

Electronic Supplementary Information (ESI) for

Homochiral Association of Binuclear *trans*-Bis(β -iminoaryloxy)palladium(II) Complexes Doubly Linked with *m*-Xylylene Spacers: Drastic Linker-Dependence of the Association Chirality of Chiral Clothespin-Shaped Molecules

Masaya Naito,^a Naruyoshi Komiya^b and Takeshi Naota^{*a}

^aDepartment of Chemistry, Graduate School of Engineering Science, Osaka University, Machikaneyama, Toyonaka, Osaka 560-8531, Japan

^bChemistry Laboratory, The Jikei University School of Medicine, Kokuryo, Chofu, Tokyo 182-8570, Japan

Table of Contents

Fig. S1	NOESY spectrum of 2 (500 MHz, CDCl ₃ , 298 K, mixing time = 0.700 s).	S2
Fig. S2	¹ H NMR spectra of 2 and 4 (500 MHz, CDCl ₃ , 298 K).	S3
Fig. S3	ORTEP representations of (<i>R</i>)- 3 and (<i>R</i>)- 4 as their racemic crystals.	S4
Fig. S4	¹ H NMR spectra of (±)- 1 and (±)- 2 at 188–223 K (400 MHz, toluene- <i>d</i> ₈ , 1.0×10 ⁻³ M).	S5

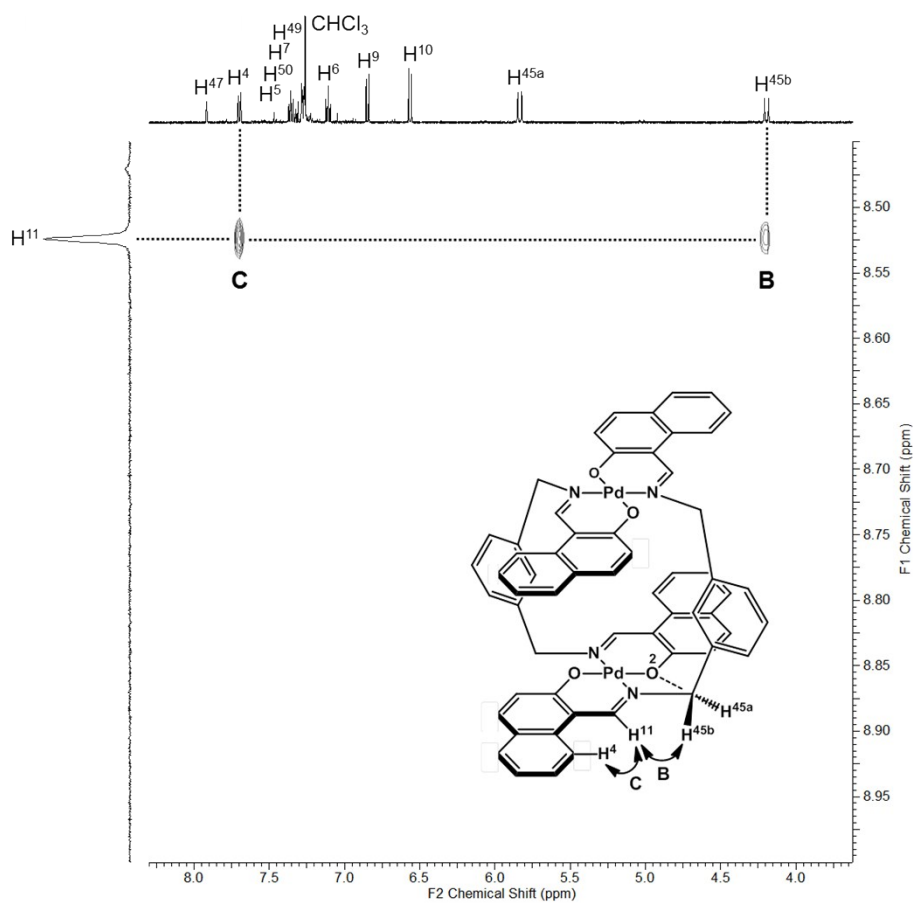


Fig. S1 NOESY spectrum (500 MHz) of **2** in CDCl_3 (298 K, mixing time = 0.700 s).

