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Computational Chemistry Study of Effect of Solvent on the Pd Metal Complex

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[Introduction]

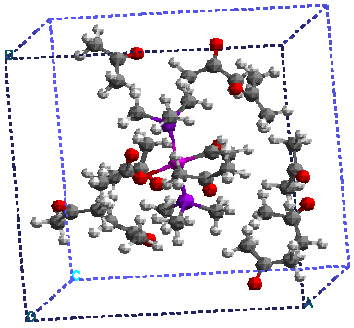
Pd complexes have extensively been utilized in organic synthesis. Several experimental studies on these complexes show that they possess remarkable catalytic properties [1]. However, the understanding of the reaction processes in the atomic and electronic levels is very difficult. On the other hand, recent progress in both computer power and theoretical methods have led to a scenario where calculations can have a significant impact in both the understanding and the optimization of catalytic cycle on complexes [2]. The hydrogenation process of carboxylic anhydrides on acetyl(acetato)bis(trimethylphosphine) palladium(II) complex using first-principles calculations have been clarified. However, the use of such regular first-principles approach can simulate only a small number of atoms owing to the computational limitation. Recently, we have succeeded to develop a tight-binding quantum chemical molecular dynamics code “Colors”, which could alleviate these problems. Hence, in the present investigation, we employed “Colors” code to study the electronic structures and the effect of solvent over above mixed-ligand palladium complex using large models.

[Method]

We employed accelerated quantum chemical molecular dynamics software “Colors”. All the parameters used for “Colors” were determined by first-principles calculations. The Amsterdam density functional (ADF) program was used to determine the parameters for Colors. The results indicate that “Colors” has the same accuracy as that of the first-principles approach.

[Results]

First, using “Colors” we performed the geometry optimization and binding energy calculations for the Pd complex. Structure, energy and charges obtained by “Colors” are in good agreement with that obtained using ADF. Next, the effect of solvent on the Pd complex was investigated. Acetone is used as solvent. Fig.1 shows the dynamic behavior of acetone towards the Pd complex, performed by classical molecular dynamics. Table.1 indicates the atomic charges of the Pd complex without solvent and with solvent, performed by single point calculation in “Colors”. It was also observed that the solvent affects significantly the energy of the complex. In the presentation, we will show more details and discuss about the effect of solvent on the complex.



[Pd(MeCOO)(MeCO)(PMe_3)$_2$]

Table.1. Change of charges by the effect of solvent

	Without solvent		Effect of solvent	
Atoms	Colors			
Pd	0.29		0.27	
P	0.12	0.13	0.11	0.12
O1	-0.27		-0.23	
O2	-0.27		-0.32	
O3	-0.21		-0.31	
C1 (methyl)	-0.15	0.13	-0.15	0.13
C2 (methyl)	-0.002		-0.06	
C3 (carbonyl)	0.2		-0.16	
H	0.005	0.027	0.0001	0.09

[References]

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