

Supporting Information for

A comparative vibrational CD study of homo- and heteroleptic complexes of the type [Cu(*trans*-1,2-diaminocyclohexane)₂L](ClO₄)₂.

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Content:

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1. Structures and spectra of $[\text{Cu}(\text{chxn})_3]^{2+}$

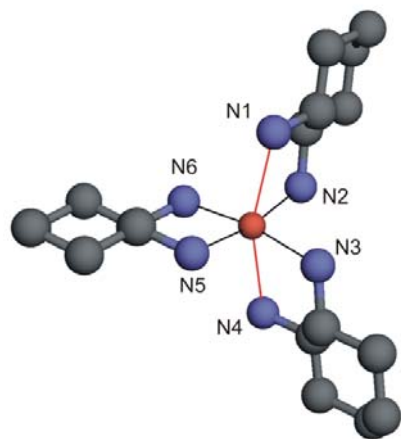


Table S1. Selected bond length (Å) and bond angles (°) of the calculated structure of $\text{Cu}(\text{chxn})_3^{2+}$

Cu-N(1)	2.556	N(1)-Cu-N(2)	75.438
Cu-N(2)	2.102	N(3)-Cu-N(4)	75.416
Cu-N(3)	2.101	N(5)-Cu-N(6)	81.735
Cu-N(4)	2.556	N(1)-Cu-N(3)	91.778
Cu-N(5)	2.103	N(1)-Cu-N(5)	96.526
Cu-N(6)	2.100	N(1)-Cu-N(4)	161.722

Fig. S1. Structure of $\Delta\text{-}[\text{Cu}(\text{chxn})_3]^{2+}$.
 The hydrogen atoms are omitted for clarity.

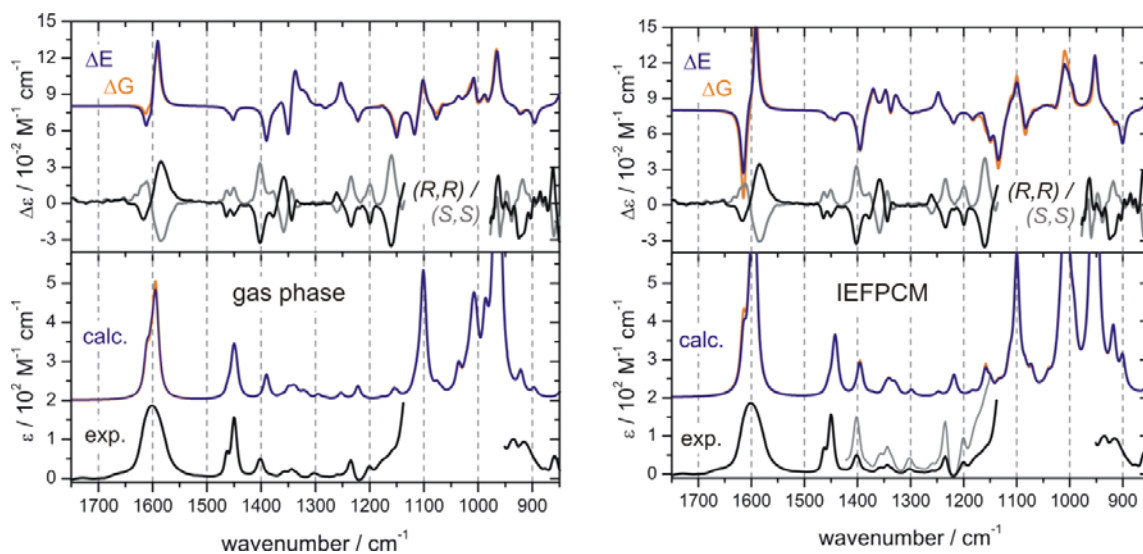


Fig. S2. Comparison of the experimental spectra with the ΔE and ΔG based population weighted spectra of $[\text{Cu}(\text{chxn})_3]^{2+}$ in the gas phase (left) and using the IEFPCM for DMSO (right).

