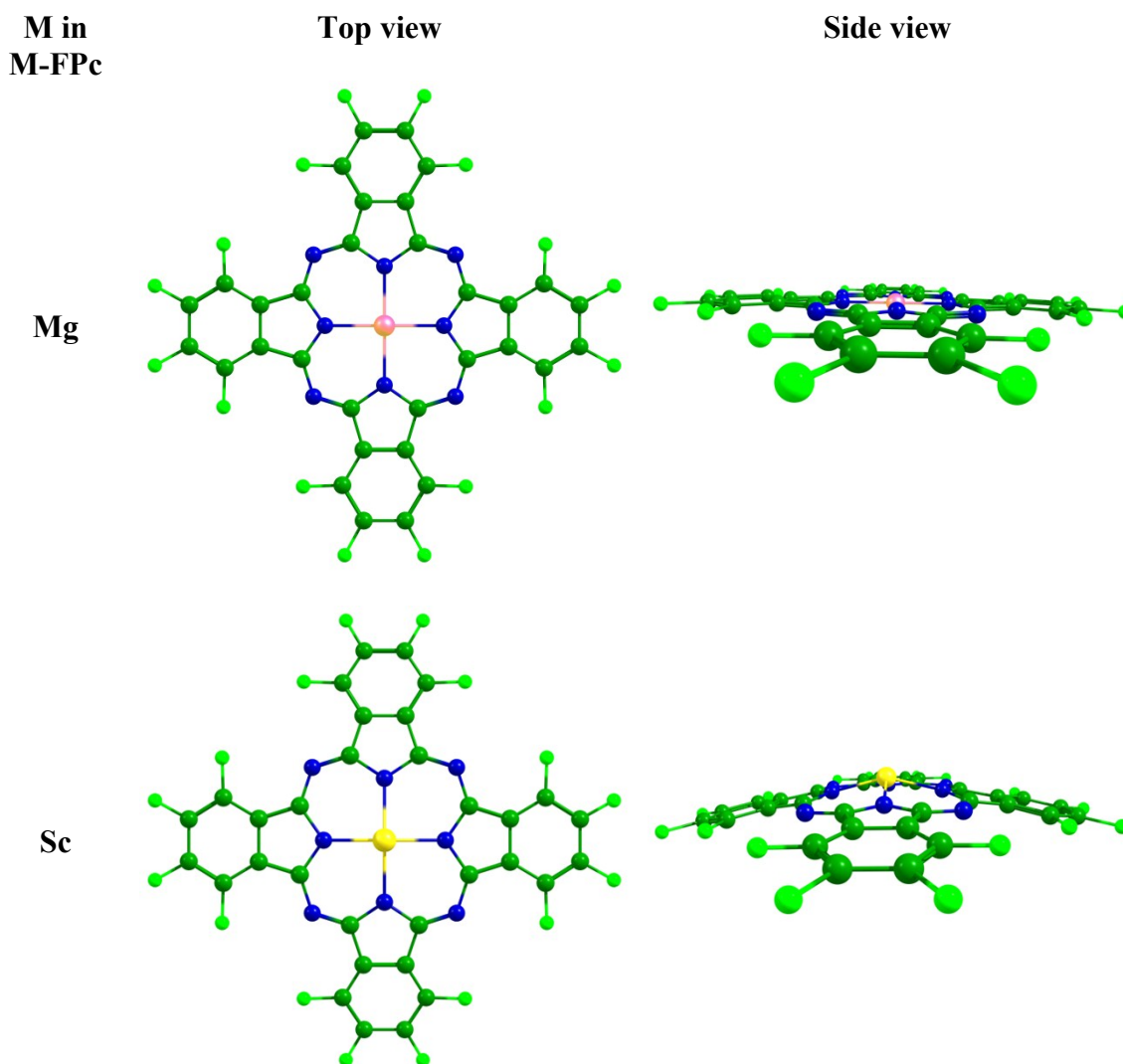


**Supplementary information:**



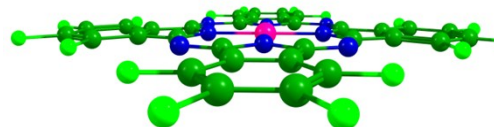
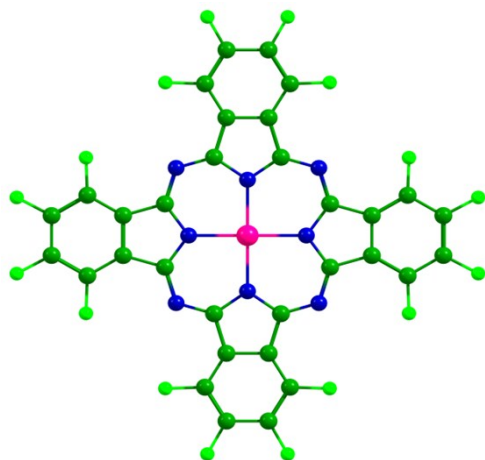
**Figure S1 Optimised configuration of fluorinated metal phthalocyanine sheets (M-FPc)**  
**(Top and side view)**

**M in  
M-FPc**

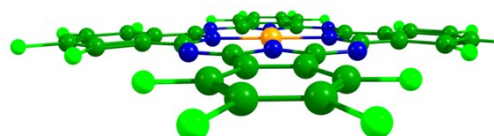
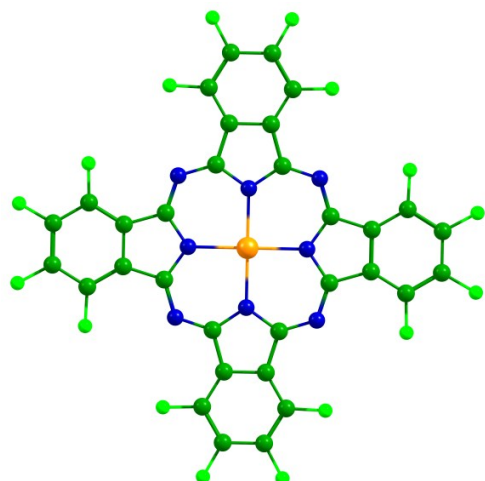
**Top view**

