Model Studies of the Cu_B Site in Cytochrome *c* Oxidase Utilizing a Zn(II) Complex Containing an Imidazole-Phenol Cross-Linked Ligand

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General

All preparations were carried out in the presence of air unless otherwise stated. ^{1}H and ^{13}C-{1H} spectra were recorded on Varian Unity 400 or 500 MHz spectrometers at room temperature and referenced internally to their respective residual solvent peaks. ^{13}C-{1H} spectra obtained in D_2O were referenced to their corresponding ^{1}H NMR spectra under identical conditions. Solvents CH_2Cl_2, CH_3CN and THF were freshly distilled over CaH_2 or Na/Benzophenone (THF) prior to use.

Table S1. Crystal Data and Structure Refinement of BPAIP-4 HBr.

	2(BPAIP-4HBr)•3 MeOH•1 H_2O
formula	$C_{53}H_{74}Br_8N_{10}O_6$
fw	1586.50
cryst system	monoclinic
space group	$P2_1/n$
Z	2
a, Å	14.088(7)
b, Å	7.523(4)
c, Å	34.71(2)
α, deg	90.00
β, deg	97.75(1)
γ, deg	90.00
V, Å^3	3645(3)
GOF (F^2)	0.963
R_1,[a] wR_2[b]	0.087, 0.19

[a] $R(F_o) = \sum[(F_o - F_c)]/\sum(F_o)$. [b] $R_w(F_o^2) = \{\sum[w(F_o^2 - F_c^2)^2/\sum[w(F_o^2)^2]\}^{1/2}$.

Table S2. Relevant Structures for Copper Complexes Used to Validate DFT Approach.

$[Cu(TEPA)(Cl)]^{+}$ – trigonal bipyramidal structure

N	-0.00629800	0.00261700	1.92053000
C	0.76422100	-2.78773600	-1.28442400
C	2.07169900	-2.11956900	0.51334600
C	1.53046200	-3.93154500	-1.48252900
H	-0.06866000	-2.55045400	-1.93476400
C	2.89842900	-3.23399200	0.35912500
H	1.27189300	-4.62115900	-2.27867400
H	3.73653300	-3.37841100	1.03333100
C	2.04299100	2.03634100	-1.28202700
C	0.81008700	2.85233500	0.50811300
C	2.66091000	3.26598400	-1.48351600
H	2.24832200	1.19186700	-1.92842700
C	1.37237400	4.12045100	0.34976800
H	3.39102900	3.37791000	-2.27767500
H	1.08240200	4.92427400	1.01885500
N	1.02666500	-1.89245800	-0.31152400
N	1.13199000	1.82768200	-0.31079700
C	2.62893100	-4.15202000	-0.65423800
H	3.26080800	-5.02504600	-0.78800800
C	2.30783400	4.33380500	-0.66120700
H	2.75595200	5.31350900	-0.79796900
C	-0.12738000	2.53762300	1.64757400
H	-1.14141400	2.34224500	1.27606900
H	-0.20034800	3.40832500	2.30615500
C	0.38904100	1.34275700	2.46486200
H	1.48021500	1.38689400	2.50107800
C	2.25408700	-1.15111000	1.65562600
H	3.04358200	-1.51854100	2.31802300
H	2.58661700	-0.17280000	1.28641300
C	0.95561700	-1.01021700	2.46539300
H	0.45039800	-1.97877800	2.49216100
C	-1.36465700	-0.32401900	2.46439600
H	-1.24325200	-0.65474800	3.50497500
H	-1.94945800	0.59865300	2.49312300
C	-2.13713100	-1.37511600	1.65244500
H	-1.45773900	-2.15462600	1.28497700
H	-2.85326900	-1.87315700	2.31295300
H	1.17891500	-0.74024700	3.50668100
H	0.03537000	1.40551600	3.50302900
C	-2.87987100	-0.72879400	0.50924300
C	-4.25860300	-0.88193000	0.35135200
C	-4.91359900	-0.18687900	-0.66361200
H	-4.80723500	-1.53350100	1.02384500
C	-2.79488700	0.73826700	-1.28799700
C	-4.16831100	0.65170800	-1.48966000
H	-5.98555000	-0.29407600	-0.80056700
H	-2.16958700	1.33945000	-1.93636100
H	-4.63202100	1.22244600	-2.28684800
N	-2.15567000	0.06017900	-0.31381400
Cu	-0.00541200	-0.00006800	-0.26544200
Cl	-0.00510800	0.00130600	-2.58456000

$[Cu(TEPA)(Cl)]^{+}$ – square pyramidal structure

Cu	0.10948000	-0.38139800	-0.37793700
N	0.04799000	-0.55831700	1.78391500
C	-0.11600400	2.55060700	-1.41151500
C	-0.65972800	2.58112000	0.84003100
C	-0.40782600	3.90204300	-1.56195600
H	0.21254500	1.94925400	-2.25331200
C	-0.98980800	3.94004600	0.76058200
H	-0.28758400	4.37675900	-2.52996800
H	-1.33769800	4.46177100	1.64714100
C	-2.83814600	-0.29451600	-1.05061400
C	-2.18956200	-2.08489300	0.29075900
C	-4.15974900	-0.72715100	-1.07063000
H	-2.51729100	0.58513800	-1.59544500
C	-3.49443100	-2.57928500	0.30989100
H	-4.90273300	-0.16786300	-1.62853600
H	-3.71632000	-3.49534700	0.84760000
N	-0.23884800	1.89079200	-0.23954400
N	-1.88100300	-0.95352900	-0.37589200
C	-0.86205200	4.61174400	-0.45145800
H	-1.11303100	5.66578200	-0.52626800
C	-4.49313800	-1.89065500	-0.37769600
H	-5.51331700	-2.26255900	-0.37927000
C	-1.03563500	-2.76230500	0.98004800
H	-0.26425500	-2.98802700	0.23112800
H	-1.35694900	-3.72366500	1.39409200
C	-0.40299300	-1.95843000	2.13149300
H	-1.10199100	-1.90838600	2.97517800
C	-0.71793800	1.90196000	2.19500900
H	0.19838400	2.14439800	2.74984800
H	-1.51937800	2.37855700	2.77213400
C	-1.00255100	0.39887900	2.28380400
H	-1.16251400	0.17447200	3.34867300
C	1.35558800	-0.26045800	2.45910000
H	1.15838600	0.18216900	3.44400900
H	1.87113200	-1.20540700	2.64258300
C	2.30764600	0.64286300	1.65701400
H	1.78603100	1.51684700	1.25916800
H	3.07539900	1.01359500	2.34377200
H	-1.93285600	0.17140800	1.76344300
H	0.46586600	-2.52390500	2.47297600
C	2.97385100	-0.11085100	0.53602500
C	4.36184600	-0.25579200	0.48853600
C	4.94422700	-1.01083300	-0.52704800
H	4.97361300	0.22188900	1.24691500
C	2.74101800	-1.41509100	-1.37544500
C	4.11422200	-1.61035200	-1.47075800
H	6.02255600	-1.12928200	-0.57624600
H	2.06108400	-1.82725700	-2.11017900
H	4.51302800	-2.21387900	-2.27878600
N	2.17365400	-0.67832800	-0.39614800
Cl	-0.00427100	-0.56777300	-2.67751800

