Supplementary Information

for

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

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Contents:

1. The experimental VCD and IR spectra of BINOL in CD3CN
2. The calculated VCD and IR spectra of R-BINOL in CH3CN
3. The calculated VCD and IR spectra of a molecular associate between R-BINOL and Δ- or Λ-[Ru(phen)3]2+ under various conformations
4. 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
5. 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+
S1. The experimental VCD and IR spectra of BINOL in CD$_3$CN

Figure S1. The observed IR (lower) and VCD (upper) spectra of BINOL in CD$_3$CN: Solid and thin lines are for the $R$ and $S$-forms, respectively.
S2. The calculated VCD and IR spectra of R-BINOL in CH₃CN

Figure S2. The calculated IR (lower) and VCD (upper) spectra of R-BINOL in CH₃CN 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 Δ- [Ru(phen)₃]²⁺ under various conformations

Figure S3. The calculated IR (lower) and VCD (lower) spectra of a molecular associate between *R*-BINOL and Δ- or Δ- [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/Δ-[Ru(phen)₃]²⁺
S4. The calculated VCD and IR spectra for the optimized structure of a molecular associate between $R$-BINOL and $\Delta$- or $\Lambda$-[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/$\Delta$-[Ru(phen)$_3$]$^{2+}$ and (b) $R$-BINOL/$\Lambda$-[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 $\Delta$- [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 $\Delta$-[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.