**Side view**

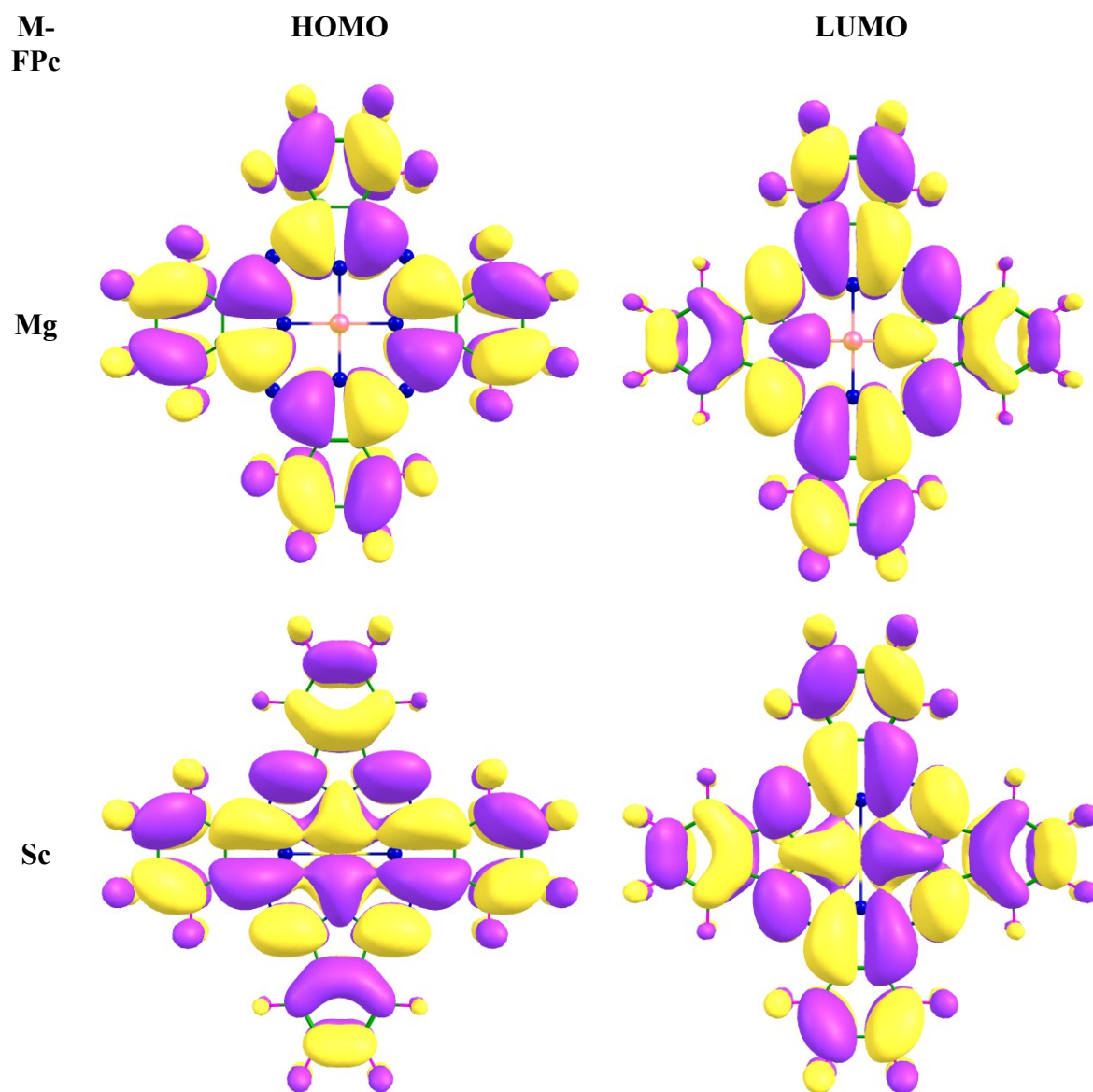
**Cu**



**Zn**



**Figure S1 Continued**



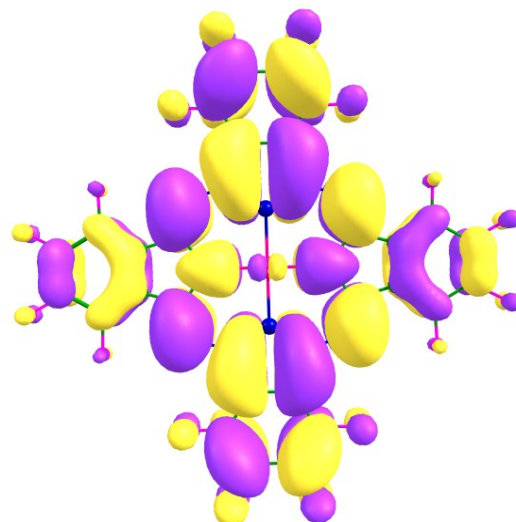
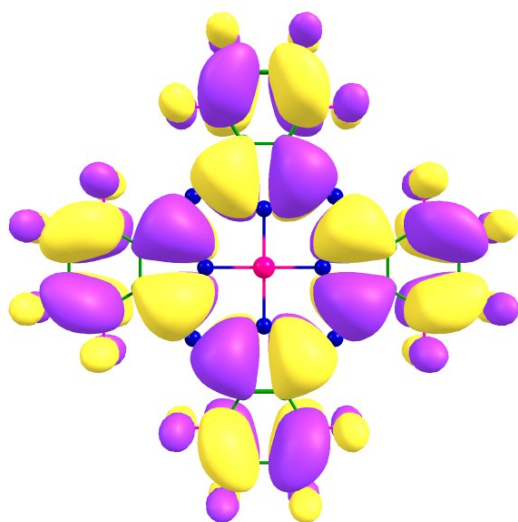
**Figure S2 HOMO and LUMO plot of fluorinated metal phthalocyanine sheets (M-FPc)**

**M-  
FPc**

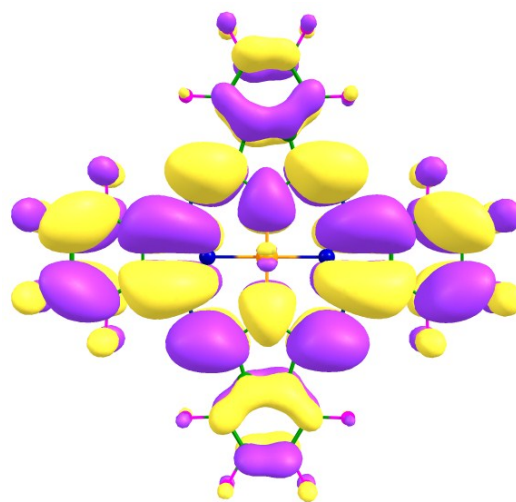
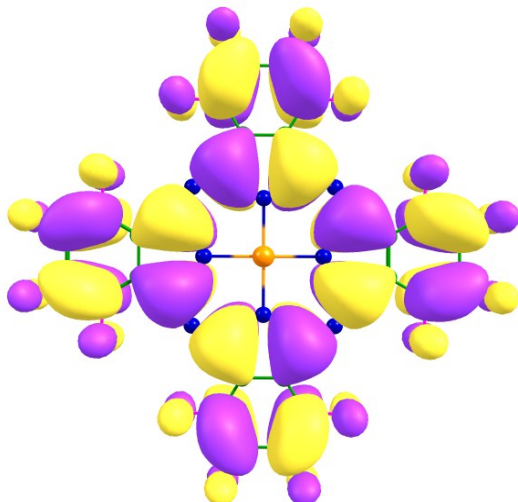
**HOMO**

