

Supporting Information

Unraveling Ligand Exchange Reactions in Linear Neutral Au(I) and Cu(I) N-heterocyclic carbene complexes for Biological Applications.

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Table S1. Comparison of calculated and experimental values for structural parameters of [Au(IMes)Cl] and [Cu(IMes)Cl] complexes^{1,2}.

Structural Parameter	[Au(IMes)Cl]		[Cu(IMes)Cl]	
	Experimental	Calculated	Experimental	Calculated
M-Cl (Å)	2.27	2.30	2.09	2.14
M-C(1) (Å)	1.99	1.98	1.96	1.90
N-C(1) (Å)	-	1.35	1.31	1.35
Cl-M-C(1) (°)	180.0	178.7	180.0	177.6

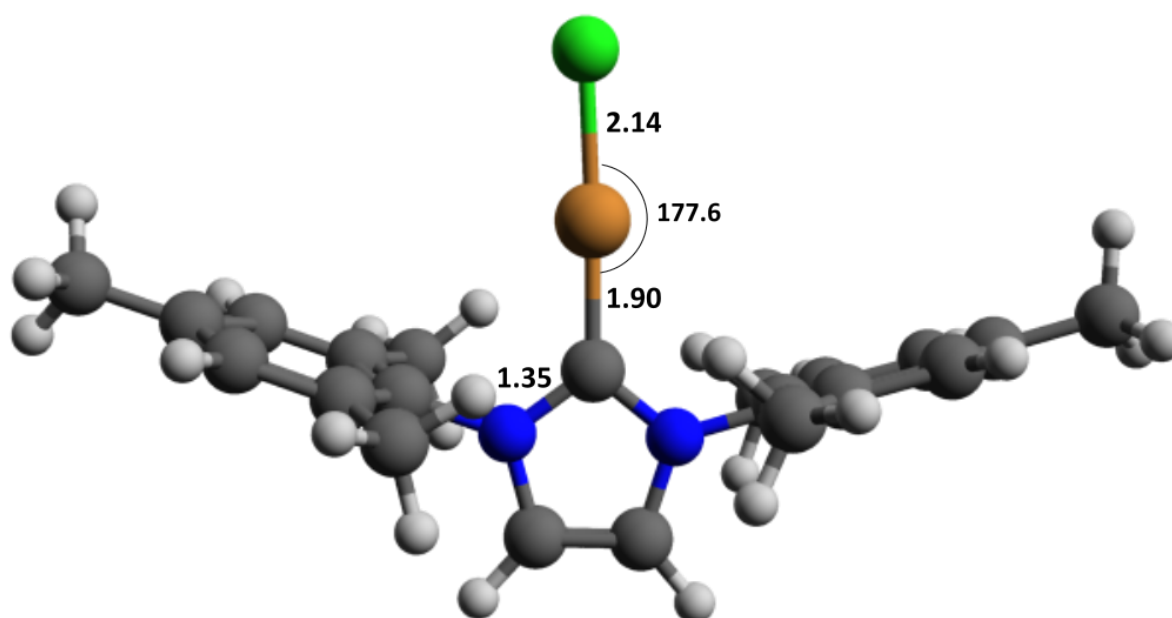


Figure S1. Optimized structures of [Cu(IMes)Cl]. The main distances (Å) and angles (degrees) are indicated. Carbon, hydrogen, nitrogen, gold and chlorine atoms are depicted by black, grey, blue, yellow and green spheres, respectively.

Table S2. Comparison of [Cu(IMes)Cl], [Cu(IMes)₂]⁺ and CuCl₂⁻ energies calculated without ZORA corrections (PBE0, def2-TZVP, def2/J, RIJCOSX) and with ZORA corrections (PBE0, SARC-ZORA-TZVP for Cu(I), ZORA-def2-TZVP for other atoms, SARC/J, RIJCOSX). Values in hartree (Eh).

Species	Without ZORA	With ZORA	Relative Error
[Cu(IMes)Cl]	-3023.551511	-3048.854815	0.83 %
[Cu(IMes) ₂] ⁺	-3486.368007	-3510.049617	0.67 %
[CuCl ₂] ⁻	-2560.716048	-2587.639161	1.04 %

Table S3. Root-mean-square deviation (RMSD) from the superposition of calculated structures [Cu(IMes)Cl], [Cu(IMes)₂]⁺ and CuCl₂⁻ without ZORA corrections (PBE0, def2-TZVP, def2/J, RIJCOSX) and with ZORA corrections (PBE0, SARC-ZORA-TZVP for Cu(I), ZORA-def2-TZVP for other atoms, SARC/J, RIJCOSX).

Species	RMSD for ZORA (Å)
[Cu(IMes)Cl]	0.033
[Cu(IMes) ₂] ⁺	0.023
[CuCl ₂] ⁻	0.019

Table S4. Comparison of [Cu(IMes)Cl], [Cu(IMes)₂]⁺, CuCl₂⁻, and the ligand scrambling TS energies calculated without D3BJ dispersion corrections (PBE0, def2-TZVP, def2/J, RIJCOSX) and with D3BJ dispersion corrections (PBE0, def2-TZVP, def2/J, RIJCOSX, D3BJ). Values in hartree (Eh).

Species	Without D3BJ	With D3BJ	Relative Error
[Cu(IMes)Cl]	-3023.551511	-3023.615549	0.002 %
[Cu(IMes) ₂] ⁺	-3486.368007	-3486.507865	0.004 %
[CuCl ₂] ⁻	-2560.716048	-2560.718264	0.0001 %
TS	-6047.054234	-6047.215027	0.003 %

Table S5. Root-mean-square deviation (RMSD) from the superposition of calculated structures of [Cu(IMes)Cl], [Cu(IMes)₂]⁺, CuCl₂⁻, and the ligand scrambling TS without D3BJ dispersion corrections (PBE0, def2-TZVP, def2/J, RIJCOSX) and with D3BJ dispersion corrections (PBE0, def2-TZVP, def2/J, RIJCOSX, D3BJ).

Species	RMSD for D3BJ (Å)
[Cu(IMes)Cl]	0.038
[Cu(IMes) ₂] ⁺	0.033
[CuCl ₂] ⁻	0.000
TS	0.585

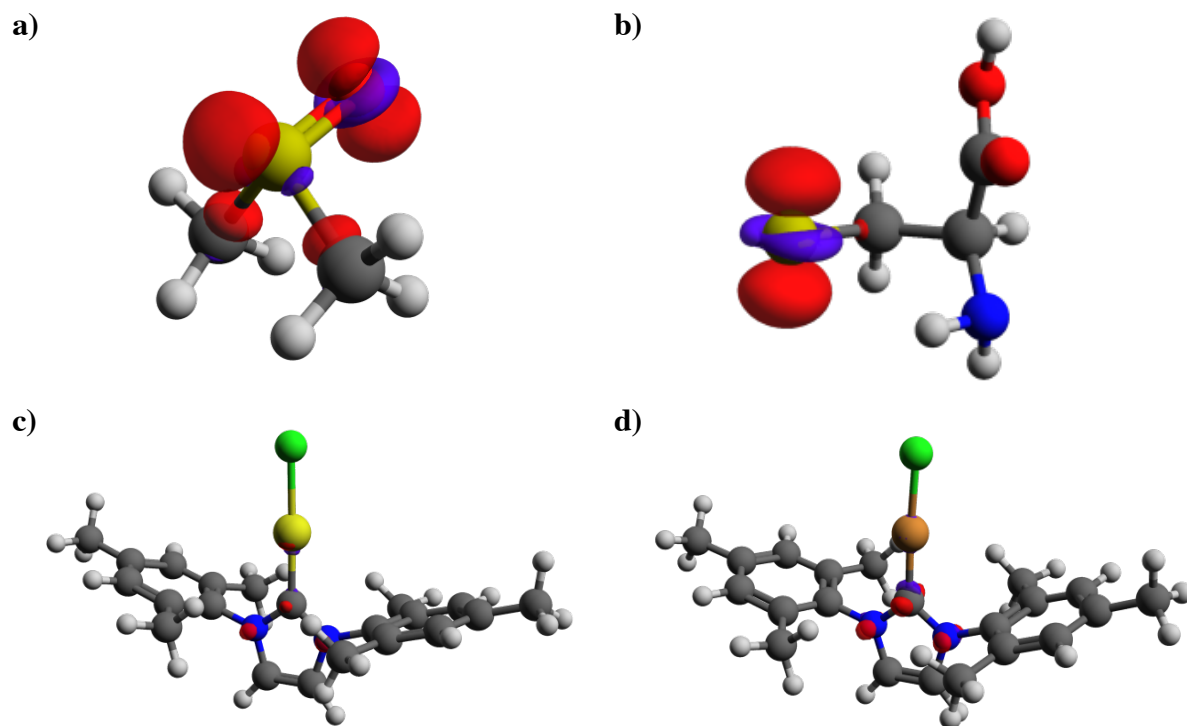


Figure S2. Calculated Fukui f^+ functions surfaces of (a) DMSO, (b) Cys⁻, (c) [Au(IMes)Cl], and (d) [Cu(IMes)Cl]. Red are positive values and blue are negative values. The surfaces were plotted using isovalues of 0.01 a.u.

