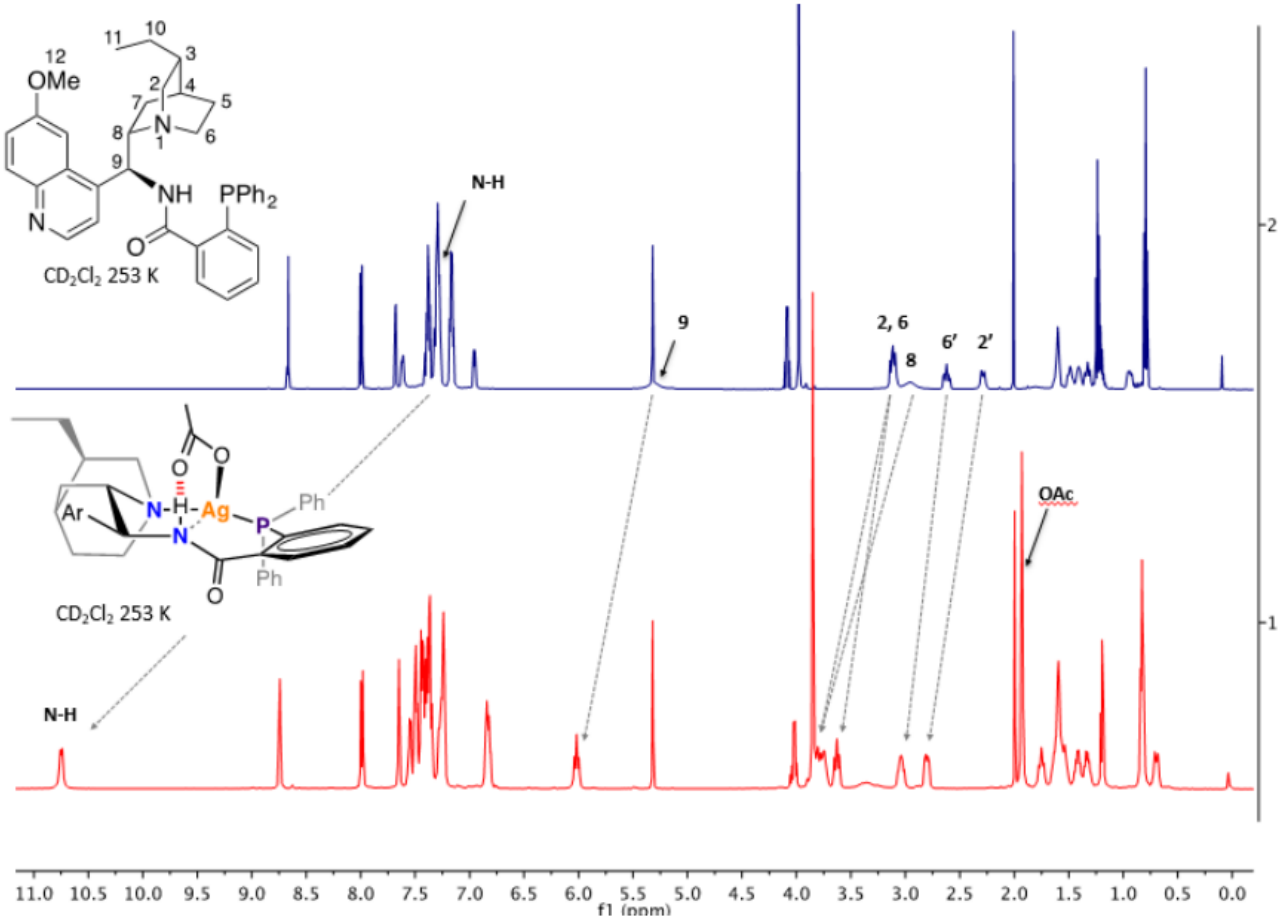


Figure S2. Crystal structure of complex **1a**·AgOAc (dimer indicating the polymeric chain structure in the solid state).

Dixon, D. J. et al *Chem. Commun.* **2016**, *52,* 10632

NCIs-Assisted Cinchona-Derived Ligands

- **Cinchona-Derived Amino Phosphine**

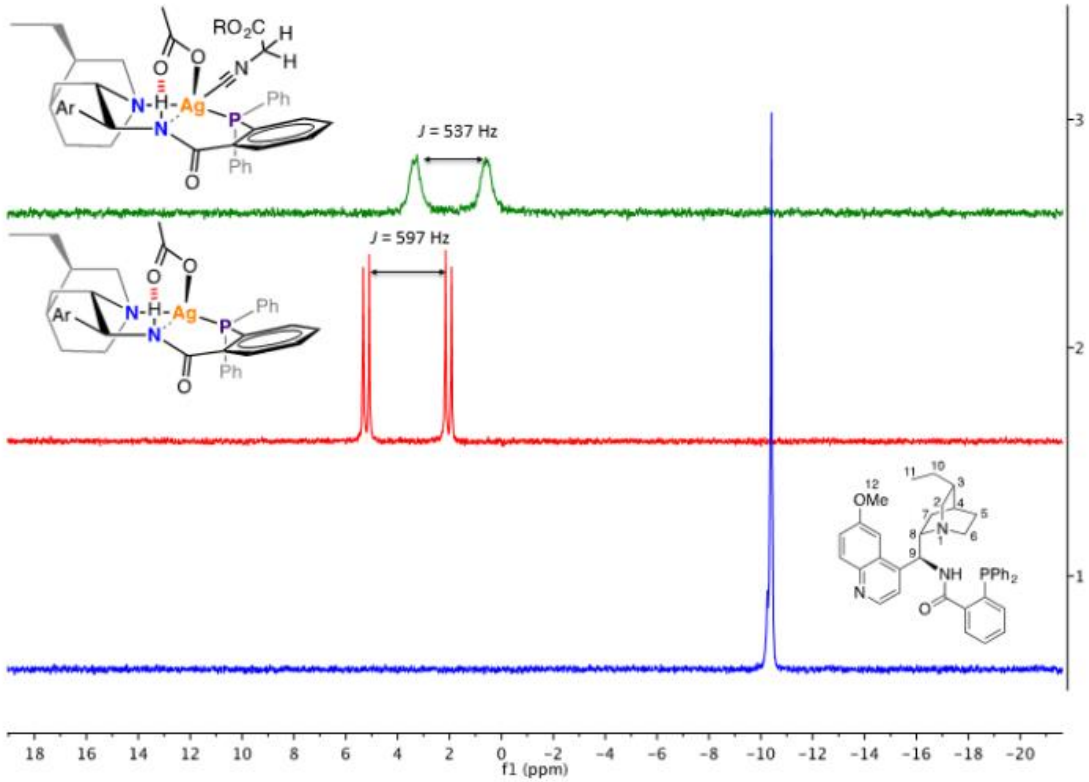


Dixon, D. J. et al *Chem. Commun.* **2016**, *52,* 10632

NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Amino Phosphine

6.2 ^{31}P-NMR spectra

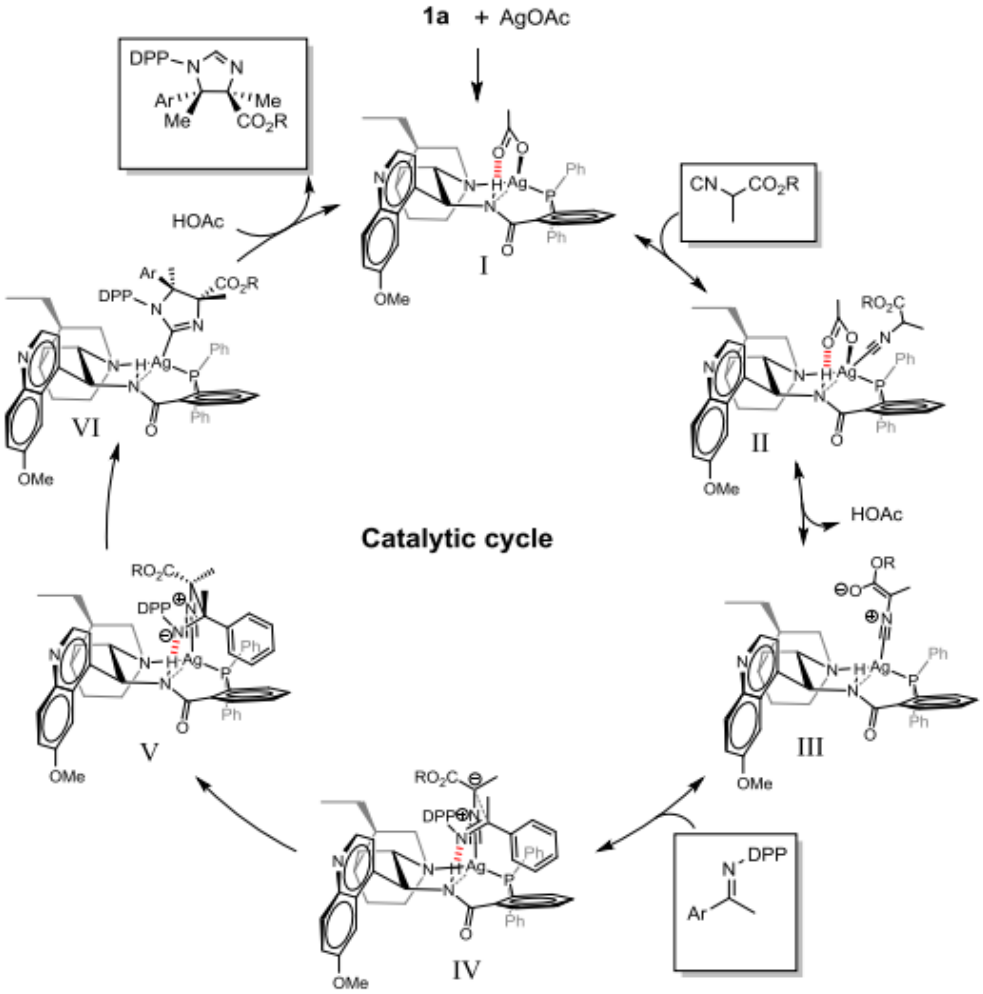


^{31}P NMR at 253 K (including proposed binding mode) of 1) Free ligand **1a**: $\delta^{31}P = -10.4$; 2) **1a**·AgOAc: $\delta^{31}P = 3.6$, $^{1}J^{107}Ag^{31}P = 597$ Hz; 3) Ligand 1 +1 eq of AgOAc + 1 eq. of methylisocyanoacetate: $\delta^{31}P = 2.0$, $^{1}J^{107}Ag^{31}P = 537$ Hz.