$[Cu(TEPA)(Br)]^{+}$ – trigonal bipyramidal structure

N	-0.00235700	-0.00658800	2.12838500
C	0.09575000	2.91278700	-1.05269400
C	-1.37771700	2.61751900	0.71633500
C	-0.28105500	4.24214700	-1.21222200
H	0.82606500	2.45496600	-1.70831400
C	-1.82140800	3.93619600	0.59923700
H	0.18800200	4.84590400	-1.98150300
H	-2.58333500	4.30841800	1.27654000
C	-2.57148100	-1.36125800	-1.05892000
C	-1.59046200	-2.49981700	0.71020200
C	-3.54005800	-2.34572800	-1.22311100
H	-2.53253800	-0.49906300	-1.71304200
C	-2.51660800	-3.53759800	0.58792800
H	-4.29462100	-2.23502100	-1.99429100
H	-2.46475300	-4.38564900	1.26318100
N	-0.44294000	2.10742700	-0.11509000
N	-1.60796500	-1.43279400	-0.11832500
C	-1.27126400	4.76048900	-0.38047800
H	-1.60447900	5.78879700	-0.48493000
C	-3.50281200	-3.46468400	-0.39401700
H	-4.23126300	-4.26279600	-0.50233200
C	-0.57849200	-2.47060300	1.82842700
H	0.44272100	-2.54263400	1.43380300
H	-0.72642200	-3.34139300	2.47409400
C	-0.74233300	-1.19269300	2.66819300
H	-1.80393800	-0.93788900	2.71792200
C	-1.85255900	1.71938500	1.83119100
H	-2.53707600	2.27560800	2.47854600
H	-2.41922700	0.86880400	1.43247800
C	-0.66102900	1.22625600	2.66895600
H	0.08908400	2.01971000	2.71544000
C	1.39261000	-0.05403700	2.67369700
H	1.36928400	0.31554400	3.70806900
H	1.70447600	-1.10051000	2.72027300
C	2.41924300	0.73261800	1.84231200
H	1.97049400	1.65348100	1.44961100
H	3.24299300	1.03987100	2.49360900
H	-0.97254100	1.02395200	3.70295100
H	-0.40962300	-1.36400500	3.70109500
C	2.95969000	-0.12195200	0.72290700
C	4.32382100	-0.39512200	0.60433200
C	4.76411800	-1.27616200	-0.38150800
H	5.02642100	0.07469400	1.28504900
C	2.48128300	-1.53243600	-1.05749500
C	3.82122100	-1.86853200	-1.21866700
H	5.82157600	-1.49967400	-0.48718900
H	1.72067800	-1.93053800	-1.71757900
H	4.11049500	-2.56988100	-1.99375400
N	2.05131300	-0.67173100	-0.11271700
Cu	0.00320900	-0.00381200	-0.08494300
Br	0.00815300	-0.00071400	-2.54656500

$[Cu(TEPA)(Br)]^{+}$ – square pyramidal structure

Cu	0.13777500	-0.34988300	-0.13696700
N	0.08220300	-0.18432200	2.05678600
C	-0.25100800	2.39490800	-1.58723800
C	-0.81892700	2.71791500	0.63470500
C	-0.64551900	3.68131000	-1.93902900
H	0.13111000	1.70318700	-2.33145400
C	-1.25649500	4.01810100	0.35114800
H	-0.54988100	4.01437500	-2.96703200
H	-1.65361200	4.63753200	1.14977200
C	-2.82648400	-0.48483100	-0.74749800
C	-2.06949800	-2.02148200	0.83099500
C	-4.12886900	-0.96385700	-0.65924500
H	-2.55675700	0.31063900	-1.43165500
C	-3.35171400	-2.55643900	0.96467000
H	-4.90861700	-0.52416000	-1.27145300
H	-3.52114700	-3.38684200	1.64237200
N	-0.33516700	1.90833400	-0.33054900
N	-1.82503800	-0.99568700	-0.01076900
C	-1.16899300	4.50966300	-0.94780700
H	-1.50211600	5.51716200	-1.17920800
C	-4.39551000	-2.01995600	0.21197800
H	-5.39878700	-2.42619000	0.29847600
C	-0.87422400	-2.53251500	1.58985200
H	-0.09555300	-2.81149300	0.86710000
H	-1.13605600	-3.44497800	2.13545200
C	-0.28441100	-1.53954000	2.60946000
H	-0.98188100	-1.40981100	3.44615900
C	-0.82439400	2.25705300	2.08007400
H	0.08452100	2.63306200	2.56865600
H	-1.64298500	2.77725100	2.59147400
C	-1.02075500	0.77416400	2.41385400
H	-1.16171600	0.71574300	3.50360700
C	1.36928800	0.29147500	2.66213600
H	1.15010600	0.88365500	3.56018400
H	1.93667500	-0.57912500	2.99790100
C	2.26692500	1.09752300	1.70732400
H	1.69163200	1.85177900	1.16482200
H	3.00813100	1.63117100	2.31093300
H	-1.93959200	0.41346300	1.95220000
H	0.61687500	-2.00113900	3.01739200
C	2.98071800	0.19730900	0.73408400
C	4.37452800	0.10987600	0.72519000
C	5.00708200	-0.78701200	-0.13221400
H	4.95170200	0.74239500	1.39169100
C	2.83819000	-1.43705100	-0.91238100
C	4.21964800	-1.58488600	-0.95812200
H	6.09024600	-0.86248300	-0.14981400
H	2.19097700	-2.00676600	-1.56661400
H	4.65725100	-2.30681600	-1.63897800
N	2.22052200	-0.56180900	-0.09002000
Br	0.02025400	-0.96631400	-2.49313400

Table S3. Relevant Structures for Complexes in Table 1 of Main Text.

$[Zn(TEPA)(Br)]^+$

Zn	0.00396900	-0.00249500	-0.29216800
Br	-0.02124700	0.00049300	-2.75996600
N	0.01608500	-0.01564100	2.27833000
C	0.20577900	2.85376200	-1.04914400
C	-1.19084200	2.64261200	0.80128800
C	-0.03693700	4.21820400	-1.14590400
H	0.83309300	2.34306300	-1.77088300
C	-1.49466000	4.00452900	0.74413400
H	0.44395000	4.79546300	-1.92785400
H	-2.17783700	4.42886000	1.47248600
C	-2.59776800	-1.22185500	-1.03915800
C	-1.70394400	-2.36050400	0.78357000
C	-3.66614200	-2.10450000	-1.13643900
H	-2.47257500	-0.41301300	-1.74967100
C	-2.73918900	-3.29597600	0.72461500
H	-4.41517600	-1.95855400	-1.90689300
H	-2.76242900	-4.11020900	1.44146700
N	-0.35677200	2.07113100	-0.10122500
N	-1.62804000	-1.33982800	-0.10473900
C	-0.91600400	4.80472700	-0.23852100
H	-1.14703500	5.86452200	-0.29123500
C	-3.73209800	-3.17241800	-0.24476200
H	-4.54080500	-3.89515300	-0.29911600
C	-0.67864900	-2.41305000	1.88869200
H	0.33470700	-2.50785900	1.47976000
H	-0.85577100	-3.30817400	2.49194100
C	-0.77339000	-1.16762900	2.79102300
H	-1.82241800	-0.86610800	2.86318300
C	-1.72377000	1.77945900	1.91715700
H	-2.40138900	2.37791800	2.53310900
H	-2.31640300	0.94708600	1.51902500
C	-0.58134900	1.24291600	2.79956500
H	0.20353400	2.00271600	2.85594500
C	1.40902500	-0.12662600	2.78766400
H	1.45581300	0.25668600	3.81819100
H	1.67770100	-1.18577700	2.84001600
C	2.43668800	0.59973600	1.89950500
H	2.00903200	1.53107000	1.50858100
H	3.29843100	0.88547600	2.50999400
H	-0.93449400	1.08541100	3.82994000
H	-0.45042800	-1.41015600	3.81471700
C	2.90864900	-0.28857000	0.77659900
C	4.23714900	-0.71499500	0.71347900
C	4.63298800	-1.61126000	-0.27684300
H	4.95013900	-0.34579800	1.44317800
C	2.38052200	-1.58661300	-1.08166000
C	3.68029200	-2.06579100	-1.18562300
H	5.66409800	-1.94704000	-0.33453700
H	1.62045400	-1.86443500	-1.80286200
H	3.93300700	-2.76581100	-1.97428000
N	1.99148600	-0.71273900	-0.12604400

