

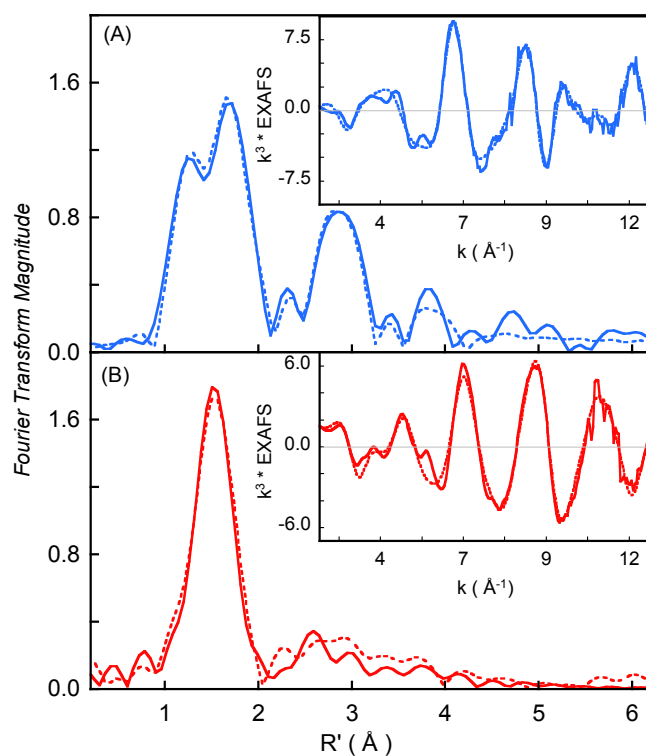
# X-ray Absorption Spectroscopy of Archetypal Chromium Porphyrin and Corrole Derivatives

Rui Cao,<sup>§</sup> Kolle E. Thomas,<sup>†</sup> Abhik Ghosh\*,<sup>†</sup> Ritimukta Sarangi\*,<sup>§</sup>

<sup>§</sup>Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, Stanford University, Menlo Park, California 94025, USA;

<sup>†</sup> Department of Chemistry, UiT – The Arctic University of Norway, N-9037 Tromsø, Norway;

Email: [abhik.ghosh@uit.no](mailto:abhik.ghosh@uit.no) (A.G.), [ritis@slac.stanford.edu](mailto:ritis@slac.stanford.edu) (R.S).



**Figure S1.** Non-phase-shift-corrected Fourier transform data and their corresponding FEFF best-fits for **2** (A) and **3** (B). The inset shows the Cr K-edge EXAFS fits. Data (solid), Fits (dashed).