Dixon, D. J. et al *Chem. Commun.* **2016**, *52,* 10632

NCIs-Assisted Cinchona-Derived Ligands

- **Cinchona-Derived Amino Phosphine**

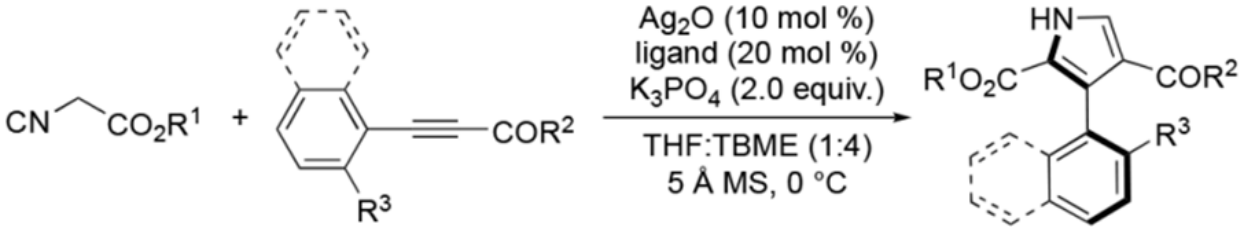


Dixon, D. J. et al *Chem. Commun.* **2016**, *52,* 10632

NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Amino Phosphine

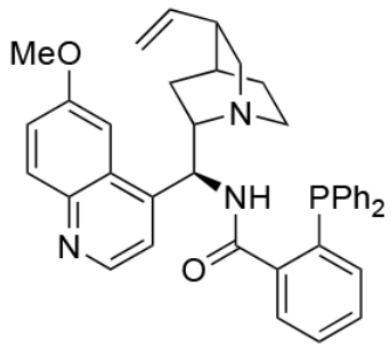
Synthesis of Axially Chiral 3-Arylpyrroles



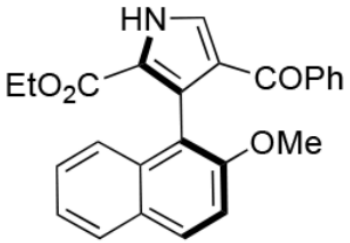
Zhu (2019)

22 examples
up to 96 % ee

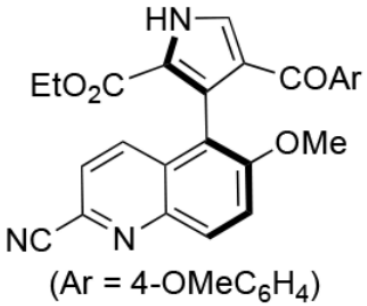
b) ligand



c) representative examples



52 % yield
91 % *ee*



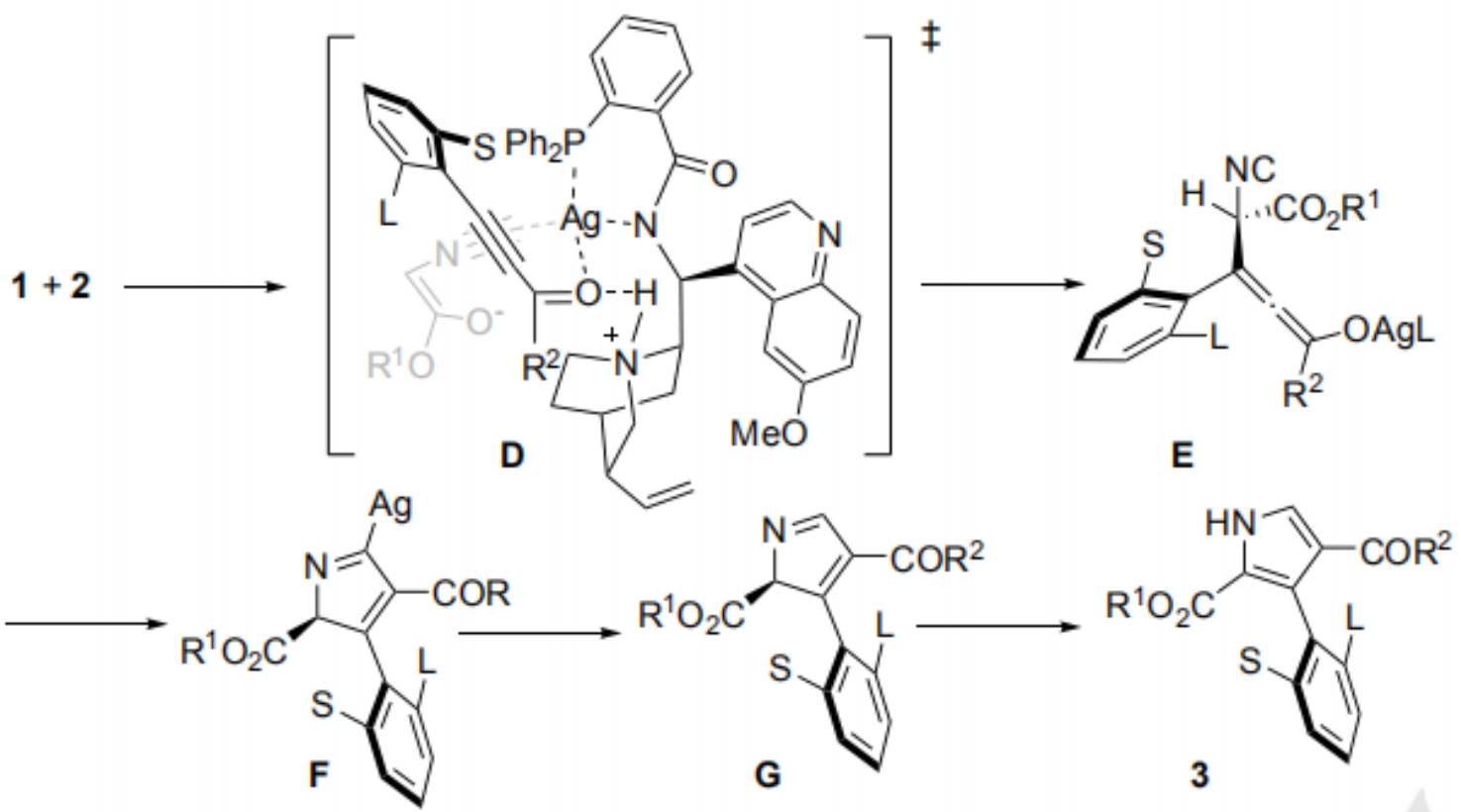
(Ar = 4-$OMeC_6H_4$)

43 % yield
91 % *ee*

Zhu, J. et al *Angew. Chem. Int. Ed.* **2019**, *58,* 1494

NCIs-Assisted Cinchona-Derived Ligands

- **Cinchona-Derived Amino Phosphine**
  - **Synthesis of Axially Chiral 3-Arylpyrroles**

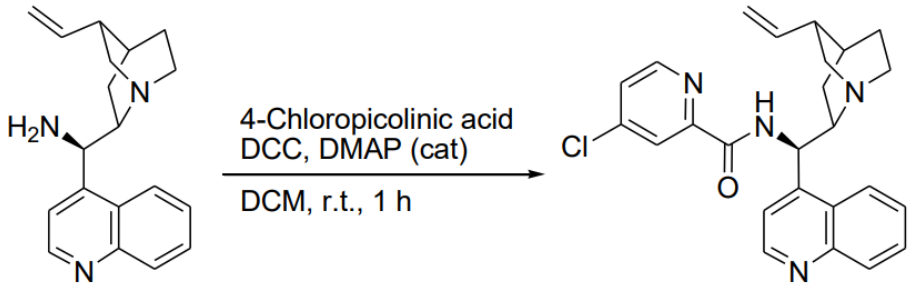


Zhu, J. et al *Angew. Chem. Int. Ed.* **2019**, *58,* 1494

NCIs-Assisted Cinchona-Derived Ligands

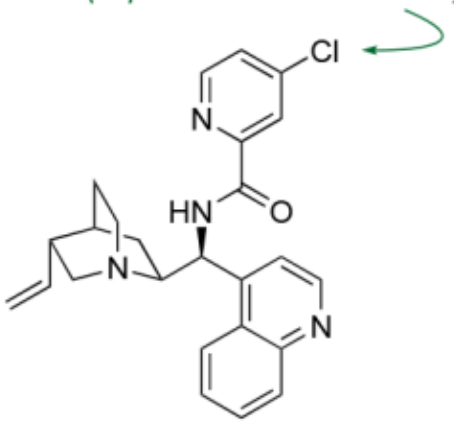
Cinchona-Derived Picolinamide

Design and synthesis of Cinchona-Derived Picolinamide



74% yield

tuning of picolinamide group
(improved enantioselectivity)

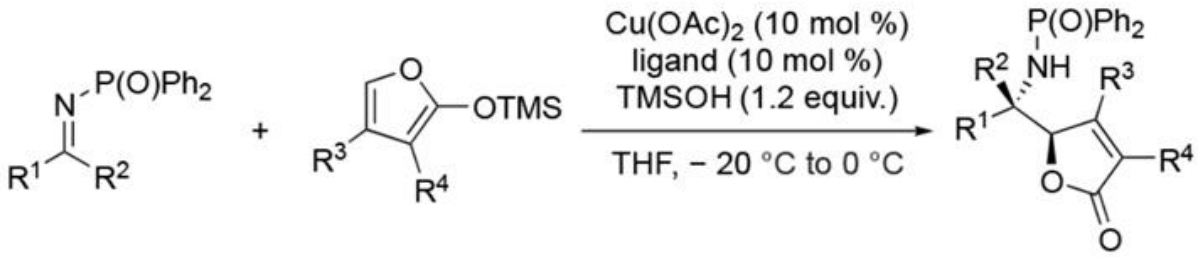


Nakamura, S. et al *Angew. Chem. Int. Ed.* **2013**, *52,* 5557

NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Picolinamide

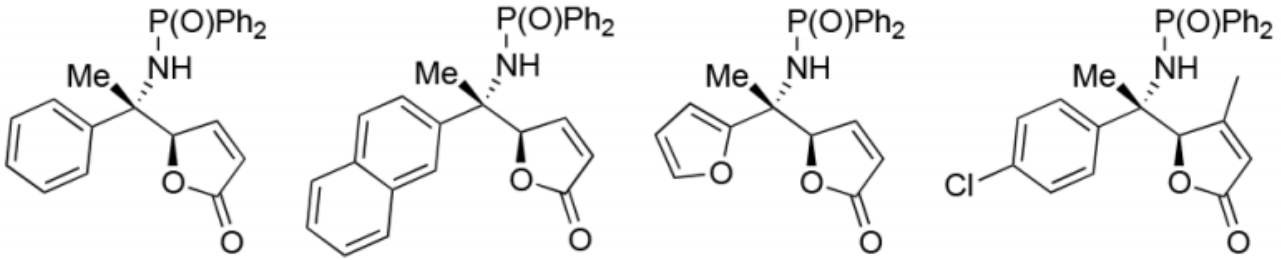
Asymmetric Aldol Reaction



Nakamura (2013)

