Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information

Vibrational circular dichroism spectroscopy of two chiral binaphthyl diphosphine ligands and their palladium complexes in solution

Zahra Dezhahang, Christian Merten, Mohammad Reza Poopari, Yunjie Xu*

Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada T6G 2G2

*Tel: 1-780-492-1244, Fax: 1-780-492-8231, Email: yunjie.xu@ualberta.ca

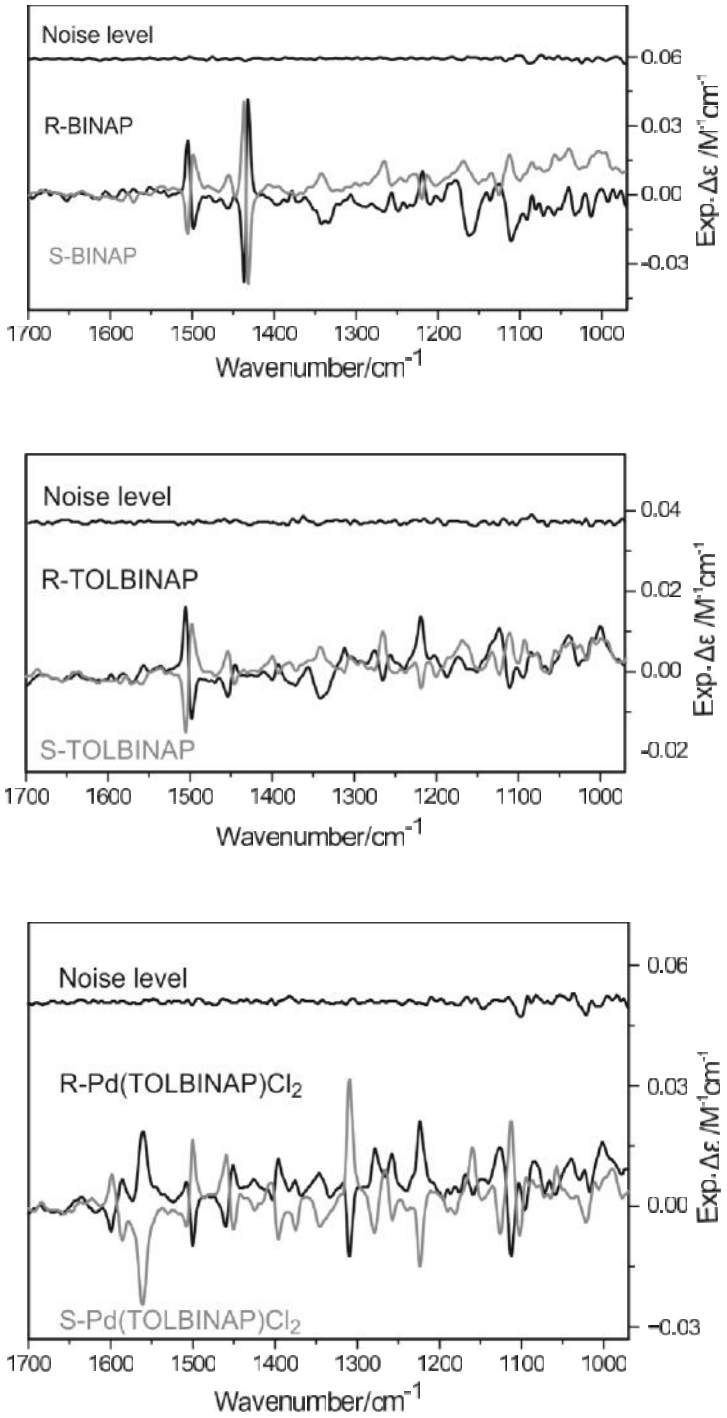

Figure S1 The experimental VCD spectra of both R and S enantiomers BINAP, TOLBINAP and Pd(TOLBINAP)Cl_2 in $CDCl_3$ solution and their related noise levels. In all the VCD spectra shown, the corresponding $CDCl_3$ spectrum obtained under identical experimental conditions was subtracted off. As one can see, good mirror images have been obtained for all the VCD spectral features measured except a few broad features at the very low wavenumber region. This is likely due to the strong absorption by the solvent starting at about 970 cm^{-1}.

