Electronic Supporting Information for:

Anti-proliferation and nuclease activities of copper(II) complexes of tripodal polyamine ligands

Doti Serre, Sule Erbek, Nathalie Berthet, Christian Philouze, Xavier Ronot, Véronique Martel-Frachet, and Fabrice Thomas

Content:

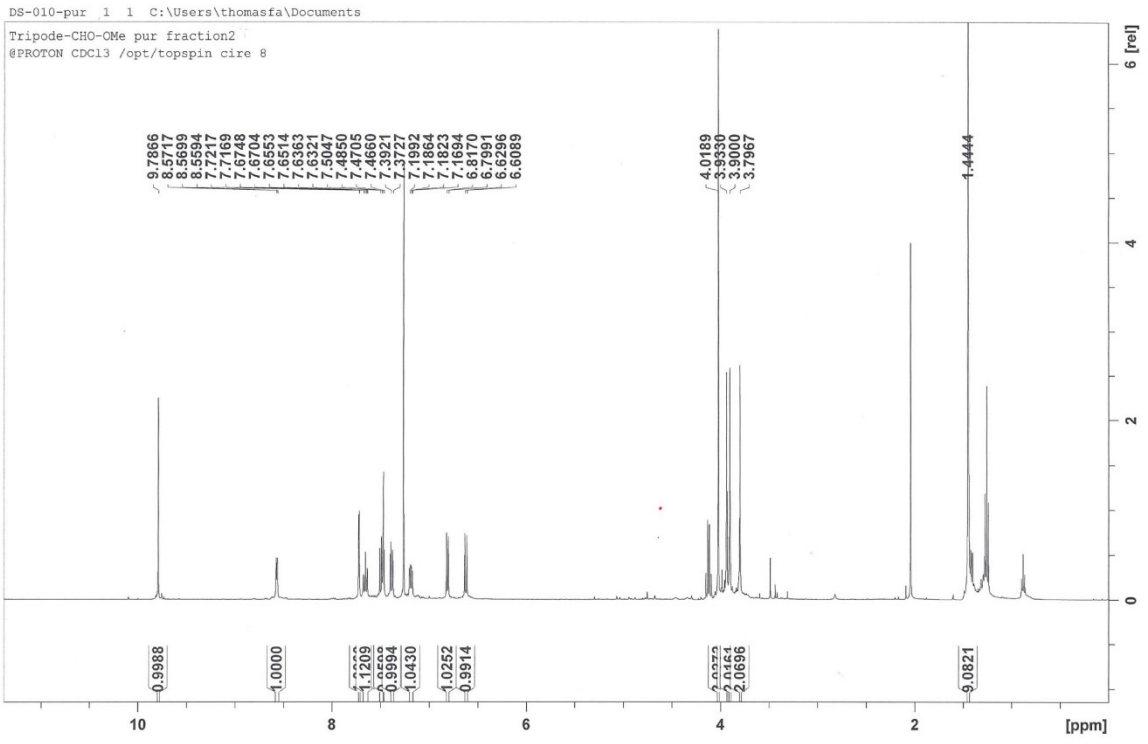

Fig. S1 ^{1}H NMR spectrum of **HL^{CHO}**

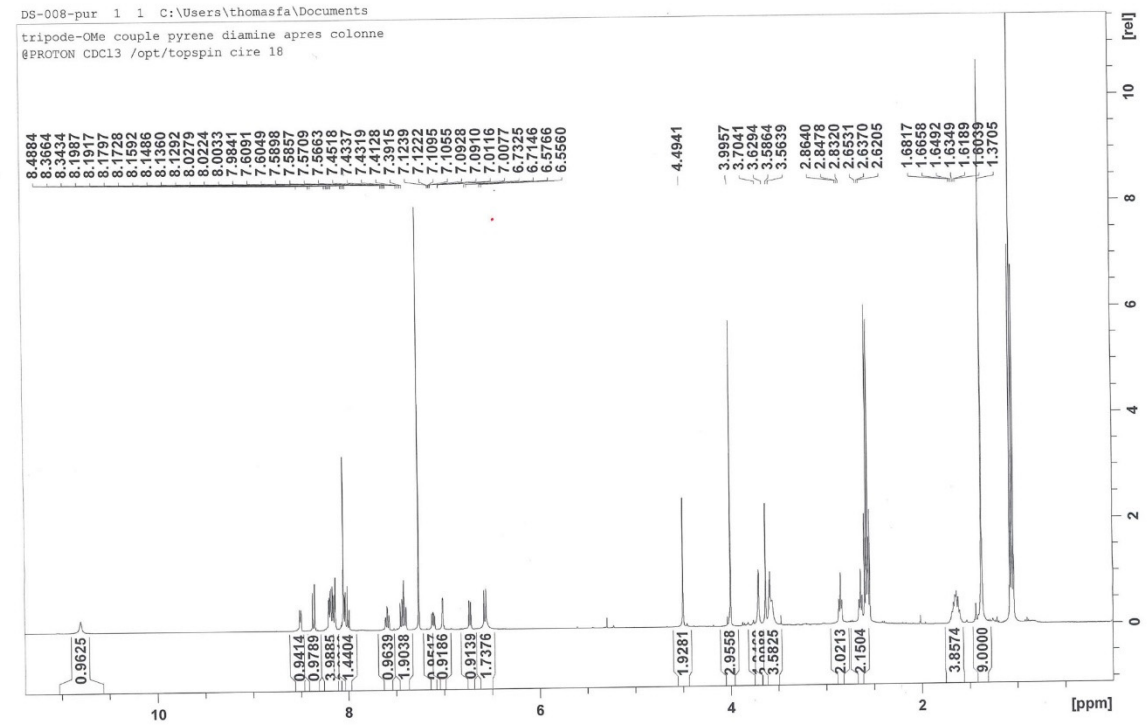

Fig. S2 ^{1}H NMR spectrum of **HL^{pyr}**

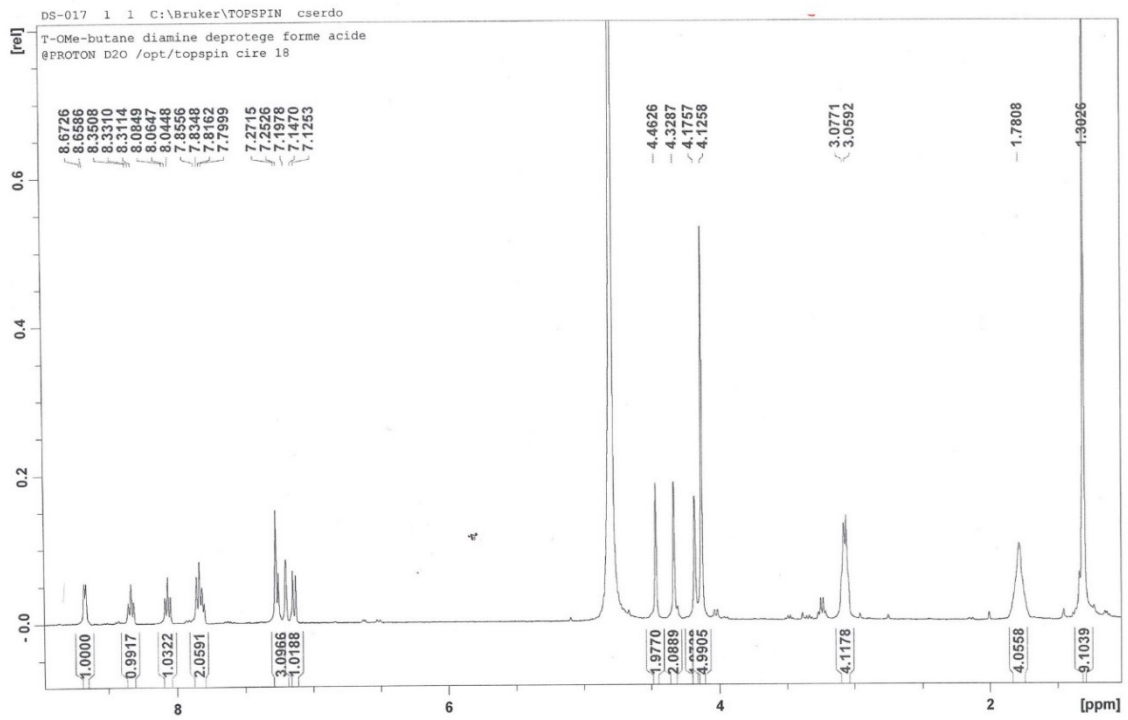

Fig. S3 ^{1}H NMR spectrum of **HL^{amine}**

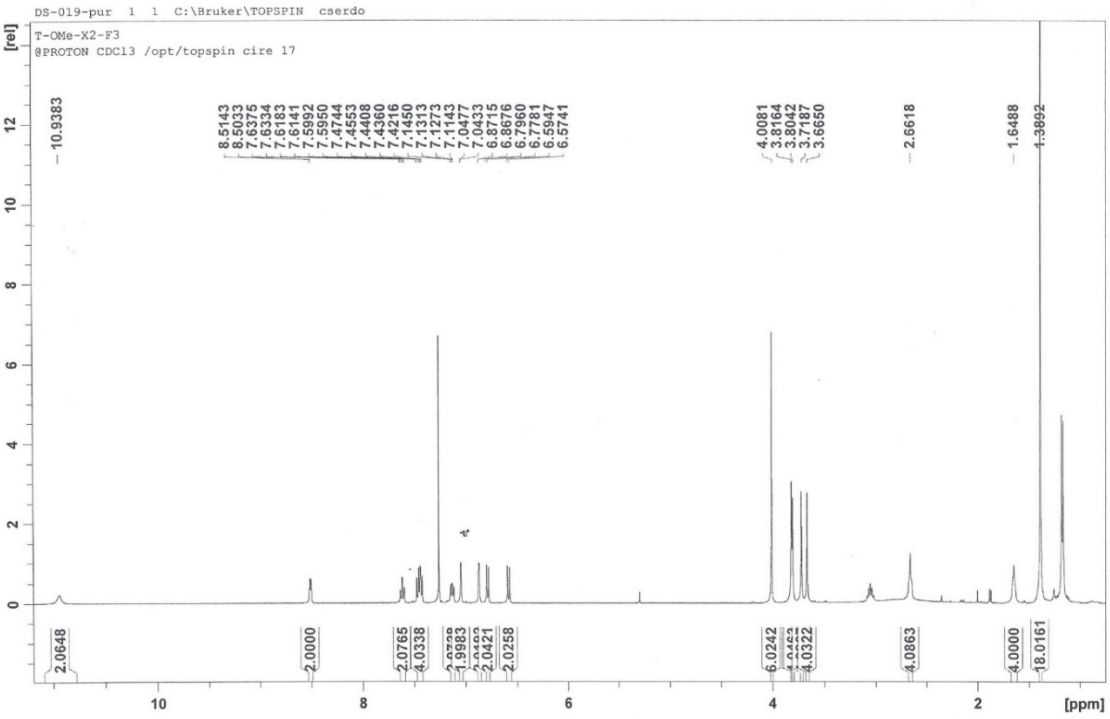

Fig. S4 ^{1}H NMR spectrum of **H$_2$L^{bis}**

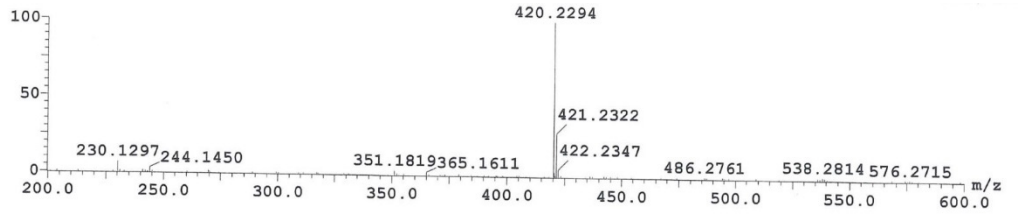

Fig. S5 HRMS of **HL^{CHO}**

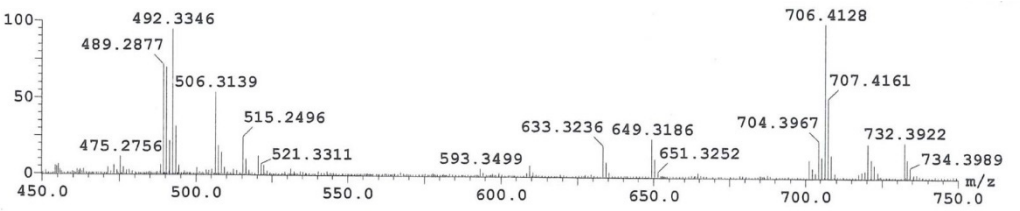

Fig. S6 HRMS of **HL^{pyr}**

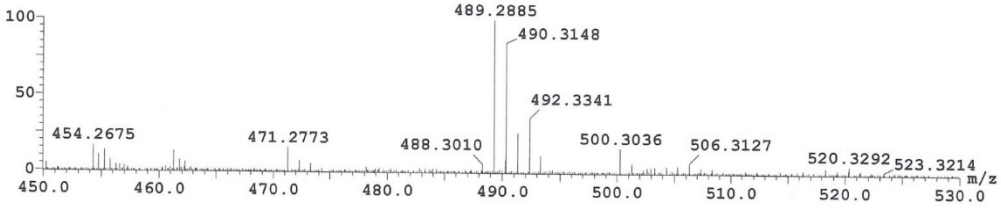

Fig. S7 HRMS of **HL^{amine}**

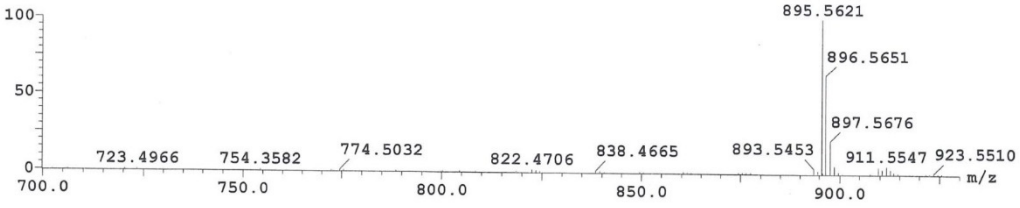

Fig. S8 HRMS of **H_2L^{bis}**

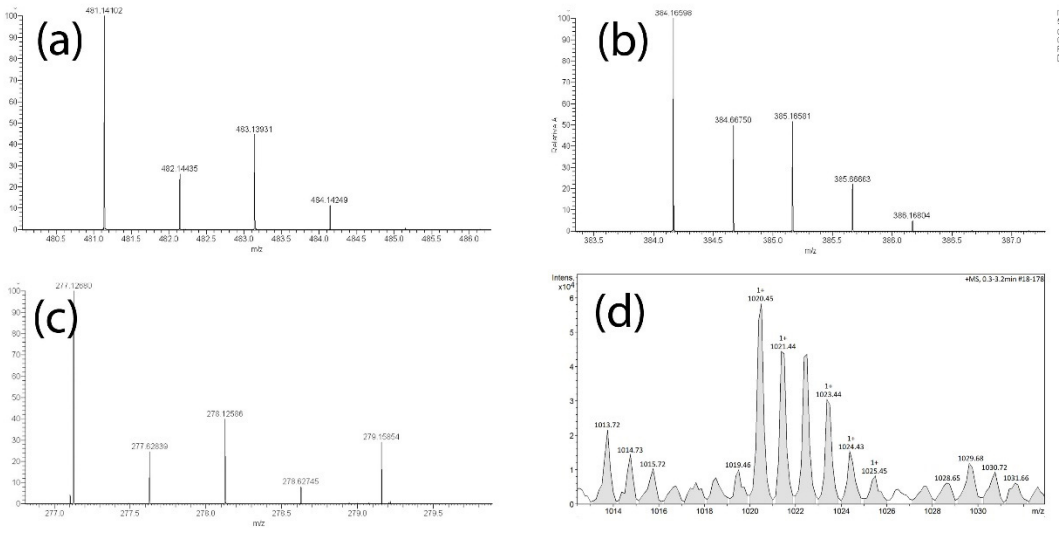

Fig. S9 Mass spectra of the complexes : HRMS of a) **1** ; b) **2** ; c) **3** ; d) ESI-MS of **4**. It was not possible to get a HRMS spectrum for **4**, only the ESI-MS spectrum is provided.

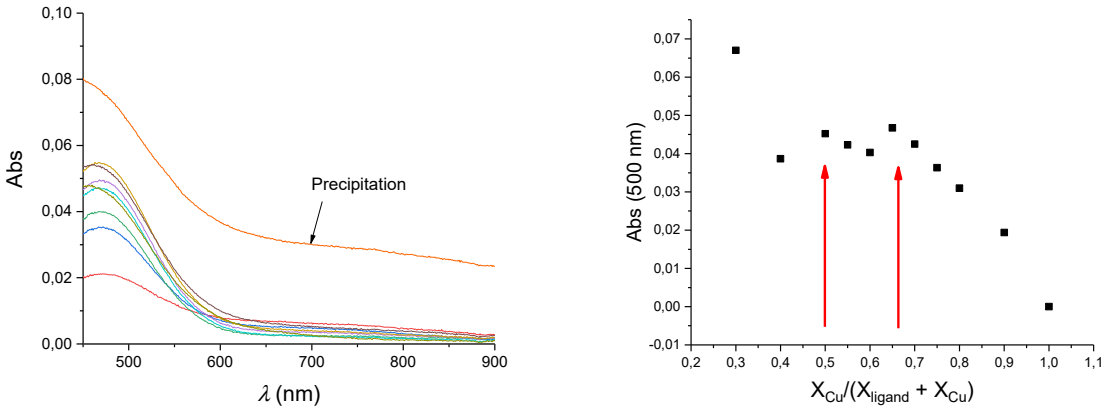

Figure S10 Job's of complex **4** : Left, evolution of the UV-Vis spectrum as a function of χ_{Cu} and χ_{ligand} ([Cu^{2+}] = 0.01-0.033 mM; [H_2L^{bis}] = 0-0.023 mM); Right, Job's plot diagram showing maximum peaks at $\chi_{Cu}/(\chi_{Cu} + \chi_{\lambda igand}) = 0.5$ (complex with 1:1 Cu:Ligand stoichiometry) and $\chi_{Cu}/(\chi_{Cu} + \chi_{\lambda igand}) = 0.66$ (complex with 2:1 Cu:Ligand stoichiometry). H_2O: DMF 90: 10 solution at pH 7. [Tris-HCl] = 0.05 M, [NaCl] = 0.02 M; T, 298 K; Note that a precipitation is observed at $\chi_{Cu}/(\chi_{Cu} + \chi_{\lambda igand}) \leq 0.3$.

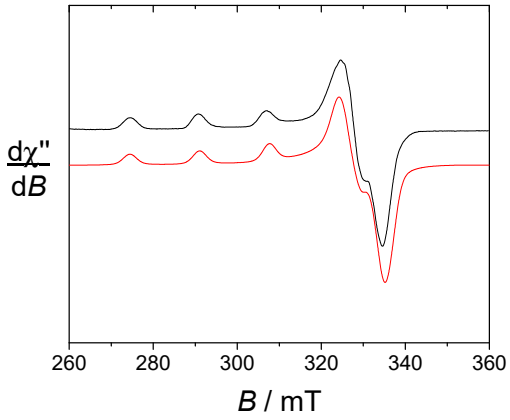

Figure S11. X-Band EPR spectra of a 0.5 mM solution of **1** in a water: DMF 90:10 medium at pH 7. Black: Experimental spectrum; Red: simulation by using the parameters given in Table 2.

