ICC Report II

Homework Report

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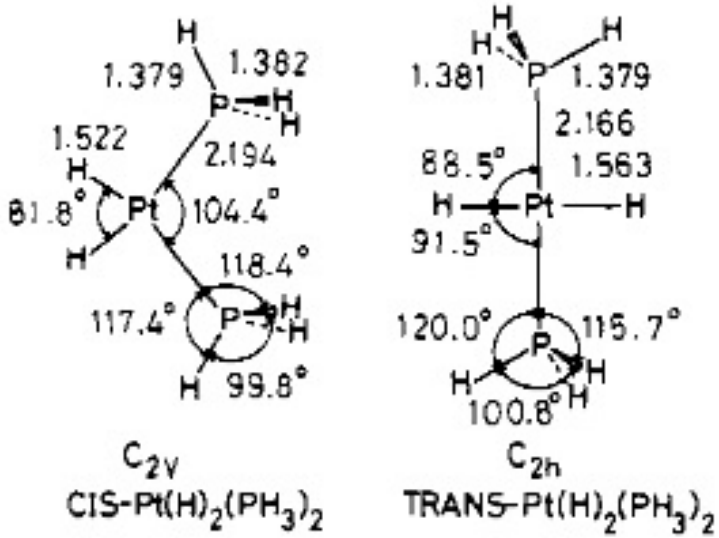
Oxidative addition of $Pt(PMe_3)_2$

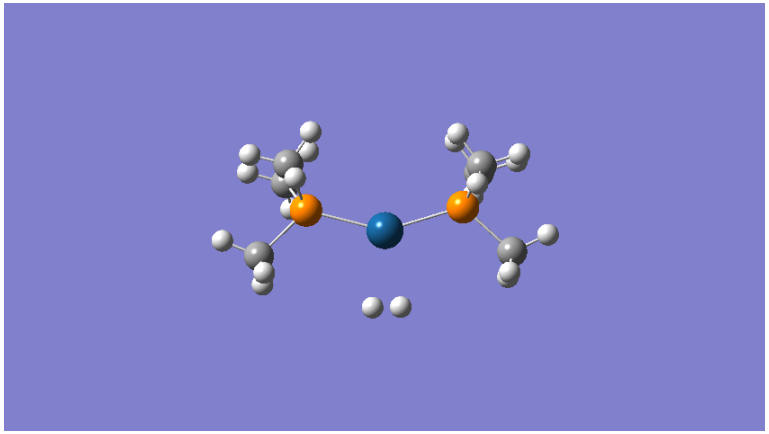
$$Pt(PMe_3)_2 + H_2 \longrightarrow Pt(PMe_3)_2H_2 \tag{1}$$

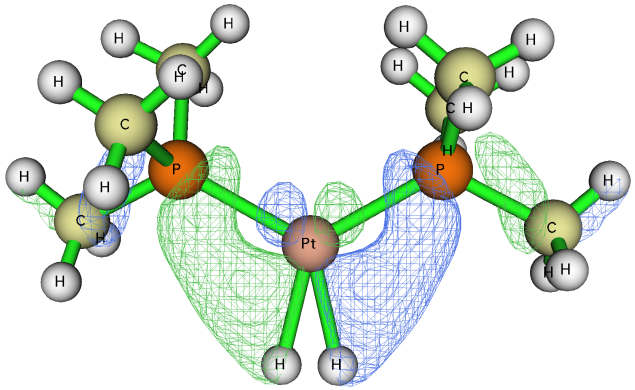
Question: *cis* or *trans* product?



Only *cis* product is symmetry allowed. (*cis* product can be converted into *trans*, although)
Kitaura, K. et al. *J. Am. Chem. Soc.* **1981**, *103*, 2891–2892

