Theoretical Study of the Copper Complexes with Lipoic and Dihydrolipoic Acids

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Electronic Supplementary Information

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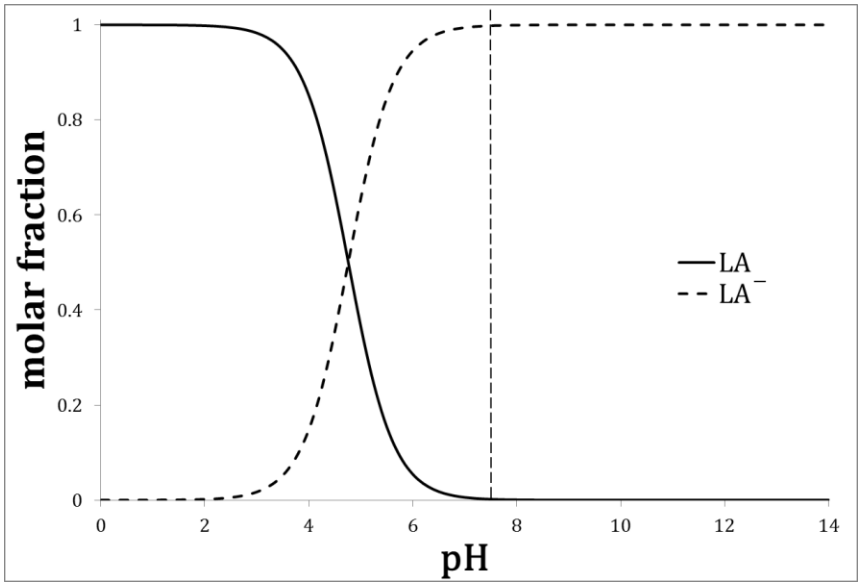

Figure S1. Distribution diagram for the acid/base species of LA as a function of pH.

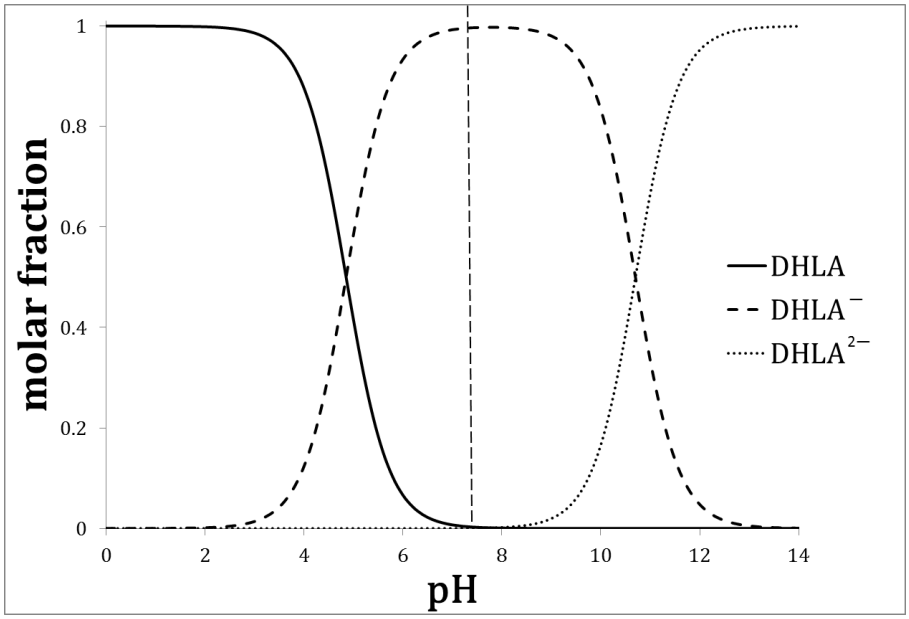

Figure S2. Distribution diagram for the acid/base species of DHLA as a function of pH.

Table S1. Absolute enthalpies and Gibbs free energies of the different species considered in this study at the M06-2X-SMD/6-31++G(d,p) level of theory in water at 298.15 K.

	Species	H° (au)	G° (au)
[1]	Cu^{2+} – LA^{-} (CO)	-3128.447001	-3128.523818
[2]	Cu^{2+} – LA^{-} (COO)	-3052.047687	-3052.121095
[3]	Cu^{2+} – LA^{-} (CO, S2 *trans*)	-3052.040074	-3052.106314
[4]	Cu^{2+} – LA^{-} (CO, S1 *cis*)	-3052.038496	-3052.105204
[5]	Cu^{2+} – LA^{-} (CO, S2 *cis*)	-3052.036201	-3052.101857
[6]	Cu^{2+} – LA^{-} (S1)	-3128.409631	-3128.486437
[7]	Cu^{2+} – LA^{-} (S2)	-3128.405430	-3128.481366
[8]	Cu^{2+} – $DHLA^{-}$ (CO)	-3129.621696	-3129.699254
[9]	Cu^{2+} – $DHLA^{-}$ (COO)	-3053.223720	-3053.296113
[10]	Cu^{2+} – $DHLA^{-}$ (CO, S2 *cis*)	-3053.221427	-3053.290923
[11]	Cu^{2+} – $DHLA^{-}$ (CO, S2 *trans*)	-3053.215262	-3053.283538
[12]	Cu^{2+} – $DHLA^{-}$ (CO, S1 *cis*)	-3053.207391	-3053.277178
[13]	Cu^{2+} – $DHLA^{-}$ (CO, S1 *trans*)	-3053.207375	-3053.276666
[14]	Cu^{2+} – $DHLA^{-}$ (S1)	-3129.584080	-3129.665061
[15]	Cu^{2+} – $DHLA^{-}$ (CO, S1, S2)	-2976.806770	-2976.868901
[16]	Cu^{2+} – $DHLA^{-}$ (S2)	-3129.581771	-3129.660084
[17]	Cu^{2+} – $DHLA^{-}$ (S1, S2 *cis*)	-3053.182286	-3053.253664
[18]	Cu^{2+} – $DHLA^{2-}$ (CO, S1 *trans*)	-3052.777637	-3052.847064
[19]	Cu^{2+} – $DHLA^{2-}$ (CO, S1 cis)	-3052.774480	-3052.844820
[20]	Cu^{2+} – $DHLA^{2-}$ (S1)	-3129.157314	-3129.236924
[21]	Cu^{2+} – $DHLA^{2-}$ (CO)	-3129.156156	-3129.232134
[22]	Cu^{2+} – $DHLA^{2-}$ (COO)	-3052.757973	-3052.829271
[23]	Cu^{2+} – $DHLA^{2-}$ (CO, S2 cis)	-3052.787975	-3052.857491
[24]	Cu^{2+} – $DHLA^{2-}$ (CO, S2 trans)	-3052.783826	-3052.851908
[25]	Cu^{2+} – $DHLA^{2-}$ (CO)	-3129.174664	-3129.249725
[26]	Cu^{2+} – $DHLA^{2-}$ (COO, S2)	-2976.384686	-2976.448570
[27]	Cu^{2+} – $DHLA^{2-}$ (S2)	-3129.157881	-3129.235813
[28]	Cu^{2+} – $DHLA^{2-}$ (COO)	-3052.757780	-3052.829498
[29]	Cu^{+} – $DHLA^{2-}$ (COO)	-3052.927833	-3053.001687
[30]	$[Cu(H_2O)_2]^{+} \cdot 2H_2O$	-1945.717783	-1945.773093
[31]	$[Cu(H_2O)_4]^{2+}$	-1945.577002	-1945.624279
[32]	$(H_2O)_2$	-152.771849	-152.804083
[33]	$(H_2O)_3$	-229.158963	-229.200715
[34]	LA^{-}	-1259.227997	-1259.284568
[35]	$DHLA^{-}$	-1260.404853	-1260.464494
[36]	S1-deprotonated $DHLA^{2-}$	-1259.937581	-1259.996159
[37]	S2-deprotonated $DHLA^{2-}$	-1259.936736	-1259.995440

M06-2X-SMD/6-31++G(d,p) Cartesian coordinates of the optimized geometries in water of the species calculated in this study.

