

## Supporting Information for

# Theoretical Investigations on the Activity Influence Factors of $\cdot\text{Mn}(\text{CO})_5$ Catalyzed Alkynes Hydrosilylation and Hydrogermylation

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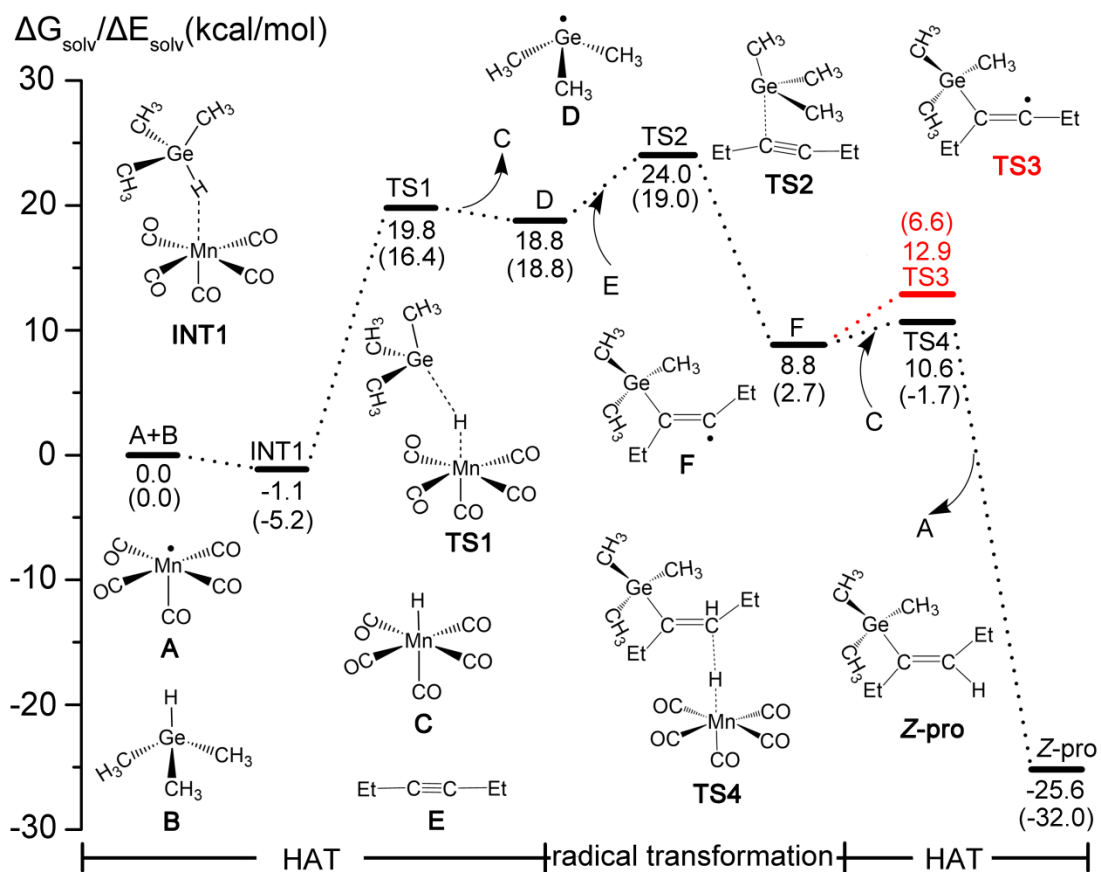
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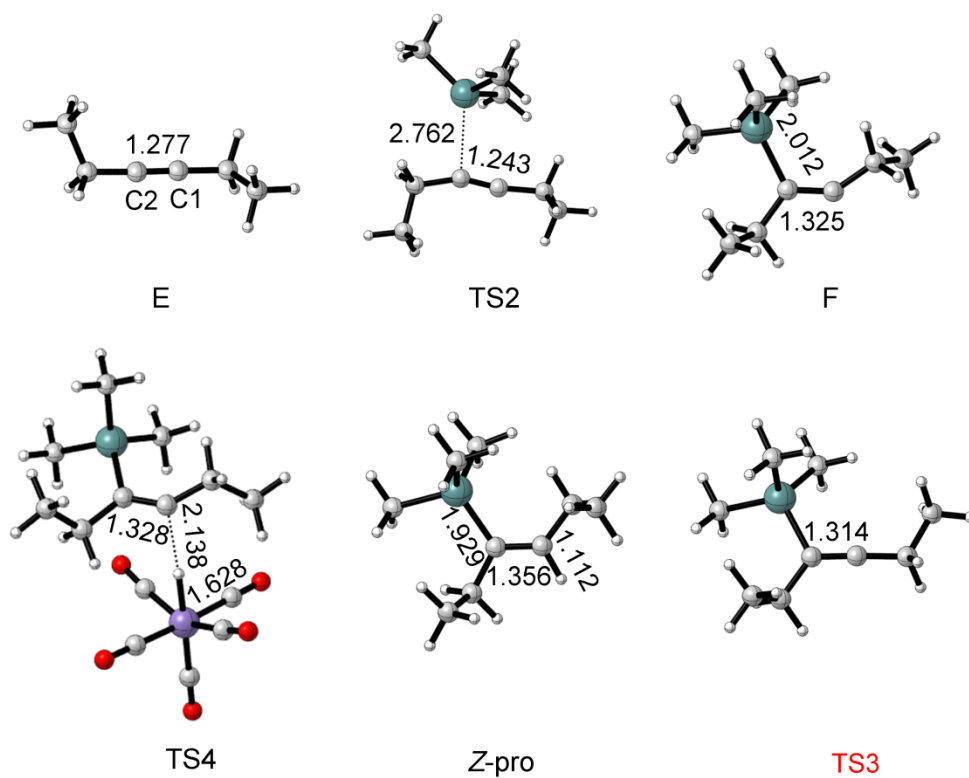
**Fig. S1.** The Gibbs-free energy profiles for hydrogermylation of internal alkyne catalyzed by  $\cdot\text{Mn}(\text{CO})_5$  (relative enthalpies are given in parentheses)