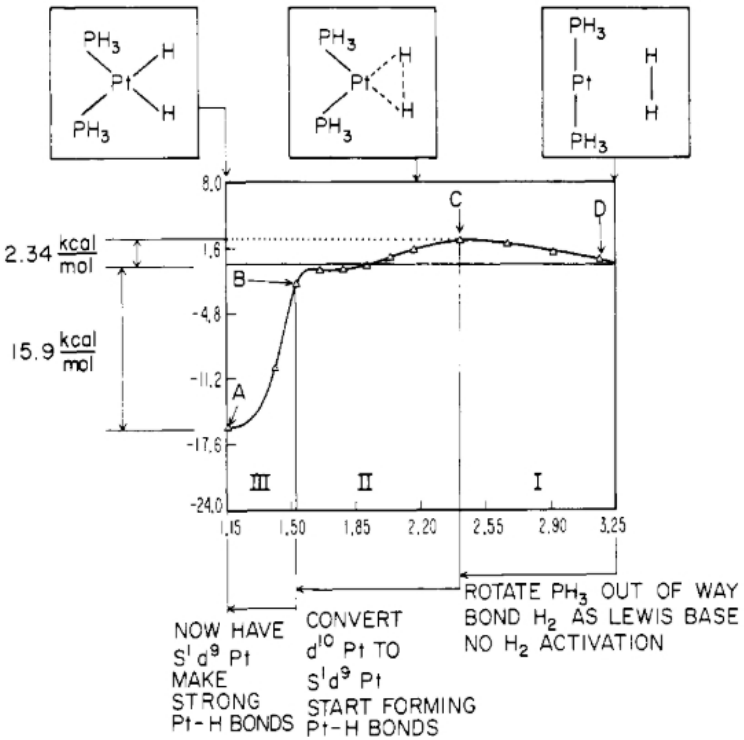
TS





Calculated at PBE0-D3/def2-TZVP.

Reaction path from literature



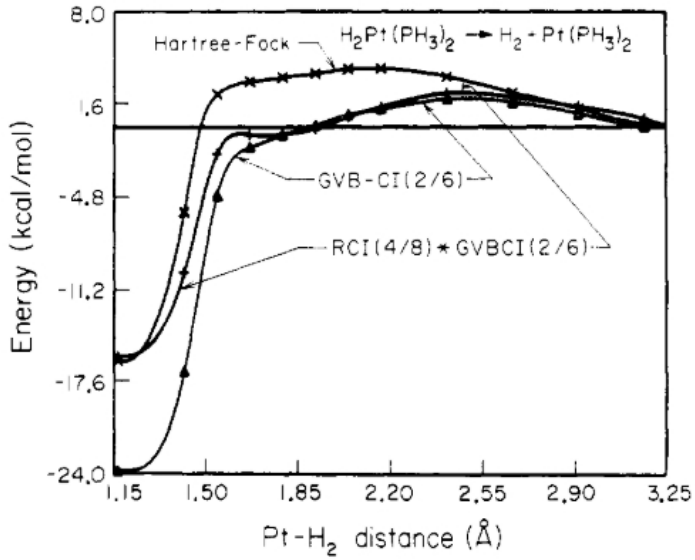
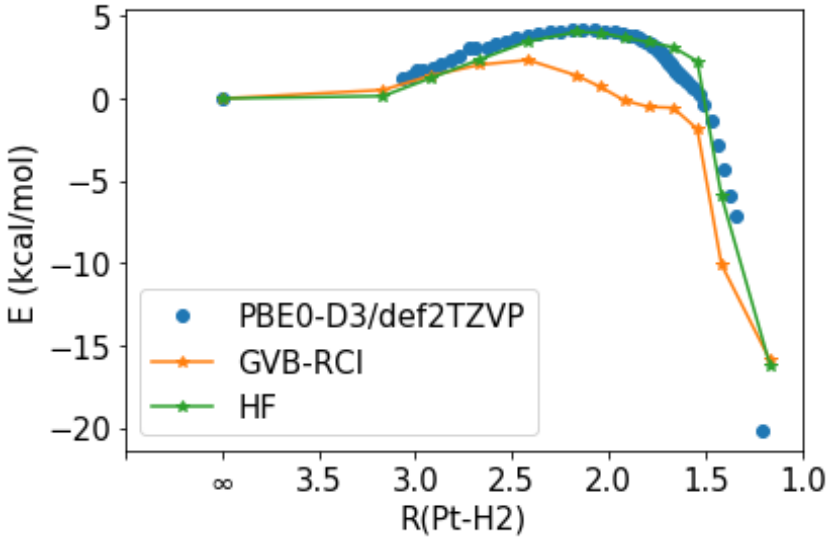
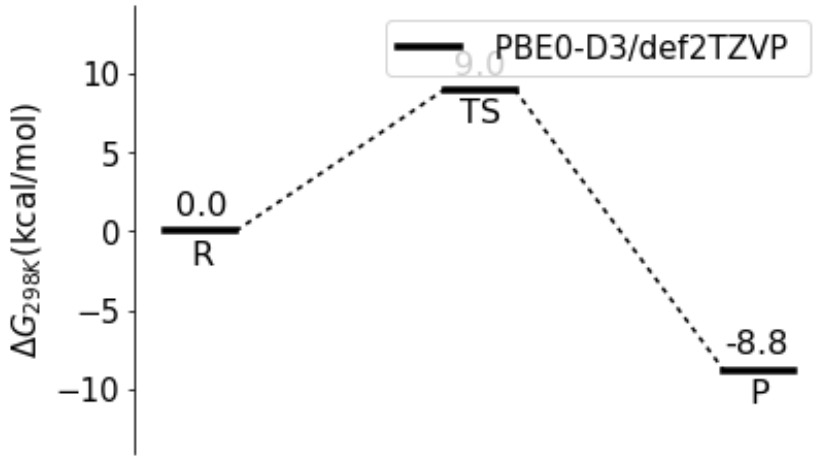