20 examples
up to 97 % ee

d) representative examples

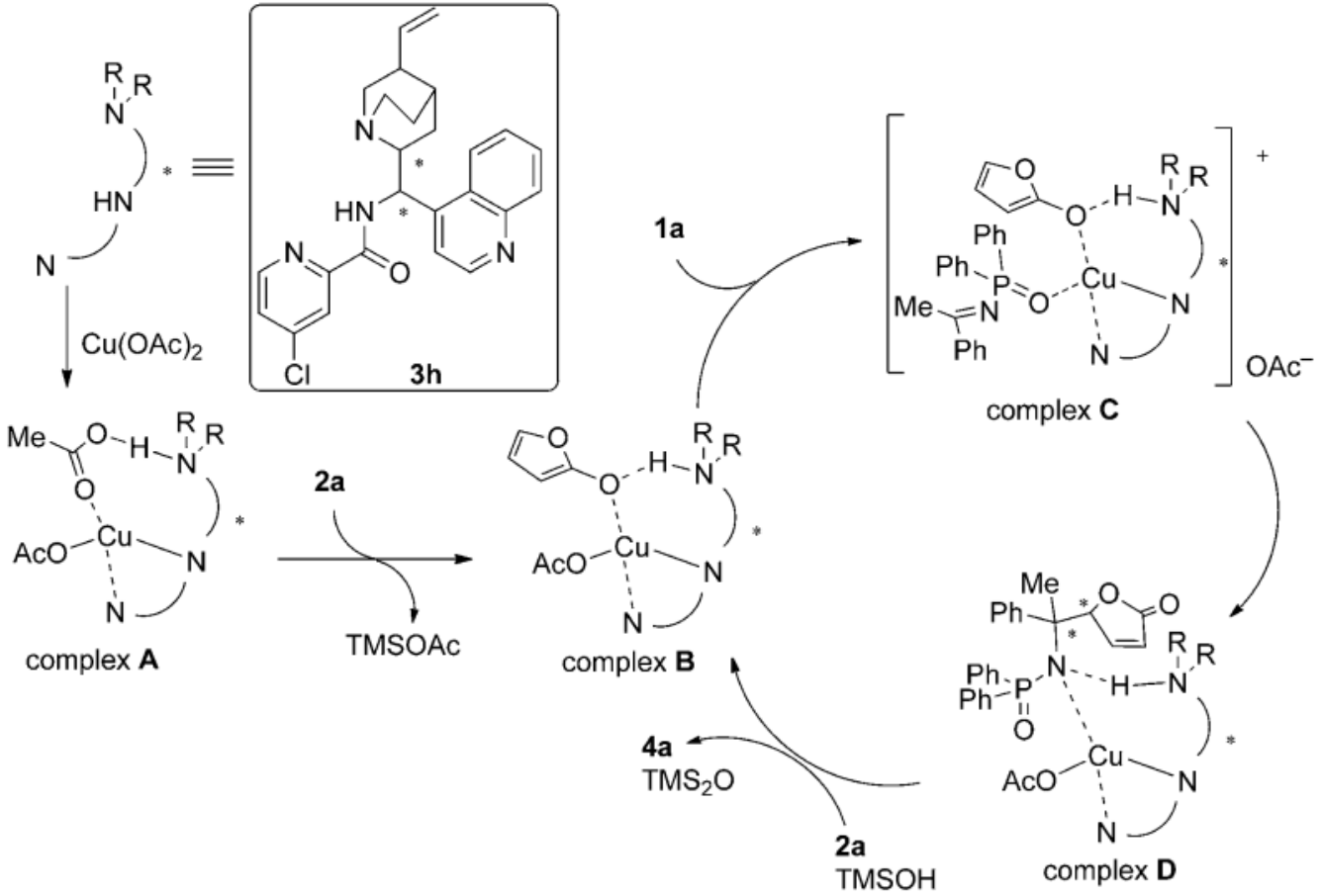


Nakamura, S. et al *Angew. Chem. Int. Ed.* **2013**, *52,* 5557

NCIs-Assisted Cinchona-Derived Ligands

Cinchona-Derived Picolinamide

Asymmetric Aldol Reaction



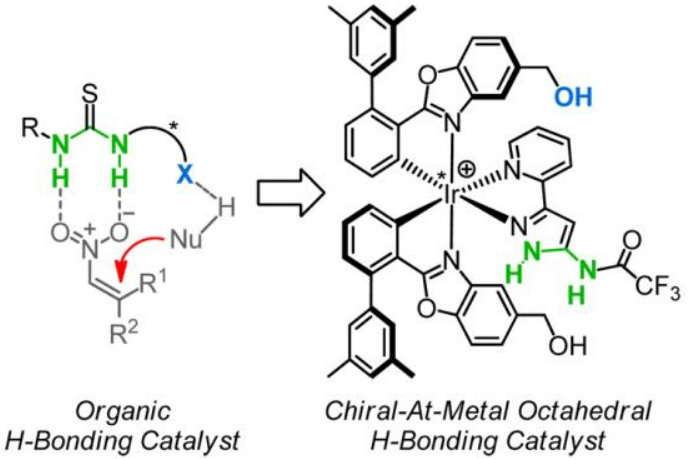
Nakamura, S. et al *Angew. Chem. Int. Ed.* **2013**, *52,* 5557

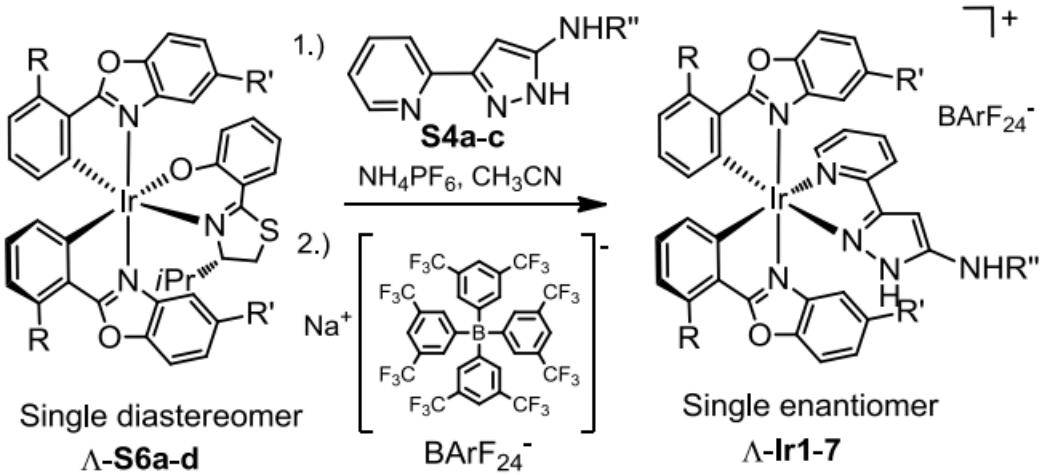
Outline

- Introduction: Noncovalent Interactions
- NCIs-Assisted Ferrocenyl Phosphine Ligands
- NCIs-Assisted Cinchona-Derived Ligands
- **NCIs-Assisted Chiral-at-Iridium Octahedral Complex**
- My Comments & Idea

NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Design and synthesis of chiral-at-iridium octahedral complex**

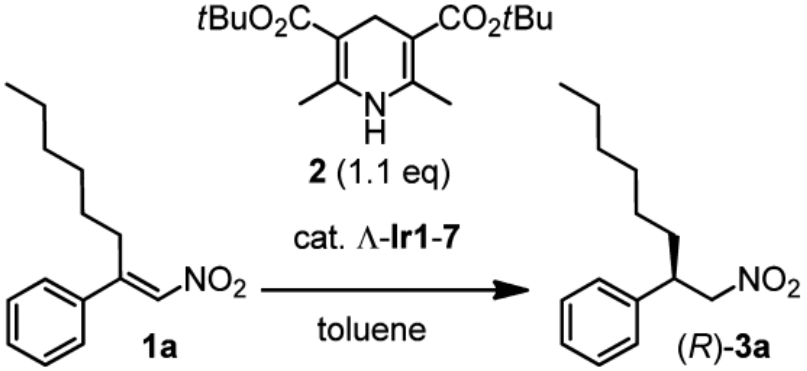




Meggers, E. et al *J. Am. Chem. Soc.* **2013**, *135,* 10598

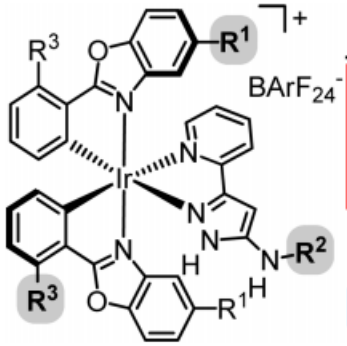
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric hydrogenation**



entry	catalyst	loading (mol %)	t (h)	conv. (%)[b]	ee (%)[c]
1	Λ-**Ir1**	20	22	92	63
2	Λ-**Ir2**	20	24	82	70
3	Λ-**Ir3**	20	20	94	84
4	Λ-**Ir4**	20	7	96	90
5	Λ-**Ir5**	20	1	100	99
6	Λ-**Ir5**	1	20	96	98
7	Λ-**Ir6**	1	14	94	99
8	Λ-**Ir7**	20	20	<20	0

[a]Reaction conditions: mixtures of **1a** (0.10 mmol), **2** (0.11 mmol), and catalyst (1–20 mol %) in toluene (0.10 mL, 1.0 M) were stirred at room temperature (18–20 °C) under argon. [b]Determined by ^{1}H NMR analysis. [c]Determined by chiral HPLC analysis.