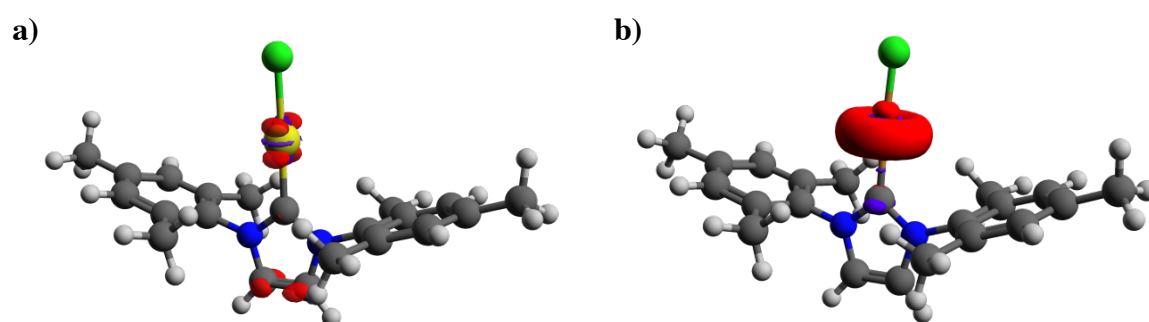


Figure S3. Calculated Fukui f^- functions surfaces of (a) [Au(IMes)Cl] and (b) [Cu(IMes)Cl]. Red are positive values and blue are negative values. The surfaces were plotted using isovalues of 0.01 a.u.

Table S6. Hirshfeld atomic charges (in a.u.) of key atoms in the reactants and products molecules for each reaction of [Au(IMes)Cl].

Atoms	Reactants [Au(IMes)Cl] and DMSO	Products [Au(IMes)DMSO]⁺ and Cl⁻
Au	0.01	0.14
Cl	-0.49	-1.00
S	0.22	0.32
Atoms	Reactants [Au(IMes)Cl] and Cys⁻	Products [Au(IMes)Cys] and Cl⁻
Au	0.01	0.00
Cl	-0.49	-1.00
S	-0.79	-0.38
Atoms	Reactants 2 [Au(IMes)Cl]	Products [Au(1)(IMes)₂]⁺ and [Au(2)Cl₂]⁻
Au(1)	0.01	0.06
Au(2)	0.01	-0.06

Table S7. Mulliken atomic charges (in a.u.) of key atoms in the reactants and products molecules for each reaction of [Au(IMes)Cl].

Atoms	Reactants [Au(IMes)Cl] and DMSO	Products [Au(IMes)DMSO]⁺ and Cl⁻
Au	0.27	0.38
Cl	-0.55	-1.00
S	0.47	0.51
Atoms	Reactants [Au(IMes)Cl] and Cys⁻	Products [Au(IMes)Cys] and Cl⁻
Au	0.27	0.22
Cl	-0.55	-1.00
S	-0.94	-0.54
Atoms	Reactants 2 [Au(IMes)Cl]	Products [Au(1)(IMes)₂]⁺ and [Au(2)Cl₂]⁻
Au(1)	0.27	0.68
Au(2)	0.27	0.19

Table S8. Bader (AIM) charges of key atoms in the reactants and products molecules for each reaction of [Au(IMes)Cl].

Atoms	Reactants [Au(IMes)Cl] and DMSO	Products [Au(IMes)DMSO]⁺ and Cl⁻
Au	0.20	3.89
Cl	-0.64	-0.64
S	1.29	1.36
Atoms	Reactants [Au(IMes)Cl] and Cys⁻	Products [Au(IMes)Cys] and Cl⁻
Au	0.20	0.09
Cl	-0.64	-0.64
S	-0.83	-0.45
Atoms	Reactants 2 [Au(IMes)Cl]	Products [Au(1)(IMes)₂]⁺ and [Au(2)Cl₂]⁻
Au(1)	0.20	2.09
Au(2)	0.20	0.19

Table S9. Coordinates (x, y, z) of optimized structures of [M(IMes)Cl], [M(IMes)DMSO]⁺, [M(IMes)Cys], [M(IMes)₂]⁺, [MCl₂]⁻ (M = Au(I), Cu(I)), DMSO and Cysteine, as also as TS, AR and AP for each reaction (Chloride substitution for DMSO, Cysteine, and Ligand Scrambling Reaction).

[Cu(IMes)Cl]

Coordinates from ORCA-job

H	6.75882048212956	2.18869711053716	-1.13893783917599
C	6.13554597820440	2.16153478448404	-0.25021444544031
Cl	4.85475942761483	-2.89803147276496	2.44225105534884
C	4.30120149015103	1.21787185349777	-1.68136110432011
C	4.83409301076773	1.68589619972638	-0.36193490516865
Cu	3.47043638784246	-1.43481610362023	1.70332340066749
H	-1.23755514082619	-3.79632267547751	-0.65247263096251
C	-0.99898754008468	-3.13534053708821	0.17523576957041
C	8.07519107259142	3.07160464550809	1.06246367008224
C	6.65671958204397	2.59821854161676	0.96383223006666
C	-1.54631242691978	-3.38602442901470	1.42837300544638
C	-2.48577149942753	-4.53380939154214	1.64317076746165
C	-0.15023820845656	-2.05673251690637	-0.05407633465749
C	0.42181168931920	-1.80942496616227	-1.41625250413548
C	-1.22000650398078	-2.53038560832865	2.47642072022805
C	0.14634915742977	-1.22266014233702	1.02313798356240
C	2.32567419587034	-0.07318247456970	1.03857644535617
C	4.04944011199219	1.65875372106058	0.79220712632648
C	-0.37781870939326	-1.43928413785159	2.29873386402672
C	5.83743509546823	2.56188188628665	2.08675098911830
H	-1.63546569043791	-2.71235467720031	3.46308641199917

N	0.99511337918437	-0.09131696470717	0.80701347802352
N	2.70455199603549	1.17924009466430	0.70116438547831
C	4.52814572112049	2.09608751445993	2.02717965946124
C	-0.04720137428518	-0.53352941121010	3.44483939046467
C	0.55116885210275	1.12606104530061	0.33403077587648
C	1.63287117591527	1.93023076625445	0.26755399274766
H	6.22388117655787	2.90936900457977	3.04007418879921
H	-0.48337177692885	1.30679335998357	0.09447660150690
H	1.73583250972229	2.95694423885727	-0.04165007391562
C	3.67191969896842	2.06485081587216	3.25569556842760
H	1.01358429045124	-0.59612824793394	3.70407922433677
H	-0.62969364134041	-0.80543498612737	4.32509844594607
H	-0.25557731863828	0.51159884420941	3.20256256171253
H	-3.52101199834804	-4.18135797149376	1.68806089351076
H	-2.27883155451896	-5.04541387520625	2.58560887604577
H	-2.41771232846381	-5.25909932661953	0.83106386273267
H	0.12829304033976	-2.60394080070081	-2.10227958345603
H	1.51369686258676	-1.76464803404233	-1.38695235117726
H	0.07379391127800	-0.85836589904520	-1.82862852261723
H	2.71362761746079	2.56364536228272	3.09067193565740
H	4.17881165938656	2.55694369300318	4.08583748644117
H	3.44985640308441	1.03547517862404	3.55237286947870
H	8.38286014618550	3.59507827566378	0.15525545041005
H	8.75485864745263	2.22382744813942	1.19507537683527
H	8.21182832080500	3.73850466022967	1.91520264241186
H	5.08954186872455	1.22466735518594	-2.43402399445014
H	3.48958700721099	1.85964361490645	-2.03525860016458

