# Supporting Information

## Diastereomers of the Pentacoordinate Chiral Phosphorus Compounds in Solution: Absolute Configurations and Predominant Conformations

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Table S1. The relative Gibbs free energies $\Delta G$ (kcal/mol), relative total energies $\Delta E$ (kcal/mol), and the normalized Boltzmann factors $B_f$ (in %) at 298.15 K based on the relative Gibbs free energy and the relative total energy of the 1:1 **3** $\Lambda_p SS$-DMSO (**1DMSO**) conformers at the B3LYP/6-311++G** level of theory.

| System | $\Delta E$ | $B_f(\Delta E)$ | $\Delta G$ | $B_f(\Delta G)$ |
|---|---|---|---|---|
| **1DMSOI** | 0 | 91.42 | 0 | 92.76 |
| **1DMSOII** | 1.40 | 8.58 | 1.51 | 7.28 |

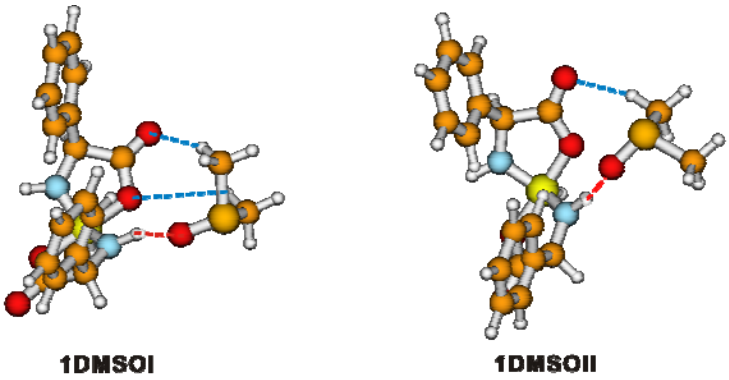


Figure S1. The optimized geometries of the 1:1 **3** $A_p$*SS*-DMSO conformers at the B3LYP/6-311++G** level of theory.

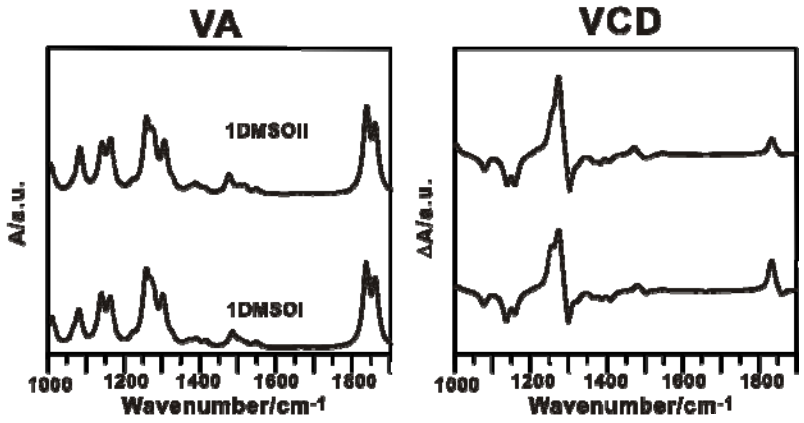


**Figure S2.** The calculated VA and VCD spectra of the 1:1 **3** $A_p$*SS*-DMSO conformers at the B3LYP/6-311++G** level of theory.

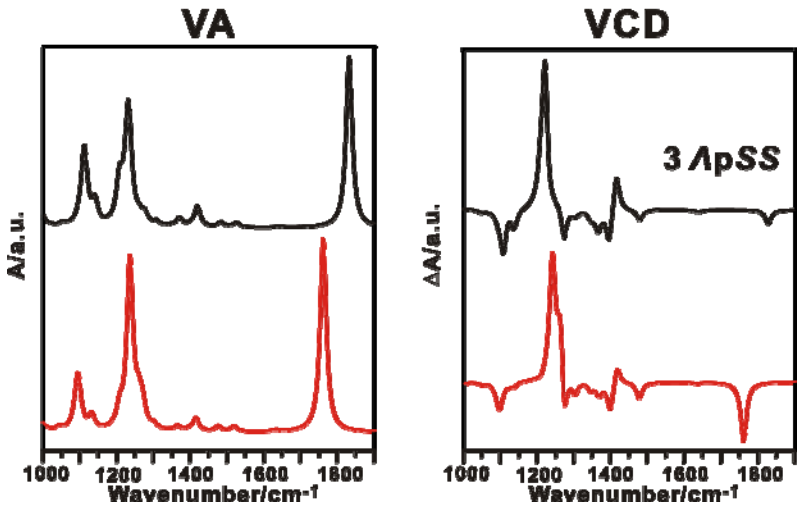


**Figure S3.** Comparison between the calculated gas phase (black) VA and VCD spectra and the IEFPCM (red) VA and VCD spectra of **3** $\Lambda_p SS$, respectively.

