

Electronic Supplementary Information

Interactions of neurokinin B with copper(II) ions and their potential biological consequences

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Supplementary Figures

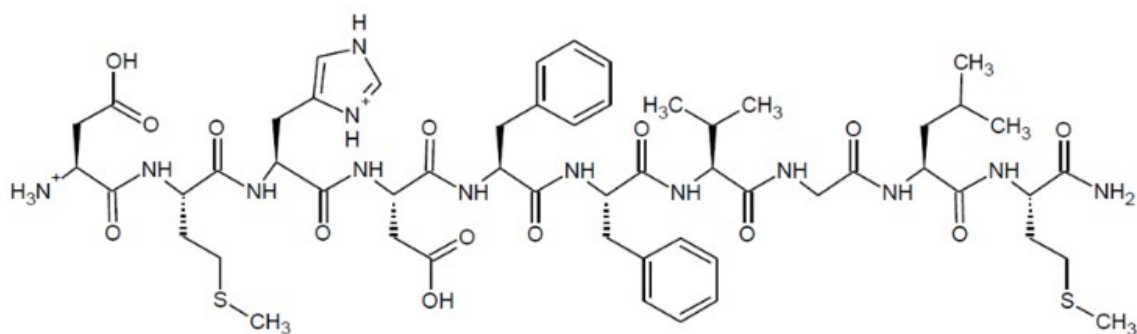


Figure S1. Molecular structure of neurokinin B (Asp-Met-His Asp-Phe-Phe-Val-Gly-Leu-Met-NH₂, DMHDFVGLM-NH₂) in its fully protonated form.

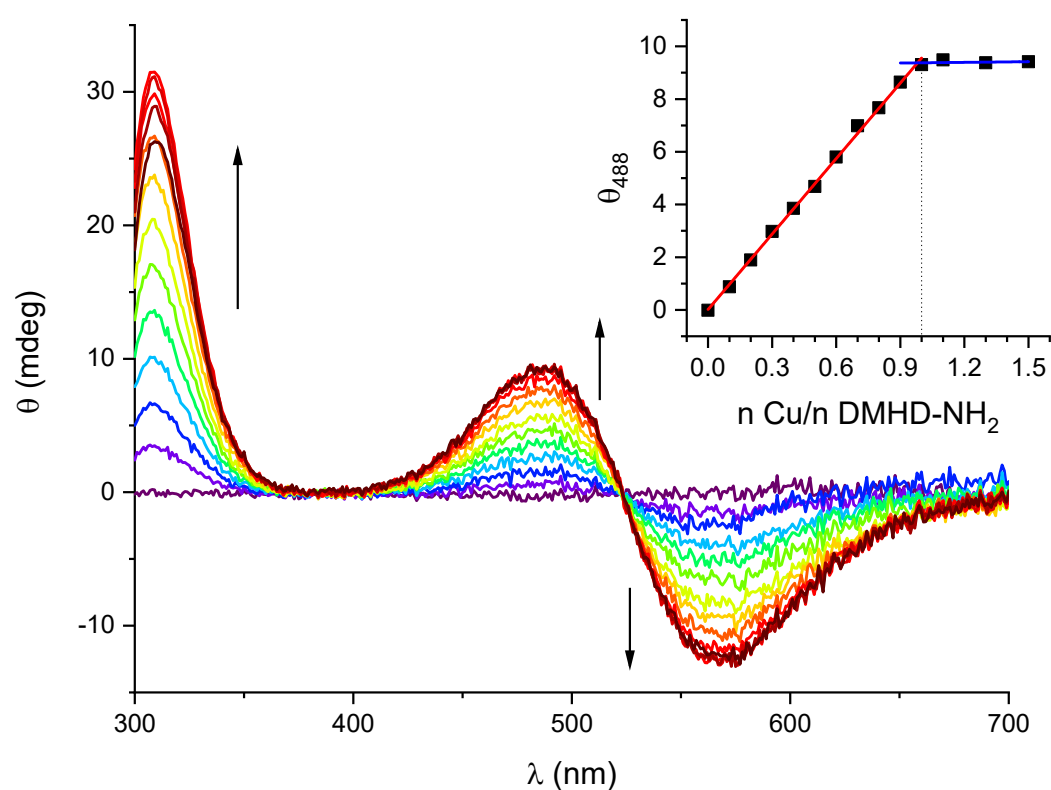


Figure S2. CD spectra of the titration of 1 mM DMHD-NH₂ with CuCl₂ at 25 °C, $l = 1$ cm. Inset presents the dependence of ellipticity at 488 nm on the Cu(II)/ DMHD-NH₂ ratio.

Supplementary Tables

Table S1. The Cu(II)..NKB distances in angstroms.

	CuHL ⁺ {1N}	CuHL ⁺ {1N}	CuL {2N}	CuH ₂ L ²⁻ {4N}
O _(COO-, Asp4)	1.879		1.901	
O _(COO-, Asp1)		1.820		
N _{1(imidazole, His3)}	1.885		1.932	1.894
O _(C=O, Met2)		1.995	2.066	
N _{2 (amide, Asp1)}				1.813
N _{3 (amide, Met2)}				1.852
N _{4 (NH2)}		1.936	1.973	1.881

Table S2. Hydrogen bonds of NKB complexes with Cu(II) cation.

	H...PA [Å]	PD-H...PA [deg]	Fragment
CuHL⁺ (the more stable form)			
Asp ₁ ..Asp ₁	1.868	136.8	N-H..O
Met ₂ ..NH ₂	2.179	152.2	N-H..N
His ₃ ..Asp ₄	1.930	149.2	N-H..O
CuHL⁺ (the less stable form)			
Met ₂ ..Asp ₄	1.841	164.9	N-H..O (helical)
Phe ₅ ..NH ₂	2.000	148.6	O..H-N
Leu ₉ ..Met ₁₀	2.058	152.2	O..H-N
CuL			
His ₃ ..Asp ₄	1.903	161.6	N-H..O
Leu ₉ ..Asp ₄	2.219	160.9	N-H..O
Val ₇ ..Leu ₉	1.936	162.2	N-H..O (helical)
CuH₂L²⁻			
Met ₂ ..Asp ₄	1.730	151.9	N-H..O (helical)
Phe ₅ ..Asp ₄	1.892	149.2	N-H..O
Asp ₄ ..Val ₇	1.618	173.9	O..H-O

Table S3. The Cartesian coordinates in angstroms and electronic energies in atomic units of the DFT optimized complexes.

CuH₂L²⁺ (1N)_a (-6344.113937 a.u.)

H	-2.93322700	6.48370700	-1.25038600
C	-1.76110900	4.83521000	-0.85153200
H	-0.76786100	4.51111500	-1.16723500
C	-2.90203600	4.05793400	-1.52075200
O	-4.00361900	4.59035800	-1.59767100
C	-1.90988500	4.71440500	0.66628300
H	-2.92570200	4.99909300	0.96547700
H	-1.77917700	3.66587400	0.94791700
C	-0.95000900	5.59759200	1.42627000
O	-0.47716800	6.63153000	0.98887900
N	-2.62677300	2.81108800	-1.93059500
H	-1.65932800	2.49586400	-1.97048000
C	-3.65498400	2.00812200	-2.57576200
H	-4.22864300	2.64161000	-3.25695900
C	-4.67461200	1.46013200	-1.57017200
O	-5.85943400	1.37339300	-1.85808100
C	-2.97556300	0.87155700	-3.34801400
H	-2.32137000	1.31988100	-4.10110300
H	-2.33187800	0.30682900	-2.66414800
C	-3.96097000	-0.08415900	-4.01033200
H	-4.51624700	-0.65595700	-3.26002800
H	-4.68852300	0.46248000	-4.61705700
S	-3.04487400	-1.25793000	-5.06263200
C	-4.31684900	-2.53325900	-5.26358000
H	-3.90252900	-3.30625600	-5.91259900
H	-4.57248200	-2.97872900	-4.29917400
H	-5.21470700	-2.12204400	-5.72930700
N	-4.13584800	1.01300500	-0.40587000
H	-3.19951800	1.32944300	-0.16510300
C	-4.95174800	0.54072300	0.69843800
H	-5.60171700	1.33089100	1.08629800
C	-4.01926800	0.16467000	1.84435400
O	-4.09627800	0.59070200	2.96377300
C	-5.82335900	-0.67409100	0.28474600
H	-6.58797800	-0.30589900	-0.39711300
H	-5.21028900	-1.37856200	-0.28835700
C	-6.45449500	-1.35712600	1.44881100
N	-5.72015500	-2.18324200	2.28711600
C	-7.72874400	-1.29979700	1.92465300
H	-8.59916700	-0.77650000	1.56647800
C	-6.53987900	-2.60947100	3.24107100
H	-6.28060700	-3.27180200	4.05121300
N	-3.06434200	-0.87420000	1.51754900
H	-2.91004200	-0.88893900	0.50610300
C	-1.76445600	-0.75510000	2.21719600
H	-1.96250800	-0.80647800	3.29029600
C	-1.18079700	0.63365000	1.89378600
O	-1.74530900	1.38809000	1.10198000

C	-0.77081600	-1.84571000	1.79498300
H	-0.45218600	-1.69841600	0.75534200
H	0.13738000	-1.73650300	2.38776000
C	-1.16226200	-3.31610900	1.93963900
O	-2.42909700	-3.63130900	1.96400200
N	-0.03835900	0.94186100	2.51964200
H	0.38028500	0.27241600	3.15028300
C	0.70676500	2.16095300	2.24009900
H	-0.01156900	2.89393600	1.88254900
C	1.60724100	1.89101900	1.02121900
O	1.16882000	2.09038900	-0.10692700
C	1.34424600	2.74642100	3.51761200
H	1.92371500	3.62388100	3.21665500
H	0.51195300	3.11366400	4.12450000
C	2.19711700	1.81605300	4.35373600
C	1.60536800	0.85206900	5.18045800
H	0.52347400	0.81522300	5.28024400
C	3.59436400	1.89692500	4.32669100
H	4.07784600	2.68046200	3.74866700
C	2.38695600	-0.03902200	5.91020900
H	1.90802200	-0.78146600	6.53966000
C	4.37841500	1.00376100	5.05329400
H	5.45953000	1.08242000	5.01042900
C	3.77608900	0.02442300	5.83755700
H	4.38478900	-0.67316200	6.40282400
N	2.82375300	1.36047100	1.27109400
C	3.80780700	1.10995500	0.23884100
H	3.25218400	0.99467900	-0.69534000
C	4.53993200	-0.21260600	0.48955200
O	5.62933000	-0.44770600	-0.03475400
C	4.79406300	2.28625900	0.06690000
H	5.35681800	2.42158500	0.99595000
H	5.50498700	2.00877600	-0.71460200
C	4.03261000	3.53538800	-0.29898900
C	3.52960300	4.38829200	0.68605200
H	3.81064900	4.23265600	1.72412100
C	3.70197700	3.78968000	-1.63177300
H	4.12587500	3.16226100	-2.41122000
C	2.66358900	5.42806000	0.35600300
H	2.26750600	6.07271000	1.13389000
C	2.84055400	4.82899000	-1.96991500
H	2.59118000	5.00482800	-3.01163200
C	2.30211200	5.64019700	-0.97222000
H	1.62206800	6.44559800	-1.22977900
N	3.90999200	-1.08127400	1.30170600
H	2.94483800	-0.89675300	1.53191100
C	4.50260600	-2.33801600	1.73085600
H	5.58561800	-2.19440700	1.66739000
C	4.13722700	-3.44413900	0.72569500
O	3.29890100	-4.31992500	0.94299000
C	4.14522700	-2.63734800	3.19706600
H	4.59924900	-1.81483700	3.76385300
C	2.64128200	-2.61523500	3.48940900