H 3.89964374605159 0.20351463501601 -1.61120821592429

[Cu(IMes)Cl] - ZORA

Coordinates from ORCA-job

H	6.76521524752041	2.16872822884449	-1.12962901010873
C	6.13728246143822	2.14946209114439	-0.24402437548552
Cl	4.82228306625881	-2.85546994879325	2.39770082265682
C	4.30217952773560	1.21672984531340	-1.68086276554619
C	4.83243653825332	1.68502462976216	-0.36084187003496
Cu	3.44867836480635	-1.40525474469163	1.67691418147544
H	-1.23079592119931	-3.79911194741883	-0.64905248750129
C	-0.99295187241582	-3.13624499008655	0.17728942904393
C	8.07968816783870	3.04059984101853	1.07617323027745
C	6.65679335414650	2.58283505574617	0.97160167908172
C	-1.53113340354403	-3.39112222911932	1.43324392853278
C	-2.45932081554109	-4.54668888613760	1.65337308963109
C	-0.15332961405661	-2.05162874695143	-0.05611210168026
C	0.41255276030410	-1.80215601452622	-1.42016459962814
C	-1.20597417277285	-2.53334051031650	2.47966047094510
C	0.14303530170280	-1.21580869885961	1.01947936332283
C	2.31790983773489	-0.06192876812632	1.03068449082037
C	4.04258039416789	1.66668908802090	0.78952529015950
C	-0.37283065511609	-1.43633281695633	2.29764120351510
C	5.83218561355873	2.55683928775329	2.09069789638946
H	-1.61427093815313	-2.71878224293145	3.46861434983219
N	0.98740556697348	-0.08174207268638	0.80055423608191
N	2.69647515392654	1.19116550402202	0.69581506030147
C	4.51933696804924	2.10266655262996	2.02564519655691
C	-0.04075698727945	-0.53048082608470	3.44285840264079

C	0.54285712694909	1.13604790597114	0.33009527553198
C	1.62382048388758	1.94123230546454	0.26434032192557
H	6.21759089155312	2.90161333068937	3.04535929011833
H	-0.49197937437465	1.31624939505554	0.09175740875069
H	1.72571951910139	2.96861177633688	-0.04277795393743
C	3.65860396826831	2.07891686452937	3.25084460944514
H	1.02022148984339	-0.59428482285257	3.70111828655423
H	-0.62247735303400	-0.80192385528323	4.32373288432572
H	-0.24829054091819	0.51474773869163	3.20074190244296
H	-3.49743932357631	-4.20345101951683	1.70245685991365
H	-2.24362223362666	-5.05510855631396	2.59552440822107
H	-2.38836874294051	-5.27232138146463	0.84188069518146
H	0.11384156622498	-2.59432832627848	-2.10660120714261
H	1.50472057242710	-1.76090353071251	-1.39551724741875
H	0.06568662566096	-0.84913583186114	-1.82868245297749
H	2.70437398175018	2.58403907003689	3.08206070744830
H	4.16601792258945	2.56839321657074	4.08214554204275
H	3.42877995980513	1.05135142298376	3.54781463363955
H	8.39674970760811	3.56153025956706	0.17079276217381
H	8.74947378584095	2.18527045321917	1.21050350748755
H	8.22028869039876	3.70500489752418	1.93016125060904
H	5.09252661646892	1.22152835711074	-2.43138965838886
H	3.49209754621257	1.85876748666209	-2.03751763132219
H	3.89952316954275	0.20283616330107	-1.61039930590436

[Cu(IMes)Cl] - D3BJ

Coordinates from ORCA-job

H	6.77949912748020	2.15333438361076	-1.09918419785519
C	6.13692072465352	2.13621824097072	-0.22433072072311
Cl	4.82824634394037	-2.84916862233417	2.41952446055976
C	4.30643392662014	1.22398682127471	-1.68669855262170
C	4.82907401594072	1.68768528100045	-0.36305166235923
Cu	3.44206851863893	-1.39587423396198	1.67297332055507
H	-1.24984189612591	-3.79256264704164	-0.63315338633079
C	-0.99665071532560	-3.12624962028363	0.18560116812258
C	8.06670678774714	2.99763097059293	1.13152832919928
C	6.64123190944155	2.55574154253372	1.00280257499213
C	-1.49691663848001	-3.38566178799342	1.45653242811638
C	-2.40758949810468	-4.54967429129398	1.70108674026464
C	-0.17387925878074	-2.03396808363892	-0.06892419932152
C	0.36564640218837	-1.77522416497555	-1.44093216665740
C	-1.15056732706760	-2.52707090418279	2.49587122602135
C	0.13928884115785	-1.19656337105562	0.99852732778080
C	2.30156844829634	-0.04309381198529	1.00171591835190
C	4.02387216812772	1.67448828319217	0.77459344716913
C	-0.33369522723014	-1.42251448627737	2.29078848668705
C	5.80148490652660	2.52922479103858	2.11087876442010
H	-1.52777315155582	-2.71924689320181	3.49562065393289
N	0.97407188974327	-0.06285917383692	0.76256035232640
N	2.67964701008879	1.20727722542023	0.66172355295422

C	4.48520541736361	2.09065308774408	2.02174565034845
C	0.03367281352594	-0.51215983299709	3.42041442732358
C	0.52902406920341	1.15155228492120	0.28223389123526
C	1.61083784143909	1.95714625963901	0.21860425573994
H	6.17795693962829	2.86025066766652	3.07372466000439
H	-0.50503779529628	1.32713956901490	0.03794268918842
H	1.71765168618183	2.98254383034607	-0.09277850135883
C	3.59987061280104	2.05569522105132	3.22795536824604
H	1.10467641102041	-0.56880605219265	3.63542291546950
H	-0.51279458907031	-0.78355520829919	4.32328970163240
H	-0.18746047502701	0.53067110580317	3.18017882505690
H	-3.44712312570597	-4.21570842855558	1.77544393639972
H	-2.16303264546523	-5.05390728003701	2.63824839707292
H	-2.34944979111583	-5.27510998059924	0.88855119149084
H	0.07392983516971	-2.57358049939160	-2.12285056865783
H	1.45696399280204	-1.71034157022791	-1.42866988073667
H	-0.00535426146463	-0.82900789647014	-1.84368079758231
H	2.65872353763626	2.58133555908559	3.04865388644526
H	4.09774571511269	2.51591076495605	4.08110513473583
H	3.34362332421570	1.02541571422150	3.49236001355157
H	8.40110859007798	3.52336549639449	0.23533014084184
H	8.72512411824875	2.13392257593613	1.26728009377918
H	8.20135123271091	3.65276405781858	1.99347737739227
H	5.10305515777508	1.21668354925089	-2.43020336676527
H	3.50664456256767	1.87472138221048	-2.05030511387099
H	3.88962951774345	0.21588017513920	-1.61429819256732

[Cu(IMes)DMSO]⁺

Coordinates from ORCA-job

H	-2.32051643387473	-6.13945630704261	1.96294251480992
H	-0.30317773032344	-5.05604695963295	1.58297047855967
H	1.71985810486829	-3.15001590290736	1.77534396596008
C	-2.97290728299913	-5.42902440208047	1.45534338524070
H	-3.71549960829217	-5.07157887098689	2.17411422604885
C	-0.79357010962170	-4.25072932613570	1.04430978887974
C	1.45747589487807	-3.18685434871158	0.71415556662036
H	-3.51809775254119	-5.96415976272284	0.67333211354940
C	-2.17337094524120	-4.29560073610550	0.88992419159365
H	1.90516582021419	-2.32213845081045	0.22291033078871
H	-6.75882806586004	-4.59130458434297	2.50810822526418
C	-0.02953926553934	-3.20666137610679	0.52897174095476
H	-8.42943397260474	-5.11050404478374	2.78353242505325
C	-7.75637015580318	-4.64452113050035	2.06399914012388
H	1.91540368642267	-4.09024157253344	0.30257283334695
C	-2.78385723192026	-3.24941239167765	0.19526226076277
H	-10.03954550758945	-3.43794645683336	2.85161316498256
H	-7.68316795847696	-5.30046764683392	1.19224016971651
C	-0.67871209457039	-2.18839168329764	-0.15859637630383
C	-8.25652835966752	-3.28454463369906	1.68522704086067
C	-9.46481632711153	-2.80590212297493	2.18149472575935
N	-4.20393474920291	-3.27456434049503	0.01587302863488
C	-5.08147058164425	-2.66309089880804	0.83715061536140
Cu	-4.68259256801140	-1.64417461229501	2.41554794594452
C	-4.85101043974446	-3.91044081747377	-1.02137212580124
C	-2.05883771576311	-2.18685583394807	-0.34081596128311
N	-6.28926100398496	-2.92479244170379	0.29822534503716

