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Supplementary Information

Catechol oxidation promoted by bridging phenoxo moieties in a bis(*μ*-phenoxo)-bridged dicopper(II) complex

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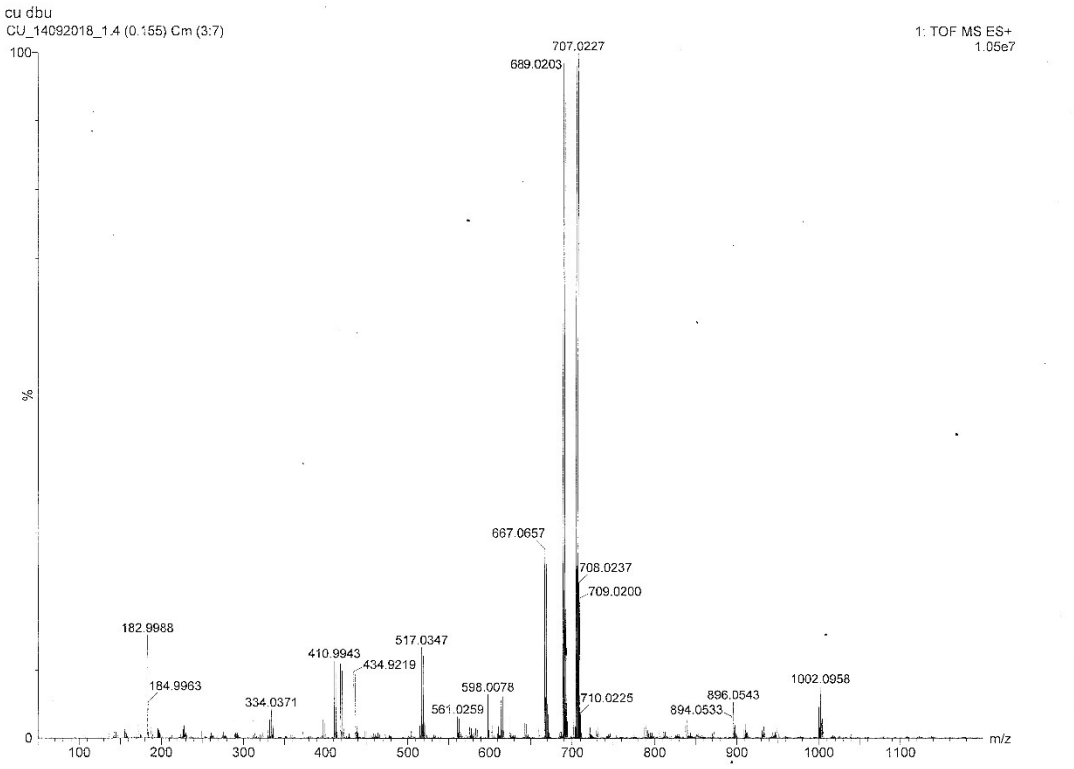

Figure S1. The ESI-MS of complex **1** in CH_3OH.

