

Electronic Supplementary Information (ESI) for *PCCP*

Strong chiroptical activity in Au₂₅ clusters protected by mixed ligands of chiral phosphine and achiral thiolate

Takumi Nashimoto and Hiroshi Yao*

Division of Chemistry for Materials, Graduate School of Engineering, Mie University, 1577 Kurimamachiya-cho, Tsu, Mie 514-8507, Japan

Comparison of CD spectra between the obtained product [Au₂₅(S-BINAP)₄(DDT)₅X₄] and pure S-BINAP.

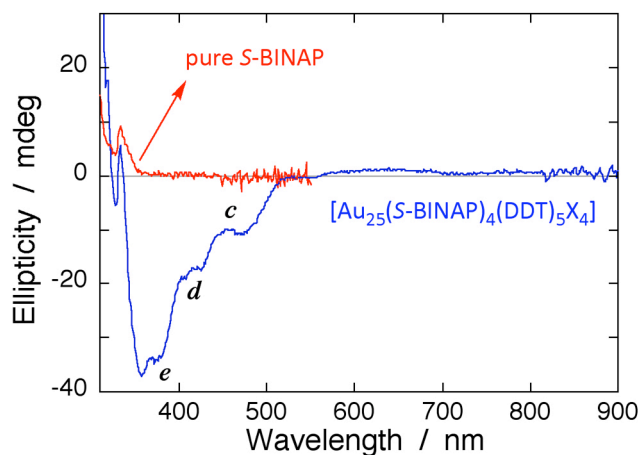


Fig. S1. CD spectra of the obtained Au₂₅ product [Au₂₅(S-BINAP)₄(DDT)₅X₄] and pure S-BINAP in DCM.

Optimize structure and theoretical absorption/CD spectra of *trans*-form of Au₂₅ model cluster having (*S*)-1,4-diphosfinobuta-1,3-diene ligands instead of PH₃.

We also optimized *trans*-form of bi-icosahedral Au₂₅ cluster having (*S*)-1,4-diphosfinobuta-1,3-diene ligands instead of monodentate PH₃, and on the basis of the structure, optical absorption and CD spectra were simulated (Fig. S2).

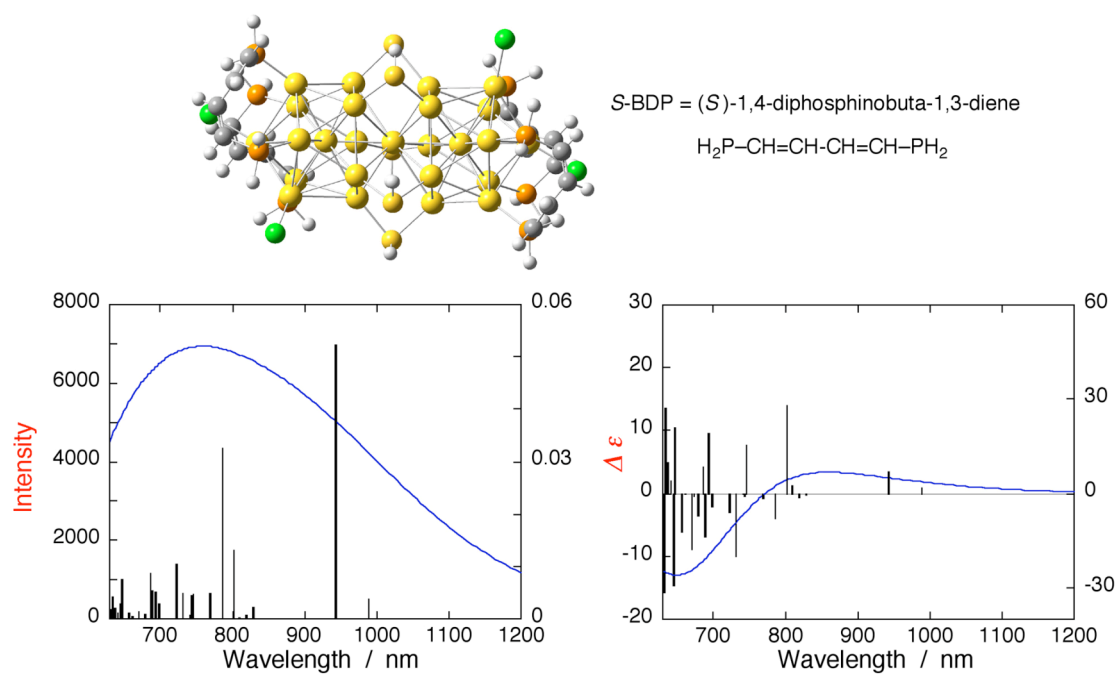


Fig. S2. Optimize structure (upper) and theoretical absorption/CD spectra (lower) of *trans*-form of Au_{25} model cluster having (*S*)-1,4-diphosfinobuta-1,3-diene ligands instead of monodentate PH_3 .