Introverted Phosphorous-Au Cavitands for Catalytic Use

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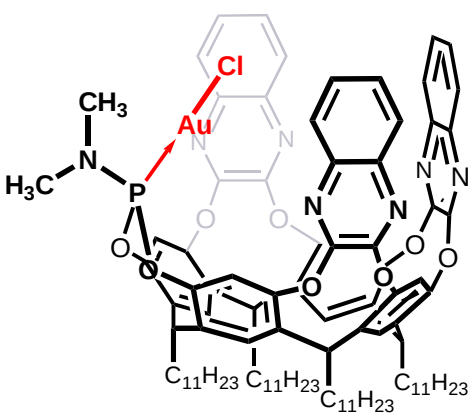
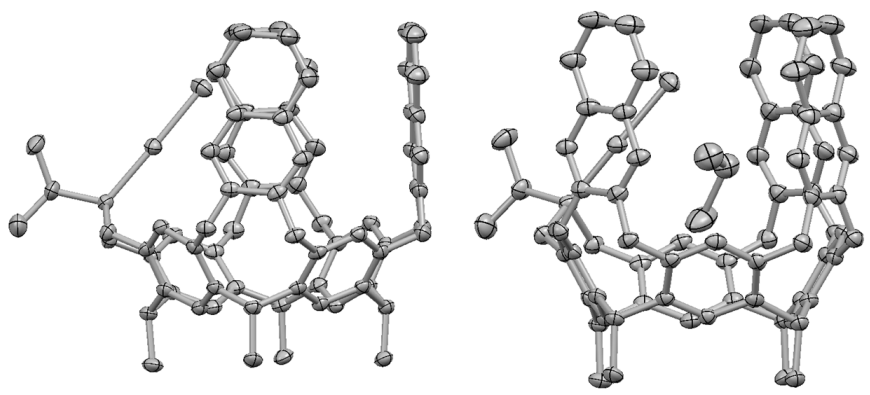
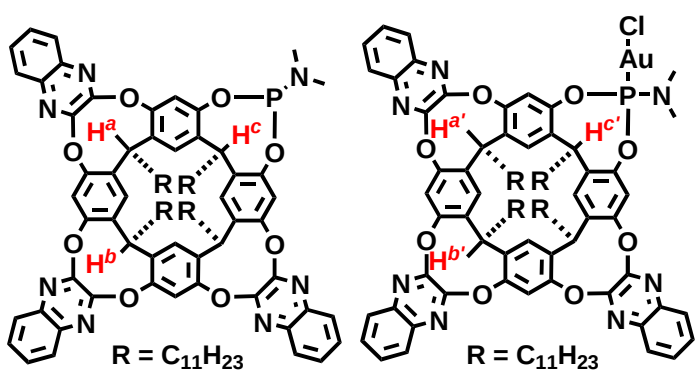
1. Summary

Schramm, M. P.; Kanaura, M.; Ito, K.; Ide, M.; Iwasawa, T. *Eur. J. Org. Chem.* 2016, 813-820.