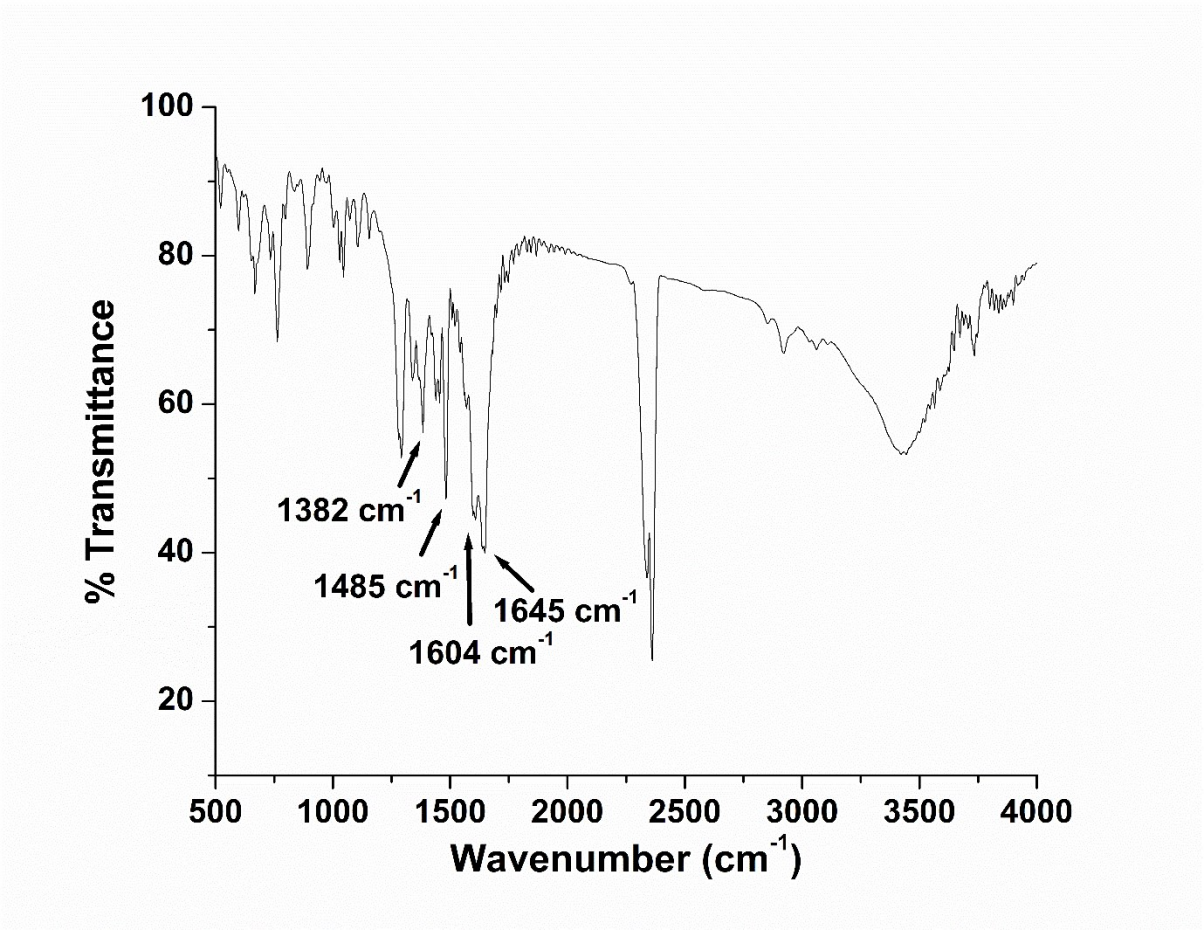

Figure S2. The FTIR spectrum of complex **1**.

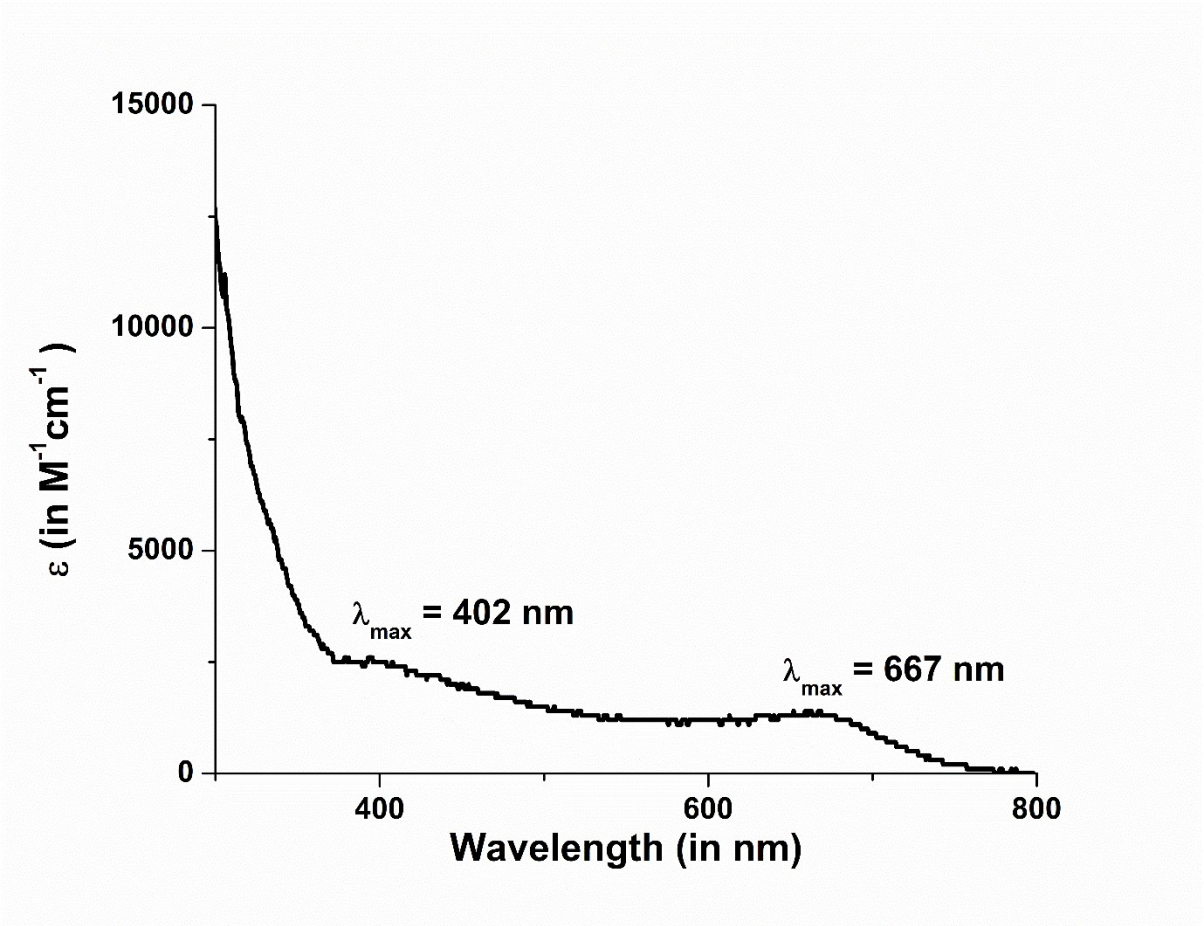

Figure S3. The UV/Vis spectrum of complex **1** in CH_3OH recorded at 298 K.

