Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Novel Ruthenium Sensitizers with A Dianionic Tridentate Ligand for Dye-Sensitized Solar Cells: Relationship Between the Solar Cell Performances and the Electron-Withdrawing Ability of Substituents at the Ligand

Hironobu Ozawa, Shunsuke Honda, Daichi Katano, Takahito Sugiura and Hironori Arakawa*

Department of Industrial Chemistry, Faculty of Engineering, Tokyo University of Science, 12-1, Ichigaya-Funagawara, Shinjuku, Tokyo, 162-0826, JAPAN
E-mail: h.arakawa@ci.kagu.tus.ac.jp; Fax: (+81) 3 5261 4631; Tel: (+81) 3 5228 8311

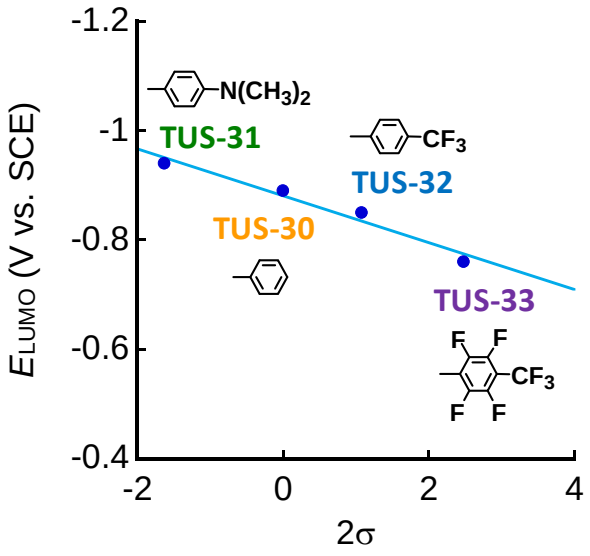

Figure S1. Relationship between the energy levels of LUMOs (E_{LUMO}) of TUS sensitizers and the Hammett constants of the substituents (2σ) at the dianionic tridentate ligands.

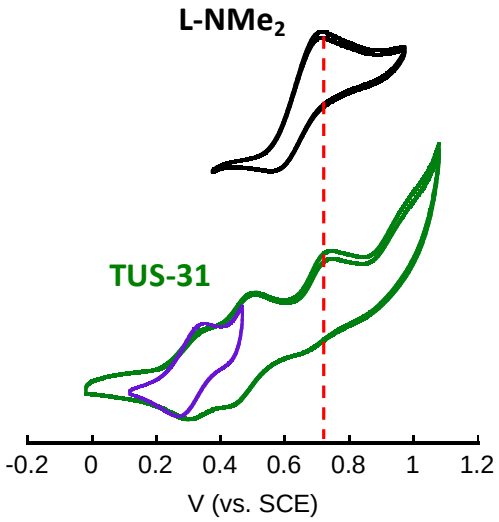

Figure S2. Cyclic voltammograms of **TUS-31** and its ligand (L-NMe2) in DMSO.

