Supporting Information for

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

Hisako Sato*[a], Ryoichi Takase,[b] Yukie Mori[c] and Akihiko Yamagishi*[b]

[a] Graduated School of Science and Engineering, Ehime University, Matsuyama, Ehime 790-8577, Japan. Fax: +81-89-927-9599; Tel: +81-89-927-9599; E-mail: sato.hisako.my@ehime-u.ac.jp
[b] Department of Chemistry, Toho University, Funabashi, Chiba 274-8510, Japan
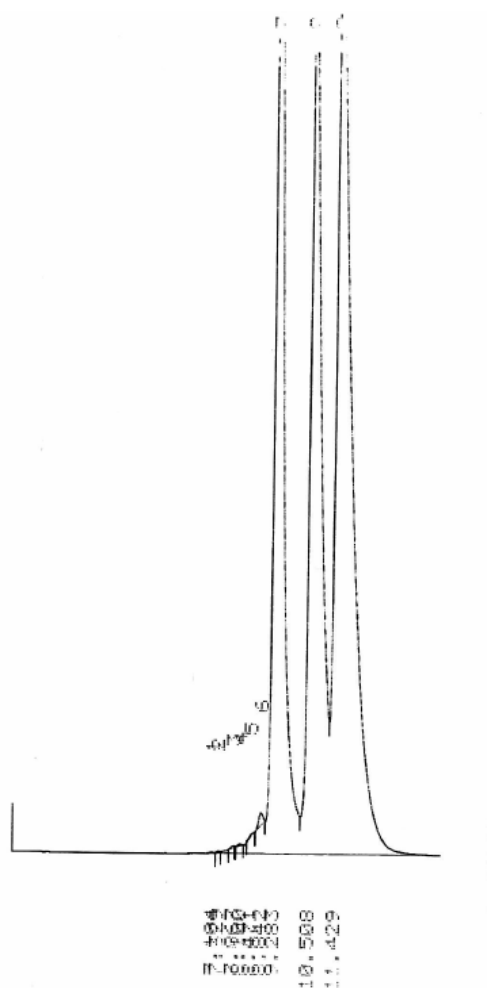[c] Department of Chemistry, Ochanomizu University, Bunkyo-ku, Tokyo, 112-8610, Japan

F1 F2 F3

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 mlmin^{-1}. The eluted solution was monitored by the absorbance at 600 nm. Peaks F$_1$, F$_2$ and F$_3$ were assigned to be meso-type, racemic and racemic dinuclear complexes, respectively (see text).
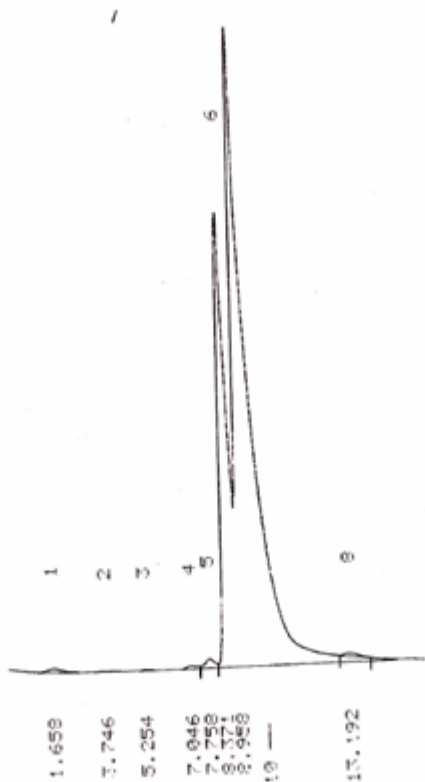
F1   F2

