Electronic Supplementary Material (ESI) for New Journal of Chemistry.


*Supporting Information*:

**Spectral properties of supramolecular systems based on cobalt(II)/manganese(III) phthalocyanine and fullero[60]pyrrolidines with PET**

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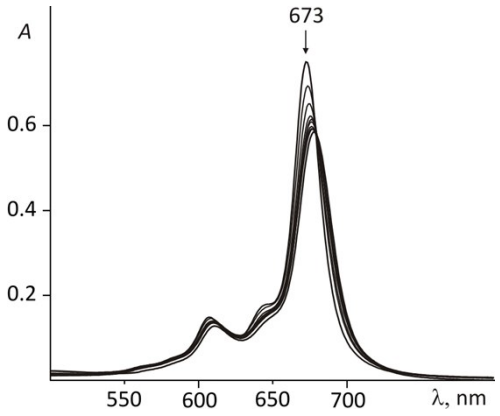
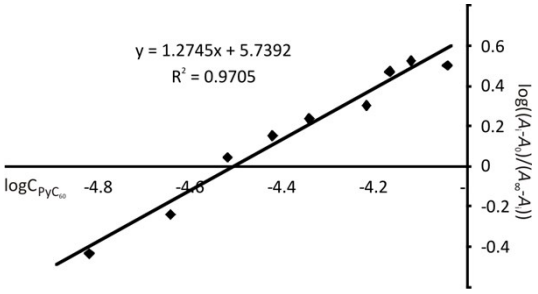
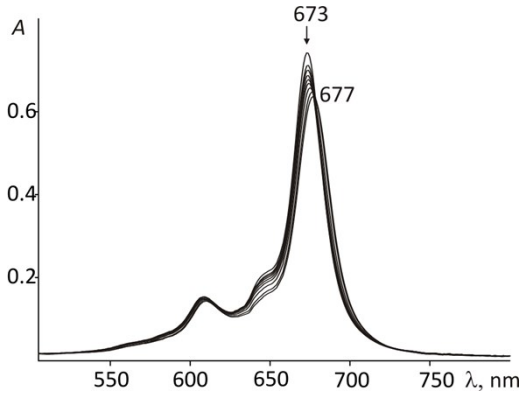
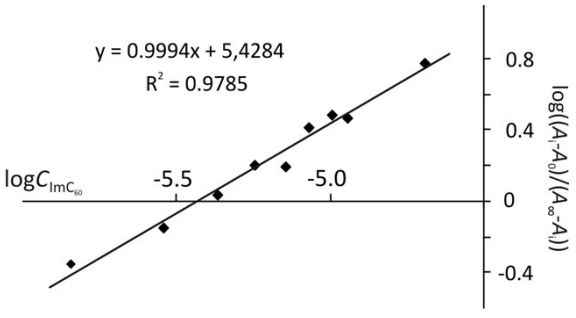
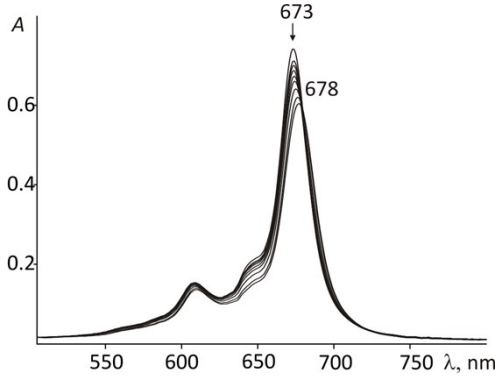
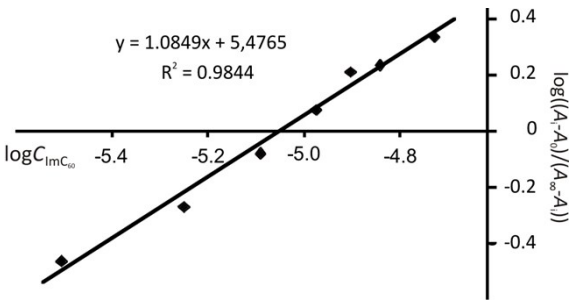
Figure S1.