H	2.46521100	-2.89795900	4.53112000
H	2.23214300	-1.60423700	3.38282000
H	2.08644600	-3.29820200	2.84203300
C	4.79571500	-3.94153900	3.66371600
H	4.33371900	-4.80505300	3.17983200
H	5.86793800	-3.95295800	3.44174800
H	4.67596800	-4.05056100	4.74509100
N	4.81184300	-3.36925100	-0.44161400
H	5.41920400	-2.57194900	-0.59414600
C	4.61458500	-4.34047700	-1.50327800
H	5.50099000	-4.36208000	-2.13545800
H	4.47364800	-5.32506000	-1.04907000
C	3.41067800	-3.99274300	-2.38307400
O	3.53816600	-3.67415300	-3.56285300
N	2.22019900	-4.04613000	-1.74170900
H	2.24793800	-4.22291300	-0.73982300
C	1.02276000	-3.42480600	-2.28249000
H	1.03728500	-3.57201200	-3.36545000
C	1.12135400	-1.92799200	-1.95091900
O	1.30424500	-1.55351000	-0.79258700
C	-0.21389400	-4.10326700	-1.68827800
H	-0.09044700	-5.17382600	-1.88215700
H	-0.20016900	-3.98004400	-0.59792600
C	-1.56323300	-3.63653000	-2.26069000
H	-1.43757200	-3.42722500	-3.33102600
C	-2.60727200	-4.74561900	-2.10798100
H	-3.57772200	-4.42674900	-2.50104600
H	-2.30706700	-5.65329200	-2.63952900
H	-2.74064100	-4.99966600	-1.04961600
C	-2.08131000	-2.36415000	-1.58706500
H	-1.36414600	-1.53913400	-1.62189500
H	-3.00691500	-2.02592400	-2.06168800
H	-2.30318300	-2.59438100	-0.53914800
N	1.05074500	-1.07932500	-3.00242500
H	0.95009100	-1.45664100	-3.93382500
C	1.46289000	0.30111600	-2.87970900
H	1.52727700	0.51001600	-1.81038200
C	0.47816700	1.25617200	-3.53959300
O	-0.05862500	0.98947400	-4.60482200
C	2.82000800	0.55234200	-3.57183600
H	2.67721900	0.48851000	-4.65619800
H	3.11804200	1.58141100	-3.35001700
C	3.89884300	-0.43173500	-3.14596100
H	3.99038800	-0.48856800	-2.05891900
H	3.66649400	-1.43389300	-3.51140200
S	5.50852800	0.06453300	-3.83654000
C	6.49305200	-1.34645000	-3.26061500
H	7.47173400	-1.28993600	-3.73900300
H	6.61726700	-1.29663800	-2.17694200
H	6.00323100	-2.28032100	-3.54733400
N	0.31484400	2.44524800	-2.89163400
H	0.88745800	2.64022400	-2.07513100
N	-1.93193000	6.25537900	-1.27348100

H	0.02585100	3.22968600	-3.46045400
O	-0.28137200	-4.15704800	1.96960400
H	-1.59562400	6.41486200	-2.22443700
H	-1.39842300	6.85456600	-0.62059500
H	3.13835100	1.31097400	2.23249600
H	-8.56145700	-2.26952000	3.62872400
N	-7.75599800	-2.09461800	3.04520700
Cu	-3.89770000	-2.61637400	2.07914700
O	-0.70321400	5.14564500	2.64618800
H	-0.12887000	5.77857400	3.10536600

CuH₂L²⁺ (1N)_b (-6344.089182 a.u.)

C	-2.46465500	3.34197600	-0.31261100
H	-1.46238800	2.89712800	-0.34139600
C	-3.42578000	2.45890600	-1.11534500
O	-4.34403400	2.98955500	-1.79357100
C	-2.90056400	3.48218100	1.16152800
H	-3.01239200	2.48856300	1.60260700
H	-2.07822300	3.96744900	1.69911400
C	-4.14934500	4.30885000	1.55561000
O	-4.63793200	5.18979200	0.71427500
N	-3.24286800	1.15705800	-1.02349700
H	-2.45365700	0.83797800	-0.45691700
C	-4.21982600	0.16777600	-1.48750800
H	-4.93806400	0.69389200	-2.11713600
C	-4.97702600	-0.27765800	-0.22139300
O	-6.13105600	0.05529400	0.00165700
C	-3.50638700	-0.92636900	-2.28282200
H	-2.81426900	-0.43213100	-2.97091000
H	-2.88425200	-1.54196700	-1.62437200
C	-4.39995200	-1.82019000	-3.13719700
H	-5.01990200	-1.22263600	-3.81147600
H	-3.75555900	-2.44194000	-3.76238200
S	-5.50806300	-2.98574800	-2.26886600
C	-7.10254300	-2.11607500	-2.29883500
H	-7.82491200	-2.78051900	-1.82211800
H	-7.05893300	-1.17821600	-1.74509700
H	-7.40695200	-1.94125500	-3.33187500
N	-4.22269900	-0.98510000	0.66101800
H	-3.23306800	-1.07450600	0.46105200
C	-4.56274400	-1.04719600	2.08221700
H	-5.18161400	-0.18209500	2.32782900
C	-3.22962100	-0.82763700	2.80580100
O	-3.01290600	0.18586700	3.45438600
C	-5.37352600	-2.30177700	2.45362700
H	-5.54264800	-2.31121300	3.53250800
H	-6.35127500	-2.19799800	1.97376000
C	-4.77457900	-3.60655800	2.05317900
N	-4.61066700	-3.98808900	0.73305500
H	-4.86659200	-3.44248500	-0.10091900

C	-4.32925000	-4.65440200	2.80235500
H	-4.26961400	-4.77933900	3.86995900
C	-4.09794600	-5.21093700	0.67835800
H	-3.86807900	-5.76108900	-0.21806000
N	-3.92683000	-5.63263600	1.92509000
H	-3.51696800	-6.52041300	2.17887500
N	-2.25526500	-1.72819200	2.51710700
H	-2.46107200	-2.63255300	2.10879400
C	-0.86547600	-1.34766600	2.61454000
H	-0.55046300	-1.27445300	3.66024700
C	-0.69416800	0.01507700	1.91703400
O	-1.35678100	0.29409800	0.91821500
C	0.03223300	-2.33588000	1.85178000
H	-0.15502600	-2.22527600	0.77884600
H	1.07792800	-2.08768700	2.01916900
C	-0.21594400	-3.78237600	2.19001200
O	-1.29551500	-4.33139600	2.06483300
N	0.23703900	0.83022500	2.43254500
H	0.76974600	0.52937400	3.23757600
C	0.43668800	2.18070500	1.93316700
H	-0.53913300	2.53484300	1.60943100
C	1.26024200	2.14758400	0.63456900
O	0.68807500	2.15773300	-0.45435900
C	0.91392100	3.13647600	3.05182000
H	1.07799200	4.11480800	2.59124500
H	0.06828100	3.24674200	3.73700100
C	2.13603700	2.71227500	3.83907600
C	2.03022000	1.76606500	4.86564200
H	1.05152100	1.39777900	5.16431000
C	3.40078800	3.24290500	3.55618800
H	3.49966000	4.02275300	2.80601600
C	3.16167400	1.31355700	5.53927000
H	3.05799500	0.57223800	6.32458600
C	4.53429700	2.79194000	4.22781800
H	5.50443900	3.21191200	3.98479900
C	4.41925300	1.81272600	5.21105700
H	5.30162000	1.45372100	5.72969000
N	2.59342000	2.05849400	0.77239000
C	3.53042400	2.05767100	-0.33920600
H	3.00761300	1.61724700	-1.19165200
C	4.70530100	1.15527400	0.07052300
O	5.84145900	1.59179500	0.20546500
C	4.00811300	3.46789100	-0.71699900
H	4.53332700	3.90107700	0.13868000
H	4.73549800	3.35981800	-1.52651900
C	2.85906100	4.34460500	-1.14644700
C	2.21819500	5.18686600	-0.23663800
H	2.60270500	5.27399100	0.77594900
C	2.37374600	4.27912200	-2.45560400
H	2.88753000	3.65265000	-3.18050600
C	1.10348200	5.93146900	-0.61658900
H	0.62427100	6.58994700	0.10137800
C	1.25804500	5.01449900	-2.84089700

H	0.89451900	4.95172300	-3.86159900
C	0.61847600	5.84341200	-1.91938000
H	-0.23326200	6.44320400	-2.22725100
N	4.36698300	-0.13470100	0.31605100
H	3.41056100	-0.44670100	0.15792600
C	5.23918300	-1.00277100	1.09750600
H	6.25174300	-0.60909000	0.96312200
C	5.20407200	-2.40448000	0.47594900
O	4.68243700	-3.38121900	1.01201900
C	4.90126600	-0.92596900	2.59981500
H	5.05063700	0.13169300	2.85467000
C	3.44512700	-1.27072000	2.91672000
H	3.24006700	-1.08589900	3.97465000
H	2.76030700	-0.64275800	2.33634700
H	3.23723500	-2.31977800	2.69474400
C	5.87698400	-1.74683400	3.44342500
H	5.73748100	-2.81697900	3.27224500
H	6.91643000	-1.49236000	3.21181400
H	5.71119700	-1.54525100	4.50575700
N	5.79230900	-2.47994100	-0.73938900
H	6.14340700	-1.63460500	-1.16292900
C	5.74022800	-3.68074700	-1.55526600
H	6.54384300	-3.65019600	-2.28898500
H	5.86992400	-4.55133300	-0.90851500
C	4.40097900	-3.73713900	-2.29281500
O	4.28915600	-3.44619900	-3.47881800
N	3.35653600	-4.07802200	-1.49720000
H	3.54490900	-4.11526400	-0.49832100
C	1.98698600	-3.80457800	-1.89615100
H	1.90556400	-4.03848300	-2.96086900
C	1.75972700	-2.30122200	-1.67557500
O	2.02919800	-1.77631800	-0.58960500
C	1.03849200	-4.70485000	-1.09632700
H	1.53120900	-5.68110500	-1.04399200
H	0.98086900	-4.33718100	-0.06558700
C	-0.36434100	-4.90832200	-1.69033800
H	-0.23731900	-5.10874200	-2.76260200
C	-1.01406300	-6.14093900	-1.05486600
H	-1.98065400	-6.35120400	-1.52394600
H	-0.38895000	-7.03061100	-1.17453100
H	-1.17522200	-5.98019100	0.01756300
C	-1.28934800	-3.69651900	-1.54109300
H	-0.88249900	-2.79265100	-2.00261200
H	-2.25435200	-3.90047800	-2.01773600
H	-1.48636300	-3.49318300	-0.48164200
N	1.31733100	-1.61224200	-2.74043200
H	1.09124500	-2.09765500	-3.59692800
C	1.19610100	-0.17546800	-2.74405100
H	1.26518400	0.15524200	-1.70512600
C	-0.15529500	0.23578000	-3.32592500
O	-0.78190300	-0.51256800	-4.07140600
C	2.30903800	0.48879900	-3.57957600
H	2.10494800	0.33930800	-4.64529000

H	2.25532500	1.56626500	-3.39541900
C	3.69729500	-0.05212200	-3.24382000
H	3.82548100	-0.16668400	-2.16403400
H	3.84920100	-1.03931700	-3.68737600
S	4.96371500	1.10156300	-3.86543100
C	6.45100000	0.33743400	-3.16661100
H	7.31464100	0.84321400	-3.60060900
H	6.48282700	0.47206500	-2.08155700
H	6.49895500	-0.72075500	-3.43421900
N	-0.53646600	1.48673700	-3.01164300
H	-0.03520600	2.02556900	-2.31525700
H	-1.35503600	1.87572000	-3.45277800
O	-4.58326100	4.16127400	2.68256000
O	0.87895200	-4.41792800	2.58953100
H	0.65528200	-5.34929800	2.74220100
H	2.98030800	2.10441600	1.70618200
H	-2.00063900	5.35915500	-0.40159600
H	-1.98737800	4.63414500	-1.86929400
N	-2.47314100	4.66245000	-0.97365600
Cu	-4.39946900	4.84309800	-1.05668000

CuHL⁺ (2N) (-6343.666641 a.u.)