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 mlmin^{-1}. The eluted solution was monitored by the absorbance at 600 nm. Peaks F$_1$ and F$_2$ were assigned to be meso-type and racemic dinuclear complexes, respectively (see text).
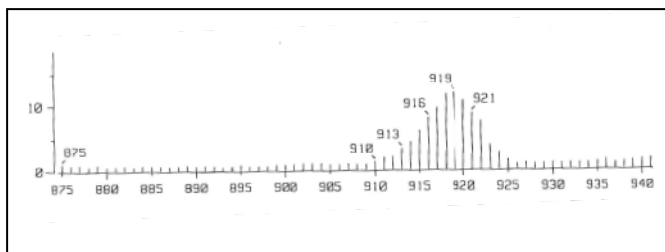
Figure S2 (a). The observed mass spectrum of fraction F_1 in the chromatogram for [Ru(III)(acac)$_2$(dabe)Ru(III)(acac)$_2$] (Figure S1(a)). The fractions F_2 and F_3 gave the same results: (m/z) obs: 919 (calc. 918.9).
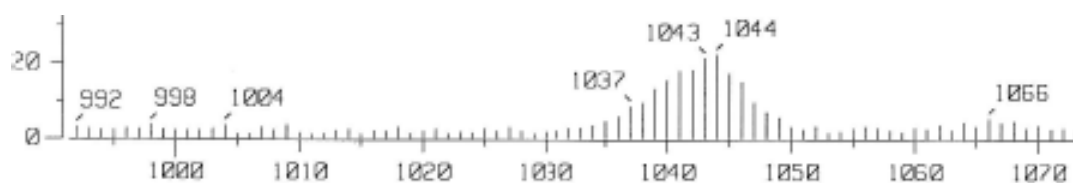

Figure S2 (b). The observed mass spectrum of fraction F_1 in the chromatogram of [Ru(III)(acac)$_2$(tbet)Ru(III)(acac)$_2$] (Figure S1(b)). The fractions F_2 gave the same results: (m/z) obs: 1044 (calc. 1043.0).

^{1}H NMR Data (400 MHz, CDCl$_3$):

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

dabeH$_2$: δ = 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)

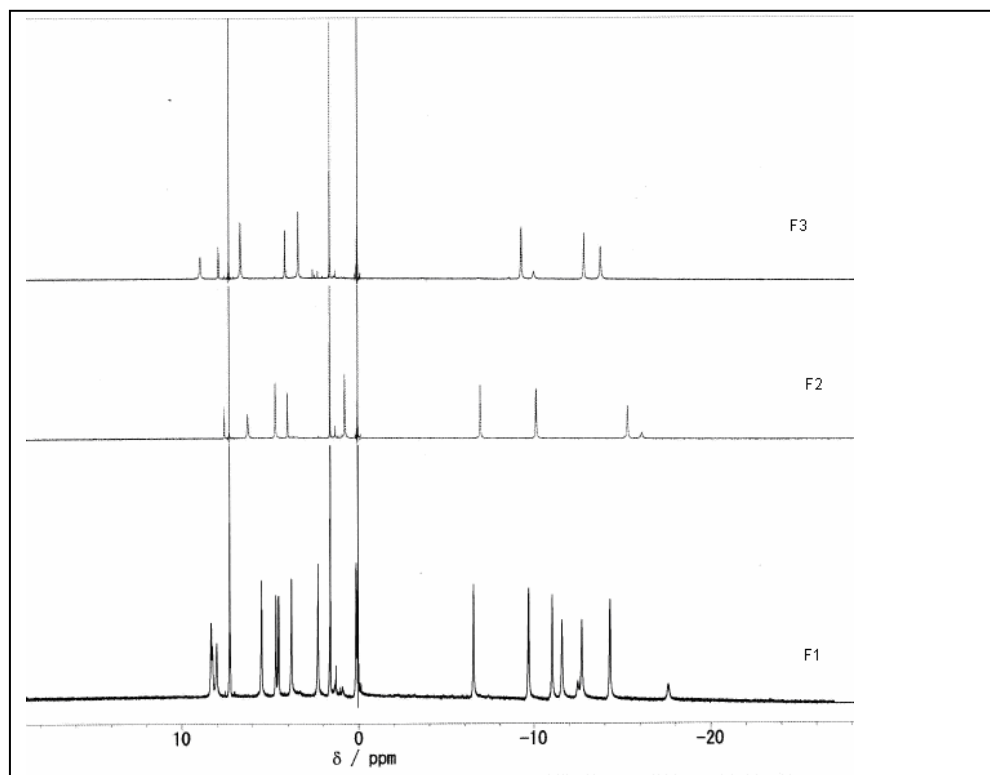**tbet H$_2$:** δ = 6.72 (2H, s, CH), 7.36 (8H, t, J = 8 Hz), 7.50 (4H, t, J = 8 Hz), 7.91 (8H,d, J = 8 Hz)

