Diels-Alder in Aqueous Molecular Hosts: Unusual Regioselectivity and Efficient Catalysis

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ERRATUM

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Reports: "Diels-Alder in aqueous molecular hosts: unusual regioselectivity and efficient catalysis" by M. Yoshizawa *et al.* (14 Apr. 2006, p. 251). Due to a nomenclature error, all references to "phthalimides" in the text and Supporting Online Material should instead refer to "maleimides." The chemical structures in the schemes and figures are all correct as drawn.

Fig. 1. Self-assembled coordination cages (1 and 2), which are prepared by simple mixing of an exo-tridentate organic ligand and an end-capped Pd(II) ion in a 4:6 ratio in water.

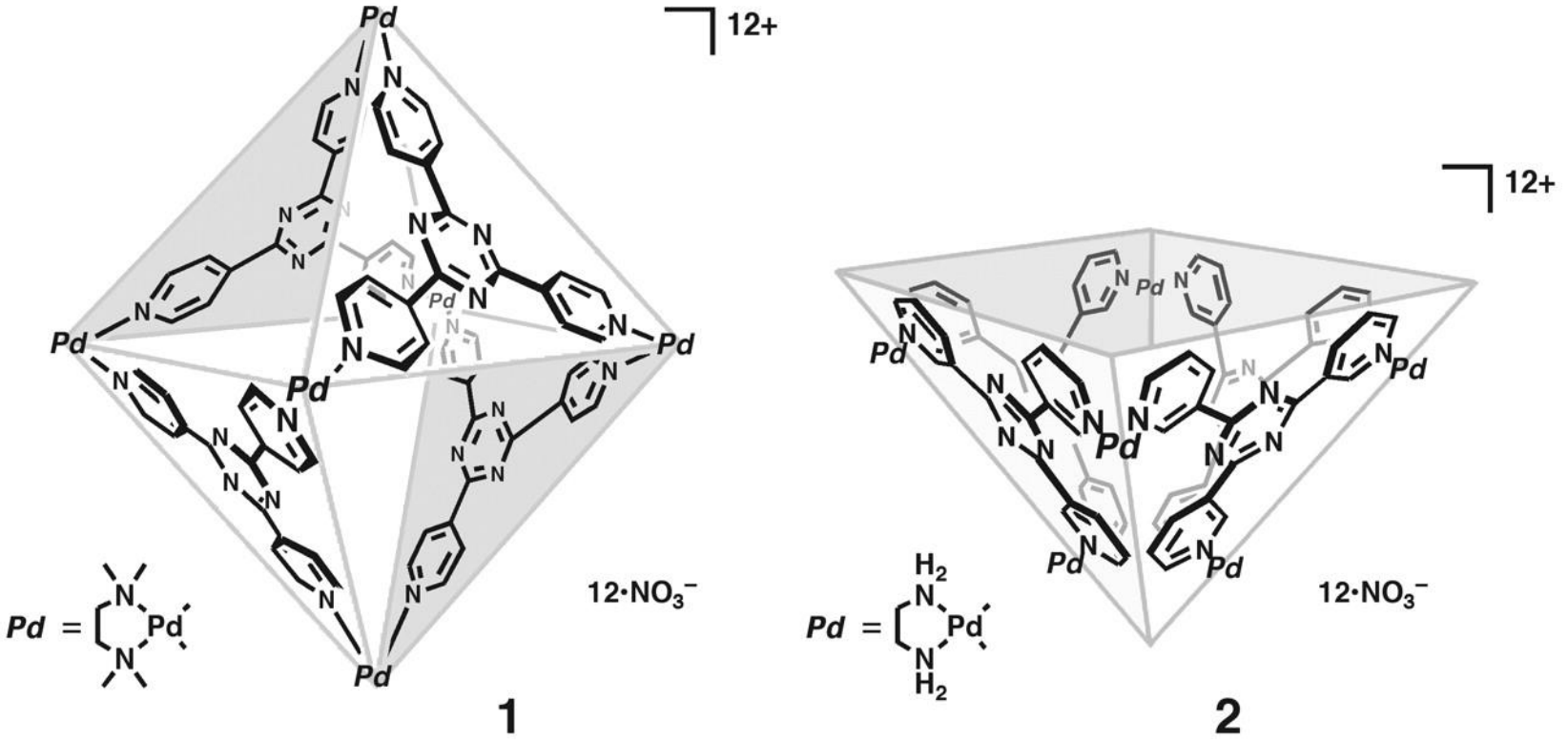
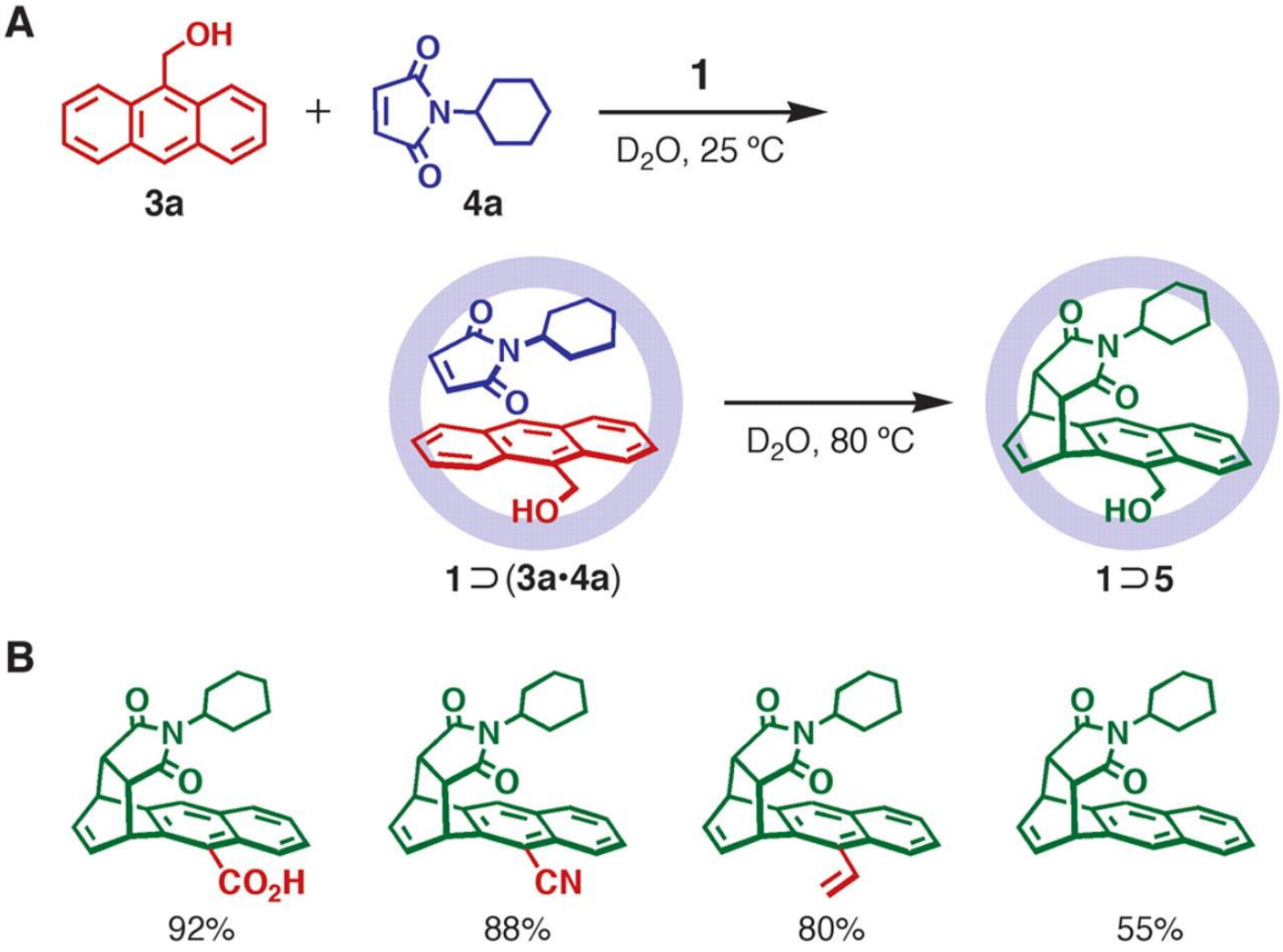