C	-7.51955700	2.77348100	-1.65369300
H	-8.12988800	3.46444200	-2.24076600
C	-6.74851300	1.89763300	-2.65439000
O	-7.39343100	1.30086600	-3.50251900
C	-6.72196500	3.56954800	-0.62095700
H	-6.06889700	4.27381000	-1.13963800
H	-7.43344600	4.15771300	-0.03248900
C	-5.87939700	2.73839900	0.35566200
O	-6.51826000	1.89688100	1.11359700
N	-5.41017500	1.70190200	-2.46151700
H	-4.94976600	2.24145700	-1.73446300
C	-4.90313500	0.33509600	-2.64161000
H	-5.55070500	-0.13609600	-3.38267200
C	-5.26405200	-0.29881200	-1.29081200
O	-6.46408700	-0.61352400	-1.09384800
C	-3.45694100	0.28909200	-3.13231200
H	-3.38030600	1.03685600	-3.92698500
H	-2.74075200	0.59506600	-2.36285200
C	-3.05945300	-1.05608600	-3.74356400
H	-3.77689100	-1.33419300	-4.52128600
H	-2.07461500	-0.96499800	-4.20803200
S	-3.01332200	-2.42584200	-2.53259500
C	-3.18769700	-3.84926100	-3.63999700
H	-3.12236400	-4.74577800	-3.02204900
H	-4.15891300	-3.82459100	-4.13732100
H	-0.46137200	-2.92280800	-4.24385000
N	-4.33679400	-0.32785900	-0.34694700
H	-3.41447500	0.06831600	-0.54494600
C	-4.54534300	-0.70245300	1.05382100

H	-5.02084900	0.13606600	1.56953200
C	-3.14906300	-0.82609800	1.66662300
O	-2.84996800	-0.25260500	2.70142100
C	-5.37524900	-2.00256100	1.23845800
H	-5.58198500	-2.44445800	0.26159900
H	-4.79023200	-2.73844000	1.79451600
C	-6.64819400	-1.77363300	1.98810300
N	-7.55889400	-0.77802800	1.67349800
C	-7.11657400	-2.44993400	3.07559500
H	-6.70607000	-3.27868900	3.62780000
C	-8.54664500	-0.86215700	2.55451500
H	-9.41497600	-0.22379200	2.59516000
N	-8.31304900	-1.86354500	3.40913400
H	-8.91470500	-2.12974600	4.17435900
N	-2.27327100	-1.58824000	0.94945100
H	-2.60779600	-1.95422000	0.06434500
C	-0.87061800	-1.24406400	0.97164100
H	-0.56235700	-1.11697500	2.01324100
C	-0.68893300	0.11017900	0.25205900
O	-1.62314600	0.67141300	-0.32565900
C	-0.04227500	-2.33484100	0.30816000
H	-0.46010200	-2.56600000	-0.67780300
H	0.99464300	-2.01386500	0.15338200
C	0.00857600	-3.59864800	1.12690900
O	-0.37552400	-3.72731600	2.26433100
N	0.52952800	0.66012600	0.33407700
H	1.26273200	0.15649600	0.81316500
C	0.81854700	1.99120500	-0.18986000
H	0.47235000	2.03835600	-1.22390200
C	2.33901300	2.14311700	-0.26044900
O	2.90533000	2.34010800	-1.32757100
C	0.10242500	3.12444900	0.60252300
H	0.50382500	4.07692900	0.24276000
H	-0.95043600	3.08377000	0.31450500
C	0.21762200	3.02124200	2.10482900
C	-0.63279500	2.17023200	2.81886700
H	-1.43111000	1.64209600	2.30705400
C	1.19249500	3.73207500	2.81319700
H	1.84064100	4.42202900	2.28119400
C	-0.48264400	1.99977800	4.19108700
H	-1.14751300	1.32389200	4.71875200
C	1.34803900	3.56186100	4.18729800
H	2.11811800	4.11635600	4.71375500
C	0.51631800	2.68545800	4.87862800
H	0.64044100	2.54451600	5.94722400
N	2.97373900	1.98089700	0.92307500
C	4.41299700	1.91784100	1.10704200
H	4.83681200	1.58781500	0.15397200
C	4.70434700	0.83498800	2.16442700
O	5.44014200	1.03767200	3.12378400
C	5.04298600	3.26658600	1.47741700
H	4.50318700	3.69345400	2.32850800
H	6.06569900	3.07155400	1.80970000

C	5.03883500	4.20292500	0.29561900
C	4.05044000	5.17272300	0.13132500
H	3.30452000	5.31659700	0.90743400
C	6.00632500	4.05691200	-0.70280000
H	6.79769800	3.32180400	-0.57324900
C	4.00875900	5.95992900	-1.01728300
H	3.22951300	6.70704300	-1.13018900
C	5.96951700	4.83853800	-1.85262200
H	6.72530400	4.70624500	-2.62022900
C	4.96242600	5.78884400	-2.01679600
H	4.92871700	6.39789300	-2.91438400
N	4.06846700	-0.33711700	1.94716700
H	3.61176200	-0.50175300	1.05208800
C	4.14201200	-1.43201200	2.90341000
H	5.17827500	-1.50990300	3.25128500
C	3.75604500	-2.69571100	2.14050400
O	2.60975100	-2.87683600	1.74020000
C	3.25782300	-1.18843200	4.15030900
H	3.70876600	-0.31906300	4.64181900
C	1.80171300	-0.84474800	3.82984900
H	1.28088700	-0.54985600	4.74506700
H	1.73117100	0.00149000	3.13859500
H	1.28172500	-1.69892000	3.38947100
C	3.35387800	-2.38339500	5.10056500
H	2.88061100	-3.26973300	4.66378000
H	4.39545000	-2.63024600	5.33034300
H	2.84346000	-2.16464200	6.04216200
N	4.74627700	-3.58310400	1.90494800
H	5.69222900	-3.35506200	2.16760000
C	4.53352700	-4.69833800	0.99704100
H	5.34731900	-5.41166200	1.11965300
H	3.58746600	-5.18447600	1.24126500
C	4.55340100	-4.16207800	-0.43580600
O	5.61018500	-3.88609000	-0.99618600
N	3.33942300	-3.94681500	-0.99617900
H	2.53104500	-4.00724500	-0.38640600
C	3.23626000	-3.09396800	-2.16361800
H	3.94736900	-3.46203300	-2.90841700
C	3.65002500	-1.67026400	-1.77705000
O	3.24114200	-1.13443800	-0.73935000
C	1.81913400	-3.15871000	-2.75487600
H	1.72076900	-4.14652700	-3.21571000
H	1.08938000	-3.12895800	-1.94246900
C	1.46580200	-2.06197500	-3.78081800
H	2.37172900	-1.79271000	-4.33973000
C	0.44017200	-2.60311800	-4.77805800
H	0.14955500	-1.83564000	-5.50189200
H	0.83008100	-3.46410000	-5.32896400
H	-2.39133700	-3.87208900	-4.38581500
C	0.91510600	-0.79158300	-3.11529900
H	1.59307100	-0.36676700	-2.37132700
H	0.71680300	-0.02241500	-3.86818700
H	-0.03408700	-1.01378600	-2.60998800

N	4.45817300	-1.06608700	-2.65722900
H	4.75257400	-1.55148200	-3.49362600
C	4.92728100	0.28884000	-2.50386500
H	4.27480700	0.77189800	-1.77745400
C	4.80491700	0.99925900	-3.85149100
O	4.95568600	0.38345500	-4.90327900
C	6.38498500	0.34920600	-2.01527900
H	7.05568600	0.01128300	-2.81274400
H	6.62031300	1.40047300	-1.81827500
C	6.59592300	-0.49609400	-0.76108700
H	5.78787800	-0.33685300	-0.04324400
H	6.59336600	-1.56190800	-1.00578900
S	8.16831600	-0.05490200	0.04432600
C	8.00733500	-1.03822000	1.55942700
H	8.95465500	-0.97082200	2.09632200
H	7.21110300	-0.64060400	2.19383600
H	7.81417900	-2.08550900	1.31575700
N	4.59659000	2.32453000	-3.76471300
H	4.29809500	2.74045300	-2.89160200
H	4.51211200	2.86181500	-4.61368800
O	-4.66156400	2.89821900	0.39270700
O	0.54889100	-4.60235800	0.41556900
H	0.60215200	-5.38045000	0.98964300
H	2.41386900	2.02987400	1.76585600
H	-9.11340500	2.29981900	-0.43981300
H	-8.92979600	1.29596800	-1.71266500
N	-8.41617500	1.78871200	-0.98103000
Cu	-7.52650100	0.53356800	0.25503100

CuH₁L⁰ (3N) (-6343.206025 a.u.)

C	-8.10744800	-1.67251900	0.31475800
H	-8.63779400	-2.29421200	1.04212000
C	-6.63966400	-2.12424200	0.27266600
O	-6.31186200	-3.29368300	0.49443700
C	-8.75042800	-1.83870100	-1.07210000
H	-8.10225600	-1.35037700	-1.81280600
H	-8.78135400	-2.90070300	-1.32166200
C	-10.16867000	-1.23110300	-1.24090400
O	-10.96851300	-1.85929100	-1.95313200
N	-5.83796300	-1.10458300	-0.07558100
C	-4.38677700	-1.21653000	-0.09538900
H	-4.02242300	-1.90694200	0.67216100
C	-3.99403400	0.18197100	0.36788400
O	-3.54457400	0.43342000	1.46937700
C	-3.81881700	-1.59995100	-1.47021800
H	-4.46598800	-1.16700600	-2.24424000
H	-2.81870300	-1.17306400	-1.59397100
C	-3.76258700	-3.11246600	-1.69259800
H	-4.70635400	-3.58309200	-1.40763200
H	-3.58193100	-3.31827800	-2.74967200

S	-2.41306700	-3.91055900	-0.74665700
C	-3.32611200	-4.85049500	0.51258200
H	-2.60255500	-5.13030300	1.28042900
H	-4.11837800	-4.23713800	0.94490400
H	-3.76489800	-5.75407900	0.08497400
N	-4.45405300	1.18424200	-0.51053200
H	-4.39938700	0.88240200	-1.48003700
C	-4.10153000	2.61840800	-0.37717300
H	-4.48891700	3.08514400	-1.28361700
C	-2.58361100	2.85067800	-0.46028100
O	-2.10304900	3.38126600	-1.45373600
C	-4.79342100	3.27449600	0.82978800
H	-4.64242800	2.66870300	1.72794100
H	-4.32647300	4.24431500	1.01424500
C	-6.24971400	3.48982500	0.56556100
N	-7.08349100	2.45639600	0.17792300
C	-6.98383400	4.63832000	0.60211300
H	-6.71367500	5.65165900	0.84798900
C	-8.28956400	2.97098900	-0.01032400
H	-9.16747300	2.42218500	-0.31826000
N	-8.26244900	4.28575900	0.23982500
H	-9.05181300	4.91033400	0.16725900
N	-1.84624400	2.44869000	0.60444300
H	-2.32661800	1.84463600	1.26463300
C	-0.43972300	2.19455200	0.40663400
H	0.01389300	3.09168200	-0.02522600
C	-0.27502400	1.06148500	-0.63919100
O	-1.23502400	0.43184000	-1.07190200
C	0.22670400	1.88498300	1.75382700
H	-0.30070200	2.41337400	2.55106700
H	0.17765700	0.81516300	1.97763600
C	1.68387000	2.26251400	1.82251400
O	2.41477800	2.38274400	0.84951200
N	0.99253300	0.88303200	-1.05200800
H	1.69714600	1.47559300	-0.61639700
C	1.32249100	0.12358500	-2.23989900
H	0.60593300	-0.69386100	-2.32261400
C	2.68074300	-0.54759500	-2.04504200
O	2.78422500	-1.77067700	-2.02554100
C	1.21358900	0.99215800	-3.52903900
H	1.64963000	0.43277800	-4.36306200
H	0.14377700	1.09733100	-3.73060500
C	1.83553100	2.36520800	-3.41334800
C	1.14616800	3.40384700	-2.77501200
H	0.12779700	3.24736100	-2.42708400
C	3.12076800	2.62445400	-3.90004900
H	3.65597200	1.84336900	-4.43054200
C	1.74606100	4.64591900	-2.59036700
H	1.19762500	5.43593800	-2.08701000
C	3.72434800	3.86697900	-3.71637200
H	4.72531700	4.03972000	-4.09801000
C	3.04059200	4.87936200	-3.05049600
H	3.50895600	5.84619800	-2.89914900

