Electronic Supplementary Material (ESI) for Chemical Communications

Intramolecular Reorganization Energy in Zinc Phthalocyanine and its Fluorinated Derivatives: A Joint Experimental and Theoretical Study

Demetrio A. da Silva Filho[*a,c], Veaceslav Coropceanu[c], Nadine E. Gruhn[b], Pedro Henrique de Oliveira Neto[a] and Jean-Luc Brédas

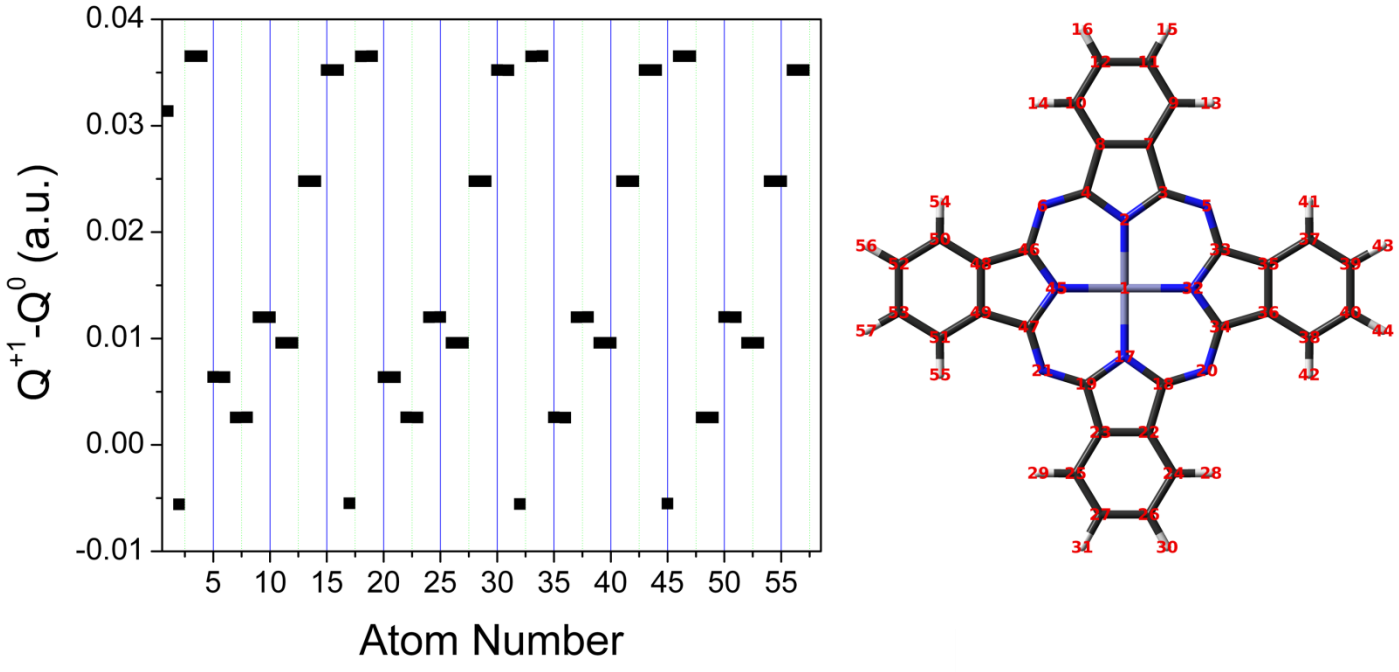
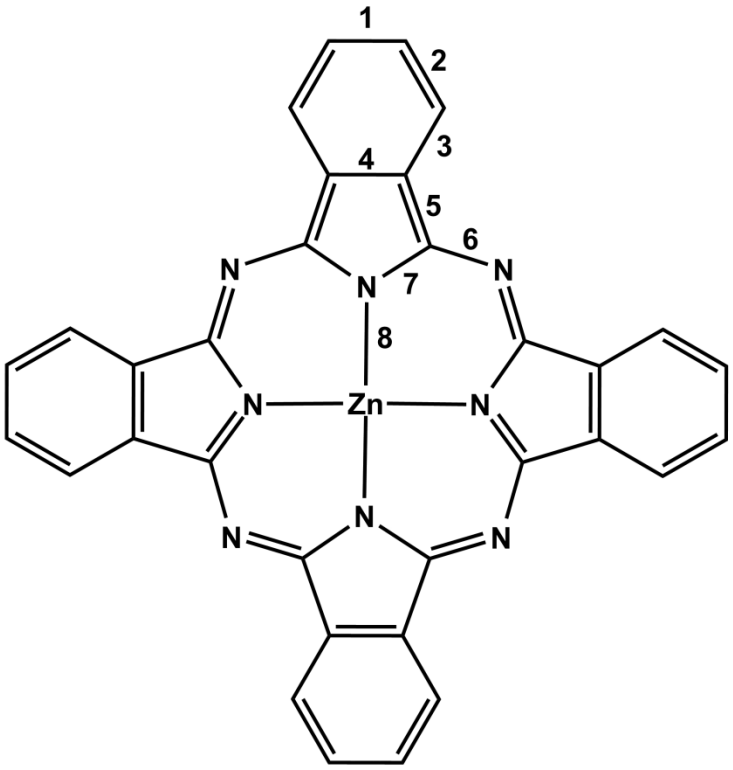