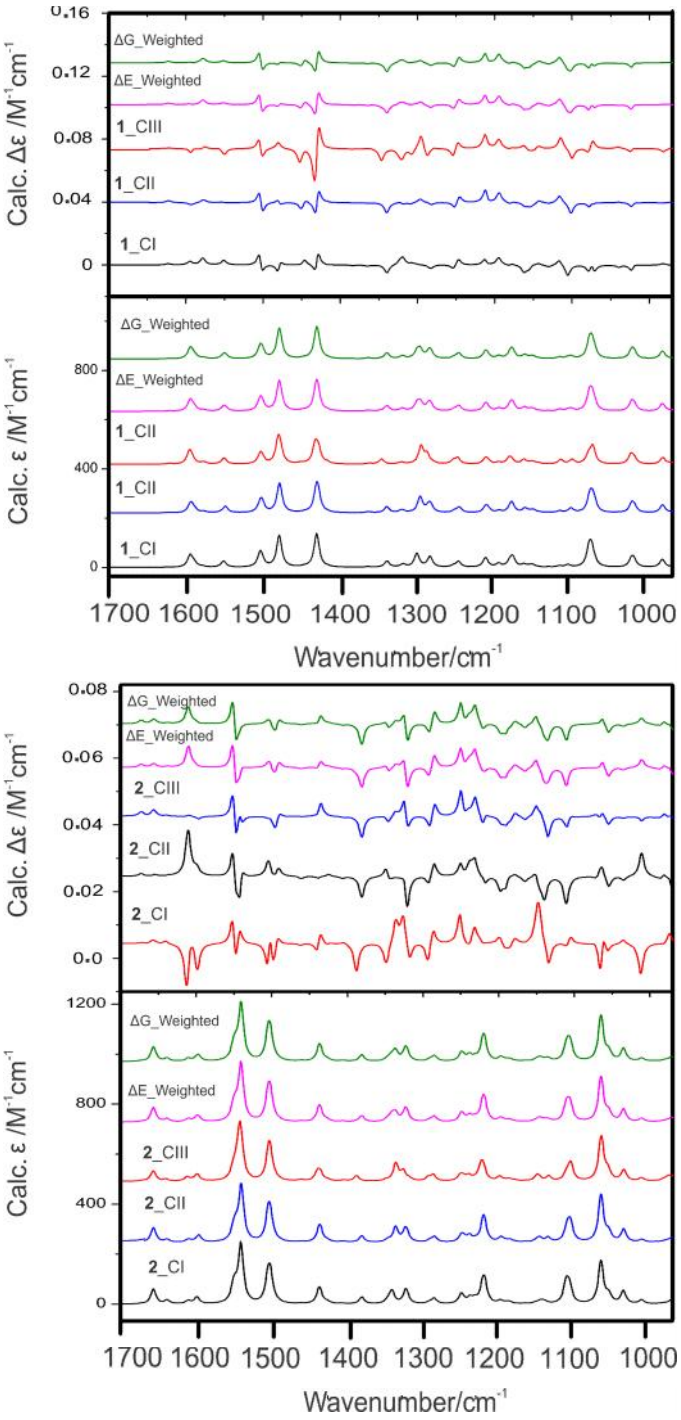

Figure S2 The calculated gas phase VA and VCD spectra of the three conformers of BINAP (top) and of the three conformers of TOLBINAP (bottom) and their corresponding population weighted spectra based on the relative energies and the relative free energies at the B3LYP/6-31G(d,p) level.

