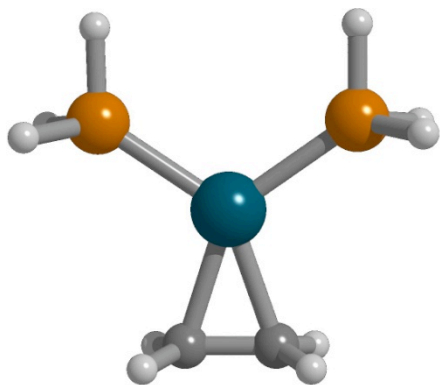
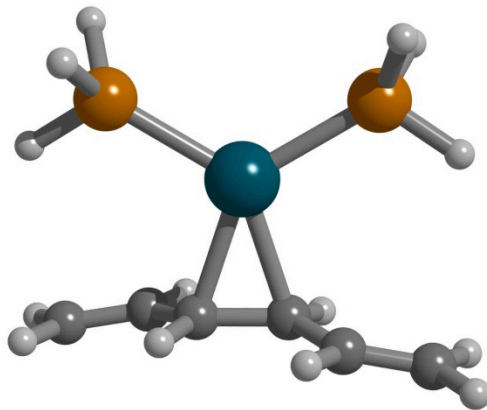


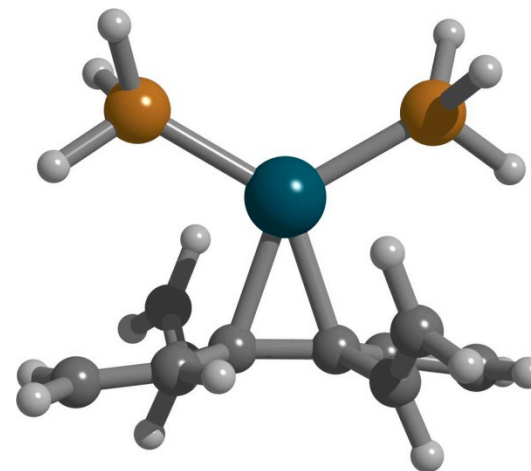
Accuracy of density functionals for $\text{Pd}(\text{PH}_3)_2\text{L}$ complexes where L is ethene or a conjugated C_nH_{n+2} system ($n = 4, 6, 8, \text{ and } 10$)



$\text{Pd}(\text{PH}_3)_2\text{C}_2\text{H}_4$



$\text{Pd}(\text{PH}_3)_2\text{C}_6\text{H}_8$



$\text{Pd}(\text{PH}_3)_2\text{C}_{10}\text{H}_{12}$

Recent studies have shown that popular density functional methods systematically underestimate the binding energy of alkenes and polyenes to Pd and Pt, and the error becomes very large when the size of the conjugated system is increased. We carried out accurate benchmark calculations and more density functional calculations and showed that the Minnesota density functionals (M06, M06-L, M06-D, M06-L-D) predict the binding energy for these systems much more accurately than older functionals. See B. Averkiev, Y. Zhao, and D. G. Truhlar, *Journal of Molecular Catalysis A* **2010**, 324, 80.

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