

Supporting information

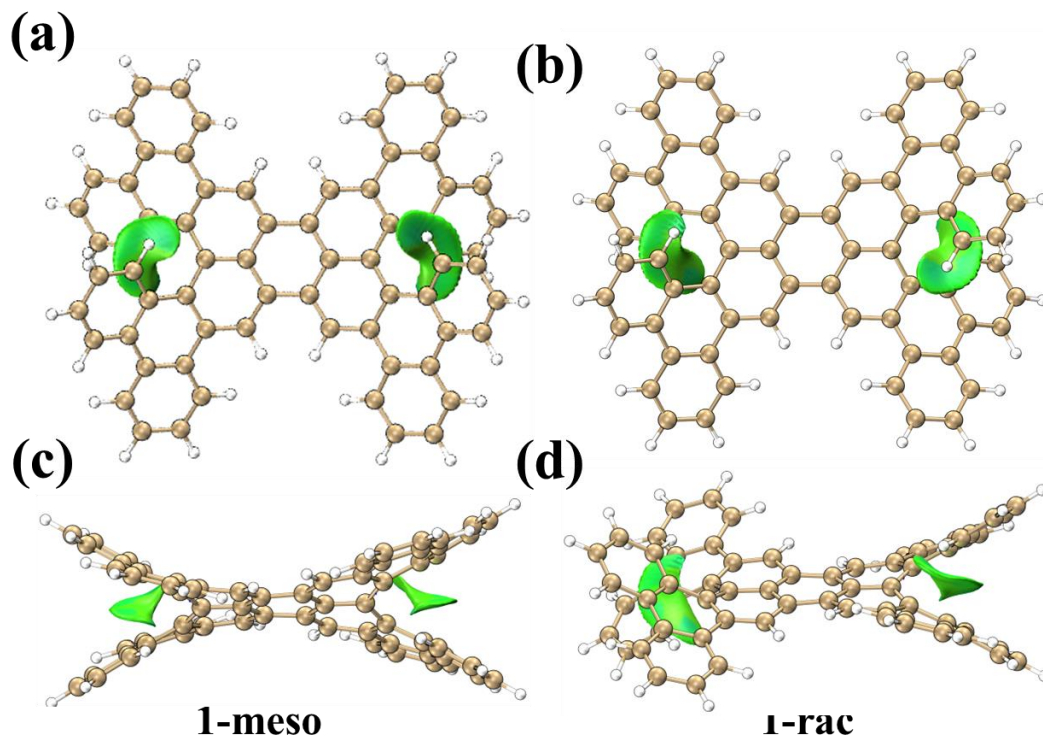


Figure S1. IGMH isosurfaces of 1-meso and 1-rac (a, b), and their side views (c, d).

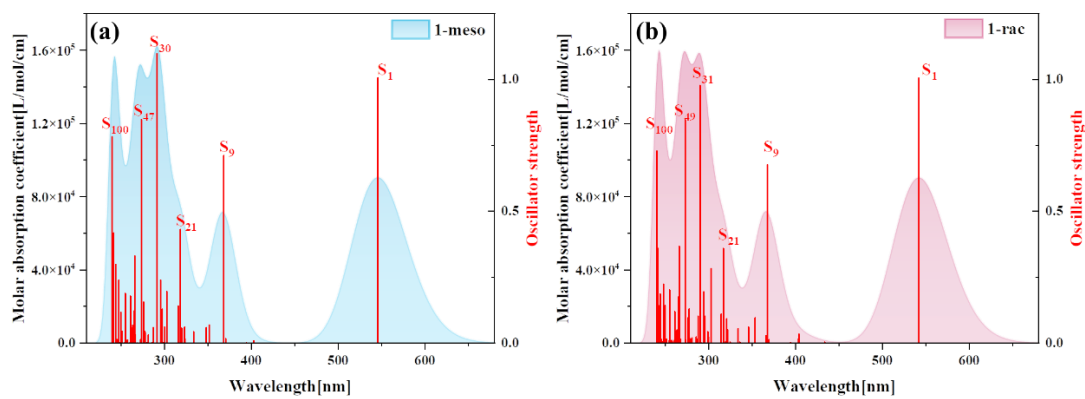


Figure S2. UV-vis spectra of 1-meso (a) and 1-rac (b).

