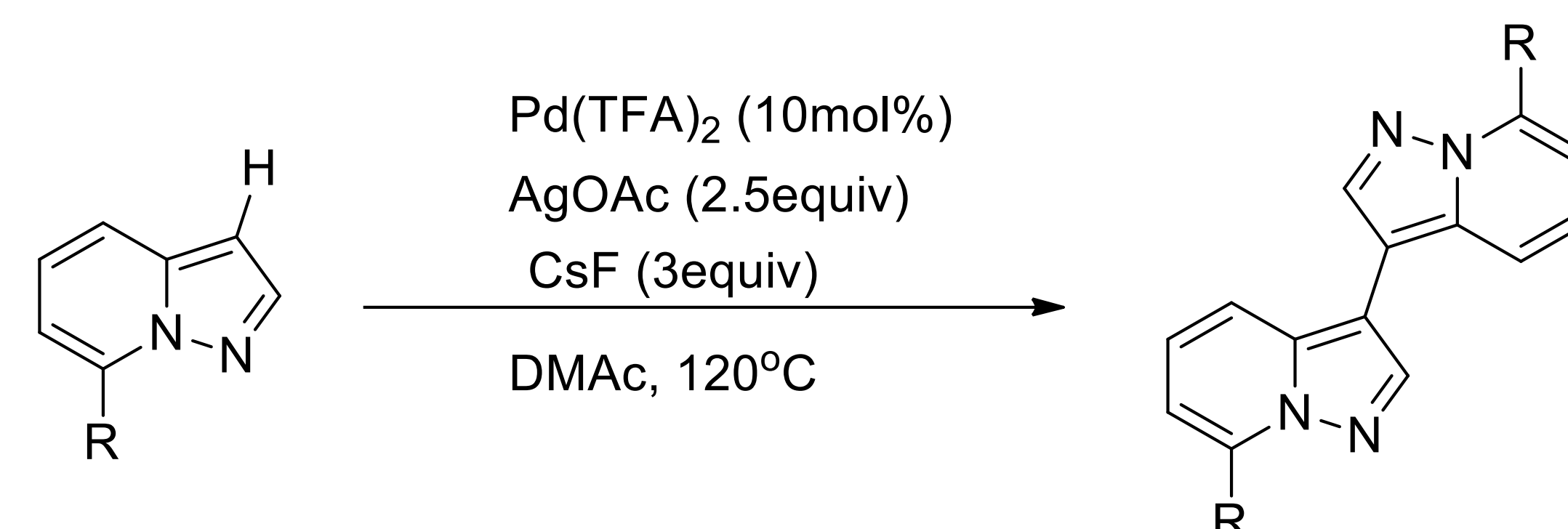


Palladium(II)-Catalyzed the Dimerization of Pyrazolo[1,5-a]pyridines via C-H Bond Activation



