

Electronic Supplementary Material

X-ray Absorption Spectroscopy of Exemplary Platinum Porphyrin and Corrole Derivatives: Metal- versus Ligand-Centered Oxidation

Benjamin D. Matson,[§] Kalle E. Thomas, Abraham B. Alemayehu,[†] Abhik Ghosh*[†]

Ritimukta Sarangi*[§]

[§]Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Stanford
University, Menlo Park, California 94025, USA;

[†] Department of Chemistry, UiT – The Arctic University of Norway, N-9037 Tromsø, Norway; Email:
abhik.ghosh@uit.no (A.G.), ritis@slac.stanford.edu (R.S)

Optimized Cartesian coordinates (Å)

Pt^{II}[TpCF₃PP]

Pt	-2.024231000	-0.004763000	-1.184205000
F	-2.672743000	-9.813141000	-0.150635000
F	-2.692277000	-9.746674000	-2.331464000
F	-0.789988000	-9.817722000	-1.263360000
F	-1.384122000	9.803899000	-0.147254000
F	-1.343915000	9.735710000	-2.327672000
F	-3.256271000	9.809126000	-1.277768000
F	-1.476763000	1.197729000	-10.930098000
F	-1.284213000	-0.975163000	-10.995545000
F	-3.265958000	-0.049976000	-10.991168000
F	-2.593108000	1.190733000	8.560487000
F	-2.758214000	-0.984360000	8.626329000
F	-0.788280000	-0.034260000	8.624540000
N	-2.016524000	1.464466000	0.285110000
N	-2.037020000	1.464621000	-2.653308000
N	-2.013898000	-1.473865000	-2.653667000
N	-2.029091000	-1.474208000	0.284919000
C	-2.027397000	-0.004358000	-4.651997000
C	-2.030169000	3.463160000	-1.183864000
C	-2.021200000	-0.005073000	2.283523000
C	-2.018199000	-3.472638000	-1.184517000
C	-2.059031000	-2.831450000	-2.437514000
C	-2.063005000	-1.257479000	-4.011056000
C	-1.990546000	1.248552000	-4.010826000
C	-1.991794000	2.822167000	-2.437019000
C	-1.979613000	-2.831577000	0.068516000
C	-1.981030000	-1.257957000	1.642381000
C	-2.062168000	1.247929000	1.642603000
C	-2.066291000	2.821921000	0.069135000
C	-2.169085000	-3.497951000	-3.714755000
C	-2.171351000	-2.534570000	-4.677744000
C	-1.883716000	2.525785000	-4.677527000
C	-1.884341000	3.488949000	-3.714344000
C	-2.175707000	3.488078000	1.346444000
C	-2.173126000	2.524746000	2.309526000
C	-1.867634000	-3.498009000	1.345466000
C	-1.868724000	-2.534884000	2.308793000
C	-2.029009000	-0.003553000	-6.146639000
C	-0.948864000	-0.537614000	-6.865411000
C	-3.112160000	0.529207000	-6.862141000
C	-0.946683000	-0.536999000	-8.257977000
C	-3.118659000	0.528457000	-8.254535000
C	-2.034203000	-0.005328000	-8.955112000
C	-2.032222000	4.957677000	-1.185047000
C	-3.111801000	5.672698000	-1.724786000
C	-0.954855000	5.677073000	-0.645094000
C	-3.117572000	7.065556000	-1.727317000
C	-0.952305000	7.069113000	-0.648240000
C	-2.036169000	7.766132000	-1.188826000