**LUMO**

**Cu**



**Zn**



**Figure S2 Continued**

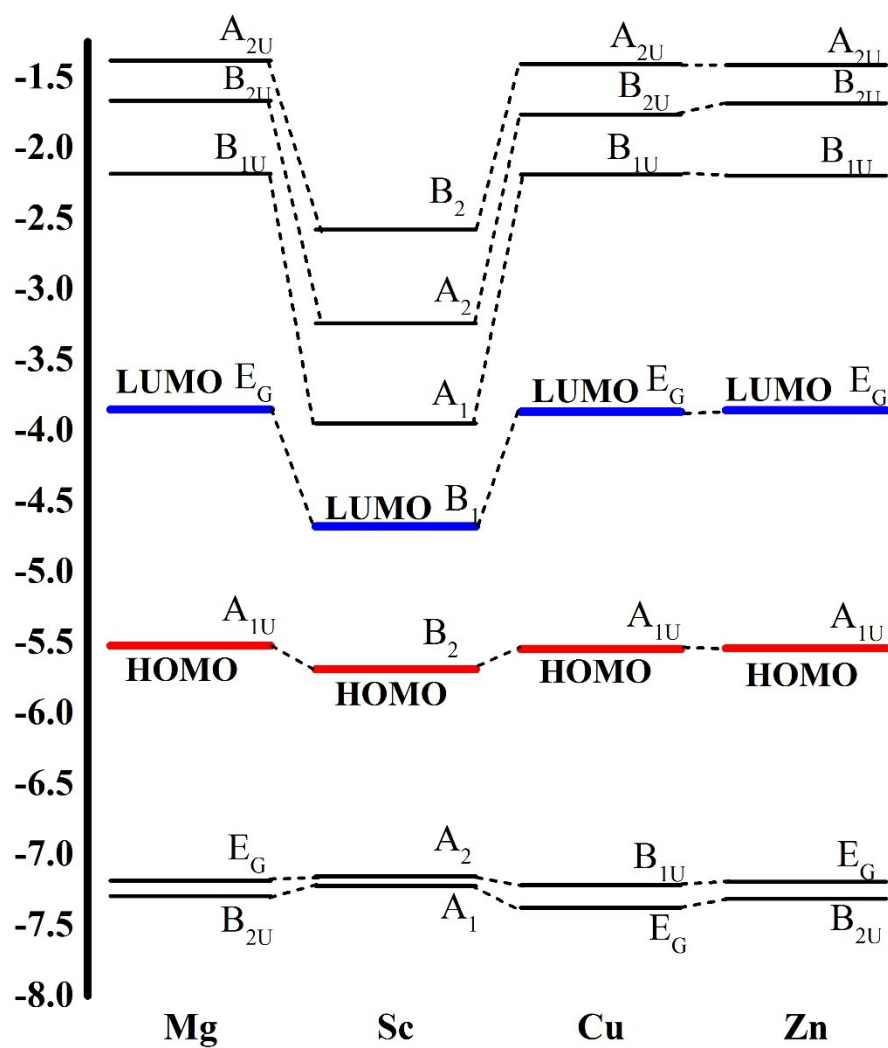


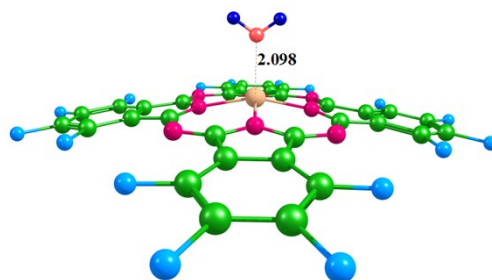
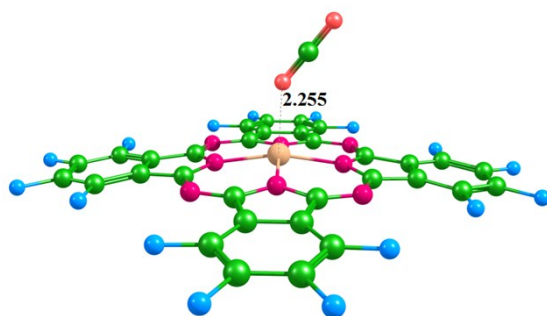
Figure S3 Molecular Orbital diagram of fluorinated metal phthalocyanine sheets (M-FPc)

FPc

CO<sub>2</sub>

H<sub>2</sub>O

Mg



Sc

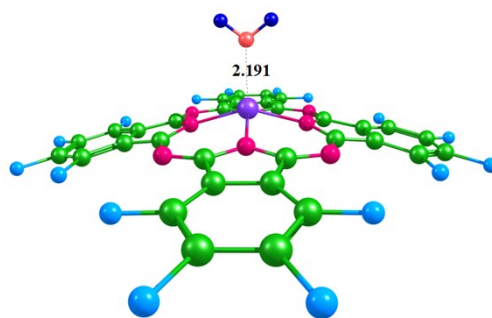
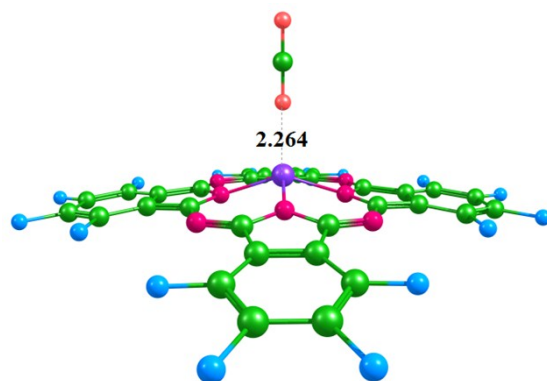