$[Zn(BPAIP)(Br)]^{+}$ - phenol

Zn	0.92403100	0.01049500	-0.33493100
Br	0.20257500	0.02761700	-2.68648500
N	1.65202900	0.14167400	2.31942200
C	1.53073400	-2.72385900	-1.13760600
C	3.15702800	-2.03785200	0.38195000
C	2.12655500	-3.96732600	-1.30354200
H	0.64683800	-2.44462300	-1.70126700
C	3.81140300	-3.26576700	0.24768600
H	1.68341300	-4.69024700	-1.97956700
H	4.72091000	-3.44663700	0.81103000
C	2.76879100	1.89977000	-1.61575800
C	2.07069800	2.79118800	0.41999900
C	3.47016400	3.05199400	-1.94514700
H	2.70853500	1.06479900	-2.30423300
C	2.73688600	3.98654600	0.13663700
H	4.00604400	3.10538600	-2.88634700
H	2.69906000	4.79892000	0.85492000
N	2.02628900	-1.77104100	-0.31623500
N	2.07944900	1.76201700	-0.46095000
C	3.29706100	-4.24288600	-0.60079700
H	3.80295600	-5.19752500	-0.71112600
C	3.44337900	4.12399200	-1.05565800
H	3.96204700	5.05044200	-1.28382000
C	1.39314100	2.58454900	1.75085300
H	0.34393000	2.29499800	1.61668000
H	1.39006300	3.53411200	2.29412900
C	2.13191100	1.51878900	2.58852900
H	3.20048400	1.57250100	2.36027400
C	3.67699500	-1.00409700	1.35043500
H	4.66212800	-1.32520700	1.70219600
H	3.82360000	-0.04300500	0.84447400
C	2.74907400	-0.82083100	2.56977000
H	2.31344800	-1.78992100	2.82968200
C	0.51611300	-0.14816100	3.23202800
H	0.90059800	-0.39054600	4.23644000
H	-0.07985500	0.76323300	3.33791500
C	-0.40582600	-1.27088300	2.73194000
H	0.19030700	-2.12144000	2.37572900
H	-0.99264800	-1.64397100	3.57814100
C	-2.71868500	-0.82661100	1.68252000
C	-2.02701100	0.08979800	-0.19973800
H	-3.42367400	-1.17920600	2.41687100
H	-2.03781000	0.53345700	-1.18377700
C	-1.35129200	-0.80522300	1.67111500
N	-0.92711600	-0.22502200	0.48069300
H	3.34006800	-0.50451700	3.44414600
H	2.03657900	1.74736300	3.66143700
N	-3.13688300	-0.25783500	0.48789400
C	-4.47748000	-0.12170400	0.00385000
C	-5.48218900	0.39723200	0.83886300
C	-4.77561900	-0.48703600	-1.31142200
C	-6.77697700	0.54182900	0.33324800
C	-6.06617700	-0.32693400	-1.81170300
H	-3.99119200	-0.90636800	-1.93436700
C	-7.06569100	0.18644700	-0.98349100

H	-7.55745800	0.94194500	0.97691900
H	-6.28862300	-0.61205600	-2.83442100
H	-8.07722600	0.30879500	-1.35820600
O	-5.14103300	0.73865900	2.11514000
H	-5.91960900	1.10226000	2.56680600

$[Zn(BPAIP)(Br)]^{+}$ - phenoxide

Zn	0.87839800	0.11971300	-0.45214300
Br	0.53932400	0.73808800	-2.78090700
N	1.50602500	-0.54044800	2.36962500
C	1.83598100	-2.27271800	-1.77774700
C	3.30379000	-1.85648300	-0.01947300
C	2.53870000	-3.40251200	-2.17706400
H	0.96635800	-1.92802300	-2.32732500
C	4.06477500	-2.97345000	-0.38199500
H	2.19449000	-3.97625200	-3.03055300
H	4.95061700	-3.22068700	0.19425400
C	2.57018700	2.51274700	-0.78042800
C	1.59274400	2.58438000	1.33243100
C	3.12953500	3.77481500	-0.63061800
H	2.67680100	1.95689800	-1.70550600
C	2.10729200	3.87037200	1.53324900
H	3.72551000	4.19812100	-1.43179200
H	1.89505900	4.38462500	2.46490900
N	2.20247800	-1.50897000	-0.72528200
N	1.81471700	1.92157800	0.17163600
C	3.68345700	-3.75684800	-1.46736100
H	4.27078000	-4.62488000	-1.75304700
C	2.88090500	4.47542600	0.54773400
H	3.27942500	5.47486300	0.69738900
C	0.85423600	1.88130100	2.44144300
H	-0.09341300	1.46667200	2.08159800
H	0.61148300	2.61333800	3.21776500
C	1.71812100	0.74913300	3.04915300
H	2.77453100	1.02679300	2.96604400
C	3.67267300	-1.06191400	1.20905600
H	4.69715000	-1.32331000	1.49426200
H	3.66551000	0.01154400	0.99245200
C	2.72753000	-1.35976400	2.39722000
H	2.44116600	-2.41525000	2.36009100
C	0.36839900	-1.26386100	2.98814200
H	0.72439800	-1.85383600	3.85025300
H	-0.33637100	-0.52722800	3.38458600
C	-0.39092200	-2.15392800	1.99230600
H	0.32363900	-2.74684600	1.40375700
H	-0.99250100	-2.87269200	2.55976700
C	-2.68731600	-1.38659300	1.13537500
C	-2.01732200	0.08766400	-0.35157500
H	-3.42661400	-1.89025200	1.73921000
H	-2.03144800	0.83149900	-1.13118400
C	-1.31745400	-1.37317800	1.11464900
N	-0.89739100	-0.43837100	0.17724000
H	3.27329000	-1.22185500	3.34601100
H	1.50920100	0.65745500	4.12743400
N	-3.11970700	-0.46193800	0.19576000

C	-4.48533200	-0.15628800	-0.11105400
C	-5.49077900	-0.43934100	0.89993300
C	-4.79167000	0.41177900	-1.35339700
C	-6.81700000	-0.01413400	0.51612200
C	-6.09361600	0.78141800	-1.66585600
H	-4.00674100	0.54002400	-2.09700500
C	-7.10153800	0.56497400	-0.70441200
H	-7.59952500	-0.18980600	1.25027700
H	-6.32618200	1.20917900	-2.63652000
H	-8.12784900	0.84951900	-0.93401000
O	-5.24276900	-0.99937400	2.00938500

$[Zn(BPAIP)(Br)]^{+}$ -phenoxyl

Zn	0.92779200	0.08103200	-0.31070300
Br	0.19817600	0.64119000	-2.60084900
N	1.62334000	-0.37426700	2.28463300
C	1.50280200	-2.40874500	-1.71279400
C	3.12560900	-2.09453700	-0.07094100
C	2.08249400	-3.59580600	-2.14101300
H	0.62902500	-1.99791600	-2.20776200
C	3.76389300	-3.27396200	-0.46485000
H	1.63602600	-4.14776100	-2.96077100
H	4.66638400	-3.58689600	0.04979200
C	2.78526900	2.19588400	-1.14942600
C	2.07518800	2.62901200	1.02675300
C	3.49160400	3.38932500	-1.21745500
H	2.72853700	1.52989700	-2.00252700
C	2.74547000	3.85497600	1.01271600
H	4.03466000	3.64277700	-2.12118000
H	2.70469700	4.49317800	1.88923000
N	2.00364300	-1.66675900	-0.69977700
N	2.08751200	1.81486300	-0.05598000
C	3.24209900	-4.03615200	-1.50719100
H	3.73459800	-4.95262100	-1.81850400
C	3.46055600	4.24391700	-0.11741200
H	3.98295200	5.19579700	-0.13670100
C	1.38932600	2.13780400	2.27625300
H	0.33803600	1.89565900	2.07821000
H	1.39122100	2.94172700	3.01807900
C	2.11503600	0.90484900	2.85517500
H	3.18495800	0.99733700	2.64638000
C	3.64863100	-1.30063500	1.10072500
H	4.62852900	-1.69957200	1.37971000
H	3.80711800	-0.25406100	0.81630400
C	2.71330600	-1.37819400	2.32524400
H	2.26996400	-2.37721000	2.36649100
C	0.48453500	-0.84788100	3.11505600
H	0.86855500	-1.30122200	4.04335500
H	-0.10727100	0.02202800	3.41540900
C	-0.44140000	-1.83469800	2.38825300
H	0.15121700	-2.59142200	1.85753200
H	-1.03189800	-2.37635400	3.13453400
C	-2.74685800	-1.15464800	1.46161800
C	-2.03158000	0.12475800	-0.19629100
H	-3.45903500	-1.62931600	2.11317600

H	-2.02417300	0.77565100	-1.05676400
C	-1.38144800	-1.14851700	1.45018800
N	-0.94441800	-0.33430100	0.40711500
H	3.29878500	-1.26275300	3.25088200
H	2.01720200	0.88686500	3.95143000
N	-3.15668700	-0.34708400	0.40270000
C	-4.48010600	-0.06823500	-0.02218400
C	-5.55347400	-0.02614600	0.98014700
C	-4.74880900	0.18503100	-1.35619600
C	-6.87824400	0.31448900	0.49459200
C	-6.05250300	0.51441600	-1.76329900
H	-3.96135200	0.11209200	-2.10019000
C	-7.11289700	0.58019500	-0.83397100
H	-7.66625000	0.34298900	1.24011700
H	-6.24198700	0.70633100	-2.81471100
H	-8.11176000	0.83184400	-1.17693000
O	-5.34042700	-0.26948200	2.19039700