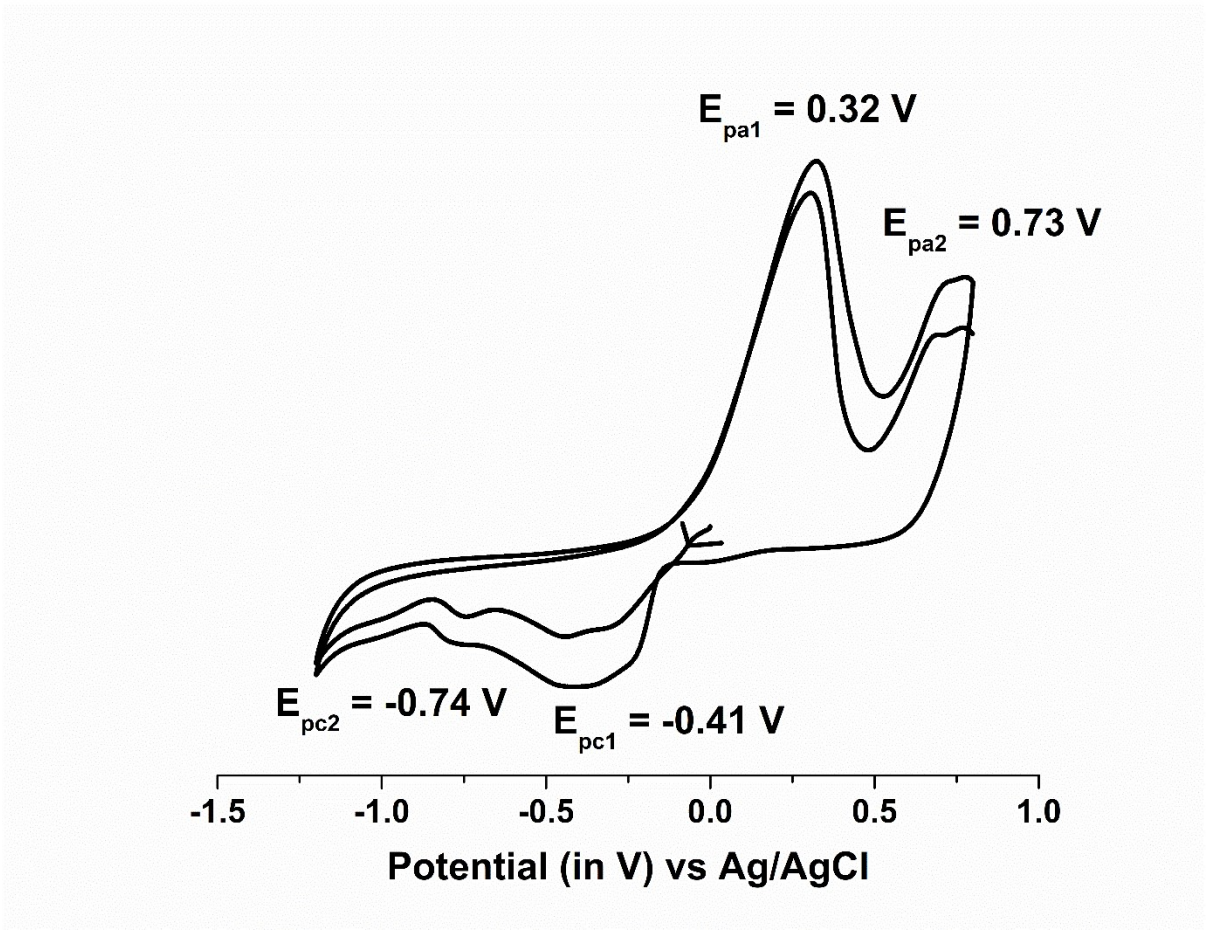

Figure S4. The cyclic voltammogram of complex **1** in CH_3OH solution (298 K) using Pt-working electrode and Ag/AgCl reference electrode.

Table S1. Table for rate dependence on different substrate concentrations:

Substrate concentration (M)	Rate of catecholase activity (in M s^{-1})	Standard deviation (in M s^{-1})
1 x 10^{-3}	1.57 x 10^{-7}	0.08 x 10^{-7}
5 x 10^{-3}	3.44 x 10^{-7}	0.17 x 10^{-7}
7 x 10^{-3}	3.96 x 10^{-7}	0.2 x 10^{-7}
10 x 10^{-3}	5.02 x 10^{-7}	0.25 x 10^{-7}
3 x 10^{-3}	7.5 x 10^{-7}	0.37 x 10^{-7}
50 x 10^{-3}	7.6 x 10^{-7}	0.38 x 10^{-7}