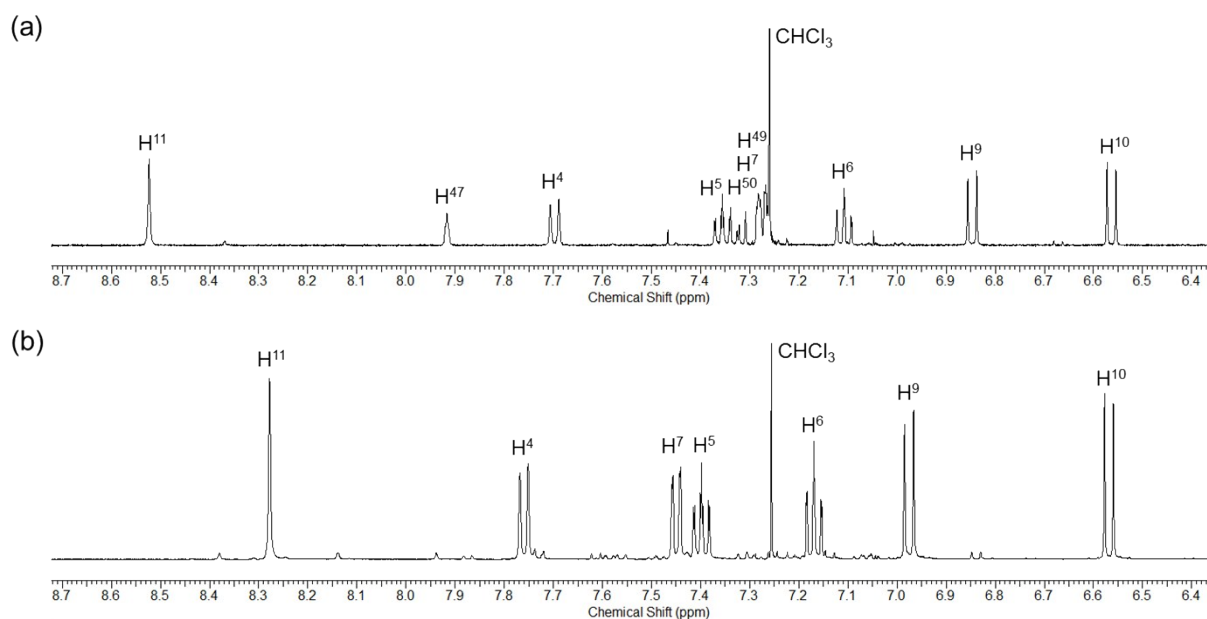


Fig. S2 ^1H NMR spectra (500 MHz) of the aromatic region of (a) *m*-xylylene-linked complex **2** and (b) pentamethylene-linked analogue **4** in CDCl_3 at 298 K. The spectrum of **4** is presented only for comparison.¹¹