Figure S4 Optimized structures of M-FPcs with guest molecules

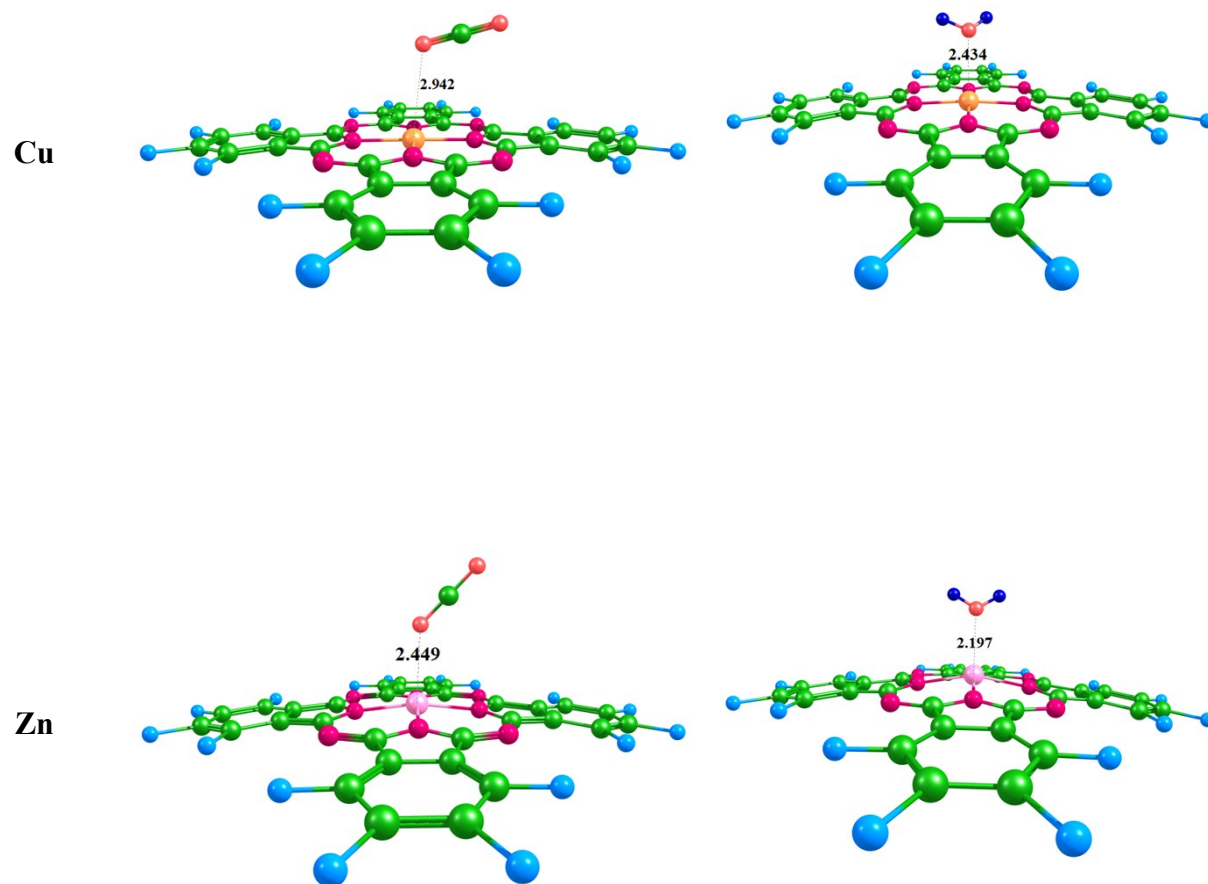
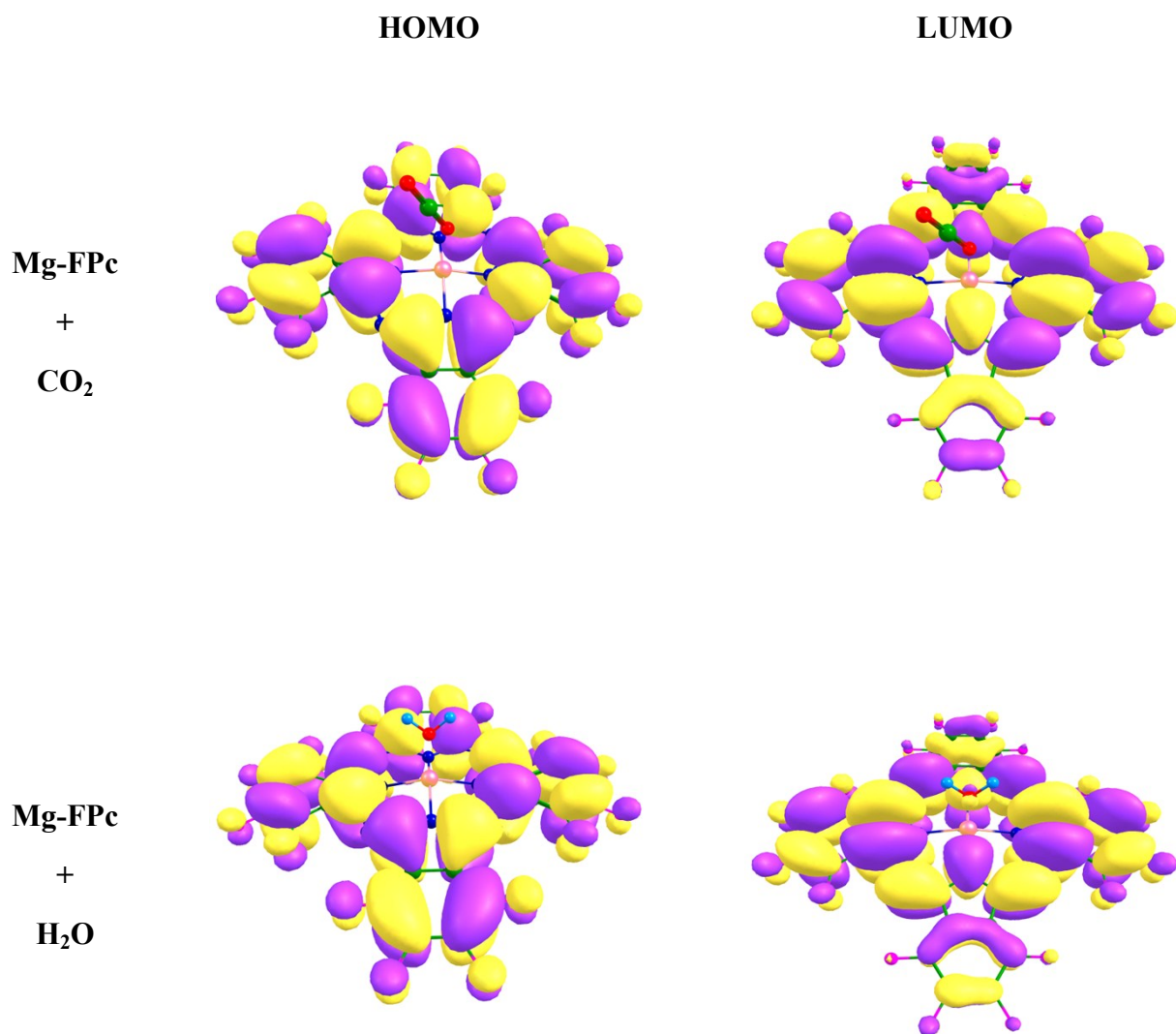