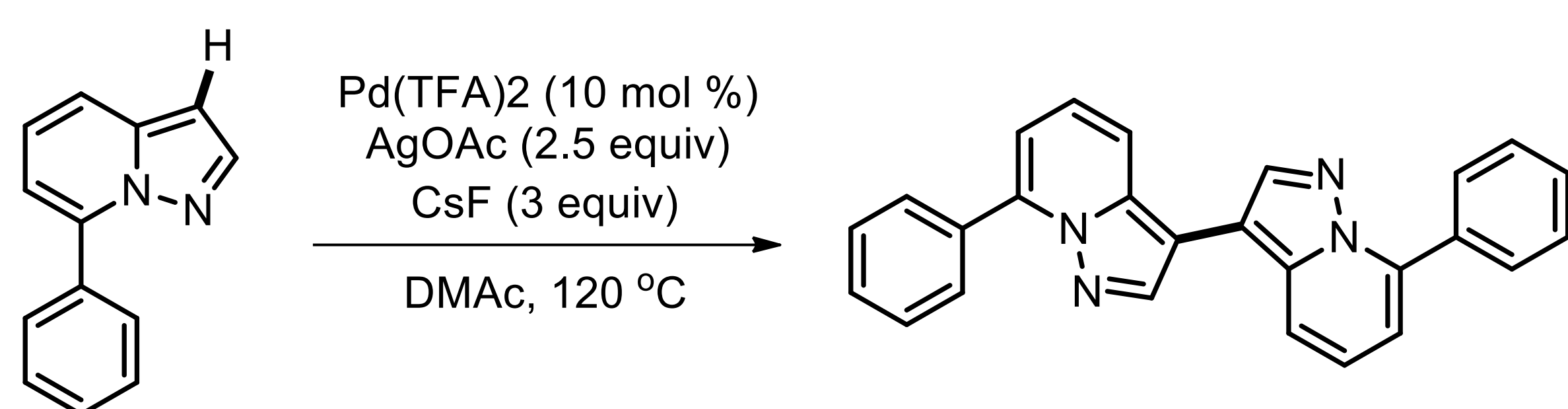
Abstract

利用鈀金屬進行碳-氫鍵活化的方式來進行Pyrazolo[1,5-a]pyridines雙聚化反應，直接經由3號碳-氫鍵來進行偶合反應進而形成各式雙聚化產物，反應具有良好官能基耐受性及產率，同時產物具有高度螢光性質。



Results

Table 1. 最佳化反應條件篩選



Entry	催化試劑	氧化試劑	鹼	溶劑	溫度	產率
1	PdCl ₂	Cu(OAc) ₂	CsF	DMAc	120°C	9%
2	Pd(TFA) ₂	Cu(OAc) ₂	CsF	DMAc	120°C	14%
3	Pd(OH) ₂	Cu(OAc) ₂	CsF	DMAc	120°C	3%
4	Pd(TFA) ₂	AgOAc	CsF	DMAc	120°C	6%
5	Pd(TFA) ₂	Ag ₂ NO ₃	CsF	DMAc	120°C	trace
6	Pd(TFA) ₂	Ag ₂ O	CsF	DMAc	120°C	3%
7	Pd(TFA) ₂	Ag ₂ CO ₃	CsF	DMAc	120°C	3%
8	Pd(TFA) ₂	O ₂	CsF	DMAc	120°C	3%

The yield was determined by ¹H NMR with 1,3,5-trimethoxybenzene as the internal standard.