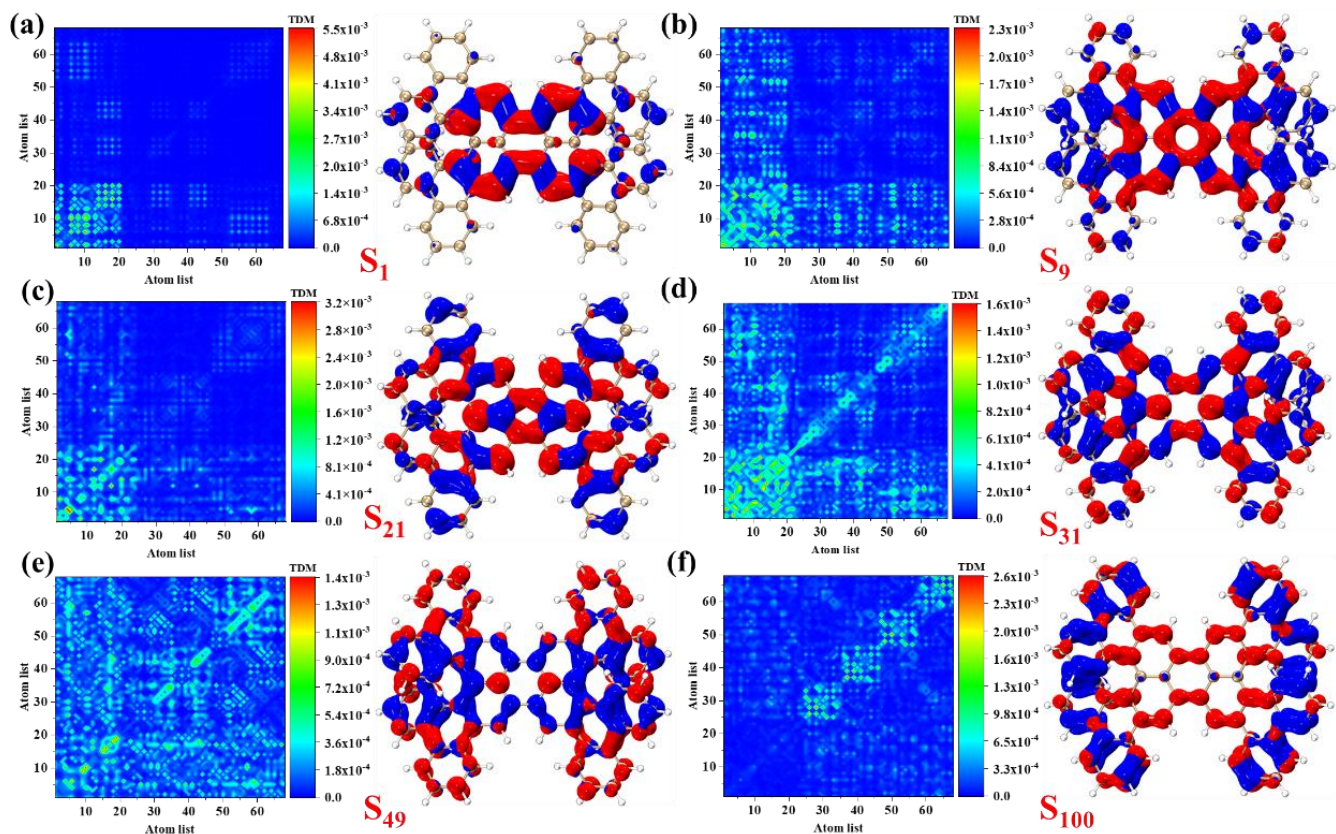


Figure S3. TDM and CDD diagrams of 1-rac under S_1 (a), S_9 (b), S_{21} (c), S_{31} (d), S_{49} (e), S_{100} (f). In CDD diagram, blue represents holes and red represents electrons. The isovalue is 0.0005.