N	3.74056400	0.27814000	-1.85197300
C	5.09766300	-0.22405800	-1.73653000
H	5.01860300	-1.24830300	-1.35845700
C	5.92369400	0.55247600	-0.70371300
O	7.15002800	0.49283700	-0.73305800
C	5.83667100	-0.26521300	-3.08706300
H	5.81890000	0.73459000	-3.53440900
H	6.88079700	-0.50208400	-2.87122000
C	5.24908200	-1.28345000	-4.03305000
C	4.52522100	-0.89937500	-5.16104800
H	4.42269800	0.15470200	-5.40214100
C	5.40115900	-2.64876900	-3.76990700
H	5.96365100	-2.96426500	-2.89400800
C	3.94753100	-1.85153100	-6.00043100
H	3.38665400	-1.53102200	-6.87271600
C	4.83204500	-3.60221100	-4.60478600
H	4.96171800	-4.65757800	-4.38635100
C	4.09665800	-3.20584300	-5.72215300
H	3.65028700	-3.95000500	-6.37392500
N	5.25619300	1.25349600	0.24377400
H	4.24543000	1.33179000	0.22035800
C	6.00122900	2.13111400	1.13900000
H	6.98381300	1.66410500	1.26090300
C	5.32094600	2.12587500	2.51105600
O	4.62916700	3.06870700	2.92110500
C	6.24542200	3.52495100	0.52357300
H	6.84268600	3.30815800	-0.37145500
C	4.97876400	4.24903700	0.06605700
H	5.25351300	5.17592000	-0.44701400
H	4.39958300	3.64592900	-0.63810200
H	4.33464100	4.49273100	0.91205600
C	7.10079300	4.39139800	1.45073900
H	6.54343500	4.67695800	2.34697000
H	8.00987900	3.86648100	1.76287900
H	7.40389600	5.30678300	0.93493000
N	5.52968100	1.02064800	3.24207700
H	6.07823200	0.26779200	2.85031000
C	4.92968600	0.79385000	4.54512300
H	5.71243000	0.61149300	5.28508300
H	4.38184000	1.69176500	4.82872000
C	4.05444200	-0.45095100	4.45535500
O	4.57291800	-1.54785700	4.26592300
N	2.71675500	-0.26840900	4.54643100
H	2.36984900	0.67777000	4.44100000
C	1.83490700	-1.32527100	4.07670700
H	2.10589900	-2.24890900	4.59572100
C	2.08891200	-1.49978700	2.57593700
O	2.29343500	-0.51983300	1.85850900
C	0.37386100	-0.98065200	4.39645300
H	0.30141200	-0.91569200	5.48702900
H	0.14135400	0.02024600	4.01171000
C	-0.66260300	-1.99048400	3.86273900
H	-0.21506400	-2.99303700	3.90120700

C	-1.89898700	-1.99994000	4.76596100
H	-2.64649600	-2.70752200	4.39429400
H	-1.64339700	-2.28097000	5.79224200
H	-2.36249300	-1.00702000	4.79234700
C	-1.08858300	-1.70507400	2.41770200
H	-0.24789200	-1.63924400	1.72303000
H	-1.74588000	-2.49820400	2.04773400
H	-1.65164900	-0.76815400	2.36267400
N	2.07827600	-2.76045000	2.11037200
H	1.85841200	-3.53862600	2.71471700
C	2.30900300	-3.03441000	0.71379900
H	2.18612400	-2.08533600	0.19231700
C	1.26061900	-4.02156100	0.20238100
O	0.65184100	-4.76598800	0.96730400
C	3.73839100	-3.54462600	0.45409500
H	3.85732800	-4.54867800	0.87749300
H	3.87938300	-3.61489900	-0.62860100
C	4.76380800	-2.59723100	1.06830500
H	4.57719200	-1.56929500	0.74097000
H	4.68490000	-2.60293100	2.15814700
S	6.45615800	-3.09370500	0.61652600
C	7.38510900	-1.94409900	1.67023000
H	8.42274500	-2.27986600	1.70024100
H	7.35902300	-0.93511600	1.25044200
H	6.97768300	-1.96049900	2.68494900
N	1.11293600	-4.01489500	-1.13490500
H	1.54932900	-3.28365300	-1.68863200
H	0.37847300	-4.57653400	-1.53843500
O	-10.38445700	-0.10911800	-0.67733600
O	2.09049100	2.47824500	3.06007400
H	3.05100200	2.74736500	3.04207500
H	3.62826300	1.25168900	-2.11256100
H	-9.08922800	0.08506400	0.34020900
H	-8.16161400	-0.16288700	1.72494300
N	-8.16670200	-0.24968800	0.71137800
Cu	-6.55413700	0.62755500	-0.01084600

CuH₂L⁻¹ (4N) (-6342.563242 a.u.)

C	-8.44167100	1.16290000	0.53051300
H	-9.29604300	1.70288400	0.11728900
C	-7.16172300	1.92299700	0.22583000
O	-7.06283500	3.14116100	0.21076800
C	-8.61870200	0.96345200	2.04558100
H	-7.66370200	0.62862700	2.47143800
H	-8.86448700	1.91823600	2.51113900
C	-9.67846000	-0.09277500	2.44376100
O	-10.30048500	0.07467700	3.49393600
N	-6.12986800	1.05296100	0.03912700
C	-4.80564400	1.45887500	-0.39809100
H	-4.87482400	2.27904600	-1.11870000

C	-4.23091500	0.22780600	-1.08242300
O	-3.39895300	0.30949300	-1.98514100
C	-3.85619600	1.82682300	0.75482600
H	-3.94488400	1.04587500	1.51684600
H	-2.82584100	1.78185000	0.38523400
C	-4.12873600	3.17863600	1.40598700
H	-5.18718600	3.27341600	1.65520800
H	-3.54344100	3.26810500	2.32442300
S	-3.70738600	4.56846400	0.29514000
C	-4.86030100	5.81535600	0.93252500
H	-4.71617700	6.72791400	0.35186700
H	-5.88580800	5.46139700	0.81074200
H	-4.66032400	6.02916400	1.98447000
N	-4.70384100	-0.90953900	-0.49383000
C	-4.19290400	-2.25826900	-0.74226700
H	-4.55524200	-2.85384900	0.09785700
C	-2.67058300	-2.46607300	-0.59251700
O	-2.27561500	-3.28893900	0.22938900
C	-4.80055800	-2.85837300	-2.02144500
H	-4.72680400	-2.13682000	-2.84095800
H	-4.27195800	-3.76559100	-2.32236100
C	-6.21954600	-3.21127600	-1.70033500
N	-6.98141300	-2.43839000	-0.83356500
C	-6.94272200	-4.32235200	-2.01041700
H	-6.70839000	-5.17012200	-2.63187900
C	-8.12850200	-3.07922600	-0.62888400
H	-8.93372400	-2.76433200	0.01711700
N	-8.13295300	-4.21285200	-1.33108200
H	-8.88394700	-4.88772400	-1.33670700
N	-1.84418300	-1.79043800	-1.41535500
H	-2.26237500	-0.99164800	-1.89395800
C	-0.44066800	-1.73304900	-1.09663900
H	-0.07073900	-2.75556300	-0.97232600
C	-0.24580200	-1.01592200	0.26391100
O	-1.15424800	-0.42547400	0.83365700
C	0.31603300	-1.05329700	-2.24523700
H	-0.20384600	-1.24140400	-3.18723700
H	0.35265900	0.02967000	-2.09955400
C	1.74587800	-1.49950300	-2.40134600
O	2.41926200	-2.00253500	-1.51394400
N	1.00172000	-1.14591000	0.76231500
H	1.66804800	-1.65761300	0.18831300
C	1.32203100	-0.84589000	2.13999600
H	0.62288500	-0.08093100	2.47786400
C	2.69843700	-0.18791100	2.20196200
O	2.82376600	0.98205400	2.55341100
C	1.15587300	-2.09104200	3.06000300
H	1.60448700	-1.86764500	4.03348000
H	0.08000100	-2.20909300	3.21752800
C	1.71577600	-3.37363500	2.48877200
C	0.99749900	-4.08919600	1.52181900
H	0.00263700	-3.75950000	1.23065100
C	2.96955100	-3.85704100	2.87690500

H	3.52470900	-3.33813800	3.65248300
C	1.54005200	-5.22795600	0.93424300
H	0.97093100	-5.76565600	0.18246500
C	3.51470000	-4.99771000	2.29039300
H	4.49165100	-5.35025500	2.60474400
C	2.80369800	-5.68103200	1.30905100
H	3.22717400	-6.56566900	0.84517000
N	3.75078100	-0.94330700	1.79740900
C	5.11630400	-0.45790900	1.86628400
H	5.05779700	0.63447400	1.82008800
C	5.95328200	-0.89847200	0.65930900
O	7.17886700	-0.91422300	0.73656600
C	5.82344700	-0.84371000	3.17898100
H	5.81939000	-1.93432300	3.28059500
H	6.86576000	-0.53240700	3.08352700
C	5.18120300	-0.19476200	4.37975700
C	4.38416400	-0.92596200	5.25956900
H	4.27304300	-1.99753900	5.12124100
C	5.34237300	1.17596500	4.60500000
H	5.96170600	1.75905900	3.92724000
C	3.74193900	-0.30366200	6.32949600
H	3.12284900	-0.89071400	7.00051900
C	4.70898300	1.80117400	5.67220200
H	4.84510300	2.86616900	5.83180800
C	3.89989700	1.06266300	6.53585400
H	3.40253800	1.55029900	7.36817400
N	5.29616200	-1.21771300	-0.48195500
H	4.28275800	-1.24923000	-0.50704100
C	6.04321300	-1.78698100	-1.59809900
H	7.04351900	-1.34612500	-1.53664900
C	5.41696600	-1.30949600	-2.91200500
O	4.70735000	-2.03776500	-3.61999200
C	6.22144400	-3.31434100	-1.46737100
H	6.79381600	-3.42783500	-0.53788900
C	4.91507800	-4.09148800	-1.30059900
H	5.13829700	-5.14687000	-1.11572600
H	4.33399300	-3.72731800	-0.44940400
H	4.29276400	-4.01327800	-2.19288100
C	7.07764900	-3.86589100	-2.60947200
H	6.54503800	-3.80637400	-3.56238000
H	8.01997300	-3.31626900	-2.70587100
H	7.32026800	-4.91571200	-2.42249700
N	5.69754000	-0.04118300	-3.24747500
H	6.26389500	0.51924400	-2.62632200
C	5.16086800	0.61555300	-4.42682100
H	5.98041400	0.98787500	-5.04571300
H	4.59519700	-0.11895000	-4.99866500
C	4.32497100	1.80538400	-3.96899800
O	4.87288400	2.76099200	-3.42706000
N	2.98442400	1.72156700	-4.14512800
H	2.60254100	0.80309500	-4.34062500
C	2.13490800	2.60422600	-3.36027300
H	2.45053600	3.63411600	-3.54809900

C	2.37316800	2.26992800	-1.88484100
O	2.53304300	1.10254100	-1.52601400
C	0.66438100	2.44856200	-3.77440400
H	0.59977900	2.77071500	-4.81887400
H	0.38830600	1.38714500	-3.76288300
C	-0.33705600	3.25205600	-2.91956900
H	0.14415700	4.19540100	-2.62803700
C	-1.57548200	3.60277100	-3.74931300
H	-2.30157400	4.15641800	-3.14589900
H	-1.31512600	4.21415300	-4.61884400
H	-2.06625700	2.69106900	-4.10854400
C	-0.77420800	2.51854400	-1.64420300
H	0.06000400	2.13922500	-1.04995500
H	-1.34542100	3.19608600	-1.00174500
H	-1.42945800	1.67662700	-1.89135800
N	2.39122700	3.30879200	-1.03340400
H	2.21615700	4.25063300	-1.35275300
C	2.56794200	3.10218300	0.38269500
H	2.39362600	2.04222300	0.56489900
C	1.53362100	3.92727600	1.14625000
O	1.06436100	4.95957400	0.67328600
C	3.99787100	3.44069900	0.84171600
H	4.15899900	4.52341900	0.78692200
H	4.09547300	3.13635900	1.88841100
C	5.02282700	2.71806400	-0.02690300
H	4.79274500	1.64882700	-0.08049500
H	4.99407600	3.10075400	-1.05018000
S	6.70632100	2.95175100	0.62609700
C	7.63825500	2.14301300	-0.70499000
H	8.69401700	2.38117900	-0.56783300
H	7.51852100	1.05806500	-0.64723300
H	7.31075200	2.52585700	-1.67541700
N	1.22864600	3.43487500	2.35932000
H	1.62207500	2.55153200	2.67014200
H	0.58641100	3.94047900	2.94875900
O	-9.78841500	-1.10563100	1.65983200
O	2.20047400	-1.30701900	-3.62788200
H	3.14348100	-1.62666200	-3.67419000
H	3.61542900	-1.94629800	1.73546200
H	-8.96828100	-0.78114900	0.53864600
H	-8.71002100	-0.12427200	-1.06207100
N	-8.32647600	-0.15711300	-0.11831300
Cu	-6.52824000	-0.69086000	-0.25793500

NiH₂L²⁺ (1N)_a (-6211.964099 a.u.)