[1] Cu^{2+} – LA^{-} (CO)

Charge = 1 Multiplicity = 2

C	-6.94300400	-0.52599400	0.31624800
H	-7.23375000	0.00992700	1.22388100
H	-7.76049600	-1.18082600	0.00493100
C	-5.63529200	-1.28199100	0.49670200
H	-5.44577700	-1.89068200	-0.39407200
H	-5.69997100	-1.95192800	1.36048800
C	-4.46148300	-0.31851300	0.70829900
H	-4.41628800	-0.01852000	1.75987800
S	-6.65363500	0.66611500	-1.03197500
S	-4.81454100	1.26857500	-0.20795200
C	-3.12554500	-0.92078700	0.28822700
H	-3.02217100	-1.88534800	0.80487400
H	-3.15414500	-1.13294400	-0.78857600
C	-1.92432300	-0.04110200	0.62016100
H	-2.02468000	0.92594100	0.10754700
H	-1.91836200	0.17200000	1.69780600
C	-0.59676000	-0.68128700	0.22063300
H	-0.60617300	-0.90520000	-0.85318900
H	-0.47808300	-1.63747300	0.74350800
C	0.57956300	0.23118500	0.53983900
H	0.46969300	1.19827200	0.03626900
H	0.61561500	0.45162200	1.61468800
C	1.94100300	-0.31568200	0.16924500
O	2.91627500	0.50812800	0.28059900
O	2.06657600	-1.50735600	-0.20689100
Cu	4.82809600	0.14924900	-0.07953300
O	4.56803900	-1.75325300	-0.69887700
H	3.57582700	-1.83169200	-0.51709200
H	5.02242900	-2.37013400	-0.10708500
O	6.83249400	-0.00710700	-0.36550700
H	7.21236200	0.81096500	-0.72019900
H	7.04533800	-0.70174100	-1.00687600
O	5.10660400	2.14113300	0.38835700
H	5.95225400	2.29998900	0.83407200
H	4.41754500	2.42719900	1.00685800

[2] Cu^{2+} – LA^{-} (COO)

Charge = 1 Multiplicity = 2

C	6.38013200	0.91951400	0.26465800
H	6.77184200	0.43709900	1.16423300
H	7.08235700	1.68650100	-0.07134400
C	4.97930900	1.47297200	0.47986300
H	4.68102800	2.04577300	-0.40491300
H	4.96514300	2.14687800	1.34286700
C	3.96474200	0.34640700	0.71707000
H	3.97438700	0.05830800	1.77279000
S	6.23285900	-0.31050900	-1.07255200
S	4.54369800	-1.18444100	-0.17895000
C	2.55041700	0.73909300	0.30599600
H	2.31373200	1.68717000	0.80936200
H	2.53541000	0.93544300	-0.77413900
C	1.49192700	-0.29834600	0.66782000
H	1.71365000	-1.24531400	0.15647400

H	1.53673600	-0.50217200	1.74624000
C	0.08313900	0.15608500	0.29537700
H	0.04087600	0.37880000	-0.77785600
H	-0.15294100	1.08663900	0.82385400
C	-0.95924200	-0.90370500	0.63479700
H	-0.75502200	-1.84638000	0.11724000
H	-0.93992300	-1.12973100	1.70961100
C	-2.37382400	-0.50762200	0.32259300
O	-3.28909900	-1.39216100	0.24059400
O	-2.70724700	0.71002400	0.16188400
Cu	-4.65431800	0.11426300	-0.10401900
O	-5.55420000	1.86541900	-0.56408900
H	-5.04613400	2.61148100	-0.21090600
H	-6.43580700	1.93041200	-0.16664900
O	-6.33318400	-1.00915500	-0.34148300
H	-7.12396900	-0.53979900	-0.03613100
H	-6.27916800	-1.81781400	0.18958400

[3] Cu^{2+} – LA^{-} (CO, S2 *trans*)

Charge = 1 Multiplicity = 2

C	-3.27328600	0.46660900	0.30521300
H	-4.02762900	0.92157800	-0.34071100
H	-3.76548600	-0.18537200	1.03094000
C	-2.38603200	1.50985700	0.98030500
H	-1.93024600	1.05914400	1.86680400
H	-3.00813500	2.34511100	1.31382900
C	-1.24307700	2.03357800	0.07236200
H	-1.42162900	3.07275300	-0.22175100
S	-2.21323800	-0.57193100	-0.75616900
S	-1.27797800	1.11812600	-1.54161900
C	0.10175700	1.89995400	0.77784300
H	0.00737400	2.39825300	1.75285100
H	0.26601900	0.83780200	0.99316300
C	1.30503900	2.48747600	0.03852000
H	1.28457800	2.17495500	-1.01468700
H	1.21732200	3.57959800	0.03640800
C	2.64356100	2.05677500	0.67249500
H	2.47194600	1.73918000	1.70760400
H	3.33581300	2.90223600	0.71688500
C	3.34841200	0.92989000	-0.09878300
H	3.71672300	1.30052800	-1.05826400
H	4.20527400	0.56135800	0.47621600
C	2.43434700	-0.24571300	-0.37303000
O	1.86138000	-0.78953100	0.63211600
O	2.27104600	-0.63167600	-1.56288300
Cu	0.08467000	-1.72135900	0.44742200
O	-0.49557700	-1.33481700	2.31367800
H	0.23430000	-0.94877300	2.82393000
H	-0.75582900	-2.14260500	2.78310300
O	0.37893800	-2.28787000	-1.41566700
H	0.66550200	-3.21286700	-1.44397300
H	1.19752100	-1.70197400	-1.62049000

[4] Cu^{2+} – LA^{-} (CO, S1 *cis*)

Charge = 1 Multiplicity = 2

C	-2.19847300	-2.13451600	-1.15494500
H	-2.65435500	-3.06759500	-0.82051100
H	-2.38329800	-1.99729200	-2.22136200
C	-0.71159400	-2.09347600	-0.82844400
H	-0.22627400	-1.28183700	-1.37290100
H	-0.26082200	-3.04533300	-1.12978800
C	-0.54969800	-1.90552700	0.67901200
H	-1.10823600	-2.70779900	1.17380000

S	-3.05730900	-0.75441600	-0.27164500
S	-1.47687600	-0.36212100	1.07023800
C	0.85089300	-1.82180800	1.31919800
H	1.17825900	-0.78261700	1.41239400
H	0.74752200	-2.19231500	2.34333000
C	1.93762800	-2.64488900	0.61290200
H	2.74279000	-2.80784500	1.33959200
H	1.53784100	-3.63725200	0.37072600
C	2.56616000	-2.03396700	-0.64804100
H	1.82762700	-1.91733100	-1.44527800
H	3.30871600	-2.74864700	-1.01917800
C	3.28183600	-0.70137100	-0.42394700
H	3.94669900	-0.74879800	0.44545100
H	3.92227500	-0.47569400	-1.28610000
C	2.40008900	0.52079000	-0.25141700
O	1.19208700	0.43854700	-0.67492900
O	2.88686200	1.55360000	0.26827400
Cu	-0.26904100	1.59574300	-0.13849300
O	0.92298400	3.27643100	-0.13311000
H	1.77835000	2.82430200	0.10373100
H	0.68917700	3.86240300	0.60097600
O	-1.98463400	2.60992600	0.18373600
H	-2.52052800	2.63753200	-0.62466800
H	-1.77602400	3.53471900	0.39091500

[5] Cu^{2+} – LA^{-} (CO, S2 *cis*)

Charge = 1 Multiplicity = 2

C	-0.36805000	-2.38407700	1.46413400
H	-0.61775400	-3.44711500	1.42869100
H	0.07518200	-2.14170600	2.43298900
C	-1.53556700	-1.47375400	1.11871700
H	-1.22959600	-0.45529100	1.34248900
H	-2.39846000	-1.72878600	1.74201800
C	-1.93736500	-1.56070300	-0.36781700
H	-2.72630400	-2.30908800	-0.48685300
S	0.89620800	-2.08772600	0.18251100
S	-0.51476900	-2.26927700	-1.34236000
C	-2.38400000	-0.24121400	-1.00955100
H	-1.50157600	0.37153700	-1.21735400
H	-2.81582800	-0.48616800	-1.98550800
C	-3.41647700	0.56241900	-0.20104700
H	-4.01565300	1.14016900	-0.91486000
H	-4.11287800	-0.12810700	0.29162600
C	-2.87359100	1.55773200	0.83849400
H	-2.39117100	1.05302300	1.67872800
H	-3.73754000	2.08242800	1.26048400
C	-1.93382300	2.62137200	0.26924600
H	-2.34069700	3.04802400	-0.65385500
H	-1.85353900	3.45459700	0.97944400
C	-0.49520900	2.22998900	-0.01887100
O	0.00445600	1.22705700	0.60692500
O	0.15447300	2.93824900	-0.82901900
Cu	1.74094900	0.38228200	0.20032900
O	2.56256300	2.19363500	-0.27658000
H	1.72778800	2.62996600	-0.62573400
H	3.18983200	2.12717800	-1.01091200
O	3.50323900	-0.54855700	-0.06481200
H	3.82178800	-1.02671900	0.71665400
H	4.20249500	0.08826900	-0.28195800

[6] Cu^{2+} – LA^{-} (S1)