C	-2.020577000	-0.004472000	3.778198000
C	-3.099275000	-0.542594000	4.496183000
C	-0.940000000	0.532358000	4.494509000
C	-3.102604000	-0.541766000	5.888694000
C	-0.934702000	0.531965000	5.886973000
C	-2.017734000	-0.005712000	6.586688000
C	-2.016240000	-4.967155000	-1.185756000
C	-0.938274000	-5.682523000	-1.728370000
C	-3.092087000	-5.686261000	-0.642484000
C	-0.932446000	-7.075315000	-1.729951000
C	-3.094550000	-7.078373000	-0.644546000
C	-2.012181000	-7.775651000	-1.187603000
C	-2.037057000	-9.280844000	-1.228086000
C	-2.010128000	9.271283000	-1.230360000
C	-2.017833000	0.035649000	-10.460493000
C	-2.036519000	0.035523000	8.092027000
H	-2.253896000	-4.566258000	-3.852605000
H	-2.257933000	-2.672185000	-5.745972000
H	-1.798874000	2.663552000	-5.745870000
H	-1.799930000	4.557293000	-3.852089000
H	-2.263442000	4.556167000	1.484454000
H	-2.258063000	2.662106000	3.377912000
H	-1.779627000	-4.566121000	1.483058000
H	-1.781820000	-2.672532000	3.376996000
H	-0.100555000	-0.948045000	-6.325317000
H	-3.961457000	0.934122000	-6.319447000
H	-0.103336000	-0.950083000	-8.802107000
H	-3.969075000	0.930559000	-8.796013000
H	-3.959273000	5.129779000	-2.133179000
H	-0.109307000	5.137279000	-0.228645000
H	-3.964809000	7.606744000	-2.135965000
H	-0.111233000	7.613641000	-0.230561000
H	-3.945580000	-0.956290000	3.955439000
H	-0.091736000	0.940303000	3.952476000
H	-3.944826000	-0.957997000	6.432202000
H	-0.086311000	0.937408000	6.429108000
H	-0.092028000	-5.139811000	-2.139583000
H	-3.936478000	-5.146261000	-0.223968000
H	-0.086290000	-7.616740000	-2.140582000
H	-3.934356000	-7.622651000	-0.224069000

Pt^{IV}[TpCF₃PP]Cl₂

Pt	-2.022510000	-0.007220000	-1.180226000
Cl	0.385880000	-0.001250000	-1.184634000
Cl	-4.431409000	-0.013726000	-1.176487000
F	-2.714876000	-9.810806000	-0.157414000
F	-2.669094000	-9.749403000	-2.338265000
F	-0.799642000	-9.820260000	-1.213485000
F	-1.356032000	9.798499000	-0.157885000
F	-1.410275000	9.737893000	-2.338579000
F	-3.275424000	9.801123000	-1.206255000
F	-1.492546000	1.199666000	-10.925600000
F	-1.255388000	-0.969044000	-10.988203000

F	-3.255676000	-0.084706000	-10.986914000
F	-2.549829000	1.195629000	8.565474000
F	-2.757688000	-0.975931000	8.629893000
F	-0.769432000	-0.064858000	8.624684000
N	-2.012821000	1.467823000	0.295320000
N	-2.038870000	1.468111000	-2.655394000
N	-2.010546000	-1.482482000	-2.655529000
N	-2.028140000	-1.482422000	0.295108000
C	-2.024473000	-0.006906000	-4.650614000
C	-2.031818000	3.463086000	-1.179894000
C	-2.015740000	-0.007458000	2.290408000
C	-2.019843000	-3.477569000	-1.180406000
C	-2.056869000	-2.834818000	-2.429934000
C	-2.058351000	-1.256494000	-4.007727000
C	-1.991537000	1.242595000	-4.007703000
C	-1.995578000	2.820471000	-2.429523000
C	-1.982327000	-2.834704000	0.069121000
C	-1.979842000	-1.256804000	1.647359000
C	-2.055164000	1.241983000	1.647711000
C	-2.063690000	2.819986000	0.069636000
C	-2.160474000	-3.497434000	-3.707272000
C	-2.161047000	-2.533774000	-4.670622000
C	-1.892240000	2.520211000	-4.670366000
C	-1.894829000	3.483622000	-3.706779000
C	-2.164963000	3.482436000	1.347244000
C	-2.159352000	2.518965000	2.310777000
C	-1.877882000	-3.497521000	1.346240000
C	-1.876307000	-2.534090000	2.309839000
C	-2.024565000	-0.006661000	-6.144836000
C	-0.930756000	-0.517280000	-6.859352000
C	-3.119762000	0.501140000	-6.859450000
C	-0.927831000	-0.517896000	-8.252004000
C	-3.124203000	0.498167000	-8.251950000
C	-2.026895000	-0.011922000	-8.950120000
C	-2.036201000	4.957302000	-1.180241000
C	-3.131823000	5.668441000	-1.691047000
C	-0.945179000	5.675125000	-0.667352000
C	-3.139980000	7.061337000	-1.689541000
C	-0.946243000	7.067345000	-0.667685000
C	-2.046074000	7.762410000	-1.177352000
C	-2.012028000	-0.006880000	3.784726000
C	-3.103704000	-0.517930000	4.502245000
C	-0.915499000	0.502259000	4.496180000
C	-3.103177000	-0.517509000	5.894842000
C	-0.907594000	0.500307000	5.888758000
C	-2.002758000	-0.010061000	6.589907000
C	-2.020733000	-4.971823000	-1.180850000
C	-0.928929000	-5.686815000	-1.694538000
C	-3.112990000	-5.685783000	-0.665247000
C	-0.925883000	-7.079752000	-1.693477000
C	-3.117025000	-7.078001000	-0.665970000
C	-2.021096000	-7.776924000	-1.178768000
C	-2.046617000	-9.282849000	-1.216856000