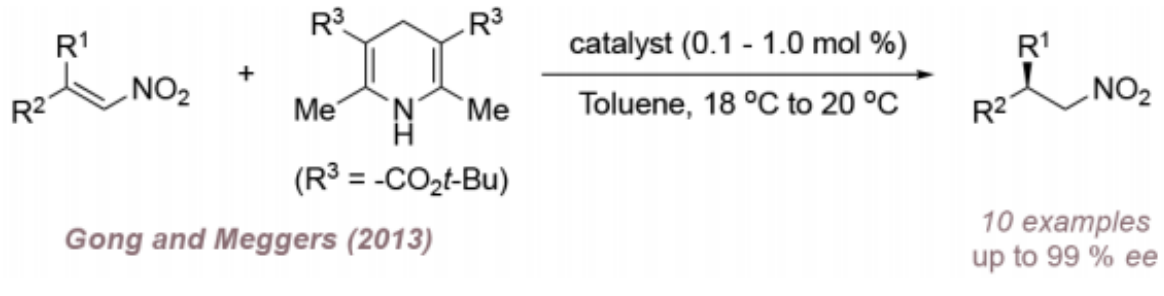


Cat	R^1	R^2	R^3
Λ-**Ir1**	CH_2OH	H	H
Λ-**Ir2**	CH_2OH	*n*Bu	H
Λ-**Ir3**	CH_2OH	Ph	H
Λ-**Ir4**	CH_2OH	$COCF_3$	H
Λ-**Ir5**	CH_2OH	$COCF_3$	Ph
Λ-**Ir6**	CH_2OH	$COCF_3$	3,5-$Me_2C_6H_3$
Λ-**Ir7**	H	Ph	H

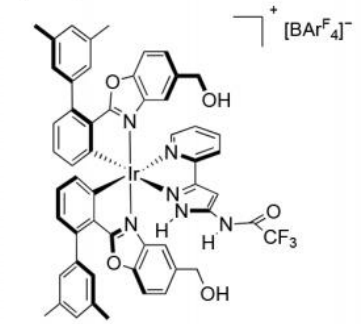
Meggers, E. et al *J. Am. Chem. Soc.* **2013**, *135*, 10598

NCIs-Assisted chiral-at-iridium octahedral complex

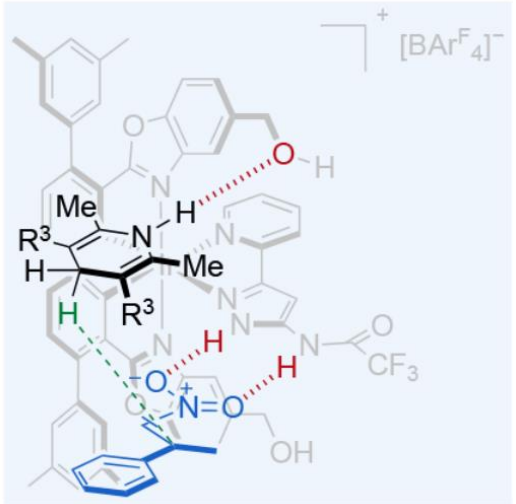
- **Chiral-at-iridium octahedral complex**
  - **Asymmetric hydrogenation**



b) catalyst



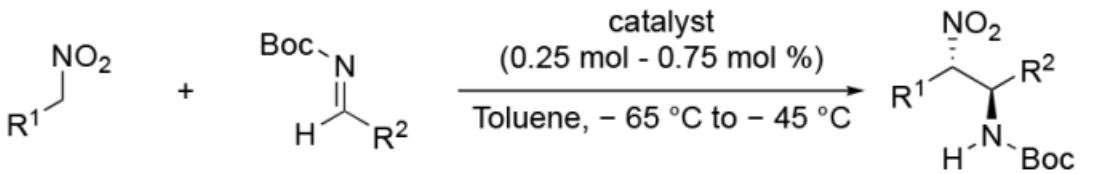
c) proposed interactions involved



Meggers, E. et al *J. Am. Chem. Soc.* **2013**, *135,* 10598

NCIs-Assisted chiral-at-iridium octahedral complex

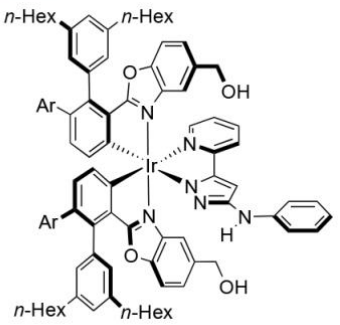
- **Chiral-at-iridium octahedral complex**
  - **Asymmetric aza-Henry reactions**



Gong and Meggers (2014)

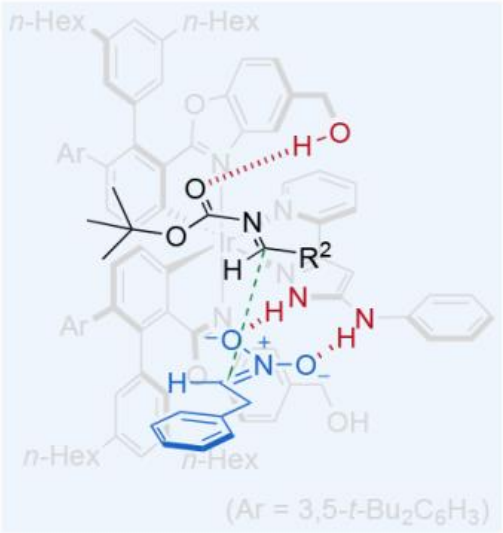
11 examples
up to 98 % ee

b) catalyst



(Ar = 3,5-*t*-$Bu_2C_6H_3$)

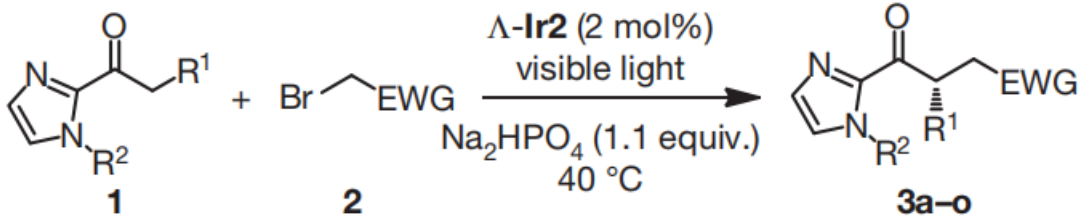
c) proposed interactions involved

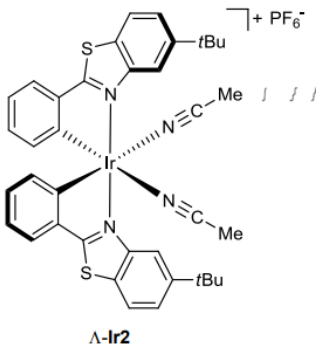


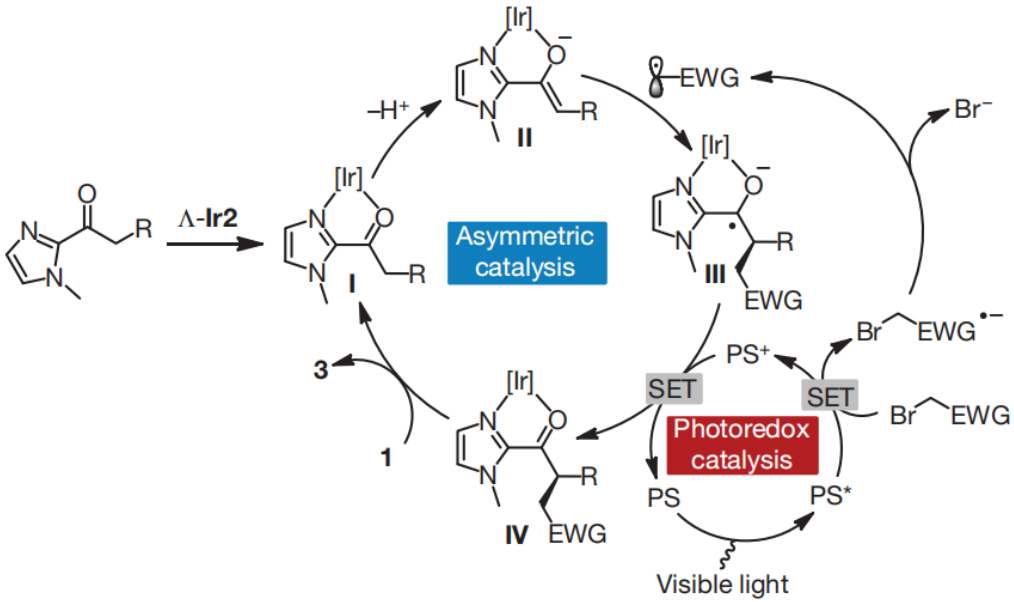
Meggers, E. et al *Nat. Commun.*. **2014**, *5*, 5431

NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric photoredox catalysis**







PS: I I

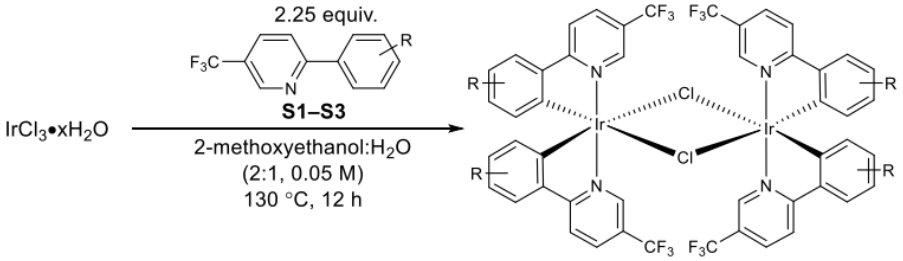
Meggers, E. et al *Nature* **2014**, *515,* 100