| | Visible absorption during titration of metallophthalocyanines with fullero[60]pyrrolidines in toluene | Plots of $\log((A_i - A_0)/(A_\infty - A_i))$ *vs* log$C_{fullerene}$ for the reaction of metallophthalocyanines with fullero[60]pyrrolidines |
|---|---|---|
| CoPc + $PyC_{60}$ |   |   at τ = ∞ |
| CoPc + $ImC_{60}$ |   |   at τ = ∞ |
| CoPc + $Py_3C_{60}$ |   |   at τ = ∞ |

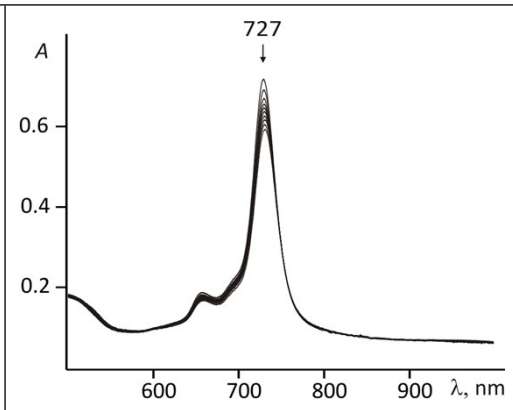
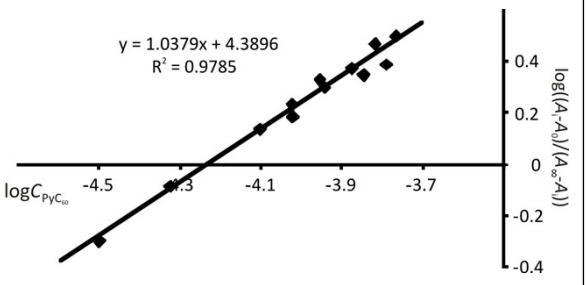
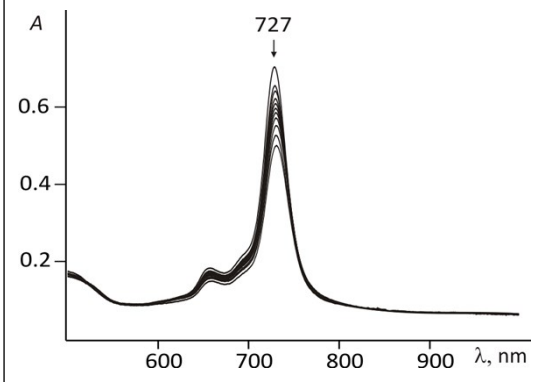
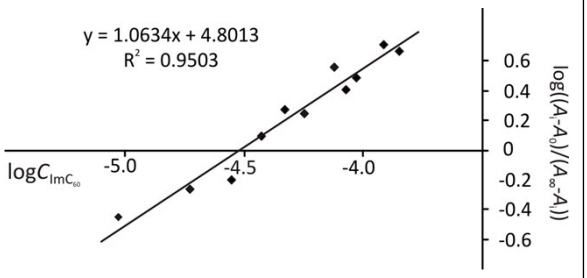
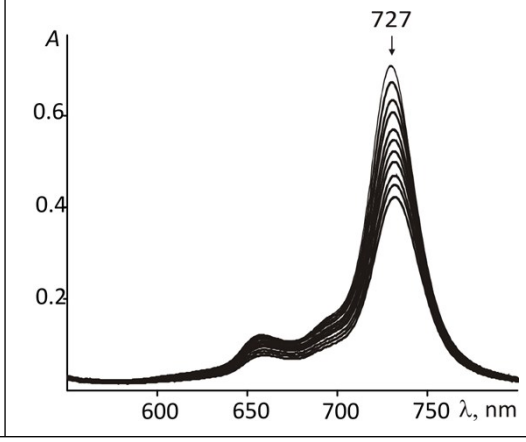
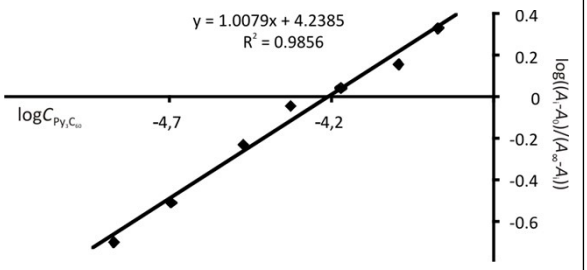
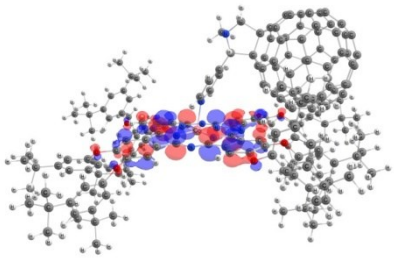
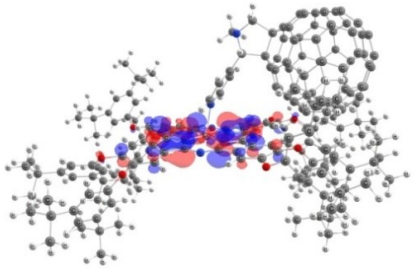
| | | |
|---|---|---|
| (AcO)MnPc + $PyC_{60}$ |  |  <br>at τ = 300 sec |
| (AcO)MnPc + $ImC_{60}$ |  |  <br>at τ = 242 sec |
| (AcO)MnPc + $Py_3C_{60}$ |  |  <br>at τ = 500 sec |