C	-2.026414000	9.268472000	-1.214869000
C	-2.010168000	0.027333000	-10.456131000
C	-2.017074000	0.030176000	8.095897000
H	-2.240693000	-4.566189000	-3.842823000
H	-2.241985000	-2.669082000	-5.739365000
H	-1.812439000	2.655997000	-5.739119000
H	-1.817565000	4.552603000	-3.842159000
H	-2.247953000	4.550968000	1.482816000
H	-2.236836000	2.653995000	3.379800000
H	-1.797662000	-4.566313000	1.481370000
H	-1.794722000	-2.669499000	3.378507000
H	-0.073529000	-0.905719000	-6.317103000
H	-3.978998000	0.885198000	-6.317250000
H	-0.074765000	-0.912038000	-8.794911000
H	-3.983149000	0.879522000	-8.794827000
H	-3.988616000	5.123641000	-2.076902000
H	-0.087347000	5.135332000	-0.276862000
H	-3.998876000	7.601765000	-2.074066000
H	-0.095553000	7.612911000	-0.271649000
H	-3.961909000	-0.907464000	3.962324000
H	-0.058021000	0.886725000	3.951501000
H	-3.954531000	-0.912021000	6.440201000
H	-0.047746000	0.882877000	6.429308000
H	-0.071071000	-5.145073000	-2.082322000
H	-3.967788000	-5.142899000	-0.272364000
H	-0.069955000	-7.623218000	-2.080352000
H	-3.968657000	-7.620619000	-0.267895000

Pt^{IV}[TpCF₃PP](Ar)(Py)

Pt	0.868841000	8.781260000	3.910413000
F	-8.733720000	7.143641000	4.485182000
F	-8.227287000	5.060612000	4.065036000
F	-8.204249000	5.803279000	6.121548000
F	9.167338000	13.660682000	2.008570000
F	10.044155000	11.671953000	2.201466000
F	9.263373000	12.332015000	0.273472000
F	3.312600000	7.473254000	13.297833000
F	2.732785000	5.408860000	12.865841000
F	4.744909000	6.102498000	12.385518000
N	-0.704857000	8.639563000	2.684511000
N	-0.170267000	8.044719000	5.479332000
N	2.562060000	9.124158000	4.964139000
N	1.649998000	9.539323000	2.232470000
N	0.141474000	10.968988000	4.493537000
N	-0.741481000	2.589956000	2.970614000
C	-0.549305000	9.193687000	1.438860000
C	-1.847835000	9.136178000	0.840432000
C	-2.722967000	8.574456000	1.765915000
C	-1.981121000	8.263238000	2.965760000
C	-2.350773000	7.759040000	4.259073000
C	-1.492358000	7.648039000	5.403745000