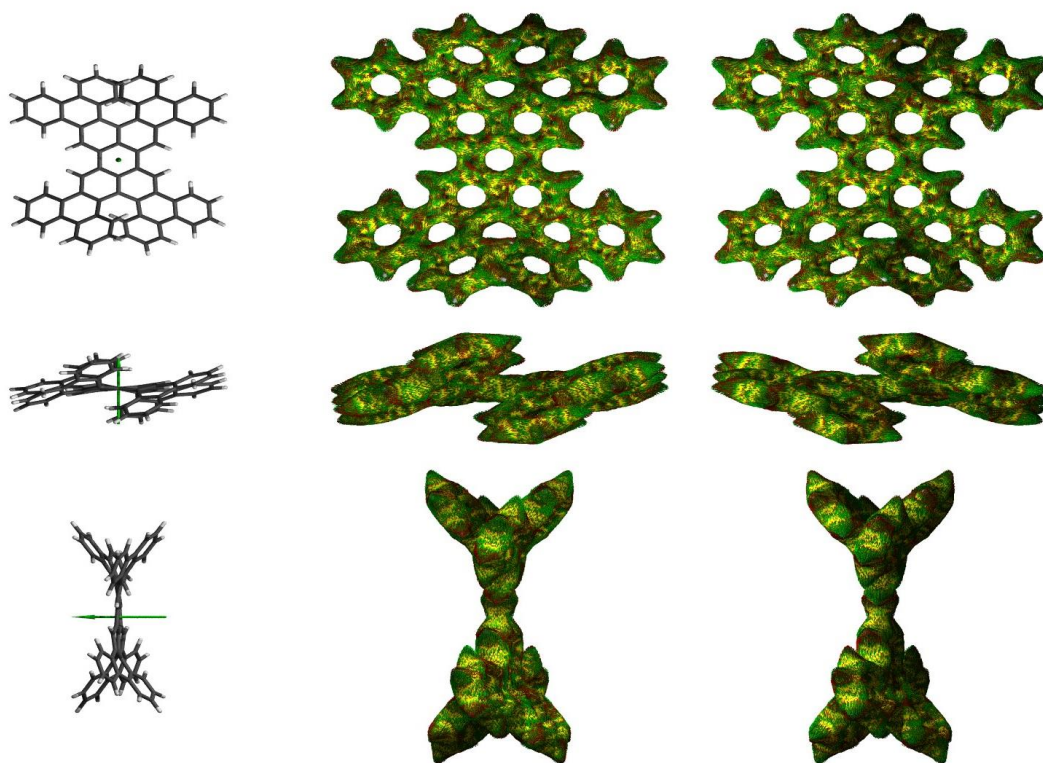


Figure S4. Magnetic induced current density of 1-meso.

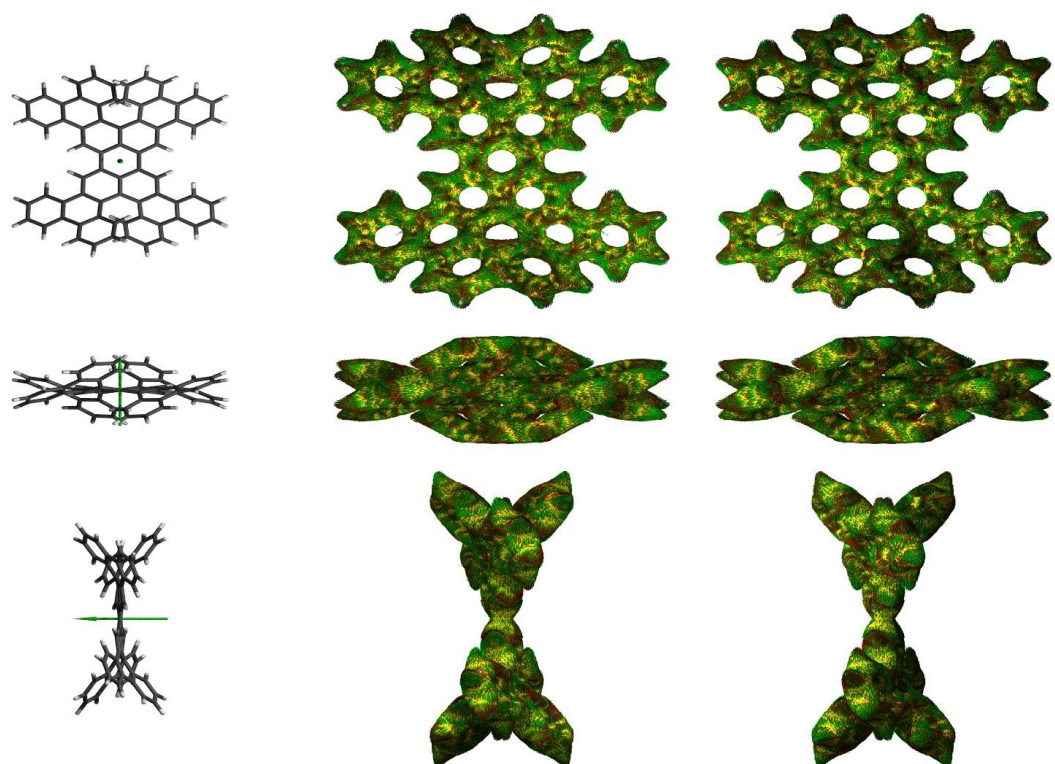


Figure S5. Magnetic induced current density of 1-rac.