Charge = 1 Multiplicity = 2

C	3.58530500	-2.21012200	-0.52251000

H	3.76069500	-1.96921100	-1.57156400
H	4.36663300	-2.88023400	-0.16251100
C	2.19233600	-2.79324900	-0.31435000
H	2.13122700	-3.32697400	0.63951700
H	1.97951300	-3.50211300	-1.12121000
C	1.15944600	-1.67645500	-0.34845000
H	1.23227500	-1.12462700	-1.29183700
S	3.74401700	-0.62485700	0.42593200
S	1.71422400	-0.51118600	0.97899600
C	-0.28063100	-2.09649700	-0.09777800
H	-0.55609900	-2.76143900	-0.92569200
H	-0.34466300	-2.68358800	0.82667700
C	-1.24738300	-0.91261000	-0.04720500
H	-1.09238700	-0.34809800	0.88377700
H	-1.02443600	-0.22438100	-0.87747700
C	-2.71022700	-1.34320300	-0.11159300
H	-2.91594100	-2.04585500	0.70502400
H	-2.88515600	-1.88721800	-1.04750700
C	-3.65994900	-0.15626900	-0.02014100
H	-3.49424400	0.39256400	0.91606700
H	-3.45596800	0.55784000	-0.82770900
C	-5.14989900	-0.49462200	-0.07972000
O	-5.95591700	0.48448600	-0.06308100
O	-5.50309000	-1.70562600	-0.13626500
Cu	0.83153600	1.71641200	-0.01715000
O	-0.28405100	2.07441700	1.60848000
H	-0.33797900	1.41722400	2.31911800
H	-0.01317700	2.90522900	2.03016400
O	0.11130900	3.46808600	-0.77066500
H	-0.07704200	4.12994400	-0.08788900
H	0.73339000	3.88598800	-1.38512500
O	1.93242700	1.28719000	-1.64184200
H	2.86171300	1.07654300	-1.44672000
H	1.94585800	2.01890500	-2.27913900

[7] Cu^{2+} – LA^{-} (S2)

Charge = 1 Multiplicity = 2

C	-1.48054600	1.90254100	0.86600800
H	-2.29372400	2.47311700	1.31948500
H	-1.18360500	1.08287200	1.52483100
C	-0.30715000	2.78297500	0.46325600
H	0.18879300	3.16586000	1.36073900
H	-0.68051900	3.63627800	-0.10908100
C	0.71800600	2.00039000	-0.37078700
H	1.19170700	2.67205500	-1.09161700
S	-2.11178500	1.21947700	-0.70669300
S	-0.18956600	0.72417600	-1.39544700
C	1.79751300	1.31393200	0.46051400
H	2.28301600	2.10082100	1.05273300
H	1.33530500	0.61203100	1.16678300
C	2.85550300	0.60868200	-0.38425100
H	2.40365100	-0.23437000	-0.92571000
H	3.22660200	1.30949900	-1.14493900
C	4.03121000	0.09965600	0.44729100
H	3.66658300	-0.59923500	1.21035800
H	4.48483700	0.94195000	0.98339400
C	5.08336000	-0.58327300	-0.41611200
H	4.64524000	-1.43347800	-0.95309200
H	5.44259300	0.10752300	-1.18994000
C	6.31861200	-1.10071100	0.32051600
O	7.16941800	-1.73248000	-0.37638800
O	6.43788400	-0.87522800	1.55763200
Cu	-3.38770500	-0.91406800	0.12491600
O	-2.24165300	-2.15980000	-0.92597000
H	-2.37705500	-2.12342200	-1.88570400

H	-1.28760300	-2.06750900	-0.77722000
O	-4.75241300	-2.37424000	0.43336600
H	-4.33909300	-3.25044000	0.46253800
H	-5.22638100	-2.26854300	1.27205000
O	-4.29473400	0.44782700	1.28555700
H	-3.85533500	0.51581500	2.14888000
H	-5.20699600	0.17493800	1.47501300

[8] Cu^{2+} – $DHLA^{-}$ (CO)

Charge = 1 Multiplicity = 2

C	-0.68777900	-3.23227500	-0.17773400
H	-1.03066900	-4.16244000	0.28135000
H	-0.68720000	-3.34922100	-1.26507400
C	0.73805100	-2.91464000	0.30470000
H	1.37179800	-3.77448500	0.05972700
H	0.74128300	-2.81910200	1.39777800
C	1.33503300	-1.65578000	-0.32327800
H	0.74888800	-0.77885600	-0.01837700
H	1.25808600	-1.72140000	-1.41778200
C	2.79860400	-1.46644000	0.07622900
H	3.35082100	-2.38877900	-0.14050100
C	3.47736500	-0.31110600	-0.66670900
C	2.74440200	1.03102400	-0.55930400
H	1.80554400	0.94376800	-1.12144500
H	3.33391300	1.80713600	-1.05983500
H	3.54305700	-0.57394000	-1.72683100
C	-1.64953500	-2.12692400	0.19998100
O	-2.22235100	-2.15627300	1.31721200
O	-1.79977300	-1.18228900	-0.65514900
C	2.43879200	1.46434200	0.86848900
H	1.84413100	0.71716000	1.39841000
H	3.36001500	1.61939700	1.43674400
H	2.86369800	-1.30734300	1.16083100
S	1.55355500	3.06234700	0.94617600
H	0.48150000	2.67054000	0.23465900
S	5.20815900	-0.20688300	-0.03907800
H	5.61946300	0.76205700	-0.87490400
Cu	-2.76287400	0.50761300	-0.33431700
O	-1.34495800	1.38962700	-1.51122300
H	-1.22552700	2.33241600	-1.32245700
H	-0.48315600	0.96870500	-1.36642800
O	-3.72375200	2.28089600	-0.14503200
H	-3.66440900	2.81075900	-0.95450200
H	-4.66963300	2.15908800	0.02779100
O	-4.13957300	-0.35954800	0.89644000
H	-4.38723100	0.23860700	1.61669800
H	-3.56480600	-1.07078600	1.28353800

[9] Cu^{2+} – $DHLA^{-}$ (COO)

Charge = 1 Multiplicity = 2

C	0.63304900	-3.19684900	0.19295700
H	1.10054000	-3.97995800	-0.41035400
H	0.59272200	-3.52180700	1.23500900
C	-0.77738600	-2.88310900	-0.33748700
H	-1.39955000	-3.77779500	-0.23297500
H	-0.71291300	-2.65364800	-1.40771700
C	-1.40946300	-1.70468800	0.39910500
H	-0.71006800	-0.85873400	0.37229900
H	-1.54802700	-1.95899300	1.45876300
C	-2.73646300	-1.26246000	-0.21298300
H	-3.44403900	-2.09983100	-0.21224700
C	-3.36567200	-0.08159800	0.53917200
C	-2.39151100	1.06772500	0.82730400

H	-1.64861500	0.69607500	1.54342000
H	-2.92413300	1.88173100	1.33130600
H	-3.74798600	-0.44406400	1.49804500
C	1.47236100	-1.95474600	0.10195400
O	1.78506600	-1.46844100	-1.03347500
O	1.83045900	-1.31517700	1.14539500
C	-1.67914900	1.61356400	-0.40670100
H	-1.28082400	0.81530000	-1.03729600
H	-2.35910900	2.20694400	-1.02270400
H	-2.56955400	-0.99188200	-1.26395400
S	-0.29822700	2.73947100	0.01033500
H	0.52166900	1.79957100	0.52277600
S	-4.82490100	0.46636700	-0.44453400
H	-5.26040900	1.39675100	0.42203400
Cu	2.59632500	0.15990800	-0.03902500
O	3.02574800	1.55803300	1.36598100
H	3.16488600	1.13587700	2.22749100
H	3.84311200	2.03972000	1.16724800
O	3.23775300	1.25590300	-1.61131000
H	3.94282800	1.87492800	-1.36873800
H	3.60929400	0.67949500	-2.29616100

[10] Cu^{2+} – $DHLA^{-}$ (CO, S2 *cis*)

Charge = 1 Multiplicity = 2

C	-0.32042500	3.19297900	-0.58863600
H	-0.75145500	3.63636900	-1.49501100
H	-0.31810200	3.97605800	0.17590600
C	1.08492200	2.66828000	-0.85770700
H	1.69685500	3.47170700	-1.28183100
H	1.02809500	1.88321100	-1.61887700
C	1.75119300	2.11706900	0.40837900
H	0.99851200	1.57639100	0.99332300
H	2.07091000	2.95322800	1.03958500
C	2.94769700	1.18921200	0.11694200
H	3.88495600	1.67680100	0.40300000
C	2.86032400	-0.15415200	0.85493500
C	1.59127600	-0.96726300	0.55777700
H	0.73369200	-0.45434200	1.00954700
H	1.66869700	-1.94215000	1.05381400
H	2.88854000	0.03389200	1.93248900
C	-1.29683800	2.12209300	-0.13887500
O	-2.29593900	2.46885600	0.54124900
O	-1.06217200	0.91563100	-0.50170000
C	1.32108500	-1.17318600	-0.92577100
H	1.20707100	-0.22585500	-1.45648300
H	2.11408800	-1.74579000	-1.41098500
H	3.01676700	1.00076000	-0.96230800
S	-0.25754000	-2.03581800	-1.24617700
H	-0.09878800	-3.06132500	-0.38781800
S	4.39181900	-1.09127600	0.43465600
H	4.13463900	-2.16891600	1.19597200
Cu	-2.01780300	-0.69227600	0.06858700
O	-2.81583100	-2.51002200	0.47727500
H	-2.40362800	-2.91547400	1.25631800
H	-3.75385400	-2.40536100	0.70228400
O	-3.55357900	0.30022000	0.98079100
H	-4.36257700	0.21128700	0.45686300
H	-3.20184800	1.24135900	0.84633500

[11] Cu^{2+} – $DHLA^{-}$ (CO, S2 *trans*)