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).
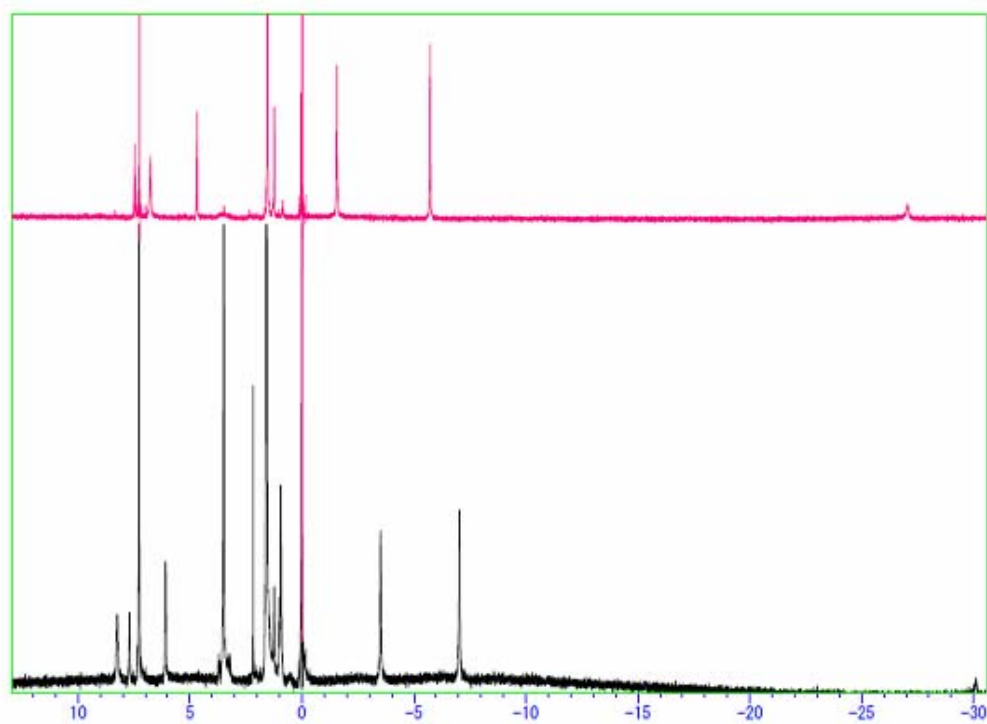
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Figure S3(b). ^{1}H NMR spectra of fractions F_1 and F_2 of [Ru(III)(acac)$_2$(tbet)Ru(III)(acac)$_2$] (400 MHz, CDCl$_3$): meso-type (F_1) (lower); racemic (F_2) (upper).