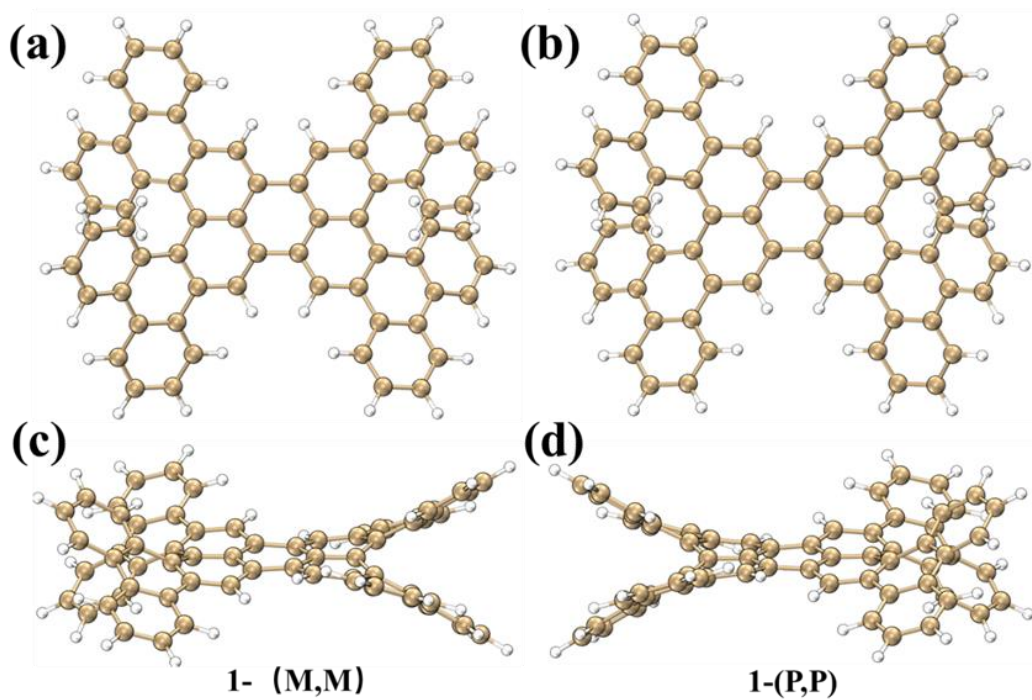


Figure S6. Structure diagram of 1- (M, M) and 1- (P, P).

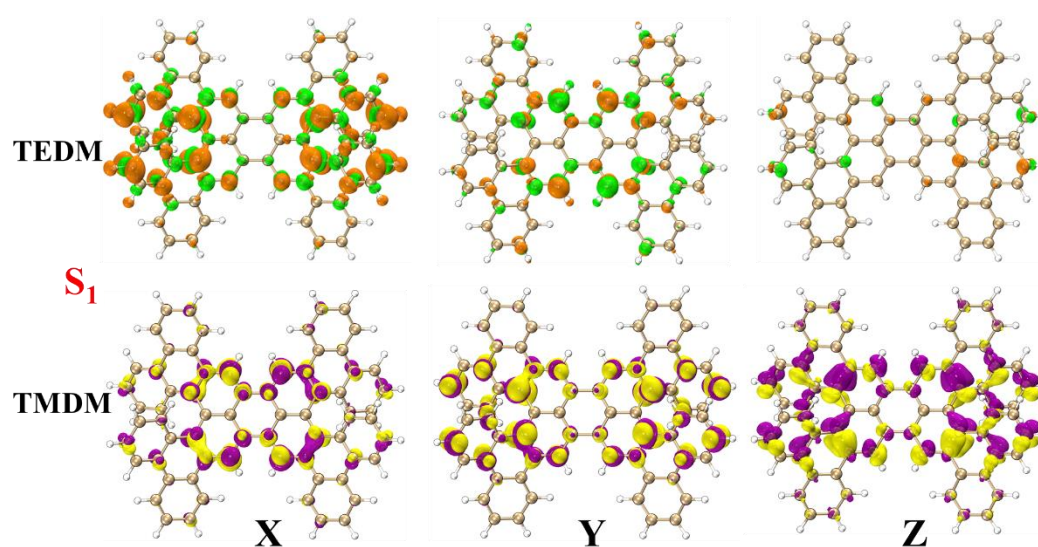


Figure S7. TEDM and TMDM of 1-meso in S_1 excited state.

