

SUPPORTING INFORMATION

Peroxo-Transition Metal Systems: Examples of Electromerism in Palladium Structures

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Table 4. Charge to the Pd, C, N, P, Cl

<i>Nr.</i>	<i>C*</i>	<i>N*</i>	<i>P*</i>	<i>Cl*</i>
1	-0.12	-		
3	-0.13			
4	-0.15			
6	-0.15	-0.37		
7	-0.22	-		
8	-0.16	-0.38		
9	-0.14	-	0.17	
11	-0.12	-	0.21	
12	-	-0.38	-	-0.49
13	-	-0.43	-	-0.45
14	-	-	-	
16	-	-0.27	-	
17	-	-0.39	-	
18_Pd1	-	-0.3	-	-
18_Pd2	-	-0.27	-	-
19	-	-0.40	-	

*sum of all atoms of C, N, P or Cl bonded to Pd