C	-6.17118877270852	-3.68904826702030	-0.84265838711975
C	-7.53063817741228	-2.45331018557387	0.83287837747350
S	-4.12572749676241	-0.48160652908575	4.21524411273581
H	-4.31879941820725	-4.45432489643278	-1.78381363447991
H	-11.25464022160988	0.00841373295939	2.55602165596738
H	-0.09798268927973	-1.36880029892019	-0.57052614737641
C	-9.94990001375993	-1.54656786433888	1.84571293652170
H	-12.06532739100499	-1.25855060780392	1.64131710091069
C	-11.27000471556685	-1.06691092119220	2.36852208103479
H	-7.02734302245619	-4.00018405490677	-1.41755728045342
C	-7.97578477653120	-1.18053993853296	0.47379594008689
C	-9.19040524162603	-0.74937193550577	0.99479701911352
C	-2.73178021756011	-1.07507711871800	-1.08553663775899
H	-7.74346123021216	0.59437323942036	-0.69584128379660
H	-1.99131747247670	-0.38142414612652	-1.48357708338122
C	-7.17386941901659	-0.29641553439946	-0.43107147557709
H	-9.55128737503765	0.23891420567370	0.72606643985343
H	-11.53935120430827	-1.57966652279754	3.29321894694033
H	-3.32989032036886	-1.45504295342588	-1.91775793977420
H	-6.24658552490817	0.02323081264191	0.05329833880751
H	-3.40898965705121	-0.51599148481540	-0.43370805625149
H	-6.89133415965243	-0.81218233549703	-1.35200931448493
C	-5.19264811173655	-0.86030780262947	5.58206974676921
H	-4.92256319158967	-0.20632534369460	6.41285663241955
H	-5.02940774630384	-1.90688514374187	5.83707974987342
H	-6.22548454616770	-0.70019139140133	5.26947857829656
C	-4.50311542254245	1.23774224664945	3.98708221028687
H	-3.87681911701206	1.59911404670571	3.17215207195703
H	-4.27859309631511	1.76171750531218	4.91756912187325

H	-5.55844994692505	1.32717723195896	3.72528851591537
O	-2.71836794988422	-0.61250608931682	4.65339690315122

[Cu(IMes)Cys]

Coordinates from ORCA-job

H	5.15508132764776	1.09512579356601	-2.61020069120096
H	4.11154036294849	0.15757024217288	-1.52840219608661
C	4.47325100193251	1.16203600308522	-1.76238492506492
H	6.92806281508652	2.27729390682472	-1.68272193589599
H	2.41156273783053	-2.04895095686570	-0.59860295692574
H	1.09017039104976	-3.04103652519518	-1.23434850332468
C	1.32419845777930	-2.13742860602256	-0.67151053277039
H	3.60511758882623	1.75051523550999	-2.07256821201720
Cu	4.14356746184478	-1.23230156698952	1.96526844055353
H	-0.15874766189941	-4.12398111692899	0.39352393556555
C	6.44107383612014	2.31632475536268	-0.71311212854769
C	5.16255716694098	1.78065123474662	-0.58523503350381
C	-0.04880863155882	-3.29365960582879	1.08461007417314
C	0.69341316168699	-2.18736121016693	0.68616752759506
H	8.79952803211985	3.44845172798850	-0.84143591296700
H	-1.08067006471349	-5.46951694537163	2.27325438018964
H	0.97096804840733	-1.27505439810641	-1.24341600872087
H	-1.48386948255157	-4.68690789755372	3.81319016643433
C	-1.46774183192416	-4.55671551165559	2.72984710110196
C	2.93769146480579	0.09103401498045	1.29069776093509
C	-0.64957469268248	-3.36386613819107	2.33771906367878
C	8.48302198214672	3.46485220092386	0.20218077033265
C	7.10518348741877	2.89579200525306	0.36098948086832
C	0.83022486702517	-1.13464870368839	1.59240303832180
C	4.55354568493216	1.84107209019102	0.66728526970360

H	9.21069717582968	2.89447372855677	0.78657354003977
N	1.59123072992303	0.01384015021790	1.20744937010182
N	3.22857229096419	1.32027788854290	0.81013143716884
C	-0.49015705738054	-2.29102561593802	3.20844899439177
C	0.24609317539877	-1.16358835399465	2.85849015671812
C	6.46154845631151	2.93176487361228	1.59521064079975
C	5.18488359761864	2.41289776658468	1.77396195028811
H	-2.50413584672820	-4.43982629770580	2.39744132022170
C	2.08661551704020	1.99782434594501	0.43581610083936
H	8.52483840414671	4.49733302963063	0.55830457868836
C	1.05020394570316	1.17116847027890	0.68733528252087
H	-0.94364910352927	-2.33215864190721	4.19417137718497
H	1.46781580740625	0.19450094752271	3.99374594688419
C	0.41155842769676	-0.02777541122582	3.82043045539294
H	6.96402191245431	3.38223011824423	2.44608513727857
H	-0.01003229064161	1.29908560677594	0.54657743037615
H	2.11573493559977	2.99468990807119	0.02860601850710
C	4.51848501745420	2.46381940010449	3.11420067371404
H	4.38393785185592	1.45794323517319	3.52260536853049
H	-0.05131153168178	-0.26903303107898	4.77726333455130
H	-0.04999982273453	0.88787456259044	3.44070063940255
H	3.52639451814456	2.91820724781729	3.05212825099662
H	5.11938740261338	3.04094769491404	3.81701096388467
O	5.01618312770536	-2.69646846862918	6.34884855790730
N	2.88463427551319	-2.99992195131068	4.65684091654325
H	2.17403448897018	-3.24206462417351	3.97432286173683
H	3.25390316956843	-2.09481487407462	4.37517308385588
C	4.96713216585455	-3.69422074522578	5.67410374723833
C	3.94377218108613	-3.98156823272795	4.59777354788451

H	3.51378951441005	-4.96132346309274	4.84093325865289
H	6.48384558331370	-4.45171549331503	6.48709455896671
O	5.84189459557672	-4.69618626849961	5.80280277833027
C	4.63943089925994	-4.13867995952886	3.23505107720077
S	5.58908576028905	-2.67729950898566	2.69215918646817
H	3.87380720851359	-4.38753885354210	2.49827853117162
H	5.33712600525399	-4.97682920766685	3.28425095313372

[Cu(IMes)₂]⁺

Coordinates from ORCA-job

H	7.43631262783403	-2.23420571572852	-2.38706546015006
C	7.15256026913118	-1.79210925654343	-1.43685434762539
C	4.86497885330446	-2.77293192733809	-1.77284985783631
C	5.85170927205793	-1.97465593410778	-0.97781636374656
H	-0.36605475527089	-5.91674564717089	2.17823931098801
C	0.16991528914989	-5.10549337826562	2.66181895879762
C	9.49404908116460	-0.90198923535744	-1.21618583739022
C	8.08992359164918	-1.05990463204147	-0.71647246190401
C	0.05245984974191	-4.93312808631116	4.03767082812501
C	-0.82417633898725	-5.83813189257282	4.84918643268888
C	0.95972273606499	-4.26895451243235	1.88176524432286
C	1.07798876298692	-4.48283834562595	0.40430762053476
C	0.75163718950785	-3.89084587515328	4.63633392302469
C	1.64488032834068	-3.23660072268619	2.52408533781427
C	3.77608463024600	-2.62014620385634	1.48042697551990
C	5.50625283137676	-1.39547231604861	0.24295734755592
C	1.55599484809685	-3.02691386803170	3.89976438396796
C	7.70091526169099	-0.49635863724999	0.49457941820004
H	0.67617161769777	-3.74491359577182	5.70958384399736
N	2.47645740542359	-2.37021947809235	1.74568382514976
N	4.17451520096251	-1.56427156211814	0.73961197854877
C	6.41390427636213	-0.65039155771342	0.99705927285609
C	2.30682437892060	-1.91923084695782	4.57276959194927
C	2.06734012714685	-1.18123781343068	1.18065050407235
C	3.14281300839413	-0.67097805864549	0.54293382665650