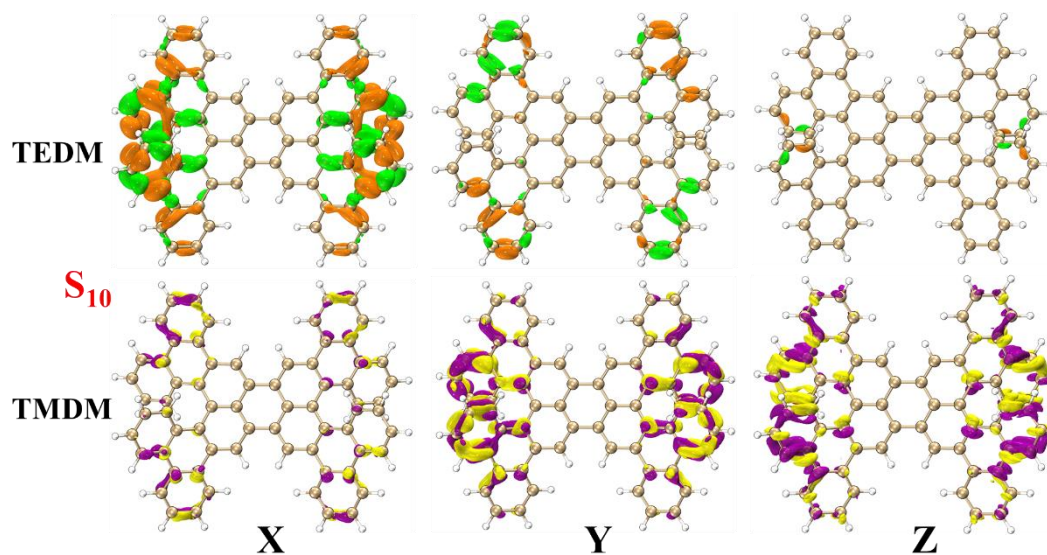


Figure S8. TEDM and TMDM of 1-meso in S_{10} excited state.

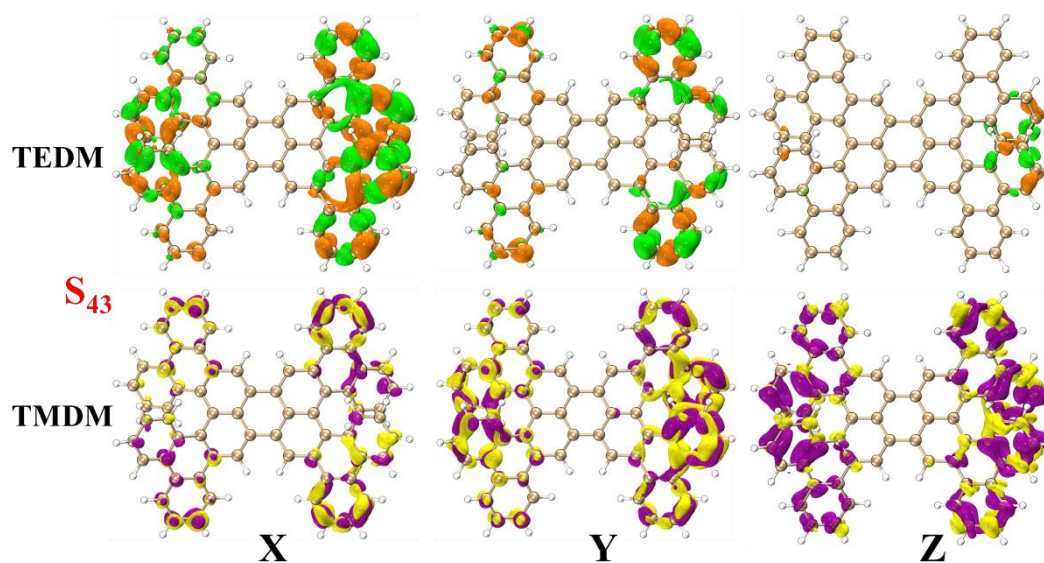


Figure S9. TEDM and TMDM of 1-meso in S_{43} excited state.

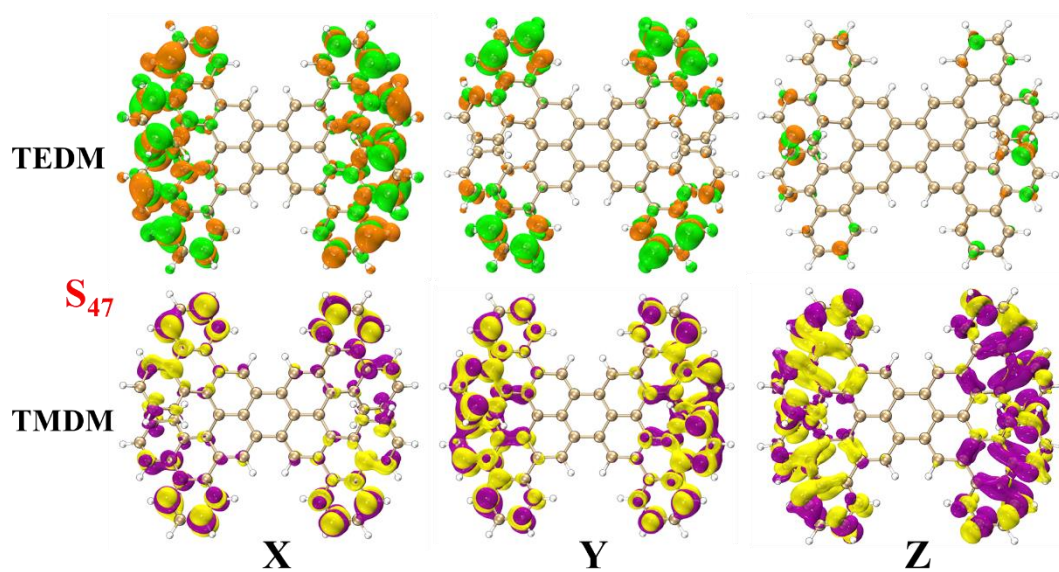


Figure S10. TEDM and TMDM of 1-meso in S_{47} excited state.