NCIs-Assisted chiral-at-iridium octahedral complex

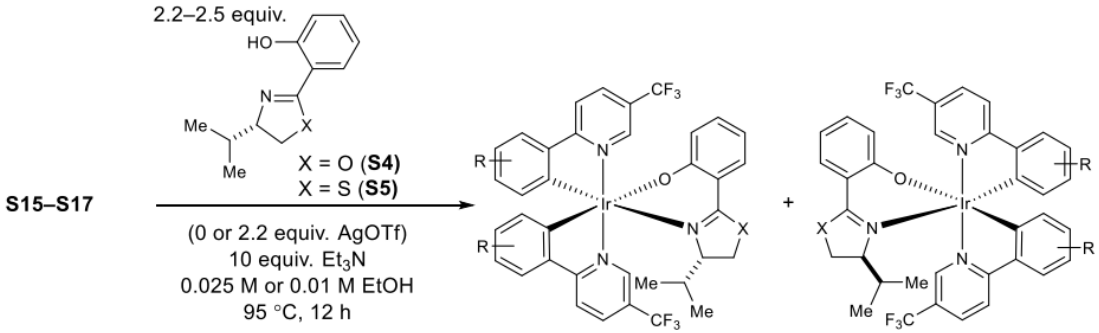
Chiral-at-iridium octahedral complex

Design and synthesis of chiral-at-iridium octahedral complex

Synthesis and Resolution of Neutral Iridium Complexes



dF(CF_3)ppy:**S15**
2,4-F/CF_3(CF_3)ppy:**S16**
tF(CF_3)ppy: **S17**



dF(CF_3)ppy, X = O:	(Λ,*S*)-**S18**	(Δ,*S*)-**S18**
dF(CF_3)ppy, X = S:	(Λ,*S*)-**S19**	(Δ,*S*)-**S19**
2,4-F/CF_3(CF_3)ppy, X = S:	(Λ,*S*)-**S20**	(Δ,*S*)-**S20**
tF(CF_3)ppy, X = S:	(Λ,*S*)-**S21**	(Δ,*S*)-**S21**

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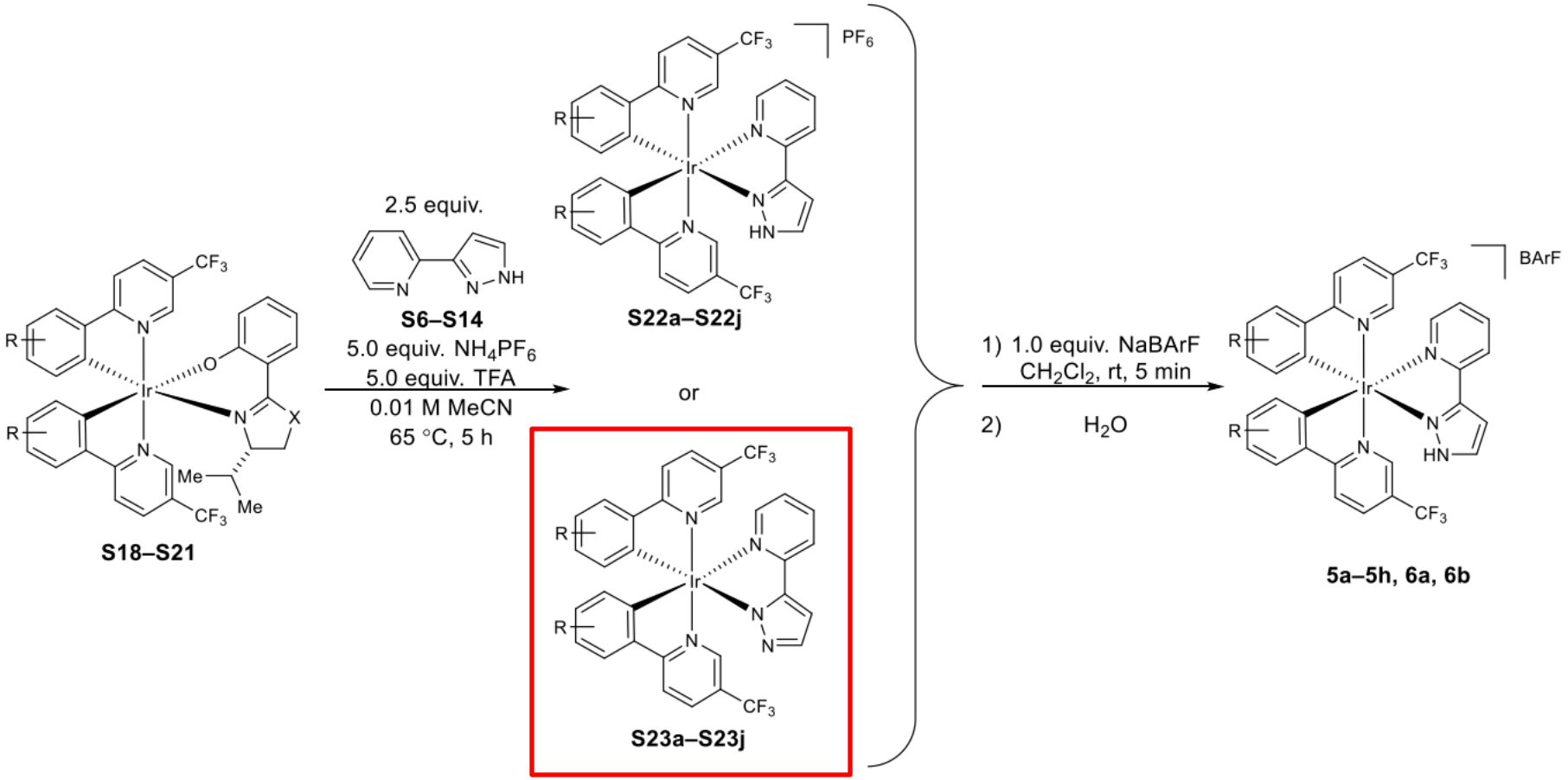
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Design and synthesis of chiral-at-iridium octahedral complex**



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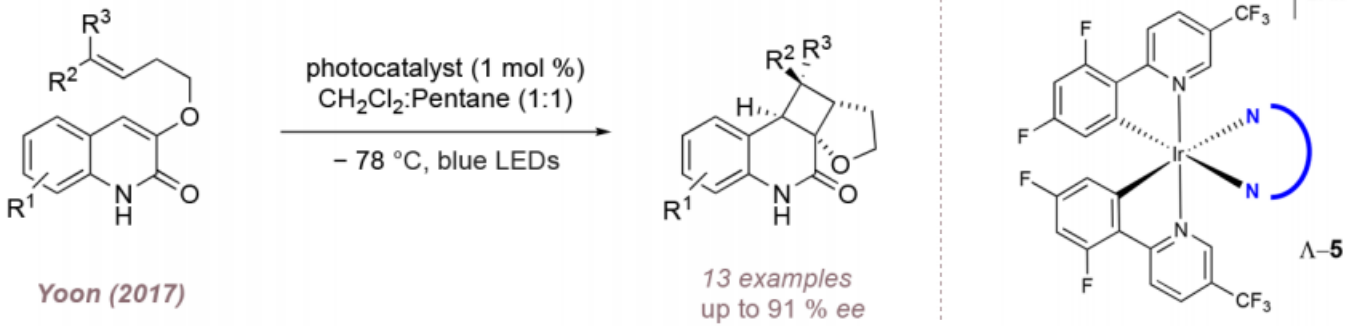
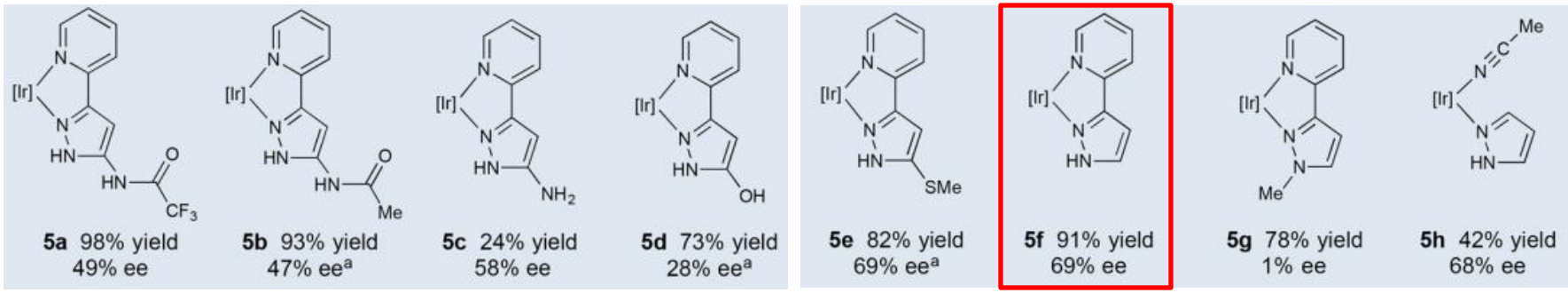
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric intramolecular [2 + 2] cycloaddition**





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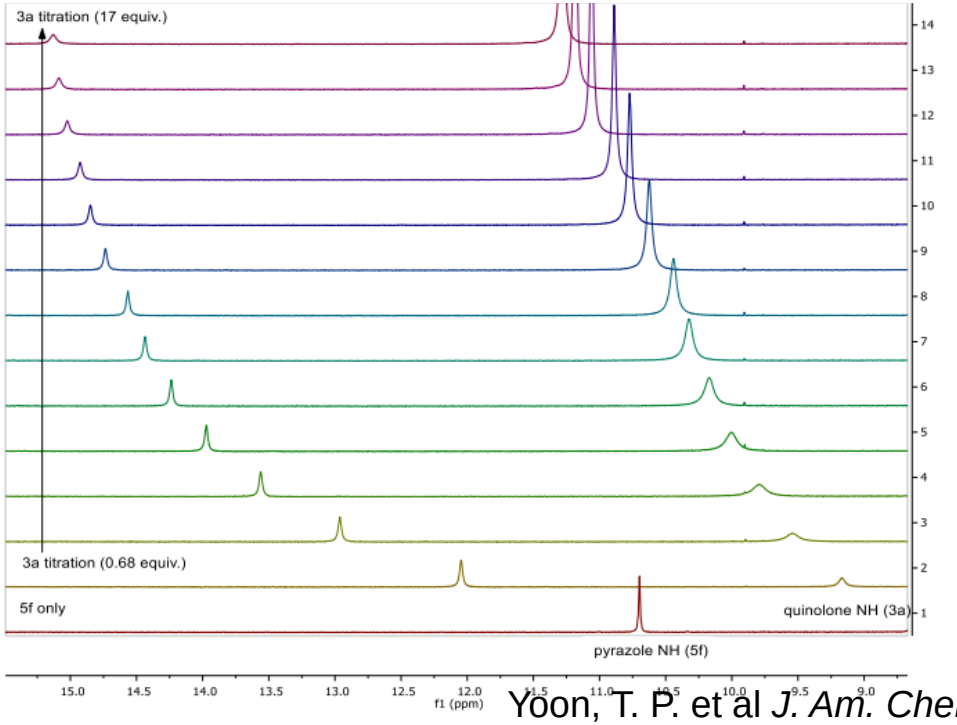
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric intramolecular [2 + 2] cycloaddition**