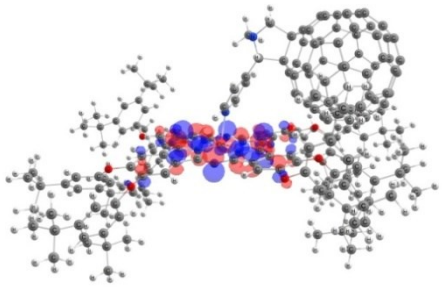
Figure S2. The shape of the frontier molecular orbitals of ($PyC_{60}$)CoPc.



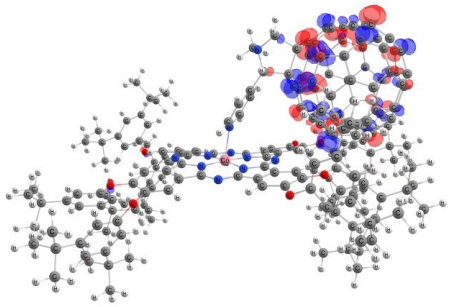
α HOMO



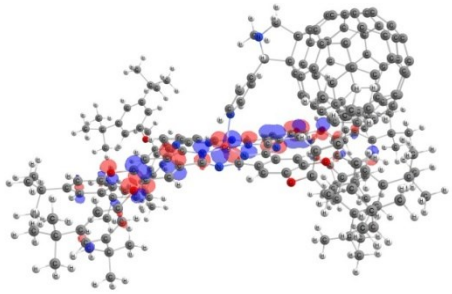
α LUMO+3



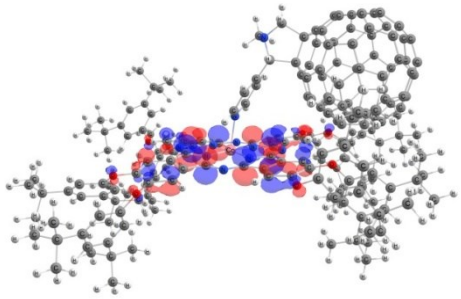
α LUMO+4



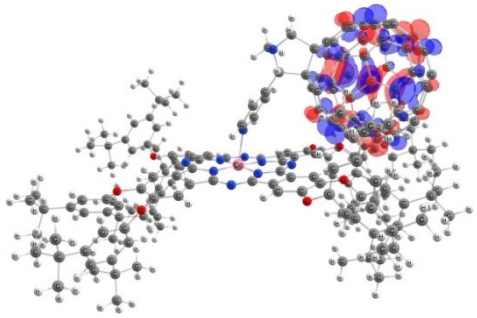
β HOMO-7



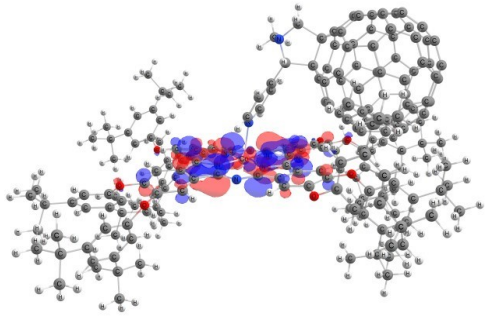
β HOMO-1



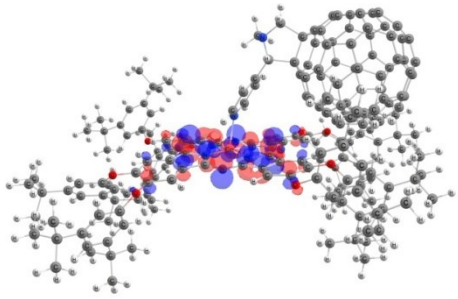
β HOMO



β LUMO



β LUMO+3



β LUMO+4

Figure S3. The shape of the frontier molecular orbitals of (AcO)(PyC$_{60}$)MnPc.