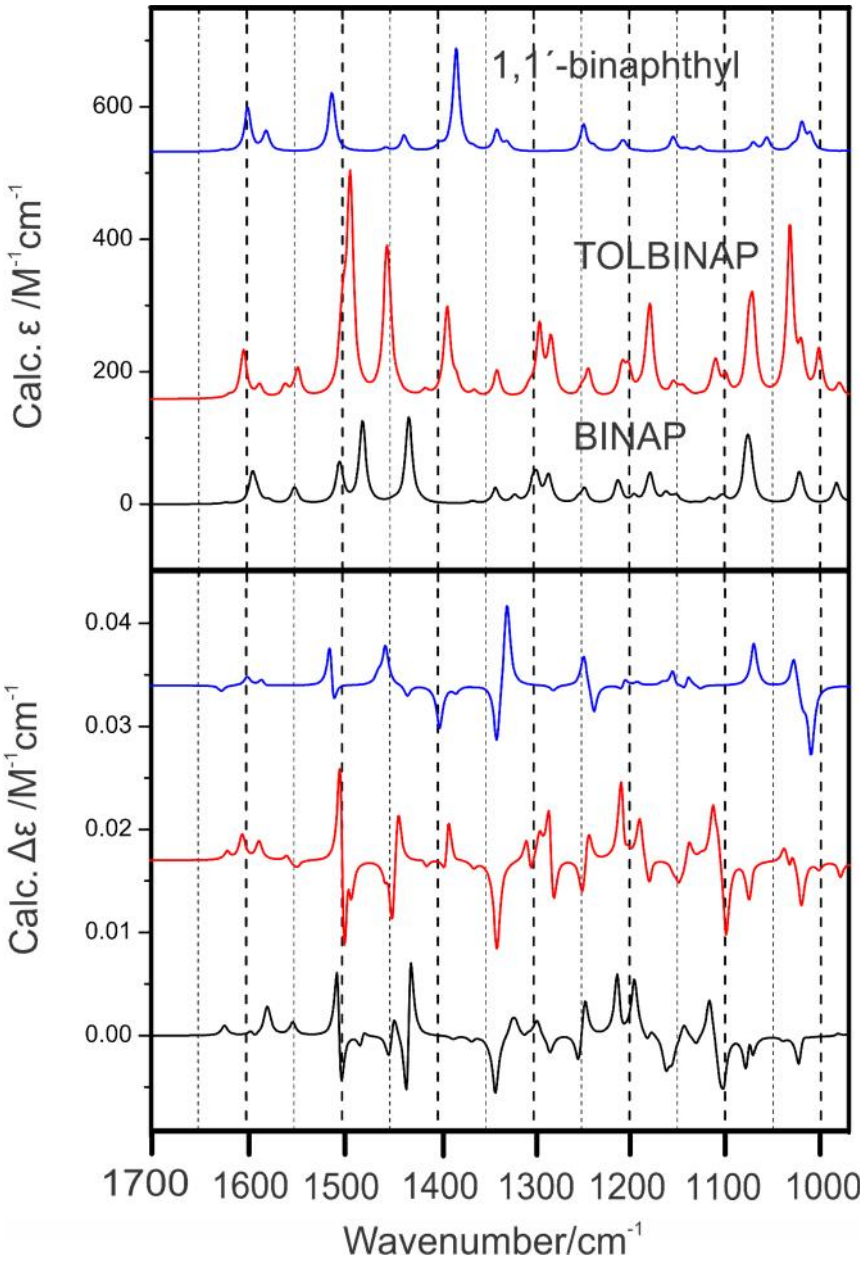

Figure S3 Comparison of the calculated gas phased VA and VCD spectra of 1,1'-binaphthyl, BINAP, and TOLBINAP at B3LYP/6-31G(d,p) level. The VA intensity of 1,1'-binaphthyl was amplified by a factor of two for easy comparison. The intense band in the 1430-1460 cm^{-1} region in BINAP and TOLBINAP corresponds to the C-C stretching and C-H bending vibrational modes of four phenyl rings bonded to phosphorous, which does not show up for 1,1'-binaphthyl. The bands at 1250 cm^{-1} corresponds to the same vibrational modes in all three systems. The related bisignated VCD feature flip going from 1,1'-binaphthyl to BINAP and TOLBINAP. The intense bands at ~1500 cm^{-1} correspond to the C=C stretching vibrational motions of phenyl rings and naphthalene rings.

