

# Supplementary Information

## Computational prediction of chiral iron complexes for asymmetric transfer hydrogenation of pyruvic acid to lactic acid

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### 1. Evaluation of basis set

In order to evaluate the influential of the basis set superposition errors (BSSE) on enantio-determining step (EDS) of our iron catalytic system, we calculated singlet point energies of the enantio-determining transition states **TS<sub>2,3-R</sub>** and **TS<sub>2,3-S</sub>** with extended basis sets (def2-TZVP for main group and def2-QZVP for Fe)[1-3]. The absolute free energies are obtained by adding the free energy corrections calculated by using small basis sets (6-31G(d)/ECP10MDF) to the corresponding electronic energies calculated by using extended basis sets (def2-TZVP/def2-QZVP):

$$G_{\text{extended}} = E_{\text{extended}} + G_{\text{correction}}(\text{small basis set})$$

As shown in Table S1, the free energy difference between **TS<sub>2,3-R</sub>** and **TS<sub>2,3-S</sub>** with extended basis set is 3.3 kcal mol<sup>-1</sup>, which is only 0.1 kcal mol<sup>-1</sup> larger than the relative free energy with small basis set. Such results indicate that the BSSE of 6-31G(d)/ECP10MDF basis sets is negligible for this iron based catalytic system.

**Table S1.** Absolute and relative energies of **TS<sub>2,3-R</sub>** and **TS<sub>2,3-S</sub>** with different basis set.

Basis set	<b>TS<sub>2,3-R</sub></b> (a.u.)	<b>TS<sub>2,3-S</sub></b> (a.u.)	$\Delta G$ (EDS) (kcal mol <sup>-1</sup> )
6-31G(d)/ECP10MDF	-2475.934071	-2475.929023	3.2
def2-TZVP/def2-QZVP	-3616.541443	-3616.536225	3.3

**Reference:**

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2. Schuchardt, K. L.; Didier, B. T.; Elsethagen, T.; Sun, L.; Gurumoorthi, V.; Chase, J.; Li, J.; Windus, T. L., Basis set exchange: A community database for computational sciences. *J. Chem. Inf. Model.*, **2007**, 47, 1045-1052.
3. Feller, D., The role of databases in support of computational chemistry calculations. *J. Comput. Chem.*, **1996**, 17, 1571-1586.