## BP86 optimized geometries (Å)

### [Cr(TPP)O]

Cr	-0.00723611393895	0.02691083320908	-0.04413889048786
O	-0.43435643858489	0.05986382277651	1.45796789463855
N	-1.79710995516894	0.00919595737986	-1.05467386897918
C	-2.58389246639765	-1.09854576128412	-1.34013448707380
C	-3.85308422378380	-0.68564460587903	-1.88243298259258
C	-3.85414749668977	0.67892519916766	-1.90044344446035
C	-2.58477238395210	1.10780455807742	-1.37121232901425
C	-2.22285941638932	2.45275703858491	-1.21847544932661
C	-3.25061995598273	3.49951010734398	-1.51671739078052
C	-3.14034039398821	4.31868560570190	-2.65367410811630
C	-4.10640202357848	5.29190406326779	-2.92671740917039
C	-5.19464500050043	5.46394222176306	-2.06510211849004
C	-5.31336071254857	4.65509145601972	-0.93030448614217
C	-4.35031900934014	3.67866445468622	-0.65937839542720
H	-5.94742323002955	6.22523599918739	-2.27782633526114
N	0.12203455480660	2.02509353508610	-0.53199289901611
C	-0.94831225931881	2.86370844247340	-0.80999725288485
C	-0.56183023828542	4.24259045734321	-0.64708435227947
C	0.75582645411518	4.24743124846343	-0.29251315613005
C	1.18056832290910	2.87132906311632	-0.23309087943094
C	2.48720973813727	2.47000287263610	0.07062887720269
C	3.51967113868898	3.52674411676026	0.31163987710408
C	4.03825768922417	3.73855524357083	1.60107566233784
C	5.00021880346301	4.72712252392319	1.82842811860228
C	5.46209446561866	5.51605988847775	0.76984258758618
C	4.95527032651604	5.31169955480050	-0.51758364450097
C	3.98998682843223	4.32615022824168	-0.74472636439037
H	6.21483835589222	6.28643794891942	0.94760252899248
N	2.04635527128453	0.02375399587720	0.03267168062708
C	2.88020736472576	1.12763130910126	0.15165025190693
C	4.24075289799082	0.70694306712306	0.36918592052286
C	4.23444497605562	-0.65705911083023	0.41234353763336
C	2.87052716814388	-1.07798777102843	0.21852365010443
C	2.46760647981692	-2.41979685579569	0.21075611450819
C	3.48984529781930	-3.46737742905750	0.52519869283448
C	3.98049743328391	-3.61432766488894	1.83436628605254
C	4.93374717390280	-4.59266543947425	2.13207033809362
C	5.41477895962804	-5.43577755404087	1.12511871004950
C	4.93611766172932	-5.29585853729048	-0.18161350765579
C	3.97936219575978	-4.32070630495844	-0.47892109594674
H	6.16059882180432	-6.19824368495044	1.35763233879496
N	0.11403929739205	-1.99127616524308	-0.44403300019105
C	1.16281110430730	-2.82847904386849	-0.09001004901373
C	0.73203435511836	-4.20386987397013	-0.09581578078238
C	-0.57841802286824	-4.20884520406607	-0.47625303251474
C	-0.95555210406757	-2.83651767375183	-0.70382251242868
C	-2.22396322603298	-2.43817961520042	-1.14280866445911
C	-3.24880399547353	-3.49403256810997	-1.41829339541431

C	-4.35688956420009	-3.64863586649018	-0.56711521384947
C	-5.31618341778261	-4.63402204765959	-0.81789027724589
C	-5.18529469815629	-5.47696870700260	-1.92627005375430
C	-4.08830989059324	-5.33005944089704	-2.78148028378811
C	-3.12618658710126	-4.34764655754253	-2.52839139937017
H	-5.93538154417095	-6.24547796777497	-2.12333469721306
H	3.67369509545660	3.12728925977586	2.42892331125891
H	5.38682881938830	4.88376198716322	2.83739713696979
H	-4.63640923354650	1.34305470180348	-2.25387852109814
H	-6.15728823167962	4.78642502750936	-0.25016110497947
H	-2.29493142830862	4.18074881571024	-3.33069752881279
H	-4.63409731564778	-1.36017984368876	-2.21845840883824
H	-4.00935808673488	5.91505615244379	-3.81800524147444
H	-4.44025440181220	3.05065355043160	0.22906736330496
H	-1.22151962020908	5.09382149701064	-0.78187530691510
H	1.38823476527030	5.10335955026962	-0.07946049219787
H	5.09113078477849	1.37530429635159	0.45868784251314
H	-4.45651815098407	-2.99395120041812	0.30086049641584
H	3.59910457486058	4.16325572205805	-1.75103359518899
H	-3.98144536138708	-5.98006622820042	-3.65222286146007
H	3.61064313408810	-4.20858629105908	-1.50045150571473
H	5.29884422675330	-4.69830976747139	3.15558118977095
H	-2.27358702020324	-4.22985329125408	-3.20023664486851
H	5.31081922006935	-5.94583833505112	-0.97483091606843
H	-6.16687148754906	-4.74563343569686	-0.14266193476657
H	-1.23986091265202	-5.06222508802921	-0.58666562514503
H	3.60195837708728	-2.95959576553637	2.62171224139035
H	5.31468489622345	5.91922313725049	-1.35056084122496
H	1.35626872972818	-5.05222587153294	0.16607714291540
H	5.07828985936859	-1.32654194186344	0.54521394420461

