Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

for

Solid State Vibrational Circular Dichroism towards Molecular Recognition: Chiral Metal Complexes Intercalated in a Clay Mineral

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Contents:

S1. The experimental VCD and IR spectra of BINOL in CD_3CN

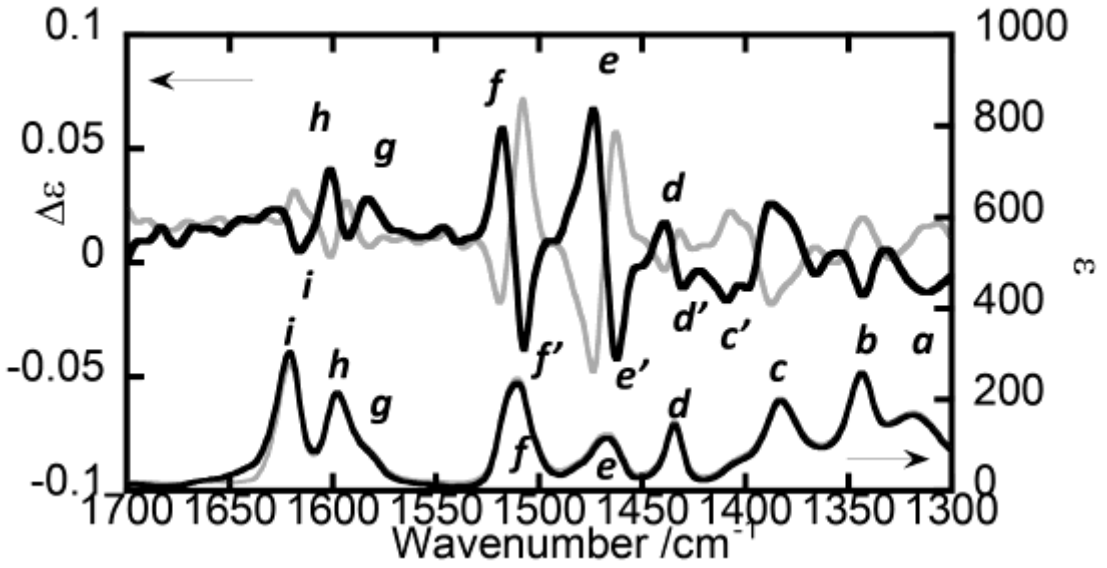

Figure S1. The observed IR (lower) and VCD (upper) spectra of BINOL in CD_3CN: Solid and thin lines are for the *R* and *S*-forms, respectively.