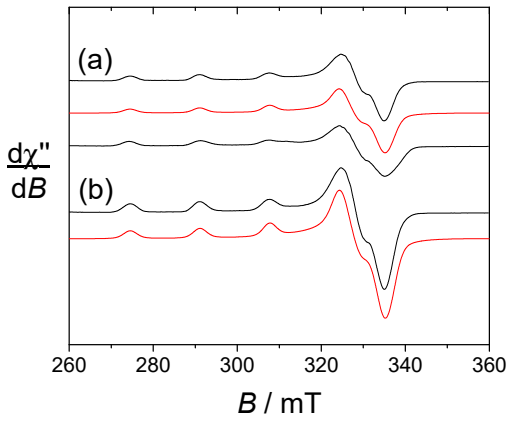

Figure S12. X-Band EPR spectra of 0.5 mM solutions of (a, top) **2** (a, bottom) **3** and (b) **4** in a water: DMF 90:10 medium at pH 7. Black: Experimental spectrum; Red: simulation by using the parameters given in Table 2. [Tris-HCl] = 0.05 M, [NaCl] = 0.02 M; *T*, 100 K; microwave frequency, 9.44 GHz; microwave power, 4 mW; mod. Freq., 100 KHz; mod. Amp. 0.4 mT.

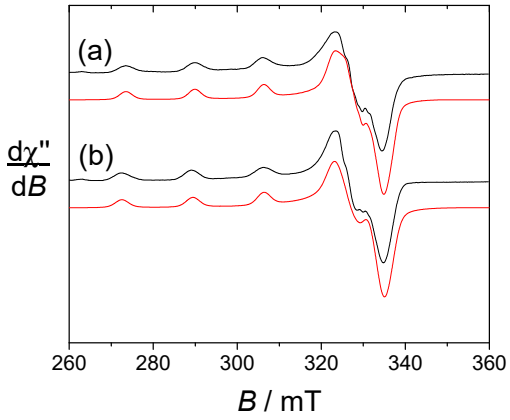

Figure S13. X-Band EPR spectra of a 0.5 mM solution of **1** in a water: DMF 90:10 medium at (top) pH = 3.80 and (bottom) pH = 1.80. Black: Experimental spectrum; Red: simulation by using the parameters given in Table 2. [NaCl] = 0.1 M; *T*, 100 K; microwave frequency, 9.44 GHz; microwave power, 4 mW; mod. Freq., 100 KHz; mod. Amp. 0.4 mT.

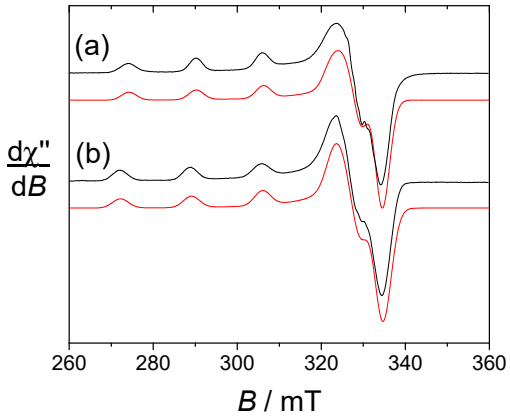

Figure S14. X-Band EPR spectra of a 0.5 mM solution of **3** in a water: DMF 90:10 medium at (top) pH = 5.26 and (bottom) pH = 3.25. Black: Experimental spectrum; Red: simulation by using the parameters given in Table 2. [NaCl] = 0.1 M; *T*, 100 K; microwave frequency, 9.44 GHz; microwave power, 4 mW; mod. Freq., 100 KHz; mod. Amp. 0.4 mT.

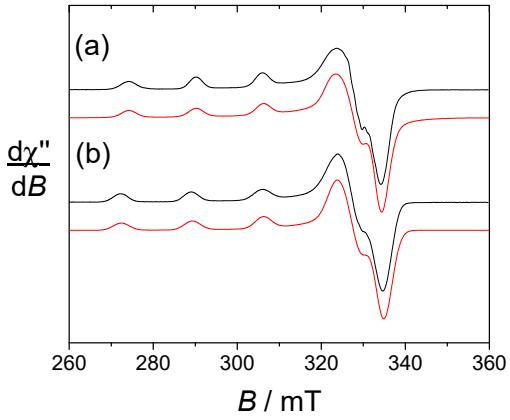

Figure S15. X-Band EPR spectra of a 0.5 mM solution of **4** in a water: DMF 90:10 medium at (top) pH = 5.35 and (bottom) pH = 3.34. Black: Experimental spectrum; Red: simulation by using the parameters given in Table 2. [NaCl] = 0.1 M; *T*, 100 K; microwave frequency, 9.44 GHz; microwave power, 4 mW; mod. Freq., 100 KHz; mod. Amp. 0.4 mT.

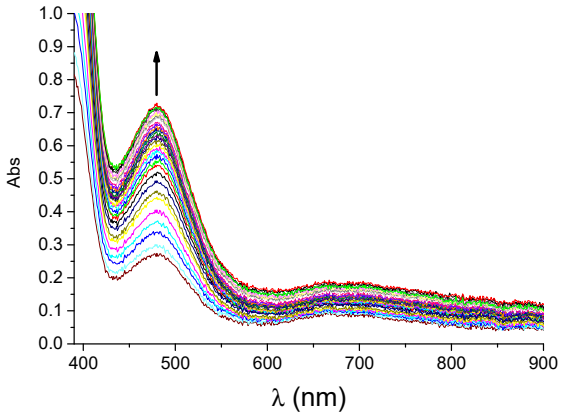

Figure S16 pH-dependence of the electronic spectrum of **1** in a 1 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm. pH varies from 2.66 to 7.33.

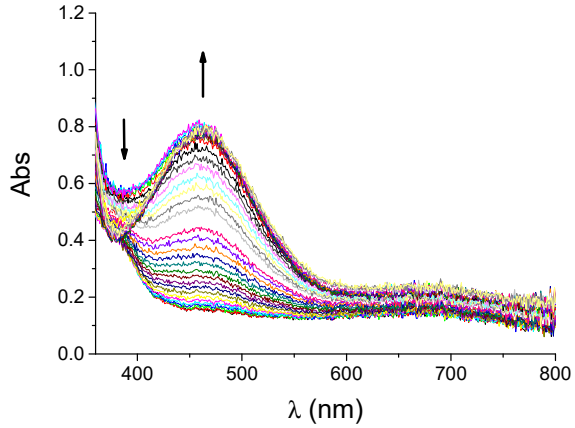

Figure S17 pH-dependence of the electronic spectrum of **3** in a 1 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm. pH varies from 2.57 to 7.37.