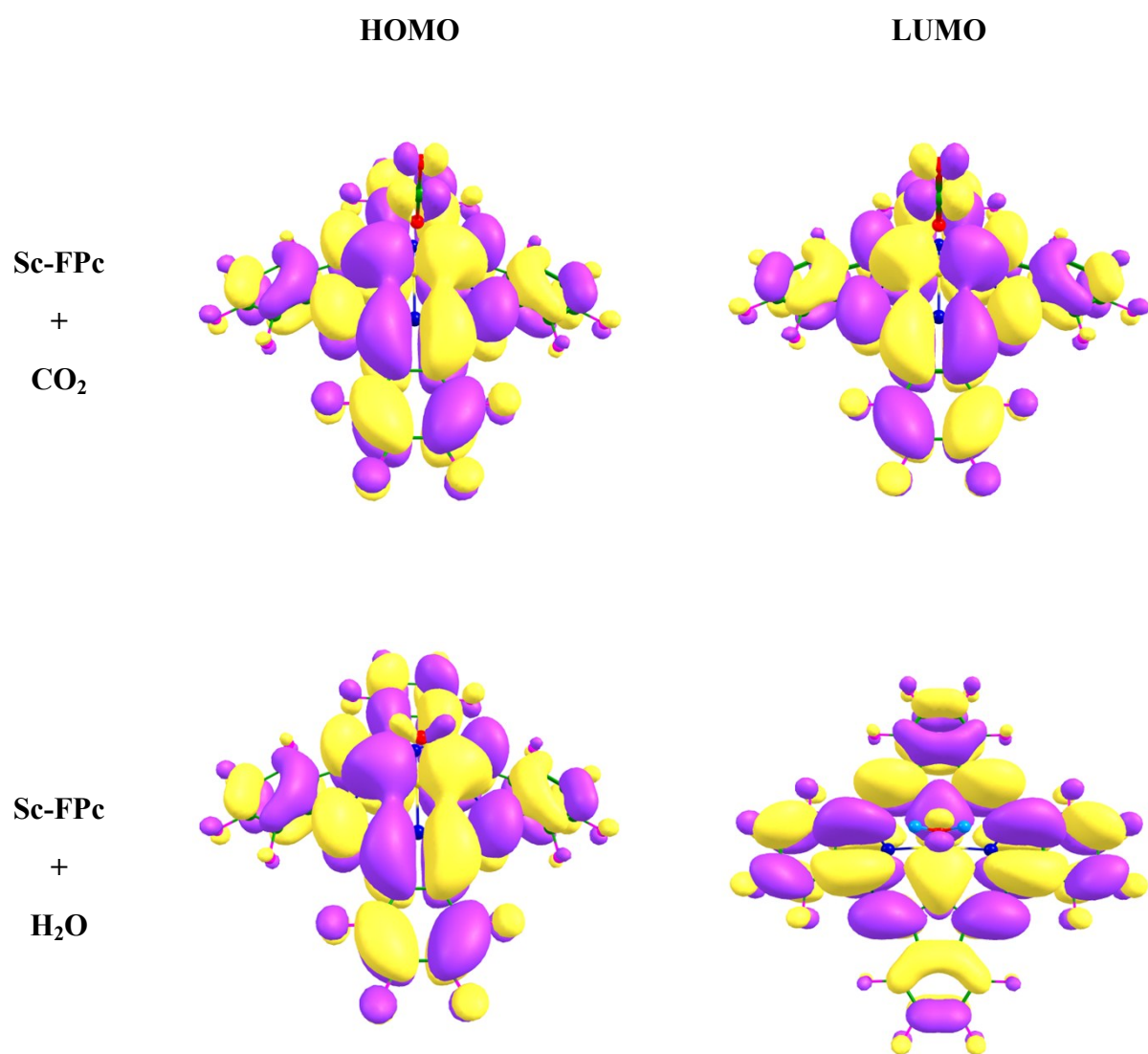
Figure S4 Continued



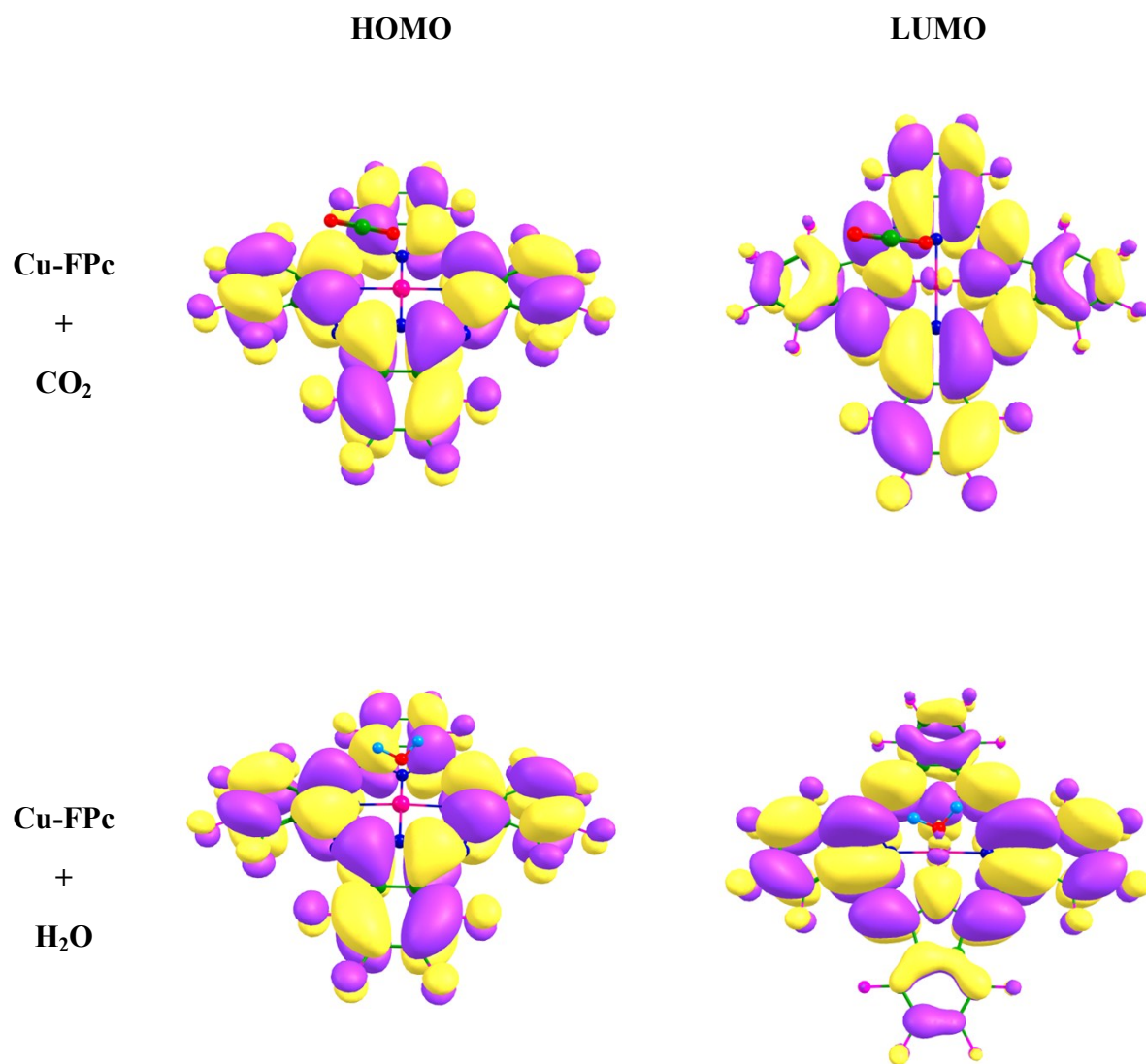


**Figure S5 (a) HOMO and LUMO plot of Mg-FPc with guest molecules**

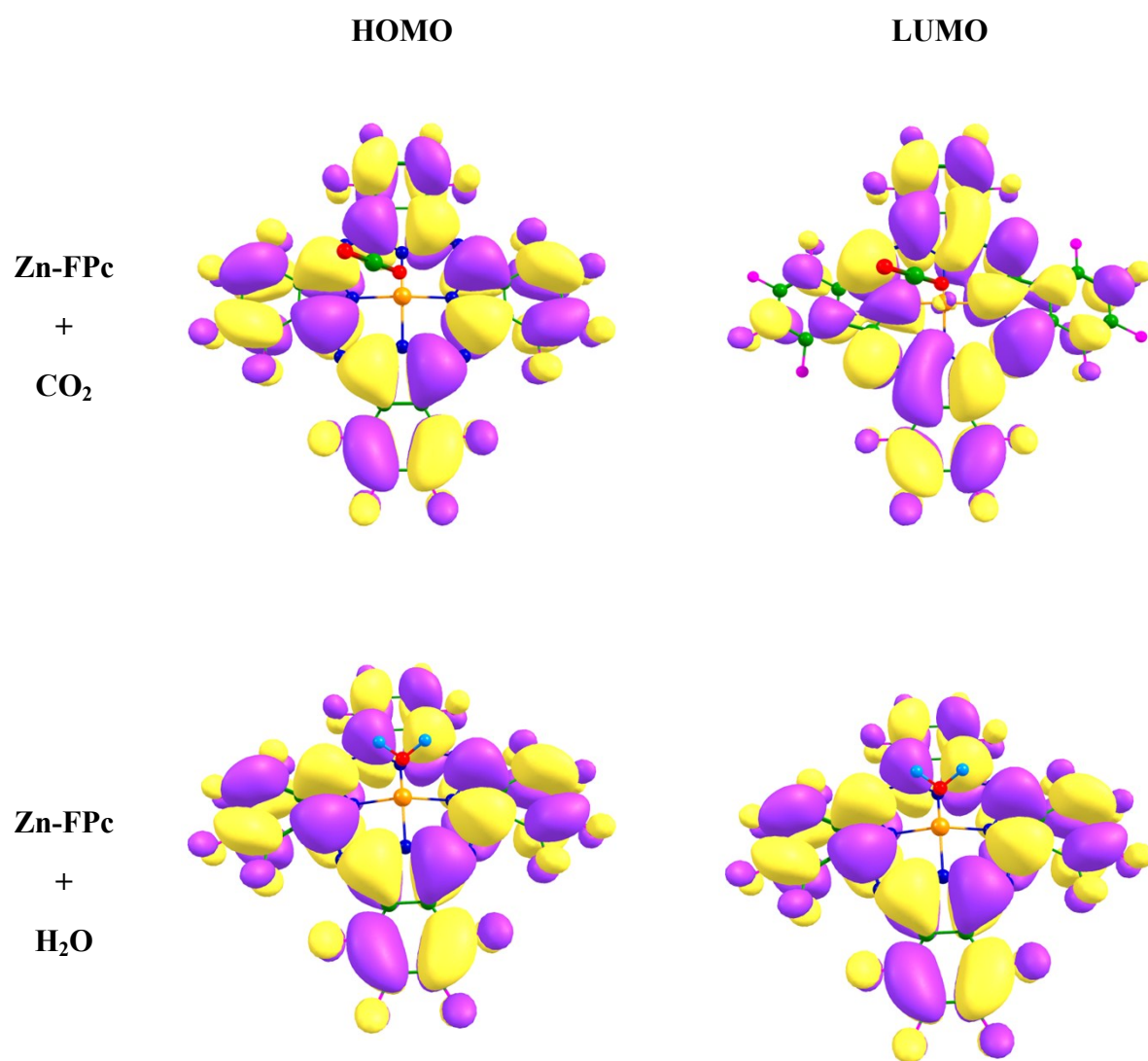




**Figure S5 (b) HOMO and LUMO plot of Sc-FPc with guest molecules**



**Figure S5 (c) HOMO and LUMO plot of Cu-FPc with guest molecules**



**Figure S5 (d) HOMO and LUMO plot of Zn-FPc with guest molecules**

### Cartesian coordinates of optimized M-FPc structures

Optimized using Heyd-Scuseria-Ernzerhof (HSE) PBE (Perdew, Burke and Ernzerhof) based hybrid functional with LANL2DZ for Mg, Sc, Cu, Zn and 6-31g(d,p) for C, N, H

Charge =0

Spin multiplicity =1 for Mg-FPc and Zn-FPc / 2 for Sc-FPc and Cu-FPc)

Mg-FPc

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 0.706411000  | 4.177834000  | 0.000000000 |
| C | 0.699145000  | 6.564084000  | 0.000000000 |
| C | -0.699145000 | 6.564084000  | 0.000000000 |
| C | -1.415198000 | 5.371222000  | 0.000000000 |
| C | -0.706411000 | 4.177834000  | 0.000000000 |
| C | -1.120292000 | 2.781847000  | 0.000000000 |
| N | 0.000000000  | 2.002449000  | 0.000000000 |
| N | -2.386276000 | 2.386276000  | 0.000000000 |
| C | 1.120292000  | 2.781847000  | 0.000000000 |
| C | 1.415198000  | 5.371222000  | 0.000000000 |
| C | 2.781847000  | -1.120292000 | 0.000000000 |
| C | 4.177834000  | -0.706411000 | 0.000000000 |
| C | 5.371222000  | -1.415198000 | 0.000000000 |
| C | 6.564084000  | -0.699145000 | 0.000000000 |
| C | 6.564084000  | 0.699145000  | 0.000000000 |
| C | 5.371222000  | 1.415198000  | 0.000000000 |
| C | 4.177834000  | 0.706411000  | 0.000000000 |
| C | 2.781847000  | 1.120292000  | 0.000000000 |
| N | 2.002449000  | 0.000000000  | 0.000000000 |
| N | 2.386276000  | 2.386276000  | 0.000000000 |
| N | -2.386276000 | -2.386276000 | 0.000000000 |