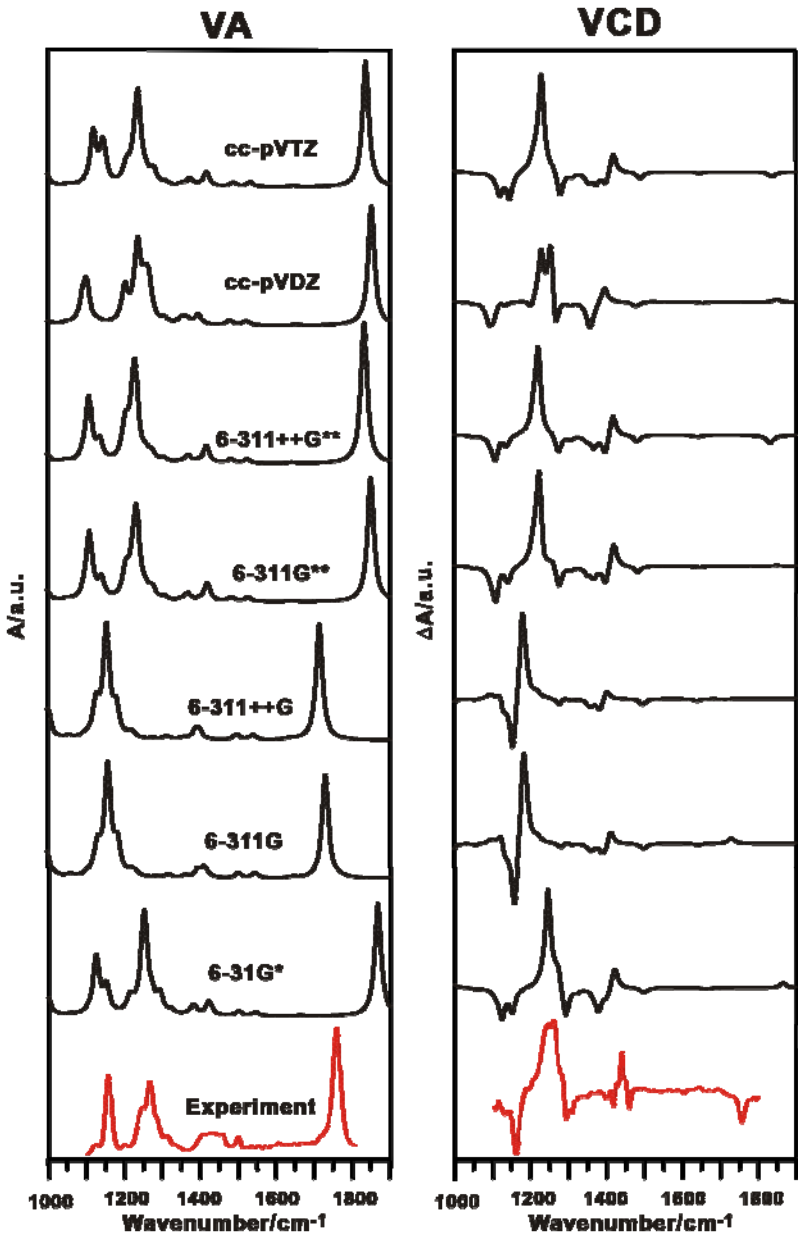


**Figure S4.** Calculated VA (left) and VCD (right) spectra of **3** $\Lambda_p SS$ using the DFT/B3LYP functional and seven different basis sets along with the experimental VA and VCD (red) spectra.