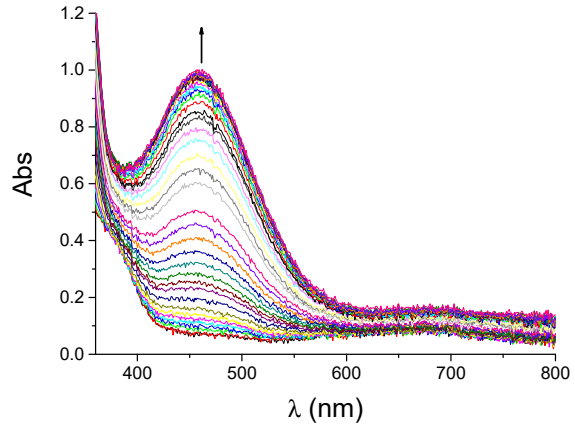

Figure S18 pH-dependence of the electronic spectrum of **4** in a 0.5 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm. pH varies from 2.64 to 7.05.

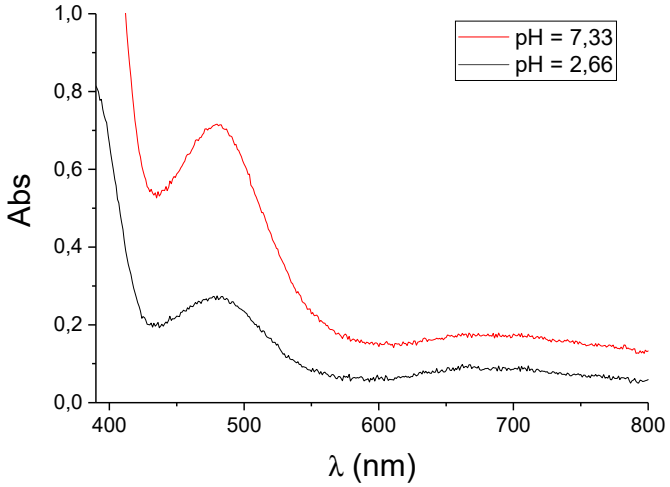

Figure S19 Electronic spectrum of **1** in a 1 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm.

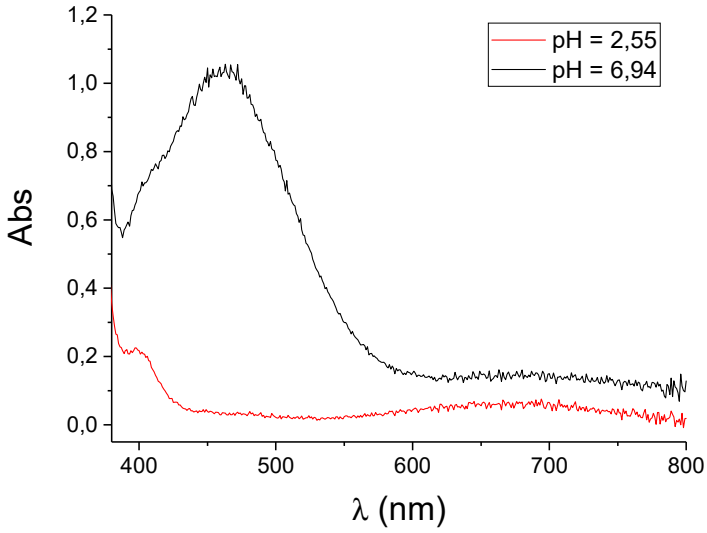

Figure S20 Electronic spectrum of **2** in a 1 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm.

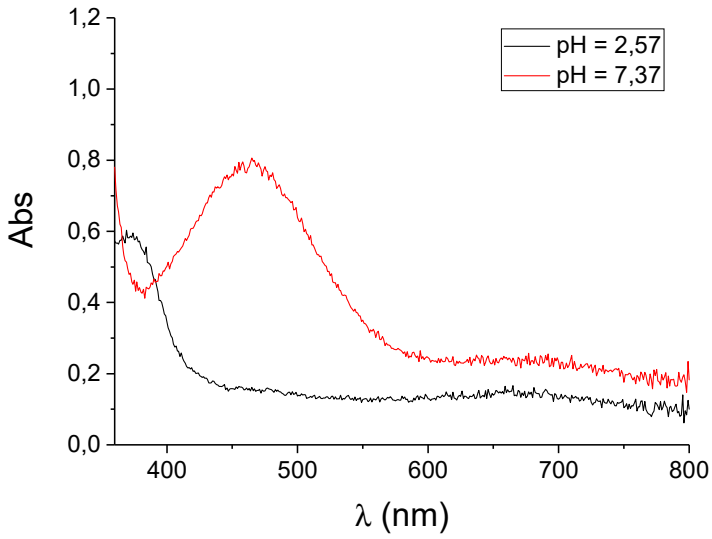

Figure S21 Electronic spectrum of **3** in a 1 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm.

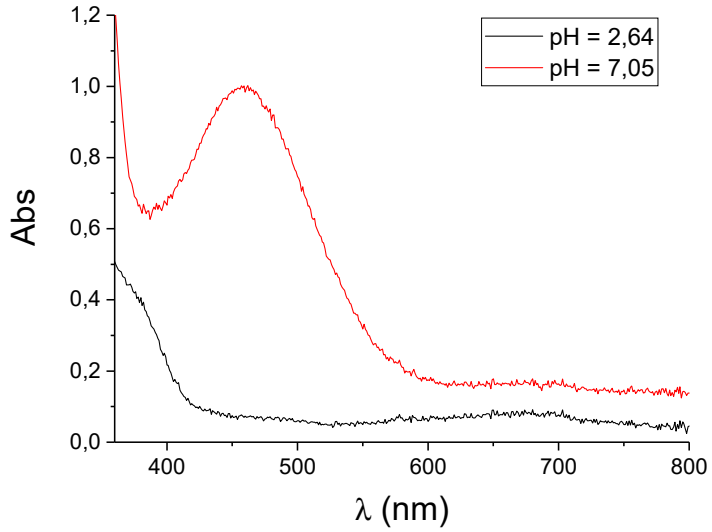

Figure S22 Electronic spectrum of **4** in a 0.5 mM H_2O: DMF 90: 10 solution. [NaCl] = 0.1 M, T = 298 K, *l* = cm.

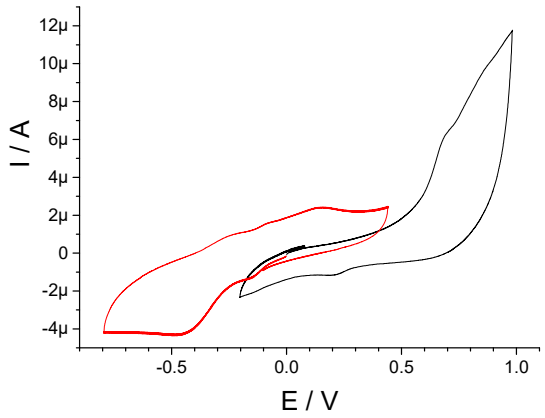

Figure S23. Cyclic voltammetry curves of **3** in a water:DMF 90:10 medium at pH 7. [Tris-HCl] = 0.05 M, [NaCl] = 0.02 M; T, 298 K; scan rate, 0.1 V sec^{-1}; The potentials are given versus the SCE reference.

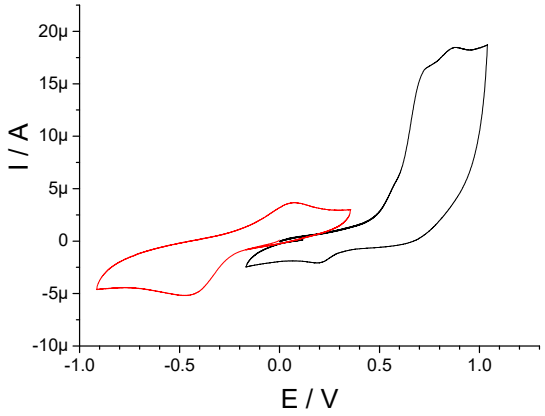

Figure S24. Cyclic voltammetry curves of **4** in a water:DMF 90:10 medium at pH 7. [Tris-HCl] = 0.05 M, [NaCl] = 0.02 M; T, 298 K; scan rate, 0.1 V sec^{-1}; The potentials are given versus the SCE reference.

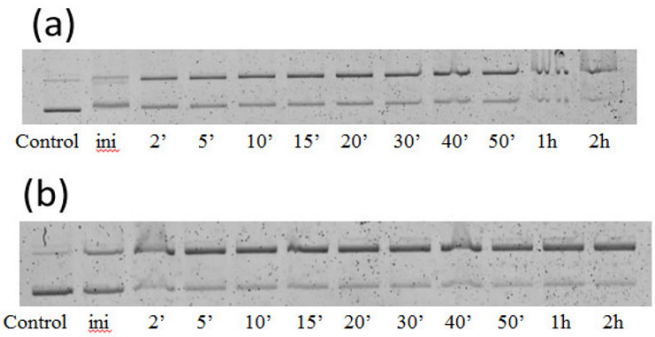

Figure S25. Agarose gel electrophoresis patterns of supercoiled ϕX174 DNA (20 µM base pairs) incubated with the copper complexes in a phosphate buffer 10 mM pH 7.2 (+ 10 % DMF) at 37°C as a function of time; (a) **2**, 10 µM; (b) **3**, 25 µM.

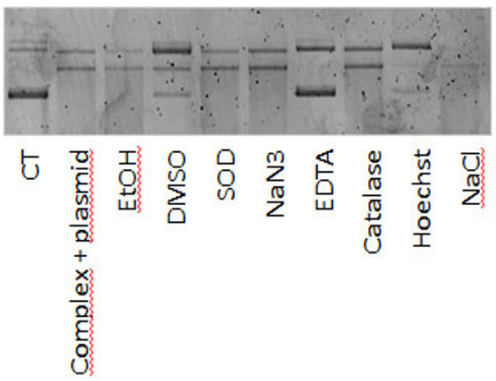

Figure S26. Agarose gel electrophoresis patterns of supercoiled ϕX174 DNA (20 µM base pairs) incubated with the copper complex **3** in a phosphate buffer 10 mM pH 7.2 (+ 10 % DMF) at 37°C for 1h. [ascorbate] = 0.8 mM; Complex concentration = 30 µM. Lane 0, DNA control; lane 1, DNA + complex (without scavenger); lanes 2-10, DNA + complex in the presence of agents: lane 2, ethanol; lane 3, DMSO (2 µL); lane 4, Superoxide Dismutase (0.5 unit); lane 5, NaN_3 (100 µM); lane 6, EDTA (10 mM); lane 7, Catalase (0.1 unit); lane 8, Hoechst 33258 (100 µM); lane 9, NaCl (350 µM).

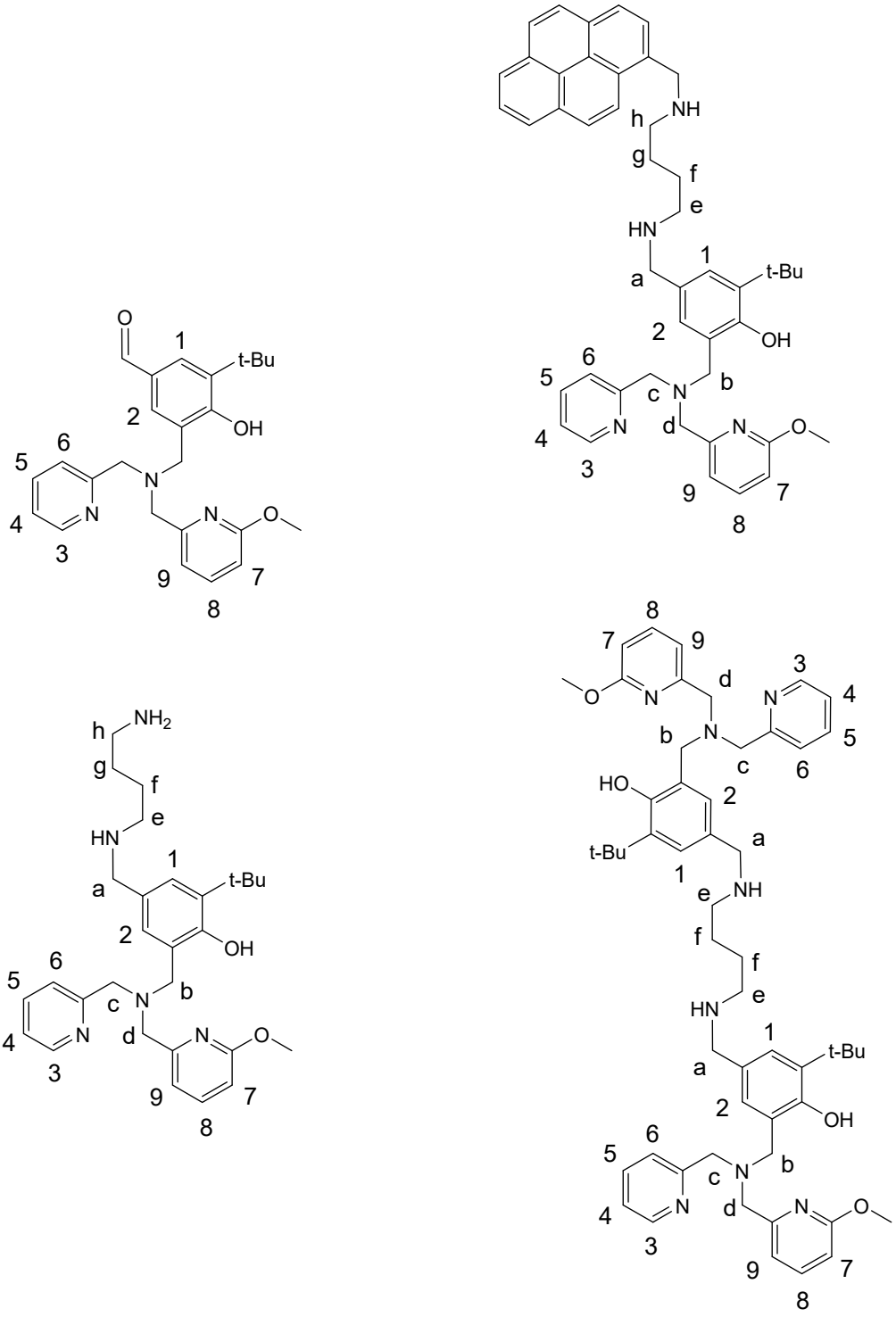

Figure S27. Selective numbering of the ligands **HL^{CHO}**, **HL^{pyr}**, **HL^{amine}** (the same numbering is used for **HL^{Boc}**) and **H$_2$L^{bis}** for the assignment of the ^{1}H NMR resonances.

