

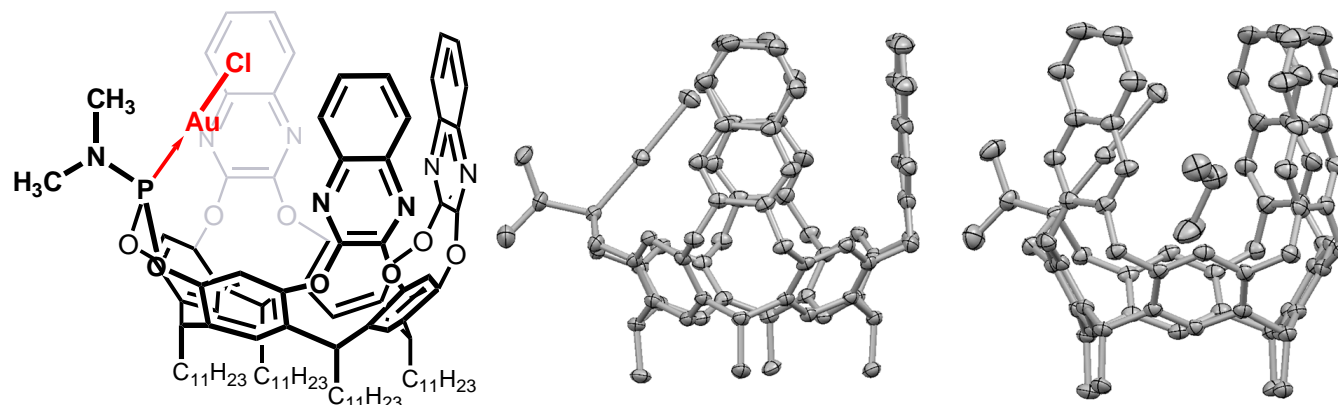
# Introverted Phosphorous-Au Cavittands for Catalytic Use

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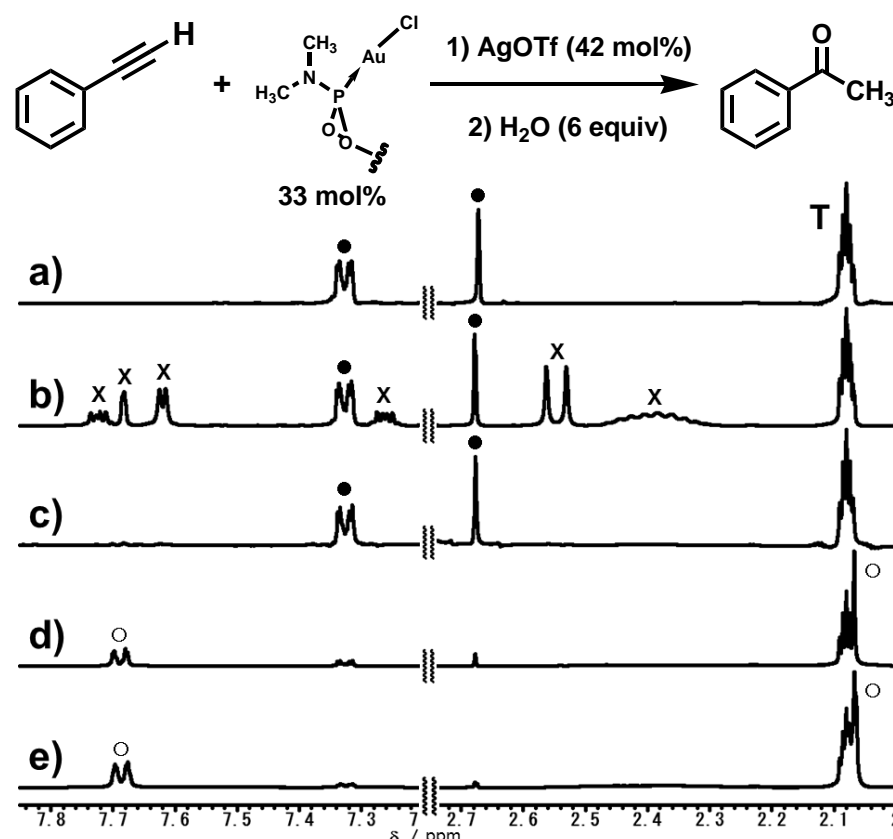
## 1. Summary Schramm, M. P.; Kanaura, M.; Ito, K.; Ide, M.; Iwasawa, T. *Eur. J. Org. Chem.* 2016, in press.



