Supporting Information for

Can a Meso-type Dinuclear Complex be Chiral?: Dinuclear β-Diketonato Ru(III) Complexes

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Figure S1 (a). The HPLC chromatogram when a solution of dinuclear Ru(III) complex, [Ru(III)(acac)2(dabe)Ru(III)(acac)2], was eluted on a silica gel column (Inertsil, GL Science Inc., (Japan)) with a solvent of 9:1 (v/v) benzene-acetonitrile at a flow rate of 0.5 ml/min. The eluted solution was monitored by the absorbance at 600 nm. Peaks F1, F2 and F3 were assigned to be meso-type, racemic and racemic dinuclear complexes, respectively (see text).
Figure S1(b). The HPLC chromatogram when a solution of dinuclear Ru(III) complex, [Ru(III)(acac)₂(tbet)Ru(III)(acac)₂], was eluted on a silica gel column (Inertsil, GL Science Inc., (Japan)) with a solvent of 95:5 (v/v) benzene-acetonitrile at a flow rate of 1 ml/min⁻¹. The eluted solution was monitored by the absorbance at 600 nm. Peaks F₁ and F₂ were assigned to be meso-type and racemic dinuclear complexes, respectively (see text).
Figure S2 (a). The observed mass spectrum of fraction F₁ in the chromatogram for [Ru(III)(acac)₂(dabe)Ru(III)(acac)₂] (Figure S1(a)). The fractions F₂ and F₃ gave the same results: (m/z) obs: 919 (calc. 918.9).

Figure S2 (b). The observed mass spectrum of fraction F₁ in the chromatogram of [Ru(III)(acac)₂(tbet)Ru(III)(acac)₂] (Figure S1(b)). The fractions F₂ gave the same results: (m/z) obs: 1044 (calc. 1043.0).
$^1$H NMR Data (400 MHz, CDCl$_3$):

[Ru(acac)$_2$(CH$_3$CN)$_2$]PF$_6$: \( \delta = -26.45 \) (6H, CH$_3$), -22.62 (6H, CH$_3$), 37.09 (6H, CH$_3$)

dabeH$_2$: \( \delta = 2.08 \) (6H, s, CH$_3$), 5.91 (2H, C-H), 7.57 (4H, t, J = 7 Hz), 7.67 (2H, tt, J = 7 and 0.6 Hz), 8.17 (4H, dd, J = 7 and 0.6 Hz)

tbet H$_2$: \( \delta = 6.72 \) (2H, s, CH), 7.36 (8H, t, J = 8 Hz), 7.50 (4H, t, J = 8 Hz), 7.91 (8H,d, J = 8 Hz)

Figure S3(a). $^1$H NMR spectra of fractions F$_1$, F$_2$ and F$_3$ in Figure S1(a) of [Ru(III)(acac)$_2$(dabe)Ru(III)(acac)$_2$] (400 MHz, CDCl$_3$): meso-type (F$_1$) (lower); racemic (F$_2$) (middle); racemic (F$_3$) (upper).
Figure S3(b). $^1$H NMR spectra of fractions F$_1$ and F$_2$ of [Ru(III)(acac)$_2$(tbet)Ru(III)(acac)$_2$] (400 MHz, CDCl$_3$): meso-type (F$_1$) (lower); racemic (F$_2$) (upper).
Figure S4(a). The HPLC chromatograms when fractions F₁, F₂ and F₃ of [Ru(III)(acac)₂(dabe)Ru(III)(acac)₂] were eluted on a chiral column (4 mm (i.d.) × 25 cm) at a flow rate of 0.5 ml/min. The column was packed with an ion-exchange adduct of Δ-[Ru(phen)₃]²⁺ (phen = 1,10-phenanthroline) and synthetic hectorite. The eluting solvent was 1:1(v/v) methanol/chloroform mixture. The elution was monitored at 600 nm.

Figure S4(b). The HPLC chromatogram when fraction F₂ of [Ru(III)(acac)₂(tbet)Ru(III)(acac)₂] were eluted on the same chiral column. The eluting solvent was 1:1(v/v) methanol/chloroform mixture. The elution was monitored at 600 nm. Fraction F₁ gave a single peak under the same eluting conditions (not shown).
Figure S5. (a) The electronic circular dichroism spectra of racemic [Ru(III)(acac)$_2$(tbet)Ru(III)(acac)$_2$]. The solid and dotted (red) curves are for the $\Delta\Delta$- and $\Lambda\Lambda$-enantiomers, respectively. (b) The UV-vis spectra of meso-type (blue) and racemic-type (black) dimers, respectively. (c) The vibrational circular dichroism spectra of racemic [Ru(III)(acac)$_2$(tbet)Ru(III)(acac)$_2$]. The black and red curves are for the $\Delta\Delta$- and $\Lambda\Lambda$-enantiomers, respectively.
Figure S6(a). The UV-vis spectrum of a methanol solution of $\Delta \Lambda$-[Ru(III)(acac)$_2$(dabe)Ru(III)(acac)$_2$]
Figure S7. The DFT-calculated VCD (upper) and IR (lower) spectra of ΔΛ−[Ru(III)(acac)$_2$(S-dabe)Ru(III)(acac)$_2$] for the theoretically optimized structure (right). The vertical axis is Δε × 10$^4$ (left) and ε (right), respectively.