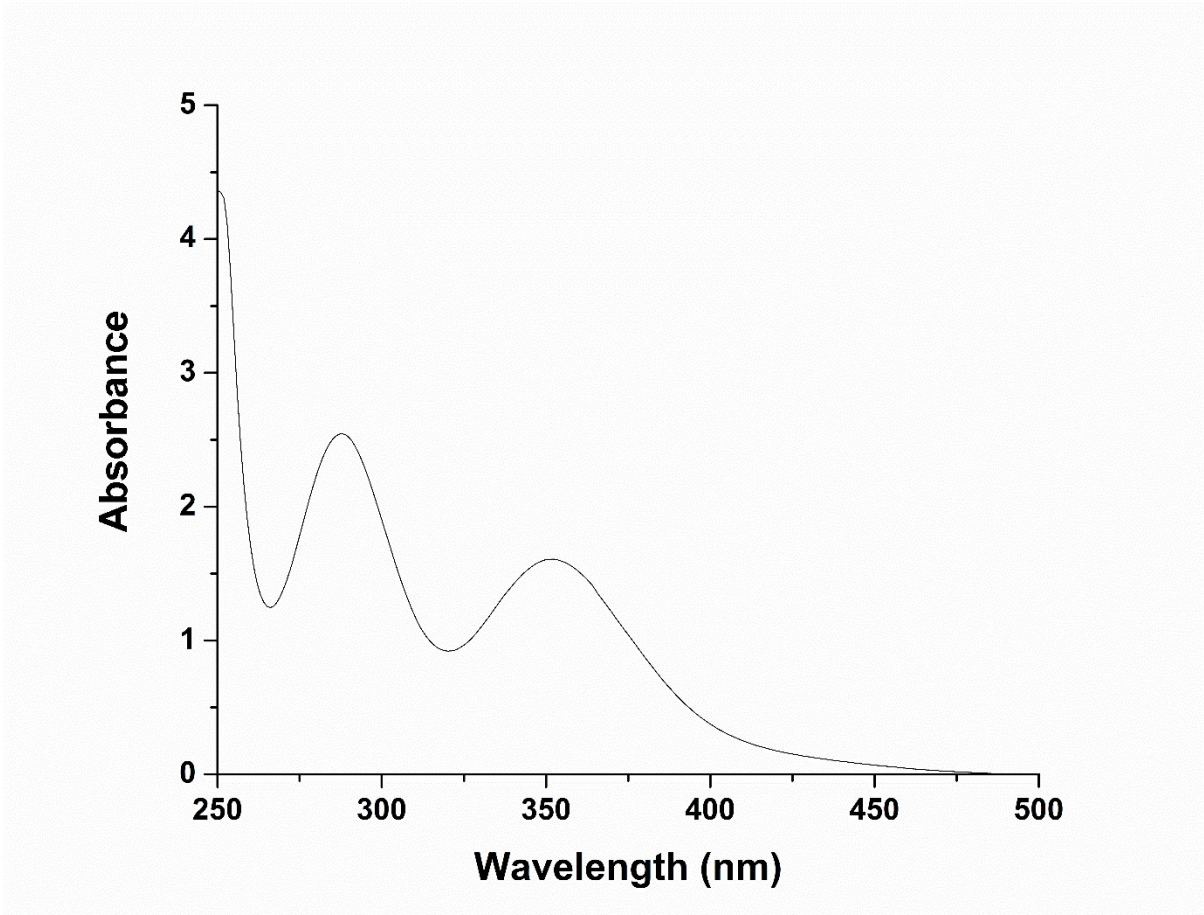

Figure S5. The formation of I_3^- as detected by the characteristic absorbance band at λ_{max} = 353 nm (298 K).

DFT calculations:

Absolute Gibbs Free Energies of all complexes at each step in the reaction pathway (Energies in Hartrees)

Phenoxide Acceptor Pathway		Solvent (MeOH) Acceptor Pathway	
Cu(II) – Cu(II) + Substrate (I)	-3150.57192	**Cu(II) – Cu(II) + Substrate (I)**	-3150.57192
Cu-Substrate + 2*MeOH (II)	-3150.568219	**Cu-Substrate + 2*MeOH (II)**	-3150.568219
Cu-Product + 2*MeOH (III)	-3150.599671	**Cu-Product + 2*MeOH2+ (III)**	-3150.030913
Cu(I) – Cu(I) + Product + 2*MeOH (IV)	-3150.610358	**Cu(I) – Cu(I) + Product + 2*MeOH2+**	-3150.043334

Coordinates of Substrate (Catechol)

38

-696.897808 Hartrees

C	1.05823900	-0.19962600	0.00000800
C	-0.25235900	-0.70138900	0.00001900
C	-1.40232300	0.10264300	0.00000200
C	-1.21942500	1.48989600	-0.00002600
C	0.06514400	2.01997700	-0.00004200
C	1.19997200	1.19980700	-0.00002800
H	-0.38512600	-1.77564300	0.00004400
H	-2.06532900	2.17153300	-0.00003400
C	2.29086900	-1.12655300	0.00002300
C	3.14246000	-0.86745400	1.26725800
H	4.02091400	-1.52497600	1.26915100
H	3.48875600	0.16684000	1.31522000
H	2.56193400	-1.07905200	2.17315100
C	3.14252600	-0.86739700	-1.26715600
H	4.02098600	-1.52491300	-1.26902800
H	2.56205100	-1.07896200	-2.17308900
H	3.48881700	0.16690200	-1.31505600

C	1.89730400	-2.61700300	-0.00001900
H	1.31678700	-2.89058000	0.88858700
H	1.31685500	-2.89054900	-0.88867900
H	2.80619500	-3.22919100	0.00000400
C	-2.79808300	-0.54927100	0.00001800
C	-3.93079300	0.49509300	0.00000100
H	-4.90225200	-0.01197300	0.00001200
H	-3.89466200	1.13616700	0.88859200
H	-3.89466500	1.13613400	-0.88861400
C	-2.95999700	-1.42974500	1.26188700
H	-3.94862400	-1.90554100	1.27354700
H	-2.20749100	-2.22390900	1.30290300
H	-2.86034300	-0.82917500	2.17330300
C	-2.96000500	-1.42979400	-1.26181600
H	-3.94863200	-1.90559000	-1.27345000
H	-2.86035700	-0.82926000	-2.17325600
H	-2.20750000	-2.22396000	-1.30280600
O	0.33583500	3.37623300	-0.00006200
H	-0.49657200	3.87113400	-0.00023000
O	2.43488200	1.79873600	-0.00005500
H	2.28135400	2.75971100	-0.00011300

Coordinates of Cu(II)-Cu(II) complex (MeOH coordinated Cu(II) dimer)

82

-2453.674112 Hartrees

Cu	1.55208200	-0.10328300	-0.34857300
O	2.61828600	0.84584500	-1.75955900
O	3.94151000	0.37493600	-3.51939400
O	-0.10907800	-1.25382700	-0.01608100