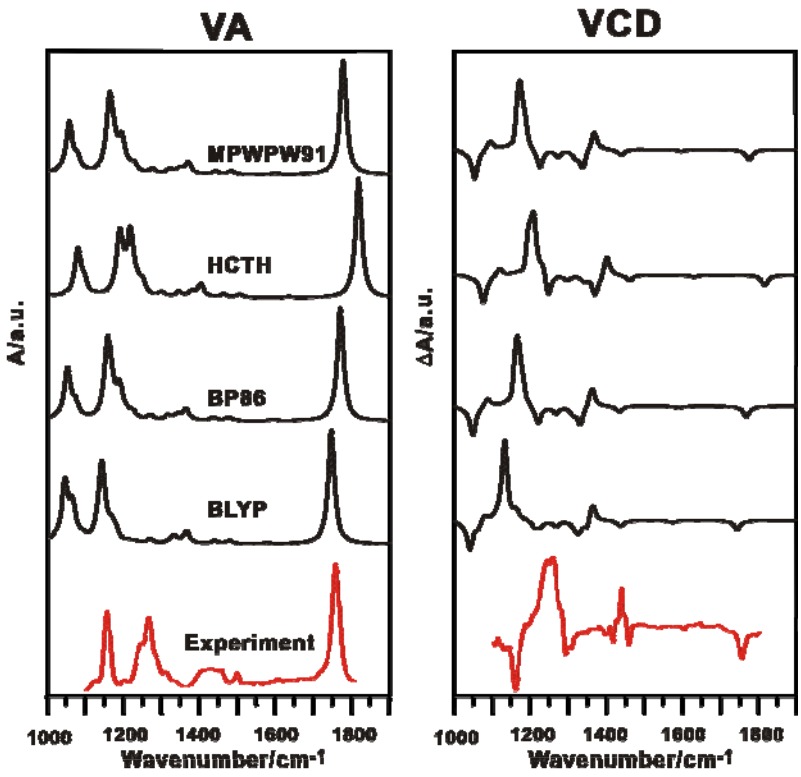


**Figure S5.** Calculated VA (left) and VCD (right) spectra of **3** $\Lambda_p SS$ using the four different GGA functionals and the 6-311++G** basis sets along with the experimental VA and VCD (red) spectra.

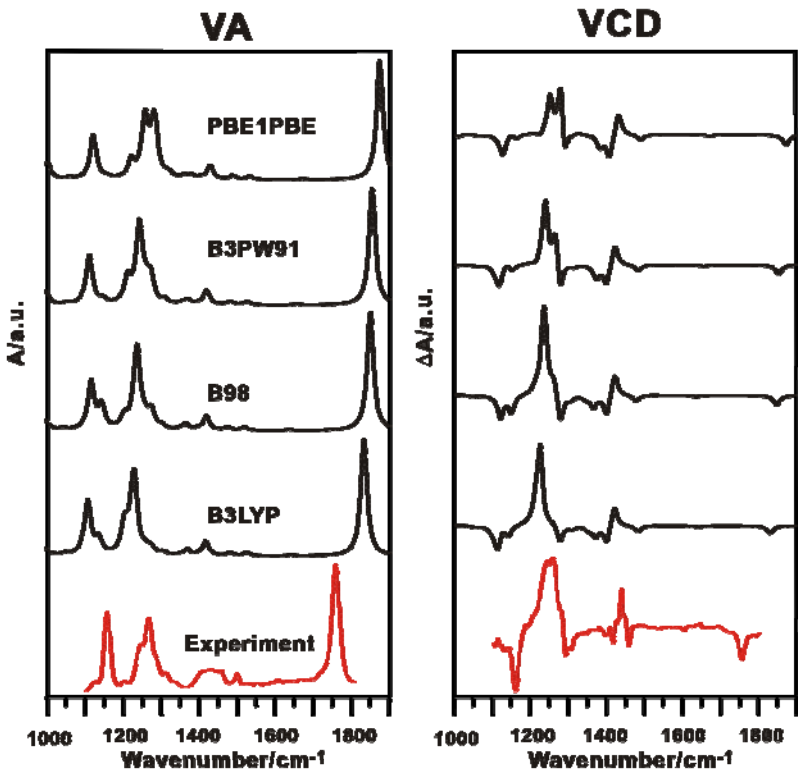


**Figure S6.** Calculated VA (left) and VCD (right) spectra of **3** $\Lambda_p SS$ using the four different HGGA functionals and the 6-311++G** basis sets along with the experimental VA and VCD (red) spectra.

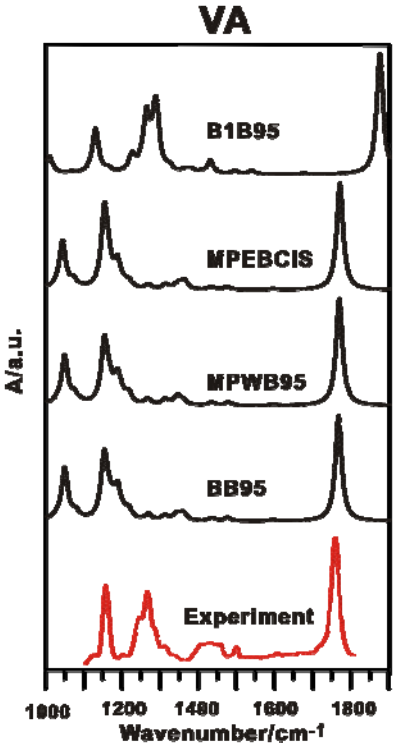


**Figure S7.** Calculated VA spectra of **3** $\Lambda_p SS$ using the three different MGGA and one HMGGA (BB95) functionals and the 6-311++G** basis sets along with the experimental VA (red) spectrum. These functionals are not implemented for VCD calculations in Gaussian03.