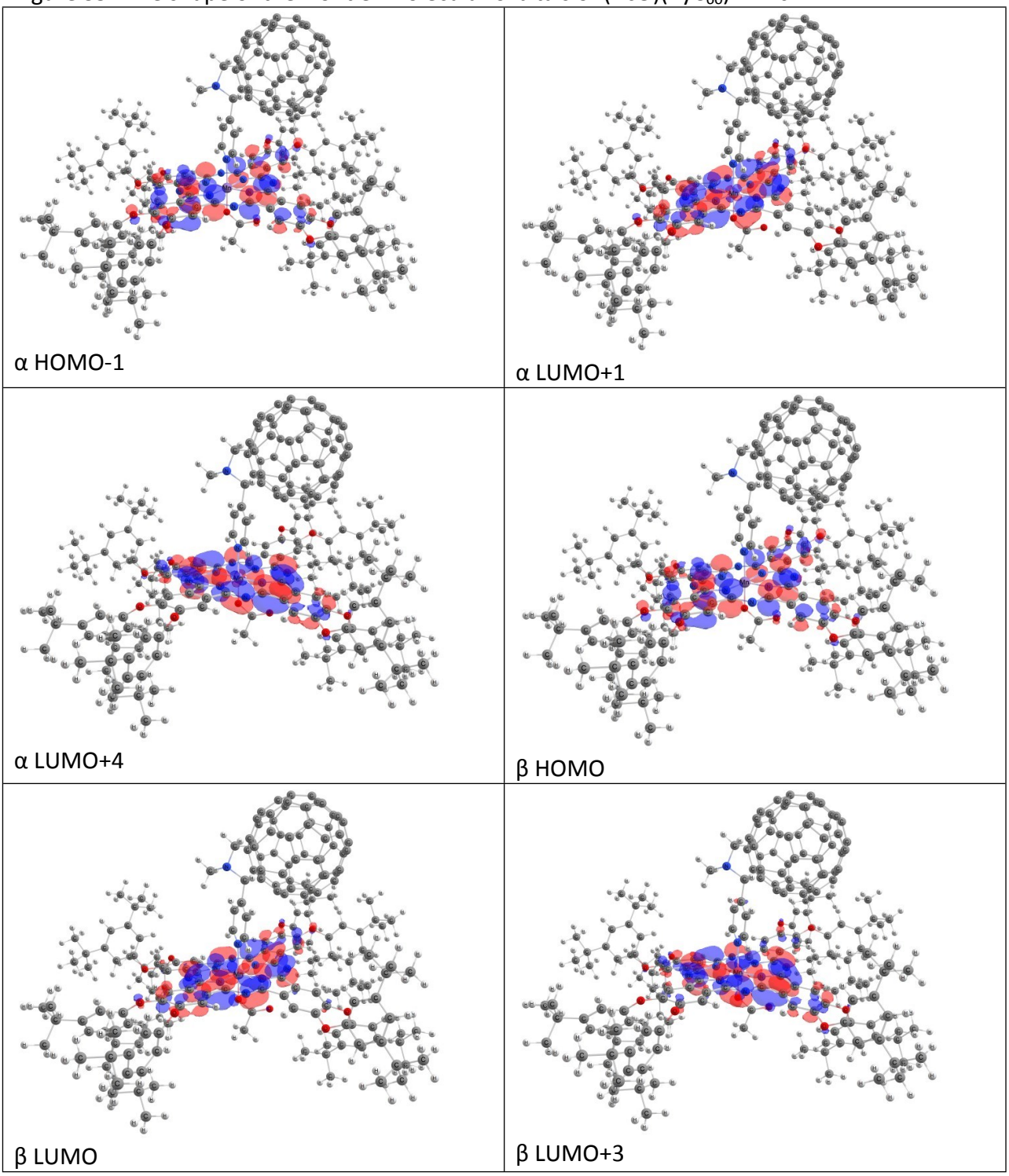
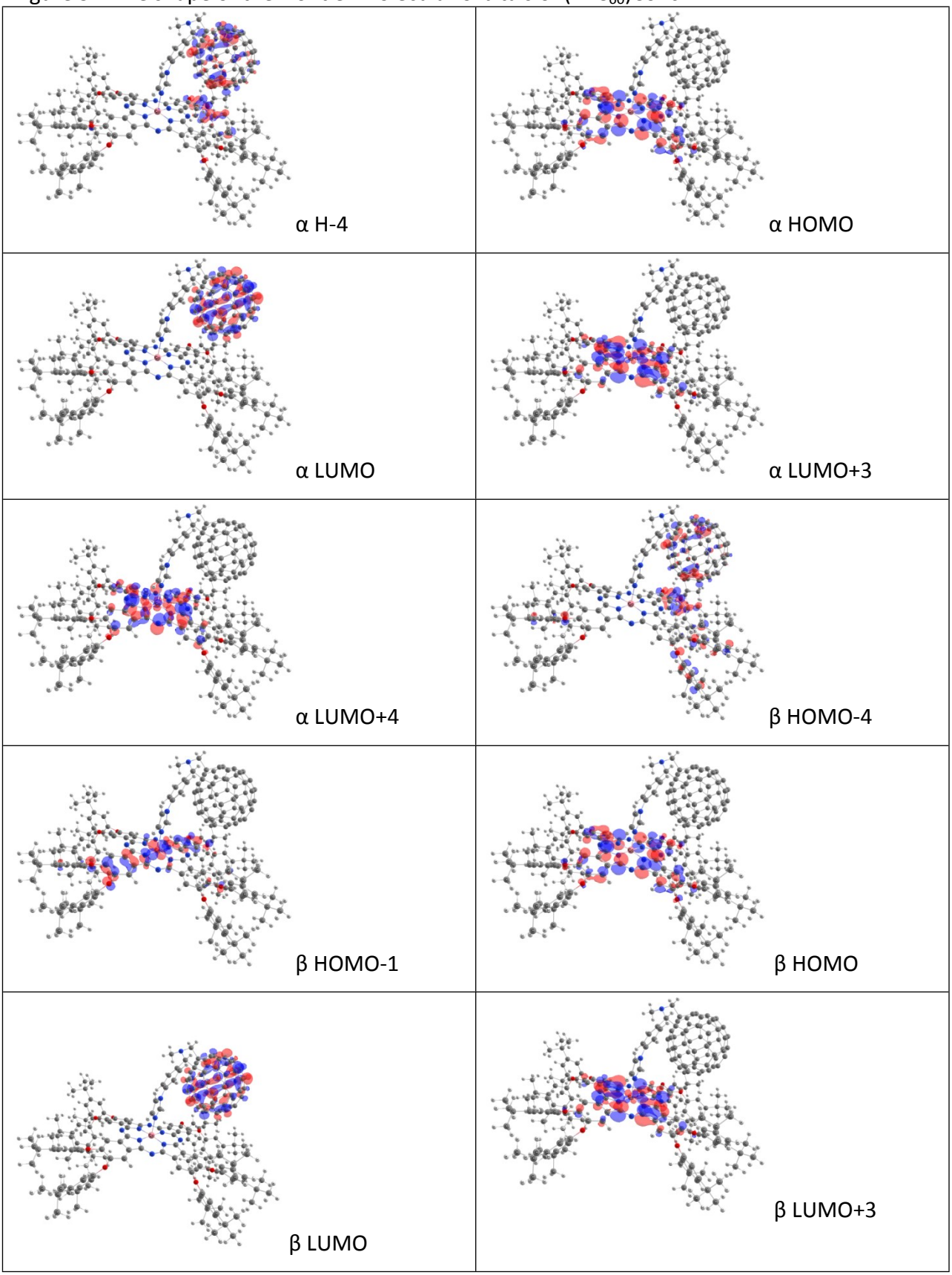
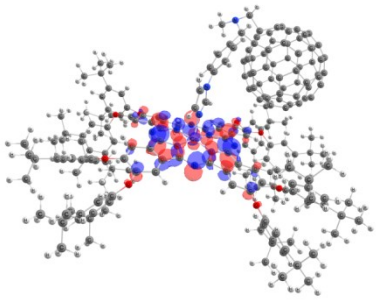