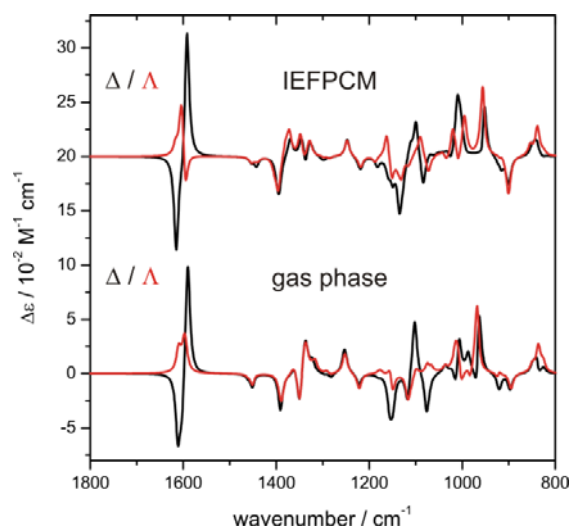


Fig. S3. VCD spectra of the Δ - and Λ -isomer of $[\text{Cu}(\text{chxn})_3]^{2+}$ calculated in the gas phase (bottom) and using the IEFPCM of DMSO (top).

2. Direct comparison of the experimental VCD spectra of all three complexes investigated

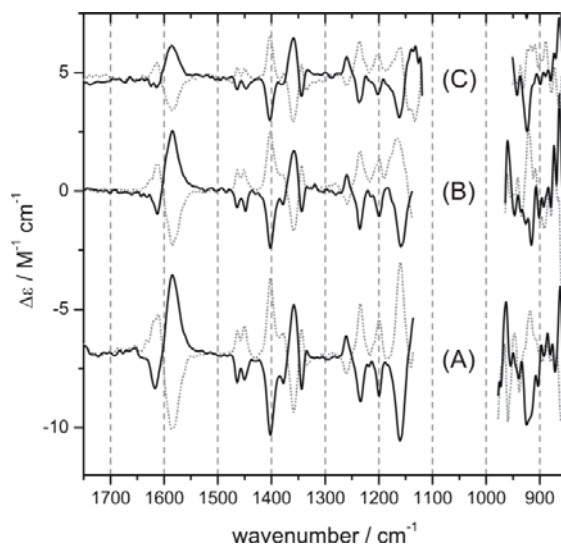


Fig. S4. Comparison of the experimental VCD spectra of (A) $[\text{Cu}(\text{chxn})_3](\text{ClO}_4)_2$, (B) $[\text{Cu}(\text{chxn})_2\text{en}](\text{ClO}_4)_2$, and (C) $[\text{Cu}(\text{chxn})_2(\text{dmen})](\text{ClO}_4)_2$

3. Structures and energies of $[\text{Cu}(\text{chxn})_2(\text{en})]^{2+}$

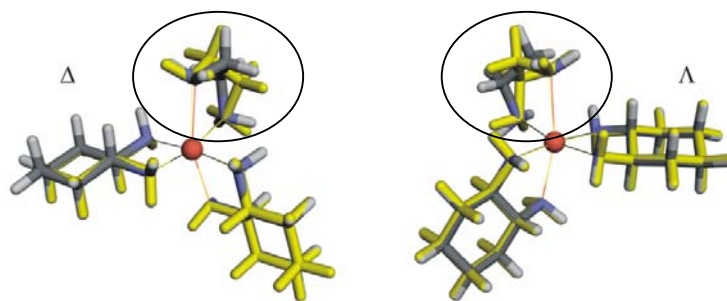


Fig. S5. Superposition of the structures of the Δ - and Λ -isomers of $[\text{Cu}(\text{chxn})_2(\text{en})]^{2+}$ showing the high similarity of the structures. The ligands of the Δ -isomers are in gray scale, while those of the Λ -isomers are in yellow. The differences are only visible for the conformation of the en-ligand highlighted with ovals.