Charge = 1 Multiplicity = 2

C	2.09867600	2.76807900	0.09195100
H	2.74842300	3.20704700	0.85659600

H	2.16618500	3.38027300	-0.81071500
C	0.65217600	2.69855000	0.60785900
H	0.27206500	3.71753000	0.73843500
H	0.64754900	2.22435400	1.59694700
C	-0.26642000	1.91434300	-0.32986000
H	0.17288400	0.92309900	-0.50384400
H	-0.31563200	2.40948700	-1.30902600
C	-1.67463700	1.73301400	0.23389800
H	-2.12875500	2.71712700	0.40195700
C	-2.59152200	0.92686400	-0.69592200
C	-2.06044000	-0.46143900	-1.07369600
H	-1.09775000	-0.31717300	-1.57930500
H	-2.72825600	-0.91799300	-1.81105600
H	-2.72630800	1.49328600	-1.62194000
C	2.60107600	1.37471100	-0.22928200
O	3.04977100	1.10796800	-1.36788600
O	2.47572100	0.49382400	0.70270100
C	-1.90513400	-1.40415300	0.12161300
H	-1.60404900	-0.87440600	1.02720700
H	-2.82635300	-1.94976600	0.32655000
H	-1.60882700	1.24662100	1.21686500
S	-0.60137200	-2.64928700	-0.26214400
H	-0.69322100	-3.35871600	0.87990000
S	-4.23938600	0.82472800	0.12325200
H	-4.83298600	0.06952300	-0.81722200
Cu	1.36657000	-1.13119700	0.33321200
O	0.70151000	-0.90491100	2.22242600
H	0.30942700	-0.02267000	2.32880500
H	0.08107400	-1.53124600	2.62426500
O	1.99115900	-1.32968200	-1.55649300
H	2.54012500	-2.11867000	-1.67942800
H	2.57806600	-0.53745400	-1.67119200

[12] Cu^{2+} – $DHLA^{-}$ (CO, S1 *cis*)

Charge = 1 Multiplicity = 2

C	2.51509300	1.21004100	-0.91926800
H	3.23300400	1.61112200	-1.63746400
H	1.89374600	0.46418700	-1.43034800
C	1.63003600	2.34448500	-0.35746400
H	2.21625500	3.26736900	-0.32915300
H	1.36170400	2.13568700	0.68722400
C	0.36018400	2.55894400	-1.18330500
H	0.62845400	2.61080000	-2.24544000
H	-0.08072600	3.52790400	-0.92072900
C	-0.71693300	1.48493900	-0.99482700
H	-0.34816500	0.49045500	-1.27881400
C	-1.30966700	1.45791600	0.42444900
C	-2.81381700	1.16108200	0.45646700
H	-3.29149600	1.98326100	-0.09061100
H	-3.18250000	1.20375300	1.48694500
H	-1.16663900	2.44143000	0.88224100
C	3.24478600	0.52667000	0.21800800
O	4.36084700	0.93296900	0.58714100
O	2.63142300	-0.43787900	0.82611100
C	-3.22042300	-0.16169900	-0.18230100
H	-2.82913700	-0.25506300	-1.19767000
H	-2.86039500	-1.01890700	0.39299600
H	-1.54008400	1.71079200	-1.68325400
S	-5.03405800	-0.38477500	-0.22309100
H	-5.30470700	0.70087300	-0.96834500
S	-0.38720200	0.32335600	1.58562800
H	-1.41578300	-0.47958100	1.91892500
Cu	1.03739100	-1.34541600	0.18228500
O	2.18426200	-2.44944700	-1.16654700

H	1.71033200	-2.61651500	-1.99502700
H	2.97056000	-1.93792100	-1.41093500
O	-0.65727700	-2.25733200	-0.40858700
H	-0.46319200	-2.96287700	-1.04598300
H	-1.16500700	-2.67774600	0.30307800

[13] Cu^{2+} – $DHLA^{-}$ (CO, S1 *trans*)

Charge = 1 Multiplicity = 2

C	-2.24310000	1.84516900	0.50443400
H	-2.57713300	2.83065400	0.83555100
H	-1.78467500	1.33154500	1.35867800
C	-1.21330300	1.98792300	-0.63273300
H	-1.57233300	2.74150600	-1.34123600
H	-1.14693200	1.04726500	-1.19653800
C	0.17983200	2.37134100	-0.12173200
H	0.08898500	3.21062900	0.57767900
H	0.79605400	2.72280200	-0.95850400
C	0.90394300	1.21159500	0.57494300
H	0.21920400	0.74567900	1.29487200
C	1.44095100	0.18111400	-0.44140000
C	2.93852300	0.32963600	-0.72967000
H	3.09373700	1.37972000	-1.01080900
H	3.20928800	-0.28048500	-1.59794500
H	0.90606600	0.29175400	-1.38937200
C	-3.44787800	1.02023200	0.08108600
O	-4.55715600	1.56448800	-0.07754900
O	-3.27626800	-0.24701500	-0.11179700
C	3.85090500	-0.02800600	0.43951500
H	3.56560300	0.49215200	1.35671700
H	3.81760500	-1.10027700	0.64788100
H	1.73746900	1.60178200	1.16618400
S	5.61030000	0.31830600	0.09057100
H	5.48628500	1.65186100	-0.01822900
S	1.03068600	-1.53487600	0.14320000
H	1.24014100	-2.17548200	-1.02278700
Cu	-1.53366300	-1.16701000	0.02125000
O	-1.58906900	-1.34709600	2.03154500
H	-1.12144900	-0.63974000	2.50297700
H	-2.51919100	-1.25454400	2.29518200
O	-1.39116700	-1.52536000	-1.97666500
H	-2.27987100	-1.51012000	-2.36642400
H	-0.88837100	-0.85246600	-2.46138700

[14] Cu^{2+} – $DHLA^{-}$ (S1)

Charge = 1 Multiplicity = 2

C	4.70849000	1.46750100	0.21758800
H	5.22268000	2.13118700	0.92248200
H	5.10034600	1.67227100	-0.78301500
C	3.20236200	1.73610900	0.25879900
H	3.01687300	2.77768300	-0.02915500
H	2.83490300	1.61702400	1.28513100
C	2.42587200	0.80359700	-0.66904300
H	2.56535500	-0.23350100	-0.33524400
H	2.83734600	0.86968200	-1.68552200
C	0.93557300	1.13882800	-0.70578800
H	0.81301000	2.18277300	-1.02113200
C	0.17099800	0.23301500	-1.67263700
C	0.20996400	-1.26233600	-1.34350700
H	1.23021500	-1.60229000	-1.55925500
H	-0.44734300	-1.80551600	-2.03106000
H	0.57893100	0.36760200	-2.67880700
C	5.05042600	0.02806100	0.60423600
O	4.60049300	-0.40281400	1.70669100

O	5.76314300	-0.65244500	-0.19006900
C	-0.13069900	-1.62738400	0.09689800
H	0.51749400	-1.10891100	0.80654700
H	-1.16837200	-1.38862800	0.35569100
H	0.51243900	1.05877000	0.30238200
S	0.00166000	-3.42631000	0.39824500
H	1.31139300	-3.52711900	0.11143400
S	-1.55141200	0.89641100	-1.81165700
H	-2.10439800	-0.13251400	-2.48035200
Cu	-2.85896000	0.56849300	0.36754600
O	-3.95259100	-0.73311800	-0.73015100
H	-3.49935400	-1.58532900	-0.83700500
H	-4.79516900	-0.93763200	-0.29360100
O	-4.08054100	0.38636600	2.02369300
H	-4.54063800	-0.46641300	2.01454800
H	-3.56526400	0.39867100	2.84479600
O	-1.66766200	1.87037000	1.35158200
H	-2.09398600	2.19622800	2.15977800
H	-1.36125200	2.65683000	0.87384800

[15] Cu^{2+} – $DHLA^{-}$ (CO, S1, S2)

Charge = 1 Multiplicity = 2

C	2.32260800	0.77527100	-0.97886600
H	3.08712600	1.01653900	-1.71941100
H	1.48945800	0.27992800	-1.49149100
C	1.83501400	2.05492400	-0.26027200
H	2.65660700	2.77694500	-0.23806800
H	1.61512300	1.83285700	0.78944000
C	0.62144500	2.71308500	-0.92581000
H	0.88284600	2.94265600	-1.96555100
H	0.42104100	3.67221700	-0.43345800
C	-0.67381800	1.89380300	-0.94875400
H	-0.48716200	0.89185700	-1.35903300
C	-1.46557200	1.78689700	0.35818500
C	-2.88646300	1.25639900	0.13194600
H	-3.44596000	2.08064500	-0.32757600
H	-3.37747900	1.04745100	1.08848800
H	-1.54566600	2.77921700	0.80944600
C	2.87718900	-0.19717000	0.04283800
O	4.10077400	-0.28230000	0.24320500
O	2.02082000	-0.87907900	0.73692800
C	-3.06340700	0.07756200	-0.81625600
H	-4.12818000	-0.12735600	-0.93788200
H	-2.65425100	0.28310300	-1.80772800
H	-1.36115400	2.37503500	-1.65569700
S	-2.30770500	-1.52817200	-0.33612500
H	-2.80089500	-1.60087600	0.91670200
S	-0.55328100	0.78501100	1.64403400
H	-1.63521300	0.28847500	2.27534800
Cu	0.15385300	-1.15918600	0.25590400
O	0.54435000	-2.78263600	-0.88790200
H	0.37740900	-2.66029400	-1.83527100
H	1.49086400	-2.98391600	-0.81192300