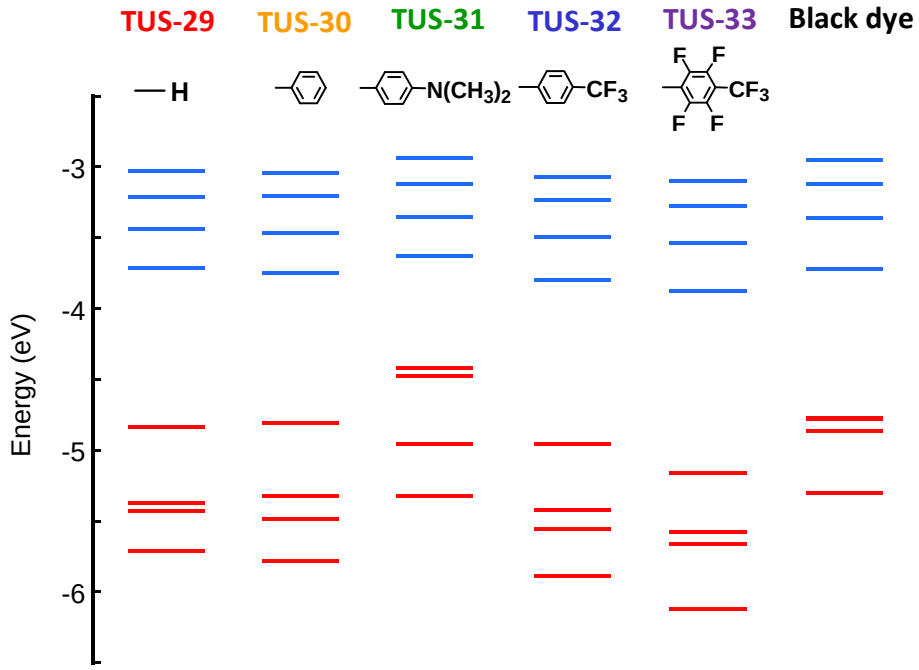

Figure S3. Energy diagrams of the frontier molecular orbitals of fully optimized structures of TUS sensitizers and Black dye in acetonitrile.