Table S2. Relative energies (ΔE) and Gibbs free energies (ΔG), as well as the corresponding percentage Boltzmann population factors at room temperature of the calculated conformers of $\text{Cu}(\text{chxn})_2(\text{en})^{2+}$ in the gas phase and using the IEFPCM for DMSO. In the C_1 conformers, en occupies an axial position, while it occupies two equatorial positions in the C_2 conformers.

		gas phase				IEFPCM (DMSO)			
conf	en	ΔE (kcal/mol)	ΔG (kcal/mol)	pop- ΔE (%)	pop- ΔG (%)	ΔE (kcal/mol)	ΔG (kcal/mol)	pop- ΔE (%)	pop- ΔG (%)
$\Lambda(\delta\text{-en}) C_1$	ax	0.00	0.23	31.05	25.87	0.27	1.11	17.14	7.38
$\Lambda(\delta\text{-en}) C_2$	eq	1.74	1.79	1.65	1.84	1.52	3.19	2.06	0.22
$\Delta(\delta\text{-en}) C_1$	ax	0.06	0.00	28.25	37.96	0.00	0.00	26.86	48.18
$\Delta(\delta\text{-en}) C_2$	eq	1.74	2.47	1.64	0.59	0.37	1.14	14.37	7.07
$\Delta(\lambda\text{-en}) C_1$	ax	0.30	0.29	18.79	23.19	0.15	0.32	20.89	27.98
$\Delta(\lambda\text{-en}) C_2$	Eq	2.12	3.02	0.86	0.23	0.99	2.09	5.09	1.42
$\Lambda(\lambda\text{-en}) C_1$	Ax	0.37	0.79	16.63	10.02	0.53	1.18	11.05	6.61
$\Lambda(\lambda\text{-en}) C_2$	Eq	1.96	2.87	1.13	0.30	1.39	2.21	2.55	1.15

4. Single-isomer spectra

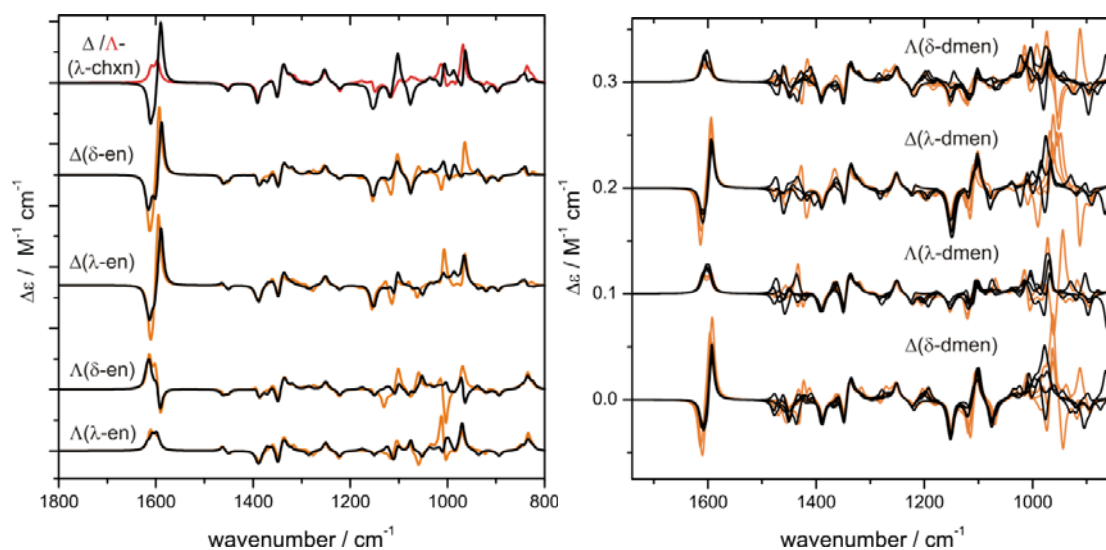


Fig. S6. Comparison of the single-isomer spectra of $[\text{Cu}(\text{chxn})_3]^{2+}$, $[\text{Cu}(\text{chxn})_2(\text{en})]^{2+}$, and $[\text{Cu}(\text{chxn})_2(\text{dmen})]^{2+}$.

