

# Theoretical Investigation on $S_N2$ with/without Solvation

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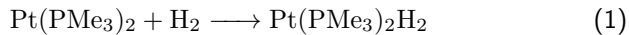
November 9, 2019

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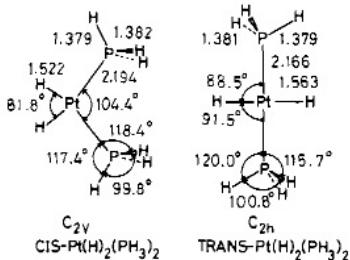
Reaction I

Reaction III

## Oxidative addition of $\text{Pt}(\text{PMe}_3)_2$



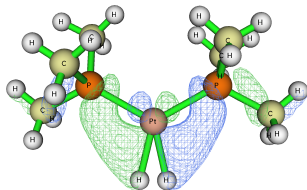
**Question:** *cis* or *trans* product?



Only *cis* product is symmetry allowed. (*cis* product can be converted into *trans*, although)

Kazuo Kitaura, Shigeru Obara, and Keiji Morokuma. In: *J. Am. Chem. Soc.* 103.10 (1981), pp. 2891–2892

TS



Calculated at PBE0/def2-TZVP.

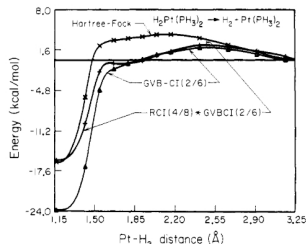
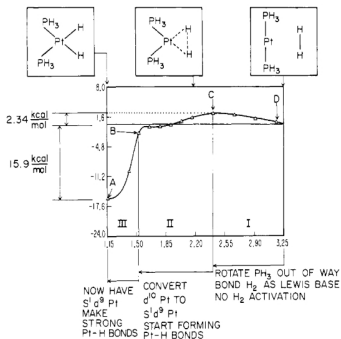
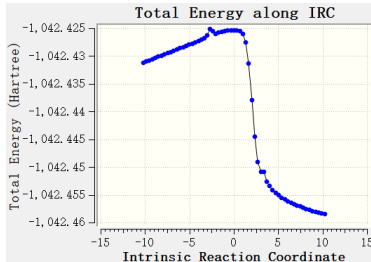


Figure 7. Plot of energy along the reaction coordinate for HF, GVB-CI(2/6), and RCI(4/8)\*GVB-CI(2/6) wave functions.

John J. Low and William A. Goddard III. In: *J. Am. Chem. Soc.* 2.21 (1984), pp. 6928–6937

	$R_{\text{PtH}}(\text{TS})$	$R_{\text{PtH}}(\text{P})$	$A_{\text{HPtH}}(\text{TS})$	$A_{\text{HPtH}}(\text{P})$
M06-2X/SDD/6-31g*	1.860		26.22	

**Table:** Bond length (Å) and bond angle (°) in configurations above

	R	TS	P
$E_{elec}(\text{B2PLYPD3/def2-TZVP})$			
$\Delta G_{freq}(\text{M06-2X/SDD/6-31g}^*)$			
$\Delta G_{sol}(\text{M06-2X/SDD/6-31g}^*)$			

**Table:** Energies