Table 2. X-ray 晶體繞射結構圖

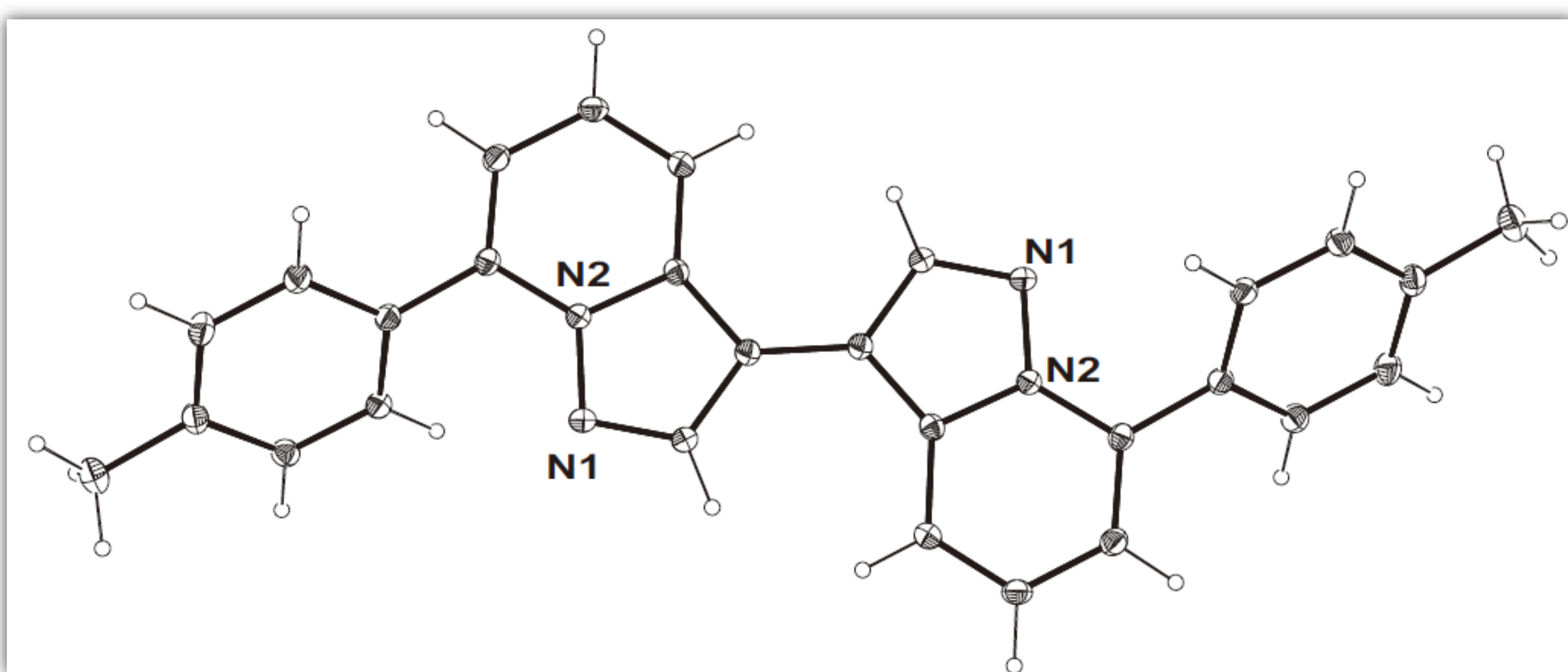
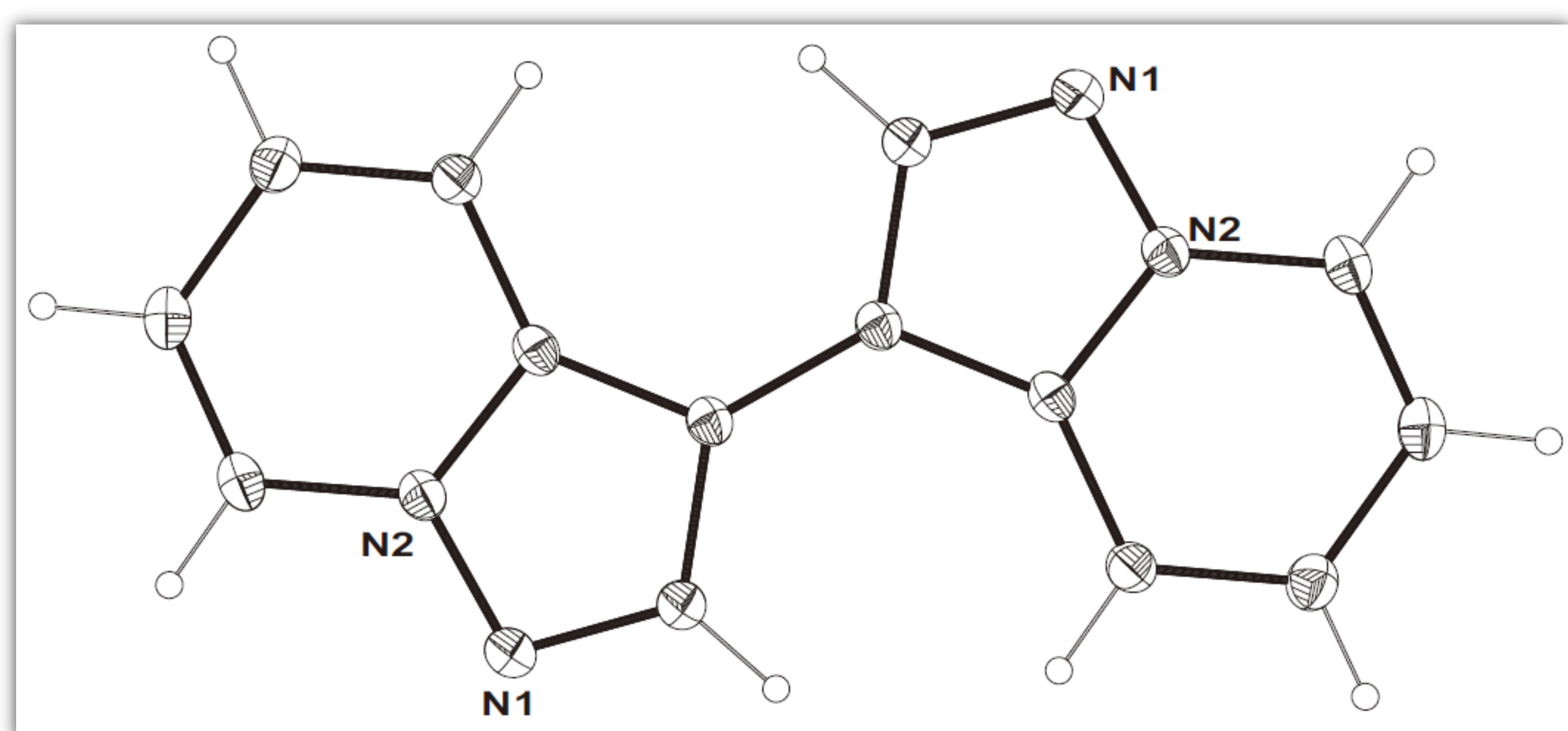


