

**The role of the [CpM(CO)₂]⁻ Chromophore in the Optical properties of the
[Cp₂ThMCp(CO)₂]⁺ complexes, where M=Fe, Ru and Os.**

Theoretical View

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Supporting Information

Optimized geometries for the three complexes [Cp₂ThMCp(CO)₂]⁺ M= Fe, Ru, Os

-Level of Theory ZORA/BP86/TZ2P

[Cp₂ThFeCp(CO)₂]⁺

Fe	-2.022305000	0.239785000	0.000000000
C	-3.131484000	-1.146368000	-1.149379000
C	-3.900901000	-0.808389000	0.000000000
C	-3.131484000	-1.146368000	1.149379000
C	-1.902051000	-1.763073000	0.714404000
C	-1.902051000	-1.763073000	-0.714404000
H	-3.423626000	-0.996205000	-2.182284000
H	-4.875976000	-0.336523000	0.000000000
H	-3.423626000	-0.996205000	2.182284000

H	-1.175034000	-2.234158000	1.373938000
H	-1.175034000	-2.234158000	-1.373938000
Th	0.684657000	-0.173675000	0.000000000
C	2.641661000	0.818242000	-1.719762000
C	2.788076000	-0.591890000	-1.793947000
C	1.641793000	-1.117917000	-2.451334000
C	0.789554000	-0.032825000	-2.791195000
C	1.402508000	1.163447000	-2.329093000
H	3.357555000	1.514357000	-1.295129000
H	3.630966000	-1.168016000	-1.424985000
H	1.460786000	-2.166375000	-2.670254000
H	-0.156109000	-0.102806000	-3.318720000
H	1.007777000	2.168273000	-2.445268000
C	2.641661000	0.818242000	1.719762000
C	2.788076000	-0.591890000	1.793947000
C	1.641793000	-1.117917000	2.451334000
C	0.789554000	-0.032825000	2.791195000
C	1.402508000	1.163447000	2.329093000
H	3.357555000	1.514357000	1.295129000
H	3.630966000	-1.168016000	1.424985000
H	1.460786000	-2.166375000	2.670254000
H	-0.156109000	-0.102806000	3.318720000
H	1.007777000	2.168273000	2.445268000
C	-1.884209000	1.442400000	1.252507000
O	-1.869426000	2.263681000	2.084483000
C	-1.884209000	1.442400000	-1.252507000
O	-1.869426000	2.263681000	-2.084483000

[Cp₂ThRuCp(CO)₂]⁺

Os	-2.095727000	0.262556000	0.000000000
C	-3.257388000	-1.373020000	-1.153620000
C	-4.038315000	-1.054365000	0.000000000
C	-3.257388000	-1.373020000	1.153620000
C	-2.016894000	-1.956737000	0.717427000
C	-2.016894000	-1.956737000	-0.717427000
H	-3.564195000	-1.248258000	-2.185418000
H	-5.034939000	-0.628611000	0.000000000
H	-3.564195000	-1.248258000	2.185418000
H	-1.276617000	-2.411582000	1.370151000
H	-1.276617000	-2.411582000	-1.370151000
Th	0.759516000	-0.202687000	0.000000000
C	2.689380000	0.828422000	-1.723286000
C	2.831328000	-0.578843000	-1.840759000
C	1.672476000	-1.083465000	-2.493154000
C	0.817052000	0.012028000	-2.786681000
C	1.439262000	1.193389000	-2.299527000
H	3.414943000	1.510984000	-1.293452000
H	3.677792000	-1.167573000	-1.500091000
H	1.483473000	-2.125298000	-2.736325000
H	-0.139146000	-0.042056000	-3.296574000
H	1.044323000	2.201663000	-2.379219000
C	2.689380000	0.828422000	1.723286000
C	2.831328000	-0.578843000	1.840759000

C	1.672476000	-1.083465000	2.493154000
C	0.817052000	0.012028000	2.786681000
C	1.439262000	1.193389000	2.299527000
H	3.414943000	1.510984000	1.293452000
H	3.677792000	-1.167573000	1.500091000
H	1.483473000	-2.125298000	2.736325000
H	-0.139146000	-0.042056000	3.296574000
H	1.044323000	2.201663000	2.379219000
C	-1.910128000	1.584389000	1.316013000
O	-1.848929000	2.400843000	2.152952000
C	-1.910128000	1.584389000	-1.316013000
O	-1.848929000	2.400843000	-2.152952000

[Cp₂ThOsCp(CO)₂]⁺

Ru	-2.079698000	0.274993000	0.000000000
C	-3.214293000	-1.376665000	-1.149857000
C	-4.001729000	-1.080310000	0.000000000
C	-3.214293000	-1.376665000	1.149857000
C	-1.967954000	-1.953032000	0.713366000
C	-1.967954000	-1.953032000	-0.713366000
H	-3.522651000	-1.259833000	-2.183074000
H	-5.005226000	-0.668865000	0.000000000
H	-3.522651000	-1.259833000	2.183074000
H	-1.230871000	-2.413423000	1.367511000
H	-1.230871000	-2.413423000	-1.367511000
Th	0.719228000	-0.187552000	0.000000000

C	2.702708000	0.781136000	-1.706141000
C	2.781429000	-0.629893000	-1.834265000
C	1.605125000	-1.076220000	-2.498777000
C	0.801657000	0.058870000	-2.786809000
C	1.473578000	1.206936000	-2.284540000
H	3.456050000	1.426664000	-1.267275000
H	3.598864000	-1.258634000	-1.494502000
H	1.371583000	-2.105797000	-2.754371000
H	-0.151650000	0.052171000	-3.304610000
H	1.126764000	2.233365000	-2.357918000
C	2.702708000	0.781136000	1.706141000
C	2.781429000	-0.629893000	1.834265000
C	1.605125000	-1.076220000	2.498777000
C	0.801657000	0.058870000	2.786809000
C	1.473578000	1.206936000	2.284540000
H	3.456050000	1.426664000	1.267275000
H	3.598864000	-1.258634000	1.494502000
H	1.371583000	-2.105797000	2.754371000
H	-0.151650000	0.052171000	3.304610000
H	1.126764000	2.233365000	2.357918000
C	-1.896044000	1.606526000	1.306787000
O	-1.846675000	2.445733000	2.116608000
C	-1.896044000	1.606526000	-1.306787000
O	-1.846675000	2.445733000	-2.116608000