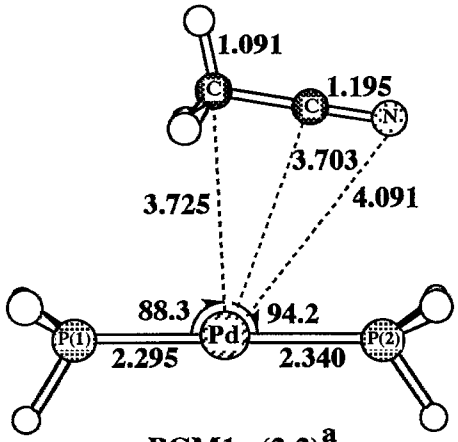
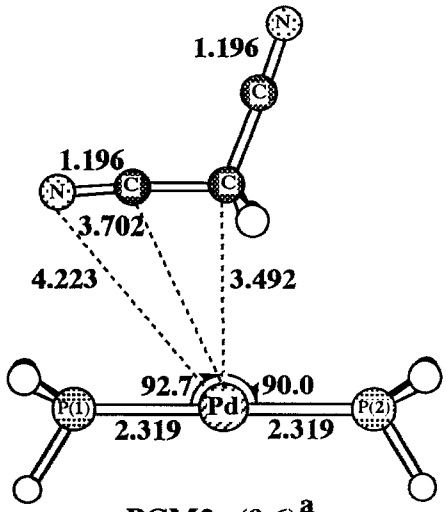
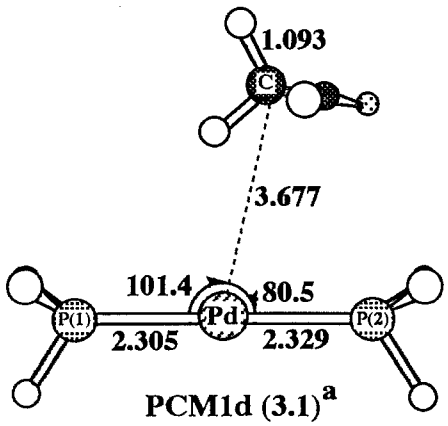
ORGANOMETALLICS
Organometallics, 1998, 17(7), 1278-1289, DOI:10.1021/om970705i



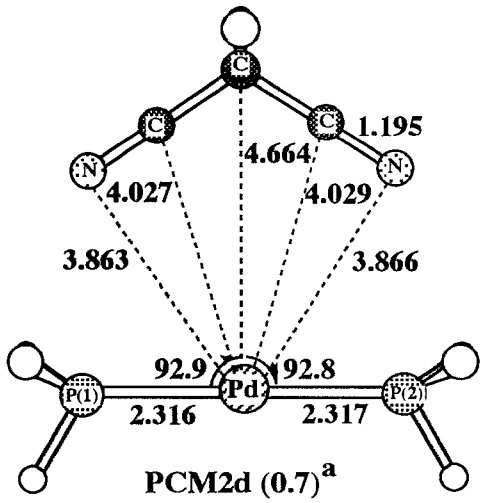
PCM1c (2.2)[a]



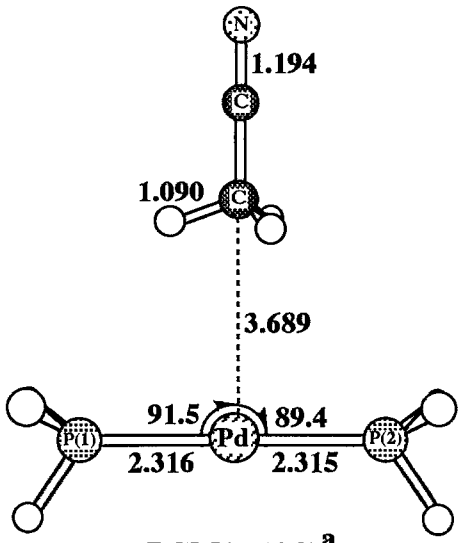
PCM2c (0.6)[a]



