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## Computational study of a self-activate Psbp-Pt Catalyzed 1,6-Enyne Cycloisomerization: The role of a novel Pincer ligand

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Antimony pincer ligands have attracted widely attention in transition metal complexes due to its non-innocent and stability in the presence of oxygen and water compared with other pincer ligands<sup>1</sup>. A newly designed PSbP-Pt complex has been used to catalyze the 1,6-enyne cycloisomerization at mild condition<sup>2</sup>. In this work, the detailed reaction mechanism was studied by density functional theory (DFT) and found that PSbP-Pt<sup>+</sup> could be the catalytic active species instead of PSbP-Pt since the energy difference between HOMO of 1,6-enyne with LUMO of PSbP-Pt is larger than that of PSbP-Pt<sup>+</sup> (Figure 1). Another similar pincer ligand PNP was also studied and found PNP-Pt<sup>+</sup> is more difficult to be formed than PSbP-Pt<sup>+</sup>. PSbP-Pt is proposed to be a self-activate system, whereas PNP-Pt need to be activated by a Lewis acid (Figure 1).

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