### Cr[TPC]O

Cr	0.03441866778815	0.00369293802808	-0.09769186242937
O	0.09285325709998	0.11994945589199	1.47161331601390
N	0.06378420714619	-1.90288988432805	-0.53374629699423
N	-1.86245763479165	0.15346519042796	-0.55620713810810
N	0.18742487517365	1.78201179773301	-0.88714067162438
N	1.86515687301411	0.01101430682093	-0.76879795365904
C	1.19273967298807	-2.74189305142045	-0.52532606634679
C	0.74515864704908	-4.08876101624731	-0.32832962268819
C	-0.62483142357924	-4.07696298001985	-0.23525346675579
C	-1.06209775071685	-2.71911043956250	-0.36897502283176
C	-2.39220024483764	-2.26565102086856	-0.35569502930525
C	-2.75888169902782	-0.91370736728578	-0.48324865310382
C	-4.09036847665757	-0.40008048237012	-0.61258829592993
C	-4.00178598195000	0.96455012179449	-0.74633608360585
C	-2.61601923540073	1.32719512472671	-0.70713768578662
C	-2.09154806440537	2.62455223414134	-0.87176277205692
C	-0.70592277041704	2.83406913932086	-0.97920218492123
C	0.05364983573291	4.02118457408085	-1.23812046671324

C	1.39506408678372	3.66430582236599	-1.32501928817481
C	1.46662479089184	2.26539473848863	-1.10339252841782
C	2.43184971847060	1.23815282857674	-1.06170547457858
C	3.81551945975993	1.05267227006923	-1.31222790158386
C	4.07139158350217	-0.30889589377814	-1.18293536829740
C	2.84154228016717	-0.96154982290812	-0.84496748426134
C	2.52774504158127	-2.32309527044577	-0.68768760612282
C	3.62786589660432	-3.32543532482691	-0.71967796186149
C	4.67315954685392	-3.26178965275100	0.22077050933516
C	5.71741438391028	-4.18987307110969	0.19164431076003
C	5.73855576994724	-5.19547222161225	-0.78018312460287
C	4.70831780013302	-5.26614962729789	-1.72382955915085
C	3.66236709661251	-4.34019850857258	-1.69448573763108
C	-3.48526275068482	-3.27777857613871	-0.22649756855848
C	-3.72292643562727	-4.21703172653261	-1.24553930859998
C	-4.74935404539969	-5.15801439151379	-1.12255086723433
C	-5.55347064315909	-5.17637392252863	0.02174915062249
C	-5.32601820831699	-4.24702999359095	1.04188345698158
C	-4.30124765783109	-3.30440759749854	0.91842739416998
C	-3.01952442927652	3.78515716111383	-0.97312589596661
C	-3.87031753877149	4.11895106524423	0.09696207874756
C	-4.73363122440710	5.21396614796067	0.00725581848641
C	-4.76328710773362	5.99397001062792	-1.15345031176693
C	-3.92395270946802	5.67097976856387	-2.22457984109005
C	-3.05851795088747	4.57725740851673	-2.13550299208191
H	4.65046593101401	-2.48589432615772	0.98805851387425
H	6.51460875902589	-4.13058983774928	0.93546404613315
H	6.55479148522969	-5.91977890410380	-0.80349745575324
H	4.72257747049476	-6.04124626638743	-2.49276388196670
H	2.86961218762849	-4.38602878442532	-2.44330228312721
H	-3.10226855272900	-4.19768949516869	-2.14346853895363
H	-4.92487931313830	-5.87550667637699	-1.92668020072698
H	-6.35443982518958	-5.91174052486251	0.11797315320518
H	-5.94524382552734	-4.25826993995027	1.94106116690978
H	-4.11918599635724	-2.58499079590484	1.71918103816829
H	-3.83831841084227	3.51957264857567	1.00868084648071
H	-5.38064847966728	5.46272562969778	0.85084934098106
H	-5.43843053141724	6.84913955849590	-1.22348389566771
H	-3.94705255182514	6.26897186896984	-3.13788311188307
H	-2.41664002587913	4.31724246899419	-2.97906879099251
H	1.40173730454789	-4.95105859597839	-0.26413236068789
H	-1.28411866568535	-4.92521093669777	-0.07973214974069
H	-4.98851741964517	-1.00975008291206	-0.62293582164519
H	-4.81624361130123	1.66717041592439	-0.89458970631000
H	-0.36630405135799	5.01603603524305	-1.35283509259812
H	2.23520081130044	4.32275426148804	-1.52818535826933
H	4.52596727122317	1.82939039372961	-1.58155357468814
H	5.02163053223489	-0.81303837572928	-1.33308382501742