Fig. 2. (A) Pair-selective encapsulation of two types of reactants, 9-hydroxymethylanthrancene (3a) andN-cyclohexylphthalimide (4a), within cage 1 and the subsequent Diels-Alder reaction leading to syn isomer of 1,4-adduct 5 within the cavity of 1.



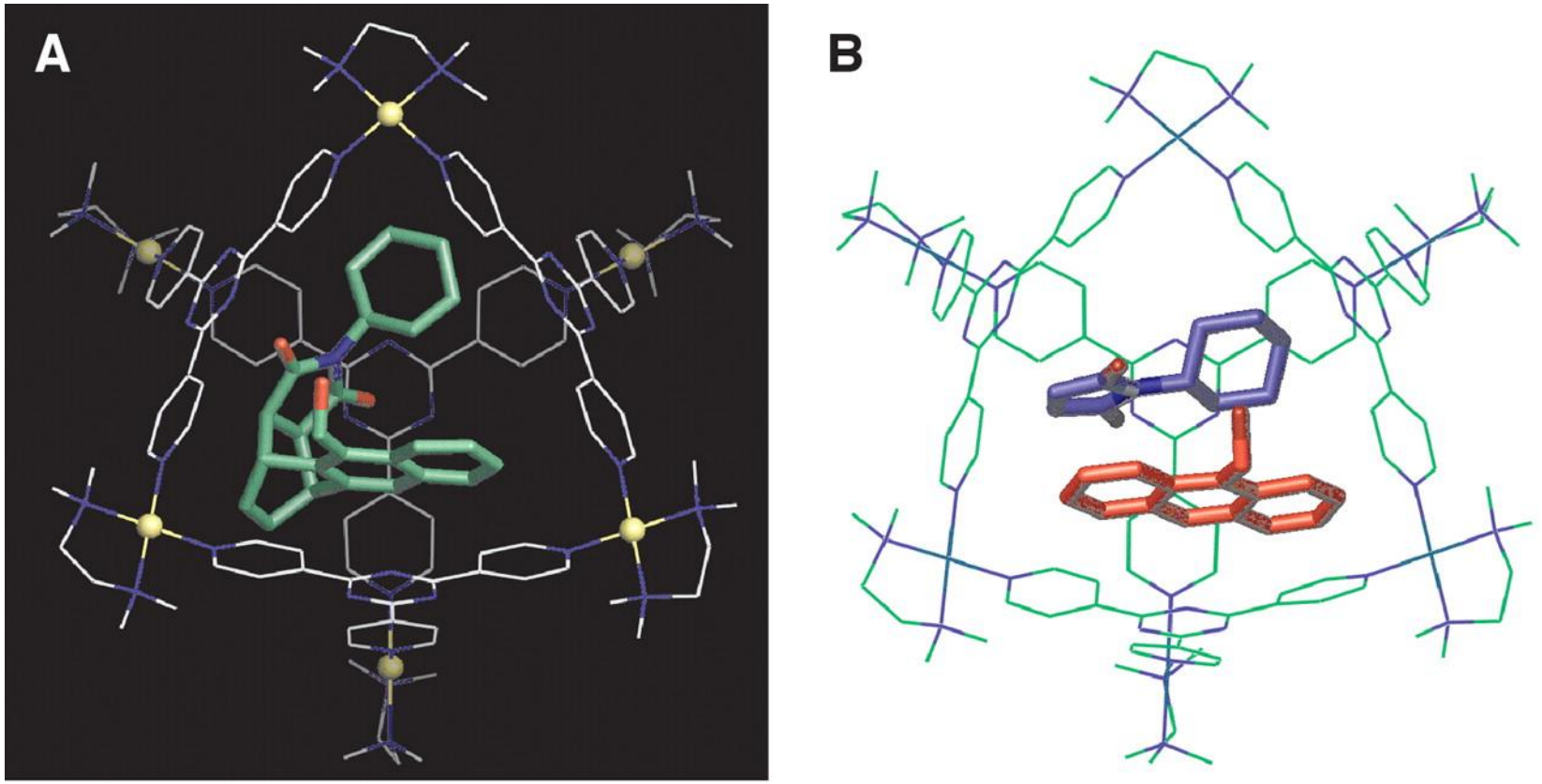
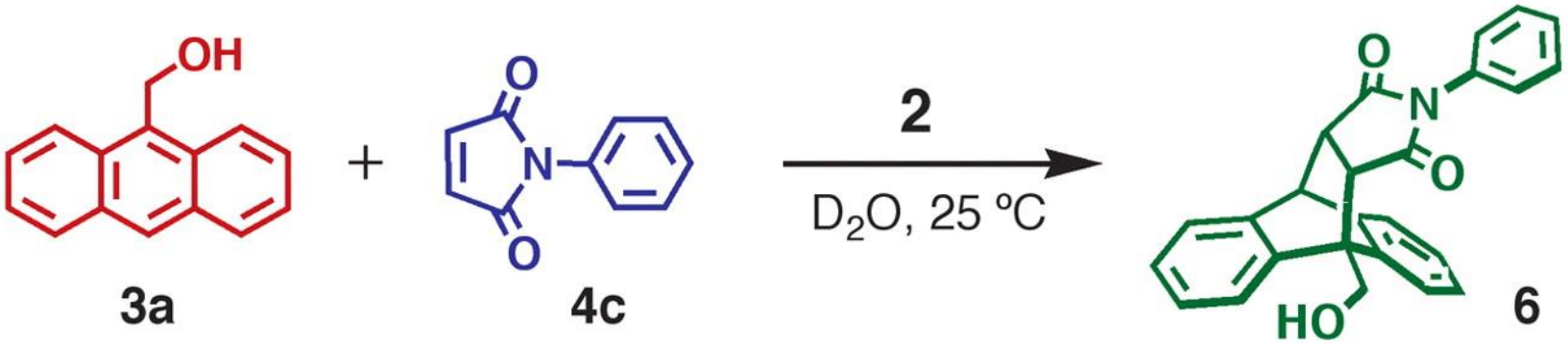