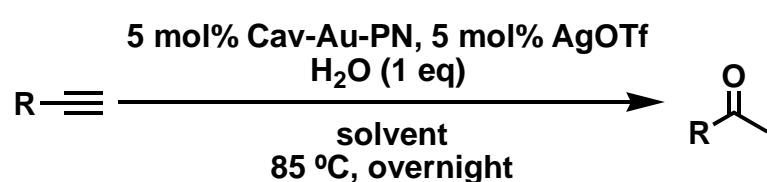
## 2. NMR chemical shifts

D-solvent	H <sup>a</sup>	H <sup>b</sup>	H <sup>c</sup>	H <sup>a'</sup>	H <sup>b'</sup>	H <sup>c'</sup>
CD <sub>2</sub> Cl <sub>2</sub>	5.32	5.66	4.57	5.64	5.76	4.55
CDCl <sub>3</sub>	5.68	5.68	4.54	5.70	5.76	4.53
[D <sub>6</sub> ]benzene	6.10	6.20	5.13	6.07	6.18	4.75
[D <sub>8</sub> ]toluene	6.04	6.12	5.02	6.05	6.09	4.74
[D <sub>10</sub> ]p-xylene	6.01	6.06	4.93	5.97	6.03	4.72
[D <sub>12</sub> ]mesitylene (5.82)	-	-	-	(5.78)	(5.54)	-

## 3. Hydration



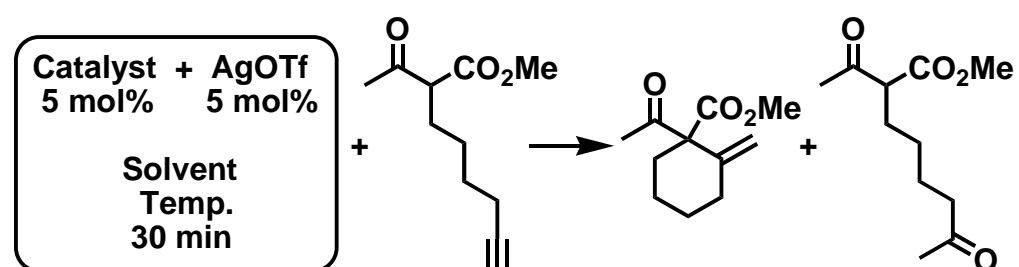
## 4. Aromatic alkynes & aliphatic alkynes



Entry	R (Ar)	Solvent	Conversion	
			1.5 h	19 h
1	Ph	[D <sub>8</sub> ]toluene	15%	43%
2	Ph	[D <sub>12</sub> ]mesitylene	14%	49%
3	1-Naphtyl	[D <sub>8</sub> ]toluene	4%	48%
4	1-Naphtyl	[D <sub>12</sub> ]mesitylene	5%	16%
5	9-Anthryl	[D <sub>8</sub> ]toluene	81%	100%
6	9-Anthryl	[D <sub>12</sub> ]mesitylene	54%	98%

Entry	R (Aliph)	Solvent	Conversion		
			1 h	4 h	16 h
1	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub>	[D <sub>8</sub> ]toluene	100%	-	-
2	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub>	CDCl <sub>3</sub> (65 °C)	25%	26%	29%
3	Ph(CH <sub>2</sub> ) <sub>2</sub>	[D <sub>8</sub> ]toluene	52%	72%	79%
4	(CH <sub>3</sub> ) <sub>3</sub>	[D <sub>8</sub> ]toluene	49%	67%	89%

## 5. Conia-Ene reaction



Entry	Catalyst	Solvent (Temp.)	Time	SM	TM	Ketone
1		[D <sub>8</sub> ]toluene (85 °C)	1 h	65%	10%	25%
			17 h	35%	34%	33%
2		CDCl <sub>3</sub> (60 °C)	1 h	69%	3%	20%
			17 h	17%	62%	28%
3		CDCl <sub>3</sub> (60 °C)	1 h	72%	3%	23%
			17 h	55%	23%	25%
4		CDCl <sub>3</sub> (60 °C)	1 h	75%	2%	23%
			17 h	42%	25%	33%