

ORGANOMETALLICS

Organometallics, 1998, 17(7), 1278-1289, DOI:[10.1021/om970705i](https://doi.org/10.1021/om970705i)

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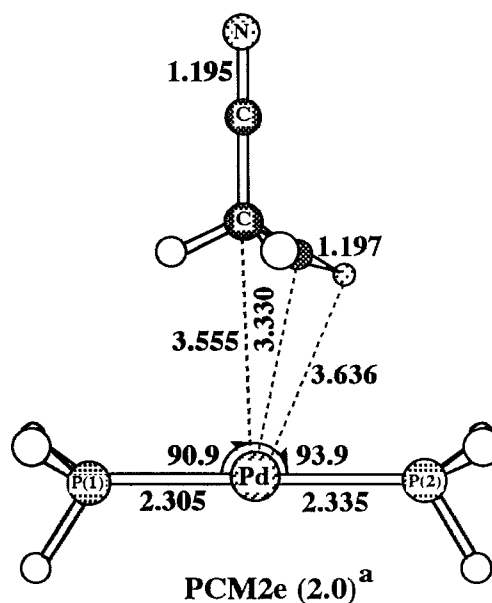
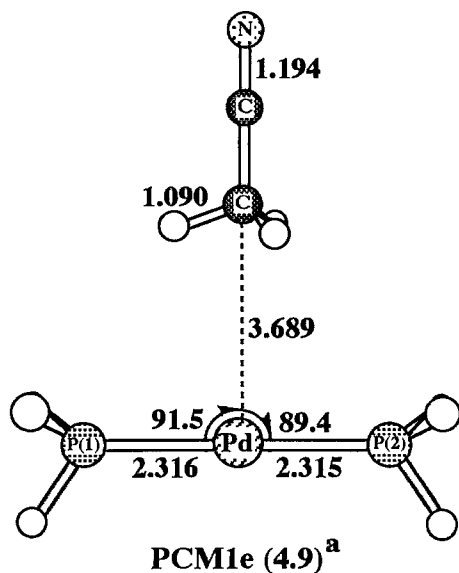
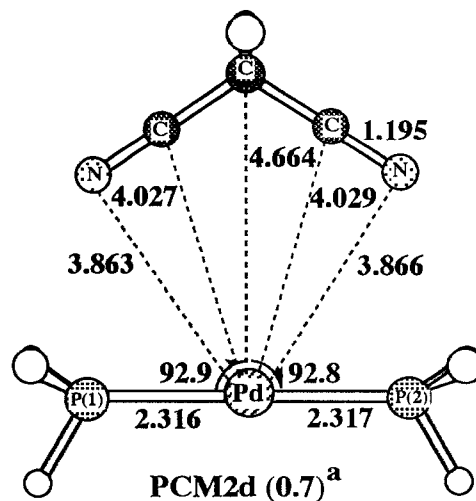
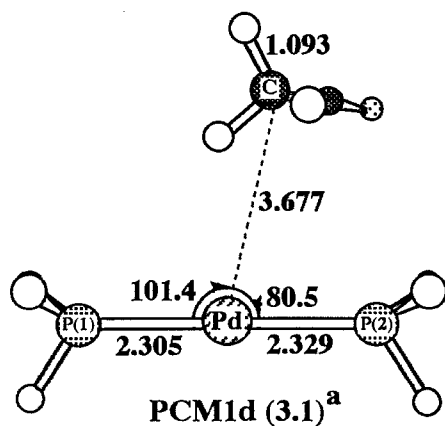
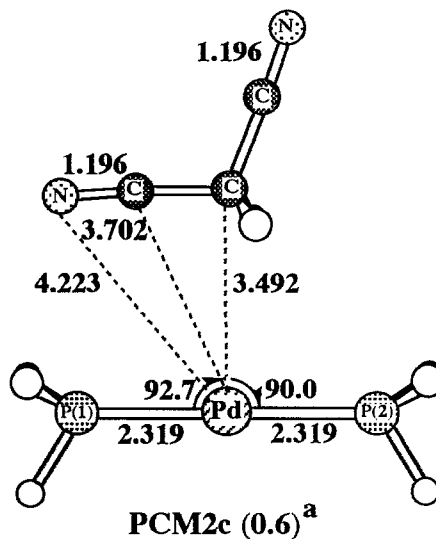
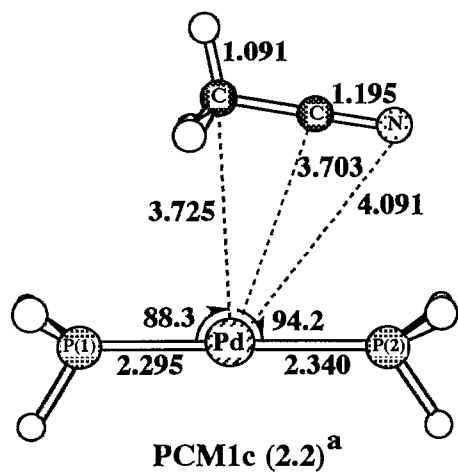
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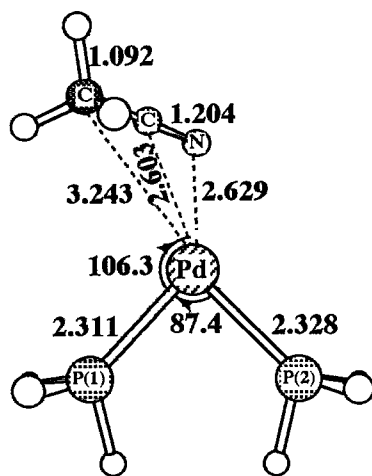
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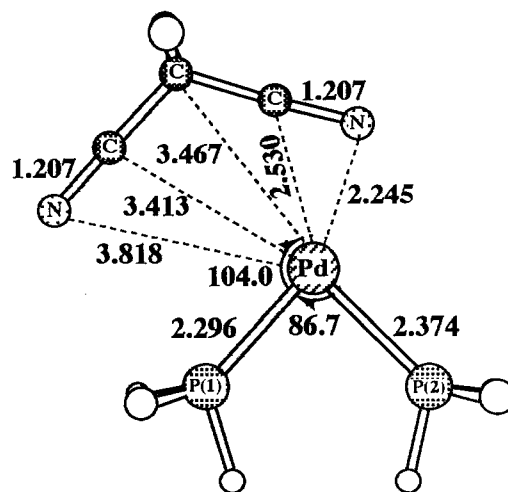
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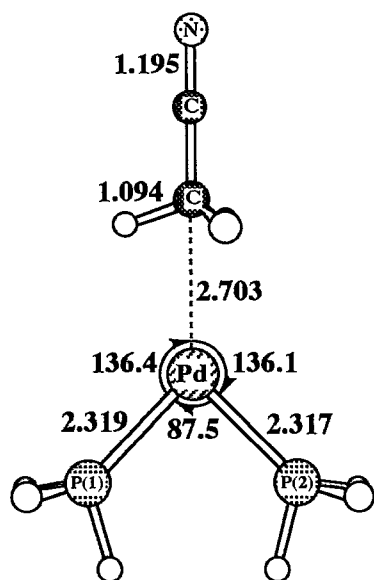
Several possible geometries of precursor complexes in the C-H activation of CH_3CN and $\text{CH}_2(\text{CN})_2$ by $\text{Pd}(\text{PH}_3)_2$. Bond length in Å and bond angle in degree. a) Relative energy to the most stable precursor complex (MP2 values are given). Unit in kcal/mol.