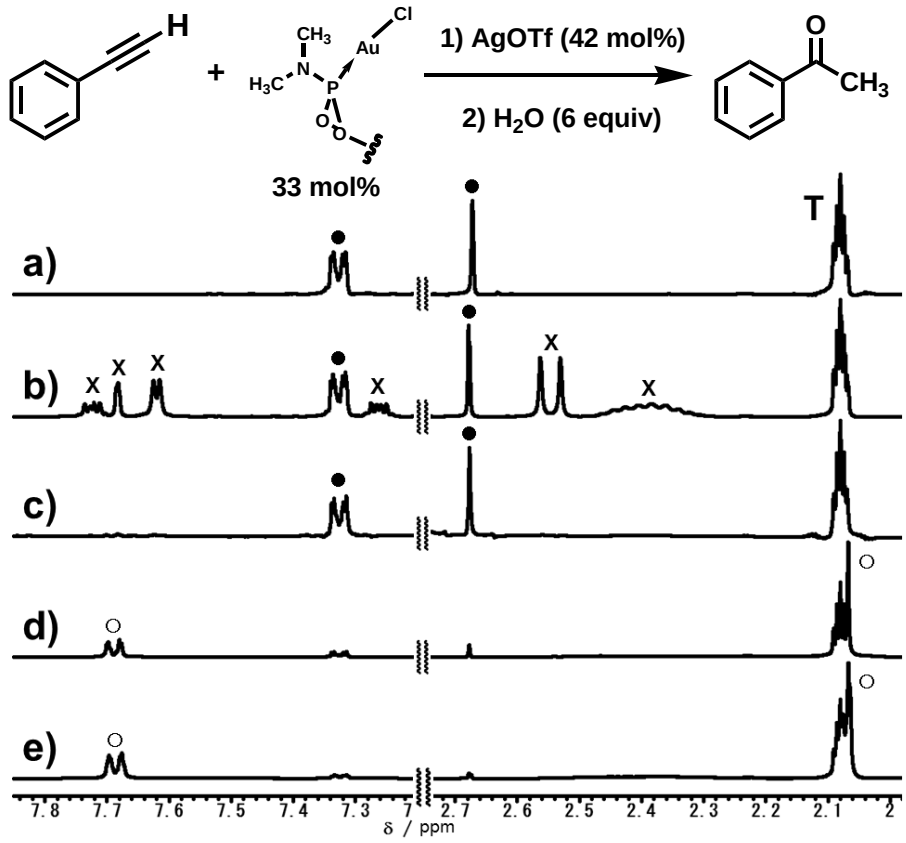
2. NMR chemical shifts



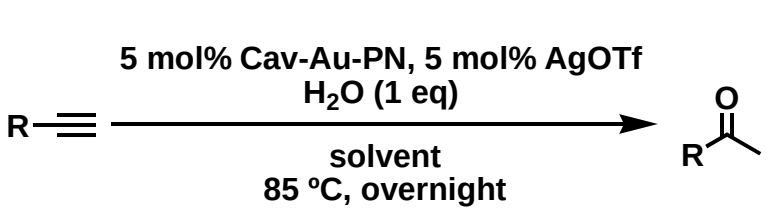
D-solvent

	H^a	H^b	H^c	$H^{a'}$	$H^{b'}$	$H^{c'}$
CD_2Cl_2	5.32	5.66	4.57	5.64	5.76	4.55
$CDCl_3$	5.68	5.68	4.54	5.70	5.76	4.53
[D_6]benzene	6.10	6.20	5.13	6.07	6.18	4.75
[D_8]toluene	6.04	6.12	5.02	6.05	6.09	4.74
[D_{10}]*p*-xylene	6.01	6.06	4.93	5.97	6.03	4.72
[D_{12}]mesitylene	(5.82)	-	-	(5.78)	(5.54)	-

3. Hydration



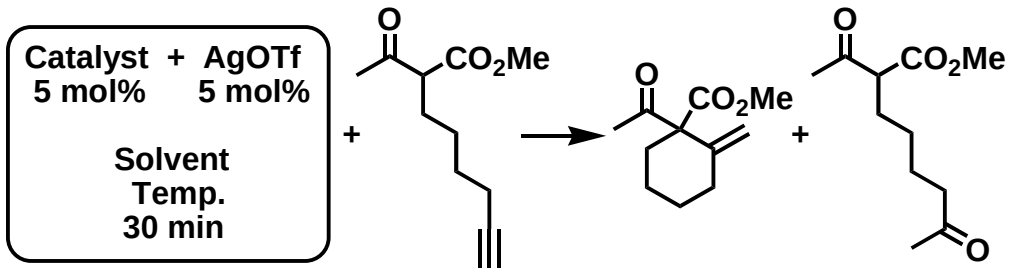
4. Aromatic alkynes & aliphatic alkynes

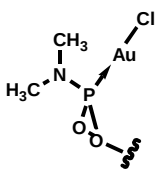
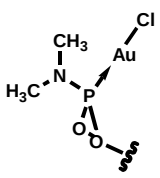
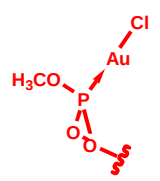
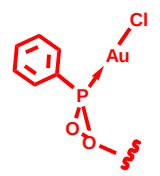


Entry	R (Ar)	Solvent	Conversion 1.5 h	Conversion 19 h
1	Ph	[D_8]toluene	15%	43%
2	Ph	[D_{12}]mesitylene	14%	49%
3	1-Naphtyl	[D_8]toluene	4%	48%
4	1-Naphtyl	[D_{12}]mesitylene	5%	16%
5	9-Anthryl	[D_8]toluene	81%	100%
6	9-Anthryl	[D_{12}]mesitylene	54%	98%

Entry	R (Aliph)	Solvent	Conversion 1 h	Conversion 4 h	Conversion 16 h
1	$CH_3(CH_2)_3$	[D_8]toluene	100%	-	-
2	$CH_3(CH_2)_3$	$CDCl_3$ (65 ℃)	25%	26%	29%
3	$Ph(CH_2)_2$	[D_8]toluene	52%	72%	79%
4	$(CH_3)_3$	[D_8]toluene	49%	67%	89%

5. Conia-Ene reaction



Entry	Catalyst	Solvent (Temp.)	Time	SM	TM	Ketone
1		[D_8]toluene (85 ℃)	1 h	65%	10%	25%
			17 h	35%	34%	33%
2		$CDCl_3$ (60 ℃)	1 h	69%	3%	20%
			17 h	17%	62%	28%
3		$CDCl_3$ (60 ℃)	1 h	72%	3%	23%
			17 h	55%	23%	25%
4		$CDCl_3$ (60 ℃)	1 h	75%	2%	23%
			17 h	42%	25%	33%