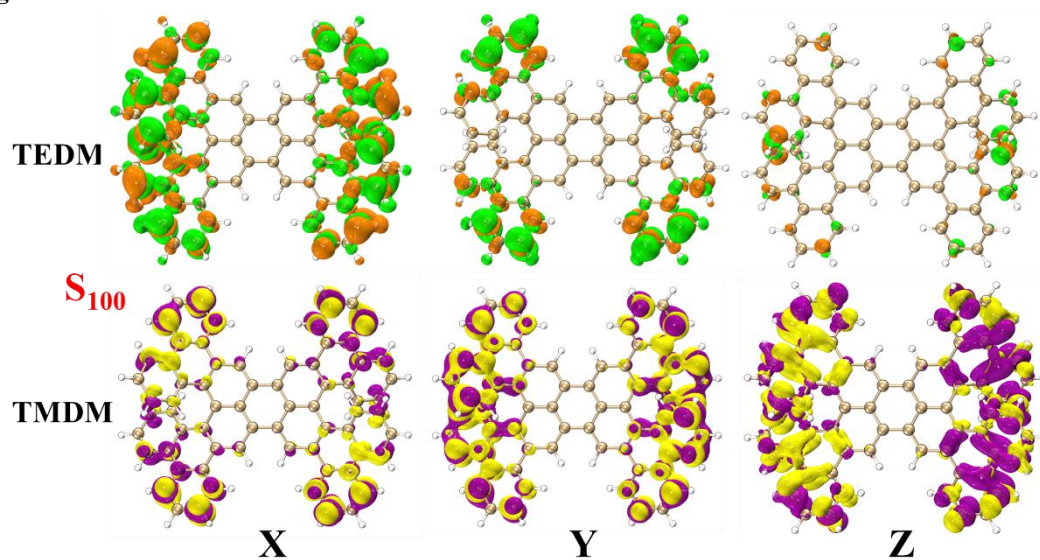


Figure S11. TEDM and TMDM of 1-meso in S_{100} excited state.

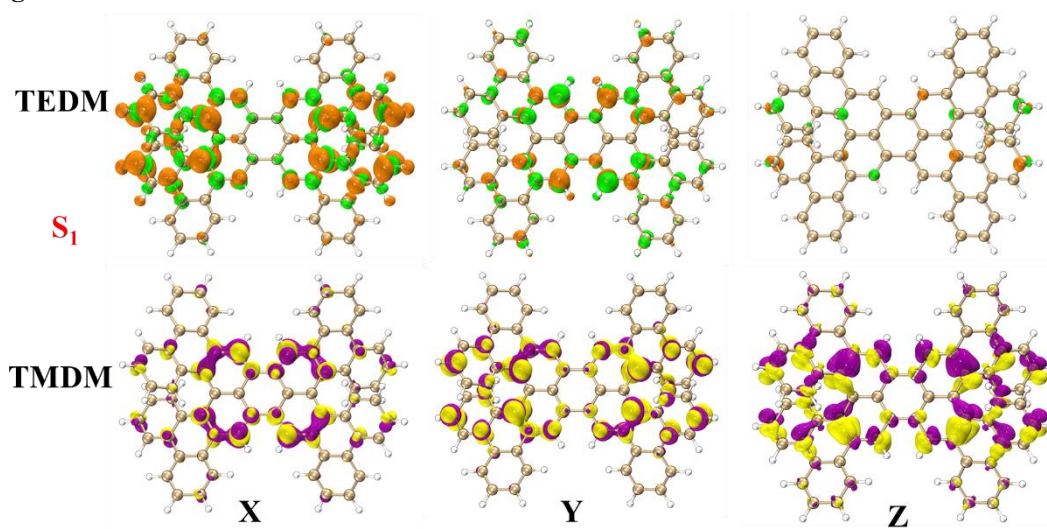


Figure S12. TEDM and TMDM of 1- (P, P) in S_1 excited state.