**Cr[TPP]Cl**

Cr	-0.02115	-0.05175	0.25108
Cl	0.08071	-0.04171	2.48347
N	-0.06880	-2.08015	-0.01040
N	1.98660	-0.09103	-0.12798
N	-0.00057	1.96709	-0.05276
N	-2.05604	-0.02040	0.06089
C	-1.18752	-2.89660	0.07912
C	-0.78488	-4.28064	0.11287
C	0.57847	-4.30443	0.04750
C	1.02423	-2.93514	-0.02704
C	2.37037	-2.54565	-0.08703
C	2.80363	-1.21281	-0.14433
C	4.18456	-0.81337	-0.25555
C	4.20750	0.55129	-0.28425
C	2.83983	1.00097	-0.20579
C	2.44988	2.34818	-0.20885
C	1.11796	2.78318	-0.14687
C	0.71320	4.16512	-0.22222
C	-0.65024	4.18886	-0.15810
C	-1.09402	2.82176	-0.04303
C	-2.44019	2.43329	0.02080
C	-2.87452	1.10041	0.06197
C	-4.25828	0.69846	0.11485
C	-4.27971	-0.66621	0.14536
C	-2.90898	-1.11316	0.12591
C	-2.51871	-2.46019	0.14656
C	3.41313	-3.62143	-0.09169
C	4.18744	-3.86647	1.05522
C	5.15939	-4.87142	1.05494
C	5.37324	-5.64311	-0.09187
C	4.60840	-5.40591	-1.23851
C	3.63411	-4.40298	-1.23829
C	3.52263	3.39122	-0.28941
C	3.87240	4.14062	0.84668
C	4.87251	5.11505	0.77463
C	5.53465	5.35556	-0.43363
C	5.19225	4.61584	-1.57018
C	4.19384	3.63957	-1.49859
C	-3.47904	3.51286	0.04182
C	-3.69408	4.26969	1.20604
C	-4.66254	5.27784	1.22942
C	-5.42730	5.54529	0.08932
C	-5.21918	4.79857	-1.07480
C	-4.25269	3.78840	-1.09831
C	-3.59394	-3.49897	0.24644
C	-4.25596	-3.72134	1.46589
C	-5.25818	-4.69127	1.56350
C	-5.61406	-5.45019	0.44381
C	-4.96170	-5.23510	-0.77446
C	-3.95745	-4.26705	-0.87252
H	-1.46450	-5.12362	0.18687

H	1.23224	-5.17067	0.05869
H	5.02655	-1.49636	-0.30621
H	5.07248	1.20298	-0.35471
H	1.39194	5.00569	-0.32636
H	-1.30614	5.05261	-0.20032
H	-5.10328	1.37948	0.12334
H	-5.14566	-1.31978	0.17577
H	4.01608	-3.26756	1.95181
H	5.74869	-5.05371	1.95578
H	6.13236	-6.42760	-0.09154
H	4.77216	-6.00110	-2.13910
H	3.04047	-4.21500	-2.13526
H	3.35919	3.94806	1.79084
H	5.13718	5.68520	1.66733
H	6.31480	6.11709	-0.48956
H	5.70118	4.80110	-2.51823
H	3.92282	3.06625	-2.38747
H	-3.10032	4.05712	2.09725
H	-4.82171	5.85364	2.14328
H	-6.18259	6.33324	0.10777
H	-5.80878	5.00433	-1.97043
H	-4.08681	3.20919	-2.00896
H	-3.97302	-3.13274	2.34077
H	-5.75956	-4.85655	2.51918
H	-6.39721	-6.20681	0.52056
H	-5.23701	-5.82036	-1.65414
H	-3.45197	-4.09541	-1.82501