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Erratum to "Theoretical Study of the Reaction of (2, 2)-Dichloro (Ethyl) Arylphosphine with Bis (2, 2)-Dichloro (Ethyl) Arylphosphine by Hydrophosphination Regioselective by the DFT Method" [Computational Chemistry 5 (2017) 113-128]

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The original online version of this article (Kouadio Valery Bohoussou[1], Anoubilé Benié[2], Mamadou Guy-Richard Koné[1], Affi Baudelaire Kakou[2], Kafoumba Bamba[1], Nahossé Ziao[1]) Theoretical Study of the Reaction of (2, 2)-Dichloro (Ethyl) Arylphosphine with Bis (2, 2)-Dichloro (Ethyl) Arylphosphine by Hydrophosphination Regio selective by the DFT Method. Computational Chemistry 5 (2017) 113-128. DOI: 10.4236/cc.2017.53010) unfortunately contains a mistake. The author wishes to correct the errors from Table 3 to Table 4, on page 121 and the beginning of page 122.

On analysis of the values in Table 3, phosphines 1a and 1b have the highest values of the local nucleophilic indices N_k. Similarly, the carbon C_1 of the compound R_2 has the highest value of the local electrophilic index (ω_k). This shows that the most favored interaction takes place between the P_1 atom of the compound 1a and the C_1 atom of the compound R_2 for the first reaction, and between the P_9 and C_1 atoms for the second reaction. Therefore, the formation of experimentally observed P_1-C_1 and P_2-C_1 bonds are correctly predicted by the Domingo model with the Mulliken and NPA approaches.

Table 3. Local reactivity descriptors on the P_1, P_2, C_1 and C_2 atoms of reactants 1a, 1b and R_2 using NPA and Mulliken population analyzes at B3LYP/6-311 + G (d, p).

		1a	1b	R_2	
Atomes		**P_1**	**P_2**	**C_1**	**C_2**
Mulliken	f_k^+			**0.352**	−0.245
	f_k^-	0.358	**0.218**		
	ω_k			**0.4872**	−0.339
	N_k	**0.904**	**0.598**		
NPA	f_k^+			**0.358**	0
	f_k^-	0.092	**0.313**		
	ω_k			**0.4880**	0.208
	N_k	**0.252**	**0.858**		

3.3.2. Prediction Using the Gazquez-Mendez Model

The prediction according to the Gazquez-Mendez model presents values of the Fukui function (f_k^+ , f_k^-), local softness S_k^+ for reactants R2 and local softness S_k^- for reactants 1a or 1b. These values of the local descriptors on the atoms P_1, P_2, C_1 and C_2 of the reactants 1a, 1b and R2 were calculated according to the Gazquez-Mendez model with the NPA population analyzes and MK at the B3LYP 6-311+G level (d, p) are given in **Table 4**. f_k^+ , f_k^-), local softness k S+ for reactants R2 and local softness kS—for reactants 1a or 1b. These values of the local descriptors on the atoms P_1, P_2, C_1 and C_2 of the reactants 1a, 1b and R2 were calculated according to the Gazquez-Mendez model with the NPA population analyzes and MK at the B3LYP 6-311+G level (d, p) are given in **Table 4**. Examination of the values in **Table 4** indicates that the phosphines 1a, and dichloroethylene R2 have similar values of local softnesses (S_k^+ , S_k^-) by the approach of Mulliken. This observation shows that the most favored interaction takes place between the P_1 atom of the compound 1a and the C1 atom of the dichloroethylene.

Table 4. Values of Fukui Functions (f_k^+ , f_k^-), local softnesses, S_k^+ for reactants R2 and local softness, S_k^- for reactants 1a and 1b calculated by NPA, MK.

Réactants		1a	1b	R_2	
Atomes		**P_1**	**P_2**	**C_1**	**C_2**
Mulliken	f_k^+			0.352	−0.245
	f_k^-	0.358	0.218		
	S_k^+			**0.052**	−0.036
	S_k^-	**0.060**	0.040		
NPA	f_k^+			0.358	0
	f_k^-	0.092	0.121		
	S_k^+			0.053	0.000
	S_k^-	0.015	0.021		

That the most favored interaction takes place between the P_1 atom of the compound 1a and the C_1 atom of the dichloroethylene for the first reaction and the P_2 atom of the compound 1b and the C_1 atom of the dichloroethylene for the second reaction.