Titration Study of (±)-5f with 3a. A solution of (±)-**5f** (1.6 mg, 0.93 μmol, 1.0 equiv.) in CD_2Cl_2 (450 μL) was transferred to an NMR tube. Separately, a stock solution of **3a** (20.6 mg in 1.5 mL CD_2Cl_2) was prepared, and increasing amounts of this solution were titrated into the catalyst solution, acquiring ^1H NMR spectra between each titration (Figure S5). The experiment was repeated with fresh stock solutions to further probe the low-concentration region. The titration was quantified by monitoring the chemical shift of the NH proton in the catalyst, which moved downfield with increasing [**3a**]. Analogous experiments were also performed for (±)-**6b** in both CD_2Cl_2 and 1:1 CD_2Cl_2:pentane.



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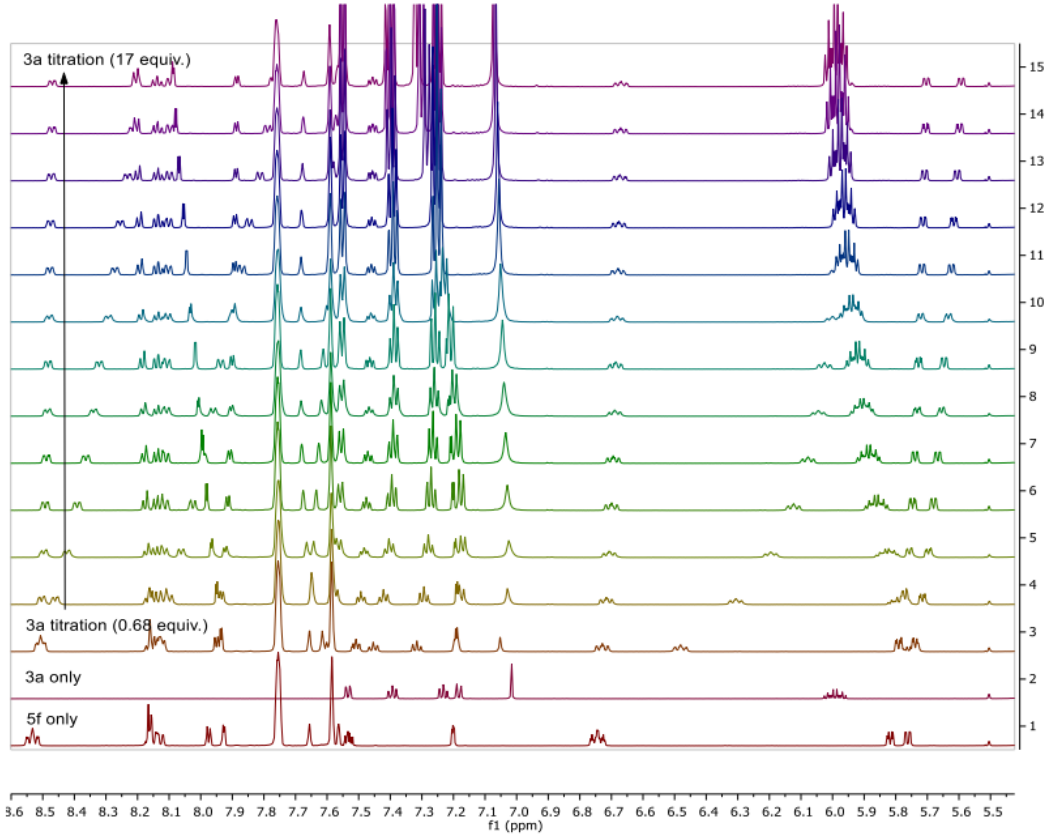
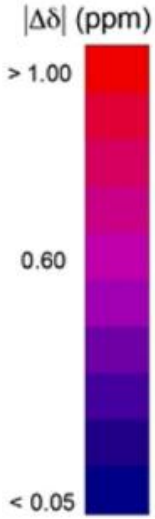
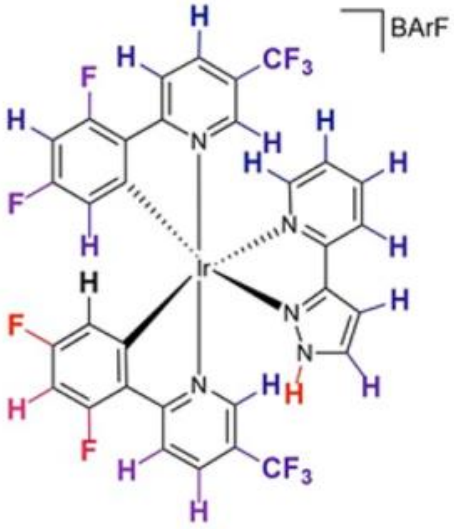
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric intramolecular [2 + 2] cycloaddition**







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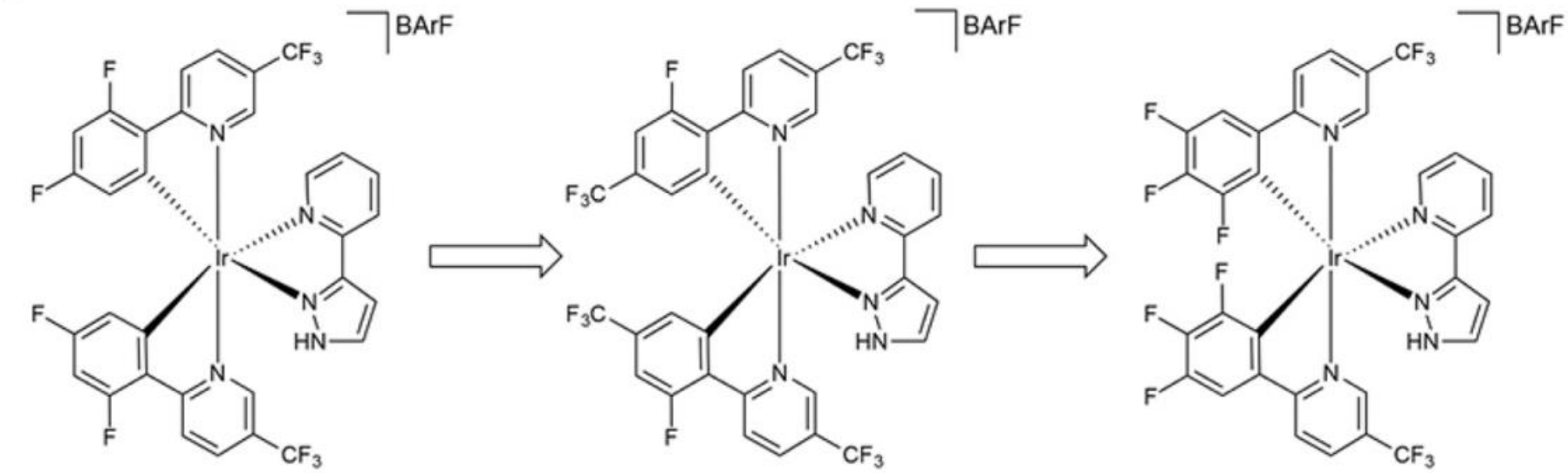
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric intramolecular [2 + 2] cycloaddition**