[16] Cu^{2+} – $DHLA^{-}$ (S2)

Charge = 1 Multiplicity = 2

C	5.39282400	-0.30939200	0.19084100
H	6.23902400	-0.39886900	0.88445500
H	5.81041100	-0.03112500	-0.78224700
C	4.41907000	0.75523300	0.68661200
H	4.95820600	1.69632600	0.84737800
H	4.01539000	0.44991600	1.65927800
C	3.26321500	0.98993200	-0.28630900

H	2.83047800	0.01995500	-0.56168300
H	3.64324000	1.43913500	-1.21358100
C	2.18572600	1.88894600	0.31953500
H	2.63161600	2.85305400	0.59183600
C	1.00210100	2.14205900	-0.61836200
C	0.32360000	0.86169800	-1.12282700
H	0.98123100	0.38278800	-1.85731300
H	-0.59866600	1.13395500	-1.65185300
H	1.34979200	2.70788700	-1.48718800
C	4.78793700	-1.71203500	0.07558300
O	3.87193900	-2.04134800	0.88287200
O	5.27128100	-2.48225200	-0.80628200
C	0.01846800	-0.12444800	-0.00102700
H	0.92593300	-0.59745800	0.37930900
H	-0.50951400	0.35611200	0.82498300
H	1.82509300	1.43551000	1.25338400
S	-1.03748300	-1.46963800	-0.67361600
H	-0.94457600	-2.31029100	0.37343300
S	-0.18591700	3.22709200	0.28391800
H	-1.00108300	3.46114200	-0.75892400
Cu	-3.31457700	-0.62075500	0.08686800
O	-3.81155100	-0.32192200	-1.84499100
H	-4.69149300	0.08220000	-1.90987000
H	-3.21080400	0.28334900	-2.30788000
O	-5.24433700	-0.31959700	0.75311700
H	-5.89165300	-0.54080400	0.06644900
H	-5.43760000	-0.90659500	1.49973900
O	-2.58353400	-0.77926000	1.95766900
H	-3.27528100	-1.12003900	2.54722000
H	-2.34061500	0.08956300	2.31574700

[17] Cu^{2+} – $DHLA^{-}$ (S1, S2 *cis*)

Charge = 1 Multiplicity = 2

C	-3.89283700	-0.50490100	0.50116200
H	-3.64990300	0.13344700	1.35623100
H	-4.28371100	-1.45706200	0.87604300
C	-2.62792000	-0.76162600	-0.32431400
H	-2.28173400	0.18753200	-0.75904900
H	-2.86317100	-1.42832100	-1.16270000
C	-1.49931400	-1.36312500	0.50971700
H	-1.81021200	-2.32928100	0.92632700
H	-1.30594900	-0.70110600	1.36598700
C	-0.22982900	-1.54651300	-0.31850200
H	-0.00366300	-0.59894000	-0.82992600
C	0.98404300	-2.02992500	0.47106400
C	2.18387400	-2.41155100	-0.39810500
H	1.90345500	-3.35118900	-0.89037200
H	3.05001000	-2.64192700	0.23223400
H	0.70629200	-2.90985300	1.05759700
C	-4.95763800	0.17406100	-0.35471700
O	-5.15167800	1.41467700	-0.19198900
O	-5.56249400	-0.53948200	-1.20804000
C	2.59293900	-1.47477600	-1.52707400
H	3.36781100	-1.95724800	-2.12454800
H	1.76084200	-1.23875400	-2.19432700
H	-0.41033800	-2.28585600	-1.10937900
S	3.28901300	0.16171400	-1.05040600
H	4.10744500	-0.26869100	-0.06854500
S	1.39424400	-0.74754400	1.76117600
H	2.70553400	-1.03103600	1.89044000
Cu	1.46547500	1.23104200	0.30040200
O	1.61870800	2.80178200	-0.97559400
H	1.19227800	2.62825900	-1.83008800
H	1.15180300	3.56758400	-0.60506200

O	-0.24705800	1.88245700	1.19507700
H	-0.30874600	2.84836000	1.12640800
H	-1.03865400	1.54181500	0.74773000

[18] Cu^{2+} – $DHLA^{2-}$ (CO, S1 *trans*)

Charge = 0 Multiplicity = 2

C	-2.22900400	1.73797700	0.59212300
H	-2.58770100	2.67347200	1.02741800
H	-1.72287500	1.16070600	1.37537800
C	-1.24947800	2.02094300	-0.55950400
H	-1.69096100	2.77327300	-1.22228600
H	-1.12724500	1.11111500	-1.16188000
C	0.12621800	2.49236600	-0.07767700
H	-0.00366700	3.33033900	0.61906300
H	0.69146100	2.88114200	-0.93472400
C	0.95127000	1.38861600	0.59703000
H	0.38130900	0.95112300	1.42329100
C	1.39193100	0.28134400	-0.39118700
C	2.89527600	0.35723300	-0.70405000
H	3.12102200	1.39078900	-1.00310100
H	3.12580400	-0.28646300	-1.56008100
H	0.88099000	0.45207200	-1.34627600
C	-3.41275600	0.91149700	0.11312500
O	-4.53820600	1.44036200	0.00039400
O	-3.20294400	-0.32623500	-0.18252200
C	3.79393300	-0.03534200	0.46231300
H	3.56476400	0.53895100	1.36312000
H	3.66686500	-1.09318400	0.70432700
H	1.83783100	1.84647100	1.05205200
S	5.57513300	0.14430600	0.08784700
H	5.55427900	1.46318100	-0.16857700
S	0.93248300	-1.42992700	0.14869000
Cu	-1.40893200	-1.20243600	-0.04599800
O	-1.74282100	-1.52889100	1.95142500
H	-0.95782300	-1.26772800	2.45817600
H	-2.46506700	-0.95739900	2.25651700
O	-1.36769700	-1.39443500	-2.09532800
H	-1.86826000	-0.67316400	-2.50707100
H	-0.45454200	-1.30834100	-2.41080000

[19] Cu^{2+} – $DHLA^{2-}$ (CO, S1 cis)

Charge = 0 Multiplicity = 2

C	-2.52178500	1.32761600	0.88924900
H	-3.19164800	1.83181400	1.58917300
H	-1.93983100	0.57939600	1.44206200
C	-1.56738300	2.34315700	0.22516500
H	-2.09092300	3.29750900	0.11186100
H	-1.30554100	2.00028200	-0.78334200
C	-0.28045600	2.53559900	1.03036600
H	-0.53339200	2.67277300	2.08990300
H	0.21616200	3.45789900	0.70432300
C	0.72137000	1.38246800	0.88939000
H	0.27805000	0.44045000	1.24091100
C	1.27916500	1.23668200	-0.54618100
C	2.80994800	1.10111800	-0.54335500
H	3.21566700	1.97785400	-0.01913000
H	3.18894700	1.13459300	-1.57084700
H	1.06218800	2.17467000	-1.07115100
C	-3.32066400	0.60601400	-0.17676400
O	-4.45706200	1.01085700	-0.49881900
O	-2.75232100	-0.39050200	-0.76511900
C	3.32029400	-0.16328900	0.13484500
H	2.87743500	-0.29825000	1.12523600

H	3.07921700	-1.04431300	-0.46494700
H	1.55847100	1.58756700	1.56961700
S	5.14232200	-0.20544900	0.29543100
H	5.26186000	0.90498700	1.04330300
S	0.50252700	-0.08521700	-1.59578100
Cu	-1.05241400	-1.22788900	-0.17077300
O	-2.17688100	-2.33541200	1.19770000
H	-1.69213000	-2.49468800	2.02117000
H	-2.97557400	-1.84806500	1.44957300
O	0.51497300	-2.37770900	0.50278100
H	0.31511900	-3.32558500	0.54282200
H	1.20572000	-2.26350300	-0.17115500

[20] Cu^{2+} – $DHLA^{2-}$ (S1)