N	2.94306600	-0.35867300	1.43110900
N	2.66800900	-1.79482900	-0.93825800
C	3.27943800	0.52472800	2.37850500
H	2.69122200	1.43750400	2.40866300
C	4.71411700	-1.79032300	2.17225500
H	5.26986900	-2.71564600	2.05171900
C	5.05064800	-0.87550600	3.16977400
H	5.87750800	-1.07975700	3.84406900
C	-0.19814700	-2.58877000	-0.10645500
C	3.64595700	-1.49912400	1.32303400
C	3.17413300	-2.48373100	0.26824600
H	3.98195300	-3.18414900	0.00916500
H	2.35496900	-3.07811500	0.68486700
C	3.77350300	-1.25172900	-1.76734600
H	4.11206000	-1.99090000	-2.50277800
H	4.61141400	-1.00867300	-1.10583200
C	3.41382400	0.07924200	-2.45814600
C	1.73883200	-2.62357600	-1.77266600
H	1.32362300	-1.93876200	-2.52235600
H	2.32471500	-3.38085200	-2.31485300
C	0.66055500	-3.31484400	-0.97936200
C	0.53571900	-4.70673100	-1.05163100
H	1.20493000	-5.25811200	-1.70895000
C	4.31956800	0.30548300	3.27939500
H	4.55417600	1.04950100	4.03337700
C	-1.24371400	-4.68106400	0.56854900
H	-1.97773100	-5.20365100	1.17656300
C	-1.12155300	-3.30079200	0.69023100
H	-1.74196400	-2.73756600	1.37835200
C	-0.42116400	-5.39614500	-0.30680300
H	-0.50792600	-6.47517600	-0.39364200
O	4.94958800	1.66753400	-0.28512100

H	4.07239600	1.59878200	-0.70655600
C	5.76504800	2.46718700	-1.12929000
H	6.78270300	2.43421200	-0.72702300
H	5.44196300	3.52019800	-1.14743900
H	5.78122000	2.09075200	-2.16123800
Cu	-1.55208200	0.10328300	0.34857300
O	-2.61828700	-0.84584500	1.75955900
O	-3.94151100	-0.37493600	3.51939300
O	0.10907800	1.25382700	0.01608200
N	-2.94306600	0.35867300	-1.43110900
N	-2.66801000	1.79482900	0.93825800
C	-3.27943700	-0.52472700	-2.37850600
H	-2.69122100	-1.43750400	-2.40866300
C	-4.71411600	1.79032300	-2.17225500
H	-5.26986800	2.71564600	-2.05172000
C	-5.05064700	0.87550700	-3.16977500
H	-5.87750700	1.07975800	-3.84407000
C	0.19814700	2.58877000	0.10645600
C	-3.64595600	1.49912400	-1.32303500
C	-3.17413300	2.48373200	-0.26824600
H	-3.98195300	3.18414900	-0.00916500
H	-2.35496800	3.07811500	-0.68486700
C	-3.77350300	1.25172900	1.76734600
H	-4.11206100	1.99090000	2.50277700
H	-4.61141400	1.00867400	1.10583100
C	-3.41382500	-0.07924300	2.45814600
C	-1.73883200	2.62357600	1.77266600
H	-1.32362400	1.93876200	2.52235700
H	-2.32471600	3.38085200	2.31485300
C	-0.66055500	3.31484400	0.97936300
C	-0.53571900	4.70673000	1.05163200
H	-1.20493000	5.25811200	1.70895100

C	-4.31956800	-0.30548300	-3.27939600
H	-4.55417500	-1.04950000	-4.03337800
C	1.24371500	4.68106400	-0.56854700
H	1.97773200	5.20365100	-1.17656100
C	1.12155400	3.30079200	-0.69023000
H	1.74196500	2.73756600	-1.37835100
C	0.42116400	5.39614500	0.30680400
H	0.50792700	6.47517600	0.39364400
O	-4.94958800	-1.66753400	0.28512000
H	-4.07239600	-1.59878200	0.70655500
C	-5.76504900	-2.46718700	1.12928900
H	-6.78270300	-2.43421200	0.72702100
H	-5.44196400	-3.52019800	1.14743700
H	-5.78122100	-2.09075200	2.16123700

Coordinates of Cu(II)-Cu(II)-Substrate complex

108

-2919.196903 Hartrees

Cu	2.06748500	-0.73705200	-0.72186400
O	0.34407100	-1.57017900	-1.58922500
O	-0.27180500	-3.51530700	-2.56372400
O	2.03760700	-0.14030800	1.26298300

N	3.96608000	-1.07446400	-1.75213300
N	2.41147600	-2.74073000	-0.21852600
C	4.55113600	-0.34493500	-2.71346000
H	4.01950700	0.55222900	-3.01823200
C	5.76218600	-2.65152700	-1.88056900
H	6.20927900	-3.57787800	-1.53220200
C	6.37523100	-1.88765600	-2.87272900
H	7.31504800	-2.21137900	-3.31070700
C	2.46716100	-0.86492900	2.30312600
C	4.55646100	-2.20928200	-1.33265500
C	3.87127900	-2.95069600	-0.19858500
H	4.12442200	-4.02138500	-0.23467100
H	4.24898600	-2.56378900	0.75483100
C	1.75462900	-3.50673600	-1.30821600
H	1.50860000	-4.52339100	-0.97598500
H	2.46145500	-3.59748300	-2.13940900
C	0.47705000	-2.84020500	-1.87926800
C	1.74704000	-3.00679700	1.09918200
H	0.69783500	-2.72442200	0.96484300
H	1.77137700	-4.08995500	1.29351700
C	2.36412200	-2.28560900	2.27212400
C	2.85698000	-3.02068200	3.35659400
H	2.79164400	-4.10647300	3.32529700
C	5.76096300	-0.71012300	-3.29911700
H	6.20147700	-0.08872600	-4.07175900
C	3.50428500	-1.00101500	4.49822100
H	3.93848800	-0.49824000	5.35858300
C	3.06011700	-0.24027200	3.42188600
H	3.12360200	0.84304600	3.42829500
C	3.41170300	-2.39612100	4.47402400
H	3.77133400	-2.99024300	5.30895500
Cu	1.30575500	1.70444400	1.13433000