Details about the DFT calculations:

Xyz coordinates

Phenol form, axial positioning of the phenol, exogeneous ligand = chloride

Cu	1.311468000	-0.495513000	-0.677699000
O	-0.209286000	1.259112000	-0.082399000
H	-0.441840000	1.882943000	-0.785740000
C	-4.623511000	-0.423636000	3.103094000
N	1.012307000	-1.261711000	1.196233000
N	-0.217785000	-1.686942000	-1.152439000
N	2.836225000	0.459760000	0.250776000
Cl	2.213657000	-0.548318000	-2.778660000
C	-1.339849000	0.912016000	0.648017000
C	-2.638538000	1.366049000	0.335106000
C	-3.667023000	0.904501000	1.171280000
H	-4.682938000	1.225336000	0.974983000
C	-3.461708000	0.052171000	2.262092000
C	-2.154472000	-0.345287000	2.540050000
H	-1.954057000	-0.980570000	3.399863000
C	-1.084700000	0.074410000	1.745432000
C	0.327453000	-0.296434000	2.126820000
H	0.953152000	0.598594000	2.161602000
H	0.326733000	-0.741859000	3.129346000
C	-2.935087000	2.343051000	-0.830325000
C	-4.439056000	2.676988000	-0.929519000
H	-5.045854000	1.785451000	-1.119886000
H	-4.596344000	3.367686000	-1.764453000
H	-4.812420000	3.165040000	-0.023291000
C	-2.537288000	1.721653000	-2.194770000
H	-1.469699000	1.497840000	-2.297419000
H	-2.793818000	2.411980000	-3.005680000
H	-3.078098000	0.784053000	-2.360843000
C	-2.201717000	3.691735000	-0.603497000
H	-2.535226000	4.153186000	0.331871000
H	-2.427745000	4.381036000	-1.424310000
H	-1.110141000	3.610992000	-0.545777000
C	3.482773000	1.604913000	-0.074992000
C	4.605672000	2.011244000	0.653594000
H	5.114755000	2.925592000	0.370057000
C	5.046271000	1.258573000	1.736530000
H	5.915330000	1.570965000	2.306933000
C	4.337655000	0.114475000	2.097521000
H	4.623345000	-0.481597000	2.957404000
C	3.239722000	-0.250453000	1.330217000
C	2.945686000	2.449197000	-1.194544000
H	2.864849000	1.872931000	-2.119527000
H	3.590112000	3.314223000	-1.364888000
H	1.945200000	2.817310000	-0.939220000
C	2.416702000	-1.479426000	1.638126000
H	2.817007000	-2.334239000	1.082445000
H	2.467433000	-1.727053000	2.705538000
C	-0.889031000	-1.676666000	-2.319366000
H	-0.501417000	-1.012142000	-3.081995000
C	-1.999310000	-2.481151000	-2.539843000
H	-2.511887000	-2.442620000	-3.494344000
C	-2.429366000	-3.325621000	-1.515180000
H	-3.296241000	-3.964192000	-1.652711000
C	-1.729963000	-3.341588000	-0.310843000
H	-2.031920000	-3.989365000	0.505341000
C	-0.622473000	-2.509866000	-0.163856000
C	0.254589000	-2.533810000	1.064931000
H	-0.331350000	-2.740719000	1.966007000
H	0.971501000	-3.354251000	0.955297000
H	-5.109942000	-1.298598000	2.652128000
H	-5.388128000	0.353585000	3.205585000
H	-4.296618000	-0.713125000	4.106913000

Phenolate form, equatorial positioning of the phenolate, exogeneous ligand = chloride:

Cu	0.685787000	-0.507423000	-0.779969000
Cl	1.000600000	-2.690547000	-1.725839000
O	-1.190295000	-0.684234000	-0.984473000
C	-2.114863000	0.201750000	-0.630049000
N	0.616501000	1.585033000	-0.759298000
N	2.689312000	-0.157447000	-0.963620000
C	-4.314437000	0.783802000	0.216306000
H	-5.277057000	0.489013000	0.622213000
C	-1.893034000	1.588763000	-0.837643000
C	-4.088610000	2.158646000	0.040466000
C	0.621717000	2.095824000	0.636797000
H	-0.425020000	2.231083000	0.927771000
H	1.098545000	3.082104000	0.682451000

C	3.000406000	1.134733000	-1.186296000
N	1.048540000	-0.159450000	1.463779000
C	2.151792000	-0.591844000	3.545665000
H	2.491555000	-1.314843000	4.279856000
C	-2.861021000	2.539017000	-0.495157000
H	-2.647501000	3.593586000	-0.665479000
C	-3.382445000	-0.210482000	-0.097423000
C	1.822436000	2.017004000	-1.506026000
H	2.051481000	3.073408000	-1.320090000
H	1.601052000	1.917045000	-2.575290000
C	1.480633000	-1.031195000	2.398712000
C	1.249031000	1.157932000	1.648512000
C	-3.721213000	-1.703192000	0.099945000
C	-5.138065000	3.175300000	0.430120000
H	-5.259986000	3.240952000	1.520087000
C	1.919435000	1.664663000	2.761331000
H	2.073302000	2.733646000	2.867695000
C	3.680469000	-1.035500000	-0.733205000
H	3.372467000	-2.061807000	-0.573046000
C	-0.616447000	2.020601000	-1.498707000
H	-0.529478000	1.576766000	-2.497423000
H	-0.602114000	3.112682000	-1.616534000
C	-3.661627000	-2.436666000	-1.262153000
H	-4.411701000	-2.029312000	-1.951723000
H	-3.874710000	-3.505414000	-1.128917000
H	-2.676886000	-2.330463000	-1.719732000
C	5.019208000	-0.659313000	-0.717208000
H	5.785866000	-1.401979000	-0.526045000
C	4.316518000	1.590557000	-1.182326000
H	4.526347000	2.639611000	-1.362441000
C	1.191948000	-2.491658000	2.175310000
H	0.128568000	-2.697997000	2.349000000
H	1.773386000	-3.117693000	2.857174000
H	1.409818000	-2.785639000	1.143988000
C	2.379100000	0.769614000	3.725177000
H	2.908736000	1.129270000	4.602408000
C	-5.135929000	-1.919889000	0.674985000
H	-5.257630000	-1.458376000	1.661987000
H	-5.315513000	-2.995132000	0.790075000
H	-5.916316000	-1.524937000	0.014160000
C	-2.720272000	-2.348661000	1.087408000
H	-1.696431000	-2.245819000	0.726300000
H	-2.943100000	-3.416361000	1.211919000
H	-2.791638000	-1.874240000	2.074361000
C	5.343040000	0.678168000	-0.944588000
H	6.377548000	1.007006000	-0.934110000
H	-6.122484000	2.921802000	0.017007000
H	-4.873855000	4.175672000	0.070777000

Phenol form, axial positioning of the phenol, exogeneous ligand = water:

Cu	1.298958000	-0.451623000	-0.780163000
O	-0.094305000	1.269612000	0.021319000
H	-0.277354000	2.065197000	-0.501204000
C	-4.549370000	-0.726043000	2.961621000
N	1.086475000	-1.390282000	0.997841000
N	-0.213371000	-1.576654000	-1.352479000
N	2.917138000	0.358363000	0.054184000
O	1.999035000	-0.413377000	-2.691987000
C	-1.234406000	0.865556000	0.712870000
C	-2.523154000	1.378927000	0.458225000
C	-3.561334000	0.829257000	1.226237000
H	-4.571436000	1.187604000	1.068895000
C	-3.374521000	-0.162227000	2.196819000
C	-2.075113000	-0.611017000	2.427705000
H	-1.888318000	-1.354582000	3.198541000
C	-0.996091000	-0.105142000	1.697649000
C	0.410809000	-0.529749000	2.035196000
H	1.047025000	0.349027000	2.167600000
H	0.411225000	-1.088358000	2.978189000
C	-2.800794000	2.502215000	-0.571080000
C	-4.300587000	2.862739000	-0.634103000
H	-4.914116000	2.009811000	-0.942923000
H	-4.444568000	3.658578000	-1.372222000
H	-4.675552000	3.231411000	0.326332000
C	-2.394729000	2.061818000	-2.000684000
H	-1.330357000	1.832221000	-2.111440000
H	-2.625462000	2.860538000	-2.714015000
H	-2.952160000	1.167399000	-2.298451000
C	-2.055470000	3.800966000	-0.163085000
H	-2.380035000	4.133249000	0.828565000
H	-2.277276000	4.597513000	-0.881559000
H	-0.963171000	3.708331000	-0.124359000
C	3.568652000	1.500699000	-0.259874000
C	4.672989000	1.913095000	0.494088000
H	5.182505000	2.831394000	0.223582000
C	5.093770000	1.156418000	1.579619000

H	5.945344000	1.472531000	2.173335000
C	4.394322000	-0.004787000	1.912400000
H	4.676172000	-0.608553000	2.767591000
C	3.313078000	-0.372986000	1.128217000
C	3.100858000	2.323037000	-1.429716000
H	3.809222000	2.248722000	-2.264026000
H	3.046920000	3.379694000	-1.151747000
H	2.116464000	2.016781000	-1.786574000
C	2.507586000	-1.623721000	1.387054000
H	2.898298000	-2.437835000	0.767667000
H	2.585206000	-1.934739000	2.434389000
C	-0.933399000	-1.429546000	-2.482411000
H	-0.605149000	-0.654255000	-3.165758000
C	-2.036858000	-2.223650000	-2.759848000
H	-2.588223000	-2.077131000	-3.681306000
C	-2.414251000	-3.192251000	-1.827903000
H	-3.277447000	-3.824289000	-2.009618000
C	-1.673955000	-3.337629000	-0.656839000
H	-1.943019000	-4.077718000	0.088872000
C	-0.570929000	-2.514301000	-0.448540000
C	0.339222000	-2.655319000	0.748573000
H	-0.221750000	-2.959974000	1.636835000
H	1.063294000	-3.448836000	0.538986000
H	-5.259938000	0.059739000	3.239945000
H	-4.223289000	-1.230429000	3.876477000
H	-5.099441000	-1.460471000	2.359022000
H	1.952642000	-1.285163000	-3.123860000
H	2.906482000	-0.098377000	-2.845640000

Phenolate form, equatorial positioning of the phenolate, exogeneous ligand = water:

Cu	0.721197000	-0.391697000	-0.802341000
O	-1.135272000	-0.558762000	-1.115799000
C	-2.077945000	0.254613000	-0.629812000
N	0.690441000	1.635834000	-0.454060000
N	2.676225000	-0.116789000	-1.153097000
C	-4.282206000	0.691137000	0.267975000
H	-5.254284000	0.338336000	0.596443000
C	-1.830950000	1.650031000	-0.574556000
C	-4.038967000	2.070667000	0.354454000
C	0.675058000	1.888167000	1.011407000
H	-0.376614000	1.949877000	1.309979000
H	1.133030000	2.856796000	1.240552000
C	3.046327000	1.179342000	-1.102020000
N	1.154168000	-0.472869000	1.398823000
C	2.204250000	-1.273519000	3.395356000
H	2.537344000	-2.116092000	3.991929000
C	-2.797653000	2.530914000	-0.078005000
H	-2.572892000	3.595776000	-0.043878000
C	-3.351845000	-0.239701000	-0.207252000
C	1.912879000	2.176539000	-1.107298000
H	2.217898000	3.125656000	-0.653285000
H	1.661647000	2.388066000	-2.153024000
C	1.586951000	-1.499881000	2.160948000
C	1.312019000	0.789709000	1.838257000
C	-3.704344000	-1.739977000	-0.296577000
C	-5.087811000	3.010484000	0.904716000
H	-5.237420000	2.866636000	1.983272000
C	1.938134000	1.087150000	3.047554000
H	2.057310000	2.118690000	3.362123000
C	3.622499000	-1.069531000	-1.237022000
H	3.270793000	-2.095203000	-1.268499000
C	-0.539819000	2.188032000	-1.127087000
H	-0.435735000	1.921377000	-2.184922000
H	-0.527077000	3.282989000	-1.054830000
C	-3.661972000	-2.198901000	-1.774409000
H	-4.415895000	-1.665073000	-2.365671000
H	-3.876567000	-3.272609000	-1.846473000
H	-2.684538000	-2.010646000	-2.223513000
C	4.977933000	-0.767572000	-1.282405000
H	5.707568000	-1.566044000	-1.354541000
C	4.386007000	1.558545000	-1.126315000
H	4.652131000	2.608905000	-1.075518000
C	1.388365000	-2.894243000	1.629459000
H	0.366824000	-3.028342000	1.260893000
H	1.581819000	-3.640364000	2.404053000
H	2.068518000	-3.095324000	0.793420000
C	2.390264000	0.033176000	3.838267000
H	2.879472000	0.228227000	4.787835000
C	-5.120046000	-2.046452000	0.235146000
H	-5.231858000	-1.773604000	1.290880000
H	-5.310178000	-3.122618000	0.150375000
H	-5.898788000	-1.529469000	-0.337020000
C	-2.711714000	-2.575624000	0.546599000
H	-1.686093000	-2.431569000	0.204264000
H	-2.957565000	-3.642616000	0.474969000
H	-2.765924000	-2.288677000	1.603933000

C	5.365346000	0.571269000	-1.220020000
H	6.415825000	0.843401000	-1.241076000
H	-6.062335000	2.854191000	0.425871000
H	-4.803496000	4.056585000	0.750000000
O	0.706083000	-2.157131000	-1.896392000
H	1.079238000	-2.056352000	-2.789457000
H	-0.263737000	-2.184012000	-2.019479000

TD-DFT results:

Phenol form, axial positioning of the phenol, exogeneous ligand = chloride:

Excited State 1: 2.002-A 1.5342 eV 808.15 nm f=0.0005 <S**2>=0.752
107B ->128B 0.14198
110B ->128B 0.11776
111B ->128B -0.24811
113B ->128B 0.24610
120B ->128B 0.54694
123B ->128B -0.15893
124B ->128B 0.40700
125B ->128B -0.50389
127B ->128B 0.25113
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3311.23663497
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.002-A 1.8752 eV 661.19 nm f=0.0006 <S**2>=0.752
104B ->128B 0.10201
108B ->128B 0.47002
111B ->128B 0.11069
112B ->128B -0.31829
113B ->128B -0.19253
118B ->128B -0.18277
119B ->128B -0.45675
120B ->128B 0.26351
121B ->128B -0.28265
124B ->128B 0.23174
125B ->128B 0.35158
127B ->128B 0.11848

Excited State 3: 2.001-A 1.9025 eV 651.69 nm f=0.0012 <S**2>=0.751
107B ->128B -0.13376
108B ->128B 0.20799
112B ->128B -0.14257
113B ->128B 0.44872
114B ->128B -0.21454
116B ->128B 0.11224
118B ->128B 0.22774
119B ->128B -0.37031
120B ->128B -0.44764
121B ->128B 0.36562
124B ->128B 0.28995
126B ->128B -0.10035

Excited State 4: 2.002-A 2.1062 eV 588.66 nm f=0.0018 <S**2>=0.752
104B ->128B 0.12453
107B ->128B -0.11009
108B ->128B 0.47248
110B ->128B -0.19036
112B ->128B 0.49476
116B ->128B -0.30761
117B ->128B 0.21601
118B ->128B 0.17804
119B ->128B 0.34384
124B ->128B 0.31311
125B ->128B 0.18219

Excited State 5: 2.013-A 2.7611 eV 449.04 nm f=0.0006 <S**2>=0.763
120B ->128B -0.19104
124B ->128B -0.10083
125B ->128B 0.12818
127B ->128B 0.95020

Excited State 6: 2.016-A 3.4155 eV 363.00 nm f=0.0015 <S**2>=0.766
108B ->128B 0.22549
119B ->128B -0.11283
120B ->128B -0.13887
124B ->128B -0.18769
125B ->128B -0.38260
126B ->128B 0.83404

Excited State 7: 2.013-A 3.4879 eV 355.47 nm f=0.0023 <S**2>=0.764
108B ->128B -0.35140
113B ->128B 0.10936
116B ->128B 0.10500
119B ->128B 0.13932

121B ->128B 0.21627
124B ->128B 0.40048
125B ->128B 0.54688
126B ->128B 0.52975

Excited State 8: 3.459-A 3.5684 eV 347.45 nm f=0.0000 <S**2>=2.742
126A ->131A -0.16527
126A ->133A -0.32870
126A ->134A -0.10022
128A ->129A 0.20578
128A ->133A 0.23415
128A ->134A -0.47353
126B ->131B 0.16387
126B ->133B 0.32966
127B ->129B -0.19983
127B ->133B -0.22884
127B ->134B 0.47493

Excited State 9: 2.027-A 3.5876 eV 345.59 nm f=0.0025 <S**2>=0.777
108B ->128B -0.21145
111B ->128B 0.13141
113B ->128B -0.24358
114B ->128B 0.10817
119B ->128B 0.10404
120B ->128B -0.39658
121B ->128B -0.32901
122B ->128B -0.17383
123B ->128B 0.29539
124B ->128B 0.58830
125B ->128B -0.29326

Excited State 10: 2.367-A 3.8044 eV 325.90 nm f=0.0010 <S**2>=1.150
123A ->129A -0.17790
123A ->130A 0.13973
113B ->128B 0.10058
120B ->128B 0.21500
121B ->128B 0.17597
122B ->128B 0.11575
123B ->128B 0.84592
123B ->129B 0.16562
123B ->130B -0.13644

Excited State 11: 3.370-A 3.8644 eV 320.83 nm f=0.0001 <S**2>=2.589
118A ->129A -0.14763
119A ->129A 0.11660
120A ->130A 0.21313
121A ->129A -0.11253
122A ->131A -0.18550
123A ->131A 0.11521
123A ->132A -0.34849
125A ->132A 0.10889
126A ->133A -0.10369
127A ->129A -0.11808
128A ->129A -0.32165
128A ->134A -0.11374
118B ->129B -0.19359
119B ->130B -0.22022
122B ->131B 0.18045
123B ->128B 0.22023
123B ->131B -0.12745
123B ->132B 0.36577
126B ->133B 0.10551
127B ->129B 0.22140
127B ->134B 0.11057

Excited State 12: 3.432-A 3.8728 eV 320.14 nm f=0.0001 <S**2>=2.694
118A ->130A 0.15947
119A ->130A -0.15449
120A ->129A -0.23991
122A ->131A 0.26195
122A ->132A 0.17859
123A ->131A 0.19244
123A ->132A -0.20836
125A ->132A 0.10693
128A ->129A 0.30898
128A ->130A 0.14877
118B ->130B 0.20325
119B ->129B 0.25158
122B ->131B -0.26875
122B ->132B -0.16828
123B ->128B 0.10898
123B ->131B -0.19084
123B ->132B 0.22693
127B ->129B -0.22608
127B ->130B -0.10165

Excited State 13: 2.939-A 3.9249 eV 315.89 nm f=0.0011 <S**2>=1.909

119A ->129A 0.10815
120A ->130A 0.12210
122A ->131A -0.24010
122A ->132A -0.10403
126A ->131A 0.12331
128A ->129A 0.76342
128A ->130A 0.23308
118B ->129B -0.10426
119B ->130B -0.13205
122B ->131B 0.24109
122B ->132B 0.10638
126B ->131B -0.13146
127B ->129B 0.10061

Excited State 14: 2.728-A 3.9391 eV 314.75 nm f=0.0015 <S**2>=1.611
122A ->131A 0.16184
126A ->131A -0.10422
128A ->129A 0.16419
122B ->131B -0.15976
127B ->129B 0.84209
127B ->130B 0.23945

Excited State 15: 2.763-A 4.0153 eV 308.78 nm f=0.0009 <S**2>=1.659
123A ->129A 0.25218
123A ->130A -0.23419
125A ->129A -0.12337
127A ->129A 0.68119
128A ->130A 0.11463
122B ->128B 0.29979
123B ->128B 0.18321
123B ->129B -0.27155
123B ->130B 0.24478
125B ->129B 0.10418
127B ->130B -0.14577

Excited State 16: 2.638-A 4.0447 eV 306.54 nm f=0.0003 <S**2>=1.490
123A ->129A -0.22390
123A ->130A 0.12797
125A ->130A -0.12087
127A ->129A 0.63226
128A ->130A -0.23384
121B ->128B 0.17306
122B ->128B -0.45320
123B ->128B -0.11388
123B ->129B 0.21145
123B ->130B -0.14433
127B ->130B 0.15700

Excited State 17: 2.942-A 4.0584 eV 305.50 nm f=0.0001 <S**2>=1.914
122A ->129A -0.10069
122A ->130A -0.11570
128A ->130A -0.33943
128A ->131A 0.22794
128A ->133A 0.28134
128A ->134A 0.10741
121B ->128B -0.12798
122B ->128B 0.61514
122B ->130B 0.11814
127B ->130B 0.29166
127B ->131B -0.22779
127B ->133B -0.28488
127B ->134B -0.10467

Excited State 18: 3.017-A 4.0698 eV 304.64 nm f=0.0003 <S**2>=2.026
123A ->129A -0.24964
123A ->130A 0.20986
125A ->129A 0.10519
125A ->130A -0.10260
127A ->129A 0.16965
128A ->130A 0.14628
128A ->131A -0.23587
128A ->133A -0.28458
128A ->134A -0.10586
122B ->128B 0.49521
123B ->128B -0.18710
123B ->129B 0.24608
123B ->130B -0.22218
127B ->130B -0.13050
127B ->131B 0.23337
127B ->133B 0.28085
127B ->134B 0.10302

Excited State 19: 3.335-A 4.1445 eV 299.15 nm f=0.0002 <S**2>=2.530
122A ->129A 0.36563
122A ->130A 0.35065
123A ->130A 0.13235
125A ->129A 0.11671

126A ->129A -0.24265
126A ->130A -0.16224
127A ->129A 0.11915
127A ->130A -0.26302
128A ->130A -0.19509
128A ->133A 0.10954
122B ->129B -0.36462
122B ->130B -0.33531
123B ->130B -0.10999
126B ->129B 0.22440
126B ->130B 0.16477
127B ->129B 0.16582
127B ->133B -0.11049

Excited State 20: 2.248-A 4.1617 eV 297.92 nm f=0.0007 <S**2>=1.014
127A ->130A 0.15673
128A ->129A -0.31562
128A ->130A 0.72044
128A ->133A 0.11413
127B ->130B 0.50534
127B ->131B -0.12142
127B ->133B -0.12953

Excited State 21: 3.060-A 4.2038 eV 294.93 nm f=0.0007 <S**2>=2.091
127A ->130A -0.45442
128A ->129A 0.14211
128A ->130A -0.17888
128A ->131A -0.19292
128A ->133A -0.22188
127B ->129B -0.28190
127B ->130B 0.65865
127B ->131B 0.17414
127B ->133B 0.21764

Excited State 22: 2.732-A 4.2364 eV 292.66 nm f=0.0012 <S**2>=1.616
122A ->129A 0.11301
122A ->130A 0.12852
125A ->129A -0.10541
127A ->130A 0.78224
128A ->130A -0.32450
122B ->129B -0.11260
122B ->130B -0.11589
127B ->130B 0.27429

Excited State 23: 2.057-A 4.2825 eV 289.51 nm f=0.0780 <S**2>=0.808
127A ->129A -0.17515
111B ->128B 0.24267
113B ->128B -0.49187
114B ->128B 0.17031
118B ->128B -0.14895
121B ->128B 0.69603
124B ->128B 0.11893
125B ->128B -0.16525

Excited State 24: 3.464-A 4.4668 eV 277.57 nm f=0.0000 <S**2>=2.750
126A ->129A -0.20571
126A ->131A -0.24906
126A ->133A -0.42556
128A ->134A 0.40795
126B ->129B 0.17458
126B ->131B 0.24694
126B ->133B 0.42675
127B ->134B -0.41050

Excited State 25: 2.007-A 4.5685 eV 271.39 nm f=0.0142 <S**2>=0.758
128A ->131A 0.65995
128A ->132A 0.11642
127B ->131B 0.69822
127B ->132B 0.12741

Excited State 26: 2.372-A 4.6178 eV 268.49 nm f=0.0120 <S**2>=1.157
126A ->129A 0.71523
126A ->130A 0.25632
125B ->129B -0.27826
126B ->129B 0.43691
126B ->130B 0.16458
127B ->131B -0.15048