H	-3.03424800	6.23213600	-1.85458700
C	-1.85458500	4.65204600	-1.25229400
H	-0.84925700	4.30988400	-1.50282800
C	-2.96842900	3.79780200	-1.87053000

O	-4.07394900	4.30555300	-2.02246500
C	-2.04337300	4.67905000	0.26644700
H	-3.07294200	4.96663200	0.51079900
H	-1.89768400	3.66681800	0.65316900
C	-1.12504900	5.65822400	0.95836700
O	-0.68094100	6.66639800	0.43846500
N	-2.66766500	2.52296100	-2.15641100
H	-1.69618500	2.22084200	-2.14409600
C	-3.67434200	1.64565500	-2.73515500
H	-4.27476500	2.22007600	-3.44480400
C	-4.66749100	1.13859400	-1.68137000
O	-5.85268500	1.00353500	-1.94836700
C	-2.97324400	0.48656900	-3.45181800
H	-2.35052000	0.90822200	-4.24575400
H	-2.29665200	-0.01593000	-2.75191000
C	-3.94508000	-0.53381600	-4.03345300
H	-4.48065800	-1.06277400	-3.23837700
H	-4.69000600	-0.04486800	-4.66793900
S	-3.01712500	-1.75907700	-5.01291900
C	-4.30063700	-3.02449700	-5.20085100
H	-3.87171500	-3.83663500	-5.78975000
H	-4.60381200	-3.41509700	-4.22663000
H	-5.17171800	-2.62581500	-5.72475000
N	-4.10773800	0.79715400	-0.49105900
H	-3.17717900	1.15307300	-0.28637200
C	-4.91433500	0.44333700	0.66379800
H	-5.56257900	1.27170700	0.96639900
C	-3.98143800	0.20226700	1.84852500
O	-4.03894300	0.77646900	2.89811000
C	-5.78846900	-0.80840600	0.39993700
H	-6.58093400	-0.52094400	-0.28782900
H	-5.18595800	-1.57194800	-0.10345600
C	-6.35170800	-1.34118700	1.66950800
N	-5.53058100	-1.97810700	2.58379700
C	-7.59826500	-1.24844000	2.21043600
H	-8.51027800	-0.82207500	1.82802800
C	-6.26925100	-2.26397400	3.64826100
H	-5.93023100	-2.76389000	4.54122600
N	-3.02606900	-0.89021700	1.65770000
H	-2.87633000	-1.01021200	0.65115000
C	-1.71259700	-0.63630300	2.30773200
H	-1.88288000	-0.62354100	3.38597600
C	-1.20267900	0.74252000	1.85813200
O	-1.78131300	1.38302300	0.98038400
C	-0.66682700	-1.69056700	1.92862000
H	-0.37400200	-1.58387600	0.87630400
H	0.24328200	-1.50941200	2.50066000
C	-1.01574200	-3.15548600	2.14462100
O	-2.27455900	-3.48402900	2.13616000
N	-0.08726100	1.16742600	2.46399400
H	0.34693000	0.58981000	3.17187100
C	0.61271700	2.37609100	2.05311000
H	-0.13555500	3.05529700	1.65363000

C	1.49313600	2.02671800	0.83883500
O	1.03620800	2.14048200	-0.29436000
C	1.26846300	3.09037000	3.25482700
H	1.85035200	3.92637600	2.85683800
H	0.44510000	3.52542300	3.82771500
C	2.11835700	2.24289200	4.17739500
C	1.51783500	1.40327000	5.12487600
H	0.43714500	1.40913200	5.24280600
C	3.51610600	2.27868900	4.11726400
H	4.00998000	2.97135600	3.44088900
C	2.28965300	0.58514900	5.94488400
H	1.80355000	-0.06284000	6.66643700
C	4.29029800	1.45791500	4.93407300
H	5.37205800	1.49859700	4.86297300
C	3.67825900	0.59995100	5.84278000
H	4.27969000	-0.04294200	6.47649400
N	2.71786400	1.52649600	1.10999200
C	3.69410500	1.20236100	0.09100300
H	3.13143700	0.98084000	-0.81889800
C	4.46846100	-0.06652300	0.46428300
O	5.56410900	-0.31547400	-0.03893400
C	4.65294500	2.37670300	-0.20769200
H	5.27418800	2.56430300	0.67363200
H	5.31688600	2.06268500	-1.01649200
C	3.86676000	3.60679300	-0.58450900
C	3.44583600	4.51233400	0.39221900
H	3.80224700	4.40175100	1.41288400
C	3.44012700	3.80118100	-1.89966700
H	3.79158000	3.12833700	-2.67699200
C	2.57315700	5.55059500	0.07670700
H	2.24346600	6.23634100	0.85057200
C	2.57412500	4.84126900	-2.22446800
H	2.25059900	4.97270700	-3.25233100
C	2.12392700	5.70974900	-1.23185500
H	1.44283400	6.51707500	-1.47809500
N	3.87171200	-0.86643000	1.36838300
H	2.89343300	-0.70934400	1.56270000
C	4.51076800	-2.05147400	1.91749900
H	5.58716100	-1.88350900	1.81771900
C	4.16001400	-3.26692900	1.04331700
O	3.31991800	-4.11301800	1.34982000
C	4.18762400	-2.20475000	3.41404000
H	4.64477800	-1.32659000	3.88638100
C	2.68969900	-2.16443400	3.73368800
H	2.53497400	-2.35532600	4.79929200
H	2.27434800	-1.16709700	3.54757300
H	2.12904900	-2.90697700	3.16022500
C	4.85984600	-3.45100400	3.99464400
H	4.39755600	-4.36191500	3.60723600
H	5.92779800	-3.47600000	3.75392100
H	4.76131400	-3.45256100	5.08367800
N	4.85012100	-3.32399700	-0.11624600
H	5.44553200	-2.54031500	-0.35789800

C	4.66290100	-4.40616000	-1.06592800
H	5.55770900	-4.50141900	-1.67905600
H	4.51113200	-5.33383700	-0.50756100
C	3.47246300	-4.15476200	-1.99448700
O	3.61765300	-3.95640200	-3.19854600
N	2.27227900	-4.14618400	-1.36920500
H	2.28447900	-4.21375900	-0.35367300
C	1.08474100	-3.58584400	-1.99076400
H	1.12964300	-3.82709300	-3.05600500
C	1.16485500	-2.06372300	-1.79830400
O	1.36525500	-1.57946700	-0.68437000
C	-0.16316900	-4.22352800	-1.37455600
H	-0.03785300	-5.30389300	-1.50105000
H	-0.16576500	-4.03549100	-0.29394200
C	-1.50051700	-3.78926400	-1.99895000
H	-1.34630700	-3.60783400	-3.07042100
C	-2.53834200	-4.90441600	-1.84972300
H	-3.49990800	-4.60321600	-2.27705100
H	-2.21480500	-5.82072800	-2.35198700
H	-2.69942200	-5.13614400	-0.79012100
C	-2.05217600	-2.50411800	-1.37736300
H	-1.33799000	-1.67579300	-1.41047800
H	-2.96170200	-2.18743100	-1.89561300
H	-2.31405200	-2.70846700	-0.33311100
N	1.05577700	-1.31608600	-2.92099600
H	0.94716200	-1.77708200	-3.81306300
C	1.45893100	0.07289100	-2.93492800
H	1.51444000	0.38772300	-1.89118700
C	0.46307200	0.94563300	-3.68577300
O	-0.05600700	0.57564800	-4.72893000
C	2.81762900	0.26254500	-3.64607200
H	2.67328500	0.09426700	-4.71911600
H	3.11654500	1.30818000	-3.52517500
C	3.89685000	-0.67427700	-3.12649800
H	4.02813300	-0.58135600	-2.04655200
H	3.63906300	-1.71227100	-3.34554900
S	5.49365400	-0.31481300	-3.92506100
C	6.46493000	-1.64763000	-3.16889400
H	7.44013600	-1.67199000	-3.65705100
H	6.60103300	-1.45359300	-2.10288300
H	5.95904300	-2.60425400	-3.32135100
N	0.26383900	2.17672000	-3.13922900
H	0.81470800	2.45572100	-2.33249900
N	-2.02937200	6.02090600	-1.81897600
H	-0.07052800	2.90039500	-3.76090800
O	-0.12136900	-3.97947200	2.24280100
H	-1.65815500	6.09385400	-2.76729800
H	-1.53249100	6.69200100	-1.20760200
H	3.04087600	1.54698300	2.06919500
H	-8.27986600	-1.94016300	4.10683400
N	-7.52117700	-1.83962400	3.44841600
Ni	-3.76354900	-2.52952800	2.32508400
O	-0.88310300	5.32559700	2.21681800

H	-0.33418400	6.01493800	2.62281400
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NiH₂L²⁺ (1N)_b (-6211.939628 a.u.)

C	-2.70134200	3.39359900	-0.51982100
H	-1.66383500	3.06814900	-0.65684900
C	-3.65446600	2.27547700	-0.95971200
O	-4.70501600	2.61537300	-1.57682800
C	-2.88040500	3.90719400	0.93329700
H	-3.24065100	3.10339000	1.58177600
H	-1.89795000	4.19939700	1.30915400
C	-3.77709300	5.15094800	1.22942800
O	-4.57513100	5.63341300	0.30900500
N	-3.32819500	1.02033800	-0.73327100
H	-2.43809200	0.80297400	-0.27525100
C	-4.18438700	-0.09964500	-1.14762200
H	-5.01793200	0.33434600	-1.70015500
C	-4.79238700	-0.70604700	0.13128800
O	-5.94804900	-0.47784500	0.45990400
C	-3.38146100	-1.03835500	-2.05341400
H	-2.79170800	-0.40935600	-2.72452600
H	-2.65692300	-1.61901900	-1.47388900
C	-4.20051600	-1.95753200	-2.95411900
H	-4.89548500	-1.37910700	-3.56975000
H	-3.50980400	-2.45527500	-3.63820600
S	-5.15377000	-3.30065500	-2.16685600
C	-6.81183600	-2.57746600	-2.00283700
H	-7.44946300	-3.36147700	-1.59119800
H	-6.81724600	-1.72270500	-1.32672000
H	-7.18974500	-2.29323900	-2.98622800
N	-3.93838800	-1.44879600	0.87949700
H	-2.95473300	-1.41425800	0.62315300
C	-4.20151100	-1.70405200	2.29639600
H	-4.86520100	-0.92225900	2.67039200
C	-2.84643700	-1.46511100	2.96945900
O	-2.64716100	-0.47997600	3.66425500
C	-4.90830100	-3.04595500	2.54963600
H	-5.06019300	-3.16917600	3.62396700
H	-5.89818100	-2.96923600	2.08974900
C	-4.22519700	-4.26335600	2.02822800
N	-4.06011700	-4.52108400	0.67893400
H	-4.37153900	-3.92606300	-0.10142400
C	-3.69555100	-5.33578400	2.68136500
H	-3.60869200	-5.54258100	3.73436200
C	-3.46839400	-5.69834700	0.51569500
H	-3.22045900	-6.15816900	-0.42578300
N	-3.24627000	-6.20915700	1.72032600
H	-2.77220200	-7.08455600	1.89247500
N	-1.83270700	-2.27932200	2.56738200
H	-2.01034200	-3.13703700	2.05960200
C	-0.48757700	-1.74532600	2.50912700

H	-0.07481500	-1.62114200	3.51458100
C	-0.56934300	-0.38743600	1.78709800
O	-1.24197800	-0.27740800	0.75673400
C	0.42441100	-2.63776000	1.65477500
H	0.12106400	-2.53361900	0.60974500
H	1.45310300	-2.29002800	1.72693100
C	0.33487000	-4.10327700	1.99022700
O	-0.67600700	-4.76522300	1.84187500
N	0.12642200	0.62096000	2.31909700
H	0.63432600	0.46878500	3.18075200
C	0.01472700	1.97492500	1.80923300
H	-1.00937600	2.09463100	1.45753400
C	0.87163700	2.13603800	0.54465300
O	0.34220000	2.19507700	-0.56476300
C	0.25863400	3.02244400	2.92641200
H	0.37578800	3.99794100	2.44561100
H	-0.65941500	3.06466300	3.51882800
C	1.42808200	2.73784600	3.84454300
C	1.27766600	1.84613100	4.91459100
H	0.29747900	1.42921000	5.13414600
C	2.68391300	3.31952300	3.63735800
H	2.81230400	4.06007000	2.85287400
C	2.36464400	1.49898200	5.71245400
H	2.22882400	0.79733700	6.52862300
C	3.77281100	2.97362100	4.43421000
H	4.73869900	3.43202900	4.25092300
C	3.61926100	2.04942600	5.46420400
H	4.46821400	1.77281900	6.08009400
N	2.19911800	2.16603800	0.74258000
C	3.18429700	2.35521800	-0.30867300
H	2.75576800	1.93553500	-1.22224100
C	4.43841900	1.55683100	0.08887000
O	5.53963800	2.08624000	0.17199300
C	3.52256200	3.83388200	-0.54802500
H	3.99343000	4.23638400	0.35334200
H	4.26964200	3.86996400	-1.34537400
C	2.30527100	4.64337800	-0.92028900
C	1.61682900	5.38420300	0.04171300
H	1.99816600	5.42916700	1.05826400
C	1.81851300	4.63181400	-2.23087000
H	2.35609700	4.07404300	-2.99384900
C	0.46622000	6.09700300	-0.29126700
H	-0.04893500	6.67801200	0.46723200
C	0.67115400	5.33954000	-2.57149400
H	0.31242000	5.32895100	-3.59572600
C	-0.00512400	6.07995300	-1.60138100
H	-0.86960900	6.67710500	-1.87935900
N	4.21165900	0.25466000	0.38890100
H	3.29557000	-0.15363900	0.22112600
C	5.18547200	-0.52352300	1.14287700
H	6.14971600	-0.03270200	0.97970900
C	5.26490400	-1.92431000	0.52623200
O	4.72609300	-2.91795700	1.01171000