|    |              |              |             |
|----|--------------|--------------|-------------|
| C  | -2.781847000 | 1.120292000  | 0.000000000 |
| C  | -4.177834000 | 0.706411000  | 0.000000000 |
| C  | -5.371222000 | 1.415198000  | 0.000000000 |
| C  | -6.564084000 | 0.699145000  | 0.000000000 |
| C  | -6.564084000 | -0.699145000 | 0.000000000 |
| C  | -5.371222000 | -1.415198000 | 0.000000000 |
| C  | -4.177834000 | -0.706411000 | 0.000000000 |
| C  | -2.781847000 | -1.120292000 | 0.000000000 |
| N  | -2.002449000 | 0.000000000  | 0.000000000 |
| C  | -1.120292000 | -2.781847000 | 0.000000000 |
| C  | -1.415198000 | -5.371222000 | 0.000000000 |
| C  | -0.706411000 | -4.177834000 | 0.000000000 |
| C  | -0.699145000 | -6.564084000 | 0.000000000 |
| C  | 0.699145000  | -6.564084000 | 0.000000000 |
| C  | 1.415198000  | -5.371222000 | 0.000000000 |
| C  | 0.706411000  | -4.177834000 | 0.000000000 |
| C  | 1.120292000  | -2.781847000 | 0.000000000 |
| N  | 0.000000000  | -2.002449000 | 0.000000000 |
| N  | 2.386276000  | -2.386276000 | 0.000000000 |
| Mg | 0.000000000  | 0.000000000  | 0.000000000 |
| F  | -5.417289000 | 2.739142000  | 0.000000000 |
| F  | -7.726409000 | 1.339805000  | 0.000000000 |
| F  | -7.726409000 | -1.339805000 | 0.000000000 |
| F  | -5.417289000 | -2.739142000 | 0.000000000 |
| F  | -2.739142000 | 5.417289000  | 0.000000000 |
| F  | -1.339805000 | 7.726409000  | 0.000000000 |
| F  | 1.339805000  | 7.726409000  | 0.000000000 |
| F  | 2.739142000  | 5.417289000  | 0.000000000 |
| F  | 5.417289000  | 2.739142000  | 0.000000000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| F | 7.726409000  | 1.339805000  | 0.000000000 |
| F | 7.726409000  | -1.339805000 | 0.000000000 |
| F | 5.417289000  | -2.739142000 | 0.000000000 |
| F | 2.739142000  | -5.417289000 | 0.000000000 |
| F | 1.339805000  | -7.726409000 | 0.000000000 |
| F | -1.339805000 | -7.726409000 | 0.000000000 |
| F | -2.739142000 | -5.417289000 | 0.000000000 |

Sc-FPc

|   |              |              |              |
|---|--------------|--------------|--------------|
| C | -0.704634000 | 4.164377000  | -0.021613000 |
| C | -0.698667000 | 6.512153000  | -0.451744000 |
| C | 0.698667000  | 6.512153000  | -0.451744000 |
| C | 1.414115000  | 5.336633000  | -0.241115000 |
| C | 0.704634000  | 4.164377000  | -0.021613000 |
| C | 1.133663000  | 2.792262000  | 0.203382000  |
| N | 0.000000000  | 2.012534000  | 0.398268000  |
| N | 2.381061000  | 2.403308000  | 0.179126000  |
| C | -1.133663000 | 2.792262000  | 0.203382000  |
| C | -1.414115000 | 5.336633000  | -0.241115000 |
| C | -2.783624000 | -1.128996000 | 0.235056000  |
| C | -4.152525000 | -0.709877000 | 0.158452000  |
| C | -5.353681000 | -1.418200000 | 0.077032000  |
| C | -6.534858000 | -0.703723000 | -0.001143000 |
| C | -6.534858000 | 0.703723000  | -0.001143000 |
| C | -5.353681000 | 1.418200000  | 0.077032000  |
| C | -4.152525000 | 0.709877000  | 0.158452000  |
| C | -2.783624000 | 1.128996000  | 0.235056000  |
| N | -1.991798000 | 0.000000000  | 0.305880000  |
| N | -2.381061000 | 2.403308000  | 0.179126000  |
| N | 2.381061000  | -2.403308000 | 0.179126000  |

|    |              |              |              |
|----|--------------|--------------|--------------|
| C  | 2.783624000  | 1.128996000  | 0.235056000  |
| C  | 4.152525000  | 0.709877000  | 0.158452000  |
| C  | 5.353681000  | 1.418200000  | 0.077032000  |
| C  | 6.534858000  | 0.703723000  | -0.001143000 |
| C  | 6.534858000  | -0.703723000 | -0.001143000 |
| C  | 5.353681000  | -1.418200000 | 0.077032000  |
| C  | 4.152525000  | -0.709877000 | 0.158452000  |
| C  | 2.783624000  | -1.128996000 | 0.235056000  |
| N  | 1.991798000  | 0.000000000  | 0.305880000  |
| C  | 1.133663000  | -2.792262000 | 0.203382000  |
| C  | 1.414115000  | -5.336633000 | -0.241115000 |
| C  | 0.704634000  | -4.164377000 | -0.021613000 |
| C  | 0.698667000  | -6.512153000 | -0.451744000 |
| C  | -0.698667000 | -6.512153000 | -0.451744000 |
| C  | -1.414115000 | -5.336633000 | -0.241115000 |
| C  | -0.704634000 | -4.164377000 | -0.021613000 |
| C  | -1.133663000 | -2.792262000 | 0.203382000  |
| N  | 0.000000000  | -2.012534000 | 0.398268000  |
| N  | -2.381061000 | -2.403308000 | 0.179126000  |
| Sc | 0.000000000  | 0.000000000  | 0.894845000  |
| F  | 5.394146000  | 2.743941000  | 0.076262000  |
| F  | 7.701012000  | 1.335586000  | -0.075498000 |
| F  | 7.701012000  | -1.335586000 | -0.075498000 |
| F  | 5.394146000  | -2.743941000 | 0.076262000  |
| F  | 2.737777000  | 5.381066000  | -0.252521000 |
| F  | 1.340877000  | 7.655305000  | -0.655597000 |
| F  | -1.340877000 | 7.655305000  | -0.655597000 |
| F  | -2.737777000 | 5.381066000  | -0.252521000 |
| F  | -5.394146000 | 2.743941000  | 0.076262000  |



|   |              |              |              |
|---|--------------|--------------|--------------|
| F | -7.701012000 | 1.335586000  | -0.075498000 |
| F | -7.701012000 | -1.335586000 | -0.075498000 |
| F | -5.394146000 | -2.743941000 | 0.076262000  |
| F | -2.737777000 | -5.381066000 | -0.252521000 |
| F | -1.340877000 | -7.655305000 | -0.655597000 |
| F | 1.340877000  | -7.655305000 | -0.655597000 |
| F | 2.737777000  | -5.381066000 | -0.252521000 |

Cu-FPc

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 0.703915000  | 4.146142000  | 0.000000000 |
| C | 0.699452000  | 6.530065000  | 0.000000000 |
| C | -0.699452000 | 6.530065000  | 0.000000000 |
| C | -1.416093000 | 5.337945000  | 0.000000000 |
| C | -0.703915000 | 4.146142000  | 0.000000000 |
| C | -1.113496000 | 2.753001000  | 0.000000000 |
| N | 0.000000000  | 1.962339000  | 0.000000000 |
| N | -2.378254000 | 2.378254000  | 0.000000000 |
| C | 1.113496000  | 2.753001000  | 0.000000000 |
| C | 1.416093000  | 5.337945000  | 0.000000000 |
| C | 2.753001000  | -1.113496000 | 0.000000000 |
| C | 4.146142000  | -0.703915000 | 0.000000000 |
| C | 5.337945000  | -1.416093000 | 0.000000000 |
| C | 6.530065000  | -0.699452000 | 0.000000000 |
| C | 6.530065000  | 0.699452000  | 0.000000000 |
| C | 5.337945000  | 1.416093000  | 0.000000000 |
| C | 4.146142000  | 0.703915000  | 0.000000000 |
| C | 2.753001000  | 1.113496000  | 0.000000000 |
| N | 1.962339000  | 0.000000000  | 0.000000000 |
| N | 2.378254000  | 2.378254000  | 0.000000000 |
| N | -2.378254000 | -2.378254000 | 0.000000000 |