Charge = 0 Multiplicity = 2

C	-4.48549600	-1.47236000	0.11499500
H	-5.00674800	-2.19690900	0.75361100
H	-4.91947900	-1.55370300	-0.88645900
C	-2.99141800	-1.78788800	0.07771900
H	-2.84936900	-2.81869600	-0.26895600
H	-2.58129800	-1.73484000	1.09350600
C	-2.21579200	-0.83524400	-0.83087700
H	-2.41089600	0.19804500	-0.51311700
H	-2.59259400	-0.92280500	-1.85973700
C	-0.71250400	-1.11347700	-0.81413800
H	-0.53778000	-2.15879400	-1.10034100
C	0.09218000	-0.20949900	-1.75228900
C	-0.08980800	1.28883900	-1.44887400
H	-1.09771600	1.58693100	-1.76812200
H	0.61680100	1.86446500	-2.05544300
H	-0.28167400	-0.36828900	-2.77069500
C	-4.80427000	-0.08523800	0.67759800
O	-4.14631900	0.31365900	1.68237800
O	-5.73185800	0.57634900	0.12455800
C	0.06860900	1.67332900	0.01858600
H	-0.67628100	1.17941300	0.64668800
H	1.05658300	1.41347100	0.41293800
H	-0.33306900	-1.00669600	0.21175000
S	-0.06515700	3.47846200	0.29090700
H	-1.30172200	3.61319300	-0.21854300
S	1.86588200	-0.71992800	-1.85688700
Cu	2.65562600	-0.58797300	0.36900300
O	3.66308000	1.15511500	-0.06986500
H	3.25000400	1.48844300	-0.88399200
H	3.51816500	1.83490900	0.60680400
O	3.30050600	-0.46036300	2.31489100
H	3.52737900	0.44735500	2.56650100
H	2.60566000	-0.74076500	2.92931700
O	1.80107300	-2.35886200	0.91651400
H	2.43852200	-2.95581800	1.33845600
H	1.48989300	-2.81221400	0.11632800

[21] Cu^{2+} – $DHLA^{2-}$ (CO)

Charge = 0 Multiplicity = 2

C	0.67514100	3.24637900	-0.14289800
H	1.01720900	4.16673000	0.33654000
H	0.68727900	3.38245100	-1.22798500
C	-0.75753300	2.92333600	0.31740200
H	-1.38893400	3.78319300	0.06519400
H	-0.77507700	2.82860700	1.41070400
C	-1.34664700	1.66293700	-0.31563800
H	-0.75959000	0.78891400	-0.00150900
H	-1.24932300	1.72551700	-1.40976200

C	-2.81639400	1.46337500	0.06183300
H	-3.37038000	2.38456600	-0.15897300
C	-3.51711100	0.30544300	-0.66474100
C	-2.72821900	-1.01242100	-0.55954400
H	-1.76839100	-0.90569900	-1.08639900
H	-3.28442400	-1.80188000	-1.07619100
H	-3.52933900	0.56202500	-1.73292200
C	1.62686600	2.12919100	0.22351500
O	2.18470600	2.12864600	1.34882100
O	1.78395200	1.20381300	-0.65140700
C	-2.45440600	-1.45047600	0.87202200
H	-1.89026100	-0.69507200	1.42444200
H	-3.39534600	-1.61841500	1.40288300
H	-2.89658800	1.31387400	1.14711400
S	-1.54242100	-3.03341000	0.98239700
H	-0.45994700	-2.63187300	0.29167600
S	-5.26901300	0.12167700	-0.11837100
Cu	2.71015200	-0.50720600	-0.35393500
O	1.28071800	-1.36298200	-1.53464600
H	1.15711400	-2.30908800	-1.36586200
H	0.42247700	-0.94120100	-1.36959900
O	3.63523100	-2.29973100	-0.17242200
H	3.57798800	-2.82408900	-0.98555800
H	4.58041300	-2.19901100	0.01691200
O	4.08752400	0.32287700	0.89754600
H	4.32711500	-0.29234800	1.60603700
H	3.51930600	1.03193600	1.29812100

[22] Cu^{2+} – $DHLA^{2-}$ (COO)

Charge = 0 Multiplicity = 2

C	0.62085200	3.20022900	-0.17961200
H	1.09216700	3.98057300	0.42438200
H	0.57231400	3.53032300	-1.21979400
C	-0.78667400	2.87942100	0.35761300
H	-1.41269800	3.77169200	0.25206800
H	-0.71629800	2.65691000	1.42922000
C	-1.41830400	1.69415000	-0.36868800
H	-0.71697300	0.84947100	-0.33063900
H	-1.54464700	1.93959600	-1.43312600
C	-2.75106400	1.24890200	0.23317200
H	-3.45150800	2.09359300	0.24718100
C	-3.41692800	0.07836500	-0.51132100
C	-2.41584900	-1.05070900	-0.82134600
H	-1.64904100	-0.67123200	-1.51070900
H	-2.93677400	-1.85810700	-1.34735600
H	-3.73879900	0.46500100	-1.48798300
C	1.46059600	1.95822900	-0.10287100
O	1.79466000	1.47218400	1.02736100
O	1.79754000	1.31546200	-1.15132700
C	-1.72730100	-1.62439500	0.41207200
H	-1.34120700	-0.83948200	1.06714200
H	-2.42506000	-2.22470500	1.00054500
H	-2.59300900	0.96772200	1.28294300
S	-0.33560900	-2.74642500	0.01023900
H	0.48467500	-1.80748700	-0.50307600
S	-4.91907900	-0.52341700	0.37161800
Cu	2.56393800	-0.16471200	0.02961200
O	2.98919600	-1.56305800	-1.37474500
H	3.11613600	-1.14160500	-2.23844700
H	3.81182500	-2.03896100	-1.18410700
O	3.20498300	-1.26394400	1.60166100
H	3.91088400	-1.88182300	1.35862700
H	3.57582100	-0.68766500	2.28697100

[23] Cu^{2+} – $DHLA^{2-}$ (CO, S2 cis)

Charge = 0 Multiplicity = 2

C	0.19037800	3.23901500	0.48668400
H	0.63819600	3.76319300	1.34025400
H	0.12359500	3.96909400	-0.32675100
C	-1.18048100	2.67828500	0.84987400
H	-1.80199800	3.47780500	1.26817000
H	-1.05680500	1.92867100	1.63921600
C	-1.88020500	2.03960900	-0.35501700
H	-1.12764000	1.50262900	-0.94108100
H	-2.26613200	2.82713100	-1.01217200
C	-3.01423100	1.07224500	0.03172700
H	-3.98840600	1.55511200	-0.10109400
C	-2.98929600	-0.22707200	-0.78558700
C	-1.67913100	-1.02429500	-0.67575300
H	-0.90214300	-0.48660700	-1.23344200
H	-1.80440700	-1.98685900	-1.18631700
H	-3.15339800	0.01702300	-1.84024300
C	1.19883700	2.17971000	0.07042700
O	2.21790600	2.54780900	-0.57733600
O	0.97290000	0.97603900	0.42100400
C	-1.17869000	-1.26475900	0.74502900
H	-1.04230500	-0.31493600	1.26658200
H	-1.91335300	-1.84820700	1.30880800
H	-2.93740500	0.82011700	1.09662700
S	0.40665800	-2.18336700	0.79994700
S	-4.44753900	-1.21888300	-0.24100900
H	-4.22301400	-2.28221700	-1.03159100
Cu	2.02921900	-0.67758600	0.01855100
O	3.28861500	-2.32936700	-0.16033600
H	2.80676800	-3.11850800	-0.45054700
H	3.96761900	-2.17105500	-0.83356500
O	3.54370700	0.38225500	-0.87421300
H	4.34466900	0.34899000	-0.33223000
H	3.15478700	1.31429400	-0.78886200

[24] Cu^{2+} – $DHLA^{2-}$ (CO, S2 trans)

Charge = 0 Multiplicity = 2

C	1.72997600	2.93158700	0.07727000
H	2.33284300	3.45128100	0.83012600
H	1.73745300	3.52946700	-0.83775600
C	0.29669800	2.73693900	0.59412500
H	-0.17771400	3.71917600	0.69818300
H	0.33006600	2.28847000	1.59494400
C	-0.53524200	1.84504700	-0.32623800
H	-0.02775800	0.87553300	-0.41857300
H	-0.57130400	2.27730300	-1.33586300
C	-1.95283700	1.60636200	0.19009700
H	-2.47813900	2.56518600	0.27817000
C	-2.77081900	0.67909600	-0.72157900
C	-2.06564000	-0.63300400	-1.08921900
H	-1.17402800	-0.37164300	-1.67015800
H	-2.70767300	-1.21073700	-1.76483000
H	-2.98994200	1.21681200	-1.64934100
C	2.38427700	1.59415600	-0.21499200
O	2.89819400	1.37794100	-1.34053500
O	2.34043200	0.71380100	0.71845700
C	-1.65809400	-1.50245700	0.10418500
H	-1.40043300	-0.86852100	0.95766600
H	-2.49966200	-2.12318600	0.42179900
H	-1.89641800	1.18604400	1.20321600
S	-0.23567400	-2.62079500	-0.25179200
S	-4.38644500	0.39273100	0.12163600
H	-4.91661800	-0.40672800	-0.82008100

Cu	1.45766600	-1.09581000	0.31576800
O	0.79519600	-0.88357400	2.25166900
H	0.40575900	-0.00195100	2.36543100
H	0.10582100	-1.52120400	2.49220200
O	2.56700500	-1.27995900	-1.42288000
H	3.35613100	-1.80801500	-1.23169800
H	2.87669100	-0.34180300	-1.52379600

[25] Cu^{2+} – $DHLA^{2-}$ (CO)