S2. The calculated VCD and IR spectra of *R*-BINOL in CH_3CN

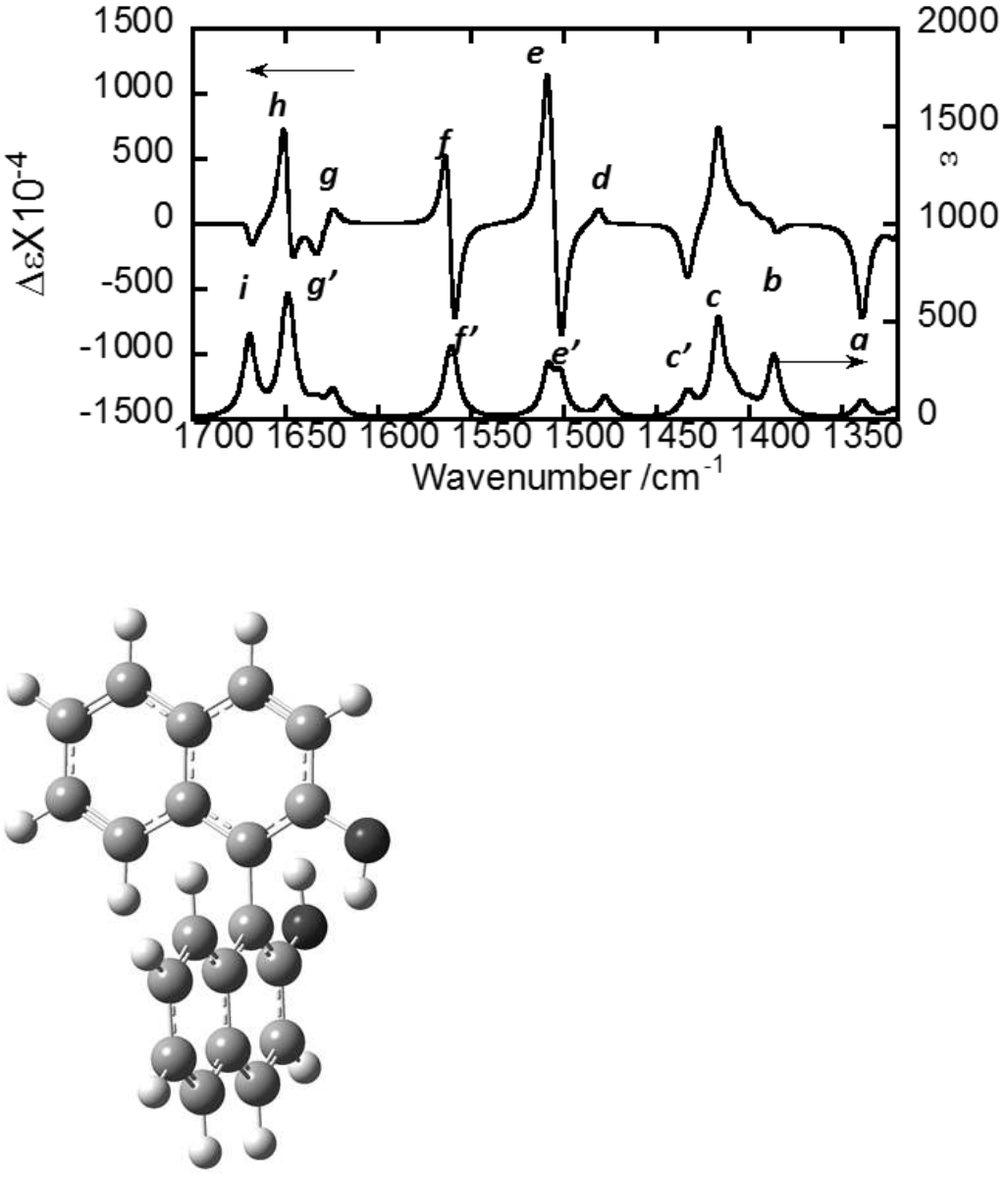

Figure S2. The calculated IR (lower) and VCD (upper) spectra of *R*-BINOL in CH_3CN together with the optimized molecular structure under the cis-cis conformation. The solvent was approximated as a dielectric continuum (see the calculation details in the text).

S3. The calculated VCD and IR spectra of a molecular associate between *R*-BINOL and Δ- or Λ- $[Ru(phen)_3]^{2+}$ under various conformations

(a)

(b)

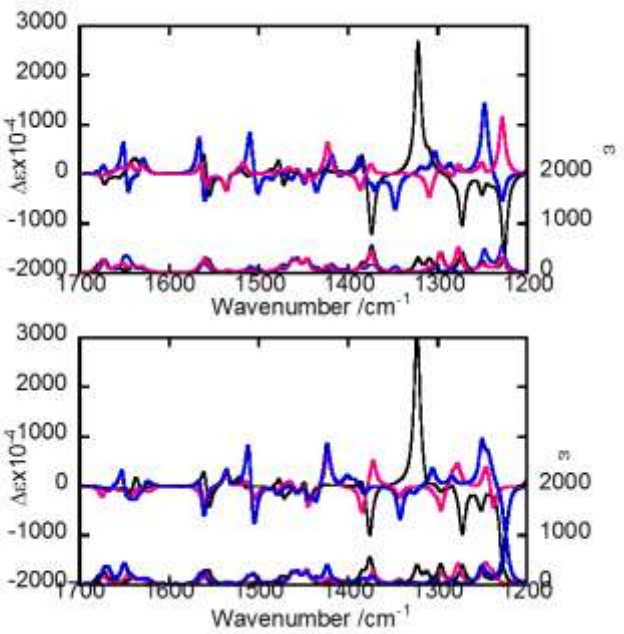

Figure S3.The calculated IR (lower) and VCD (lower) spectra of a molecular associate between *R*-BINOL and Δ- or Λ-$[Ru(phen)_3]^{2+}$ under various conformations. The structure of *R*-BINOL was assumed to take the conformation of cis-cis (blue) or trans-trans (black) or cis-trans (red), respectively: (a) *R*-BINOL/Δ-$[Ru(phen)_3]^{2+}$ and (b) *R*-BINOL/Λ-$[Ru(phen)_3]^{2+}$