H	8.41818356894141	0.08248143125755	1.06853829217339
H	1.06034120964929	-0.81194135857621	1.28083455304633
H	3.26625569501898	0.23529014926949	-0.02615364886164
C	6.02728370604787	-0.03942056310249	2.30869743286636
H	3.38526731207603	-2.02514603209809	4.42527393655858
H	2.10600252334754	-1.91952202007065	5.64403840336823
H	2.02421347916249	-0.94218704522466	4.17205124329251
H	-1.87076019748622	-5.52474607300372	4.78187290550140
H	-0.54194376346679	-5.82231137872978	5.90298368764419
H	-0.77102061085931	-6.86743913693911	4.48857502084466
H	0.42754347140695	-5.29640159196393	0.08311580081245
H	2.10491067708178	-4.73538361614210	0.12503063490277
H	0.80654267629335	-3.58346551663029	-0.15435928065255
H	5.19138770523270	0.65638499652277	2.19853178187029
H	6.86891648857441	0.50514331198446	2.73662622038565
H	5.71421653689943	-0.80435942859941	3.02492744387314
H	9.54470095880238	-1.01274604600571	-2.30052984696134
H	10.14657736711272	-1.66300110831275	-0.77613718838432
H	9.90327233539989	0.07281385113827	-0.94427800630915
H	5.30990106761189	-3.10270228914228	-2.71167203217642
H	3.96891555555316	-2.19030332100995	-2.00268460588677
H	4.53755780331626	-3.65767747074222	-1.21954551209332
Cu	4.79270432761688	-4.15972640225607	2.00730558192116
H	0.79932007229711	-7.86134198959645	-1.60259862512273
H	8.42663818217324	-0.44427061073522	6.10993547252927
H	9.93751368058338	-0.72440707946833	5.23314978096327
C	1.42497244154804	-8.71487402803560	-1.32214748848698
C	9.18859153291900	-1.19207801253834	5.87324685105219
C	8.57688659236318	-2.38793778826069	5.20843993359202

C	2.52450859495103	-8.28228049217610	-0.40032381246830
C	8.95332321845511	-2.76487500746133	3.92522694173685
H	9.70367765127872	-2.18359445754237	3.39802338895735
H	0.77774915490247	-9.45381545514430	-0.84698587279015
C	3.72288773167566	-7.78781570386215	-0.90520129909204
H	7.98728295478012	-4.14045270222565	1.19893420645739
H	1.82533490330357	-9.14094149519538	-2.24395118779484
H	3.87047074629531	-7.74158390668691	-1.97998519267577
C	2.36413555066477	-8.34428565800220	0.97967514444534
C	7.61424596046278	-3.14892343434768	5.86690757495361
H	6.15638980155396	-5.76523339681091	-0.40617296029220
C	5.78885161987222	-5.70908514704174	2.54205846623520
H	9.63428200367133	-3.61035990920311	1.56532408685967
C	8.39812946074343	-3.87262248831546	3.29042146884514
H	1.43792429980948	-8.73283498822430	1.39210979707397
H	3.25929863773593	-7.01644567614965	3.80587954203449
H	7.30636909445412	-2.86934374637847	6.87008699647592
C	8.81756363649669	-4.24852716411720	1.90294667590536
C	4.74807207501773	-7.35380438701773	-0.07204724185318
H	5.05469791359614	-5.09575678383757	5.44163058476572
H	6.02986658752274	-6.93183906289104	-1.73027410199522
C	3.35890316766714	-7.92214672173160	1.85567909897648
C	7.03017922829102	-4.26254119849105	5.27680279621316
C	6.02642944646610	-6.82451804256288	-0.64556921043481
H	9.66775030976325	-1.47053129330934	6.81566651630617
C	7.43994655951565	-4.60644497049835	3.98685255256328
C	4.54195727992015	-7.42784534874848	1.30630836894156
C	3.15485915003283	-7.99927632619776	3.33765718412092
C	5.99206276497797	-5.06055437061832	6.00367883139911

H	2.16003242252509	-8.38266661513638	3.56468124680421
N	6.85989768052733	-5.75595344658387	3.36207651503022
N	5.58507858289211	-6.99538606314037	2.18552587560674
H	5.79054386960356	-4.62242463248393	6.98110765967500
H	9.14786509822057	-5.28905613999316	1.85085005487629
H	6.89560385606043	-7.35169232087946	-0.24391741675056
H	3.88848325757496	-8.65776554513856	3.81034305218032
H	6.31346806011708	-6.09483615553690	6.15301028208884
C	7.31955572547745	-7.04671803637521	3.51590419051859
C	6.51247172028231	-7.83148360385133	2.77025627004026
H	8.16933509633045	-7.28563845629482	4.13334663672273
H	6.51462238830015	-8.89575438353371	2.60361325095693

[Cu(IMes)₂]⁺ - ZORA

Coordinates from ORCA-job

H	7.43848092440838	-2.24269062073157	-2.39006533641108
C	7.15842251368504	-1.80450060692875	-1.43700110479675
C	4.86748127606757	-2.77653144214477	-1.77174749662207
C	5.85863746583036	-1.98567020852302	-0.97537692285228
H	-0.36012610162332	-5.92337248004917	2.19591186159763
C	0.17992695685212	-5.11416687805270	2.67826292385992
C	9.50221101782139	-0.92155512479943	-1.21834560384570
C	8.09925665279017	-1.07791838359840	-0.71571253245140
C	0.07000832411926	-4.94407471031248	4.05473438513894
C	-0.80389430254235	-5.84874297985619	4.86903396736236
C	0.96758259716671	-4.27788869248207	1.89606255105863
C	1.07676293146225	-4.48816419676896	0.41767750118987
C	0.77386213836571	-3.90436342682848	4.65201610347434
C	1.65858156153324	-3.24899630380069	2.53696809961272
C	3.78740533987948	-2.63563727060355	1.48692005664146
C	5.51818689498757	-1.41183257845557	0.24914627176183
C	1.57648274492481	-3.04121249280540	3.91320816805404
C	7.71518137565703	-0.51890591452857	0.49863593135977
H	0.70361057275038	-3.76005107011199	5.72578515773463
N	2.48919180591237	-2.38356438603740	1.75654216664978
N	4.18713302463135	-1.57885257374282	0.74823716057019
C	6.42943693214507	-0.67259094516188	1.00403945148991
C	2.33267143443104	-1.93645351355240	4.58443289951308
C	2.08226818586720	-1.19221144779151	1.19612021146852
C	3.15729342291987	-0.68289943908979	0.55722238015687

H	8.43543017728980	0.05557713137539	1.07313927760880
H	1.07657822454976	-0.82063116568495	1.30022685501824
H	3.28167023382212	0.22468127460035	-0.00944970932137
C	6.04845172970670	-0.06731060293841	2.31962383410409
H	3.41038660609828	-2.04614112846657	4.43452842809804
H	2.13438221063545	-1.93628501551426	5.65613452242350
H	2.05251872109929	-0.95841205963060	4.18457127143760
H	-1.84836701022320	-5.52532724772569	4.81868417489470
H	-0.50797005392721	-5.84516025661306	5.91916811049773
H	-0.76459955774867	-6.87495686494923	4.49822838978378
H	0.42910559115782	-5.30508790129863	0.09954665744275
H	2.10309284443021	-4.73343514452008	0.13022071624743
H	0.79511639980747	-3.58943119176767	-0.13698679146403
H	5.21274599153814	0.62967888311212	2.21607599491765
H	6.89227773218841	0.47460703773169	2.74651863625131
H	5.73808980241583	-0.83521964735889	3.03379230601304
H	9.54753661092364	-1.01259032043306	-2.30476239512392
H	10.15039958482163	-1.69590090752289	-0.79552172103630
H	9.92013122762345	0.04473385585648	-0.93011969041753
H	5.30941951783295	-3.10422244366752	-2.71265718243604
H	3.97354195146152	-2.18919150854837	-1.99764544117945
H	4.53756802141715	-3.66214583014398	-1.22147820814148
Cu	4.79118130397909	-4.15936857028931	2.00352697303052
H	0.78917811813208	-7.87452730944054	-1.60898676575791
H	8.40111007491088	-0.41727688892488	6.08866803256228
H	9.92565375011534	-0.71473565368458	5.24177368715719
C	1.42191026389072	-8.72316955388659	-1.32969703451939
C	9.16158626555548	-1.17232683610003	5.87110310830000
C	8.55343075651701	-2.36806697160620	5.20346663217359

C	2.51944372141211	-8.28230598618785	-0.40982284978956
C	8.95213520481798	-2.75768071896258	3.93102826843831
H	9.71698091778669	-2.18624288521337	3.41409916021699
H	0.78136970946938	-9.46723088296519	-0.85357571265672
C	3.71204079906290	-7.77674957092420	-0.91678086505334
H	8.02241097904449	-4.16934079818945	1.20113130202399
H	1.82408511041495	-9.14592450507161	-2.25219977787923
H	3.85662903446066	-7.72741693187989	-1.99178494233457
C	2.36257250930580	-8.34813215841916	0.97014688229338
C	7.57197491872186	-3.11576313258075	5.84879702675634
H	6.12918459497439	-5.73535401731393	-0.42111965722518
C	5.77667129870587	-5.69151655221679	2.52862864542258
H	9.65721638502185	-3.61302030716805	1.58298357651804
C	8.40030207958092	-3.86555130955440	3.29411993485057
H	1.44058666398011	-8.74500706943245	1.38398351811114
H	3.25939114142186	-7.01877434634448	3.79683984965600
H	7.24711647718401	-2.82605936714066	6.84366661550476
C	8.84356659641520	-4.25611706647439	1.91848073235873
C	4.73539270025989	-7.33586405109758	-0.08535126577617
H	5.00479017362362	-5.04230742415623	5.39401669687099
H	6.00977121735933	-6.90191423452121	-1.74575044114679
C	3.35572471014056	-7.91917949398955	1.84430854679821
C	6.99096016315756	-4.22929806803582	5.25605265890761
C	6.00780305338324	-6.79549489946958	-0.66098208566961
H	9.62135729397269	-1.44775937309524	6.82398920977246
C	7.42266452171547	-4.58587220283899	3.97699020322098
C	4.53308364189176	-7.41412990478080	1.29308686259067
C	3.15566128669254	-8.00054562084038	3.32637694960063
C	5.93424261642012	-5.01469463535004	5.96938239973913