$[Zn(BPAIP)(Br)]^{+}$ - no phenol

Zn	-0.00982300	-0.08978800	-0.40831800
Br	-0.17471900	0.14330400	-2.84839000
N	0.05431700	-0.52178400	2.28857800
C	2.07264800	1.87944300	-0.91641800
C	1.08110800	2.37359600	1.13311900
C	2.92919000	2.96915700	-0.83079500
H	2.06970200	1.23278700	-1.78771200
C	1.90580400	3.49356400	1.27126600
H	3.63634600	3.16193200	-1.63002600
H	1.80953900	4.11853500	2.15303100
C	-2.66902700	1.09049900	-0.82602200
C	-2.84008400	-0.62850100	0.73647200
C	-4.04288300	1.29203500	-0.83880600
H	-2.01364800	1.65938400	-1.47531200
C	-4.23052400	-0.49292600	0.75054400
H	-4.46826600	2.06120000	-1.47385200
H	-4.82216200	-1.14299600	1.38662800
N	1.16382000	1.57888800	0.03837300
N	-2.07029100	0.15210700	-0.05903700
C	2.83974100	3.79920200	0.28423900
H	3.48138300	4.66957200	0.38484700
C	-4.84261600	0.47405900	-0.04333400
H	-5.92284900	0.58539100	-0.03938000
C	-2.14736700	-1.58679300	1.67119400
H	-1.49447400	-2.27277700	1.11795300
H	-2.90195000	-2.20392200	2.16774100
C	-1.32948200	-0.82270100	2.73411800
H	-1.84091300	0.11743200	2.96038600
C	0.11507300	1.99997600	2.23061100
H	0.07984200	2.82009600	2.95389500
H	-0.89943300	1.89246500	1.83013600
C	0.53143900	0.70824600	2.96481200
H	1.62301000	0.67522900	3.02601200
C	0.92413900	-1.66494900	2.66799100
H	1.15720600	-1.61171100	3.74393300
H	0.36053800	-2.59057000	2.51643400

C	2.22282900	-1.75119700	1.85167900
H	2.68825900	-0.76031100	1.77240700
H	2.93634100	-2.38033700	2.39440000
C	2.58612400	-3.45760700	-0.04990800
C	1.16887300	-2.58598300	-1.50851800
H	3.32050900	-4.14654200	0.33786400
H	0.62258900	-2.40804100	-2.42354100
C	2.00974100	-2.34050800	0.49395500
N	1.11956100	-1.80544300	-0.43123600
H	0.16604300	0.73391000	4.00351400
H	-1.30395000	-1.39188100	3.67605100
N	2.04008600	-3.59254900	-1.31139400
H	2.26536500	-4.31103100	-1.98638100

BPAIP

N	-1.71917700	-0.01547400	-0.23673400
C	-2.52798600	5.58458200	-0.20661800
C	-3.36659900	3.44509900	-0.34740100
C	-3.71408700	6.08956100	0.32921600
H	-1.67934900	6.24556400	-0.38050400
C	-4.59243500	3.86121900	0.18973900
H	-3.80281100	7.14308600	0.57729500
H	-5.39349500	3.14129600	0.33228900
C	-6.13313000	-3.52121000	0.28095700
C	-3.89672800	-3.16918000	-0.13749300
C	-5.91068300	-4.80959400	0.77021700
H	-7.14405100	-3.11654800	0.24057000
C	-3.57800200	-4.44741400	0.34085800
H	-6.74044700	-5.41991000	1.11421600
H	-2.54408800	-4.78093400	0.34753400
N	-2.34682700	4.30267300	-0.53889700
N	-5.16369700	-2.71480000	-0.16238300
C	-4.76912600	5.20122500	0.53103900
H	-5.71360900	5.54432300	0.94570200
C	-4.59852300	-5.27906800	0.79926700
H	-4.37232700	-6.27531400	1.17078600
C	-2.83398300	-2.21673900	-0.63685700
H	-3.10296600	-1.86420100	-1.63915300
H	-1.87546200	-2.74090100	-0.72158100
C	-2.69602400	-0.98107600	0.27272700
H	-3.67832700	-0.50233300	0.31819900
C	-3.10982600	2.00390300	-0.72640700
H	-4.04481800	1.43475400	-0.67423300
H	-2.75682200	1.95717500	-1.76297100
C	-2.03119100	1.35856500	0.16425300
H	-1.12822000	1.96803300	0.07018300
C	-0.33880600	-0.39150300	0.08671100
H	-0.05099800	-0.05628900	1.10169800
H	-0.26264600	-1.48249900	0.09101400
C	0.67805700	0.13549500	-0.94205100
H	0.36831200	-0.22351200	-1.93148600
H	0.65564400	1.23107700	-0.98072000
C	3.18157400	0.42946300	-0.34721600
C	3.67993000	-1.72132600	-0.33343400
H	3.34125100	1.49580300	-0.29797900

H	4.27610900	-2.61650300	-0.23987000
C	2.07352000	-0.32309800	-0.64028600
N	2.40158800	-1.66982500	-0.61992600
H	-2.33817100	1.41442600	1.22669100
H	-2.45467200	-1.29971200	1.30535300
N	4.22610800	-0.47009900	-0.15624400
C	5.54908300	-0.13744300	0.23406100
C	5.76489000	0.86982800	1.18012000
C	6.66058200	-0.78896400	-0.33697600
C	7.05523500	1.24552100	1.55233800
H	4.90193600	1.34945200	1.63112600
C	7.95124400	-0.41868800	0.05008400
C	8.15138000	0.59617600	0.98562500
H	7.19824500	2.03099600	2.28784300
H	8.80348100	-0.92763800	-0.39687900
H	9.16295300	0.87128700	1.26945200
O	6.42762400	-1.76861500	-1.26037500
H	7.27819300	-2.09138400	-1.59712200

BPAIP - phenoxide

N	-1.70725200	0.03042900	-0.30622000
C	-3.32277300	5.53549600	-0.30033100
C	-3.74809500	3.27232500	-0.30723300
C	-4.42750500	5.81405900	0.50594900
H	-2.67658200	6.34274900	-0.64448300
C	-4.87691600	3.45756100	0.50562100
H	-4.65438000	6.83529500	0.79837400
H	-5.47284900	2.59977000	0.80539600
C	-5.61848400	-4.11173300	0.20205700
C	-3.48233000	-3.35960000	-0.21506200
C	-5.16521500	-5.29551200	0.78557700
H	-6.68776800	-3.91530200	0.12056400
C	-2.93604900	-4.51808600	0.35786500
H	-5.87044900	-6.03054800	1.16307900
H	-1.85762600	-4.64132100	0.39990500
N	-2.98264100	4.30662700	-0.70163100
N	-4.81294800	-3.16329400	-0.28700100
C	-5.22111700	4.74343900	0.91654500
H	-6.09372800	4.90651500	1.54457700
C	-3.78746200	-5.49791300	0.86359500
H	-3.38192000	-6.40328100	1.30850700
C	-2.60316300	-2.25428200	-0.74919000
H	-2.98184500	-1.92353500	-1.72222200
H	-1.58494600	-2.62749800	-0.90069200
C	-2.58088500	-1.03182800	0.19157000
H	-3.60669000	-0.65564600	0.26391800
C	-3.30882800	1.89693900	-0.74937200
H	-4.16013400	1.20698300	-0.70972400
H	-2.96331200	1.94068700	-1.78696000
C	-2.14745600	1.35885100	0.11437800
H	-1.30902800	2.05281700	0.00725400
C	-0.29373900	-0.22249200	0.02624500
H	-0.06485200	0.09347900	1.06180400
H	-0.11450700	-1.30007100	-0.01085200
C	0.70516100	0.42126700	-0.94817300

H	0.39904400	0.14059100	-1.96593600
H	0.65891100	1.51696900	-0.89419700
C	3.22066000	0.70995400	-0.37374500
C	3.72039100	-1.43085300	-0.38170900
H	3.37100500	1.77675400	-0.32106400
H	4.35537500	-2.30087400	-0.33569000
C	2.10634100	-0.04054800	-0.66563100
N	2.42684700	-1.38235200	-0.66551700
H	-2.43857700	1.38015700	1.18412200
H	-2.29235000	-1.35179500	1.21195300
N	4.26238000	-0.18617100	-0.18691500
C	5.61643500	0.13157400	0.16210100
C	5.88724500	1.35540800	0.77544400
C	6.66763300	-0.83435600	-0.13559300
C	7.19047600	1.74850400	1.09193800
H	5.05856000	2.01350400	1.03170800
C	7.99108600	-0.36050600	0.19672700
C	8.24057800	0.86936400	0.78409000
H	7.37536500	2.70582500	1.57353700
H	8.80537000	-1.04543500	-0.03340400
H	9.26812900	1.15358800	1.01772400
O	6.45739500	-1.98115600	-0.63227300