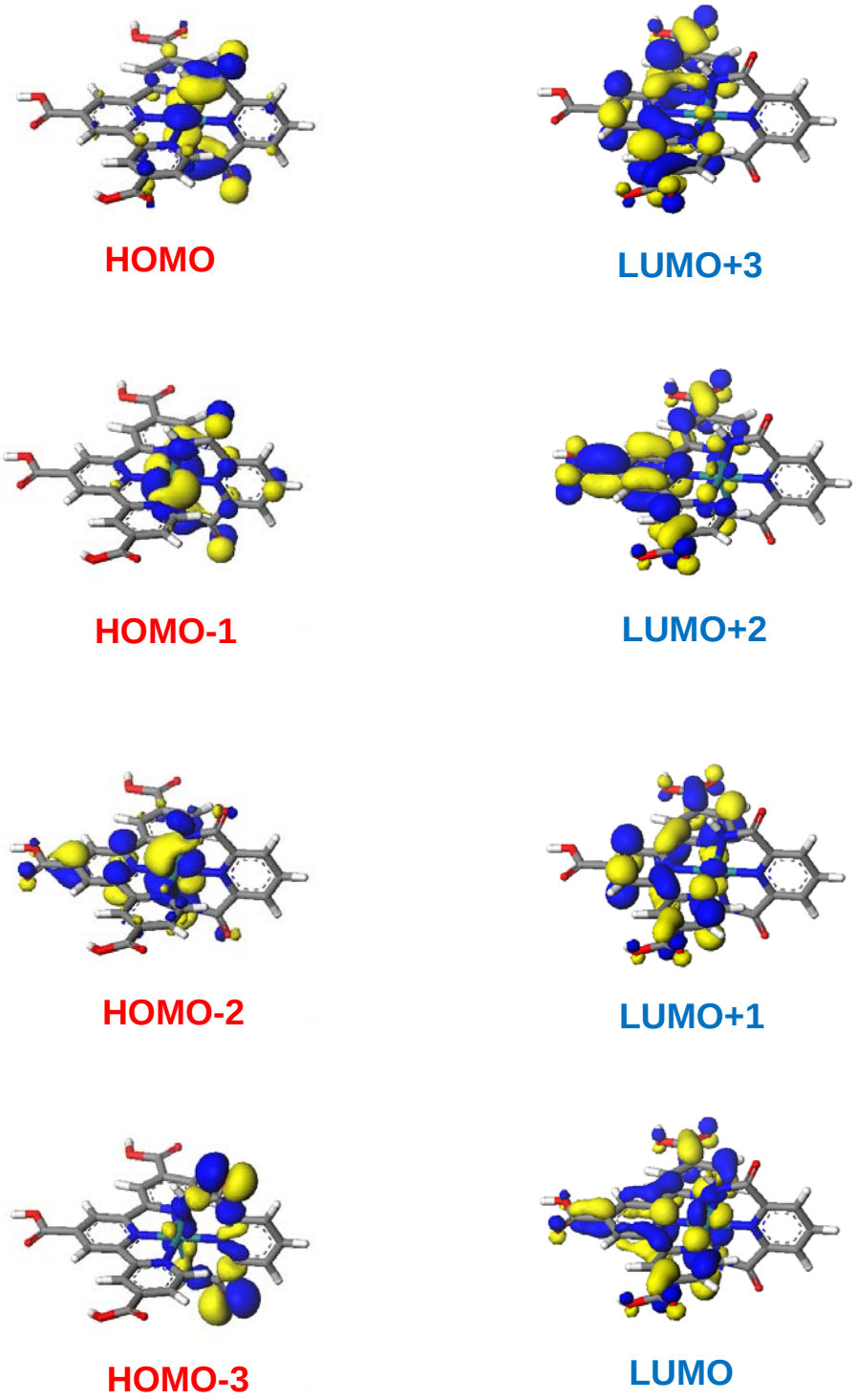

Figure S4. Frontier molecular orbitals (occupied and unoccupied MOs) of a fully optimized structure of **TUS-29** in acetonitrile.

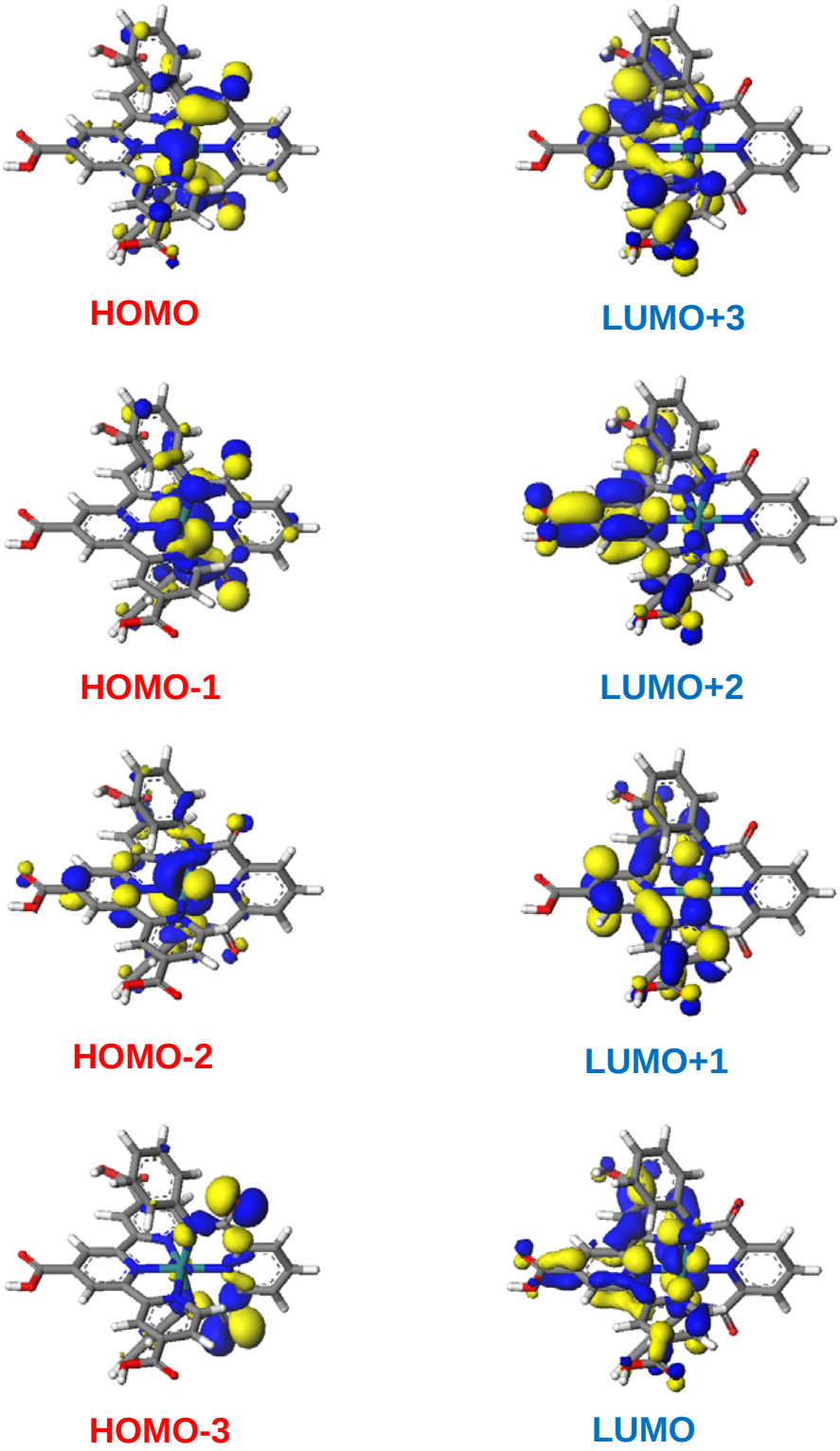

Figure S5. Frontier molecular orbitals (occupied and unoccupied MOs) of a fully optimized structure of **TUS-30** in acetonitrile.