O	2.27724900	2.65283600	2.56338100
O	2.50513900	4.69111600	3.47937200
O	1.53602100	1.17433400	-0.83210300
N	-0.88951500	1.59271500	1.66229500
N	0.66334100	3.58931700	0.55627100
C	-1.54352900	0.75969600	2.48034400
H	-0.96644600	-0.06975700	2.87741100
C	-2.89022700	2.88522500	1.40966600
H	-3.39157100	3.74008500	0.96577400
C	-3.57111600	2.01425300	2.25999000
H	-4.61968300	2.17976700	2.48918400
C	1.38288200	1.91798800	-1.93085100
C	-1.54767900	2.63540400	1.12727900
C	-0.75909200	3.48576800	0.15211400
H	-1.20602900	4.48601500	0.05502200
H	-0.80110200	3.00625900	-0.83087200
C	0.84974700	4.42268300	1.77365300
H	1.02049000	5.47109800	1.50339000
H	-0.06982600	4.37580400	2.36491600
C	1.99330300	3.91419300	2.68698100
C	1.57460000	4.05137700	-0.53790700
H	2.59106100	3.93105900	-0.14284800
H	1.41439400	5.12844600	-0.69539800
C	1.39804200	3.33710500	-1.85442500
C	1.23735000	4.07997100	-3.02868300
H	1.23378800	5.16608400	-2.96382100
C	-2.88795300	0.92989600	2.80651700
H	-3.38047500	0.22472100	3.46647900
C	1.06389000	2.07037000	-4.34195900
H	0.92031200	1.57320100	-5.29783100
C	1.18439800	1.30380900	-3.18685200
H	1.10841000	0.22149400	-3.22365700

C	1.09209900	3.46571500	-4.27302800
H	0.98105000	4.06740300	-5.16997200
C	-4.13822800	-1.93003200	0.24072900
C	-5.31882900	-1.29430200	-0.16644600
C	-5.34716100	-0.17814400	-1.01832400
C	-4.12371500	0.29738500	-1.49229200
C	-2.92025400	-0.29563900	-1.10840100
C	-2.91733000	-1.38841900	-0.22015100
H	-6.26264200	-1.69209700	0.18442900
H	-4.05509500	1.13522300	-2.17655100
C	-4.16907700	-3.19549200	1.12730100
C	-3.43053100	-2.95003100	2.46549900
H	-3.44317800	-3.86240100	3.07569400
H	-2.39144600	-2.65813400	2.30448600
H	-3.92992000	-2.16011200	3.04088000
C	-3.50539400	-4.37197100	0.36817200
H	-3.50452000	-5.27291700	0.99576800
H	-4.06248200	-4.59978400	-0.54793500
H	-2.47607700	-4.14165800	0.08807100
C	-5.60781300	-3.62908400	1.47655600
H	-6.14422300	-2.86267500	2.04862100
H	-6.19528400	-3.86407500	0.58191700
H	-5.57152500	-4.53440700	2.09371600
C	-6.69521400	0.45471600	-1.41174800
C	-6.52085700	1.66130500	-2.35380700
H	-7.50149300	2.08382200	-2.60264400
H	-5.92475400	2.45617500	-1.89042500
H	-6.03447200	1.37595600	-3.29331000
C	-7.43021500	0.94327600	-0.14069700
H	-8.39806900	1.39096500	-0.40069500
H	-7.61890200	0.12309500	0.55993300
H	-6.83643900	1.70114000	0.38490700

C	-7.57404400	-0.59302700	-2.13582300
H	-8.54027800	-0.15629100	-2.41964200
H	-7.08084500	-0.95131800	-3.04651700
H	-7.77443900	-1.46322800	-1.50210500
O	-1.75943500	0.26705000	-1.58161000
H	-1.06674600	-0.40973800	-1.75696100
O	-1.72976400	-1.91703100	0.22359100
H	-0.99128700	-1.62790500	-0.35274800

Coordinates of Cu(I)-Cu(I)-Product complex (Phenoxide acceptor)

108

-2919.228355 Hartrees

Cu	2.51032000	0.94089600	-0.38387300
O	0.91153400	-0.03762800	-1.91966900
O	0.47661200	-1.78375300	-3.29314600
O	2.11977000	-0.56436800	1.34364300
N	4.51726200	1.35268300	-0.42373500
N	3.48825500	-1.05072000	-1.55144700
C	4.95055100	2.42013700	0.27649300
H	4.18847200	3.16455700	0.49365900
C	6.74065300	0.46851000	-0.41268000
H	7.42187100	-0.32600600	-0.70430400
C	7.18832700	1.56060700	0.32781600
H	8.23006300	1.62954100	0.62945500
C	3.22171900	-1.33030800	1.64314800
C	5.39592300	0.40039600	-0.78341800
C	4.90135700	-0.69237900	-1.72137200
H	5.03738300	-0.31009400	-2.74099400

