Supporting Information

Theoretical Study on Electronic Structural Properties of Catalytically Reactive Metalloporphyrin Intermediates

Meijuan Cao[1], Aijing Gao[1], Yuanyuan Liu[2], Yang Zhou[2*], Zhicheng Sun[1*], Yaling Li, [1] Furui He[2], Luhai Li[1*], Lixin Mo[1], Ruping Liu[1], Yumeng Han[1] and Yonggang Yang[1]

[1] Beijing Engineering Research Center of Printed Electronics, Beijing Institute of Graphic Communication, Beijing 102600,China. Email: sunzhicheng@bigc.edu.cn and liluhai@bigc.edu.cn

[2] School of Chemical Engineering and Technology and Key Laboratory of Advanced Materials of Tropical Island Resources of Ministry of Education, Hainan University, Haikou, Hainan 570228, China. Email: yzhou@hainanu.edu.cn

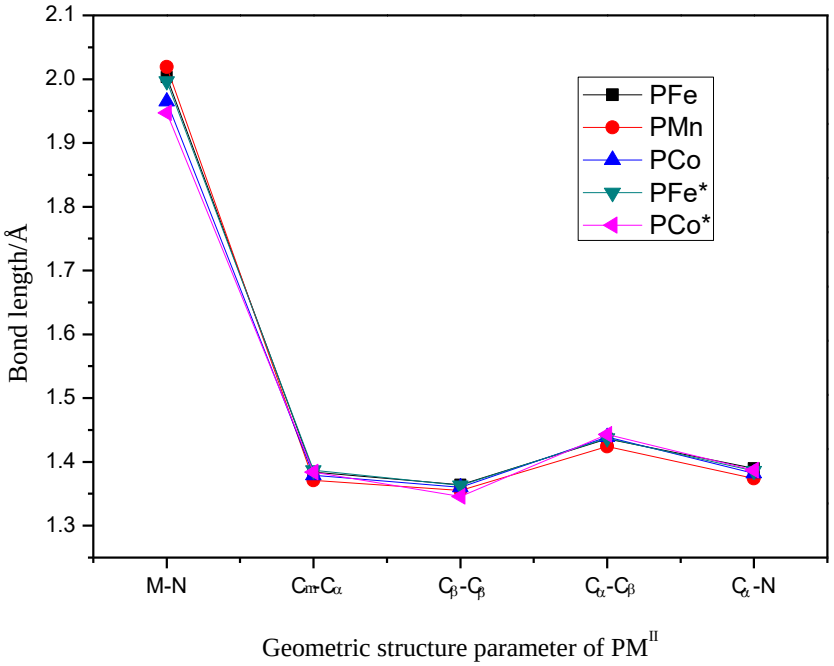

Figure S1. Geometric parameters of the ground state for PM^{II} (* presents the experimental value).

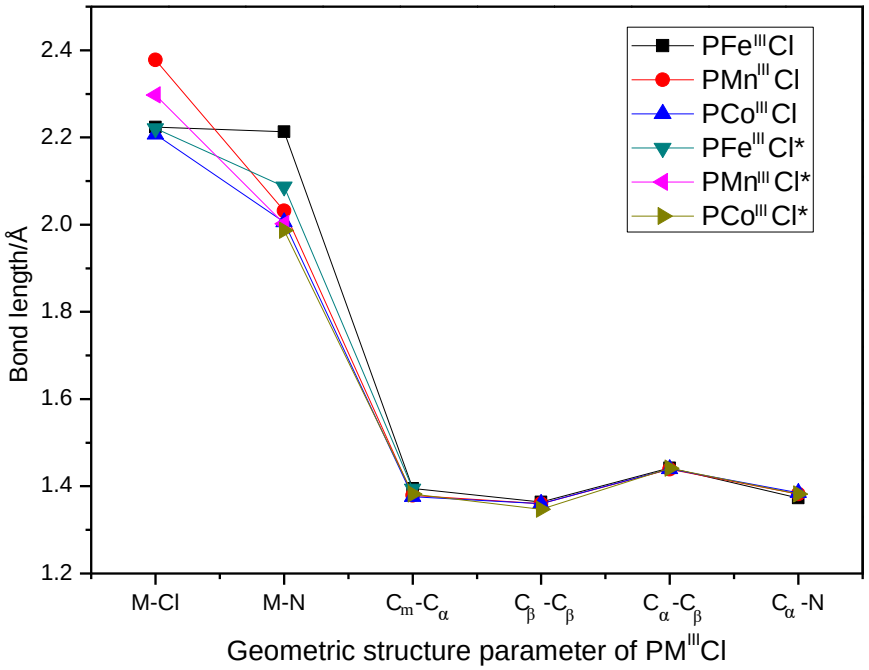

Figure S2. Geometric parameters of the ground state for $PM^{III}Cl$ (* presents the experimental value).

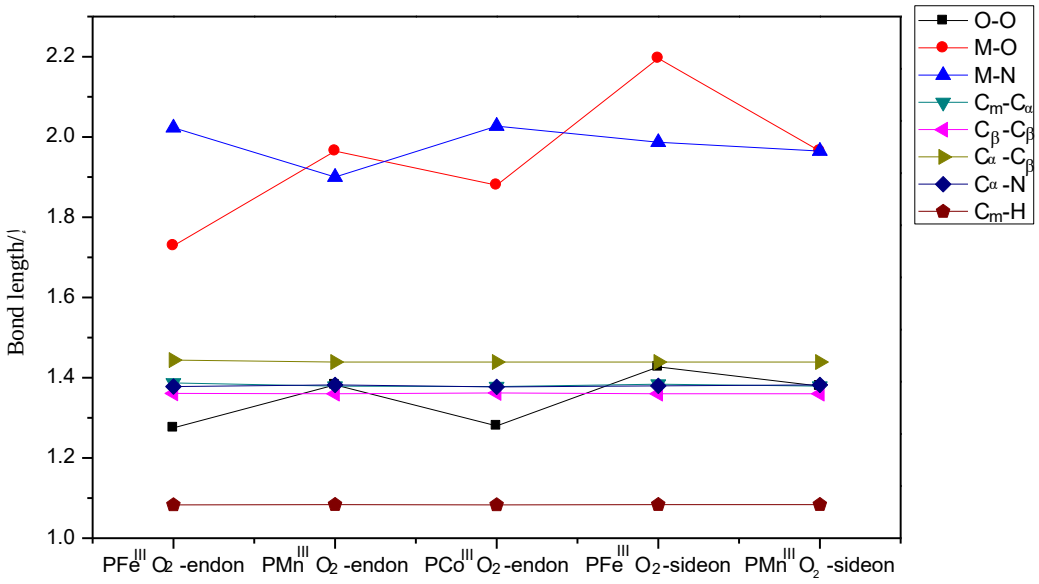

Figure S3. Geometric parameters of side-on and end-on PM^{II}-O_2 intermediates.