BPAIP – phenoxyl

N	1.69305500	-0.01535600	0.22768800
C	2.47212000	5.58211000	0.14300800
C	3.32936400	3.45168600	0.30582400
C	3.65897900	6.09480900	-0.38370000
H	1.61573700	6.23629900	0.30402700
C	4.55660900	3.87570700	-0.22138900
H	3.74046000	7.14755600	-0.63736900
H	5.36579600	3.16254000	-0.35118700
C	6.11245200	-3.50278100	-0.27934900
C	3.87669800	-3.16651600	0.15421900
C	5.90009000	-4.80598500	-0.73259700
H	7.11876700	-3.08538700	-0.26059200
C	3.56787800	-4.46009700	-0.28731200
H	6.73334600	-5.41528700	-1.06978600
H	2.53811800	-4.80599100	-0.27393600
N	2.29946200	4.30056600	0.48138300
N	5.13811400	-2.69660900	0.15353800
C	4.72425700	5.21523900	-0.56926100
H	5.66963800	5.56462600	-0.97644400
C	4.59347500	-5.29140800	-0.73522500
H	4.37526100	-6.29947100	-1.07842100
C	2.80873700	-2.21409200	0.64362300
H	3.07444900	-1.85209800	1.64358300
H	1.85266300	-2.74235200	0.73197300
C	2.66800300	-0.98678000	-0.27607000
H	3.64986100	-0.50820900	-0.32802400
C	3.08261100	2.01086300	0.69383100
H	4.02033400	1.44647200	0.64036100
H	2.73540700	1.96790400	1.73264400
C	2.00294600	1.35543600	-0.18748100
H	1.09970200	1.96530900	-0.09748500

C	0.31177600	-0.39335000	-0.08279700
H	0.01067900	-0.05492800	-1.09263200
H	0.23604100	-1.48429300	-0.08870400
C	-0.69085600	0.13388800	0.96205700
H	-0.37520000	-0.23909100	1.94432000
H	-0.65815400	1.22851000	1.01022400
C	-3.19458000	0.44542400	0.40143400
C	-3.70207800	-1.71751700	0.39076100
H	-3.33559900	1.51373600	0.37668700
H	-4.30981300	-2.60284300	0.30755500
C	-2.09084400	-0.31142700	0.67402300
N	-2.42563400	-1.66461000	0.64791500
H	2.30691600	1.40040900	-1.25104900
H	2.42374700	-1.31363600	-1.30523500
N	-4.25612100	-0.44738900	0.22405700
C	-5.56364200	-0.11704000	-0.13646300
C	-5.84417700	1.11788600	-0.72660400
C	-6.66455400	-1.06470200	0.12359600
C	-7.14942600	1.47397300	-1.06212200
H	-5.03409100	1.80241200	-0.95267800
C	-7.99791700	-0.63342800	-0.25915300
C	-8.23236000	0.59355900	-0.82356700
H	-7.33084500	2.43827800	-1.52755800
H	-8.79469000	-1.34422900	-0.06420000
H	-9.23991500	0.89330000	-1.09741200
O	-6.48051200	-2.18356200	0.65544200

BPAIP – no phenol

N	0.00131700	0.22409600	0.12429800
C	5.35850400	-1.59296500	0.00109400
C	3.11333300	-2.00856100	0.29619500
C	5.61518100	-2.89638700	-0.42800200
H	6.16866600	-0.86720300	0.06614600
C	3.27575100	-3.33509900	-0.12607500
H	6.62174100	-3.19925900	-0.70080200
H	2.41800500	-4.00089400	-0.16251300
C	-4.23022500	-3.52709300	0.07489500
C	-3.48551100	-1.36013400	0.29899100
C	-5.48603300	-3.12252900	-0.38135500
H	-4.00003600	-4.58687900	0.18057900
C	-4.71458800	-0.86200400	-0.15434200
H	-6.24408100	-3.85771500	-0.63468500
H	-4.86908500	0.21061300	-0.23109600
N	4.14830900	-1.14973800	0.35523900
N	-3.25054600	-2.68113000	0.40830200
C	4.54338600	-3.78525300	-0.49183400
H	4.69040600	-4.81128100	-0.81944400
C	-5.72858500	-1.75484000	-0.49771600
H	-6.69004400	-1.38830400	-0.84834500
C	-2.34361800	-0.44349300	0.67604900
H	-2.00068200	-0.68616100	1.68844400
H	-2.69075200	0.59579800	0.68967700
C	-1.14178700	-0.60051600	-0.27460700
H	-0.84564400	-1.65298700	-0.24906100
C	1.76195400	-1.45684500	0.69121500

H	1.03092900	-2.27148300	0.74755200
H	1.82816800	-1.00886100	1.68935900
C	1.28087800	-0.36326400	-0.28107700
H	2.04367900	0.42017900	-0.28989300
C	-0.13554900	1.61998900	-0.30366000
H	0.20704300	1.76358200	-1.34634500
H	-1.19506400	1.89064400	-0.28826700
C	0.60230600	2.60025400	0.62605000
H	0.23450500	2.43256500	1.64608000
H	1.67755200	2.38533500	0.63819100
C	1.31641600	4.96518000	-0.16282700
C	-0.71551500	5.83045500	-0.19495800
H	2.39010900	4.92096600	-0.26862200
H	-1.49958900	6.56464600	-0.32678900
C	0.38691400	4.03026600	0.22753300
N	-0.88050900	4.58782700	0.19972000
H	1.23621000	-0.76871200	-1.31042700
H	-1.45505700	-0.38814000	-1.31510900
N	0.59920300	6.11614000	-0.42958300
H	0.97934500	7.00021900	-0.73387100

TEPA

N	-0.00050600	-0.00491400	0.14645900
C	-3.84117200	-4.15482700	0.02329300
C	-3.31330200	-1.92998000	0.29016700
C	-5.12962000	-3.86667300	-0.43032700
H	-3.50839400	-5.18870500	0.11020500
C	-4.58440800	-1.54610200	-0.15802500
H	-5.81124900	-4.66773100	-0.70040300
H	-4.84330800	-0.49256300	-0.21543100
C	-1.68578500	5.39130100	0.04454600
C	-0.01455500	3.82687800	0.28898400
C	-0.80030900	6.36768700	-0.41537100
H	-2.74737900	5.61591500	0.14332300
C	0.94537800	4.74061200	-0.16660100
H	-1.15955000	7.35812400	-0.67851700
H	1.98765700	4.44212500	-0.23596700
N	-2.94991700	-3.22322800	0.37599700
N	-1.31645000	4.15382900	0.38934300
C	-5.50523200	-2.52750900	-0.52187100
H	-6.49735800	-2.25062300	-0.86920600
C	0.54737600	6.02842500	-0.52240300
H	1.27692500	6.75285100	-0.87537700
C	0.35214100	2.41255100	0.67945100
H	-0.01260500	2.20809700	1.69268500
H	1.44243200	2.30362300	0.69741200
C	-0.28149000	1.37359000	-0.26458100
H	-1.36264500	1.53562000	-0.24416700
C	-2.26689200	-0.91297700	0.68732700
H	-2.71453100	0.08680700	0.71898200
H	-1.90256600	-1.13928700	1.69602200
C	-1.05536100	-0.93586600	-0.26349000
H	-0.65421300	-1.95294600	-0.25022800
C	1.33152000	-0.45141800	-0.27116100
H	1.32674300	-0.83309700	-1.31042900

H	2.01153700	0.40459400	-0.25903600
C	1.92165600	-1.51400300	0.67459700
H	1.92730500	-1.09145400	1.68626600
H	1.28590500	-2.40634500	0.69920600
H	-1.38808300	-0.74400200	-1.30191100
H	0.04450400	1.56316600	-1.30552900
C	3.33043200	-1.90005800	0.28377700
C	3.65280000	-3.19826000	-0.13486500
C	4.96830200	-3.49477600	-0.48786600
H	2.88054500	-3.96124600	-0.17820100
C	5.51278300	-1.22050600	0.00765200
C	5.92640500	-2.48529500	-0.41612500
H	5.23887900	-4.49663700	-0.81201500
H	6.23099000	-0.40390100	0.07734500
H	6.96433200	-2.66691400	-0.67884100
N	4.25546000	-0.92457900	0.34979600

Table S4. Relevant Structures for Complexes in Table 2 of Main Text.