5. Cartesian coordinates of $[\text{Cu}(\text{chxn})_3]^{2+}$ and $[\text{Cu}(\text{chxn})_2(\text{en})]^{2+}$

Δ - $[\text{Cu}(\text{chnx})_3]^{2+}$

Cu	0.00000000	0.00000000	0.08877600
N	0.00000000	2.52506600	-0.31163800
H	0.88552900	2.99579700	-0.48634100
N	-1.51196700	0.30894500	-1.33668900
H	-2.29294100	-0.32121000	-1.15948200
N	1.51196700	-0.30894500	-1.33668900
H	2.29294100	0.32121000	-1.15948200
N	0.00000000	-2.52506600	-0.31163800
H	0.40575300	-3.04192600	0.46795200
H	-0.88552900	-2.99579700	-0.48634100
N	1.37529500	0.00085700	1.67830700
H	1.79960900	-0.92061200	1.78217700
N	-1.37529500	-0.00085700	1.67830700
H	-1.79960900	0.92061200	1.78217700
H	-2.15228800	-0.64254600	1.53218000
H	-1.18327300	0.04072500	-2.26399900
H	1.18327300	-0.04072500	-2.26399900
H	2.15228800	0.64254600	1.53218000
H	-0.40575300	3.04192600	0.46795200
C	0.67538900	0.35489100	2.95355500
C	-0.67538900	-0.35489100	2.95355500
C	0.87827700	-2.70579000	-1.49859100
C	2.04322200	-1.71097900	-1.42907700
C	-0.87827700	2.70579000	-1.49859100
C	-2.04322200	1.71097900	-1.42907700
H	-0.49785100	-1.43506600	2.91016400
H	0.49785100	1.43506600	2.91016400
H	-0.27277300	2.45114200	-2.37770100
H	-2.59182400	1.89123300	-0.49741700
H	2.59182400	-1.89123300	-0.49741700
H	0.27277300	-2.45114200	-2.37770100
C	-3.00648800	1.86725200	-2.61179100
H	-3.84539900	1.17475800	-2.49479000
H	-2.48307500	1.57622500	-3.53193100
C	-1.39317000	4.14278600	-1.66354600
H	-0.53925200	4.81746400	-1.76751800
H	-1.91161300	4.43549900	-0.74111700
C	1.39317000	-4.14278600	-1.66354600
H	0.53925200	-4.81746400	-1.76751800
H	1.91161300	-4.43549900	-0.74111700
C	3.00648800	-1.86725200	-2.61179100
H	3.84539900	-1.17475800	-2.49479000
H	2.48307500	-1.57622500	-3.53193100
C	1.48344300	0.03018300	4.21154300
H	2.42430000	0.58696100	4.20179100
H	1.74414300	-1.03588400	4.20267500
C	-1.48344300	-0.03018300	4.21154300
H	-2.42430000	-0.58696100	4.20179100
H	-1.74414300	1.03588400	4.20267500
C	0.67946800	0.35304800	5.47968500
C	-0.67946800	-0.35304800	5.47968500
C	3.51344600	-3.30728200	-2.75163500
C	2.34709100	-4.29223700	-2.85317500
C	-3.51344600	3.30728200	-2.75163500
C	-2.34709100	4.29223700	-2.85317500
H	-1.25771100	-0.06135700	6.35775500
H	-0.53438000	-1.43615700	5.55268600
H	0.53438000	1.43615700	5.55268600
H	1.25771100	0.06135700	6.35775500
H	1.80030600	-4.12228200	-3.78711600
H	2.71798400	-5.31756300	-2.89779300
H	4.14057900	-3.56105100	-1.89010800
H	4.15551700	-3.38044700	-3.63099200
H	-4.14057900	3.56105100	-1.89010800
H	-4.15551700	3.38044700	-3.63099200
H	-2.71798400	5.31756300	-2.89779300
H	-1.80030600	4.12228200	-3.78711600