Figure S1. (left) Difference between the Mulliken population of each atom in the cation and neutral state of ZnPc. (right) ZnPc molecule with the atom labels used in the plot.



Bond Length	Change (10^{-4}Å)
1	-62
2	71
3	-52
4	-19
5	38
6	1
7	6
8	-37

Figure S2. (left) ZnPc molecule with the bond labels used on the table. (right) Table with the differences between the bond lengths in the cation and neutral state. The bond lengths of equivalent (D_{4h}) bonds were averaged to simplify the table.

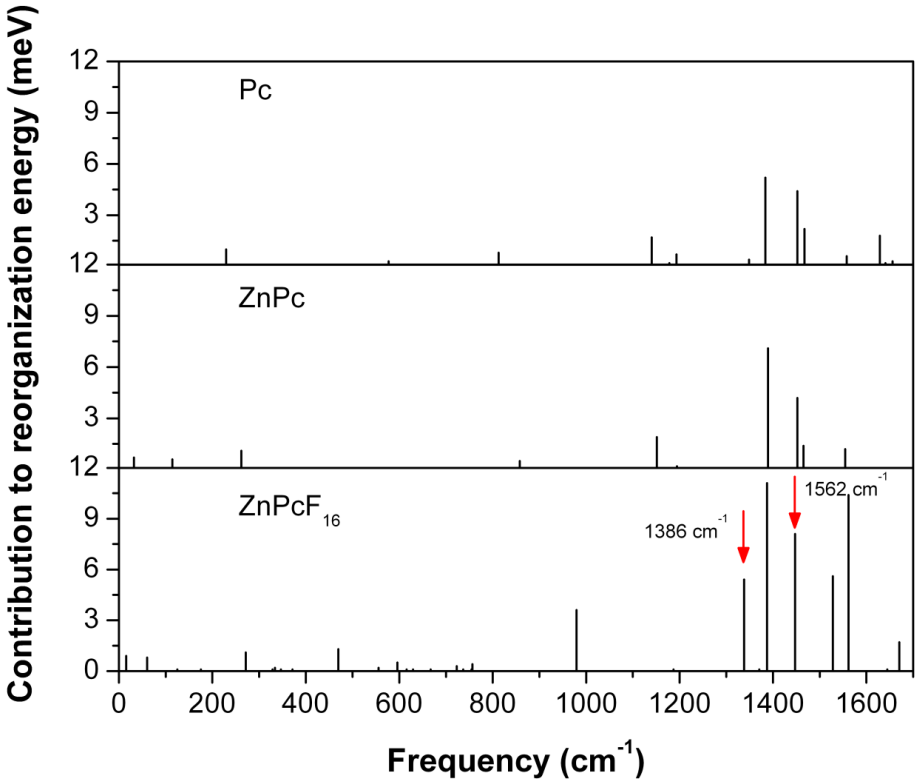


Figure S3. Contribution of the vibrational modes of the Pc (top), ZnPc (center) and $ZnPcF_{16}$ (bottom) molecules to the reorganization energy associated with the formation of a positive polaron, as calculated at the DFT/UB3LYP level.

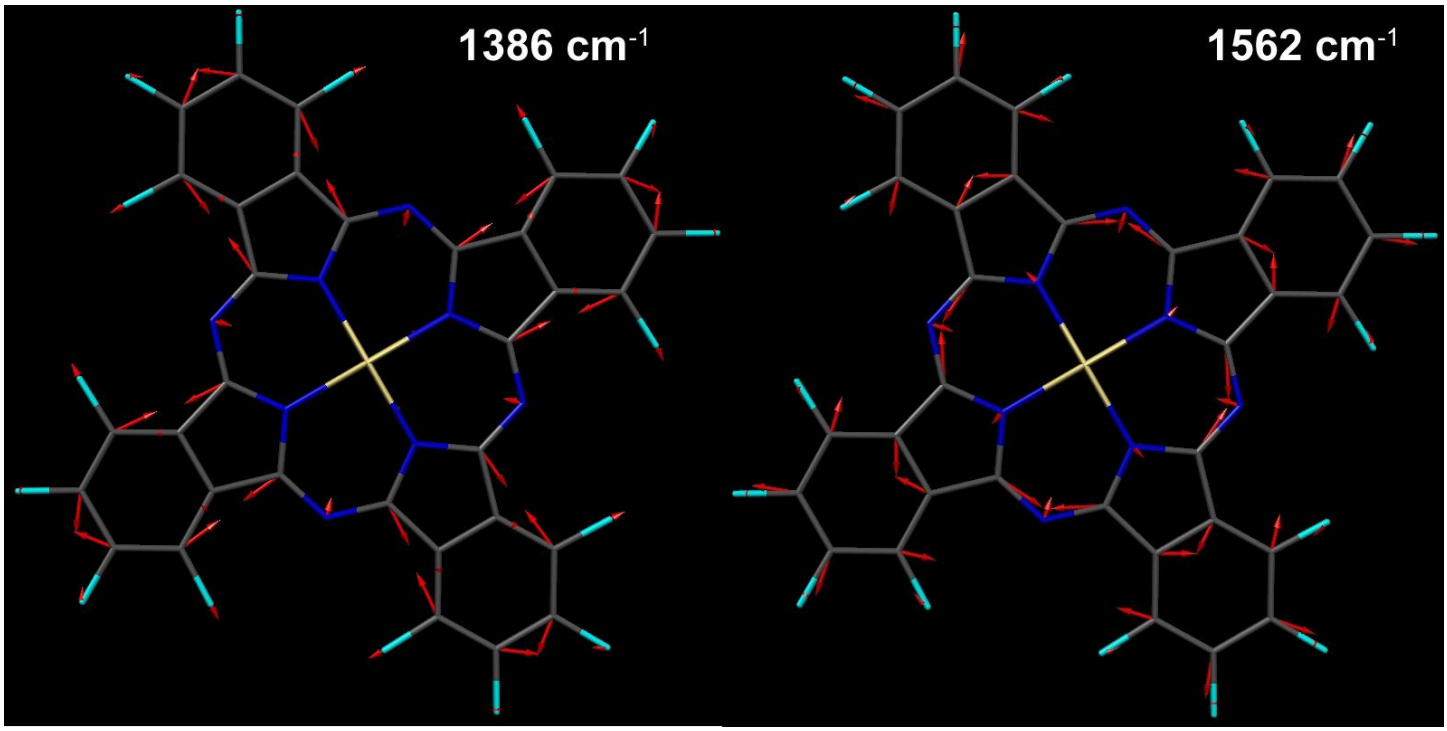


Figure S4. Vibrational modes identified on Figure S3.

