

Supplementary Information

Table S1. Compiled Dimer Classification of 1,3-bis(4-ethynyl-3-iodopyridinium)-benzene Halogen Bond Donors.

Anion (solvent)	Dimer	Receptor Conformation
Tetrafluoroborate	centered antiparallel	Bidentate
Bromide	centered antiparallel	Bidentate
Iodide	centered antiparallel	Bidentate
Nitrate (Methanol)	centered antiparallel	Bidentate
Perrhenate	centered antiparallel	Bidentate
Triflate (DMF)	'slipped' centered antiparallel	Bidentate
Chloride	'slipped' centered antiparallel and off-centered antiparallel	Bidentate
Hydrogen Sulfate	centered parallel dimer and off-centered antiparallel	W
Triflate	off-centered antiparallel	W
Triiodide	off-centered antiparallel	W
Thiocyanate (Methanol)	off-centered antiparallel	W
Thiocyanate (DCM)	off-centered antiparallel	S

Images of reported structures with atomic numbering scheme.

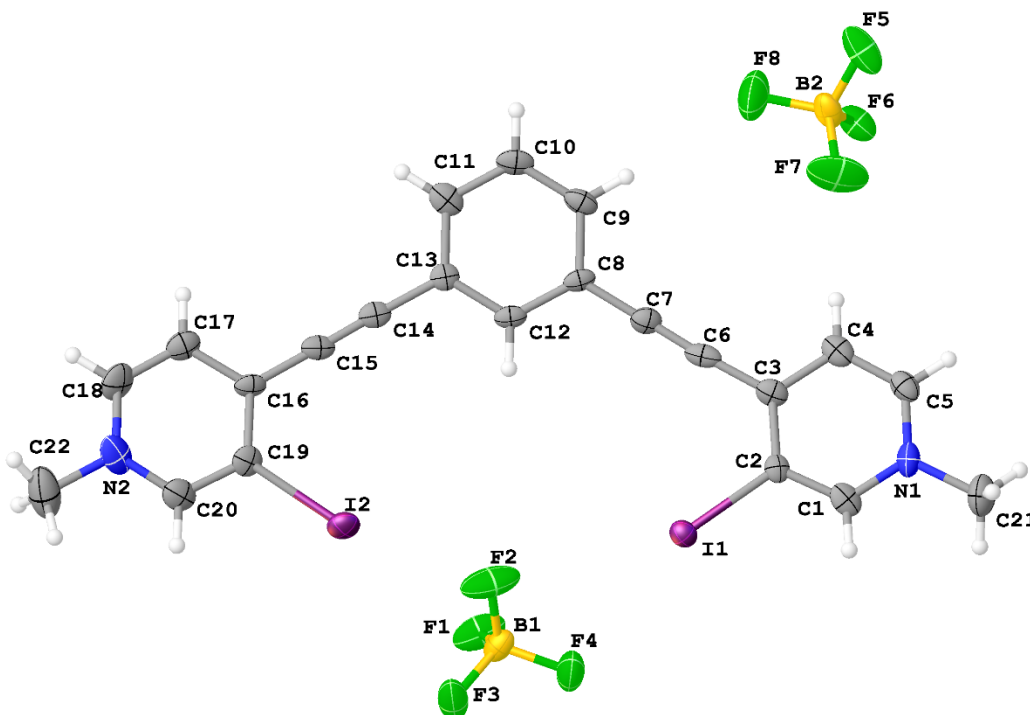


Figure S1. Complex 1 with atomic numbering scheme. Thermal ellipsoids drawn at the 50% probability level. Anion disorder omitted for clarity.