Zn(TEPA)(OH)

Zn	0.00933800	-0.09606800	-0.50184300
N	-0.07703600	-0.45700100	1.84432000
C	-2.78747200	-0.28836000	-1.53830400
C	-2.56879800	-1.83722100	0.18240100
C	-4.08519500	-0.70389400	-1.81666600
H	-2.27539500	0.46960500	-2.12234000
C	-3.85789600	-2.31974700	-0.05361700
H	-4.64765300	-0.22803000	-2.61282600
H	-4.25012600	-3.13118200	0.55101200
C	2.49591700	-1.14908600	-1.76268900
C	2.92094600	-1.10337900	0.51914200
C	3.74742000	-1.68966000	-2.03858600
H	1.77795400	-0.87465100	-2.53220200
C	4.18847500	-1.65422600	0.31360900
H	4.03134600	-1.89115800	-3.06606300
H	4.83742700	-1.83531000	1.16451000
N	-2.04443200	-0.83860700	-0.55629300
N	2.07540900	-0.86801800	-0.50861300
C	-4.62765600	-1.74510100	-1.06421900
H	-5.63326600	-2.10578100	-1.25968000
C	4.61005300	-1.95738500	-0.97911400
H	5.59322500	-2.38567900	-1.15137100
C	2.48235500	-0.71552300	1.90805600
H	2.53893700	0.37578400	2.00702500
H	3.21066500	-1.10974500	2.62398500
C	1.10329000	-1.23357700	2.33405900
H	0.99106400	-2.26579800	1.98853700
C	-1.70553800	-2.35936500	1.30330900
H	-2.26072300	-3.11344700	1.86967000
H	-0.82189100	-2.87128200	0.89928500
C	-1.29074600	-1.23036800	2.26233400
H	-2.12733300	-0.53433200	2.35481700
C	-0.11475800	0.84658500	2.57813000
H	-0.41030500	0.65269800	3.62051600
H	0.89584000	1.25702900	2.61339600
C	-1.04720800	1.90607700	1.96628700
H	-1.98078600	1.44402000	1.62117300
H	-1.33013000	2.60528600	2.75916800
H	-1.11205400	-1.63853000	3.26817500
H	1.06242500	-1.26237400	3.43438300
C	-0.42709000	2.68497600	0.83087000
C	-0.34762800	4.07854100	0.86460700
C	0.21100400	4.76209300	-0.21443600
H	-0.72475400	4.61806000	1.72740500
C	0.55849200	2.64577800	-1.27967700
C	0.66778300	4.03193500	-1.30968800
H	0.27928900	5.84595700	-0.20081100
H	0.84289600	2.01901900	-2.11943200
H	1.09541800	4.52098200	-2.17821400
N	0.03443500	1.98287000	-0.22611800
O	-0.01478000	0.05483700	-2.40127000
H	-0.41711100	-0.66706400	-2.90258600

Zn(BPAIP)(OH) phenol

Zn	-0.89420500	-0.00841500	-0.43284300
N	-1.73056600	-0.48800500	1.95109900
C	-1.20367900	2.73965100	-1.19965000
C	-2.74024100	2.34687300	0.50942500
C	-1.55411800	4.08332400	-1.27671700
H	-0.48038200	2.27980600	-1.86899700
C	-3.13462300	3.68703000	0.48368500
H	-1.06984100	4.72657700	-2.00355400
H	-3.91188800	4.03009800	1.15882600
C	-2.82692700	-1.16650600	-2.28480000
C	-2.78927600	-2.54529800	-0.40801900
C	-3.75542200	-1.97611200	-2.92847300
H	-2.38820600	-0.28900500	-2.75080600
C	-3.71127700	-3.41051000	-1.00316600
H	-4.10654800	-1.71484600	-3.92096800
H	-4.03652500	-4.29787200	-0.46976600
N	-1.77391100	1.88971200	-0.31691800
N	-2.35744000	-1.43860900	-1.04898900
C	-2.53353700	4.56844500	-0.41307900
H	-2.83376000	5.61194200	-0.44096300
C	-4.20330500	-3.12365200	-2.27521300
H	-4.92130700	-3.78745300	-2.74793600
C	-2.26722000	-2.77969300	0.98702100
H	-1.17595800	-2.89378700	0.96700600
H	-2.66921700	-3.72479700	1.36492700
C	-2.66762300	-1.64656600	1.95148900
H	-3.66471000	-1.29408800	1.67632200
C	-3.40505900	1.36433600	1.44474600
H	-4.18433500	1.89353400	2.00210400
H	-3.92348000	0.60063200	0.85180700
C	-2.46113800	0.70080600	2.46621100
H	-1.73030500	1.44263200	2.79513400
C	-0.63208300	-0.83115300	2.90421600
H	-1.05832800	-0.89993800	3.91926200
H	-0.26959600	-1.83111100	2.64679600
C	0.56904200	0.12297500	2.93776200
H	0.23495200	1.15851800	3.08488700
H	1.15385600	-0.12381700	3.83097700
C	2.82900400	0.01250700	1.68684300
C	2.01380300	-0.00336900	-0.36507900
H	3.58032600	0.00252300	2.45909600
H	1.92402200	0.00659900	-1.44188200
C	1.46170900	0.03731600	1.74167300
N	0.96500300	0.01998000	0.44941400
H	-3.03951500	0.41316800	3.35962600
H	-2.75239000	-2.04194400	2.97596000
N	3.17009200	-0.00812900	0.34119900
C	4.48302600	0.01529300	-0.22577900
C	5.47693000	-0.85864700	0.24970500
C	4.76779100	0.89500900	-1.27282000
C	6.74374000	-0.83299500	-0.34012300
C	6.02934900	0.90538700	-1.86493000
H	3.99441600	1.57824300	-1.61023100
C	7.01675900	0.03946800	-1.39260300

H	7.51460900	-1.50745200	0.02659200
H	6.24028600	1.59203500	-2.67792500
H	8.00653600	0.04242000	-1.83870600
O	5.15321800	-1.69955700	1.27403800
H	5.92035300	-2.25588000	1.48452600
O	-0.19714500	0.22460400	-2.19723100
H	-0.12151200	-0.55281800	-2.76585000

Zn(BPAIP)(OH) phenoxyl

Zn	-0.89247600	-0.03703400	-0.41326700
N	-1.68896800	-0.39716300	1.97187900
C	-1.20941200	2.66035000	-1.34824400
C	-2.71147500	2.37286700	0.41200700
C	-1.55809500	3.99839500	-1.49618000
H	-0.50015900	2.15932500	-2.00309400
C	-3.10269400	3.71072600	0.31681500
H	-1.08760400	4.59686300	-2.26887600
H	-3.86487700	4.09555900	0.98653400
C	-2.85253300	-1.25533900	-2.20516500
C	-2.80292900	-2.55298800	-0.27226000
C	-3.78766600	-2.08870500	-2.80713200
H	-2.42027500	-0.39844000	-2.71279600
C	-3.73124400	-3.44047300	-0.82312800
H	-4.14649800	-1.86846500	-3.80676900
H	-4.05459000	-4.30332700	-0.24987500
N	-1.76312200	1.86534900	-0.40587100
N	-2.37343000	-1.47572500	-0.96301900
C	-2.51797500	4.53636400	-0.64181500
H	-2.81583500	5.57765700	-0.72382400
C	-4.23242100	-3.20679500	-2.10237500
H	-4.95550300	-3.88822600	-2.54093500
C	-2.27091400	-2.72803000	1.12788500
H	-1.18216900	-2.86435500	1.10414700
H	-2.68583800	-3.64582100	1.55562200
C	-2.64231200	-1.54240800	2.03897400
H	-3.63768800	-1.18944600	1.75888900
C	-3.36072500	1.44635200	1.41283200
H	-4.11982400	2.01114700	1.96303700
H	-3.90303100	0.66094100	0.87184000
C	-2.39855900	0.82383800	2.44278000
H	-1.65441100	1.57397200	2.71820000
C	-0.58619700	-0.71285200	2.93244500
H	-1.00926400	-0.74275400	3.95030400
H	-0.23167300	-1.72378700	2.70921900
C	0.62215000	0.23317600	2.93293600
H	0.29856400	1.27524100	3.05440600
H	1.21107700	0.00464200	3.82804800
C	2.86797800	0.06169000	1.66942400
C	2.02084600	-0.01182500	-0.37874400
H	3.62776600	0.05198900	2.43057600
H	1.89966600	-0.05746400	-1.45208100
C	1.50432900	0.10593800	1.73391400
N	0.98965700	0.04690800	0.44654500
H	-2.95848800	0.58524900	3.36173900
H	-2.71907100	-1.88514400	3.08245000
N	3.19606900	-0.00287200	0.31505400