H	5.55997200	-1.57016100	-1.63462200
C	2.77170600	-1.19712200	-2.82538700
H	2.97392800	-2.15792100	-3.32409300
H	3.09448400	-0.39330100	-3.49685400
C	1.25094800	-1.06295400	-2.69706200
C	3.29826100	-2.26700300	-0.72369800
H	2.22472100	-2.46731600	-0.68950000
H	3.77279500	-3.13201300	-1.22129900
C	3.84187900	-2.15426500	0.68207700
C	4.97684100	-2.87958100	1.06745900
H	5.44764900	-3.53729100	0.33934300
C	6.27895500	2.56211100	0.66900900
H	6.58598700	3.43809900	1.23155800
C	4.90687700	-1.92671400	3.27913000
H	5.31451500	-1.83068400	4.28215700
C	3.76353700	-1.21056100	2.92599900
H	3.26367000	-0.55561100	3.63301800
C	5.51361300	-2.77487900	2.35113400
H	6.39587300	-3.34812200	2.62192400
Cu	-1.09814600	1.49215400	0.36091200
O	0.93825400	2.16078100	0.08081500
O	2.16734100	4.05126600	-0.07001700
O	-1.53655100	0.42190100	-1.31189000
N	-2.26012200	2.57024800	1.84694900
N	-1.37646500	3.46390400	-0.58176400
C	-2.38702000	2.22809300	3.13577200
H	-1.91935300	1.28718800	3.41314900
C	-3.49529600	4.57308500	2.26914400
H	-3.91387500	5.50152800	1.89150200
C	-3.63576300	4.21495200	3.60967600
H	-4.17096900	4.86439800	4.29686000
C	-2.42677400	0.91855500	-2.17339400

C	-2.80025300	3.72135700	1.40757600
C	-2.63615100	4.01522500	-0.07403600
H	-2.72378600	5.09987300	-0.25411000
H	-3.45312900	3.53117800	-0.62310600
C	-0.20672300	4.25557000	-0.15587000
H	-0.03528500	5.11224800	-0.82362600
H	-0.40480600	4.65999600	0.84322700
C	1.09955000	3.43666100	-0.05337800
C	-1.36686800	3.23382800	-2.05383500
H	-0.37377600	2.82777200	-2.27482200
H	-1.45262800	4.20008000	-2.57891000
C	-2.43691500	2.29199000	-2.55173700
C	-3.41782500	2.75152000	-3.44074800
H	-3.41150200	3.80294600	-3.72547000
C	-3.07056600	3.01997700	4.05623100
H	-3.14911700	2.70902900	5.09304300
C	-4.35961900	0.54737700	-3.62305500
H	-5.09298500	-0.13765000	-4.04333700
C	-3.40326700	0.06600600	-2.73404700
H	-3.36887500	-0.98393000	-2.45812300
C	-4.38082600	1.89922300	-3.98047700
H	-5.12612700	2.27985200	-4.67302000
C	-1.79373300	-3.62280000	0.29415900
C	-3.14576900	-3.52365100	0.46196800
C	-3.86306300	-2.34432200	0.92628700
C	-3.14469100	-1.23300400	1.25216800
C	-1.71170400	-1.20773800	1.12751500
C	-0.98815700	-2.42753500	0.60437600
H	-3.75267200	-4.39100800	0.23358000
H	-3.61035100	-0.31951500	1.60220700
C	-1.11089000	-4.91161900	-0.19359200
C	-0.07686800	-5.38898100	0.85765200

H	0.40128300	-6.31379900	0.51210900
H	0.69969800	-4.64107800	1.02495800
H	-0.56516100	-5.60269900	1.81652300
C	-0.40806300	-4.65356100	-1.54829100
H	0.08733300	-5.57169800	-1.88864700
H	-1.13002400	-4.35319300	-2.31534100
H	0.33942600	-3.86403400	-1.47692900
C	-2.12329400	-6.05548400	-0.40265900
H	-2.65241700	-6.31488400	0.52246100
H	-2.86667600	-5.81379100	-1.17145800
H	-1.58865100	-6.95123000	-0.73741800
C	-5.39297600	-2.41437700	1.01057800
C	-6.00691900	-1.09853100	1.52365000
H	-7.09763900	-1.19377000	1.56771100
H	-5.65476600	-0.85167500	2.53189100
H	-5.77356000	-0.25778500	0.86100000
C	-5.81131800	-3.55186900	1.97459400
H	-6.90485300	-3.61310000	2.03008400
H	-5.44302900	-4.53024100	1.64884400
H	-5.42961700	-3.36902000	2.98568200
C	-5.96468300	-2.69404400	-0.40202100
H	-7.05935500	-2.74822000	-0.36015800
H	-5.68765900	-1.89457500	-1.09815700
H	-5.60225400	-3.64134700	-0.81503200
O	-1.03024300	-0.20153900	1.46575500
O	0.25112600	-2.39094900	0.49498700
H	-0.10545200	0.06647800	-1.79225700
H	1.35473800	-1.11633000	1.03055000

Coordinates of Cu(I)-Cu(I) complex (After product elimination)