Excited State 27: 3.111-A 4.6257 eV 268.04 nm f=0.0094 <S**2>=2.169
118A ->129A 0.11798
119A ->129A -0.10721
120A ->130A -0.17258
121A ->129A 0.10725
122A ->131A -0.11770
123A ->132A -0.18332
125A ->129A -0.16606
126A ->129A 0.14043

126A ->130A 0.10464
128A ->131A -0.19061
128A ->133A 0.11537
118B ->129B 0.14946
119B ->130B 0.18299
121B ->129B -0.10870
122B ->131B 0.11505
123B ->132B 0.18671
125B ->129B 0.54053
126B ->129B 0.44561
126B ->130B 0.13008
127B ->133B -0.10838

Excited State 28: 3.389-A 4.6587 eV 266.13 nm f=0.0008 <S**2>=2.621
118A ->130A 0.16632
119A ->130A -0.15650
120A ->129A -0.29219
121A ->129A -0.12522
121A ->130A 0.12763
122A ->131A -0.11308
123A ->131A -0.15622
123A ->132A 0.21297
124A ->129A -0.14774
125A ->129A -0.12228
125A ->132A -0.10071
126A ->130A -0.11560
128A ->131A -0.22037
128A ->132A -0.14592
128A ->133A 0.13310
118B ->128B -0.16420
118B ->130B 0.20943
119B ->128B 0.12271
119B ->129B 0.29298
121B ->130B -0.11187
122B ->131B 0.11579
123B ->131B 0.15754
123B ->132B -0.22635
124B ->129B 0.17986
125B ->129B 0.14436
125B ->130B 0.17297
126B ->130B 0.12762
127B ->131B 0.16944
127B ->132B 0.14227
127B ->133B -0.13136

Excited State 29: 3.200-A 4.6911 eV 264.30 nm f=0.0003 <S**2>=2.310
128A ->131A 0.42228
128A ->132A 0.12851
128A ->133A -0.28586
128A ->134A -0.10051
125B ->129B 0.54340
127B ->131B -0.41132
127B ->132B -0.12851
127B ->133B 0.29912

Excited State 30: 3.287-A 4.6980 eV 263.91 nm f=0.0002 <S**2>=2.451
122A ->129A -0.17726
122A ->130A -0.15379
125A ->129A -0.20746
126A ->129A -0.41088
126A ->130A -0.17824
126A ->133A 0.12239
128A ->131A 0.10966
122B ->129B 0.18806
122B ->130B 0.14550
124B ->129B 0.15314
125B ->129B -0.35282
126B ->129B 0.56166
126B ->130B 0.20246
126B ->133B -0.12111
127B ->131B -0.10280
127B ->134B 0.10289

Phenolate form, equatorial phenolate, exogeneous ligand = chloride:

Excited State 1: 2.003-A 1.1607 eV 1068.17 nm f=0.0014 <S**2>=0.753
109B ->128B 0.22734
110B ->128B -0.18248
118B ->128B 0.17271
122B ->128B 0.33540
124B ->128B 0.17957
125B ->128B 0.63765
127B ->128B 0.52455
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -3310.79830182
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.003-A 1.5385 eV 805.90 nm f=0.0007 <S**2>=0.753
108B ->128B 0.15847
109B ->128B -0.14946
110B ->128B -0.25539
113B ->128B 0.10719
114B ->128B -0.13324
116B ->128B 0.19343
117B ->128B 0.11678
118B ->128B -0.40446
120B ->128B -0.29288
124B ->128B 0.57208
125B ->128B 0.19665
127B ->128B -0.37733

Excited State 3: 2.002-A 1.7871 eV 693.78 nm f=0.0050 <S**2>=0.752
107B ->128B -0.24829
108B ->128B -0.24549
109B ->128B 0.11029
110B ->128B -0.13714
111B ->128B -0.12749
112B ->128B 0.18224
113B ->128B -0.25842
114B ->128B 0.10853
115B ->128B 0.12406
116B ->128B 0.42603
117B ->128B 0.15120
120B ->128B -0.28849
121B ->128B -0.13263
122B ->128B -0.42471
123B ->128B -0.22568
124B ->128B -0.20713
125B ->128B 0.27901

Excited State 4: 2.001-A 1.8742 eV 661.53 nm f=0.0027 <S**2>=0.751
107B ->128B 0.32790
108B ->128B 0.23988
110B ->128B 0.13438
111B ->128B 0.11371
112B ->128B -0.10571
113B ->128B 0.31968
116B ->128B 0.43363
117B ->128B 0.12194
118B ->128B 0.49306
122B ->128B -0.28404
123B ->128B 0.24817
124B ->128B 0.15828

Excited State 5: 2.031-A 2.2660 eV 547.16 nm f=0.0433 <S**2>=0.781
109B ->128B -0.21773
114B ->128B -0.16545
116B ->128B 0.12198
117B ->128B 0.14660
118B ->128B -0.35376
120B ->128B -0.12899
122B ->128B -0.18960
125B ->128B -0.32632
127B ->128B 0.74259

Excited State 6: 3.193-A 2.8149 eV 440.46 nm f=0.0012 <S**2>=2.298
128A ->129A 0.90574
127B ->129B -0.38698

Excited State 7: 2.301-A 2.8533 eV 434.52 nm f=0.0115 <S**2>=1.074
128A ->129A 0.39408
127B ->129B 0.90789

Excited State 8: 3.276-A 3.2695 eV 379.22 nm f=0.0002 <S**2>=2.433
128A ->130A 0.84772
127B ->130B -0.46808

Excited State 9: 2.181-A 3.3010 eV 375.60 nm f=0.0051 <S**2>=0.939
128A ->130A 0.48191
127B ->130B 0.86094

Excited State 10: 2.020-A 3.3520 eV 369.88 nm f=0.0292 <S**2>=0.770
109B ->128B -0.12769
118B ->128B -0.24666
123B ->128B 0.70787
124B ->128B -0.52652
125B ->128B 0.23122
126B ->128B 0.18230

Excited State 11: 3.077-A 3.4163 eV 362.92 nm f=0.0005 <S**2>=2.117
126A ->133A -0.11645
128A ->131A -0.48218
128A ->133A -0.29193

128A ->134A 0.20229
126B ->128B 0.51544
126B ->133B 0.10997
127B ->131B 0.42972
127B ->133B 0.24119
127B ->134B -0.21145

Excited State 12: 2.530-A 3.4541 eV 358.95 nm f=0.0004 <S**2>=1.350
128A ->131A 0.29586
128A ->134A -0.19188
123B ->128B -0.12271
125B ->128B -0.11486
126B ->128B 0.80858
127B ->131B -0.34756
127B ->134B 0.16605

Excited State 13: 2.028-A 3.5255 eV 351.68 nm f=0.0035 <S**2>=0.779
127A ->129A 0.17473
128A ->131A 0.68232
127B ->131B 0.68292

Excited State 14: 2.404-A 3.5637 eV 347.91 nm f=0.0041 <S**2>=1.195
123A ->129A 0.15683
127A ->129A 0.93073
127B ->131B -0.20521

Excited State 15: 3.377-A 3.5826 eV 346.07 nm f=0.0013 <S**2>=2.601
126A ->133A -0.27039
127A ->129A -0.15931
128A ->131A 0.32624
128A ->134A 0.52294
126B ->133B 0.26848
127B ->131B -0.28942
127B ->133B -0.10368
127B ->134B -0.50614

Excited State 16: 2.910-A 3.7004 eV 335.06 nm f=0.0058 <S**2>=1.866
128A ->131A 0.18502
128A ->133A -0.46802
107B ->128B -0.10956
108B ->128B -0.13032
113B ->128B -0.11790
116B ->128B -0.14670
120B ->128B 0.24308
122B ->128B -0.32305
123B ->128B 0.26090
124B ->128B 0.29657
125B ->128B 0.10028
127B ->131B -0.22198
127B ->133B 0.47146

Excited State 17: 2.695-A 3.7138 eV 333.84 nm f=0.0113 <S**2>=1.565
128A ->131A -0.20923
128A ->133A 0.40688
107B ->128B -0.13131
108B ->128B -0.15852
113B ->128B -0.13713
116B ->128B -0.17753
120B ->128B 0.28407
122B ->128B -0.37242
123B ->128B 0.29866
124B ->128B 0.35579
126B ->128B 0.13031
127B ->131B 0.16208
127B ->133B -0.39611

Excited State 18: 2.113-A 3.7437 eV 331.18 nm f=0.0348 <S**2>=0.866
107B ->128B 0.21951
108B ->128B 0.22052
109B ->128B -0.21906
112B ->128B -0.14112
113B ->128B 0.16941
114B ->128B -0.11909
116B ->128B -0.12183
118B ->128B -0.17722
120B ->128B 0.30803
122B ->128B -0.40330
123B ->128B -0.42069
124B ->128B -0.17066
125B ->128B 0.43611

Excited State 19: 3.417-A 3.8016 eV 326.14 nm f=0.0018 <S**2>=2.668
115A ->129A -0.10530
118A ->129A -0.18289
118A ->130A -0.19482
118A ->131A -0.12162
120A ->132A -0.15220

121A ->129A 0.11683
122A ->130A -0.17470
122A ->131A 0.25106
122A ->132A 0.29296
128A ->132A 0.16586
116B ->129B -0.10755
117B ->129B 0.16163
117B ->130B 0.16422
117B ->131B 0.11417
118B ->130B -0.10449
119B ->131B 0.12600
119B ->132B -0.16960
121B ->129B -0.11446
121B ->130B -0.18472
121B ->131B 0.24583
121B ->132B 0.29686
122B ->129B -0.10746
124B ->129B -0.11240
125B ->129B -0.23218
127B ->132B -0.13520

Excited State 20: 3.426-A 3.8690 eV 320.45 nm f=0.0018 <S**2>=2.684
114A ->129A 0.14163
115A ->129A -0.15130
117A ->129A -0.17474
118A ->130A 0.19905
119A ->131A 0.19413
120A ->130A -0.11756
120A ->131A 0.27837
122A ->132A -0.29048
123A ->129A 0.11187
109B ->129B -0.12421
113B ->129B 0.14919
114B ->130B -0.10330
117B ->130B -0.17094
118B ->129B 0.17140
119B ->129B -0.13117
119B ->130B -0.13549
119B ->131B 0.33169
121B ->132B -0.29298
122B ->129B -0.10847
124B ->129B -0.20449

Excited State 21: 3.154-A 3.9184 eV 316.41 nm f=0.0024 <S**2>=2.237
125A ->129A -0.15547
128A ->132A 0.25491
122B ->129B 0.11190
124B ->129B 0.26868
125B ->129B 0.78378
125B ->130B 0.13319
127B ->132B -0.15185

Excited State 22: 2.036-A 3.9541 eV 313.56 nm f=0.0016 <S**2>=0.787
128A ->132A 0.65015
127B ->132B 0.74829

Excited State 23: 3.366-A 3.9659 eV 312.63 nm f=0.0002 <S**2>=2.583
122A ->130A 0.10085
128A ->132A 0.65604
125B ->129B -0.21652
126B ->129B -0.10493
127B ->132B -0.58270

Excited State 24: 3.438-A 4.0749 eV 304.26 nm f=0.0002 <S**2>=2.705
120A ->130A -0.12310
122A ->129A 0.37260
122A ->130A 0.29455
122A ->131A 0.22985
125A ->129A -0.13475
126A ->129A 0.31338
126A ->130A 0.13588
128A ->132A -0.11985
119B ->130B -0.13449
121B ->129B 0.37737
121B ->130B 0.28884
121B ->131B 0.23517
126B ->129B -0.31198
126B ->130B -0.12558
127B ->132B 0.13337

Excited State 25: 2.521-A 4.1208 eV 300.87 nm f=0.0008 <S**2>=1.339
123A ->129A -0.17421
125A ->129A 0.14439
127A ->129A 0.10100
127A ->130A 0.90351
124B ->129B 0.22632

Excited State 26: 3.356-A 4.1566 eV 298.28 nm f=0.0000 <S**2>=2.566
119A ->129A 0.23443
120A ->129A 0.34986
120A ->130A -0.13615
122A ->129A 0.22107
124A ->129A 0.20432
126A ->129A -0.36405
127A ->130A 0.18006
119B ->128B 0.15901
119B ->129B 0.38664
119B ->130B -0.16750
121B ->128B 0.23815
121B ->129B 0.20232
123B ->129B -0.22319
126B ->129B 0.29418

Excited State 27: 2.937-A 4.1729 eV 297.12 nm f=0.0034 <S**2>=1.907
125A ->129A -0.35633
125A ->130A -0.10481
126A ->129A -0.10758
127A ->130A -0.14701
124B ->129B 0.69077
124B ->130B 0.10327
125B ->129B -0.43874
125B ->130B 0.17404

Excited State 28: 2.554-A 4.1877 eV 296.07 nm f=0.0051 <S**2>=1.381
121A ->129A 0.17237
121A ->130A 0.11336
125A ->129A 0.66456
125A ->130A 0.11374
127A ->130A -0.25029
121B ->128B 0.13167
124B ->129B 0.49148
125B ->130B -0.17354
126B ->129B -0.12334