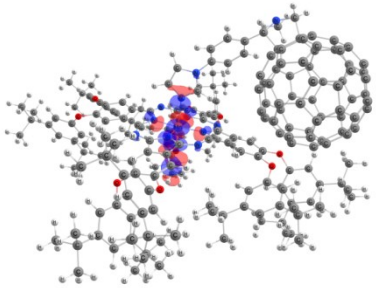
Figure S4. The shape of the frontier molecular orbitals of ($ImC_{60}$)CoPc.



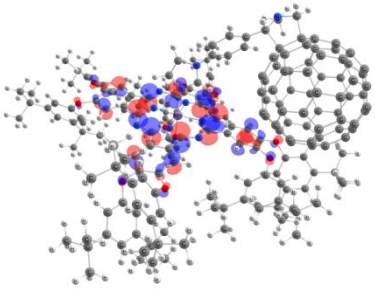


β LUMO+4

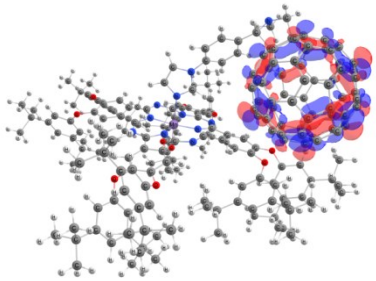
Figure S5. The shape of the frontier molecular orbitals of (AcO)(Im$C_{60}$)MnPc.



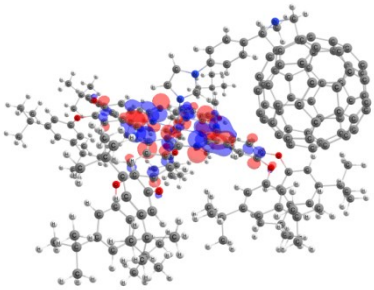
α HOMO-1



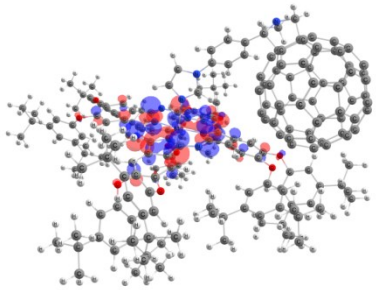
α HOMO



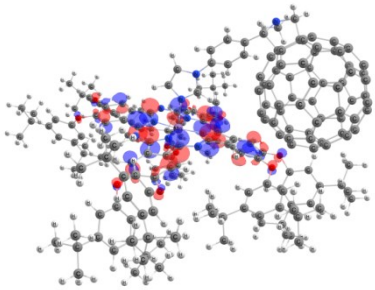
α LUMO+1



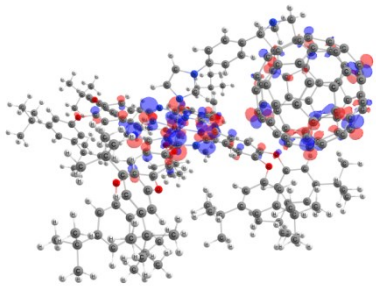
α LUMO+2



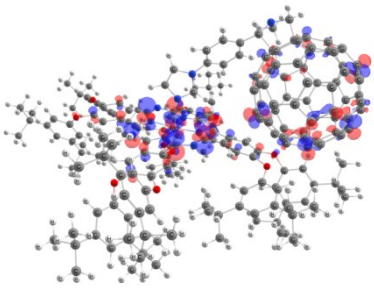
α LUMO+3



β HOMO



β LUMO+2



β LUMO+3

Figure S6. Fluorescence spectra ($\lambda_{exc}$ = 395 nm) of (AcO)MnPc ($C_{(AcO)MnPc}$ = 4.4 × $10^{-6}$ M) and dyads (AcO)($PyC_{60}$)MnPc ($C_{(AcO)MnPc}$ = 4.7 × $10^{-6}$ M, $C_{PyC_{60}}$ = 1.3 × $10^{-4}$ M), (AcO)($ImC_{60}$)MnPc ($C_{(AcO)MnPc}$ = 4.4 × $10^{-6}$ M, $C_{ImC_{60}}$ = 1.4 × $10^{-4}$ M), (AcO)($Py_3C_{60}$)MnPc ($C_{(AcO)MnPc}$ = 4.6 × $10^{-6}$ M, $C_{Py_3C_{60}}$ = 1.4 × $10^{-4}$ M).