D



5f 91% yield
69% ee

6a 76% yield
75% ee

6b 38% yield
89% ee

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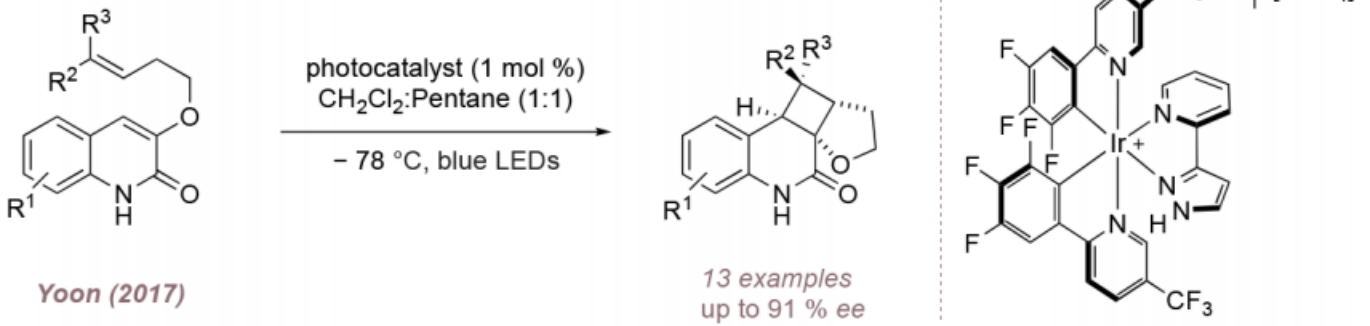
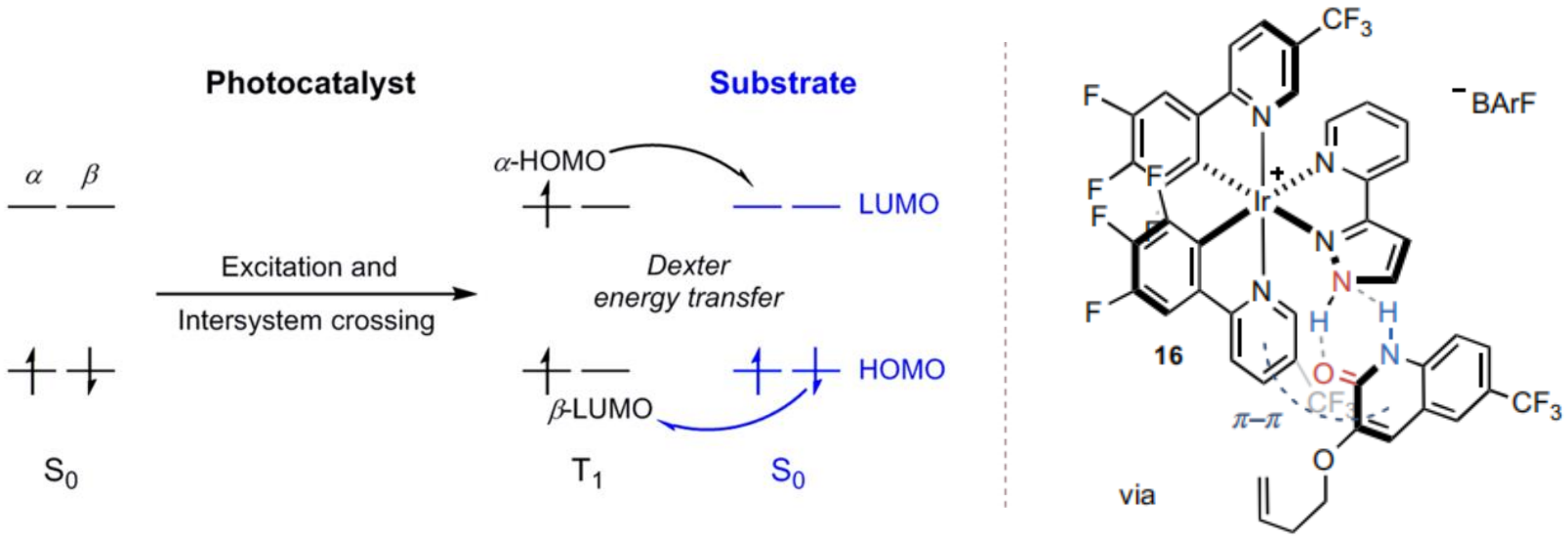
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric intramolecular [2 + 2] cycloaddition**





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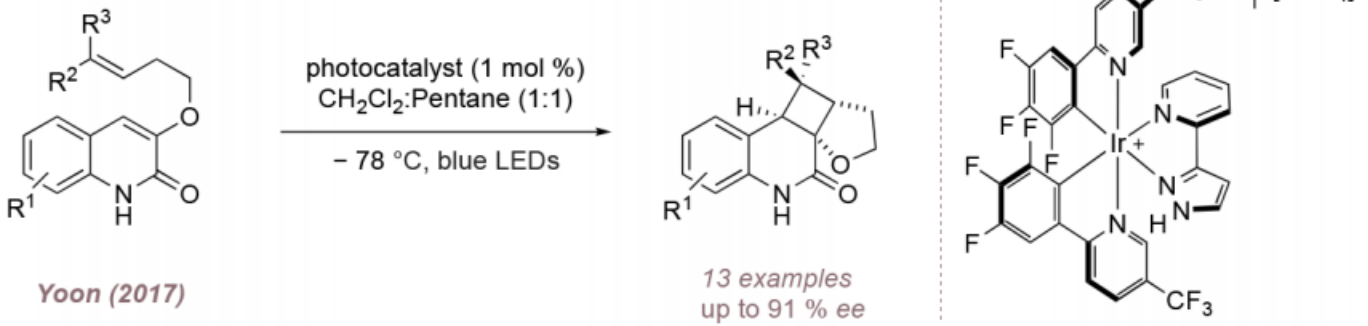
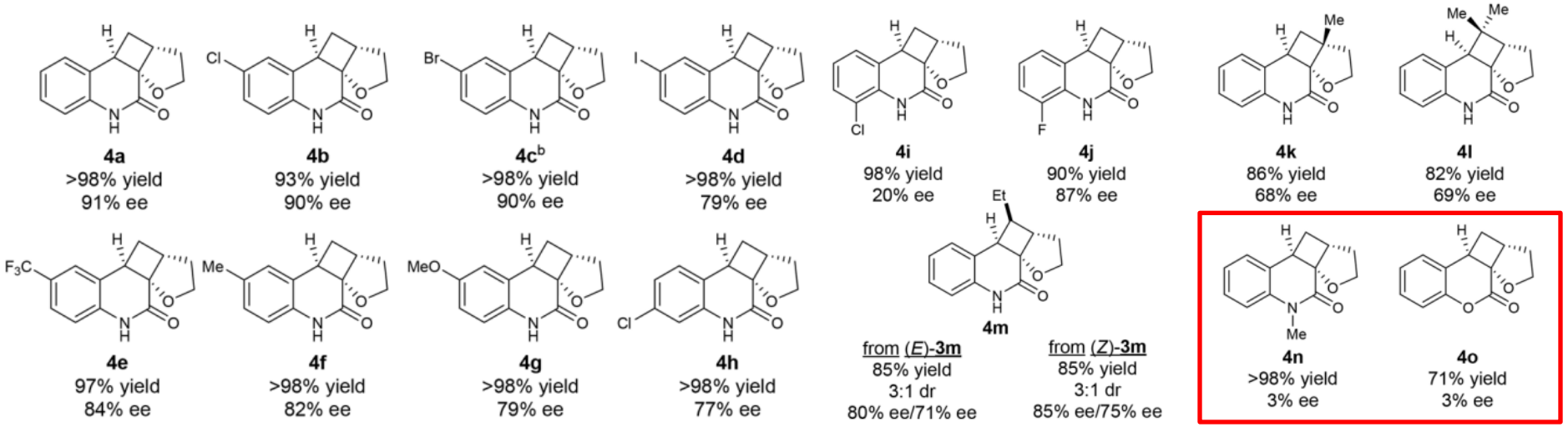
NCIs-Assisted chiral-at-iridium octahedral complex

- **Chiral-at-iridium octahedral complex**
  - **Asymmetric intramolecular [2 + 2] cycloaddition**





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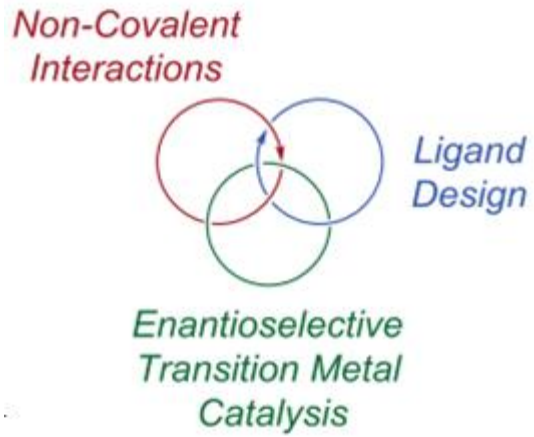
My Comments



- 在过渡金属的配体上引入非共价作用，是一种全新的策略来控制对映体的选择性。这种策略在设计配体的过程中，越来越成为一种主流的控制因素。
- 目前在配体上引入的非共价相互作用主要集中于氢键、离子相互作用。还有一些非共价相互作用值得开发：例如卤键、离子-π相互作用等。
- 目前主要是在过渡金属催化的配体上引入非共价相互作用，而像Yoon教授报道的在光催化剂上引入非共价相互作用并不多见，因此将非共价作用引入光催化领域还有很大的发展空间。

Thanks for your attention !

(图1)：从二茂铁的中轴线一端观察，如果两个取代基的优先顺序为顺时针，手性面为R_p；如果为逆时针，手性面则为S_p。在系统命名中一般以“p”表示面手性，以“P”表示的是膦手性。有时，为了避免造成混淆，当二茂铁中同时含有面手性和膦手性中心时，我们以“Fc”表示面手性。