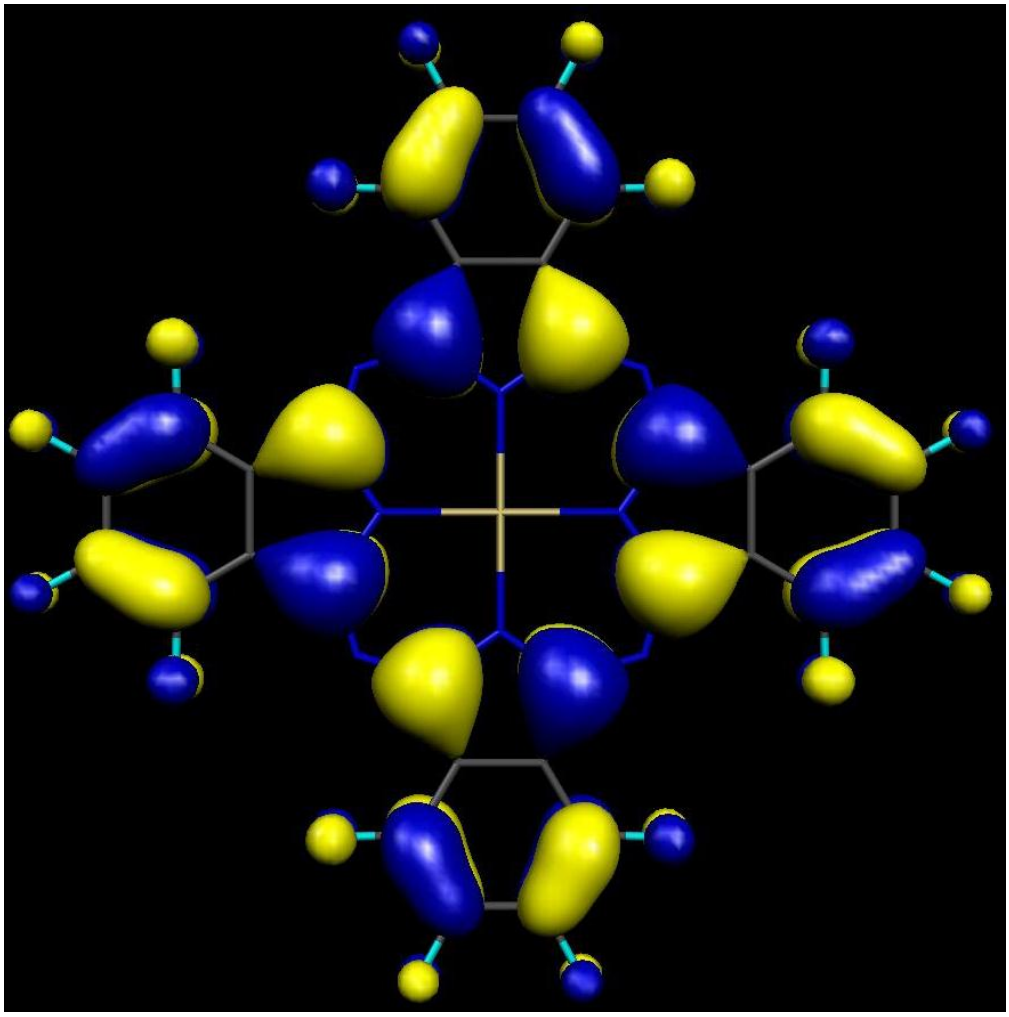


Figure S5. HOMO level of $ZnPcF_{16}$, as calculated at the DFT/B3LYP level.