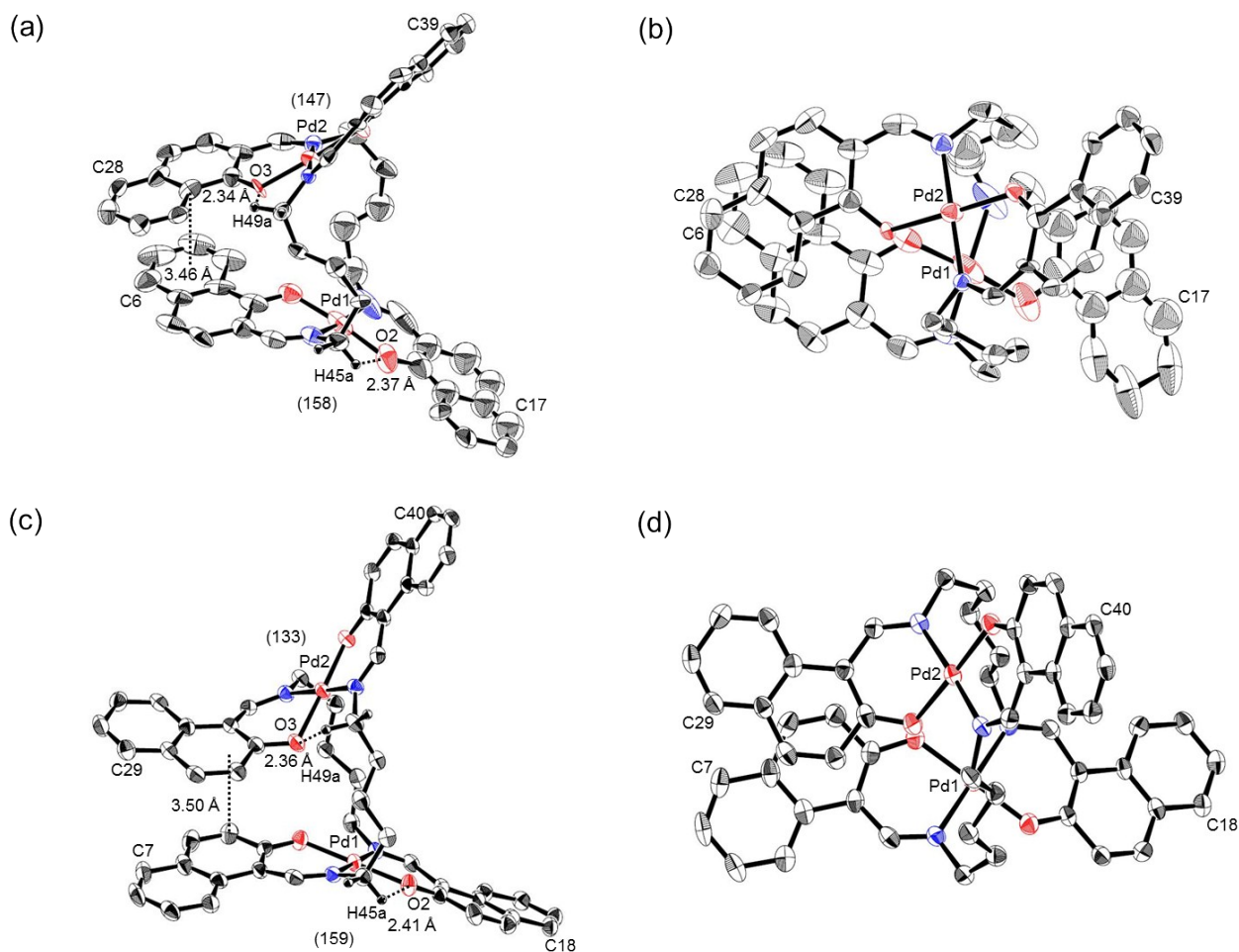
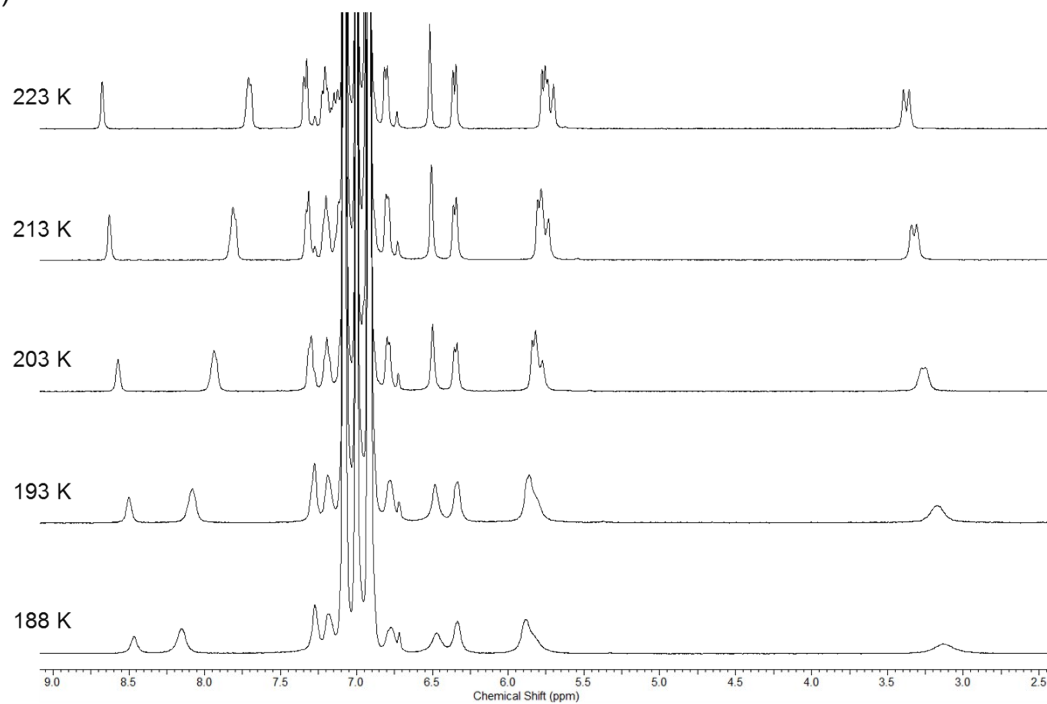