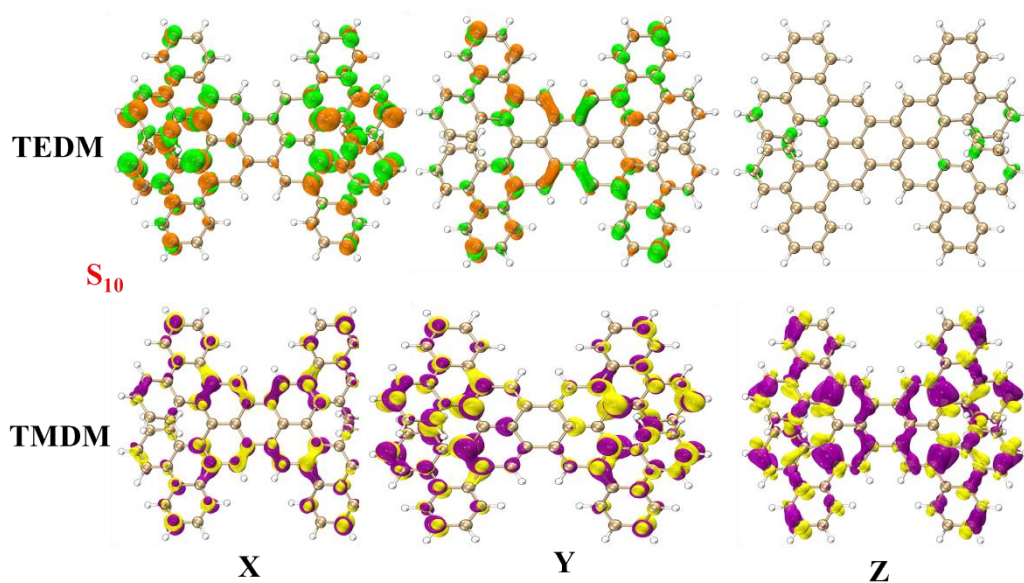


Figure S13. TEDM and TMDM of 1- (P, P) in S_{10} excited state.

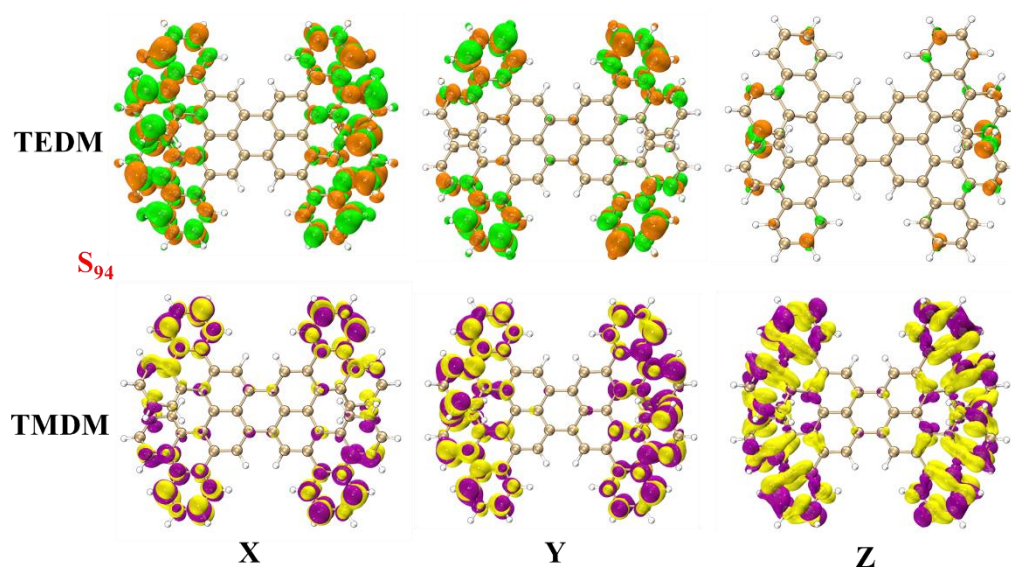


Figure S14. TEDM and TMDM of 1- (P, P) in S_{94} excited state.

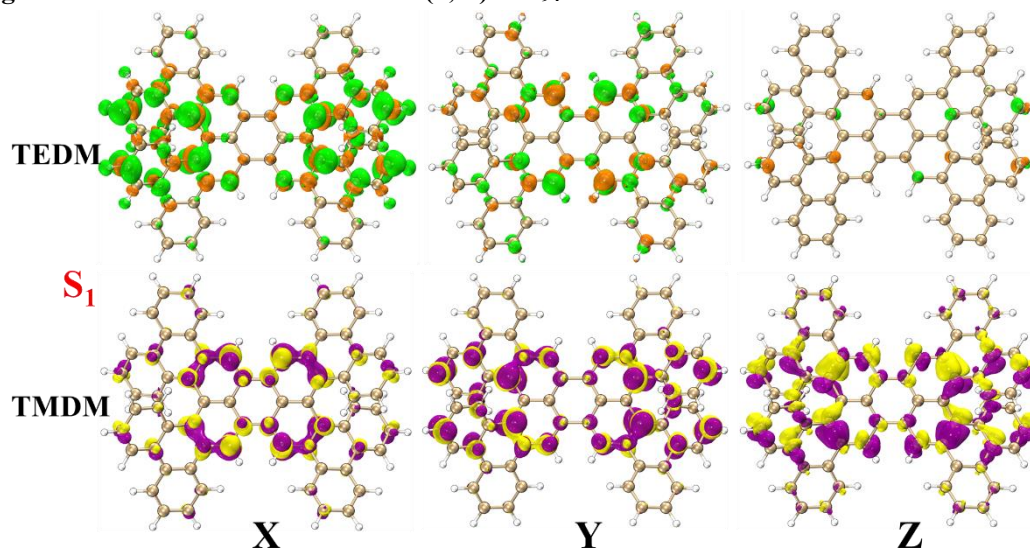


Figure S15. TEDM and TMDM of 1- (M, M) in S_1 excited state.