H	2.16207048824823	-8.38629190051335	3.55465469372893
N	6.84670033161267	-5.73617894047157	3.35004541833942
N	5.57545253906492	-6.97791677368684	2.17126038170565
H	5.72306382935542	-4.57170481372554	6.94252675144332
H	9.18786899902997	-5.29297049996900	1.88662734344238
H	6.88216191186869	-7.31572998832133	-0.26163145183133
H	3.89147548799221	-8.65916571825164	3.79540952470997
H	6.24369012577241	-6.05154396464877	6.12587285040772
C	7.30818471348977	-7.02574145322709	3.50378942095093
C	6.50360547162909	-7.81167537906200	2.75704928072833
H	8.15746151942891	-7.26309498966300	4.12243348470245
H	6.50770228204591	-8.87584753944755	2.59022993927182

[Cu(IMes)₂]⁺ - D3BJ

Coordinates from ORCA-job

H	7.87574873015953	-2.21577713104791	-1.68250568522177
C	7.45199748564500	-1.74233414825358	-0.80227641331736
C	5.24224133482653	-2.76834534908379	-1.42113430983163
C	6.10016245443175	-1.92410106764994	-0.53110950615978
H	-0.46316257127049	-5.96631933221467	1.44945038401122
C	0.09935729824601	-5.27954835487378	2.07389110909065
C	9.73177768144506	-0.83585497599035	-0.26286771558084
C	8.26880074742101	-0.97715561167357	0.02254560620665
C	0.04696104690394	-5.41196487675332	3.45830556740744
C	-0.79463438481887	-6.47928076330666	4.08720568565689
C	0.87818459935660	-4.30735691751821	1.46148596971008
C	0.97215165532911	-4.21857404270296	-0.02932461977628
C	0.79600671293857	-4.53908746978397	4.23833344224048
C	1.60548599052508	-3.44625600280971	2.28262458612327
C	3.77122808642506	-2.65441407718956	1.51558049341010
C	5.57971990868923	-1.30912540072740	0.60598597531437
C	1.58465680725140	-3.54278381512932	3.67179574399195
C	7.70544082285361	-0.37728774196261	1.14403430142194
H	0.77502861708735	-4.63800662793016	5.31909166891347
N	2.44823636072468	-2.46420477338800	1.67827274870388
N	4.20561848568981	-1.51998319616446	0.93307361236241
C	6.36297621474350	-0.53632170184569	1.46235517622039
C	2.40633120785366	-2.62806604326163	4.52555195983761
C	2.05510941147497	-1.22952489532068	1.20564353947272
C	3.17095785150550	-0.63044539051324	0.73170645225943

H	8.33181428161428	0.21445410492004	1.80402504301002
H	1.03218655366395	-0.89517907161562	1.24769065413621
H	3.32041060906072	0.33387147939021	0.27613155675147
C	5.78786163341392	0.07290733045590	2.70262218670787
H	3.47425742923029	-2.79260150895747	4.35438472298368
H	2.19849579393287	-2.80021135981816	5.58130150727970
H	2.20660607331122	-1.57839644667287	4.29645048073170
H	-1.85861649163432	-6.24275820801817	3.99317241775973
H	-0.56677776093274	-6.58813737163376	5.14821474726615
H	-0.63442780006318	-7.44257151560580	3.59716794408185
H	0.34568611071506	-4.97818274722820	-0.49645142078999
H	2.00300595965277	-4.37129859368603	-0.36222047266677
H	0.65872680510524	-3.23847452307586	-0.39704243655923
H	5.02614177199051	0.82100711902690	2.46848945708308
H	6.57123416247145	0.55399189092512	3.28781360895797
H	5.30989107871421	-0.68809615779569	3.32561390634376
H	9.94882491921172	-1.00549445698659	-1.31852638055203
H	10.30543403800056	-1.56821568656923	0.31435587023053
H	10.09628906582637	0.15447033886857	0.01621351530842
H	5.78777099554033	-3.05276848353422	-2.32068556681965
H	4.33136264028320	-2.24168550210256	-1.71578080939748
H	4.92871063890217	-3.68205977119095	-0.90719699196549
Cu	4.79344145933859	-4.18460503900753	1.99946750181765
H	0.23962220807343	-7.55992094861594	-0.73951916085577
H	8.56311877777309	-0.03929841298915	4.91860305569977
H	10.12177014424640	-0.50543916456595	4.22529425501075
C	0.85620609944897	-8.45562683914911	-0.61165973351686
C	9.32593544289195	-0.82272597630372	4.90005823953065
C	8.73484299425076	-2.12833216189687	4.46540306549965

C	2.10672152682448	-8.12271462551827	0.14236308769840
C	9.17622518462795	-2.76242111391978	3.31132904273386
H	9.96244220921811	-2.30584322661814	2.71920951137608
H	0.25373182542935	-9.19111156065358	-0.07560572510262
C	3.27548080039419	-7.78213598400825	-0.53041987613958
H	8.22768833444645	-4.69337414071110	0.89545455130120
H	1.08228902202220	-8.84390323946383	-1.60589113653491
H	3.28873850104609	-7.79094258255403	-1.61588571046737
C	2.11138712329852	-8.10961537307705	1.53299400183959
C	7.71310442236781	-2.72188725529166	5.20246800501911
H	5.92207144270046	-5.98808976175358	-0.41905558790904
C	5.82094197858760	-5.70628618217215	2.49666334225125
H	9.83747841447905	-3.99177429783818	1.11860906055163
C	8.61678959152845	-3.95809975589877	2.87194273309868
H	1.20625682163360	-8.37037358521639	2.07161760680174
H	3.47016908761543	-6.69000032428543	4.10840915377811
H	7.35397272145472	-2.23680768680938	6.10493329892879
C	9.06389337964619	-4.59486286156013	1.59332592875578
C	4.43398643171213	-7.42550982659239	0.15056609197562
H	5.10850200144281	-4.60789876856795	5.01829432294452
H	5.55093522992678	-7.19617820841263	-1.65854341822215
C	3.24103438643756	-7.75099534811330	2.25789969961942
C	7.13218168020507	-3.92090384108978	4.81197332600877
C	5.67817853441011	-7.04127555445581	-0.58739462311962
H	9.73878007996630	-0.89403352784185	5.90970822014331
C	7.60239733090702	-4.51893143457776	3.64224106276995
C	4.39023242770476	-7.41892156768445	1.54320913975943
C	3.21401286290758	-7.69197730093648	3.75295864714246
C	6.02693388928790	-4.54100808725969	5.60808586004786

H	2.22168647585790	-7.94305103910985	4.12653816107839
N	6.97607297823138	-5.72025189157549	3.18949709396021
N	5.55202383814908	-7.00449341410526	2.26331451070480
H	5.81931466398254	-3.95049455201902	6.50016827976610
H	9.46233132977803	-5.59870889551165	1.75998404473672
H	6.53913557089386	-7.62417104864804	-0.25139084905660
H	3.93488336130182	-8.38332794606544	4.19699916093488
H	6.28151152484133	-5.55825900787091	5.91715442045065
C	7.42591814067064	-7.00836997757240	3.39073776132272
C	6.52149359715345	-7.82410198189673	2.80236955208684
H	8.33490386340385	-7.22394901744168	3.92664407435282
H	6.48013922403526	-8.89704681477310	2.71882763707721

[CuCl₂]⁻

Coordinates from ORCA-job

Cu	-3.54983717975127	2.02441716106685	-0.00006866322912
Cl	-5.69015015349822	1.98027048915220	0.00004041848680
Cl	-1.40949266675050	2.06837234978094	0.00002824474232

[CuCl₂]⁻ - ZORA

Coordinates from ORCA-job

Cu	-3.54980611211791	2.02437856532145	-0.00003169996541
Cl	-5.66681632700999	1.98049465937340	0.00000994852657
Cl	-1.43285756087210	2.06818677530515	0.00002175143884

