Supplementary material to:

S. Mahata, I. Mitra, S. Mukherjee, V. Pera Reddy B., G. Kr. Ghosh, W. Linert and S. Ch. Moi,

Speciation Study of L-ascorbic Acid and its Chelated Cu(II) & Ni(II) Complex: an Experimental and Theoretical Model of Complex Formation,

S. Afr. J. Chem., 2019, **72**, 229–236.

Cartesian coordinates of the optimized structures

Table S1 Cartesian coordinates of complex **1** [Cu(L-asa)$(H_2O)_3$(OH)].

Optimized at B3LYP/lanl2dz/6-31g(d) level of theory

C	0.40992900	1.58760300	-0.02054500
C	0.54942300	0.23934200	0.19159400
C	1.69038000	2.23801100	0.11180700
O	2.64723800	1.27396300	0.40332400
C	2.02870300	-0.02946200	0.40697500
C	2.70141800	-0.89153400	-0.68789700
H	2.19624900	-0.48788100	1.39024500
C	4.22591600	-0.97002200	-0.51680800
O	4.55579600	-1.84382500	0.57064300
H	4.66529500	0.02374900	-0.38716100
H	4.65421200	-1.43210700	-1.41109600
H	4.50769300	-1.33625900	1.39621700
O	2.17274900	-2.20851200	-0.69133300
H	2.47095600	-0.43803400	-1.65921500
H	2.69316700	-2.68217300	-0.01431700
O	2.00661500	3.41353200	0.02649700
O	-0.74105600	2.30577700	-0.26284900
O	-0.32173300	-0.72191500	0.22443400
Cu	-2.19788800	-0.48323000	-0.02730300
O	-2.50382600	1.16300200	1.47180300
H	-1.92066600	1.82559300	1.02440800
H	-3.38120900	1.57608900	1.51943400
O	-4.05638000	-0.90917700	-0.75789800
H	-3.90286800	-0.30169200	-1.51699200
H	-4.83868300	-0.57068400	-0.28833500
O	-2.35402500	-2.07931800	1.20853200
H	-2.83052000	-2.83029000	0.81529300
H	-1.43121500	-2.37050300	1.32522500
O	-2.14752300	0.61009500	-1.58744500
H	-1.54376900	0.20994900	-2.23398100
H	-1.29733500	1.75530600	-0.92436400

Table S2 Cartesian coordinates of complex **2** $[Cu(L\text{-}asa)_2(H_2O)_2]^{2-}$.

Optimized at B3LYP/lanl2dz/6-31g(d) level of theory

C	-3.73466300	-2.12685100	0.04396800
O	-4.67692700	-1.17436900	0.36084400
C	-2.42530500	-1.44227700	-0.02929300
C	-2.63324400	-0.07088100	0.25188600
C	-4.09939700	0.15852300	0.49032500
O	-1.26610700	-1.91808000	-0.27629600
O	-1.66841200	0.75572000	0.28021100
C	-4.77876000	1.11328700	-0.52190200
H	-4.28930500	0.50748200	1.51175300
C	-6.29877500	1.19107100	-0.31764300
O	-4.02746100	-3.28974700	-0.12035100
O	-4.21586200	2.40468800	-0.39027400
H	-4.56443600	0.75329100	-1.53405600
H	-4.71667600	2.82181600	0.33768100
O	-6.59149100	1.95813900	0.85406500
H	-6.74975000	0.19466900	-0.27918300
H	-6.72963700	1.74026500	-1.15979500
H	-6.62295900	1.36091200	1.61785200
Cu	-0.01794200	-0.25395900	-0.16346500
O	1.46746100	-1.36006400	-0.61284300
O	2.97435100	1.05314700	-1.71292200
C	2.70202500	-1.04650700	-0.50586300
C	3.40174700	0.09438700	-1.03219100
C	3.69487200	-1.87522300	0.22566800
O	4.91959900	-1.25645200	0.16916900
C	4.84250200	-0.01892200	-0.57355000
C	5.29784900	1.17780900	0.29528600
H	5.51282100	-0.09559600	-1.43579700
C	4.55349000	1.31431200	1.62680500
O	5.18730500	2.37397000	-0.46932700
H	6.35950400	1.03357700	0.52757900
H	4.41008900	2.28623800	-1.05625100
O	3.17459500	1.66115400	1.44895400
H	5.05328600	2.08185400	2.22903100
H	4.56872000	0.37458300	2.18267600
H	3.13528500	2.52409400	1.00349600
O	3.53182800	-2.92438000	0.80691800
O	0.79398600	0.33990300	1.62868800
H	1.67464600	0.79564200	1.61014600
H	0.19257300	0.94180400	2.09782700
O	0.27351300	0.92286300	-1.83382500
H	1.25344200	1.04896600	-1.94493200
H	-0.11235400	1.81093300	-1.75259900

Table S3 Cartesian coordinates of complex **3** $[Cu(L\text{-}asa)_4]^{2-}$.