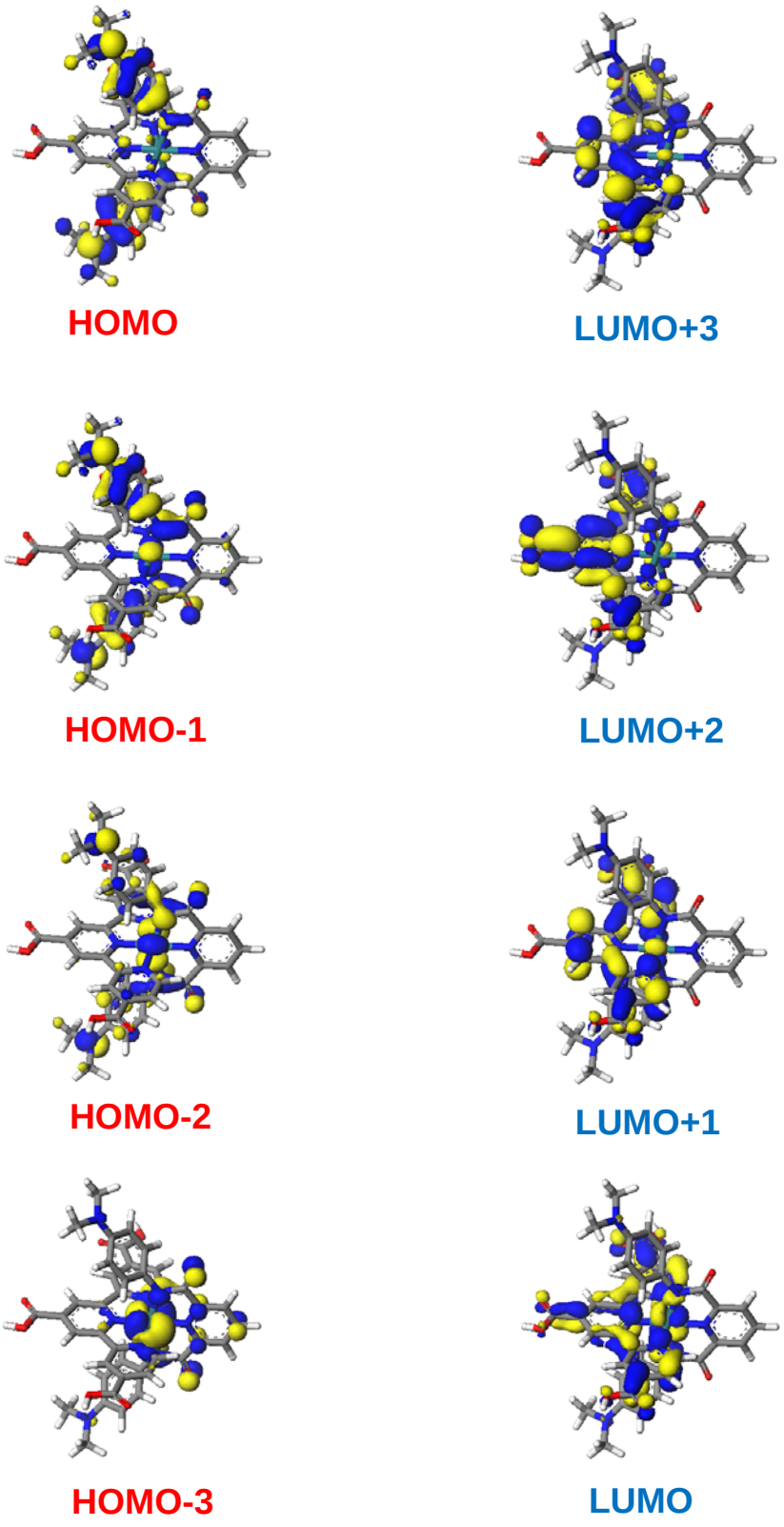

Figure S6. Frontier molecular orbitals (occupied and unoccupied MOs) of a fully optimized structure of **TUS-31** in acetonitrile.