Charge = 0 Multiplicity = 2

C	0.62328700	3.32174600	-0.49166200
H	0.97115100	4.29283600	-0.13110500
H	0.59243900	3.33358200	-1.58445800
C	-0.77853400	3.02630800	0.07124200
H	-1.43668500	3.86570200	-0.17867200
H	-0.72197300	2.98093700	1.16634900
C	-1.37816600	1.72898800	-0.46938800
H	-0.67256700	0.90331500	-0.31135600
H	-1.51602900	1.81833600	-1.55605500
C	-2.71021400	1.38775000	0.19747700
H	-3.37237100	2.26167800	0.15829100
C	-3.41765700	0.20302100	-0.46846400
C	-2.54165800	-1.04598800	-0.63361800
H	-1.77858000	-0.81094300	-1.38810900
H	-3.14827000	-1.85432300	-1.05993900
H	-3.75119600	0.51900200	-1.46210700
C	1.58920600	2.25643100	-0.02428600
O	2.07938700	2.34798900	1.13280000
O	1.82053600	1.28091500	-0.81908200
C	-1.85300700	-1.54714900	0.63330700
H	-1.24841600	-0.74383700	1.06954800
H	-2.60917700	-1.81291600	1.37902400
H	-2.53443400	1.17091800	1.25961800
S	-0.77189700	-3.00511600	0.32964100
S	-4.94657500	-0.13276300	0.50912200
H	-5.43581600	-1.09376300	-0.29289000
Cu	2.45456000	-0.51856900	-0.21753600
O	1.06997400	-1.38783100	-1.38615900
H	0.44760600	-1.98250200	-0.81062700
H	0.50623100	-0.69174500	-1.75866800
O	3.23780800	-2.36715100	0.15744400
H	3.16217300	-2.93942500	-0.62090200
H	4.18343900	-2.31230800	0.36148700
O	3.63915700	0.30359900	1.21209600
H	3.59447900	-0.21563800	2.02782100
H	3.10689600	1.14884400	1.35662500

[26] Cu^{2+} – $DHLA^{2-}$ (COO, S2)

Charge = 0 Multiplicity = 2

C	-0.88294800	3.14040700	-0.13679200
H	-1.28482900	3.80911300	-0.90576200
H	-1.10472600	3.57524600	0.84110500
C	0.62564900	2.93249700	-0.34011000
H	1.14160300	3.88954000	-0.21425900
H	0.79140400	2.61163500	-1.37419300
C	1.19730300	1.87254100	0.61162700
H	0.44269800	1.09103700	0.75140500
H	1.37364100	2.30408400	1.60428900
C	2.47764600	1.21644000	0.08427200
H	3.33226000	1.88769800	0.22902500
C	2.77915700	-0.13478500	0.74911700
C	1.61801000	-1.14134300	0.69442000
H	0.84108000	-0.79442400	1.38615800

H	1.95965000	-2.10559900	1.08963400
H	3.03377900	0.03424000	1.80010100
C	-1.59264300	1.81246400	-0.23518500
O	-1.26360900	0.98774700	-1.15349200
O	-2.44034600	1.44235600	0.63335900
C	0.99519700	-1.34786200	-0.68602500
H	0.78290900	-0.38754100	-1.16232200
H	1.69045500	-1.88623500	-1.33659300
H	2.37892000	1.06441600	-0.99799900
S	-0.57380100	-2.30939600	-0.62794300
S	4.30109600	-0.78856000	-0.06456000
H	4.40111200	-1.91253500	0.66547100
Cu	-2.03100400	-0.56156500	-0.06671100
O	-3.31859300	-1.63512000	1.06354900
H	-4.20031600	-1.23210600	1.04841500
H	-3.44108600	-2.55790000	0.79490800

[27] Cu^{2+} – $DHLA^{2-}$ (S2)

Charge = 0 Multiplicity = 2

C	5.31836100	-0.05894300	-0.50090300
H	6.34296800	0.15779500	-0.17211200
H	5.34477600	-0.11761300	-1.59400700
C	4.37355000	1.04807200	-0.04322600
H	4.76854000	2.01931600	-0.36449900
H	4.33845400	1.06525100	1.05249800
C	2.95993700	0.87058000	-0.59589900
H	2.61605000	-0.14968200	-0.38248700
H	2.98143200	0.97343800	-1.68973600
C	1.97774900	1.88422000	-0.00755600
H	2.37956600	2.89557900	-0.14253300
C	0.59779900	1.80979400	-0.66321000
C	-0.05606500	0.42518200	-0.59518700
H	0.47757400	-0.25200600	-1.27356700
H	-1.07838900	0.51121700	-0.98967700
H	0.69199500	2.10636200	-1.71200600
C	4.97999500	-1.44711200	0.05067500
O	4.44084900	-1.52660800	1.19148800
O	5.29823100	-2.44694700	-0.65953400
C	-0.08257800	-0.18964800	0.80423300
H	0.92479500	-0.50341300	1.09521700
H	-0.40434800	0.54931800	1.54630400
H	1.88961200	1.71911200	1.07493800
S	-1.16320200	-1.66707400	0.91617400
S	-0.48745800	3.09018000	0.12186800
H	-1.36850700	3.18324600	-0.88992500
Cu	-3.11577900	-0.67839800	0.04304900
O	-3.39975300	-2.40129200	-1.04484500
H	-3.85052000	-2.28065900	-1.89445300
H	-2.52348900	-2.76575400	-1.24595500
O	-4.71150600	0.19161000	-0.94336900
H	-5.29562200	-0.45947700	-1.35974600
H	-5.27797500	0.72118500	-0.36305800
O	-2.95485700	0.97992500	1.26731600
H	-3.75822300	1.52171700	1.24569600
H	-2.22675600	1.58254100	1.02003400

[28] Cu^{2+} – $DHLA^{2-}$ (COO)

Charge = 0 Multiplicity = 2

C	0.57681200	3.14697600	-0.25592100
H	1.06451600	3.93826800	0.32322000
H	0.56407600	3.44398900	-1.30730200
C	-0.84216600	2.89148700	0.26970800
H	-1.42666900	3.81340900	0.18736600

H	-0.78387300	2.64012100	1.33502100
C	-1.52667300	1.75308500	-0.48710300
H	-0.81240800	0.92806600	-0.60747300
H	-1.79034900	2.08333100	-1.50055400
C	-2.76439200	1.22544000	0.23573900
H	-3.49303500	2.03592000	0.36162600
C	-3.42779500	0.05808900	-0.50403000
C	-2.45733400	-1.06678900	-0.89256700
H	-1.80933900	-0.68070100	-1.68981700
H	-3.02567500	-1.89104500	-1.34156400
H	-3.89094600	0.44329000	-1.41822900
C	1.40502000	1.89886900	-0.11697400
O	1.48822300	1.30411700	1.00817800
O	2.00647000	1.37680700	-1.11025200
C	-1.57741000	-1.61475900	0.22977600
H	-1.06419400	-0.78633400	0.73236600
H	-2.21350700	-2.09083500	0.98441400
H	-2.47163700	0.90242200	1.24351400
S	-0.31686300	-2.81368400	-0.37275000
S	-4.80735900	-0.53712600	0.56810000
H	-5.25555900	-1.49099000	-0.26587500
Cu	2.60999700	-0.16204900	0.12484900
O	3.63860500	-1.31993200	-1.16861800
H	4.02902400	-0.78314500	-1.87478600
H	4.37648100	-1.77473300	-0.73527400
O	2.98959400	-1.29636500	1.75655000
H	3.68719500	-1.94727700	1.58532000
H	3.31403000	-0.74275700	2.48316900

[29] Cu^{+} – $DHLA^{2-}$ (COO)

Charge = -1 Multiplicity = 1

C	0.22899500	3.56692900	0.24757800
H	0.39914400	4.43665200	0.89145600
H	0.28403000	3.89558400	-0.79378200
C	-1.14485200	2.95554200	0.54553400
H	-1.92342200	3.69092800	0.31253900
H	-1.21926600	2.73678700	1.61765600
C	-1.38615200	1.67286500	-0.24744500
H	-0.57956000	0.96028700	-0.02041000
H	-1.32303600	1.88476200	-1.32408400
C	-2.73420000	1.03056600	0.07547100
H	-3.53679400	1.75327800	-0.11686900
C	-2.99850600	-0.23549100	-0.74770700
C	-1.85255100	-1.25393700	-0.70928700
H	-0.99785500	-0.80732000	-1.23358600
H	-2.13592600	-2.14067900	-1.28920900
H	-3.15880100	0.05762800	-1.79001400
C	1.33644500	2.55707600	0.51368000
O	2.11342600	2.25979100	-0.45911600
O	1.42343700	2.04262600	1.65585600
C	-1.40676100	-1.68030900	0.68641400
H	-1.23314400	-0.80366700	1.31683000
H	-2.19608100	-2.26800400	1.16457900
H	-2.77140000	0.79462100	1.14707400
S	0.12037700	-2.70910500	0.66502800
S	-4.59441000	-0.94577500	-0.15242900
H	-4.63634900	-1.97722000	-1.01284300
Cu	1.71801100	-1.15991800	0.31805000
O	3.80582700	-2.13354500	-1.71582400
H	3.01872300	-2.61277300	-1.41978800
H	3.76272100	-1.29743600	-1.21863000
O	3.27620100	0.07849200	0.01242700
H	3.78574100	0.14844700	0.83155700
H	2.85326400	1.00762300	-0.15495000