Λ -[Cu(chnx)₃]²⁺

Cu	0.00000000	0.00000000	0.16179100
N	0.00000000	1.37316900	1.75219100
H	-0.62488000	2.16607600	1.62208900
N	0.00000000	-1.37316900	1.75219100
H	0.62488000	-2.16607600	1.62208900
N	0.24393400	-1.49310200	-1.29317900
H	-0.48271500	-1.41993200	-2.00336900
N	2.53108600	-0.16874100	-0.16056000
H	2.90243000	0.61264500	-0.70042400
H	3.13697500	-0.21591900	0.65600200
N	-0.24393400	1.49310200	-1.29317900
H	-0.08721900	2.40702800	-0.86822900
N	-2.53108600	0.16874100	-0.16056000
H	-2.90243000	-0.61264500	-0.70042400
H	-3.13697500	0.21591900	0.65600200
H	-0.93513300	-1.77213200	1.83968900
H	0.08721900	-2.40702800	-0.86822900
H	0.48271500	1.41993200	-2.00336900
H	0.93513300	1.77213200	1.83968900
C	-1.57720900	1.53168500	-1.98387100
C	-2.70914400	1.41269300	-0.95613300
C	2.70914400	-1.41269300	-0.95613300
C	1.57720900	-1.53168500	-1.98387100
C	-0.35159500	0.67687200	3.02971800
C	0.35159500	-0.67687200	3.02971800
H	-2.61348500	2.25095500	-0.25375800
H	-1.61113200	0.64803700	-2.63197700
H	-1.43252900	0.50258100	2.99004300
H	1.43252900	-0.50258100	2.99004300
H	1.61113200	-0.64803700	-2.63197700
H	2.61348500	-2.25095500	-0.25375800
C	0.02076400	-1.48416500	4.28648400
H	0.57256100	-2.42804300	4.27695700
H	-1.04638000	-1.73947700	4.27683600
C	-0.02076400	1.48416500	4.28648400
H	-0.57256100	2.42804300	4.27695700
H	1.04638000	1.73947700	4.27683600
C	4.08012900	-1.50873800	-1.64072700
H	4.86236900	-1.47205100	-0.87798100
H	4.21748200	-0.62087200	-2.27165700
C	1.72097700	-2.78762700	-2.85185700
H	0.92295700	-2.80900600	-3.59991000
H	1.58099900	-3.67125700	-2.21560600
C	-1.72097700	2.78762700	-2.85185700
H	-0.92295700	2.80900600	-3.59991000
H	-1.58099900	3.67125700	-2.21560600
C	-4.08012900	1.50873800	-1.64072700
H	-4.86236900	1.47205100	-0.87798100
H	-4.21748200	0.62087200	-2.27165700
C	-3.09425100	2.86425200	-3.52880100
C	-4.22157100	2.77048100	-2.49857300
C	3.09425100	-2.86425200	-3.52880100
C	4.22157100	-2.77048100	-2.49857300
C	0.34776200	-0.68223600	5.55488100
C	-0.34776200	0.68223600	5.55488100
H	-5.19259800	2.76766100	-2.99638800
H	-4.20841100	3.65659800	-1.85451500
H	-3.18975700	2.05349500	-4.25928000
H	-3.16641000	3.79551600	-4.09312000
H	4.20841100	-3.65659800	-1.85451500
H	5.19259800	-2.76766100	-2.99638800
H	3.18975700	-2.05349500	-4.25928000
H	3.16641000	-3.79551600	-4.09312000
H	1.43185400	-0.54537100	5.63014700
H	0.05030800	-1.25807800	6.43258900
H	-0.05030800	1.25807800	6.43258900
H	-1.43185400	0.54537100	5.63014700