C	4.48467900	-0.04644400	-0.26683200
C	5.58997100	-0.66101400	0.48348900
C	4.69740400	0.46010600	-1.53918200
C	6.87582800	-0.71905800	-0.18737700
C	5.96407000	0.36951700	-2.13605200
H	3.88999800	0.94743800	-2.07648000
C	7.05109700	-0.22322600	-1.45699500
H	7.68507600	-1.17306700	0.37528700
H	6.10683300	0.77697600	-3.13206200
H	8.02208600	-0.27525400	-1.93993300
O	5.43762000	-1.11459100	1.64117400
O	-0.16874100	0.08057600	-2.18121400
H	-0.17168400	-0.71474800	-2.72950300

Zn(BPAIP)(OH) phenoxide

Zn	0.93118000	0.03573500	-0.71154000
N	1.66136100	-0.06846900	2.07981800
C	2.06331700	-2.34274100	-1.82047300
C	3.48241900	-1.78254200	-0.06078400
C	2.80277900	-3.48031400	-2.12660100
H	1.21807800	-2.00562000	-2.41535700
C	4.27080000	-2.90787900	-0.32061400
H	2.50135300	-4.11192000	-2.95546900
H	5.14899100	-3.09616400	0.28902400
C	2.07141800	2.49759000	-1.69137700
C	1.57049300	2.88796600	0.55342300
C	2.53191200	3.79747600	-1.87055500
H	1.99283800	1.76757900	-2.49792800
C	2.00997600	4.21062100	0.43290700
H	2.89185900	4.11302000	-2.84425500
H	1.95745300	4.86942400	1.29385900
N	2.38468400	-1.51584800	-0.80146100
N	1.61148900	2.04515100	-0.50316000
C	3.92638200	-3.77189700	-1.35783200
H	4.53258100	-4.64934600	-1.56559800
C	2.50107200	4.67159000	-0.78622200
H	2.84288100	5.69806300	-0.88714000
C	1.05546700	2.36744500	1.87254300
H	0.05212900	1.94732800	1.74034100
H	0.95597000	3.21158200	2.56225400
C	1.98291900	1.30697600	2.50537000
H	3.01788100	1.53094900	2.22640700
C	3.83298900	-0.84679200	1.06973200
H	4.83661400	-1.09703300	1.42913400
H	3.87889900	0.18339300	0.69755700
C	2.84396200	-0.93173800	2.25096700
H	2.50616300	-1.96728400	2.35213400
C	0.54021700	-0.59222100	2.90110300
H	0.93161100	-0.95918500	3.86626100
H	-0.13684800	0.23407700	3.13511700
C	-0.27545400	-1.68674200	2.19525600
H	0.40284300	-2.42272100	1.74024300
H	-0.85287300	-2.22871700	2.95228600
C	-2.60485400	-1.17429200	1.21562700
C	-1.95683700	-0.06525000	-0.56577100
H	-3.33398500	-1.54183600	1.92071300

H	-1.99734500	0.51314300	-1.47394900
C	-1.23376800	-1.13726100	1.18612300
N	-0.83085000	-0.43511400	0.06243400
H	3.36772500	-0.68463600	3.19140100
H	1.93759400	1.38387100	3.60538500
N	-3.05330200	-0.49710900	0.09150100
C	-4.42079000	-0.29238400	-0.28092500
C	-5.42687600	-0.33239300	0.76780200
C	-4.72941900	-0.04779400	-1.62405400
C	-6.75531300	-0.02222700	0.29097200
C	-6.03323200	0.22480800	-2.01924900
H	-3.94298500	-0.10191800	-2.37597100
C	-7.04117000	0.24126100	-1.03392900
H	-7.53881300	-0.02041400	1.04479600
H	-6.26732100	0.39927000	-3.06529400
H	-8.06904800	0.45345400	-1.32619900
O	-5.17519100	-0.60758500	1.97782000
O	0.77907200	0.06921000	-2.59522800
H	-0.06483600	0.36870700	-2.95886300

Zn(BPAIP)(OH) no phenol

Zn	0.04498100	-0.11261200	-0.65224000
N	0.05581900	-0.83876000	1.75806100
C	1.09705000	2.52709200	-1.09586200
C	0.45344300	2.42006300	1.14230100
C	1.59486800	3.81694500	-0.94484000
H	1.08314600	2.00867100	-2.05188200
C	0.93813800	3.71196700	1.36012900
H	2.02425700	4.33290900	-1.79687900
H	0.85175500	4.15815500	2.34559100
C	-2.70958100	0.51598200	-1.40943900
C	-2.81551800	-1.20348600	0.15690100
C	-4.09055800	0.53259200	-1.56550600
H	-2.04629600	1.15075600	-1.98913900
C	-4.20697600	-1.25088100	0.03851100
H	-4.54974700	1.23160000	-2.25622800
H	-4.77175200	-1.96998700	0.62296600
N	0.54916900	1.83544900	-0.07197200
N	-2.08318100	-0.32725900	-0.56231400
C	1.52099400	4.41848000	0.30942000
H	1.90092600	5.42349200	0.46860500
C	-4.85400500	-0.37230600	-0.82869100
H	-5.93516700	-0.39727000	-0.92863200
C	-2.06861100	-2.09514800	1.11671300
H	-1.38182800	-2.75035700	0.56568700
H	-2.78201900	-2.75399800	1.62106700
C	-1.30287300	-1.28814100	2.18234200
H	-1.89790100	-0.40980700	2.44274900
C	-0.22076400	1.64931600	2.25319000
H	-0.22799000	2.27526400	3.15096800
H	-1.27348900	1.49122000	1.98814400
C	0.45027200	0.31150100	2.61795200
H	1.53244300	0.43996900	2.55257500
C	0.97831200	-1.98526500	2.02941600
H	0.97919100	-2.18102300	3.11455800
H	0.55224700	-2.87189500	1.54989000

C	2.43334500	-1.83583100	1.56605800
H	2.87446300	-0.91387100	1.96629400
H	3.00040700	-2.65122000	2.02935800
C	3.61925700	-2.51010800	-0.63468900
C	2.24990400	-1.45373000	-2.01960300
H	4.46286100	-3.11083900	-0.33115000
H	1.78808200	-1.02920200	-2.90143000
C	2.62682100	-1.89560900	0.08439900
N	1.77789300	-1.24627800	-0.79482700
H	0.22520100	0.06940800	3.66941500
H	-1.21171200	-1.88316100	3.10420500
N	3.36314800	-2.21309700	-1.96023700
H	3.91311900	-2.51258700	-2.75363500
O	0.04233600	0.23845100	-2.53295400
H	-0.59937200	-0.22647000	-3.08543800

Table S5. Relevant Energies for TEPA and BPAIP Complexes.

	Complex			*Br*			*Zn*		
	Ee	*Gcorr*	*G*	*Ee*	*Gcorr*	*G*	*Ee*	*Gcorr*	*G*
				BPAIP complex					
phenol	-5668.64755	0.429439	-5668.218111	-2571.464366	-0.016176	-2571.480542	-1778.430125	-0.015877	-1778.446002
phenolate	-5668.182753	0.415039	-5667.767714	-2571.464366	-0.016176	-2571.480542	-1778.430125	-0.015877	-1778.446002
phenoxyl	-5668.010706	0.415868	-5667.594838	-2571.464366	-0.016176	-2571.480542	-1778.430125	-0.015877	-1778.446002
no phenol	-5362.382564	0.353072	-5362.029492	-2571.464366	-0.016176	-2571.480542	-1778.430125	-0.015877	-1778.446002
TEPA	-5384.439236	0.369358	-5384.069878	-2571.464366	-0.016176	-2571.480542	-1778.430125	-0.015877	-1778.446002

	ligand			*delta*	*delta*
	Ee	*Gcorr*	*G*	*Ee*	*G*
			BPAIP complex		
phenol	-1317.853808	0.417416	-1317.436392	-564.29	-536.63
phenolate	-1317.302052	0.404041	-1316.898011	-618.86	-591.84
phenoxyl	-1317.223383	0.404143	-1316.81924	-560.26	-532.79
no phenol	-1011.59426	0.341168	-1011.253092	-560.88	-533.29
TEPA	-1033.663689	0.357993	-1033.305696	-552.87	-525.63