Optimized at B3LYP/lanl2dz/6-31g(d) level of theory

Cu	0.65296200	0.19732600	-0.30217200
O	1.79212800	0.04222000	-1.92764800
O	-1.24958700	-2.09493200	1.89850800
O	-0.74445700	1.20003800	-1.30685200
O	2.22178400	-0.45888300	0.72539000
O	-0.50404400	-1.68523900	-0.97055800
O	-0.09816300	0.98694400	1.33570400
C	3.15300100	-0.60381600	-0.12559200
C	2.93316500	-0.34947800	-1.49852500
C	4.19356700	-0.61466600	-2.22599300
O	5.12118600	-1.01338000	-1.29052000
C	4.58121900	-1.02717100	0.06874700
C	5.44700900	-0.09763600	0.93658100
H	4.65824600	-2.05597300	0.43681300
O	6.80376500	-0.52184600	0.88491100
C	5.05644400	-0.13173000	2.41412900
H	5.34963800	0.93045200	0.56108400
O	5.90127300	0.72736100	3.16310800
H	5.11583800	-1.16955000	2.77802800
H	4.03037000	0.22009500	2.54661200
H	7.14639100	-0.32781100	-0.00276100
H	6.80888700	0.48503800	2.90968500
O	4.45700500	-0.53070500	-3.40276900
C	-1.46897700	-2.26893200	-0.52837100
C	-1.87335700	-2.46301700	0.93137700
C	-2.52141000	-3.00512000	-1.35432300
O	-3.43048500	-3.53812700	-0.50563800
C	-3.19965200	-3.19796100	0.90360100
O	-2.56142600	-3.13043500	-2.54912100
C	-4.41043700	-2.36101900	1.41066600
H	-3.14514600	-4.14414000	1.44614400
C	-4.24746400	-0.86268200	1.09123600
O	-3.53985800	-0.61401700	-0.13660800
H	-3.64395900	-0.39575900	1.87334600
H	-5.23226700	-0.38648200	1.08158700
H	-4.16661100	-0.61567600	-0.87932300
O	-5.61179700	-2.93588900	0.93845400
H	-4.44343900	-2.46277100	2.49959900
H	-5.55019000	-3.02212700	-0.02829100
C	-1.06486300	1.73379000	0.94217100
C	-1.39891400	1.83191700	-0.42419400
C	-1.99275500	2.59271800	1.70729700
O	-2.86158500	3.15330300	0.80231300
C	-2.56212700	2.77205900	-0.57021900
O	-2.06628000	2.81117500	2.89469300
C	-2.22880100	4.01423300	-1.40139800
H	-3.44626800	2.27770800	-0.98142700
O	-1.11186600	4.62434100	-0.79367700
O	-3.37464000	4.82609500	-1.40745600
H	-1.97904000	3.68203300	-2.41903700
H	-3.26851100	5.49944200	-2.09904000
H	-0.68735000	5.20994200	-1.44104300

Table S4 Cartesian coordinates of complex **4** $[Ni(L\text{-}asa)(H_2O)_2]$.

Optimized at B3LYP/lanl2dz/6-31g(d) level of theory

C	0.30044600	1.22277400	-0.03984300
C	-0.21580000	-0.00916300	-0.26090200
C	-0.75946000	2.19795900	-0.04669500
O	-1.95609400	1.50591600	-0.28472100
C	-1.70590500	0.08087500	-0.41562900
C	-2.52996600	-0.67252300	0.64945900
H	-2.03851500	-0.22829500	-1.41615800
C	-4.03564100	-0.39823300	0.54165600
O	-4.58177900	-1.07854300	-0.59581200
H	-4.24163700	0.67652400	0.50992500
H	-4.53500300	-0.82764000	1.41516700
H	-4.44246400	-0.52342800	-1.37944000
O	-2.30132300	-2.07007300	0.53080300
H	-2.17346200	-0.35903000	1.63752000
H	-2.93257800	-2.36320200	-0.15405400
O	-0.77717800	3.40986600	0.10234800
O	1.63937900	1.35148500	0.12995900
O	0.59758800	-1.05337700	-0.31452100
O	4.01107100	0.40548300	0.16778000
H	3.84996800	1.36202800	0.27962700
H	4.52914500	0.13140200	0.94601500
O	2.94463200	-2.13176500	-0.24861600
H	2.16721000	-2.69348200	-0.42693700
H	3.37948800	-2.52728200	0.52842100
Ni	2.26805100	-0.35320300	-0.01450500

Table S5 Cartesian coordinates of complex **5** $[Ni(L\text{-}asa)_2]^{2-}$.