$\Delta(\delta)$ -[Cu(chnx)₂(en)]²⁺

Cu	-0.07962400	0.67996100	-0.08225600
N	1.27267000	-0.90615100	-1.40533600
H	1.32023900	-0.78587000	-2.41534600
N	1.70490200	0.57974200	0.99757700
H	1.53336500	0.59252100	2.00196500
N	0.56644800	2.38010800	-1.19215300
H	-0.04743000	2.50369500	-1.99575900
N	-0.94894600	2.84666500	1.29359300
H	-1.91209400	2.90910200	1.61426000
H	-0.39160700	3.02236500	2.12725000
N	-1.84378900	0.49132900	-1.17704600
H	-2.43734100	1.30904900	-1.03711500
N	-1.06861500	-0.67903000	1.18628700
H	-0.65164300	-1.60729800	1.12034100
H	-0.99823800	-0.41769800	2.16781200
H	2.26113600	1.41701900	0.82567400
H	1.48363600	2.20132200	-1.59687100
H	-1.68921000	0.43194400	-2.18216800
H	0.95813500	-1.86853800	-1.28451500
C	-2.59124100	-0.72516200	-0.72153400
C	-2.51371100	-0.76967600	0.80093200
C	-0.69340100	3.91859200	0.30745300
C	0.60952900	3.66909500	-0.43582500
C	2.64709100	-0.79200500	-0.84443300
C	2.56214900	-0.61330800	0.67549300
H	-2.98859500	0.13454800	1.19638800
H	-2.04169700	-1.58393700	-1.12235300
H	3.08216500	0.12314700	-1.26657700
H	2.04264600	-1.48248900	1.09492900
H	0.81624100	4.50096600	-1.11291900
H	-0.65027200	4.91356000	0.75992900
C	3.95013700	-0.50142900	1.31664800
H	3.84848900	-0.42358400	2.40303100
H	4.42065100	0.42973800	0.97510000
C	3.55618400	-1.97328000	-1.20769400
H	3.63337100	-2.04407600	-2.29586700
H	3.07691300	-2.90001800	-0.86648600
C	-4.03734100	-0.77891900	-1.21749800
H	-4.05513200	-0.78783900	-2.31062500
H	-4.55900200	0.13191600	-0.89739400
C	-3.22792400	-1.99918700	1.36564800
H	-3.19391000	-1.97862500	2.45812800
H	-2.69077100	-2.90146300	1.04666800
C	-4.76249500	-2.01114400	-0.65601500
C	-4.68150700	-2.06423300	0.87232900
C	4.84782900	-1.68843800	0.94477400
C	4.94590100	-1.85383600	-0.57355700
H	-5.14692900	-2.97835500	1.24405800
H	-5.25008300	-1.23331000	1.30344100
H	-4.32283100	-2.91883000	-1.08287400
H	-5.80447100	-1.99430600	-0.97905100
H	4.44912500	-2.60452500	1.39371200
H	5.83799100	-1.54021700	1.37876000
H	5.53729700	-2.73676900	-0.82136000
H	5.47568100	-0.99827100	-1.00640200
H	-1.52446600	3.93799900	-0.40333700
H	1.44181600	3.61723000	0.27023000