Fig. S3 ORTEP representations of (a,b) (*R*)-**3** and (c,d) (*R*)-**4** as their racemic crystals, showing (a,c) side and (b,d) overhead views. The angles of (a) C(6)–Pd(1)–C(17)/C(28)–Pd(2)–C(39) and (c) C(7)–Pd(1)–C(18)/C(29)–Pd(2)–C(40) are provided in parentheses. Stacking and hydrogen-bonding distances are indicated for each structure. Thermal ellipsoids are shown at the 50% probability level. The structures of **3** and **4** are presented only for comparison with those of *m*-xylylene-linked analogues **1** and **2** shown in Fig. 2.¹¹

(a)



(b)

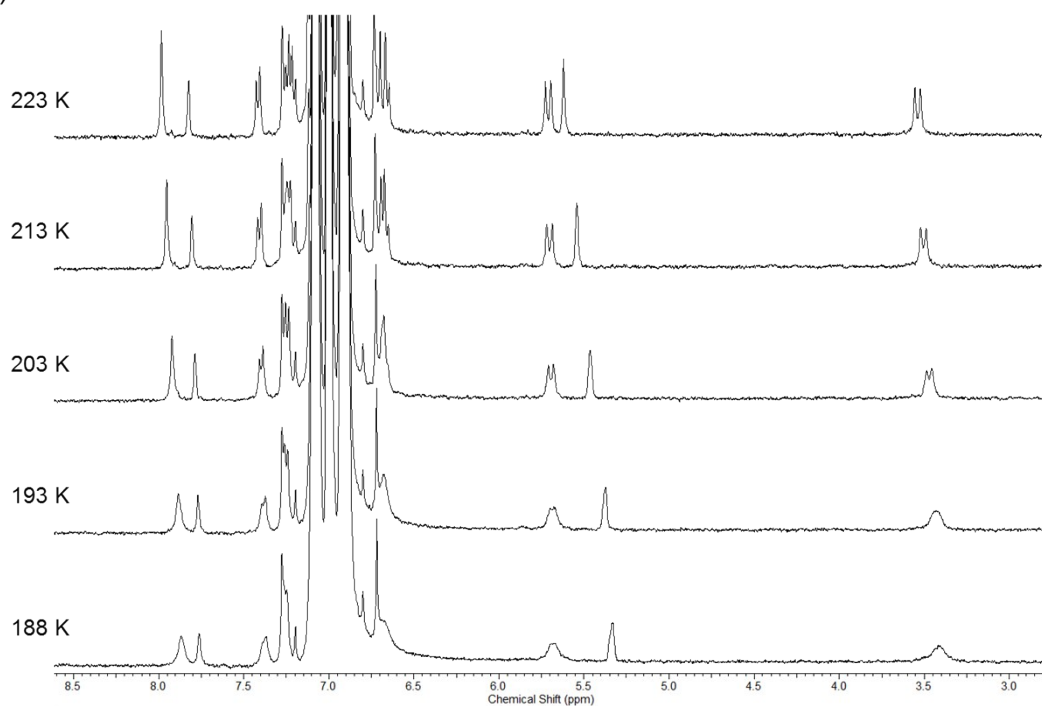


Fig. S4 Variable-temperature ¹H NMR spectra (400 MHz) of (a) (±)-**1** and (b) (±)-**2** in toluene-*d*₈ (1.0×10^{-3} M) at 188–223 K.