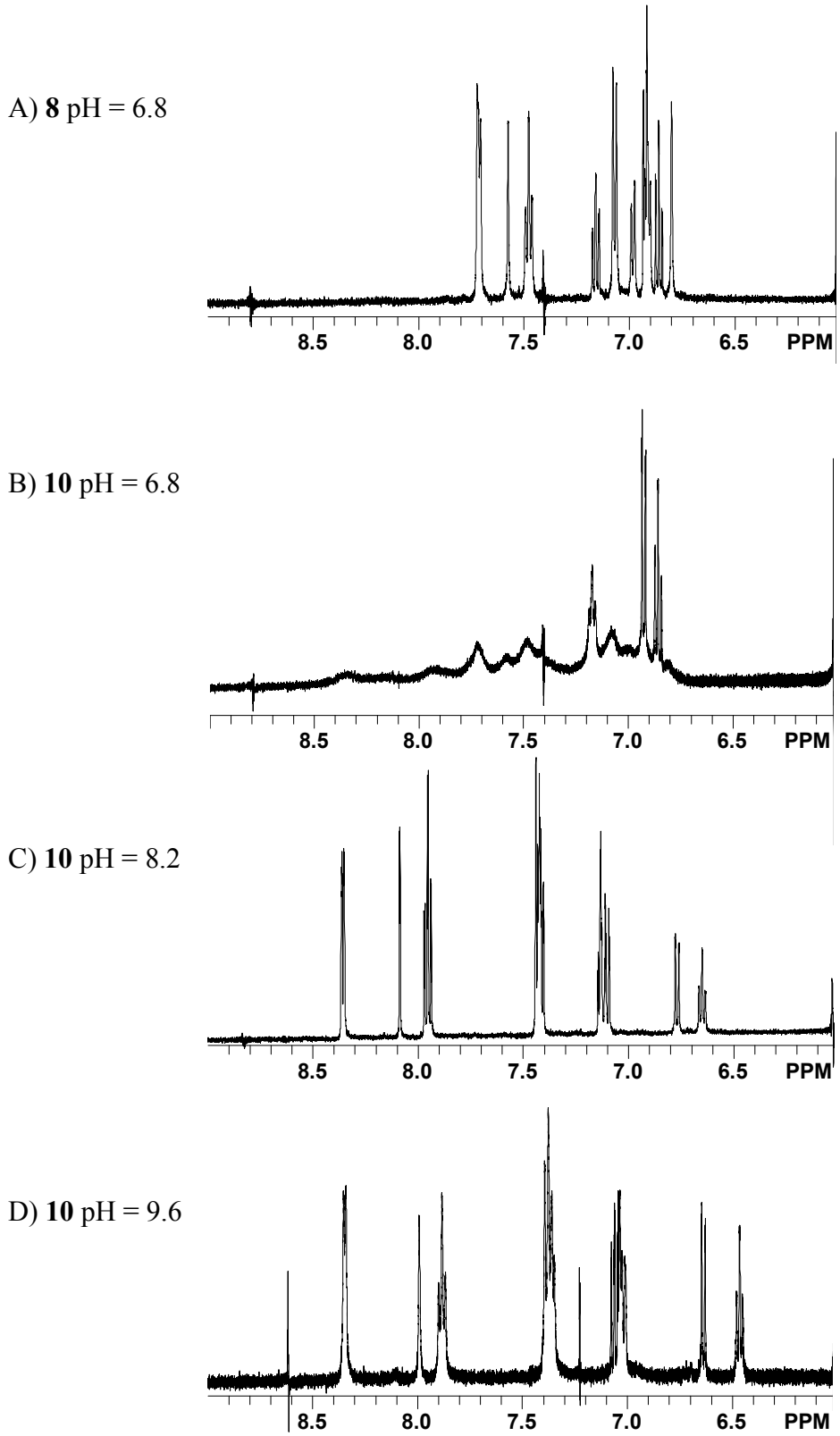
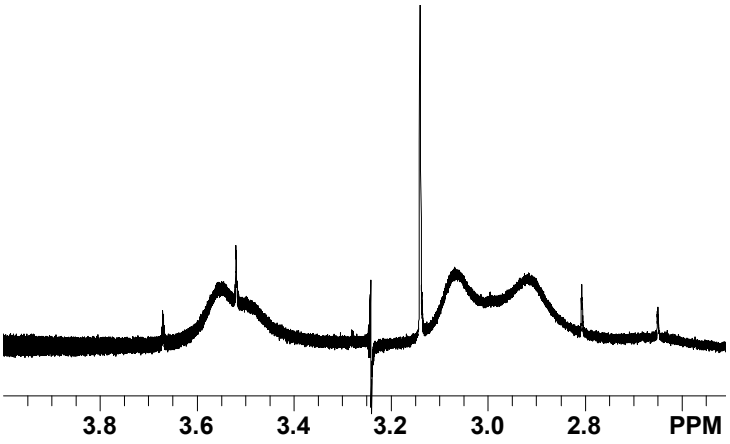


Figure S1. ^{1}H NMR spectra (aromatic region) of **8** (BPAIP-HBr) and **10** as a function of pH in buffered D_2O solutions. Chemical shifts are in ppm.

A) **10** pH = 6.8



B) **10** pH = 8.2

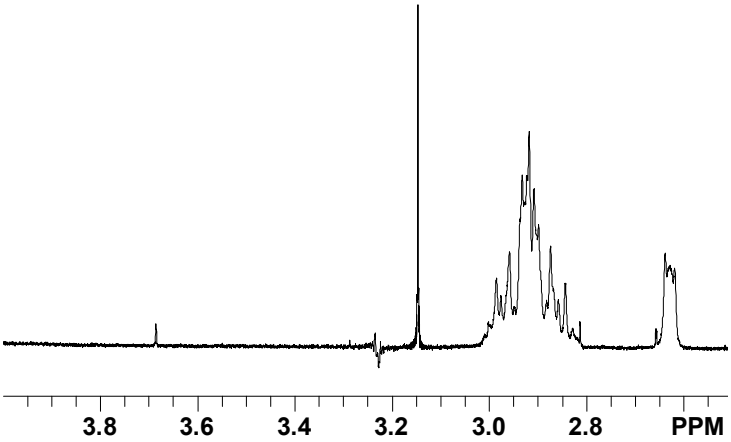
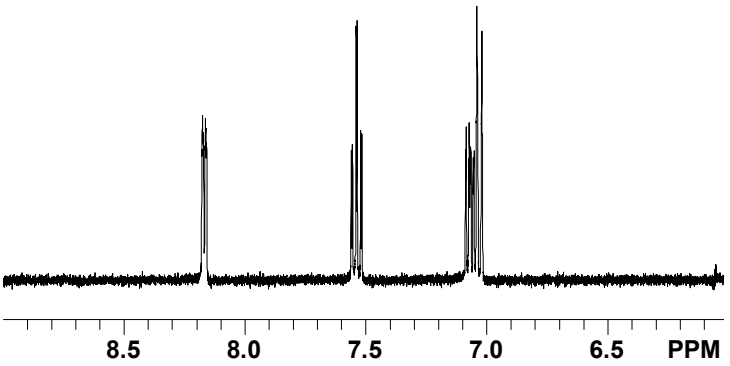


Figure S2. ^{1}H NMR spectra (alkyl region) of **10** in buffered D_2O at (A) pH 6.8 and (B) pH 8.2.

The data in Figures S1 and S2 was obtained in a phosphate buffer system (NaH_2PO_4/Na_2HPO_4), but similar results were obtained in Tris buffer.

A) **9** pH = 9.6



B) **11** pH = 9.6

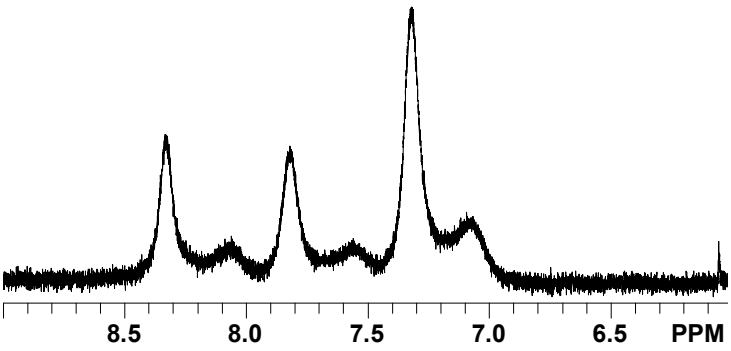


Figure S3. ^{1}H NMR spectrum (aromatic region) of free TEPA (**9**) (top) and complexed to Zn(II) (**11**) (bottom) in buffered D_2O at pH 9.6.