$\Delta(\lambda)$ - $[\text{Cu}(\text{chmx})_2(\text{en})]^{2+}$

Cu	-0.07851400	0.67618800	-0.07593300
N	1.27827200	-0.88950700	-1.41676400
H	1.32562900	-0.75593400	-2.42508300
N	1.70570500	0.56292300	1.00663700
N	0.52960100	2.37564300	-1.20945100
N	-0.80416400	2.83637800	1.38479000
N	-1.85066900	0.49869100	-1.16065400
H	-2.44465200	1.31568900	-1.01983200
N	-1.06273600	-0.69376800	1.18617600
H	-0.64808500	-1.62196400	1.10558900
H	-0.98457600	-0.44464400	2.17024900
H	1.51844800	0.55143900	2.00807600
H	-1.69622800	0.44472300	-2.16594700
H	0.96913000	-1.85525600	-1.30879100
C	-2.59836600	-0.71961800	-0.71075100
C	-2.51083000	-0.77742900	0.81072700
C	-0.10134000	3.91027900	0.64960000
C	-0.14899300	3.65877500	-0.84941100
C	2.65330000	-0.77550300	-0.85634500
C	2.56951300	-0.61979400	0.66625500
H	-2.98078100	0.12439000	1.21784900
H	-2.05357000	-1.57639200	-1.12222800
H	3.08073300	0.14828300	-1.26635400
H	2.05522600	-1.49804800	1.07317900
C	3.95766900	-0.51095900	1.30747700
H	3.85694200	-0.45002100	2.39500400
H	4.42345900	0.42747500	0.97950800
C	3.56765700	-1.94655300	-1.23852300
H	3.64407100	-2.00045200	-2.32773300
H	3.09368500	-2.88092900	-0.91096100
C	-4.04767300	-0.76524000	-1.19791100
H	-4.07256100	-0.76447000	-2.29093400
H	-4.56479000	0.14412800	-0.86636900
C	-3.22432400	-2.01026200	1.36905800
H	-3.18306100	-1.99986700	2.46141800
H	-2.69152600	-2.91081300	1.03811600
C	-4.77248100	-2.00040400	-0.64244200
C	-4.68130700	-2.06730500	0.88482000
C	4.86048600	-1.68783800	0.91647000
C	4.95758100	-1.82973200	-0.60432300
H	-5.14652300	-2.98358500	1.25144800
H	-5.24491900	-1.23889200	1.32711700
H	-4.33847100	-2.90545700	-1.08054200
H	-5.81657400	-1.97765000	-0.95821900
H	4.46652800	-2.61249700	1.35182200
H	5.85046200	-1.54172800	1.35161200
H	5.55320100	-2.70576700	-0.86610400
H	5.48242400	-0.96496400	-1.02470500
H	-0.55553300	2.88665100	2.36972800
H	-1.80524200	3.02016700	1.36603000
H	0.93840200	3.93583600	0.98759100
H	-0.51448300	4.90334500	0.84853900
H	0.31006500	4.49492700	-1.38170100
H	-1.18524300	3.59303800	-1.18852700
H	0.37953800	2.19138100	-2.19966800
H	1.53603100	2.50953400	-1.12722000
H	2.26233700	1.40584100	0.86676100

$\Lambda(\delta)$ -[Cu(chnx)₂(en)]²⁺

Cu	0.07251600	0.61132900	-0.09004400
N	-1.27462600	-1.03388500	-1.34827400
H	-0.83450100	-1.90569600	-1.63577900
N	-1.69808900	0.52794700	1.00569800
H	-1.96341800	1.45112600	1.34500400
N	0.82075200	2.79439400	1.36491500
N	-0.57744100	2.30323200	-1.20059100
N	1.84791500	0.47851400	-1.17246600
H	1.67580300	-0.10583500	-1.99132900
N	1.08468700	-0.75563500	1.15519600
H	1.39556800	-0.24745100	1.98369900
H	0.52088000	-1.52889300	1.50282000
H	-1.54621500	-0.01603900	1.85489900
H	2.19114600	1.36361700	-1.54018200
H	-1.65291000	-0.64795500	-2.21327000
C	2.91908300	-0.15920300	-0.34210200
C	2.28175400	-1.30251400	0.44136400
C	0.09225400	3.59566700	-0.85656100
C	0.08063500	3.85127000	0.64268200
C	-2.41487700	-1.35266200	-0.44374100
C	-2.86337300	-0.07544600	0.27439400
H	1.89569100	-2.03748900	-0.27385100
H	3.24500200	0.60690700	0.36993500
H	-2.02741000	-2.04527200	0.31386400
H	-3.16072900	0.65566200	-0.48683300
C	-4.05094700	-0.32871200	1.21006600
H	-4.36856800	0.61430500	1.66463600
H	-3.71999300	-0.97934900	2.02988900
C	-3.59417700	-2.02256200	-1.16092100
H	-3.25226400	-2.95576500	-1.61613200
H	-3.91689800	-1.37256500	-1.98456100
C	4.12505800	-0.63710800	-1.15253100
H	4.58236500	0.20866700	-1.67322100
H	3.78140000	-1.33826000	-1.92338200
C	3.29722900	-1.98468500	1.35977800
H	2.82398700	-2.82216400	1.87928400
H	3.61807900	-1.27201600	2.12976500
C	5.15253600	-1.32982600	-0.24536800
C	4.51810800	-2.46716800	0.56139700
C	-5.22156000	-0.99266800	0.47486500
C	-4.77742600	-2.28109200	-0.22125400
H	5.24960600	-2.89807900	1.24667900
H	4.21550800	-3.27544900	-0.11294300
H	5.59353800	-0.59297300	0.43461300
H	5.97234600	-1.71153500	-0.85576600
H	-5.63419700	-0.29550700	-0.26236800
H	-6.02358300	-1.19787700	1.18568200
H	-5.60515800	-2.71117800	-0.78739900
H	-4.49617800	-3.02906200	0.52802500
H	-1.58234200	2.42023900	-1.08188900
H	-0.45652600	2.12583800	-2.19638000
H	1.12091300	3.54664100	-1.22108300
H	-0.39220900	4.42438600	-1.37784200
H	-0.95066900	3.86293000	1.00757500
H	0.48098200	4.85280800	0.82542700
H	1.81858900	2.98554600	1.30153500
H	0.61122100	2.85747200	2.35839600