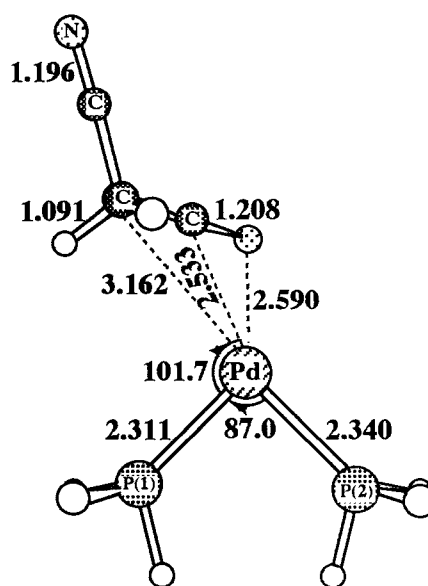
PCM3c (15.9)^a



PCM4c (7.0)^a



PCM3d (20.6)^a



PCM4d (14.4)^a

Several possible geometries of precursor complexes in the C-H activation of CH_3CN and $\text{CH}_2(\text{CN})_2$ by $\text{Pd}(\text{diPE})$. Bond length in Å and bond angle in degree. a) Relative energy to the most stable precursor complex (MP2 values are given). Unit in kcal/mol.