Table 3. 雙芳香基取代之Pyrazolo[1,5-a]pyridines雙聚物

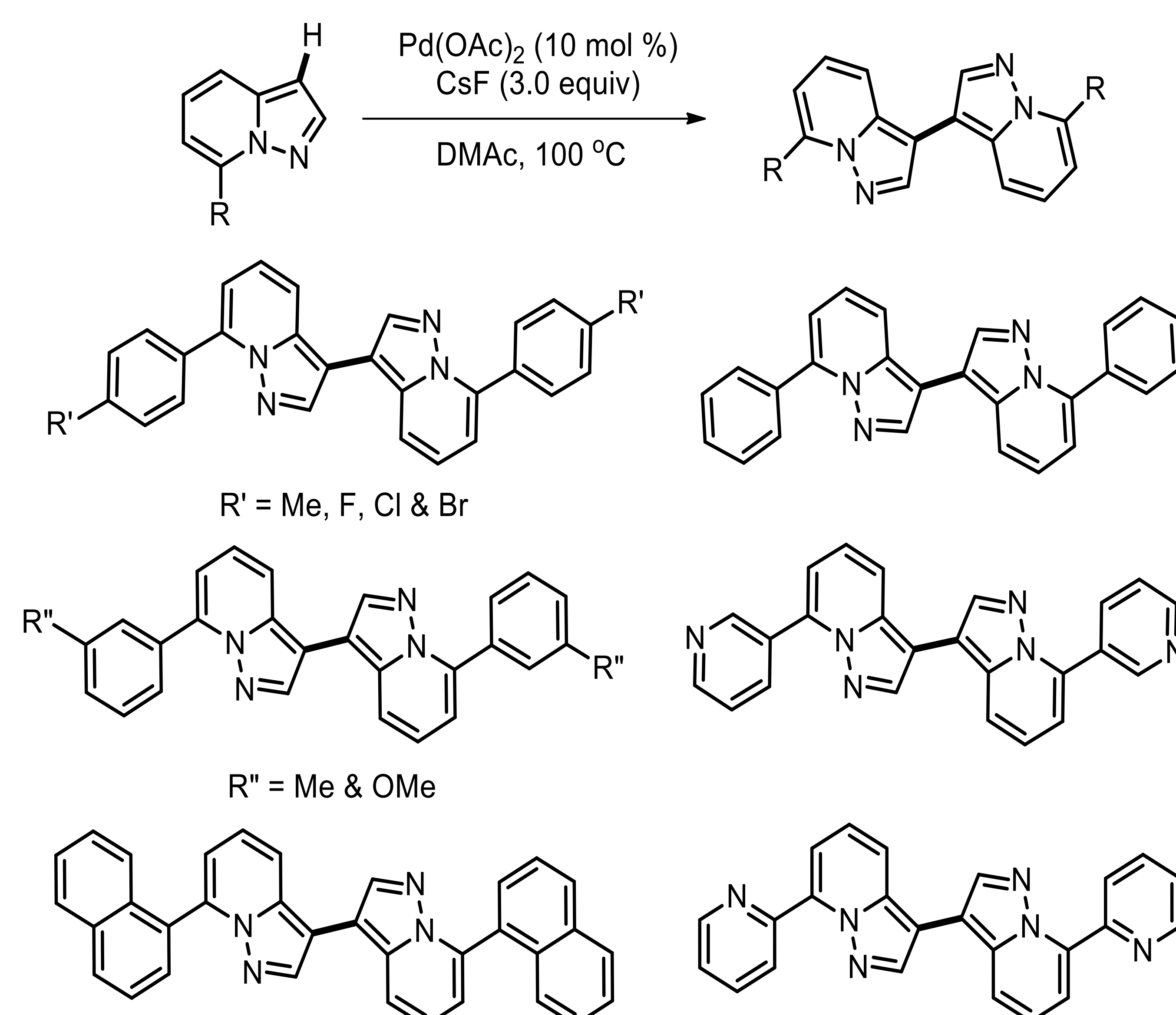
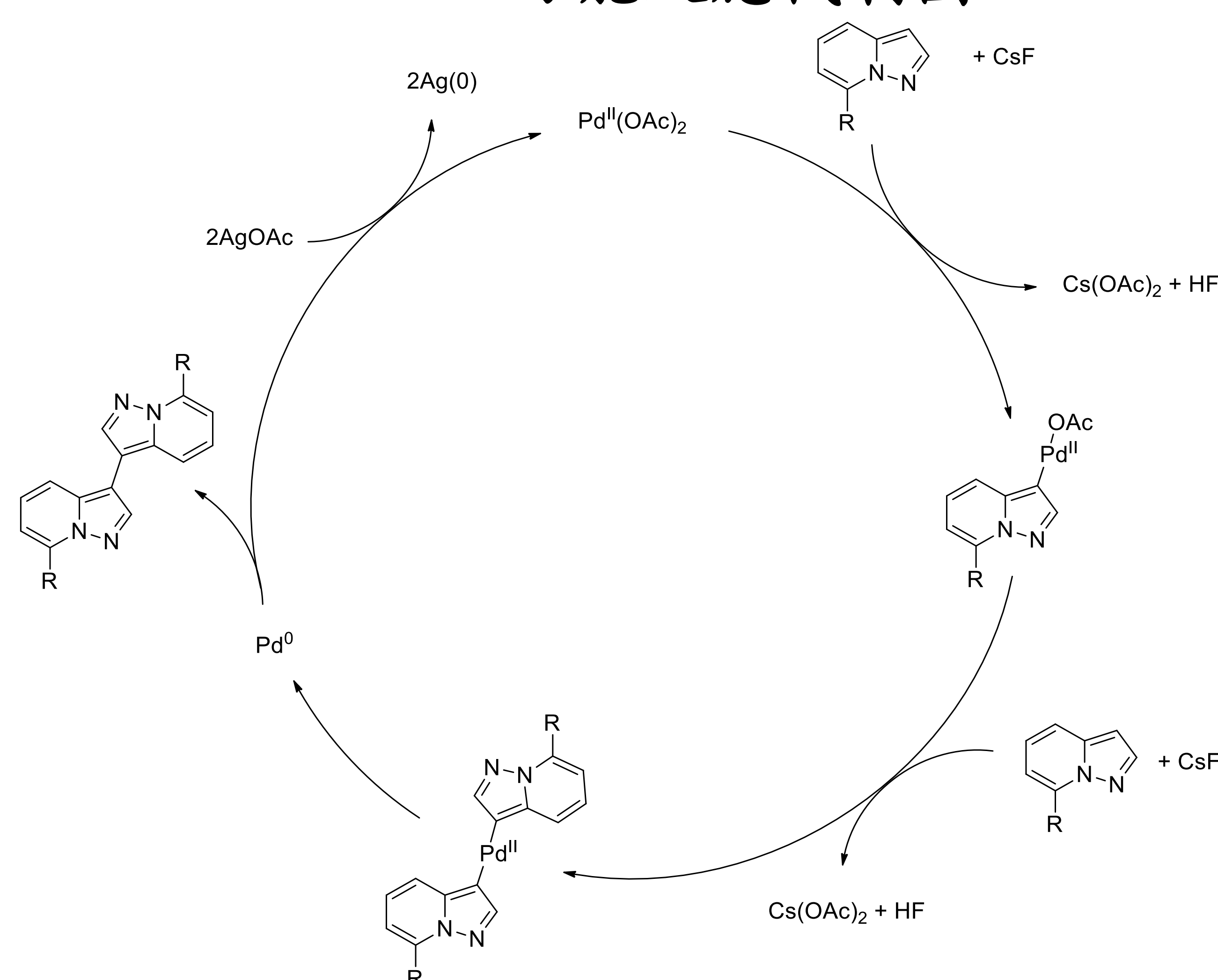


Table 4. 可能反應機制圖



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 Wang, C.-M.; Lee, L.-W.; Chang, T.-Y.; Fan, B.-L.; Wang, C.-L.; Lin, H.-M.; Lu, K.-L. *Chem. Eur. J.* 2016, 22, 16099-16102. b) Panahi, L.; Naimi-Jamal, M. R.; Mokhtari, J.; Morsali, A. *Microporous and Mesoporous Materials* 2017, 244, 208-217.