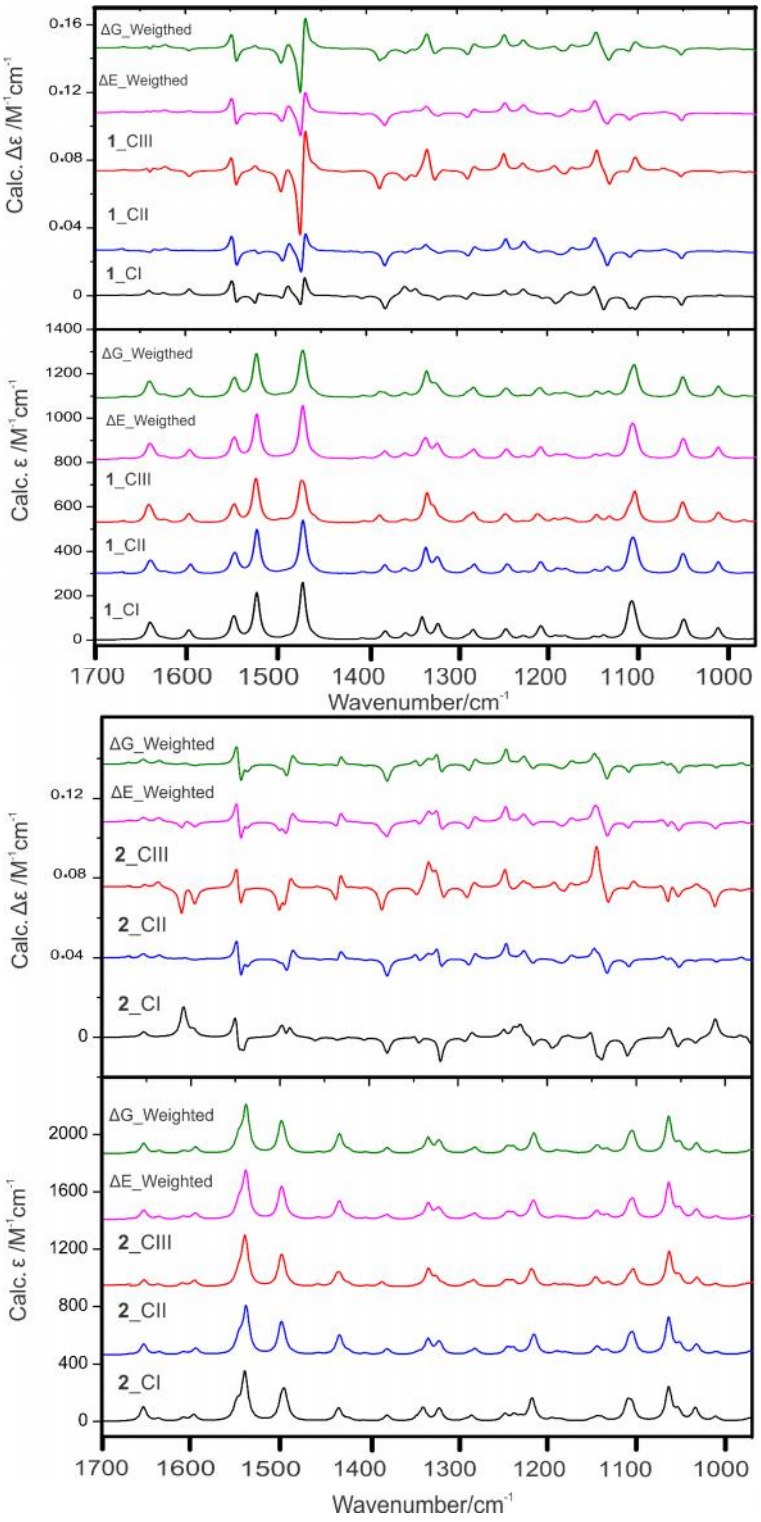

Figure S4 The calculated VA and VCD spectra with PCM of chloroform of the three conformers of BINAP (top) and of the three conformers of TOLBINAP (bottom) and their corresponding population weighted spectra based on the relative energies and the relative free energies at the B3LYP/6-31G(d,p) level.