[30] $[Cu(H_2O)_2]^{+} \cdot 2H_2O$

```
Charge = 1 Multiplicity = 1
 Cu                 0.01047600   -0.03949600    0.15124100
 O                 -1.59124200    1.12649400    0.27849500
 H                 -2.38928300    0.60386200    0.01969200
 H                 -1.53619600    1.86887600   -0.33860200
 O                  1.62124100   -1.19796400    0.05402900
 H                  1.76555600   -1.67032600    0.88546500
 H                  2.40271100   -0.60682200   -0.07372200
 O                  3.59303700    0.57380600   -0.42562000
 H                  4.48179400    0.20582000   -0.52252100
 O                 -3.67002900   -0.47490000   -0.32935600
 H                 -4.51279100   -0.15525500    0.02075100
 H                 -3.80386000   -0.54363000   -1.28462000
 H                  3.66419300    1.22338400    0.28719700
```

[31] $[Cu(H_2O)_4]^{2+}$

```
Charge = 2 Multiplicity = 2
Cu                -0.22194400   -0.40244900    0.49999500
 O                 -0.16283600    1.61946000    0.18639500
 H                  0.51837700    1.83503000   -0.46890700
 H                 -0.99845600    1.92689800   -0.19710000
 O                  0.33530700   -0.84982100   -1.38819000
 H                 -0.09832600   -1.65213200   -1.71576500
 H                  0.11602200   -0.14410000   -2.01495600
 O                 -0.78231000    0.04111000    2.38730300
 H                 -0.55851800   -0.66236900    3.01491600
 H                 -0.35817300    0.84794700    2.71609600
 O                 -0.28118900   -2.42569200    0.81240500
 H                  0.55531000   -2.73275500    1.19428200
 H                 -0.96085500   -2.64106400    1.46935600
```

[32] $(H_2O)_2$

```
Charge = 0 Multiplicity = 1
 O                  1.48346800   -0.09697500   -0.04698000
 H                  0.51257900    0.00644900   -0.03865100
 H                  1.83807100    0.79971300   -0.08379100
 O                 -1.32778400    0.05426100   -0.01967500
 H                 -1.69576800   -0.59333600   -0.63582400
 H                 -1.65821500   -0.21250500    0.84863700
```

[33] $(H_2O)_3$

```
Charge = 0 Multiplicity = 1
 O                  0.00021800    1.10996700   -0.00001800
 H                  0.77856700    0.52344100   -0.00717500
 H                 -0.77824600    0.52363600    0.00715500
 O                  2.30693800   -0.53095900   -0.01237900
 H                  2.93697900   -0.27385900   -0.69863100
 H                  2.79218000   -0.44249300    0.81879400
 O                 -2.30714700   -0.53081500    0.01245100
 H                 -2.79205600   -0.44266300   -0.81894200
 H                 -2.93749200   -0.27360400    0.69837100
```

[34] LA^{-}

```
Charge = -1 Multiplicity = 1
 C                  4.09469500    0.94933200   -0.12034300
 H                  4.81442200    1.38165800    0.57779900
 H                  4.45859100    1.10244900   -1.13727600
 C                  2.67905200    1.54204300    0.04959200
```

H	2.39835700	2.04684500	-0.87993700
H	2.67214100	2.28783800	0.84992100
C	1.61097600	0.48313400	0.36845800
H	1.61963200	0.25327700	1.43950300
S	4.06568100	-0.85296400	0.22142100
S	2.12103000	-1.06299600	-0.48906300
C	0.21222500	0.91290700	-0.05751100
H	0.00663500	1.87214700	0.43622400
H	0.20826200	1.10767200	-1.13833700
C	-0.88805100	-0.08393900	0.29912500
H	-0.72338400	-1.02839000	-0.23767100
H	-0.83162900	-0.31862000	1.37089900
C	-2.28034600	0.44606000	-0.03713200
H	-2.32574200	0.69328100	-1.10555000
H	-2.45403300	1.38134400	0.50827000
C	-3.37603100	-0.55716100	0.29984600
H	-3.19729100	-1.50773400	-0.21597700
H	-3.35814600	-0.78852200	1.37348100
C	-4.80292400	-0.11506600	-0.02538400
O	-5.70319200	-1.00530100	0.04493700
O	-5.01840400	1.09383400	-0.32231100

[35] DHLA^{-}

Charge = -1 Multiplicity = 1

C	3.39553800	-1.28183200	-0.00250900
H	4.18892700	-1.77661300	-0.57697700
H	3.55028100	-1.53960900	1.04983700
C	2.02826800	-1.76955900	-0.47796000
H	1.98507900	-2.86178100	-0.39021200
H	1.90351600	-1.53172200	-1.54112700
C	0.87950800	-1.15163000	0.31766600
H	0.96318400	-0.05750500	0.27512500
H	0.97115900	-1.43489200	1.37545400
C	-0.48561300	-1.58796800	-0.21251100
H	-0.52878700	-2.68397100	-0.23142200
C	-1.65226100	-1.06733500	0.63209800
C	-1.66782700	0.45465200	0.81996300
H	-0.81416500	0.72410800	1.45487400
H	-2.57030700	0.74056600	1.37166100
H	-1.59637900	-1.52796700	1.62299700
C	3.60538100	0.22474400	-0.17467900
O	3.18781400	0.76369400	-1.24069300
O	4.21138400	0.84471200	0.74829500
C	-1.59279700	1.24622900	-0.47946200
H	-0.67470700	1.02966600	-1.03048600
H	-2.43748400	1.00893700	-1.13224700
H	-0.59571400	-1.25063200	-1.25174600
S	-1.68967000	3.05277900	-0.21324200
H	-0.58961400	3.15409400	0.55228000
S	-3.20517600	-1.68401500	-0.14942600
H	-4.04952200	-1.19646700	0.77548900

[36] S1-deprotonated DHLA^{2-}

Charge = -2 Multiplicity = 1

C	3.40680400	-1.28689000	0.00904100
H	4.20071400	-1.78970000	-0.55812000
H	3.55363400	-1.54017700	1.06370200
C	2.03801100	-1.76731300	-0.47106000
H	1.98741300	-2.85871100	-0.37316500
H	1.92475300	-1.54116300	-1.53843600
C	0.88307900	-1.13560900	0.30550000
H	0.97169900	-0.04186500	0.24628600

```
 H                  0.97297200   -1.39902900    1.36972100
 C                 -0.48429800   -1.57589500   -0.22110600
 H                 -0.51887600   -2.67272900   -0.24905900
 C                 -1.68388100   -1.08366100    0.60149400
 C                 -1.65604100    0.44108500    0.81804200
 H                 -0.77977400    0.71079400    1.42530000
 H                 -2.54286100    0.73104300    1.39181200
 H                 -1.58891500   -1.52902100    1.60131500
 C                  3.62854600    0.21690900   -0.16884400
 O                  3.23151200    0.75208300   -1.24474100
 O                  4.22371900    0.83982400    0.75961100
 C                 -1.61577700    1.24271400   -0.47528300
 H                 -0.71478700    1.02716200   -1.05526700
 H                 -2.48191700    1.00087700   -1.09731500
 H                 -0.59611900   -1.24277000   -1.26210700
 S                 -1.70163500    3.05214100   -0.20999400
 H                 -0.60549700    3.15071700    0.56137800
 S                 -3.28294000   -1.66366400   -0.11315200
```

[37] S2-deprotonated DHLA^{2-}

```
Charge = -2 Multiplicity = 1
 C                  3.38782100   -1.04997100    0.11342400
 H                  4.22287100   -1.50726800   -0.43276400
 H                  3.51141800   -1.31450700    1.16838300
 C                  2.06148500   -1.58443500   -0.42161400
 H                  2.06749800   -2.67987400   -0.36842000
 H                  1.96112500   -1.32007200   -1.48107800
 C                  0.85774300   -1.04807800    0.35158200
 H                  0.88904400    0.04967500    0.35356700
 H                  0.92554800   -1.36870900    1.40058600
 C                 -0.46573100   -1.52504200   -0.24532600
 H                 -0.44500600   -2.61954500   -0.32857100
 C                 -1.68106300   -1.11485500    0.59002800
 C                 -1.80723300    0.39637800    0.82705300
 H                 -1.00428200    0.69483400    1.51450800
 H                 -2.74841200    0.59366600    1.35544100
 H                 -1.61429200   -1.61331700    1.56261600
 C                  3.55279400    0.46459200   -0.03452600
 O                  3.12566500    1.00936900   -1.09332600
 O                  4.14124100    1.08478100    0.90011800
 C                 -1.73867300    1.27268900   -0.42098700
 H                 -0.75671100    1.14979800   -0.89307300
 H                 -2.48188000    0.91984500   -1.14520200
 H                 -0.56675500   -1.13184300   -1.26539600
 S                 -2.01910700    3.05655300   -0.06570900
 S                 -3.16934200   -1.81731000   -0.24946200
 H                 -4.08309600   -1.30145000    0.58998900
```