Optimized at B3LYP/lanl2dz/6-31g(d) level of theory

C	-3.42443600	-2.04650600	0.61611600
O	-4.30827100	-0.98765000	0.67444100
C	-2.10909600	-1.45970400	0.31812000
C	-2.23941200	-0.08030400	0.20859500
C	-3.67270400	0.30267800	0.40410700
O	-0.92674900	-1.97213800	0.16258300
O	-1.17083500	0.59628800	-0.03098700
C	-4.34042800	0.95930700	-0.82861800
H	-3.81492200	0.93432900	1.28780000
C	-5.83886400	1.21615600	-0.61119000
O	-3.77167600	-3.19056700	0.79576300
O	-3.67996700	2.17857600	-1.10587200
H	-4.20238100	0.29491800	-1.68815700
H	-4.11886000	2.83753200	-0.53294600
O	-6.01568300	2.32736700	0.27117300
H	-6.35006500	0.31811600	-0.25055100
H	-6.27807000	1.50958200	-1.56903800
H	-6.05736300	1.99972200	1.18320100
O	1.62435200	-1.77561600	-0.27577600
O	1.40982000	0.80012600	-0.49046300
C	2.70236200	-1.09274400	-0.49981700
C	2.58362600	0.28875800	-0.60513500
C	4.11841600	-1.46296000	-0.65612200
O	4.80405800	-0.27893500	-0.85512100
C	3.92959700	0.89139700	-0.85754800
C	4.39593700	1.94236000	0.18048300
H	3.98484300	1.34476600	-1.85249600
C	4.53030100	1.39059700	1.60050400
O	3.51353700	3.05264700	0.10120800
H	5.37692200	2.30939000	-0.13795400
H	2.62616300	2.75320900	0.36572200
O	3.29496400	0.88321200	2.10631600
H	4.92631300	2.18435400	2.24488900
H	5.24255300	0.56050100	1.60622100
H	2.79679100	1.61809300	2.49687500
O	4.67449300	-2.53566200	-0.63018800
Ni	0.23114100	-0.59071100	-0.16268400

Table S6 Cartesian coordinates of complex **6** $[Ni(L\text{-}asa)_3]^{2-}$.

Optimized at B3LYP/lanl2dz/6-31g(d) level of theory

O	1.45260700	0.38306300	-1.23542900
O	-1.79080000	0.02215300	0.62025900
O	0.02782000	1.93162500	0.24555900
O	-0.03738500	-1.68257500	-0.46081600
O	-2.48117700	-0.57703400	-2.25611900
O	2.06597400	-0.03838500	1.38051400
C	1.20478700	-1.87612900	-0.74441600
C	2.00175400	-0.80373700	-1.10686400
C	3.34966000	-1.28361400	-1.40213500
O	3.33495800	-2.65614900	-1.20677500
C	2.01917200	-3.13547700	-0.78865600
C	2.18722600	-3.86650900	0.55268200
H	1.66793500	-3.83763600	-1.55299100
O	3.12149000	-4.93130300	0.40989800
C	0.89297000	-4.51375100	1.04234100
H	2.53758300	-3.14317400	1.30199800
O	1.11615100	-5.19321800	2.26855500
H	0.51740900	-5.20044000	0.26718000
H	0.13051600	-3.75195100	1.22383100
H	3.99764200	-4.53945800	0.26154300
H	1.90367100	-5.74467500	2.11881700
O	4.35550800	-0.69967100	-1.74238000
C	-3.21471600	-0.59817500	-1.30295700
C	-2.87828100	-0.30355100	0.15083200
C	-4.70635800	-0.95016700	-1.29072600
O	-5.15035300	-0.90058000	-0.01115800
C	-4.12898400	-0.49818300	0.95322300
O	-5.39534600	-1.23768200	-2.23073100
C	-4.63162400	0.77570100	1.70391900
H	-4.01268900	-1.32246600	1.66231000
C	-4.30522900	2.05412000	0.89443300
O	-4.10244700	1.79124000	-0.50477900
H	-3.36411400	2.47727800	1.25200700
H	-5.09969200	2.78980900	1.04505600
H	-4.93947100	1.91153800	-0.98396800
O	-5.98923600	0.61365400	2.04042800
H	-4.09851700	0.82587000	2.65710600
H	-6.49509900	0.46905400	1.22227500
C	2.19125800	1.17292600	1.14248800
C	1.21331000	2.13151100	0.64181700
C	3.43406100	1.98609700	1.42601000
O	3.15945300	3.30600400	1.23165100
C	1.80840600	3.51211700	0.75347100
O	4.51330600	1.59360600	1.79810000
C	1.82825200	4.27882900	-0.57536600
H	1.27077300	4.10980800	1.49757100
O	2.67258200	3.58476900	-1.46270400
O	2.29034800	5.57296600	-0.28005100
H	0.80013300	4.30561400	-0.96213700
H	2.22944000	6.10418300	-1.09145000
H	2.34064700	3.70165800	-2.36669000
Ni	-0.15313500	0.18903900	-0.31018600