**Fig. S2.** Geometries and key bond lengths (in Å) of stationary points on the PES of hydrogermylation of internal alkyne catalyzed by  $\cdot\text{Mn}(\text{CO})_5$ .

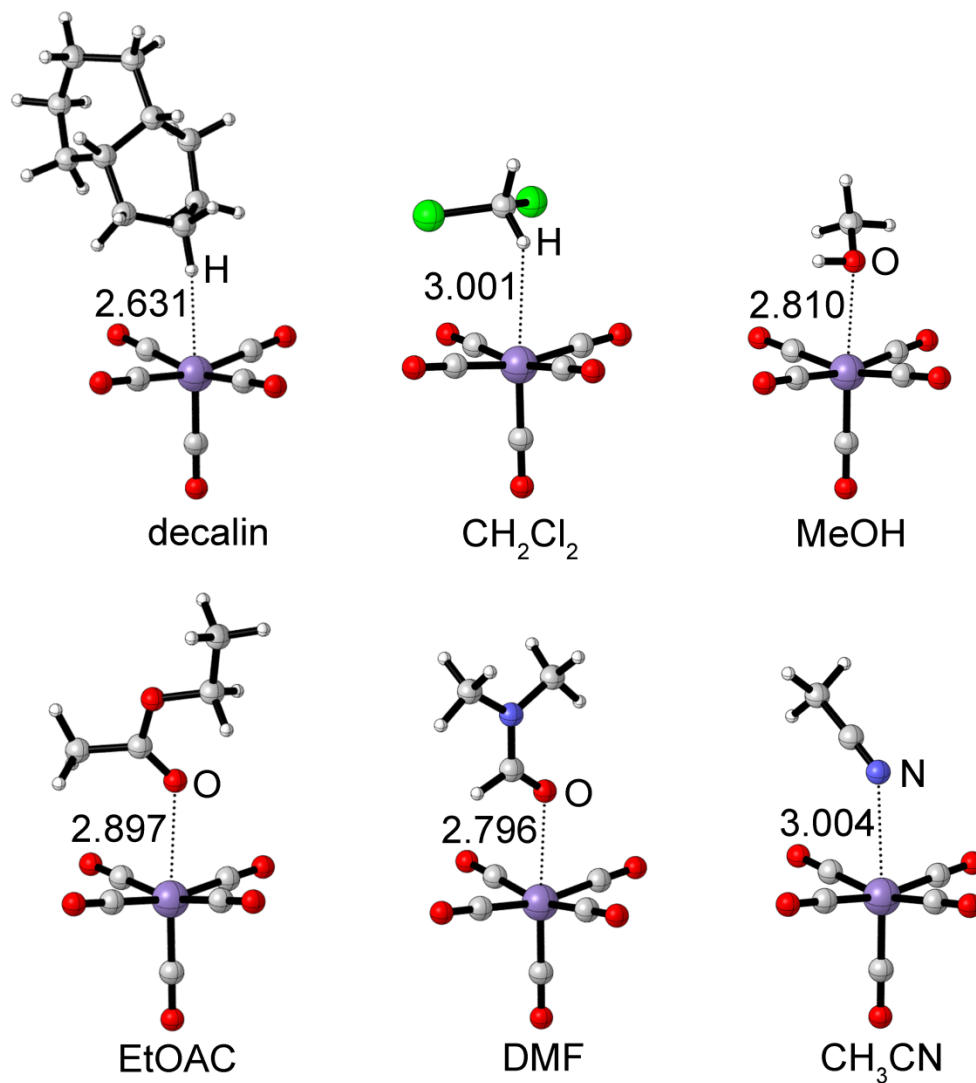
**Fig. S3.** Geometries and key bond lengths (in Å) of stationary points of the complexes formed between  $\cdot\text{Mn}(\text{CO})_5$  and the solvents.



**Fig. S1.** The Gibbs-free energy profiles for hydrogermylation of internal alkyne catalyzed by  $\cdot\text{Mn}(\text{CO})_5$  (relative electronic energies are given in parentheses).



**Fig. S2.** Geometries and key bond lengths (in Å) of stationary points on the PES of hydrogermylation of internal alkyne catalyzed by  $\cdot\text{Mn}(\text{CO})_5$ .



**Fig. S3.** Geometries and key bond lengths (in Å) of stationary points of the complexes formed between  $\cdot\text{Mn}(\text{CO})_5$  and the solvents.