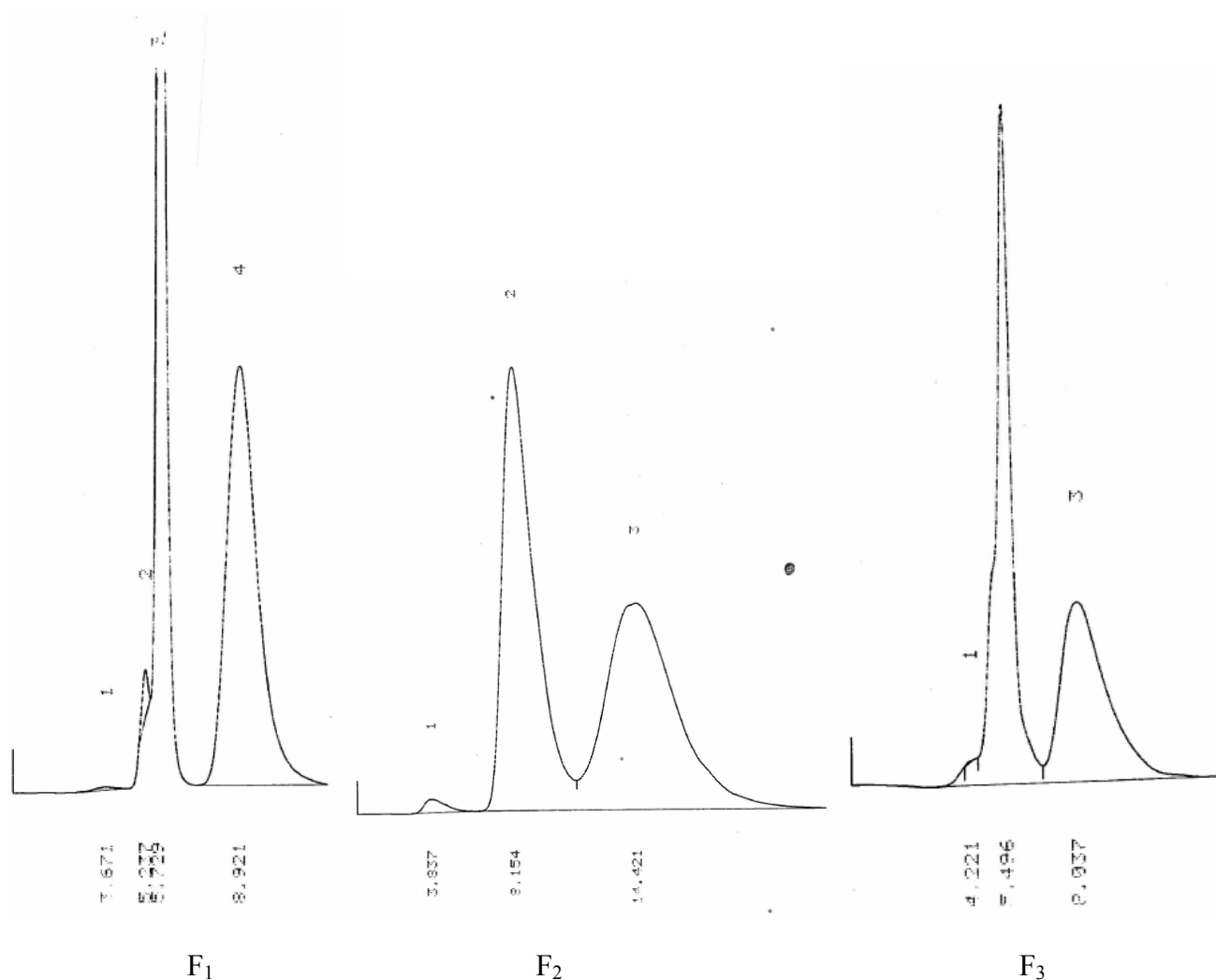F₁   F₂   F₃

Figure S4(a). The HPLC chromatograms when fractions F_1, F_2 and F_3 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 F_2 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 F_1 gave a single peak under the same eluting conditions (not shown).
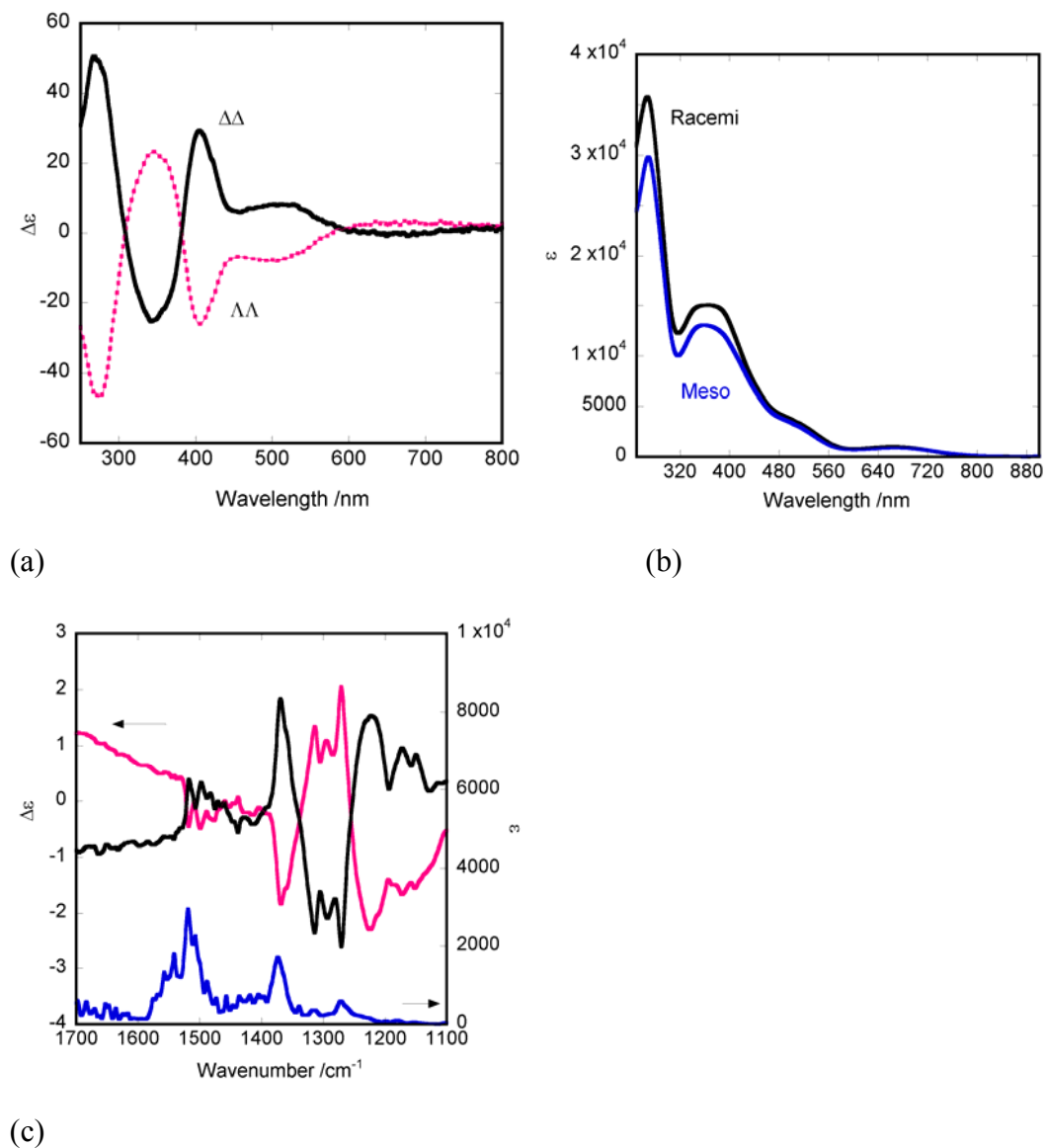
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(a)