C	4.89694300	-0.47667800	2.65718800
H	4.96379500	0.59026800	2.90952800
C	3.49473900	-0.95008400	3.04127500
H	3.30053100	-0.72553500	4.09378100
H	2.72852400	-0.43452700	2.45203800
H	3.38863500	-2.02553000	2.88589300
C	5.97848900	-1.21408000	3.44764300
H	5.93497500	-2.28971300	3.25543100
H	6.97903300	-0.85540700	3.18532500
H	5.83440600	-1.05376900	4.51987000
N	5.96991100	-1.97477500	-0.62638000
H	6.33528800	-1.11810700	-1.01295000
C	6.03016700	-3.17232300	-1.44596300
H	6.88258100	-3.09990400	-2.11934200
H	6.15260000	-4.04067300	-0.79490000
C	4.75261300	-3.28043400	-2.27924300
O	4.70041800	-2.91526900	-3.44922600
N	3.68944200	-3.76214700	-1.58845400
H	3.80172000	-3.81183200	-0.57861800
C	2.33718300	-3.59792300	-2.08900900
H	2.36730800	-3.77806600	-3.16691400
C	1.93550400	-2.13914400	-1.82688600
O	2.15824200	-1.60871600	-0.73450000
C	1.42727200	-4.63544000	-1.42090500
H	1.98100100	-5.57878500	-1.46616400
H	1.32832100	-4.39446300	-0.35668300
C	0.04459800	-4.85946100	-2.05494200
H	0.18152800	-4.89414000	-3.14404300
C	-0.49673500	-6.21956200	-1.60346900
H	-1.46845900	-6.42180000	-2.06559800
H	0.18017000	-7.03254700	-1.88159600
H	-0.61727500	-6.23832900	-0.51361000
C	-0.98113500	-3.76680300	-1.73677700
H	-0.65914100	-2.77318500	-2.05803800
H	-1.92635600	-3.98310000	-2.24627000
H	-1.19029500	-3.73948000	-0.66075900
N	1.38458600	-1.48728200	-2.86394900
H	1.18911800	-1.97439000	-3.72723600
C	1.08901600	-0.07712400	-2.82234000
H	1.07324400	0.21981600	-1.77111200
C	-0.28128400	0.17735500	-3.44464900
O	-0.81858700	-0.64884600	-4.17607000
C	2.15065900	0.74752000	-3.58164100
H	1.99399400	0.64377000	-4.66081600
H	1.99046900	1.80346000	-3.33952700
C	3.57091500	0.31273700	-3.22851300
H	3.68461000	0.17194000	-2.15026300
H	3.80813200	-0.64549600	-3.69679900
S	4.76765400	1.56562200	-3.78826300
C	6.28569100	0.83233300	-3.11908000
H	7.13444500	1.33112300	-3.58866400
H	6.34164000	0.98888900	-2.03830300
H	6.32395600	-0.23287100	-3.36145000

N	-0.79858200	1.38852900	-3.16601100
H	-0.35678600	1.99997200	-2.49138600
H	-1.62979800	1.68970300	-3.65021200
O	-3.67383900	5.63620700	2.34133900
O	1.48235400	-4.61291900	2.42203800
H	1.35594200	-5.56079500	2.58357900
H	2.53722400	2.14505200	1.69600300
H	-2.56411400	5.35168500	-1.20050900
H	-2.83397900	4.28129200	-2.41210600
N	-3.05886300	4.49503100	-1.44111100
Ni	-4.85551400	4.46407400	-1.03735100

NiHL⁺ (2N) (-6211.518132 a.u.)

C	-8.30400000	1.89900000	2.22700000
H	-9.03900000	2.61900000	2.59100000
C	-7.08500000	2.71800000	1.79800000
O	-7.27000000	3.82500000	1.31900000
C	-8.13200000	0.76700000	3.24600000
H	-7.46200000	1.08100000	4.04800000
H	-9.11200000	0.57300000	3.69300000
C	-7.64900000	-0.56600000	2.66100000
O	-8.39300000	-1.06700000	1.69600000
N	-5.87100000	2.09000000	1.74600000
H	-5.76900000	1.19700000	2.21400000
C	-5.07300000	2.30800000	0.53800000
H	-5.57500000	3.11900000	0.00700000
C	-5.35500000	1.04900000	-0.29200000
O	-6.51300000	0.91900000	-0.78100000
C	-3.62300000	2.73800000	0.77700000
H	-3.62800000	3.36700000	1.67100000
H	-2.95200000	1.90300000	1.00300000
C	-3.06900000	3.58800000	-0.37000000
H	-3.65300000	4.51000000	-0.46200000
H	-2.03400000	3.86100000	-0.15600000
S	-3.15600000	2.72400000	-1.97800000
C	-2.68100000	4.03600000	-3.13000000
H	-2.86100000	3.65100000	-4.13500000
H	-3.30000000	4.92000000	-2.97100000
H	-0.44900000	5.03100000	-1.46400000
N	-4.39800000	0.14400000	-0.38300000
H	-3.53300000	0.30800000	0.13800000
C	-4.43800000	-1.17800000	-1.00400000
H	-4.71800000	-1.90100000	-0.23300000
C	-3.00500000	-1.57500000	-1.37700000
O	-2.64900000	-2.73500000	-1.24600000
C	-5.40500000	-1.31900000	-2.20200000
H	-5.64600000	-0.33900000	-2.61500000
H	-4.90600000	-1.88700000	-2.99000000
C	-6.62500000	-2.08300000	-1.80600000
N	-7.43000000	-1.75300000	-0.72700000
C	-7.05900000	-3.27100000	-2.31500000

H	-6.68600000	-3.87100000	-3.12900000
C	-8.32700000	-2.72500000	-0.60400000
H	-9.09400000	-2.77100000	0.15100000
N	-8.13300000	-3.65000000	-1.54900000
H	-8.68200000	-4.48800000	-1.66400000
N	-2.18300000	-0.58300000	-1.82400000
H	-2.56400000	0.35700000	-1.87500000
C	-0.78800000	-0.64800000	-1.46600000
H	-0.46000000	-1.68200000	-1.61000000
C	-0.65100000	-0.35700000	0.04700000
O	-1.62500000	-0.07700000	0.74900000
C	0.07300000	0.27600000	-2.32700000
H	-0.47200000	1.19500000	-2.57300000
H	0.97900000	0.59100000	-1.79700000
C	0.52300000	-0.40100000	-3.59800000
O	0.11100000	-1.46100000	-4.00500000
N	0.58300000	-0.52300000	0.54700000
H	1.33900000	-0.73300000	-0.08900000
C	0.88800000	-0.49300000	1.97100000
H	0.49300000	0.43200000	2.39600000
C	2.40700000	-0.39300000	2.12400000
O	2.91400000	0.55500000	2.70700000
C	0.27000000	-1.68600000	2.76000000
H	0.74400000	-1.70500000	3.74600000
H	-0.78400000	-1.44400000	2.91100000
C	0.37600000	-3.03000000	2.07700000
C	-0.56900000	-3.39200000	1.11200000
H	-1.40400000	-2.73200000	0.90100000
C	1.41000000	-3.93000000	2.35900000
H	2.13700000	-3.69000000	3.13000000
C	-0.46700000	-4.59400000	0.42300000
H	-1.21100000	-4.83700000	-0.32800000
C	1.51900000	-5.13600000	1.66900000
H	2.33100000	-5.81600000	1.90100000
C	0.58200000	-5.46900000	0.69400000
H	0.66800000	-6.40600000	0.15300000
N	3.10900000	-1.39000000	1.53100000
C	4.56100000	-1.48100000	1.51100000
H	4.94100000	-0.45700000	1.53100000
C	4.99300000	-2.13700000	0.18400000
O	5.79700000	-3.06100000	0.15600000
C	5.14500000	-2.24400000	2.71000000
H	4.67500000	-3.23100000	2.76600000
H	6.20600000	-2.40700000	2.50600000
C	4.96900000	-1.48000000	3.99700000
C	3.94000000	-1.77800000	4.89100000
H	3.28800000	-2.62500000	4.70000000
C	5.81700000	-0.40800000	4.28800000
H	6.64100000	-0.18500000	3.61300000
C	3.74000000	-1.00300000	6.03100000
H	2.93100000	-1.24700000	6.71300000
C	5.62300000	0.36900000	5.42500000
H	6.29000000	1.20000000	5.63100000

C	4.57400000	0.07800000	6.29700000
H	4.41900000	0.68400000	7.18300000
N	4.40900000	-1.64200000	-0.93600000
H	3.81700000	-0.81700000	-0.86300000
C	4.47000000	-2.39600000	-2.18700000
H	5.50100000	-2.76100000	-2.28500000
C	4.23900000	-1.43700000	-3.36500000
O	3.37100000	-1.60800000	-4.22000000
C	3.56000000	-3.64200000	-2.14200000
H	3.92800000	-4.20300000	-1.27400000
C	2.08600000	-3.32700000	-1.89600000
H	1.52200000	-4.25400000	-1.76800000
H	1.94300000	-2.74900000	-0.97600000
H	1.65300000	-2.77400000	-2.73100000
C	3.75700000	-4.53200000	-3.37100000
H	3.35800000	-4.05500000	-4.26900000
H	4.81800000	-4.74800000	-3.53700000
H	3.24100000	-5.48500000	-3.22700000
N	5.10700000	-0.40400000	-3.39600000
H	5.78800000	-0.33000000	-2.65300000
C	5.04500000	0.69000000	-4.34800000
H	5.98700000	0.77400000	-4.89200000
H	4.24000000	0.48900000	-5.05400000
C	4.83600000	1.96100000	-3.53300000
O	5.79700000	2.55800000	-3.05800000
N	3.55100000	2.30000000	-3.26600000
H	2.81600000	1.65700000	-3.54500000
C	3.29600000	3.12400000	-2.09900000
H	3.94900000	3.99800000	-2.16400000
C	3.69600000	2.31300000	-0.86200000
O	3.34600000	1.13300000	-0.72100000
C	1.84000000	3.60600000	-2.05200000
H	1.72500000	4.33500000	-2.86000000
H	1.16900000	2.77600000	-2.29100000
C	1.41700000	4.22700000	-0.70200000
H	2.30500000	4.64400000	-0.21100000
C	0.43700000	5.37900000	-0.92400000
H	0.10100000	5.79900000	0.02900000
H	0.89100000	6.18200000	-1.51100000
H	-1.62600000	4.29400000	-3.03300000
C	0.80800000	3.17600000	0.23700000
H	1.49600000	2.35400000	0.45000000
H	0.51900000	3.62700000	1.19100000
H	-0.09300000	2.74100000	-0.21600000
N	4.44500000	2.98500000	0.02100000
H	4.69800000	3.94600000	-0.16300000
C	4.92000000	2.43200000	1.26400000
H	4.31900000	1.54900000	1.47300000
C	4.70500000	3.47400000	2.36200000
O	4.81700000	4.67200000	2.11700000
C	6.40800000	2.04500000	1.19700000
H	7.02500000	2.94900000	1.16400000
H	6.65200000	1.52200000	2.12800000

C	6.70500000	1.16500000	-0.01700000
H	5.90800000	0.43100000	-0.16300000
H	6.75400000	1.77000000	-0.92600000
S	8.27400000	0.27000000	0.21400000
C	8.26000000	-0.74000000	-1.29200000
H	9.21100000	-1.27200000	-1.34000000
H	7.45400000	-1.47800000	-1.25600000
H	8.17400000	-0.10800000	-2.18000000
N	4.46000000	2.96300000	3.58100000
H	4.19800000	1.99100000	3.68500000
H	4.31300000	3.59300000	4.35400000
O	-6.65400000	-1.11200000	3.11600000
O	1.49100000	0.29100000	-4.21800000
H	2.00200000	-0.34500000	-4.75700000
H	2.60200000	-2.23200000	1.28300000
H	-9.70500000	0.97800000	1.03500000
H	-8.84200000	2.11900000	0.25300000
N	-8.76200000	1.34800000	0.91700000
Ni	-7.78000000	-0.15000000	0.20800000

NiH₁L⁰ (3N) (-6211.079262 a.u.)