Figure 7. Plot of energy along the reaction coordinate for HF, GVB–CI(2/6), and RCI(4/8)*GVB–CI(2/6) wave functions.

Low, J. J.; Goddard III, W. A. *J. Am. Chem. Soc.* **1984**, *2*, 6928–6937

Reaction Path





	R_{PtH}	A_{HPtH}	R_{PtP}	A_{PPtP}
pre-R	∞	-	2.247	180.0
TS	2.167	20.66	2.244	148.7
P	1.615	83.42	2.290	102.6

Table: Bond lengts (Å) and bond angles (°), at PBE0-D3/def2TZVP

Question: Do we need triplet and MECP calculation?

Charge Transfer

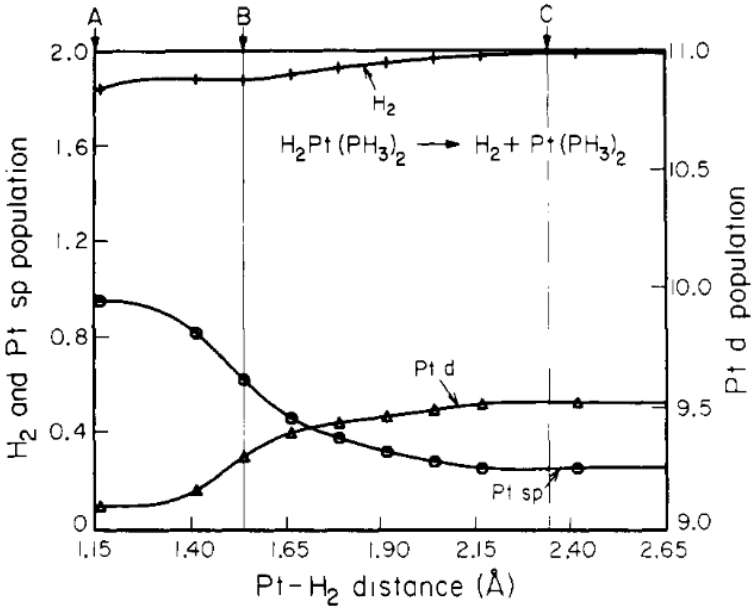


Figure 9. Muliken population along the reaction coordinate.

Low, J. J.; Goddard III, W. A. *J. Am. Chem. Soc.* **1984**, *2*, 6928–6937

Natural Electron Configuration from NBO

	R	TS	P
Pt 5d	9.51	9.52	9.26
Pt 6s	1.12	0.91	0.83
H 1s		1.00	1.23

Natural Bonding

	R	TS	P
Pt-P	$sd^{0.27} - sp^{1.94}(1.97)$	$sd^{0.13} - sp^{1.94}(1.94)$	
Pt-P	$sd^{0.27} - sp^{1.94}(0.45)$	$sd^{0.13} - sp^{1.94}(0.40)$	
Pt-H			$sd^{1.10} - s(1.91)$
Pt-H			$sd^{1.10} - s(0.47)$