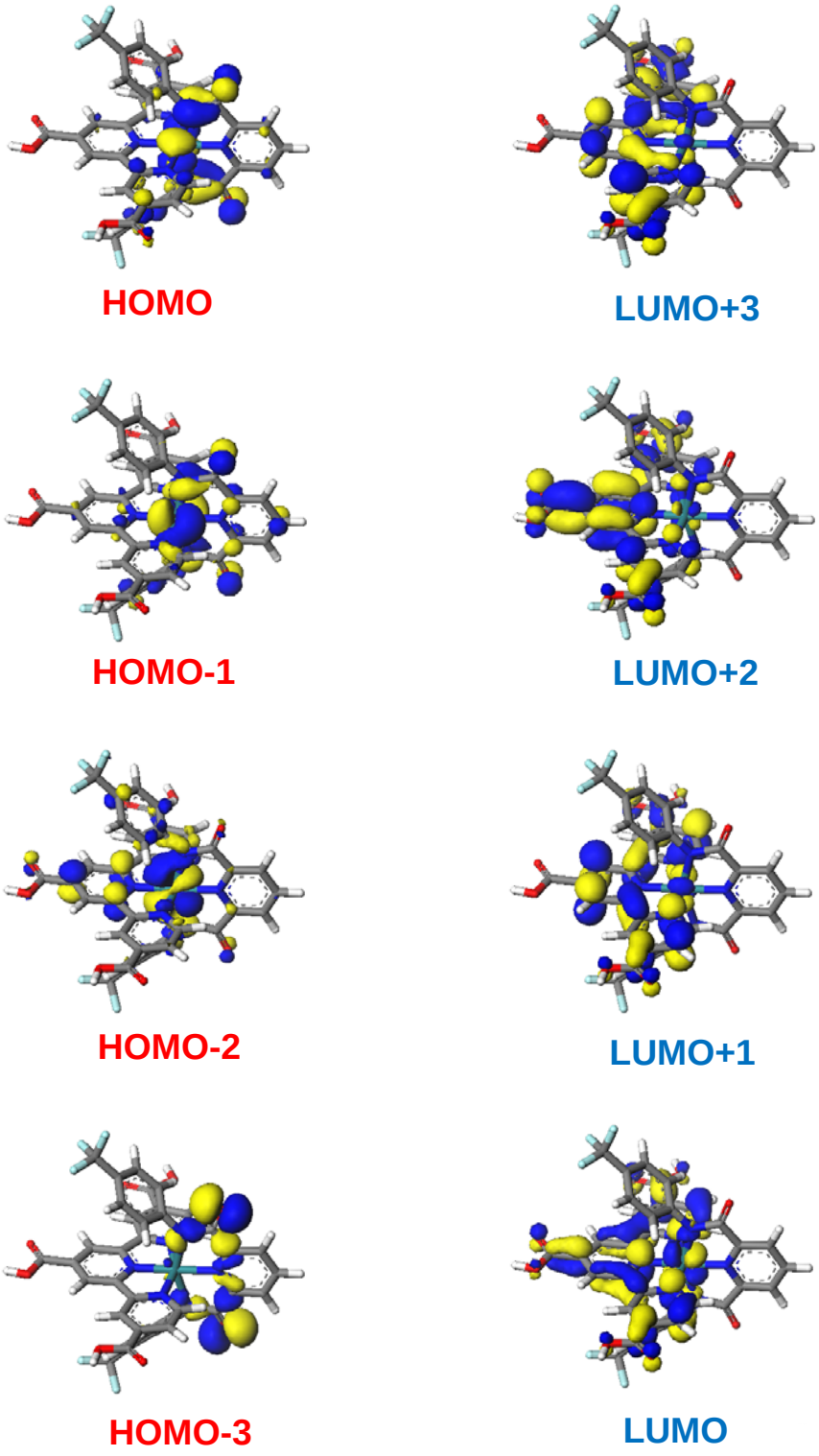

Figure S7. Frontier molecular orbitals (occupied and unoccupied MOs) of a fully optimized structure of **TUS-32** in acetonitrile.