(b)

(c)

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 ΔΔ- and ΛΛ-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 ΔΔ- and ΛΛ-enantiomers, respectively.
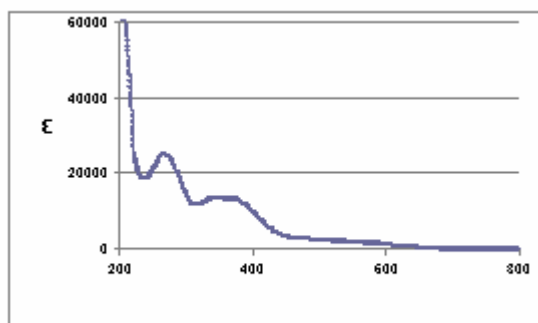
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Figure S6(a). The UV-vis spectrum of a methanol solution of $\Delta\Lambda$-[Ru(III)(acac)$_2$(dabe)Ru(III)(acac)$_2$]
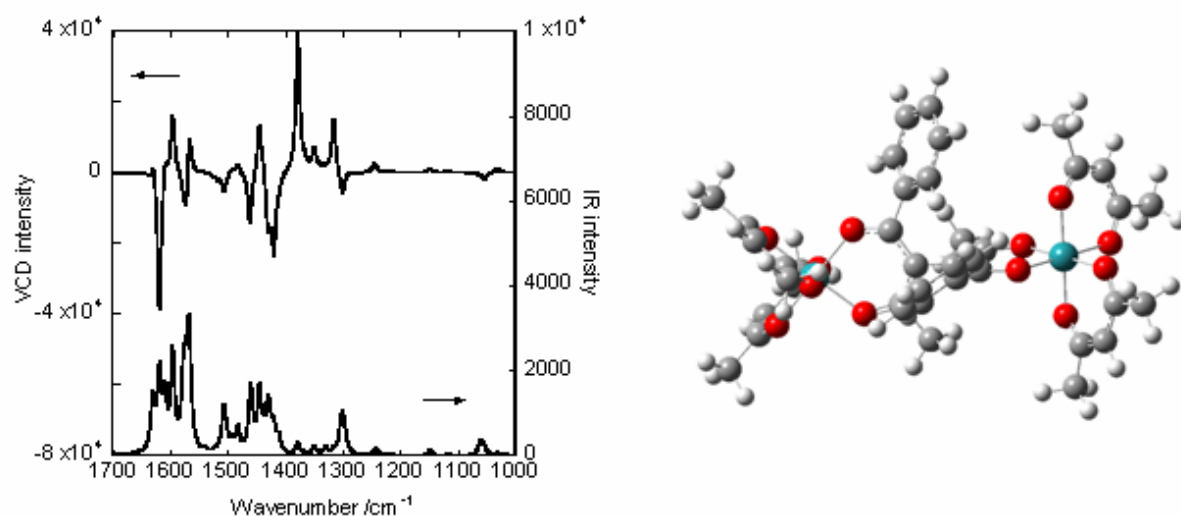
Figure S7. The DFT-calculated VCD (upper) and IR (lower) spectra of $\Delta\Lambda-[Ru(III)(acac)_2(S$-dabe)$Ru(III)(acac)_2]$ for the theoretically optimized structure (right). The vertical axis is $\Delta\varepsilon \times 10^4$ (left) and ε (right), respectively.