S4. The calculated VCD and IR spectra for the optimized structure of a molecular associate between *R*- BINOL and Δ- or Λ-$[Ru(phen)_3]^{2+}$ in a gaseous state

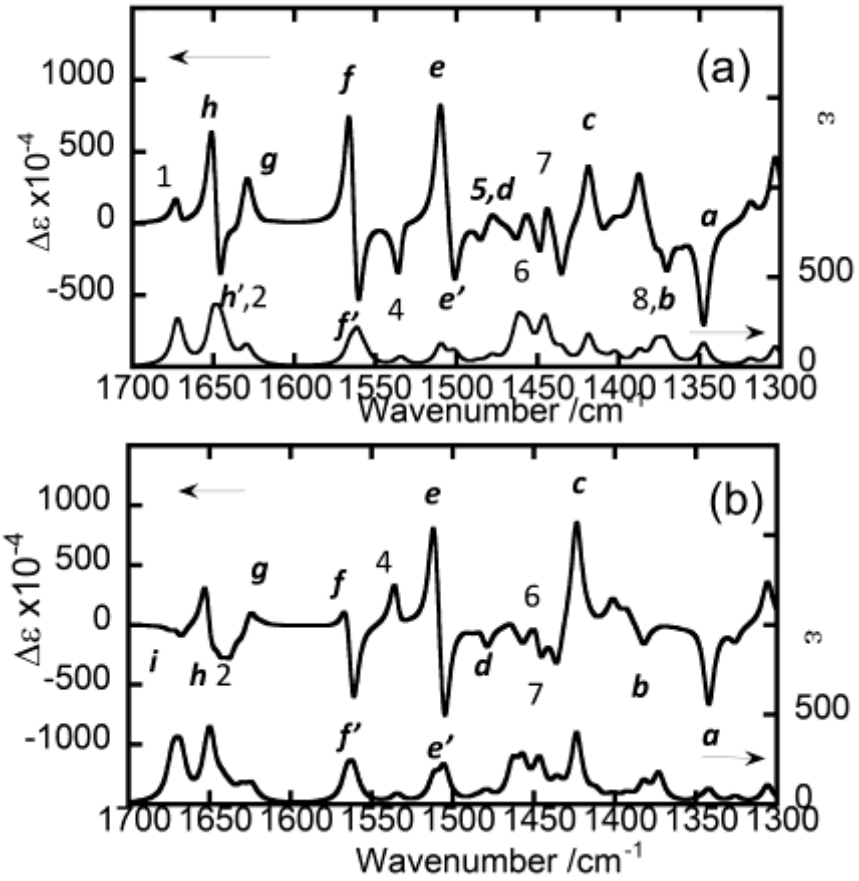

Figure S4. The calculated VCD (upper) and IR (lower) spectra for a molecular associate between BINOL and $[Ru(phen)_3]^{2+}$: (a) *R*-BINOL/Δ-$[Ru(phen)_3]^{2+}$ and (b) *R*-BINOL/Λ-$[Ru(phen)_3]^{2+}$. The structure of each associate was energetically optimized in a gaseous state. Accordingly BINOL took a cis-cis conformation. The main peaks were assigned to either BINOL or $[Ru(phen)_3]^{2+}$ as indexed in terms of alphabets or numbers, respectively.

S5. The snapshot of the animation of molecular motion for the selected vibrations of a molecular associate between *R*-BINOL and Δ- $[Ru(phen)_3]^{2+}$

(a)

(b)

Figure S5. The snapshots of the animation for the vibrational motion in a molecular associate between *R*-BINOL and Δ-$[Ru(phen)_3]^{2+}$. The selected vibrations were (a) peak No. **5** and ***d*** around 1485 cm^{-1} and (b) peak No. **8** and ***b*** around 1370 cm^{-1} in the calculated spectrum in Figure S4 (a), respectively.