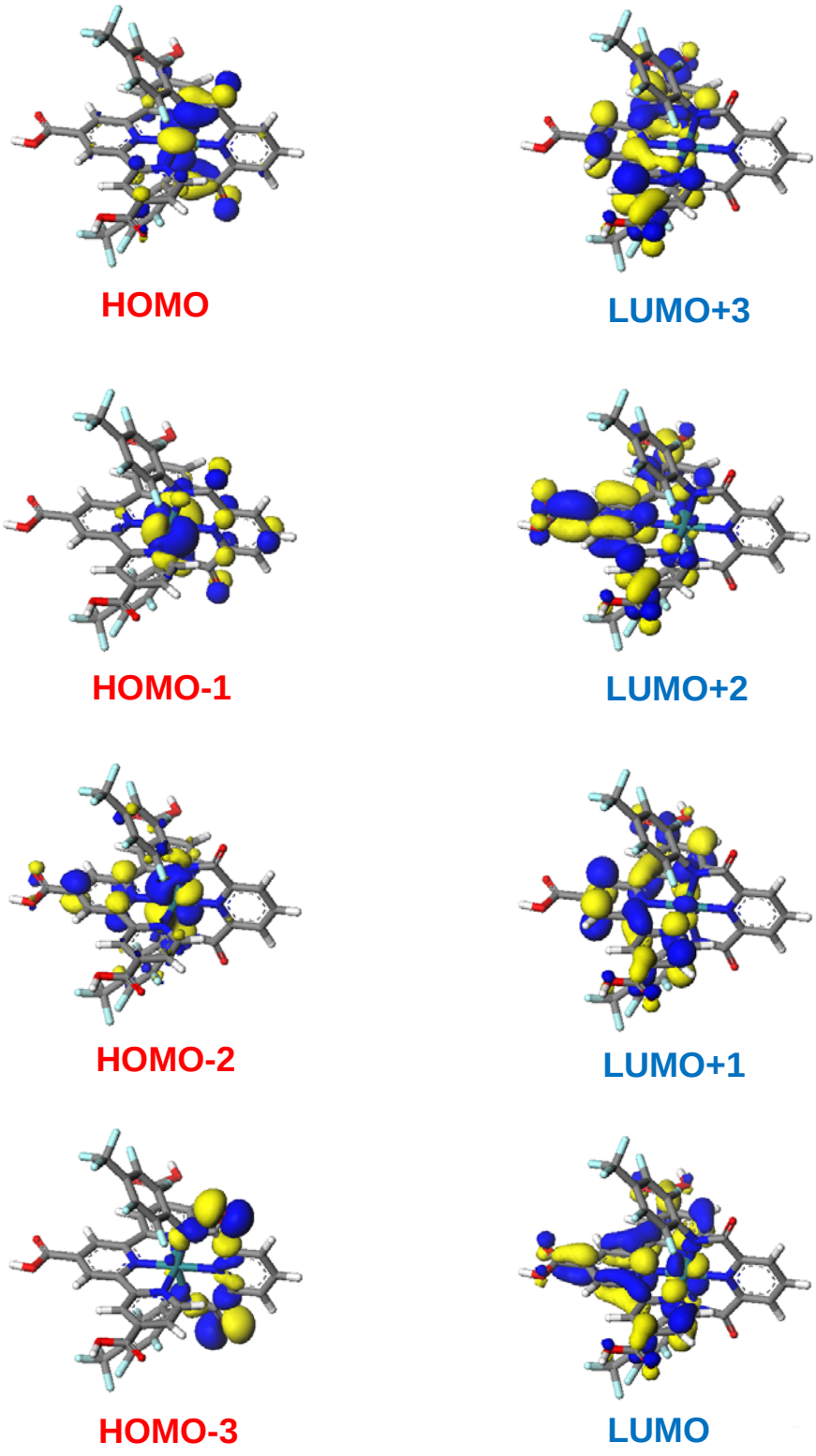

Figure S8. Frontier molecular orbitals (occupied and unoccupied MOs) of a fully optimized structure of **TUS-33** in acetonitrile.