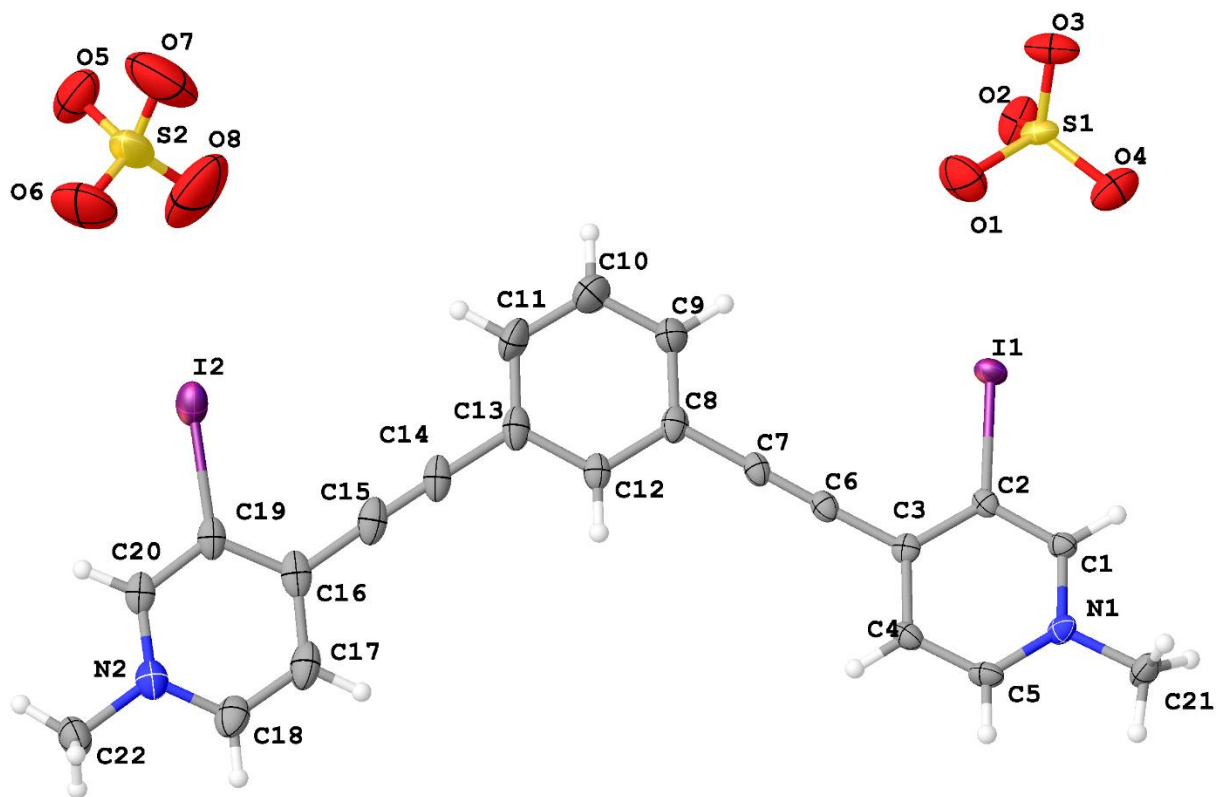


Figure S2. Complex 2 with atomic numbering scheme. Thermal ellipsoids drawn at the 50% probability level. Anion disorder omitted for clarity.

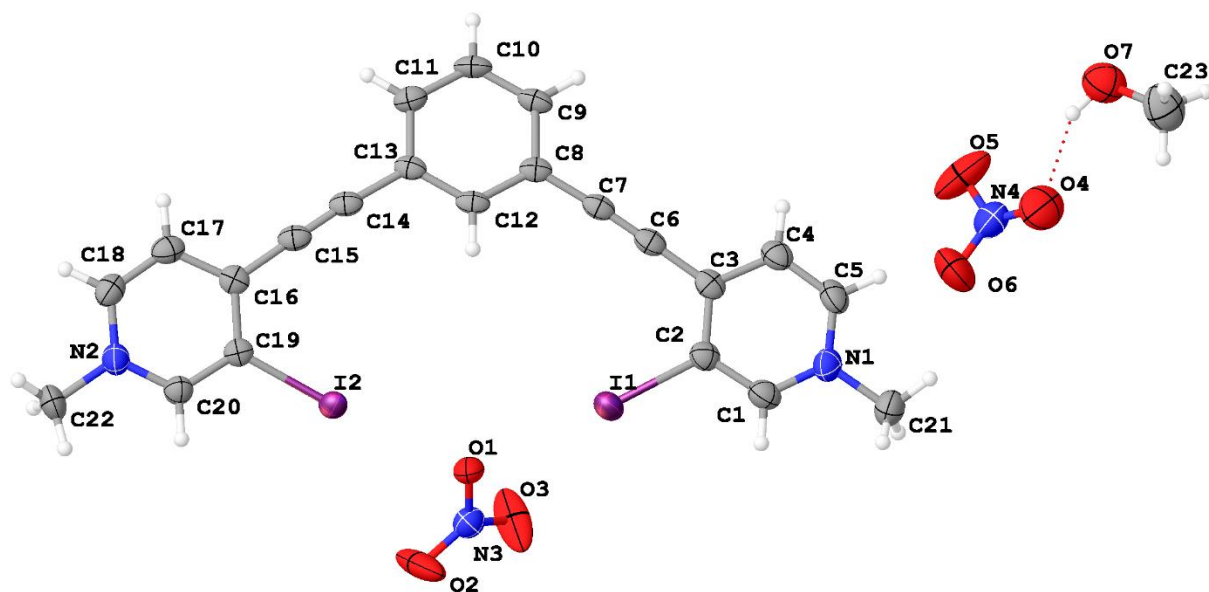


Figure S3. Complex 3•MeOH with atomic numbering scheme. Thermal ellipsoids drawn at the 50% probability level. Anion disorder omitted for clarity.