Excited State 29: 2.036-A 4.2263 eV 293.37 nm f=0.0168 <S**2>=0.786
126A ->129A 0.72859
126B ->129B 0.65332

Excited State 30: 3.159-A 4.2417 eV 292.30 nm f=0.0010 <S**2>=2.245
119A ->129A -0.10524
120A ->129A -0.14807
122A ->129A 0.15724
122A ->130A 0.26517
122A ->131A 0.12049
125A ->129A 0.22039
126A ->129A -0.30170
126A ->133A 0.18551
128A ->134A 0.15775
119B ->129B -0.16626
121B ->128B -0.43691
121B ->129B 0.14934
121B ->130B 0.24278
121B ->131B 0.11939
123B ->129B 0.11558
126B ->129B 0.45948
126B ->133B -0.18431
127B ->134B -0.14247

Phenol form, axial phenol, exogeneous ligand = water

Excited State 1: 2.002-A 1.5979 eV 775.92 nm f=0.0008 <S**2>=0.752
103B ->124B 0.13264
104B ->124B 0.14748
109B ->124B -0.33367
112B ->124B -0.10853
113B ->124B -0.13251
116B ->124B -0.15954
119B ->124B 0.77936
123B ->124B 0.35258
This state for optimization and/or second-order correction.
Total Energy, E(TD-HF/TD-KS) = -2927.25643912
Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State 2: 2.003-A 1.9526 eV 634.98 nm f=0.0017 <S**2>=0.753
98B ->124B 0.12742
108B ->124B 0.30841
109B ->124B -0.18471
110B ->124B 0.20665
111B ->124B -0.12565
112B ->124B 0.17071
113B ->124B 0.60391
114B ->124B 0.13607

117B ->124B 0.24005
118B ->124B 0.26571
119B ->124B 0.21896
123B ->124B -0.38608

Excited State 3: 2.001-A 1.9909 eV 622.76 nm f=0.0002 <S**2>=0.751
105B ->124B -0.13368
108B ->124B 0.59031
109B ->124B 0.19824
110B ->124B -0.10278
111B ->124B 0.14653
112B ->124B -0.29067
113B ->124B -0.27991
117B ->124B -0.26822
118B ->124B 0.49691

Excited State 4: 2.009-A 2.1947 eV 564.93 nm f=0.0005 <S**2>=0.759
105B ->124B -0.17554
108B ->124B 0.14084
112B ->124B 0.14169
113B ->124B 0.26919
117B ->124B 0.12087
118B ->124B 0.20398
119B ->124B -0.21111
122B ->124B -0.10710
123B ->124B 0.83307

Excited State 5: 2.002-A 2.3481 eV 528.03 nm f=0.0012 <S**2>=0.752
96B ->124B 0.11286
97B ->124B -0.14127
99B ->124B 0.10617
100B ->124B 0.40238
101B ->124B -0.10312
103B ->124B -0.32427
104B ->124B -0.25670
105B ->124B 0.64056
108B ->124B 0.26969
112B ->124B -0.22459
113B ->124B 0.14165
123B ->124B 0.14319

Excited State 6: 2.011-A 2.7932 eV 443.88 nm f=0.0002 <S**2>=0.761
122B ->124B 0.98756

Excited State 7: 2.011-A 3.3889 eV 365.86 nm f=0.0002 <S**2>=0.761
121B ->124B 0.99704

Excited State 8: 3.462-A 3.5360 eV 350.63 nm f=0.0000 <S**2>=2.747
123A ->127A -0.12120
123A ->129A -0.28772
123A ->130A 0.10863
124A ->125A 0.40153
124A ->127A 0.10109
124A ->129A 0.25089
124A ->130A 0.26238
124A ->131A -0.29028
122B ->127B 0.11972
122B ->129B 0.29088
122B ->130B -0.10075
123B ->125B -0.34979
123B ->127B -0.10011
123B ->129B -0.24501
123B ->130B -0.31346
123B ->131B 0.24090

Excited State 9: 2.022-A 3.6165 eV 342.83 nm f=0.0002 <S**2>=0.772
119B ->124B -0.11395
120B ->124B 0.98283

Excited State 10: 2.249-A 3.7043 eV 334.70 nm f=0.0019 <S**2>=1.015
124A ->125A 0.82062
124A ->126A 0.23908
123B ->125B 0.44345
123B ->126B 0.12627

Excited State 11: 3.309-A 3.7316 eV 332.26 nm f=0.0003 <S**2>=2.487
123A ->129A -0.21544
124A ->125A -0.27769
124A ->130A 0.16953
124A ->131A -0.16047
122B ->129B 0.21517
123B ->125B 0.76970
123B ->126B 0.21398
123B ->130B -0.20361
123B ->131B 0.13446

Excited State 12: 3.462-A 3.8304 eV 323.68 nm f=0.0000 <S**2>=2.746

117A ->126A 0.12933
119A ->125A 0.17686
119A ->126A -0.17125
121A ->125A 0.25854
121A ->126A -0.21321
121A ->127A 0.23869
121A ->128A 0.37143
122A ->125A 0.12546
122A ->126A -0.10329
122A ->128A 0.13227
124A ->126A -0.11129
117B ->125B -0.10178
117B ->126B 0.12894
118B ->125B -0.18365
118B ->126B 0.17492
121B ->125B 0.28060
121B ->126B -0.22812
121B ->127B 0.25117
121B ->128B 0.39718
123B ->126B 0.10193

Excited State 13: 3.456-A 3.9209 eV 316.22 nm f=0.0001 <S**2>=2.735
117A ->125A 0.21582
117A ->126A 0.16773
119A ->125A 0.16469
119A ->126A 0.17487
120A ->127A -0.39976
120A ->128A 0.26183
121A ->128A -0.10562
123A ->127A 0.14011
124A ->125A 0.12857
124A ->126A -0.23251
117B ->125B 0.20287
117B ->126B 0.15409
118B ->125B -0.15979
118B ->126B -0.17898
120B ->127B 0.40169
120B ->128B -0.26476
122B ->127B -0.13995
123B ->125B -0.11565
123B ->126B 0.14630

Excited State 14: 3.400-A 3.9413 eV 314.58 nm f=0.0003 <S**2>=2.641
120A ->127A -0.13898
120A ->128A 0.11132
121A ->127A 0.10381
124A ->125A -0.15378
124A ->126A 0.71517
124A ->127A -0.15431
124A ->129A -0.15890
124A ->130A 0.10151
120B ->127B 0.14234
120B ->128B -0.10908
123B ->126B -0.40698
123B ->127B 0.14429
123B ->129B 0.15919
123B ->130B -0.10099

Excited State 15: 2.120-A 3.9866 eV 311.00 nm f=0.0035 <S**2>=0.873
124A ->125A -0.16248
124A ->126A 0.52749
123B ->125B -0.21332
123B ->126B 0.78858

Excited State 16: 3.461-A 4.0348 eV 307.29 nm f=0.0001 <S**2>=2.745
119A ->126A -0.10032
120A ->125A -0.15853
121A ->125A -0.31713
121A ->126A 0.38158
121A ->127A 0.19297
121A ->128A 0.20348
122A ->125A -0.13423
122A ->126A 0.11865
123A ->125A 0.20325
124A ->127A 0.13051
124A ->129A 0.11872
118B ->126B 0.10201
120B ->125B 0.14547
121B ->125B -0.34147
121B ->126B 0.38417
121B ->127B 0.20582
121B ->128B 0.21458
122B ->125B -0.18484
123B ->127B -0.13373
123B ->129B -0.12090

Excited State 17: 3.458-A 4.0642 eV 305.06 nm f=0.0000 <S**2>=2.739

120A ->125A 0.40182
120A ->126A 0.35061
121A ->125A -0.21066
123A ->125A -0.31652
123A ->126A -0.22572
120B ->125B -0.39773
120B ->126B -0.34476
121B ->125B -0.18549
122B ->125B 0.28523
122B ->126B 0.20870
123B ->126B 0.11066

Excited State 18: 3.460-A 4.1305 eV 300.17 nm f=0.0000 <S**2>=2.743
121A ->125A -0.10101
124A ->125A 0.12399
124A ->126A -0.24665
124A ->127A -0.39168
124A ->129A -0.39579
124A ->130A 0.17530
121B ->125B -0.10623
121B ->126B 0.10107
123B ->125B -0.14142
123B ->126B 0.30336
123B ->127B 0.38445
123B ->129B 0.39883
123B ->130B -0.16933

Excited State 19: 2.038-A 4.3415 eV 285.58 nm f=0.0079 <S**2>=0.788
123A ->125A 0.72201
123A ->126A 0.20895
122B ->125B 0.60199
122B ->126B 0.20041

Excited State 20: 2.493-A 4.3937 eV 282.19 nm f=0.0066 <S**2>=1.303
120A ->125A 0.17072
122A ->125A -0.18660
123A ->125A 0.26684
123A ->129A 0.11093
124A ->127A -0.22627
124A ->130A 0.10415
109B ->124B 0.17477
113B ->124B -0.20257
116B ->124B 0.15090
117B ->124B 0.59730
118B ->124B 0.18013
119B ->124B 0.15438
120B ->125B -0.12346
122B ->125B -0.23508
122B ->129B -0.11376
123B ->127B -0.23371
123B ->130B -0.11375

Excited State 21: 2.499-A 4.3992 eV 281.83 nm f=0.0073 <S**2>=1.312
120A ->125A 0.13254
123A ->125A 0.16497
123A ->129A 0.14261
124A ->127A 0.55932
124A ->128A -0.13164
120B ->125B -0.12799
122B ->125B -0.33934
122B ->129B -0.11184
123B ->127B 0.57191
123B ->128B -0.19824
123B ->130B -0.13779

Excited State 22: 2.755-A 4.4012 eV 281.70 nm f=0.0050 <S**2>=1.648
120A ->125A -0.14202
122A ->125A -0.20509
123A ->125A -0.25672
123A ->129A -0.14661
124A ->127A 0.28081
124A ->128A -0.12335
124A ->130A -0.15068
124A ->131A 0.12174
109B ->124B 0.10976
113B ->124B -0.16726
116B ->124B 0.10157
117B ->124B 0.46633
118B ->124B 0.16064
119B ->124B 0.10228
120B ->125B 0.16950
120B ->126B 0.11166
122B ->125B 0.38183
122B ->129B 0.17061
123B ->127B 0.28237
123B ->130B 0.14803

Excited State 23: 3.453-A 4.4892 eV 276.19 nm f=0.0002 <S**2>=2.730
120A ->125A 0.19574
120A ->126A 0.14525
123A ->125A 0.24515
123A ->126A 0.27008
123A ->127A -0.20151
123A ->129A -0.33185
123A ->130A 0.11087
124A ->128A -0.11320
124A ->130A -0.22671
124A ->131A 0.19762
120B ->125B -0.18624
120B ->126B -0.14278
122B ->125B -0.31505
122B ->126B -0.26192
122B ->127B 0.19872
122B ->129B 0.33516
122B ->130B -0.10184
123B ->128B 0.11135
123B ->130B 0.25763
123B ->131B -0.15981

Excited State 24: 3.440-A 4.5301 eV 273.69 nm f=0.0002 <S**2>=2.709
122A ->125A -0.13729
124A ->127A 0.48119
124A ->128A -0.22418
124A ->129A -0.40089
124A ->130A 0.16485
123B ->127B -0.46161
123B ->128B 0.22163
123B ->129B 0.40453
123B ->130B -0.16186

Excited State 25: 2.082-A 4.5345 eV 273.42 nm f=0.0092 <S**2>=0.833
121A ->125A -0.11181
122A ->125A 0.37996
122A ->126A 0.14209
105B ->124B 0.15826
108B ->124B -0.30908
109B ->124B -0.21476
112B ->124B 0.22426
113B ->124B -0.12975
114B ->124B -0.10280
115B ->124B -0.12525
116B ->124B -0.32054
118B ->124B 0.62984

Excited State 26: 2.262-A 4.5541 eV 272.25 nm f=0.0099 <S**2>=1.029
121A ->125A -0.20454
122A ->125A 0.76803
123A ->126A 0.14103
109B ->124B 0.28469
116B ->124B 0.23691
117B ->124B 0.17748
118B ->124B -0.17025
119B ->124B 0.18896

Excited State 27: 2.067-A 4.6177 eV 268.50 nm f=0.0113 <S**2>=0.818
122A ->125A -0.13943
122A ->126A 0.10192
123A ->126A -0.16007
103B ->124B -0.17377
104B ->124B -0.17066
108B ->124B -0.23122
109B ->124B 0.45031
110B ->124B -0.12286
112B ->124B 0.31129
113B ->124B 0.17798
115B ->124B 0.23925
116B ->124B 0.10422
117B ->124B -0.37344
118B ->124B 0.15621
119B ->124B 0.39901

Excited State 28: 2.180-A 4.6265 eV 267.99 nm f=0.0010 <S**2>=0.939
122A ->125A -0.12642
123A ->125A -0.24541
123A ->126A 0.73546
108B ->124B -0.18002
117B ->124B -0.11239
118B ->124B 0.16380
122B ->125B -0.13024
122B ->126B 0.44890