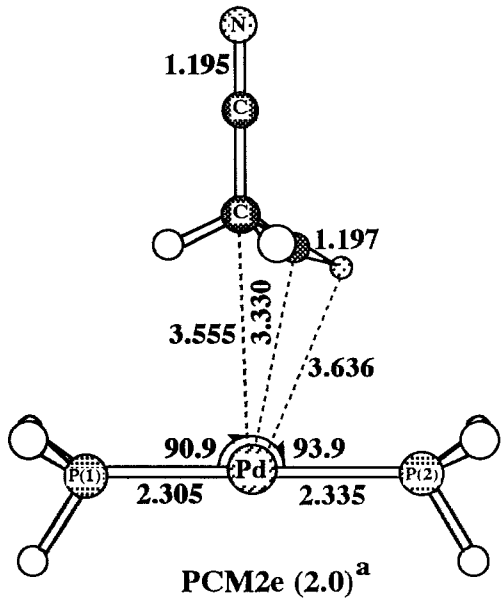
PCM1d (3.1)[a]



PCM2d (0.7)[a]

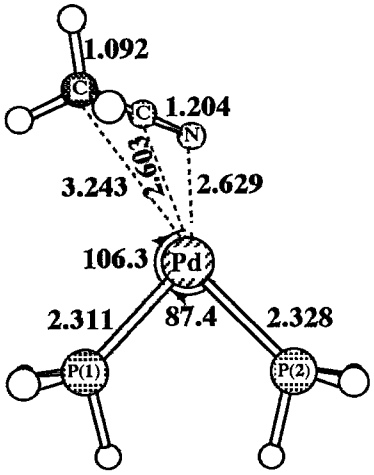


PCM1e (4.9)[a]

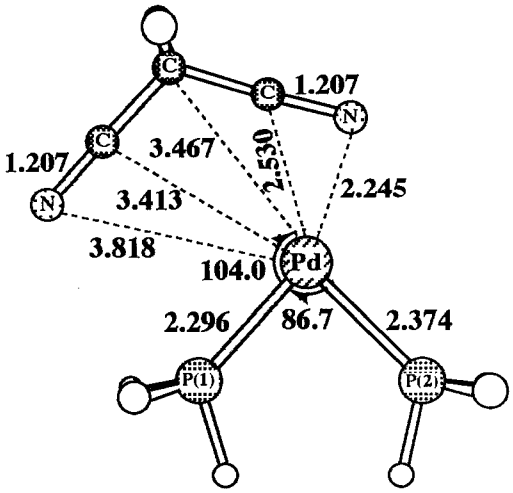


PCM2e (2.0)[a]

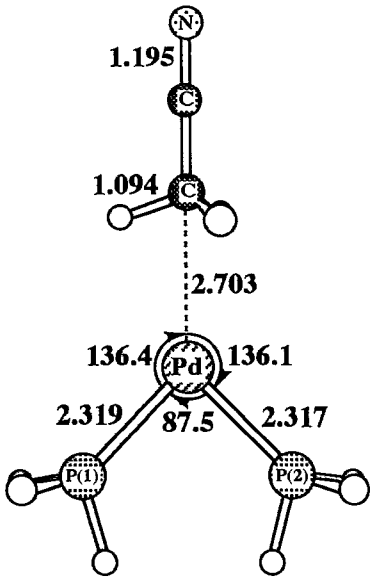
Several possible geometries of precursor complexes in the C-H activation of CH_3CN and $CH_2(CN)_2$ by $Pd(PH_3)_2$. Bond length in Å and bond angle in degree. a) Relative energy to the most stable precursor complex (MP2 values are given). Unit in kcal/mol.



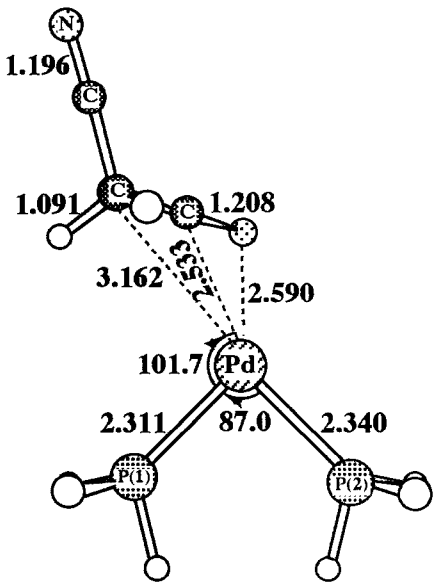
PCM3c (15.9)[a]



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 $CH_2(CN)_2$ by Pd(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.