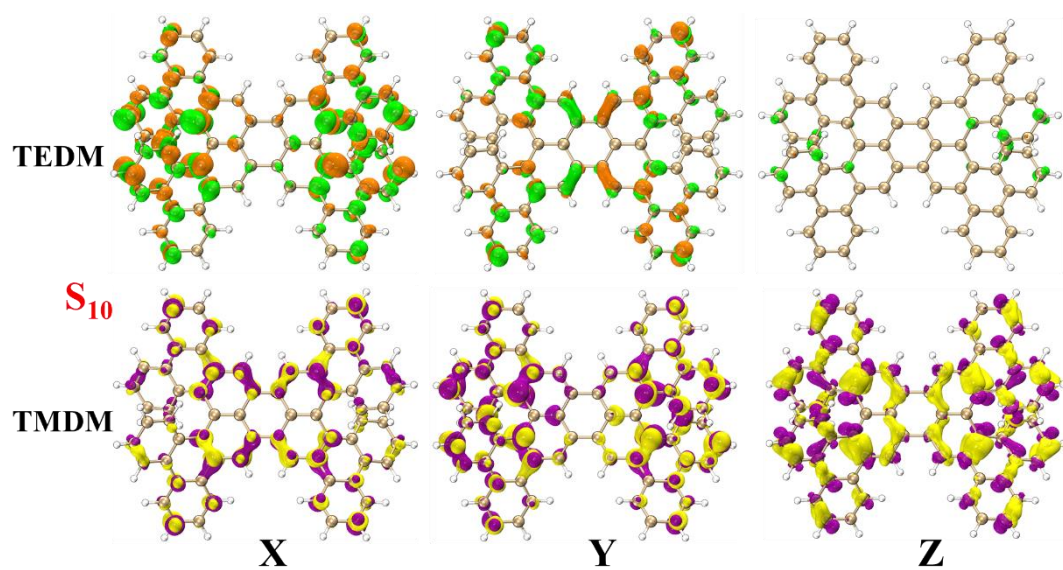


Figure S16. TEDM and TMDM of 1- (M, M) in S_{10} excited state.

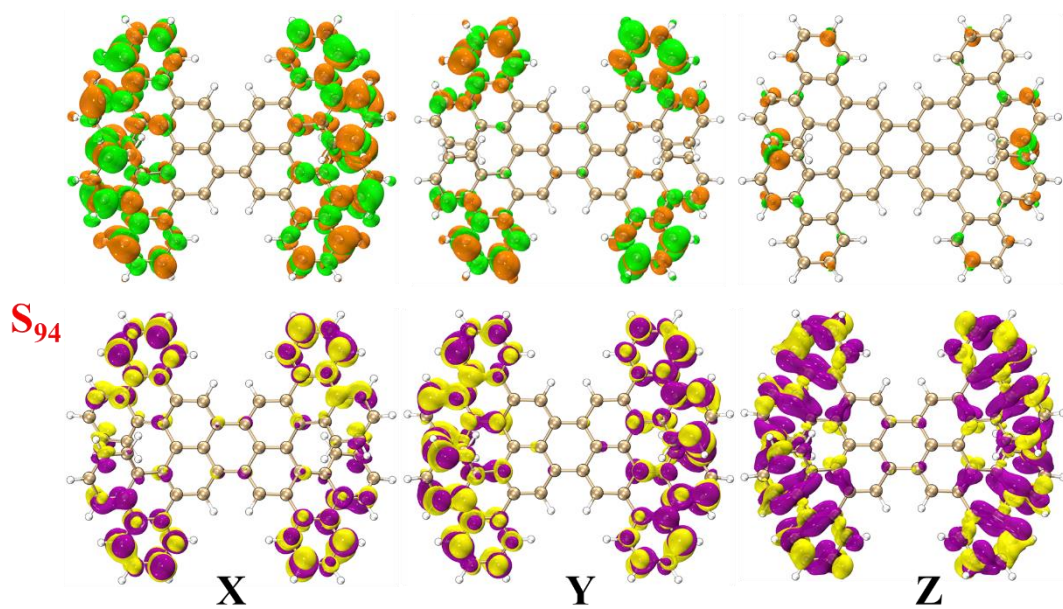


Figure S17. TEDM and TMDM of 1- (M, M) in S_{94} excited state.