C	8.15977100	-1.60175500	-0.24838200
H	8.79038900	-2.17311800	-0.93535000
C	6.73985500	-2.16844400	-0.27319200
O	6.49372100	-3.36452300	-0.45074100
C	8.74980700	-1.65772200	1.16866900
H	8.02041900	-1.21668700	1.86148200
H	8.88105400	-2.70189800	1.45752100
C	10.08778600	-0.89968000	1.37771800
O	10.89305100	-1.39119800	2.18248800
N	5.86255100	-1.17875700	-0.03799500
C	4.42195100	-1.34162200	-0.12208600
H	4.12824500	-1.98456100	-0.95890800
C	4.03645800	0.08007200	-0.51366600
O	3.51540900	0.40625000	-1.55422300
C	3.75276700	-1.82881200	1.17241600
H	4.32729300	-1.44915000	2.02692500
H	2.74368700	-1.41363600	1.24530300
C	3.69105200	-3.35364000	1.27891600
H	4.67407400	-3.79332100	1.09850500
H	3.36202500	-3.63445700	2.28151100
S	2.51802900	-4.08449200	0.07680800
C	3.63230900	-5.06497000	-0.97242000
H	3.07132200	-5.34147700	-1.86699100
H	4.50500000	-4.46910300	-1.24603200
H	3.95757600	-5.97148400	-0.45844500
N	4.58868200	1.03821200	0.40942500
H	4.47875500	0.69302300	1.36348800
C	4.20566600	2.47892900	0.36101800
H	4.62980300	2.90122600	1.27287500
C	2.69456400	2.69706500	0.53331100

O	2.26711800	3.10853500	1.60462400
C	4.85215700	3.19436900	-0.83499900
H	4.68573800	2.62897500	-1.75623700
H	4.38020300	4.17052000	-0.96303100
C	6.30834800	3.38415200	-0.56106100
N	7.08486400	2.32089900	-0.14237400
C	7.07659800	4.51030600	-0.54610500
H	6.85054900	5.53487600	-0.78935700
C	8.29509600	2.79359700	0.12021900
H	9.13651900	2.21173300	0.47504700
N	8.32159700	4.11206800	-0.11968800
H	9.12476600	4.70957000	0.00615200
N	1.90198300	2.43831100	-0.53578500
H	2.33265500	1.89525000	-1.27653200
C	0.49844200	2.20040700	-0.29364600
H	0.09642100	3.05640000	0.25599100
C	0.35741300	0.96584700	0.63260300
O	1.32148900	0.27165400	0.93873100
C	-0.24832200	2.06165800	-1.62585800
H	0.23817200	2.68467700	-2.37987100
H	-0.22121000	1.02962700	-1.98769200
C	-1.70339600	2.45350900	-1.56266400
O	-2.36666400	2.49198100	-0.53566800
N	-0.88798400	0.77249800	1.10009700
H	-1.59746200	1.43029200	0.78096400
C	-1.16663900	-0.10498400	2.21715000
H	-0.45159500	-0.92689200	2.17809900
C	-2.53378300	-0.75200100	2.00981200
O	-2.63572900	-1.96245900	1.83191700
C	-0.98983100	0.61898700	3.58448100
H	-1.39163000	-0.02687400	4.37203700
H	0.08911500	0.69705200	3.74612300
C	-1.60320700	1.99906000	3.64780900
C	-0.93873300	3.09299900	3.07901300
H	0.05759900	2.96576100	2.66223000
C	-2.85797400	2.21346000	4.22728900
H	-3.36971100	1.38615700	4.70914600
C	-1.53698800	4.34883100	3.04770400
H	-1.01037900	5.18246100	2.59397600
C	-3.45948200	3.47030700	4.19787000
H	-4.43700600	3.60948200	4.64778400
C	-2.80383100	4.53985900	3.59606600
H	-3.27247200	5.51774500	3.56227000
N	-3.60287200	0.08354700	1.98090700
C	-4.96159800	-0.41560300	1.87761700
H	-4.89655900	-1.38698300	1.37713500
C	-5.84813600	0.46629000	0.99078300
O	-7.07046400	0.39007400	1.08587000
C	-5.62452600	-0.62743100	3.25224700
H	-5.60424400	0.31655200	3.80757900
H	-6.67321200	-0.86884700	3.06613000
C	-4.95993500	-1.72715100	4.04319800
C	-4.17908900	-1.44837700	5.16423000

H	-4.08988900	-0.42536100	5.51842000
C	-5.09502600	-3.05891100	3.63733900
H	-5.70189400	-3.29227300	2.76532000
C	-3.52595000	-2.46970900	5.85395000
H	-2.92038700	-2.23079900	6.72258500
C	-4.45089700	-4.08127000	4.32306800
H	-4.56618500	-5.10882500	3.99262000
C	-3.65706400	-3.78834900	5.43231200
H	-3.15018400	-4.58616000	5.96569900
N	-5.24282500	1.27850900	0.09113000
H	-4.23279100	1.36498200	0.05809600
C	-6.05424800	2.22135000	-0.66986700
H	-7.03577800	1.74918400	-0.77265100
C	-5.46417800	2.36502500	-2.07462400
O	-4.70911200	3.29465900	-2.38979700
C	-6.27772200	3.55040900	0.08276800
H	-6.83466500	3.24960000	0.97937700
C	-4.99427200	4.24028200	0.54664200
H	-5.24926200	5.11360300	1.15528100
H	-4.38030200	3.57927800	1.16437800
H	-4.39199900	4.56652800	-0.30242500
C	-7.17429100	4.48807500	-0.72884800
H	-6.65507300	4.85738800	-1.61757200
H	-8.09253500	3.98538800	-1.05050500
H	-7.46094000	5.35257600	-0.12351600
N	-5.83416100	1.41599300	-2.94771500
H	-6.42463700	0.65977800	-2.63185300
C	-5.30813200	1.32608500	-4.29810100
H	-6.13208800	1.21010000	-5.00498900
H	-4.78038400	2.25337000	-4.51894100
C	-4.42181000	0.08817000	-4.38252400
O	-4.91945600	-1.02942700	-4.27900000
N	-3.09369500	0.29828900	-4.53009100
H	-2.74181000	1.23073100	-4.35014000
C	-2.17365000	-0.79068600	-4.24815400
H	-2.48347900	-1.65588600	-4.84114000
C	-2.30049100	-1.12995100	-2.75989800
O	-2.44422300	-0.23881100	-1.92234200
C	-0.74810700	-0.39071200	-4.64926900
H	-0.78048300	-0.17962500	-5.72321600
H	-0.48236000	0.55296500	-4.15633300
C	0.33327800	-1.45174800	-4.36044100
H	-0.12098800	-2.44538200	-4.47620600
C	1.46442800	-1.33611400	-5.38588200
H	2.24648600	-2.07567800	-5.18897500
H	1.09593800	-1.49161100	-6.40436400
H	1.92389700	-0.34207400	-5.33898600
C	0.90892000	-1.34610400	-2.94342100
H	0.14175600	-1.38369800	-2.16599500
H	1.60678600	-2.16597000	-2.74821200
H	1.46719400	-0.41173600	-2.82747400
N	-2.25032600	-2.43487600	-2.44252700
H	-2.08665300	-3.13805900	-3.14821100

C	-2.36801500	-2.86993100	-1.07268900
H	-2.20722200	-1.98620700	-0.45556100
C	-1.27881800	-3.89829100	-0.77040400
O	-0.74951200	-4.55240300	-1.66586300
C	-3.76928300	-3.42758300	-0.76204300
H	-3.90720300	-4.39073200	-1.26689300
H	-3.82924600	-3.59930400	0.31690800
C	-4.84830100	-2.44659100	-1.20939900
H	-4.65130700	-1.44999700	-0.80105000
H	-4.85198400	-2.34894900	-2.29773100
S	-6.49474100	-3.01515000	-0.67935200
C	-7.51361600	-1.76627700	-1.51383200
H	-8.54817100	-2.11235800	-1.49602700
H	-7.45611900	-0.81139600	-0.98487300
H	-7.19254300	-1.65965500	-2.55362400
N	-1.00180600	-4.03256100	0.53904500
H	-1.39616500	-3.38127200	1.21139500
H	-0.23627100	-4.63227700	0.80893800
O	10.23547800	0.19715400	0.74248900
O	-2.18626300	2.78481900	-2.74484300
H	-3.14856200	3.02432700	-2.63835000
H	-3.47933300	1.01738000	2.35693600
H	8.96057400	0.23534000	-0.31146700
H	8.08555400	-0.13344600	-1.69904500
N	8.07587500	-0.18837600	-0.68229100
Ni	6.46379800	0.55081200	-0.05961900

NiH₂L⁻¹ (4N) (-6210.430717 a.u.)

C	-8.46915500	1.20726800	0.29279600
H	-9.26428200	1.78832800	-0.17982800
C	-7.14582900	1.94861500	0.15433500
O	-7.04270000	3.16997200	0.14852000
C	-8.80942300	0.93882900	1.76809000
H	-7.91559200	0.53649100	2.26252200
H	-9.05004500	1.88319600	2.25796700
C	-9.95604600	-0.07607000	2.01888500
O	-10.65713800	0.09714100	3.02161600
N	-6.11299400	1.06713800	0.09007200
C	-4.77153700	1.47190000	-0.28858500
H	-4.80384600	2.34930300	-0.94138500
C	-4.20970000	0.29144100	-1.06215000
O	-3.38579200	0.42766300	-1.96015800
C	-3.84650000	1.73815300	0.91045200
H	-3.94468100	0.89593800	1.60365900
H	-2.80609500	1.73893300	0.56751700
C	-4.16743100	3.02816100	1.65858600
H	-5.24104300	3.09821200	1.84730100
H	-3.64375200	3.04203100	2.61729000
S	-3.68549300	4.50547300	0.69484500
C	-4.90113300	5.69061300	1.33339500

H	-4.74644300	6.63650100	0.81162200
H	-5.90850900	5.32111900	1.13152200
H	-4.76587400	5.85066600	2.40495900
N	-4.73107300	-0.89856700	-0.60323800
C	-4.16837100	-2.24068900	-0.79316700
H	-4.44830300	-2.77896300	0.11491200
C	-2.64106400	-2.45055500	-0.76468100
O	-2.21472400	-3.34200900	-0.03442700
C	-4.86536600	-2.96059000	-1.96251300
H	-4.87746000	-2.31031100	-2.84289000
H	-4.32803500	-3.87468700	-2.22491200
C	-6.24434400	-3.32282500	-1.50596100
N	-6.96078000	-2.49269800	-0.65822700
C	-6.96047400	-4.46936100	-1.67324200
H	-6.75001600	-5.36432700	-2.23421400
C	-8.07926700	-3.12779400	-0.32487400
H	-8.85267800	-2.75033800	0.33221700
N	-8.10579900	-4.32038800	-0.92671200
H	-8.84298100	-5.00288700	-0.82980600
N	-1.84646500	-1.71959200	-1.57163400
H	-2.28162700	-0.89297000	-1.98187000
C	-0.43958600	-1.65380300	-1.26402800
H	-0.04847300	-2.67351100	-1.19863600
C	-0.25502900	-1.01382100	0.13700000
O	-1.18346300	-0.50488000	0.75275700
C	0.29858400	-0.90046000	-2.37706300
H	-0.21656800	-1.05618100	-3.32761300
H	0.30666200	0.17498500	-2.18087600
C	1.73848200	-1.30609800	-2.55366300
O	2.41594100	-1.85765700	-1.69867500
N	0.99967300	-1.12198500	0.62077000
H	1.68325700	-1.56740300	0.01269300
C	1.29795700	-0.92496100	2.02265900
H	0.61449200	-0.16436800	2.40063600
C	2.69212200	-0.32015500	2.16595400
O	2.84826400	0.79327300	2.66012400
C	1.07171100	-2.22472800	2.85016800
H	1.46643000	-2.06708500	3.85917400
H	-0.01235000	-2.34030400	2.93872400
C	1.65965100	-3.47040500	2.22894600
C	0.98955300	-4.13108700	1.19152300
H	0.00135900	-3.79662700	0.88348200
C	2.90140800	-3.96614000	2.63917200
H	3.41632100	-3.48762500	3.46615200
C	1.57120600	-5.22438700	0.55620500
H	1.04105900	-5.71854500	-0.25192800
C	3.48559100	-5.06091400	2.00542700
H	4.45261700	-5.42340000	2.33874600
C	2.82476200	-5.68660200	0.95271300
H	3.27810500	-6.53547800	0.45163600
N	3.72436800	-1.05273600	1.67585200
C	5.10432300	-0.62099500	1.80246400
H	5.08235000	0.47146200	1.87274600