[CuCl₂]⁻ - D3BJ

Coordinates from ORCA-job

Cu	-3.54983619439439	2.02441614692252	-0.00006760665869
Cl	-5.69003157939371	1.98027344676261	0.00003988988613
Cl	-1.40961222621189	2.06837040631486	0.00002771677256

[Au(IMes)Cl]

Coordinates from ORCA-job

H	6.80634604880788	2.10716850136532	-1.09586984630956
C	6.15989865027997	2.12390901503212	-0.22384171642987
Cl	4.70644264610742	-3.47014408776745	1.98556437842777
C	4.37503120485235	1.06287502907177	-1.63918365872633
C	4.86619073463427	1.62565833658130	-0.34139890404944
Au	3.43423852033526	-1.63454103740819	1.44675462777431
H	-1.18876440373969	-3.84594408915124	-0.61076221109309
C	-0.96727109984717	-3.16010079946328	0.20087947689363
C	8.04785876227109	3.14765702117258	1.08198793716661
C	6.64184806470375	2.64091975507589	0.97309015490890
C	-1.50880349586143	-3.39430966515906	1.45902050896321
C	-2.37717927622075	-4.58790609351112	1.71691137503330
C	-0.14232585049052	-2.06827178262603	-0.05313732003726
C	0.43982127966802	-1.84641017231117	-1.41469491293556
C	-1.21732031272175	-2.49915861533657	2.48472061273582
C	0.12894312544372	-1.20395567053207	1.00475088291125
C	2.31363211976852	-0.07749736370765	0.95436428129022
C	4.05330421503746	1.66237581769356	0.78981048579742
C	-0.40199125904310	-1.39402959961936	2.28210140271340
C	5.79379786803260	2.66119325281475	2.07640464946681
H	-1.63496703032771	-2.66397254486400	3.47338800298285
N	0.97636695711437	-0.07193199718299	0.78050797328420
N	2.70680024662923	1.18533907087126	0.69381489280578
C	4.49269855839264	2.17879744309032	2.00979927823484
C	-0.10337405728465	-0.44498033947755	3.40097488992173

C	0.53580255632504	1.18089056190640	0.41180532824707
C	1.62614533502228	1.97344038094743	0.35737405491261
H	6.15070857254586	3.06921030861128	3.01702945785533
H	-0.50434362568546	1.38917262272049	0.22590484279410
H	1.73454523530418	3.01692561234938	0.11378845591286
C	3.59767172187446	2.21675307718887	3.20972403577176
H	0.97326042646553	-0.34929336534956	3.56426947878648
H	-0.56233829819249	-0.79141621901094	4.32672688438879
H	-0.48504551880690	0.55679939569448	3.18567293192756
H	-2.61684011912588	-5.11076749173649	0.79039625947894
H	-3.31206616789859	-4.29742186560861	2.20256847054324
H	-1.87539087844308	-5.29491131302822	2.38404794242768
H	0.07381205509648	-2.59913416119638	-2.11274209956056
H	1.53181581215419	-1.90490109218544	-1.38895707987393
H	0.18077429537572	-0.85931152031044	-1.80602196235983
H	2.70089009620151	2.81332537904833	3.02125644940471
H	4.12165902811349	2.64913347161213	4.06192307657641
H	3.26176781961420	1.21349179301604	3.48537170917340
H	8.46362733430860	3.37716658127720	0.09985212666235
H	8.69325805775934	2.39675324223139	1.54844775788151
H	8.09786582483947	4.04559334929719	1.70113140902132
H	5.12943908327849	1.18317312217958	-2.41649358770725
H	3.45742665452226	1.55536214046956	-1.97080661020343
H	4.14972248280931	-0.00344339477480	-1.54299657379215

[Au(IMes)DMSO]⁺

Coordinates from ORCA-job

H	-2.29160028672319	-5.99897593087884	1.98328506766177
H	-0.32130863408679	-4.80648624477147	1.67794045522838
H	1.64143824448896	-3.05930570805217	1.81581014176764
C	-2.97020460854134	-5.29031606830444	1.50885213663469
H	-3.67414452112365	-4.93470010848119	2.26705705814728
C	-0.82936516554265	-4.04660260378968	1.09202655390777
C	1.38553651917251	-2.91089317835069	0.76409902877986
H	-3.55434746555034	-5.82428026071344	0.75521722110191
C	-2.20195241223123	-4.15434453725684	0.90764935854117
H	1.77710339501656	-1.94396093432127	0.44585024877968
H	-6.73718226310163	-4.43269114242354	2.74801847295654
C	-0.09531065797606	-2.99400418757891	0.55226498128206
H	-8.36863443630971	-5.10116866285788	2.88207380369598
C	-7.67500501535192	-4.59697187836619	2.20948203182398
H	1.90321689475711	-3.68825846427215	0.19442943964510
C	-2.83295090268201	-3.16103380532110	0.15750535264362
H	-10.00247169672219	-3.45831178658848	2.95671974861815
H	-7.45373752620633	-5.26938280889804	1.37680027453554
C	-0.76536021943171	-2.03248674907502	-0.19462812273504
C	-8.26151513808459	-3.30529096275342	1.73082599600666
C	-9.48248165002242	-2.85450788600771	2.21926993724838
N	-4.25134665902273	-3.23308578781016	-0.03559964823315
C	-5.15468567533364	-2.70016904056209	0.80666055348207
Au	-4.72725744887843	-1.80295622248204	2.55492775335573
C	-4.87957884837538	-3.81601805487012	-1.11262990306265

C	-2.13858476778564	-2.09385423439226	-0.40934078650826
N	-6.35470075125581	-2.94735818139520	0.25319445099875
C	-6.20574443917629	-3.63538707968851	-0.93082658543405
C	-7.61077128720426	-2.51012625955702	0.78774937855481
S	-4.11581761139537	-0.88499539839355	4.56841141819397
H	-4.33000862529685	-4.30050169554091	-1.90206845359453
H	-11.51763521756675	-0.14090532369997	2.19300933910095
H	-0.20786373161266	-1.20500431947951	-0.62215792775212
C	-10.05164270606857	-1.66035354211939	1.78833166201301
H	-12.19422438872242	-1.71203132439537	1.76439569816465
C	-11.38442159184954	-1.21734798230998	2.30994380453164
H	-7.05083210689436	-3.93005500596573	-1.52996803727693
C	-8.14259275511438	-1.30670196329337	0.32612912453805
C	-9.36703932798759	-0.90138483016825	0.84570014176720
C	-2.83601865064826	-1.03924461949053	-1.21185611674148
H	-7.98573330125097	0.44371621282353	-0.88998658450909
H	-2.11962695788891	-0.30127134623132	-1.57204928915251
C	-7.42742993807979	-0.47047916490032	-0.68961059651362
H	-9.79442912372196	0.03567266978458	0.50244710492924
H	-11.50139045693526	-1.47276606266864	3.36484159597501
H	-3.34889590876528	-1.46752338312865	-2.07697487704043
H	-6.42712707414918	-0.19400771061589	-0.34562134479193
H	-3.59185704673731	-0.52021513621712	-0.61579917979654
H	-7.30445436587523	-1.00716336964703	-1.63417862882756
C	-5.53866537347118	-0.35213659744060	5.47801582183352
H	-5.18464766513007	0.14018690079666	6.38528310404489
H	-6.12239749608158	-1.24110533667988	5.71369615767729
H	-6.11332138699908	0.33064504750474	4.85096727752910
C	-3.28740080829266	0.65529740405382	4.28864077772353

H	-2.37549622345319	0.43188698792061	3.73605584028607
H	-3.06165871218707	1.09418561416730	5.26184266651539
H	-3.94386120777614	1.29867367328288	3.70151532909673
O	-3.27876281676119	-1.74211162812738	5.42451977265166

[Au(IMes)Cys]