|    |              |              |             |
|----|--------------|--------------|-------------|
| C  | -2.753001000 | 1.113496000  | 0.000000000 |
| C  | -4.146142000 | 0.703915000  | 0.000000000 |
| C  | -5.337945000 | 1.416093000  | 0.000000000 |
| C  | -6.530065000 | 0.699452000  | 0.000000000 |
| C  | -6.530065000 | -0.699452000 | 0.000000000 |
| C  | -5.337945000 | -1.416093000 | 0.000000000 |
| C  | -4.146142000 | -0.703915000 | 0.000000000 |
| C  | -2.753001000 | -1.113496000 | 0.000000000 |
| N  | -1.962339000 | 0.000000000  | 0.000000000 |
| C  | -1.113496000 | -2.753001000 | 0.000000000 |
| C  | -1.416093000 | -5.337945000 | 0.000000000 |
| C  | -0.703915000 | -4.146142000 | 0.000000000 |
| C  | -0.699452000 | -6.530065000 | 0.000000000 |
| C  | 0.699452000  | -6.530065000 | 0.000000000 |
| C  | 1.416093000  | -5.337945000 | 0.000000000 |
| C  | 0.703915000  | -4.146142000 | 0.000000000 |
| C  | 1.113496000  | -2.753001000 | 0.000000000 |
| N  | 0.000000000  | -1.962339000 | 0.000000000 |
| N  | 2.378254000  | -2.378254000 | 0.000000000 |
| Cu | 0.000000000  | 0.000000000  | 0.000000000 |
| F  | -5.383745000 | 2.739733000  | 0.000000000 |
| F  | -7.692439000 | 1.339572000  | 0.000000000 |
| F  | -7.692439000 | -1.339572000 | 0.000000000 |
| F  | -5.383745000 | -2.739733000 | 0.000000000 |
| F  | -2.739733000 | 5.383745000  | 0.000000000 |
| F  | -1.339572000 | 7.692439000  | 0.000000000 |
| F  | 1.339572000  | 7.692439000  | 0.000000000 |
| F  | 2.739733000  | 5.383745000  | 0.000000000 |
| F  | 5.383745000  | 2.739733000  | 0.000000000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| F | 7.692439000  | 1.339572000  | 0.000000000 |
| F | 7.692439000  | -1.339572000 | 0.000000000 |
| F | 5.383745000  | -2.739733000 | 0.000000000 |
| F | 2.739733000  | -5.383745000 | 0.000000000 |
| F | 1.339572000  | -7.692439000 | 0.000000000 |
| F | -1.339572000 | -7.692439000 | 0.000000000 |
| F | -2.739733000 | -5.383745000 | 0.000000000 |

# Zn-FPc

|   |              |              |             |
|---|--------------|--------------|-------------|
| C | 0.706396000  | 4.178540000  | 0.000000000 |
| C | 0.699088000  | 6.564891000  | 0.000000000 |
| C | -0.699088000 | 6.564891000  | 0.000000000 |
| C | -1.415088000 | 5.371879000  | 0.000000000 |
| C | -0.706396000 | 4.178540000  | 0.000000000 |
| C | -1.121148000 | 2.782430000  | 0.000000000 |
| N | 0.000000000  | 2.006147000  | 0.000000000 |
| N | -2.386143000 | 2.386143000  | 0.000000000 |
| C | 1.121148000  | 2.782430000  | 0.000000000 |
| C | 1.415088000  | 5.371879000  | 0.000000000 |
| C | 2.782430000  | -1.121148000 | 0.000000000 |
| C | 4.178540000  | -0.706396000 | 0.000000000 |
| C | 5.371879000  | -1.415088000 | 0.000000000 |
| C | 6.564891000  | -0.699088000 | 0.000000000 |
| C | 6.564891000  | 0.699088000  | 0.000000000 |
| C | 5.371879000  | 1.415088000  | 0.000000000 |
| C | 4.178540000  | 0.706396000  | 0.000000000 |
| C | 2.782430000  | 1.121148000  | 0.000000000 |
| N | 2.006147000  | 0.000000000  | 0.000000000 |
| N | 2.386143000  | 2.386143000  | 0.000000000 |
| N | -2.386143000 | -2.386143000 | 0.000000000 |

|    |              |              |             |
|----|--------------|--------------|-------------|
| C  | -2.782430000 | 1.121148000  | 0.000000000 |
| C  | -4.178540000 | 0.706396000  | 0.000000000 |
| C  | -5.371879000 | 1.415088000  | 0.000000000 |
| C  | -6.564891000 | 0.699088000  | 0.000000000 |
| C  | -6.564891000 | -0.699088000 | 0.000000000 |
| C  | -5.371879000 | -1.415088000 | 0.000000000 |
| C  | -4.178540000 | -0.706396000 | 0.000000000 |
| C  | -2.782430000 | -1.121148000 | 0.000000000 |
| N  | -2.006147000 | 0.000000000  | 0.000000000 |
| C  | -1.121148000 | -2.782430000 | 0.000000000 |
| C  | -1.415088000 | -5.371879000 | 0.000000000 |
| C  | -0.706396000 | -4.178540000 | 0.000000000 |
| C  | -0.699088000 | -6.564891000 | 0.000000000 |
| C  | 0.699088000  | -6.564891000 | 0.000000000 |
| C  | 1.415088000  | -5.371879000 | 0.000000000 |
| C  | 0.706396000  | -4.178540000 | 0.000000000 |
| C  | 1.121148000  | -2.782430000 | 0.000000000 |
| N  | 0.000000000  | -2.006147000 | 0.000000000 |
| N  | 2.386143000  | -2.386143000 | 0.000000000 |
| Zn | 0.000000000  | 0.000000000  | 0.000000000 |
| F  | -5.417757000 | 2.739025000  | 0.000000000 |
| F  | -7.727063000 | 1.339946000  | 0.000000000 |
| F  | -7.727063000 | -1.339946000 | 0.000000000 |
| F  | -5.417757000 | -2.739025000 | 0.000000000 |
| F  | -2.739025000 | 5.417757000  | 0.000000000 |
| F  | -1.339946000 | 7.727063000  | 0.000000000 |
| F  | 1.339946000  | 7.727063000  | 0.000000000 |
| F  | 2.739025000  | 5.417757000  | 0.000000000 |
| F  | 5.417757000  | 2.739025000  | 0.000000000 |

|   |              |              |             |
|---|--------------|--------------|-------------|
| F | 7.727063000  | 1.339946000  | 0.000000000 |
| F | 7.727063000  | -1.339946000 | 0.000000000 |
| F | 5.417757000  | -2.739025000 | 0.000000000 |
| F | 2.739025000  | -5.417757000 | 0.000000000 |
| F | 1.339946000  | -7.727063000 | 0.000000000 |
| F | -1.339946000 | -7.727063000 | 0.000000000 |
| F | -2.739025000 | -5.417757000 | 0.000000000 |