A
B

Fig. 4. Catalytic Diels-Alder reaction of 9-hydroxymethylanthracene (3a) and N-phenylphthalimide (4c) in the aqueous solution of bowl 2, leading to 9,10-adduct 6.



3a 4c 6

Fig. 5. The 1H NMR spectra (500 MHz, room temperature) of the catalytic Diels-Alder reaction of 9-hydroxymethylanthrancene (3a) and N-phenylphthalimide (4c) in an aqueous solution of bowl 2.

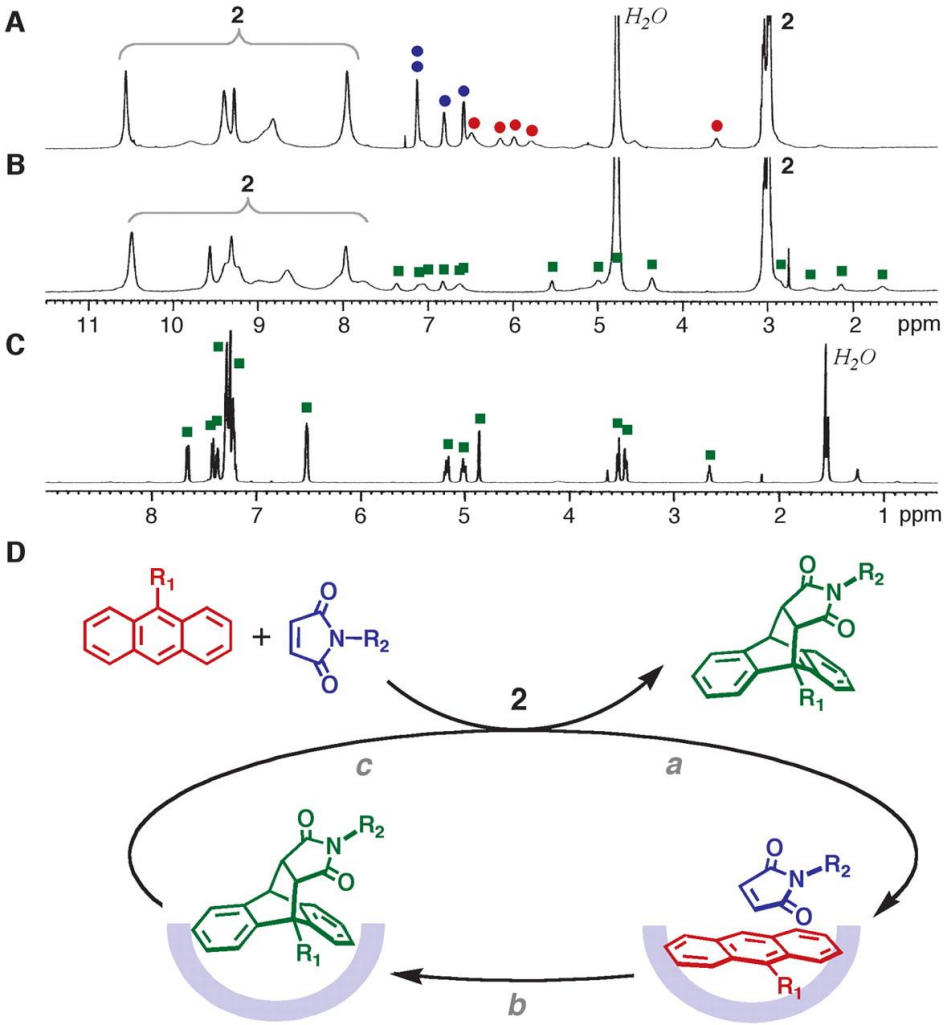
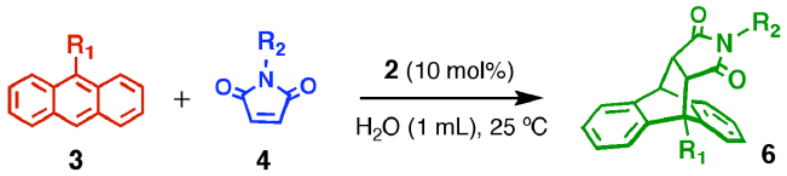


Table S1. Catalytic Diels-Alder reaction of **3** and **4** in the presence of **2** (10 mol%) in H_2O (1 mL) and control experiments in H_2O or $CDCl_3$ (1 mL) without **2**.



3 + **4** → **6**

Entry	Substrate		Time	Yield(%) of **6**		
	3 (R_1)	**4** (R_2)		with **2**	without **2**	in $CHCl_3$[†]
1	$-CH_2OH$	propyl	5 h	>99	8	0
2	$-CH_2OH$	cyclohexyl	15 h	98	0	6
3	$-CH_2OH$	phenyl	5 h	>99[*,†]	3	9
4	$-CH_2OH$	phenyl	15 h	6	7	21
5	$-CH_2OH$	benzyl	5 h	>99	trace	0
6	$-CH_2OH$	xylyl	15 h	94	0	17
7	$-CH_3$	cyclohexyl	7 h	>99	0	5
8	$-CH_3$	phenyl	3 h	>99	5	17
9	$-CH{=}CH_2$	phenyl	1 d	88	0	trace
10	$-CH{=}CH_2$	benzyl	1 d	97	5	4
11	$-CO_2H$	benzyl	1 d	12	0	0
12	$-CH_2OH$	phenyl	1 d	>99[‡]	—	—

[*] $(en)Pd(NO_3)_2$: 10 mol% [†] without **2** [‡] **2** : 1 mol%, hexane (1 mL)