Excited State 29: 2.988-A 4.6623 eV 265.93 nm f=0.0093 <S**2>=1.982
117A ->126A 0.12713
119A ->125A 0.17806

```
  119A ->126A       -0.11610
  123A ->126A       -0.18061
  108B ->124B       -0.12867
  112B ->124B       -0.15866
  116B ->124B        0.10152
  117B ->126B        0.10690
  118B ->125B       -0.15927
  118B ->126B        0.11223
  123B ->127B        0.27795
  123B ->128B        0.77410

Excited State  30:  2.629-A     4.6680 eV  265.60 nm  f=0.0070  <S**2>=1.477
  117A ->126A       -0.10970
  119A ->125A       -0.15499
  123A ->126A       -0.12257
  124A ->127A        0.22518
  124A ->128A        0.69662
  117B ->126B       -0.10586
  118B ->125B        0.15439
  118B ->126B       -0.10441
  122B ->126B        0.29191
  123B ->128B        0.34414
```

- Phenolate form, equatorial positioning of the phenolate, exogeneous ligand = water.

```
Excited State   1:  2.005-A     1.0839 eV 1143.89 nm  f=0.0021  <S**2>=0.755
  107B ->124B        0.21778
  108B ->124B        0.15635
  117B ->124B        0.14772
  120B ->124B        0.30618
  121B ->124B        0.61461
  123B ->124B        0.60480
 This state for optimization and/or second-order correction.
 Total Energy, E(TD-HF/TD-KS) =  -2926.85255517
 Copying the excited state density for this state as the 1-particle RhoCI density.

Excited State   2:  2.004-A     1.6239 eV  763.47 nm  f=0.0008  <S**2>=0.754
  106B ->124B        0.16105
  108B ->124B        0.35679
  113B ->124B       -0.16601
  115B ->124B       -0.13302
  117B ->124B       -0.40821
  120B ->124B        0.68714
  123B ->124B       -0.29419

Excited State   3:  2.002-A     1.9318 eV  641.82 nm  f=0.0007  <S**2>=0.752
  111B ->124B        0.10187
  112B ->124B        0.34750
  113B ->124B       -0.13216
  115B ->124B        0.66445
  116B ->124B        0.51898
  117B ->124B       -0.17719
  118B ->124B       -0.17935

Excited State   4:  2.012-A     2.0484 eV  605.28 nm  f=0.0128  <S**2>=0.762
  103B ->124B       -0.12077
  104B ->124B       -0.10214
  106B ->124B       -0.41492
  107B ->124B       -0.18934
  109B ->124B       -0.31338
  111B ->124B       -0.33088
  113B ->124B       -0.16207
  115B ->124B       -0.15815
  117B ->124B       -0.43883
  121B ->124B       -0.19752
  123B ->124B        0.43965

Excited State   5:  2.022-A     2.1533 eV  575.78 nm  f=0.0454  <S**2>=0.772
  106B ->124B        0.50898
  107B ->124B       -0.11486
  109B ->124B        0.19493
  111B ->124B        0.27485
  113B ->124B       -0.10147
  121B ->124B       -0.46216
  123B ->124B        0.57750

Excited State   6:  3.141-A     2.9521 eV  419.98 nm  f=0.0006  <S**2>=2.217
  124A ->125A        0.92922
  123B ->125B       -0.32678

Excited State   7:  2.373-A     2.9836 eV  415.55 nm  f=0.0046  <S**2>=1.158
  124A ->125A        0.33793
  123B ->125B        0.92957

Excited State   8:  2.046-A     3.0873 eV  401.60 nm  f=0.0021  <S**2>=0.797
```

122B ->124B 0.99133

Excited State 9: 3.382-A 3.4026 eV 364.38 nm f=0.0001 <S**2>=2.609
124A ->126A 0.70060
124A ->129A -0.14190
124A ->131A 0.13144
123B ->125B 0.10154
123B ->126B -0.61668
123B ->129B 0.13721
123B ->131B -0.12944

Excited State 10: 2.030-A 3.4431 eV 360.10 nm f=0.0053 <S**2>=0.780
124A ->126A 0.64519
123B ->126B 0.74101
123B ->127B 0.12245

Excited State 11: 3.390-A 3.5384 eV 350.39 nm f=0.0000 <S**2>=2.623
123A ->129A -0.24634
124A ->126A -0.19478
124A ->127A -0.34623
124A ->128A 0.12704
124A ->129A -0.22586
124A ->131A 0.42679
122B ->129B 0.24462
123B ->126B 0.12242
123B ->127B 0.36698
123B ->128B -0.12362
123B ->129B 0.22489
123B ->131B -0.41255

Excited State 12: 2.079-A 3.6262 eV 341.92 nm f=0.0519 <S**2>=0.831
124A ->127A 0.38810
106B ->124B -0.34216
107B ->124B 0.15909
108B ->124B -0.16461
113B ->124B 0.12916
115B ->124B 0.13084
117B ->124B 0.32593
119B ->124B -0.11923
120B ->124B 0.47845
121B ->124B -0.46215
123B ->127B 0.14355

Excited State 13: 3.260-A 3.6616 eV 338.61 nm f=0.0003 <S**2>=2.407
123A ->129A 0.18317
124A ->127A -0.23747
124A ->129A -0.10838
124A ->131A -0.31340
122B ->129B -0.18476
123B ->126B -0.13023
123B ->127B 0.76942
123B ->129B 0.11348
123B ->131B 0.29749

Excited State 14: 2.215-A 3.6799 eV 336.92 nm f=0.0258 <S**2>=0.977
124A ->126A -0.12514
124A ->127A 0.76145
124A ->131A 0.15370
106B ->124B 0.14977
117B ->124B -0.14598
120B ->124B -0.21380
121B ->124B 0.21710
123B ->127B 0.41018
123B ->131B -0.11572

Excited State 15: 3.357-A 3.8184 eV 324.70 nm f=0.0002 <S**2>=2.568
118A ->127A -0.13626
122A ->125A 0.19300
124A ->126A 0.11468
124A ->127A -0.21288
124A ->129A 0.55641
124A ->130A -0.11550
124A ->131A 0.13090
118B ->127B 0.13661
119B ->124B -0.11890
123B ->126B -0.10094
123B ->127B 0.21216
123B ->129B -0.54098
123B ->130B 0.12220
123B ->131B -0.11093

Excited State 16: 3.386-A 3.8286 eV 323.84 nm f=0.0001 <S**2>=2.617
114A ->125A 0.14298
117A ->125A 0.13181
117A ->126A 0.21019
117A ->127A 0.14954
118A ->126A -0.13114

118A ->127A 0.17654
118A ->128A 0.13294
120A ->125A -0.10291
121A ->125A -0.11750
121A ->126A -0.15646
121A ->127A 0.17563
121A ->128A -0.35535
122A ->125A -0.19598
124A ->129A 0.13005
113B ->125B -0.10842
115B ->125B -0.14112
116B ->126B 0.14580
117B ->126B 0.13858
117B ->127B 0.10564
118B ->126B 0.13625
118B ->127B -0.17176
118B ->128B -0.12952
119B ->124B -0.11995
119B ->125B 0.10289
119B ->126B 0.15526
119B ->127B -0.17616
119B ->128B 0.35591
120B ->125B 0.11338
121B ->125B 0.11809
123B ->129B -0.12436

Excited State 17: 3.199-A 3.8573 eV 321.43 nm f=0.0013 <S**2>=2.308
114A ->125A -0.12419
115A ->125A -0.10327
117A ->126A 0.18231
118A ->126A 0.11110
118A ->127A -0.24163
121A ->128A -0.28523
122A ->125A 0.41644
124A ->127A 0.16860
124A ->129A -0.19970
112B ->125B -0.10827
115B ->126B -0.11211
116B ->126B 0.10067
117B ->125B 0.12731
118B ->126B -0.10769
118B ->127B 0.23945
119B ->124B -0.27135
119B ->128B 0.28325
120B ->125B -0.11944
123B ->127B -0.12233
123B ->129B 0.19783

Excited State 18: 2.223-A 3.8931 eV 318.47 nm f=0.0005 <S**2>=0.986
121A ->128A -0.12202
122A ->125A 0.18405
119B ->124B 0.92026
119B ->128B 0.12586
120B ->124B 0.11619

Excited State 19: 2.748-A 3.9671 eV 312.53 nm f=0.0057 <S**2>=1.638
114A ->125A 0.15119
118A ->126A -0.13570
118A ->127A 0.22836
119A ->125A -0.20026
122A ->125A 0.76694
123A ->125A -0.22468
118B ->126B 0.14311
118B ->127B -0.22702
120B ->125B 0.12117

Excited State 20: 3.444-A 4.0644 eV 305.05 nm f=0.0000 <S**2>=2.715
121A ->125A 0.28445
121A ->126A 0.35227
121A ->127A 0.23769
123A ->125A -0.33199
123A ->126A -0.14858
124A ->128A 0.23940
119B ->125B -0.28205
119B ->126B -0.33319
119B ->127B -0.23993
122B ->125B 0.29941
122B ->126B 0.14460
123B ->128B -0.29182

Excited State 21: 2.062-A 4.1054 eV 302.00 nm f=0.0029 <S**2>=0.813
124A ->128A 0.62815
123B ->128B 0.76253

Excited State 22: 3.374-A 4.1240 eV 300.64 nm f=0.0000 <S**2>=2.596
118A ->125A -0.16829
121A ->125A -0.18379

121A ->126A -0.13869
121A ->127A -0.13051
124A ->128A 0.62239
124A ->129A 0.11324
118B ->124B 0.15654
118B ->125B 0.14962
119B ->125B 0.18945
119B ->126B 0.13430
119B ->127B 0.13348
121B ->125B -0.10401
123B ->128B -0.50584
123B ->129B -0.11410

Excited State 23: 3.265-A 4.1417 eV 299.35 nm f=0.0009 <S**2>=2.416
118A ->125A 0.47887
118A ->126A -0.12763
121A ->125A 0.13728
123A ->125A 0.30158
124A ->128A 0.29944
118B ->124B -0.40681
118B ->125B -0.42955
118B ->126B 0.12997
119B ->124B 0.10464
119B ->125B -0.13936
121B ->125B 0.13775
122B ->125B -0.19004
123B ->128B -0.13583

Excited State 24: 3.210-A 4.1897 eV 295.93 nm f=0.0031 <S**2>=2.326
120A ->125A -0.13668
121A ->126A -0.12296
121A ->127A -0.11892
123A ->125A -0.41387
119B ->127B 0.10379
120B ->125B 0.25654
120B ->126B 0.14036
121B ->125B 0.67213
121B ->126B 0.15352
122B ->125B 0.22639

Excited State 25: 2.120-A 4.2013 eV 295.11 nm f=0.0115 <S**2>=0.873
122A ->125A 0.19261
123A ->125A 0.67046
121B ->125B 0.16232
122B ->125B 0.66101

Excited State 26: 3.283-A 4.2353 eV 292.74 nm f=0.0017 <S**2>=2.444
118A ->125A 0.20564
121A ->126A -0.26218
122A ->125A -0.12651
123A ->125A -0.23155
123A ->129A 0.11234
124A ->131A 0.14059
118B ->124B -0.21090
118B ->125B -0.18571
119B ->125B 0.11017
119B ->126B 0.26572
119B ->127B 0.10720
120B ->125B -0.14142
121B ->125B -0.41906
122B ->125B 0.53709
122B ->129B -0.11311
123B ->131B -0.11917

Excited State 27: 3.398-A 4.4302 eV 279.86 nm f=0.0015 <S**2>=2.637
123A ->125A -0.20636
123A ->126A 0.23088
123A ->129A -0.48028
123A ->130A 0.10255
124A ->131A -0.30956
116B ->124B -0.11259
122B ->125B 0.27124
122B ->126B -0.20966
122B ->129B 0.48194
122B ->130B -0.11006
123B ->131B 0.27745

Excited State 28: 2.779-A 4.4679 eV 277.50 nm f=0.0023 <S**2>=1.681
118A ->125A 0.20011
120A ->125A -0.34525
120A ->126A -0.23779
120A ->127A -0.11769
122A ->126A 0.14571
118B ->124B 0.53012
118B ->125B -0.22484
119B ->125B -0.10093
120B ->125B 0.13127

120B ->126B 0.20788
120B ->127B 0.11948
121B ->125B -0.30840
121B ->126B 0.31544
121B ->127B 0.14154

Excited State 29: 2.634-A 4.4734 eV 277.16 nm f=0.0021 <S**2>=1.484
118A ->125A 0.21700
120A ->125A 0.26317
120A ->126A 0.20305
121A ->125A 0.11598
122A ->126A -0.21423
116B ->124B 0.11191
118B ->124B 0.63210
118B ->125B -0.22365
119B ->126B 0.11054
120B ->125B -0.18908
120B ->126B -0.16948
121B ->125B 0.29865
121B ->126B -0.24055

Excited State 30: 2.534-A 4.5072 eV 275.08 nm f=0.0032 <S**2>=1.356
119A ->125A 0.12050
120A ->125A -0.17658
122A ->126A 0.82078
123A ->126A -0.22778
120B ->125B -0.28608
120B ->126B -0.13967
121B ->126B -0.21195