C	-1.788673000	7.090703000	6.704716000
C	-0.660405000	7.176500000	7.487426000
C	0.392921000	7.771861000	6.697619000
C	1.749337000	8.052286000	7.053587000
C	2.755319000	8.660632000	6.240414000
C	4.154256000	8.878443000	6.525746000
C	4.736174000	9.447777000	5.416199000
C	3.726020000	9.606946000	4.394105000
C	3.875876000	10.110280000	3.057738000
C	2.867273000	10.111198000	2.033272000
C	2.786081000	10.682606000	0.709008000
C	1.516452000	10.428424000	0.196588000
C	0.778425000	9.704322000	1.184874000
C	-3.764797000	7.325906000	4.419674000
C	-4.327355000	6.384492000	3.542005000
C	-5.654760000	5.982779000	3.672396000
C	-6.448077000	6.519583000	4.687295000
C	-5.906433000	7.458985000	5.570746000
C	-4.580991000	7.855129000	5.436122000
C	2.169822000	7.648826000	8.426435000
C	2.095428000	6.307974000	8.839224000
C	2.487631000	5.928669000	10.119577000
C	2.963774000	6.888756000	11.016452000
C	3.047603000	8.226543000	10.623078000
C	2.652644000	8.598958000	9.341190000
C	5.194232000	10.690262000	2.692738000
C	5.801196000	11.683565000	3.482505000
C	7.028910000	12.234122000	3.129658000
C	7.679344000	11.804194000	1.969855000
C	7.092959000	10.819853000	1.170301000
C	5.864793000	10.273034000	1.528996000
C	1.501857000	6.849530000	3.374111000
C	2.828852000	6.619016000	3.013548000
C	3.236304000	5.330087000	2.650958000
C	2.331021000	4.275598000	2.638247000
C	0.994940000	4.516702000	2.995051000
C	0.578556000	5.810931000	3.364872000
C	-1.132450000	11.197067000	4.856999000
C	-1.595221000	12.465160000	5.194705000
C	-0.707902000	13.538689000	5.154252000
C	0.612204000	13.302373000	4.775741000
C	0.997431000	12.004773000	4.453528000
C	-7.892862000	6.125471000	4.834906000
C	9.027700000	12.367455000	1.611342000
C	3.429976000	6.472360000	12.385236000
C	0.039671000	3.451846000	2.981163000
H	-2.106665000	9.480167000	-0.152313000
H	-3.780587000	8.404674000	1.617314000
H	-2.739617000	6.669440000	6.999494000
H	-0.569000000	6.857818000	8.516280000
H	4.653767000	8.616133000	7.447935000
H	5.779149000	9.711149000	5.307195000
H	3.574809000	11.225412000	0.206251000

H	1.148857000	10.736141000	-0.773526000
H	3.554256000	7.425294000	3.009980000
H	4.272843000	5.156975000	2.374923000
H	2.641656000	3.275274000	2.354953000
H	-0.459121000	5.968576000	3.634614000
H	-1.787415000	10.332191000	4.871497000
H	-2.633349000	12.600108000	5.480837000
H	-1.039254000	14.540720000	5.411125000
H	1.338844000	14.106995000	4.726418000
H	2.013691000	11.773309000	4.151952000
H	-3.709102000	5.945700000	2.764589000
H	-6.067652000	5.242572000	2.995212000
H	-6.523890000	7.881636000	6.357935000
H	-4.170805000	8.595543000	6.116777000
H	2.426811000	4.887756000	10.421576000
H	1.739031000	5.556225000	8.141107000
H	2.701516000	9.643068000	9.045703000
H	3.405549000	8.975275000	11.322670000
H	7.598048000	10.480488000	0.271484000
H	7.474739000	13.009872000	3.744389000
H	5.291238000	12.039248000	4.372971000
H	5.421215000	9.498315000	0.910713000