72

-2223.550621

Cu	2.23777000	-0.49830500	-0.31522300
O	1.15983100	-1.53667300	1.10099100
O	0.97619200	-1.76288900	3.33469700
O	1.21146000	1.33568900	-0.34567800
N	4.08117400	-1.10179200	-0.92037200
N	3.37992700	0.17389900	1.51031900
C	4.34513800	-1.93535900	-1.94356000
H	3.52532800	-2.11378900	-2.63234500
C	6.32475900	-1.41951000	-0.14145300
H	7.08634600	-1.19378400	0.59935800
C	6.59348200	-2.28319100	-1.20199500
H	7.57133600	-2.74555600	-1.30158000
C	1.96959600	2.46275000	-0.22073900
C	5.06240500	-0.83424000	-0.02771500
C	4.77089800	0.18622500	1.06840200
H	5.48617800	0.04150400	1.89612100
H	4.97180900	1.17945400	0.64708100
C	3.04699800	-0.90117500	2.46166800
H	3.21018000	-0.59547100	3.50507100
H	3.70981300	-1.75142900	2.25854700
C	1.59119500	-1.43241400	2.32679000
C	2.86626700	1.49042100	1.95490400
H	1.84154300	1.30788400	2.29733100
H	3.43787800	1.85754600	2.82515100
C	2.84777600	2.55871200	0.88107300
C	3.64054000	3.70769000	0.99143600
H	4.31280300	3.79891900	1.84273000
C	5.58299000	-2.54412600	-2.12646100
H	5.74118400	-3.20870100	-2.96955100
C	2.68140100	4.62836000	-1.02012300

H	2.61152500	5.42594000	-1.75530500
C	1.88478800	3.49246200	-1.16485100
H	1.19676200	3.38027900	-1.99883700
C	3.56760100	4.73975200	0.05361600
H	4.19035800	5.62278500	0.16495700
Cu	-2.23776900	0.49830900	0.31522000
O	-1.15983100	1.53667300	-1.10099500
O	-0.97619600	1.76289300	-3.33470100
O	-1.21146000	-1.33568700	0.34567900
N	-4.08117300	1.10179000	0.92037400
N	-3.37992800	-0.17389800	-1.51032000
C	-4.34513700	1.93535300	1.94356500
H	-3.52532700	2.11378400	2.63234900
C	-6.32476000	1.41950400	0.14146000
H	-7.08634800	1.19377800	-0.59935000
C	-6.59348400	2.28318200	1.20200500
H	-7.57133900	2.74554300	1.30159200
C	-1.96959600	-2.46274900	0.22073900
C	-5.06240600	0.83423800	0.02771900
C	-4.77089800	-0.18622500	-1.06840200
H	-5.48617900	-0.04150200	-1.89611900
H	-4.97180800	-1.17945500	-0.64708300
C	-3.04700000	0.90117700	-2.46166900
H	-3.21018400	0.59547300	-3.50507200
H	-3.70981500	1.75143100	-2.25854700
C	-1.59119700	1.43241600	-2.32679400
C	-2.86626600	-1.49041800	-1.95490500
H	-1.84154200	-1.30788100	-2.29733100
H	-3.43787600	-1.85754400	-2.82515200
C	-2.84777500	-2.55871000	-0.88107400
C	-3.64053800	-3.70768900	-0.99143900
H	-4.31280000	-3.79891700	-1.84273300

C	-5.58299100	2.54411600	2.12647000
H	-5.74118500	3.20868900	2.96956200
C	-2.68140000	-4.62836000	1.02012000
H	-2.61152300	-5.42594000	1.75530200
C	-1.88478800	-3.49246100	1.16484900
H	-1.19676200	-3.38027900	1.99883600
C	-3.56759900	-4.73975100	-0.05361900
H	-4.19035600	-5.62278500	-0.16496200
H	-0.29146100	-1.49625500	0.79963200
H	0.29146200	1.49625700	-0.79963300

Coordinates of Product (*Ortho*-Quinone)

36

-695.688421 Hartrees

C	1.10102200	-0.12967100	0.00001200
C	-0.16393100	-0.61936200	0.00005300
C	-1.40717900	0.17388400	0.00000400
C	-1.33828500	1.52640600	-0.00005600
C	-0.04996200	2.21794300	-0.00005800
C	1.24929300	1.35364300	-0.00012500
H	-0.29609600	-1.69443300	0.00012700
H	-2.21439000	2.16430300	-0.00009200
C	2.35478700	-1.01531400	0.00005300
C	3.19857100	-0.72197100	1.26647400
H	4.08943800	-1.36133600	1.27169000
H	3.52290100	0.31955500	1.29727700

H	2.62594600	-0.93725600	2.17662800
C	3.19872800	-0.72183300	-1.26623100
H	4.08962000	-1.36116400	-1.27138500
H	2.62623100	-0.93705600	-2.17648000
H	3.52302400	0.31970900	-1.29689800
C	1.99933500	-2.51415800	-0.00004600
H	1.42638800	-2.80263700	0.88933500
H	1.42658000	-2.80256800	-0.88957400
H	2.92219900	-3.10399400	0.00002900
C	-2.73160800	-0.60000300	0.00004100
C	-3.95251800	0.33775400	0.00003400
H	-4.87214400	-0.25730100	0.00005500
H	-3.97289800	0.97925000	0.88775800
H	-3.97291400	0.97921600	-0.88771300
C	-2.80432200	-1.49025500	1.26590100
H	-3.74590800	-2.05144600	1.27082600
H	-1.98772200	-2.21792800	1.31466500
H	-2.76773000	-0.88110100	2.17586800
C	-2.80435900	-1.49031800	-1.26577200
H	-3.74595100	-2.05150000	-1.27064600
H	-2.76778200	-0.88121100	-2.17577100
H	-1.98776800	-2.21800200	-1.31451800
O	0.05131600	3.43410300	-0.00020900
O	2.32137700	1.93545100	-0.00015200