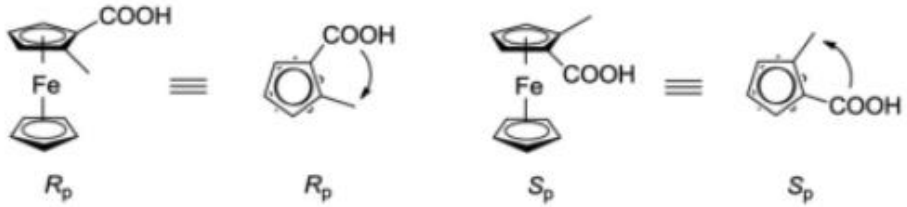
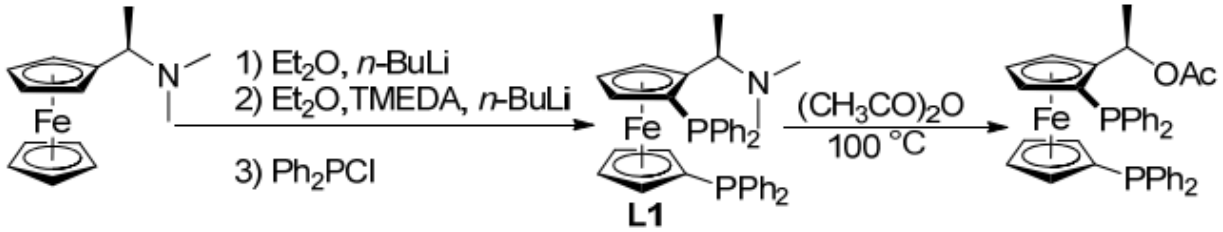
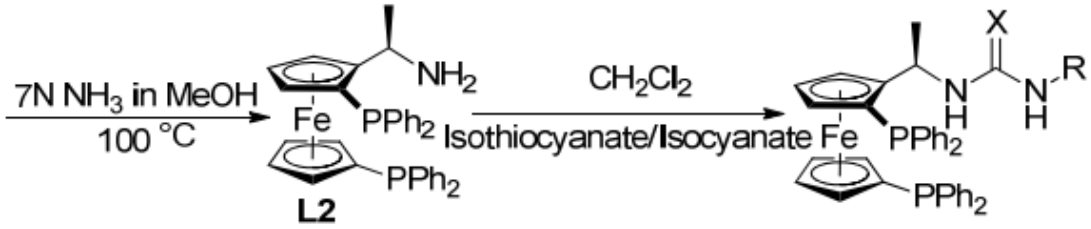
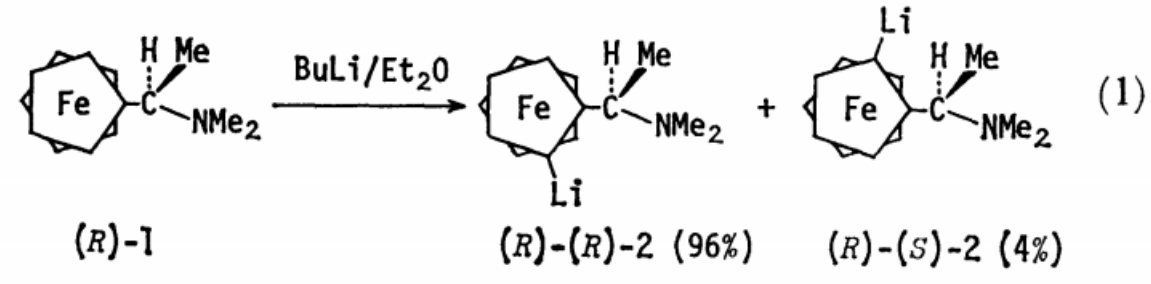
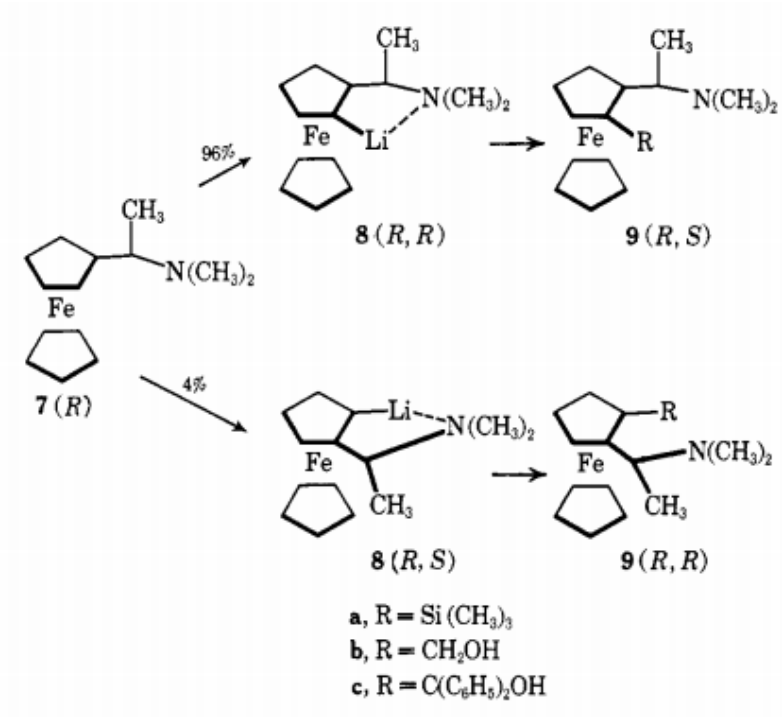


图1　二茂铁衍生物面手性的命名规则






Fe
H Me
C
NMe2
BuLi/Et2O
Li
+
(1)
(R)-1
(R)-(R)-2 (96%)
(R)-(S)-2 (4%)

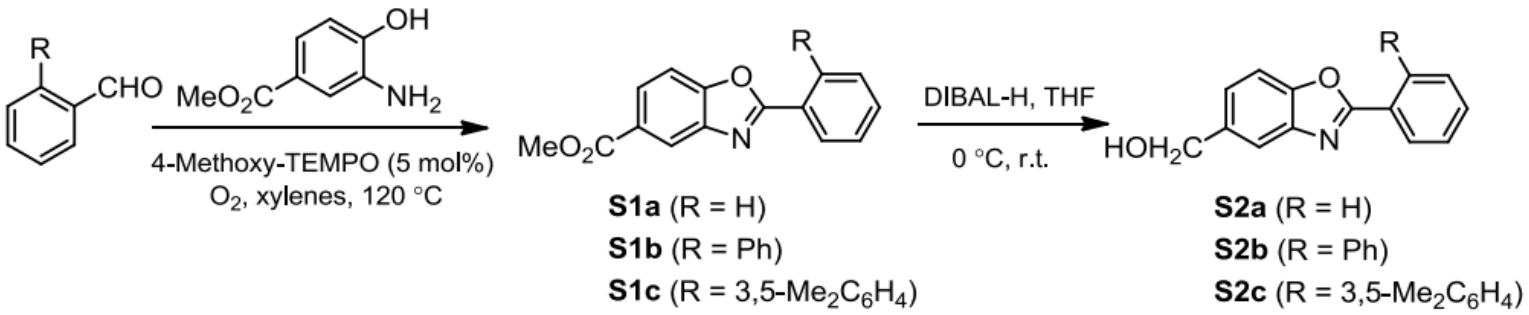

CH3
N(CH3)2
Fe
Li
R
96%
4%
7 (R)
8 (R, R)
9 (R, S)
8 (R, S)
9 (R, R)
a, R = Si (CH3)3
b, R = CH2OH
c, R = C(C6H5)2OH

8 X-Ray data for the crystal of complex 1a·AgOAc (CCDC 1493438)

Crystal growing of complex 1a·AgOAc

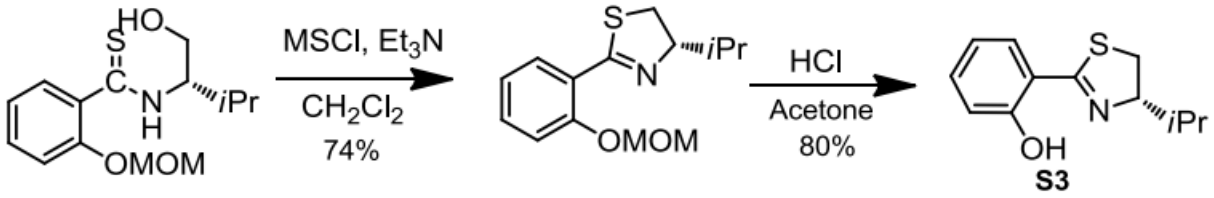
A 1:1 mixture of amino phosphine **1a** and AgOAc was dissolved in degassed CH_2Cl_2 and filtered through a microfilter to remove residual silver source. This mixture was added to a vial with a small hole in the lid to allow slow diffusion. This vial was placed within a Schlenk tube, hexane was added between the vial and the Schlenk tube, and the Schlenk tube was evacuated and purged with Argon three times. After 4 weeks in the dark at room temperature, several brown crystals of X-ray quality were present on the surface of the glass.

2.1. Synthesis of the Benzoxazole Ligands



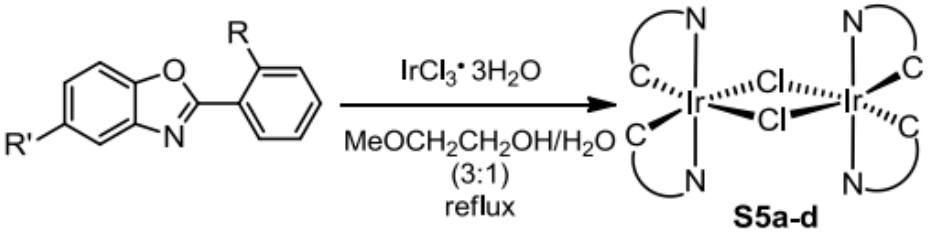
Scheme S1. Synthesis route to benzoxazole ligands.

2.2. Synthesis of the Auxiliary (*S*)-4-Isopropyl-2-(2'-hydroxyphenyl)-2-thiazoline



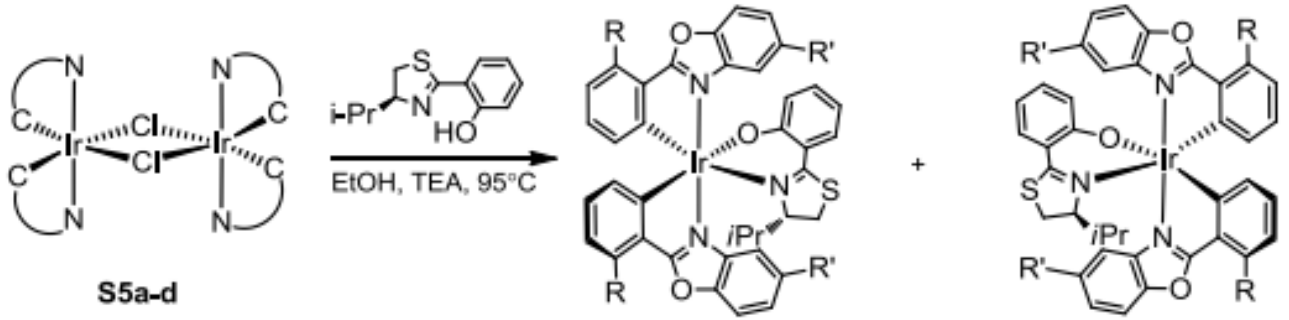
3.1. Synthesis of Iridium Complex Precursor Complexes

S2a (R = H, R' = CH_2OH)
S2b (R = Ph, R' = CH_2OH)
S2c (R = 3,5-$Me_2C_6H_4$, R' = CH_2OH)
S2d (R = H, R' = H)



S5a-d

3.2. Preparation of Iridium Auxiliary Complexes



S5a-d

Λ-**S6a** (R = H, R' = CH_2OH)
Λ-**S6b** (R = Ph, R' = CH_2OH)
Λ-**S6c** (R = 3,5-$Me_2C_6H_4$, R' = CH_2OH)
Λ-**S6d** (R = H, R' = H)

isolated for futher use

Δ-**S6a**
Δ-**S6b**
Δ-**S6c**
Δ-**S6d**

分子间作用力 (Intermolecular Forces)

Type of interaction 类型	Typical energy(kJ/mol) 作用力大小	Interacting species 分子类型
dipole-dipole 取向力	0～3	polar molecules 极性分子
Induced-dipole 诱导力	0～1	polar and nonpolar molecules 极性分子与非极性分子之间
Dispersion 色散力	8～25	all types of molecules 所有类型分子
Hydrogen bonds 氢键	5～30	N, O, F; the link is a shared H atom

化学键能约为：100～600 (kJ/mol^{-1})