C	5.93826700	-0.95385900	0.55881500
O	7.16376000	-0.98090700	0.63585000
C	5.79155300	-1.17139100	3.06687300
H	5.70461700	-2.26350400	3.07277200
H	6.85376000	-0.93317800	2.97906400
C	5.22266400	-0.58308600	4.33478900
C	4.45494900	-1.34601300	5.21340800
H	4.30487100	-2.40401400	5.01898100
C	5.43968700	0.76590600	4.63482700
H	6.04011600	1.37333000	3.96126900
C	3.89268000	-0.77407700	6.35448700
H	3.29355500	-1.38439200	7.02284300
C	4.88541400	1.34051100	5.77173100
H	5.06138100	2.38996300	5.98619800
C	4.10232700	0.57200500	6.63336700
H	3.66458100	1.02094000	7.51917600
N	5.28388100	-1.16769000	-0.60820600
H	4.27062100	-1.18977500	-0.64362600
C	6.03632200	-1.64000200	-1.76530400
H	7.03496100	-1.20227000	-1.66574100
C	5.41167700	-1.06085600	-3.03815800
O	4.70363500	-1.73171100	-3.80234900
C	6.22071700	-3.17235700	-1.75734100
H	6.78560500	-3.35784800	-0.83495300
C	4.91718600	-3.96700900	-1.66700900
H	5.14474000	-5.03148400	-1.55317900
H	4.31964300	-3.66659600	-0.80210400
H	4.30949400	-3.82927100	-2.56212300
C	7.09020900	-3.62562200	-2.93217300
H	6.56544400	-3.49627300	-3.88248100
H	8.02854200	-3.06263100	-2.97645400
H	7.34023500	-4.68484800	-2.82518700
N	5.69108500	0.23020200	-3.27207800
H	6.25601400	0.74033600	-2.60750400
C	5.14975300	0.98083500	-4.39209000
H	5.96685500	1.40887700	-4.97703400
H	4.58702600	0.29430600	-5.02345300
C	4.30908800	2.12284600	-3.83252500
O	4.85514400	3.03600900	-3.22006300
N	2.96785600	2.04215500	-4.00306400
H	2.58993500	1.14090000	-4.27216600
C	2.11765900	2.85594400	-3.14815300
H	2.43559000	3.89708500	-3.25017700
C	2.35533700	2.40077700	-1.70525300
O	2.51755600	1.20830200	-1.44223200
C	0.64786300	2.73888000	-3.57778700
H	0.58512100	3.16098600	-4.58611800
H	0.37358400	1.68110800	-3.67113000
C	-0.35948300	3.45408300	-2.65440600
H	0.11185300	4.37400500	-2.28309400
C	-1.60316600	3.86015300	-3.45036600
H	-2.33857800	4.34368400	-2.79966400
H	-1.35260100	4.55380400	-4.25868000

H	-2.07900800	2.97738900	-3.89247700
C	-0.78723800	2.61018700	-1.44536600
H	0.05038900	2.17483700	-0.89620000
H	-1.34932500	3.23021800	-0.74007200
H	-1.44922300	1.79712000	-1.76071900
N	2.37355500	3.36741300	-0.77242200
H	2.18832000	4.33104100	-1.01121400
C	2.55006900	3.04632800	0.62179800
H	2.36932100	1.97609800	0.71631700
C	1.52080000	3.81333000	1.45028700
O	1.03956300	4.87099100	1.05145600
C	3.98189100	3.33893800	1.10674100
H	4.14496500	4.42180300	1.15211500
H	4.08096900	2.93840400	2.12011300
C	5.00492000	2.69730700	0.17461300
H	4.77427900	1.63754100	0.02423000
H	4.97603500	3.17174800	-0.80930500
S	6.68749800	2.87139400	0.84801000
C	7.62490800	2.19231300	-0.54937300
H	8.67915300	2.42327200	-0.39004700
H	7.51184800	1.10594500	-0.59335400
H	7.29593700	2.65976400	-1.48139800
N	1.23479900	3.24135900	2.63269300
H	1.64276500	2.34532400	2.88340600
H	0.59826700	3.70383700	3.26234900
O	-10.05518700	-1.04777500	1.19151900
O	2.19454700	-1.02089500	-3.76113200
H	3.14185100	-1.32543100	-3.82767000
H	3.56072100	-2.04057100	1.51496400
H	-9.05030000	-0.70172200	0.05657500
H	-8.50485800	0.00738600	-1.39798300
N	-8.30702400	-0.08719600	-0.40345100
Ni	-6.49803000	-0.68653400	-0.22067200

(DMHD-NH₂) CuHL⁰ (2N) (-3762.937427 a.u.)

N	0.74650000	2.62161000	1.76963800
C	1.77845100	2.94504600	0.76638200
C	1.30196100	2.74033100	-0.67586900
O	1.63884200	3.47634100	-1.58239900
C	2.94437200	1.93381300	0.95222400
C	3.83217800	1.83625200	-0.27494000
O	4.84094900	2.48553400	-0.39526900
O	3.45332100	1.06571400	-1.32165500
N	0.64315500	1.54682800	-0.83637300
C	1.10931900	0.55376600	-1.79027200
C	0.10922300	-0.60846300	-1.90557200
O	0.03134500	-1.29406600	-2.91423000
C	2.48978800	0.00501500	-1.31716400
C	3.04599800	-1.08468700	-2.22790500
S	4.64450900	-1.76834500	-1.70404800
C	4.17228500	-2.52598200	-0.12533100

N	-0.60031800	-0.84371200	-0.77837300
C	-1.41335600	-2.00418000	-0.51370300
C	-2.91386900	-1.74301400	-0.70720500
O	-3.72789000	-2.63800000	-0.53543900
C	-1.27728400	-2.37768200	0.99422900
C	0.08835700	-2.23663700	1.58751500
C	0.99426200	-3.21151000	1.88792100
C	1.76752500	-1.27443100	2.58607600
N	2.03912800	-2.58591400	2.51894400
N	-3.25598800	-0.44289200	-0.92935300
C	-4.48336000	0.10888200	-0.37450300
C	-5.53902500	0.48649000	-1.41567300
O	-6.58070000	1.03232000	-1.06546400
C	-4.13615900	1.32261200	0.50913300
C	-2.97899400	0.94277400	1.43542500
O	-1.83603600	1.42804700	1.09777900
O	-3.18173400	0.15879900	2.37062500
H	-1.62973000	-3.40200100	1.11754000
H	-1.95418700	-1.73375000	1.56886900
H	0.97336900	-4.27626600	1.72536500
H	2.42496200	-0.55350200	3.04611100
H	-1.08974100	-2.82341900	-1.15816500
H	-0.49270000	-0.24256600	0.02855700
H	-5.02089000	1.59624500	1.08533200
H	-3.84701000	2.16995200	-0.11802000
H	-4.93127600	-0.67184800	0.24844800
H	-2.48228900	0.20614700	-0.99969500
H	1.14677800	2.79919900	2.68921900
H	-0.02109400	3.28534300	1.68197500
H	2.14467100	3.97028400	0.85648300
H	3.57287700	2.24052800	1.78853900
H	2.49424400	0.97036800	1.19907400
H	0.42043200	1.16112900	0.07830200
H	1.21444300	1.01242700	-2.77451100
H	2.35916400	-0.38968500	-0.30272000
H	3.20610300	-0.67365000	-3.22799700
H	2.32147500	-1.89558000	-2.31480800
H	4.02199400	-1.77297300	0.65068200
H	3.26675200	-3.12692300	-0.23959500
H	4.99314700	-3.17692800	0.17888600
H	-4.37146900	-0.27291400	-2.92216300
H	-5.90768600	0.38394500	-3.41742100
N	-5.24444100	0.17237300	-2.68946500
N	0.59300000	-1.01257500	2.02760000
Cu	-0.23768400	0.68220200	1.88811100
H	2.86630600	-3.03179800	2.88673500

(DMHD-NH₂) CuH₂L⁻² (4N) (-3761.985891 a.u.)

N	1.30231000	3.05877800	0.58962200
C	2.46849800	2.75114900	-0.23371100
C	2.36850300	1.38244100	-0.89825600

O	2.69000200	1.24743100	-2.07296100
C	3.75056700	2.81369100	0.61371000
C	5.02445900	2.63277300	-0.24963800
O	5.30691100	3.58941600	-1.01454900
O	5.64145300	1.54572700	-0.12915300
N	2.03773800	0.29780300	-0.08919400
C	1.45898600	-0.74663400	-0.70943500
C	0.15639000	-2.70722900	0.08505100
O	-0.08952000	-3.91964000	0.10573200
C	1.57373400	-2.16443200	-0.19809100
C	2.37952500	-3.05027400	-1.15558400
S	3.27042200	-4.42003300	-0.35154700
C	4.69270500	-3.50613400	0.30759100
N	-0.68755900	-1.69514000	0.35212000
C	-1.97053200	-1.99284200	0.94288100
C	-3.14354700	-1.27130700	0.27388200
O	-4.28720800	-1.37555200	0.71164200
C	-1.95823100	-1.56525600	2.42908100
C	-1.81669500	-0.08430300	2.62496600
C	-2.56566800	0.72661900	3.42834300
C	-1.02039400	1.92830700	2.42215800
N	-2.04301200	1.99149900	3.28995600
N	-2.83546100	-0.46922700	-0.77529200
C	-3.71936300	0.62270000	-1.13354000
C	-4.91487700	0.19215100	-1.98728200
O	-5.91057500	0.90497100	-2.06872100
C	-2.93466600	1.71291300	-1.89159000
C	-1.64724700	2.12578500	-1.15429800
O	-0.70035000	1.27093900	-1.21098500
O	-1.60557100	3.21945000	-0.56846100
H	-1.12505600	-2.09026300	2.90875100
H	-2.88208900	-1.88948200	2.91326600
H	-3.40230600	0.51539900	4.07378600
H	-0.41507600	2.76437900	2.11281100
H	-2.16989700	-3.06897800	0.89355900
H	-3.59208700	2.57330000	-2.02287800
H	-2.65721700	1.32564400	-2.87790900
H	-4.14989500	1.05216400	-0.22158000
H	-1.84849300	-0.30394400	-0.95791300
H	1.41178300	4.00654400	0.94094500
H	0.44796200	3.05649600	0.02713100
H	2.59954800	3.45274300	-1.06903800
H	3.77983200	3.80244900	1.08860900
H	3.69855500	2.05324600	1.39830900
H	1.20141400	-0.64395100	-1.76800100
H	2.08253800	-2.12017200	0.77363200
H	3.11769500	-2.45415400	-1.70113800
H	1.71639400	-3.51073300	-1.89170200
H	4.37104100	-2.71493200	0.98907600
H	5.30862100	-4.21597900	0.86220000
H	5.28547800	-3.07209900	-0.50063900
H	-3.94851100	-1.53673800	-2.51189800
H	-5.50691800	-1.29630000	-3.25125000

N	-4.75621800	-0.95640400	-2.67237100
N	-0.84878000	0.68958900	1.99824300
Cu	0.14069900	0.03896500	0.40319100
H	-2.36752200	2.82497700	3.75471000

Table S4. Excitation energies and oscillator strengths of the 4N Cu complexes.

Cu²⁺..NKB CuH₂L⁻¹

Excited State 1:	Singlet-A	2.2204 eV	558.38 nm	f=0.0016
Excited State 2:	Singlet-A	2.4852 eV	498.89 nm	f=0.0112
Excited State 3:	Singlet-A	3.1712 eV	390.97 nm	f=0.0569

Cu²⁺..DMHD-NH₂ CuH₂L⁻²

Excited State 1:	Singlet-A	3.4831 eV	355.96 nm	f=0.0334
Excited State 2:	Singlet-A	3.6917 eV	335.85 nm	f=0.0016
Excited State 3:	Singlet-A	3.9038 eV	317.60 nm	f=0.0623