$\Lambda(\lambda)$ -[Cu(chnx)₂(en)]²⁺

Cu	0.07207620	0.63817333	-0.08507652
N	-1.24810101	-1.04250411	-1.33906208
H	-0.79206137	-1.91095002	-1.61147827
N	-1.70696412	0.54128776	1.00002526
H	-1.99370824	1.46451274	1.32069737
N	0.92738483	2.79935233	1.28629369
H	1.89409271	2.85849878	1.59668085
N	-0.61605512	2.31944614	-1.18949257
H	-0.03930757	2.43635364	-2.02110184
H	-1.54976268	2.13466527	-1.55079967
N	1.85593674	0.50655004	-1.16445219
H	1.68399155	-0.05813100	-1.99717470
N	1.07376510	-0.74357022	1.15113027
H	1.39409906	-0.24531474	1.98204173
H	0.50154655	-1.51209605	1.49543256
H	-1.55534878	0.01321356	1.85934613
H	0.37974679	2.98905809	2.12346310
H	2.21484291	1.39454771	-1.51000243
H	-1.62659755	-0.67641037	-2.21248848
C	2.91589248	-0.15876721	-0.34086964
C	2.26132789	-1.30081783	0.42958483
C	-0.63678143	3.61576794	-0.44356902
C	0.67295010	3.86154747	0.28913695
C	-2.38755903	-1.36736042	-0.43604015
C	-2.85773909	-0.09003909	0.26788569
H	1.86288360	-2.02116282	-0.29353535
H	3.25391894	0.59377735	0.37969679
H	-1.99445997	-2.04724395	0.33009460
H	-3.16322097	0.63009908	-0.50028136
H	1.50038231	3.86738578	-0.42587312
H	-1.46580939	3.57891195	0.26689158
C	-4.04559438	-0.35256504	1.20082640
H	-4.37879779	0.58966730	1.64575773
H	-3.70871107	-0.99122419	2.02765361
C	-3.55431820	-2.06093006	-1.15177188
H	-3.19668294	-2.99316209	-1.59679284
H	-3.88226899	-1.42331307	-1.98299438
C	4.11468264	-0.64571773	-1.15669736
H	4.58466693	0.19908227	-1.66762703
H	3.76075080	-1.33260265	-1.93577297
C	3.26629865	-2.00938711	1.33965471
H	2.78027521	-2.84554649	1.84945553
H	3.59792520	-1.31094797	2.11812005
C	5.13154047	-1.36386947	-0.25739652
C	4.48009716	-2.50086037	0.53605043
C	-5.20354649	-1.03962207	0.46681569
C	-4.73829822	-2.32789507	-0.21553837
H	5.20481491	-2.95030134	1.21662976
H	4.16603735	-3.29683132	-0.14763529
H	5.58284499	-0.64126665	0.43108272
H	5.94606670	-1.75050901	-0.87175177
H	-5.62249786	-0.35497878	-0.27852344
H	-6.00576779	-1.24946463	1.17604990
H	-5.55718297	-2.77457122	-0.78171222
H	-4.45027438	-3.06515286	0.54174317
H	-0.84062779	4.44338780	-1.12667744
H	0.63991552	4.86176102	0.73087013