Coordinates from ORCA-job

H	5.26266613998771	0.89221836280298	-2.52017724495390
H	4.26221680786911	-0.05286969966485	-1.40603410775788
C	4.56503055212494	0.95988263683614	-1.68556026861988
H	7.02934489654126	2.05566841200429	-1.56396648721170
H	2.09748795633549	-1.84776666248975	-0.87270412939873
H	0.71373919161371	-2.78423813486614	-1.45708226896465
C	1.00705643854346	-1.92602850556062	-0.85267156539591
H	3.66732485610694	1.47851966304618	-2.03274479276423
Au	4.14762883364737	-1.29040428848074	1.93543008708123
H	-0.46249761724324	-3.94416899819658	0.17195979237106
C	6.48869416195948	2.18363838725840	-0.63128420238520
C	5.19770048281599	1.67362977055853	-0.53141977473509
C	-0.25168716682989	-3.18428052824656	0.91833609086684
C	0.49927624639042	-2.07484614560890	0.54811254096140
H	8.88514035910651	3.22710846651141	-0.70815600014735
H	-1.24636643003199	-5.42600942983883	2.02735724757171
H	0.61230148012020	-1.02341872494927	-1.32683299591036
H	-1.51195752299976	-4.74884577608932	3.64512368592890
C	-1.56629623976539	-4.53804495193969	2.57590763272402
C	2.88040579302064	0.11007625157142	1.25191334055061
C	-0.73391530102913	-3.34604139315299	2.21329928015462
C	8.49359066393670	3.38247782846642	0.29774050442101
C	7.09951041750109	2.84727901752266	0.42548399833887
C	0.76565539716086	-1.11537684977732	1.52557230262563
C	4.52241225064550	1.84890598160067	0.67443077715711

H	9.16703623921337	2.89049770773819	1.00510932739167
N	1.53638560605741	0.03606568500652	1.16649154173177
N	3.18961939219989	1.34090654130718	0.79444691968284
C	-0.44510932226049	-2.36495970265146	3.15540108885260
C	0.30331015096789	-1.23685113849026	2.83517622135312
C	6.38668441326043	3.00231530576264	1.61136218638307
C	5.09508074778233	2.51320485977808	1.76044303448252
H	-2.61780698496389	-4.36303149243087	2.32731335878370
C	2.05220903707236	2.03013543407005	0.42836986156498
H	8.52457176621354	4.45293982773125	0.51721116854849
C	1.00937606306132	1.20738562684302	0.66307873304336
H	-0.80722398182365	-2.47886319803112	4.17260960074891
H	1.68752592812220	-0.09829621512776	4.01992951632989
C	0.60892175104827	-0.19966369200705	3.87076359910809
H	6.84729741354278	3.52006800194964	2.44739987376864
H	-0.04940059238358	1.34419673804158	0.52097446600601
H	2.09125219728811	3.03325959307310	0.03809880689896
C	4.34833650531913	2.69329197632755	3.04543187532051
H	4.07262777867746	1.72876463247176	3.48072274936562
H	0.15499075851693	-0.46822077482422	4.82452225347944
H	0.23216678170490	0.78360777123026	3.57695277689356
H	3.42139570559964	3.25287093506485	2.89341734574488
H	4.95906723414033	3.23419907314629	3.76811929768310
O	5.23963871223425	-2.55511532089413	6.33198742586769
N	3.02975892618403	-3.05282588276351	4.80528167601709
H	2.31353562793826	-3.33444377149784	4.14408378345977
H	3.35614260069887	-2.14004269406253	4.49857840789829
C	5.19278237539793	-3.60065232219680	5.73447622561226
C	4.11968990588160	-3.99962764536010	4.74661299494671

H	3.74164463753678	-4.97359182719072	5.08221595486705
H	6.78733340390579	-4.24156907809300	6.49740294736523
O	6.11391926298037	-4.55754798913415	5.87506750201503
C	4.74043274650466	-4.23809952603964	3.36009198148164
S	5.67622824074007	-2.83229938609635	2.67327158865234
H	3.94150413484127	-4.53036392382452	2.67728540952537
H	5.44633218926965	-5.06860881814300	3.42178505661663

[Au(IMes)₂]⁺

Coordinates from ORCA-job

H	7.49367141733352	-2.06669373648359	-2.27422252630100
C	7.17027569506595	-1.64495666469181	-1.32756294491577
C	4.90983632152361	-2.64725919970399	-1.76356655594167
C	5.85631083000755	-1.85055541519119	-0.92015861805795
H	-0.50120424781668	-5.87289479149609	1.90761115384048
C	0.03319985631992	-5.08705649577370	2.43284512443921
C	9.49094634804522	-0.73605507863146	-1.00611292508740
C	8.07199110170890	-0.91635721999672	-0.55983236262929
C	-0.11606710703685	-4.96136709937705	3.81040830254407
C	-1.02552184121874	-5.88100897559277	4.56679821492637
C	0.85479671999987	-4.23645831093258	1.70290508713146
C	1.01194983182459	-4.40413652314611	0.22350125371153
C	0.58332990980036	-3.95251921218363	4.46340293030402
C	1.53562267590560	-3.23735944852484	2.39906373679649
C	3.70028585538540	-2.56064343440887	1.45254448454486
C	5.46193128963876	-1.29790970032867	0.29757478280685
C	1.41603463497682	-3.07399886199407	3.77827599247034
C	7.63293575632333	-0.37765156115656	0.64537502072886
H	0.48373004612832	-3.84390739084191	5.53900060671184
N	2.38820476360036	-2.34699677798114	1.67045405948168
N	4.11497926430453	-1.49272747310333	0.74341697744410
C	6.33058585850529	-0.55465136630904	1.09710158714147
C	2.16321676622806	-2.00064322891223	4.50752363693414
C	1.98374232511613	-1.15758697436594	1.10394142627952
C	3.07393137782456	-0.61850331168211	0.51791120016398

H	8.32175900612436	0.19869121742583	1.25543738235695
H	0.96675877258226	-0.80871469093389	1.16848518600535
H	3.20387942612884	0.29758573737973	-0.03336706014620
C	5.88698453611357	0.03056064337553	2.40195635164133
H	3.24405980244514	-2.12564457841935	4.39728652158633
H	1.92290733985242	-2.02522330883118	5.57026578658688
H	1.91484094404465	-1.00778789812476	4.12331387820637
H	-2.06414780325213	-5.54369136929836	4.49281978660012
H	-0.76390174358414	-5.91423547777525	5.62546334277190
H	-0.98523812527157	-6.89527434723723	4.16462000772248
H	0.35966704712294	-5.19730996770946	-0.14163962655259
H	2.04257400197368	-4.66371732053369	-0.03539761821197
H	0.76852913353577	-3.48417683420537	-0.31399452818073
H	5.07597486923221	0.75075221599733	2.26411616055553
H	6.71655548751961	0.54218786486312	2.88973721235389
H	5.51606461876063	-0.74400098106088	3.07876795229711
H	9.58106994877056	-0.83233989809989	-2.08918874641314
H	10.13592777598709	-1.49565872762104	-0.55280839902596
H	9.87910778257682	0.23954030527556	-0.70762469786952
H	5.38697959327306	-2.93775257382616	-2.69941949178332
H	4.00595834022287	-2.07974671585423	-1.99995900651154
H	4.59089327796018	-3.55665078853673	-1.24610486650352
Au	4.79562278642279	-4.15894900049559	2.02542234065425
H	0.69655003668718	-7.87807201030068	-1.32562762083726
H	8.70432216454564	-0.47508450406451	5.95624227782120
H	10.20370871590848	-0.81723226772780	5.08231190902456
C	1.30425784283038	-8.74543398416616	-1.04819340438617
C	9.44475093685682	-1.24900166072267	5.73559074202304
C	8.79776961505555	-2.44240020727209	5.10136507214961

C	2.45398964600815	-8.32679477263349	-0.18366192710469
C	9.14196680399454	-2.84476708198609	3.81709540264290
H	9.89245850857144	-2.28589428102840	3.26663703476876
H	0.65278426460931	-9.44929833579969	-0.52779544628133
C	3.64870897096416	-7.89464804217157	-0.75035885185875
H	8.09399649896432	-4.22451539244596	1.12923201893531
H	1.65218179225672	-9.20822760013388	-1.97344127981845
H	3.75536791057049	-7.88829106748186	-1.83085961528566
C	2.34470936850847	-8.33883039633349	1.20252728153530
C	7.83355578486118	-3.17409069490224	5.78993180677080
H	6.16655914565765	-5.94390422128652	-0.40939815251376
C	5.88033917455733	-5.77272347768650	2.57363069591559
H	9.76196714853807	-3.73793961628964	1.45922209682480
C	8.55296447006893	-3.94974639740070	3.20915643589013
H	1.42202833393478	-8.67995209276328	1.66193765677255
H	3.42379294938942	-6.95298961886350	3.94464173563341
H	7.55109490230528	-2.87401810799829	6.79457673197566
C	8.93463223664130	-4.35023007218717	1.81801110448136
C	4.71991846902483	-7.47140437058034	0.02771286687301
H	5.23022899342951	-5.07520680098851	5.44482154597423
H	5.94846421250351	-7.14416063784687	-1.69043608110886
C	3.38609818413459	-7.92392755834228	2.02547350931263
C	7.21748798944179	-4.28458735176384	5.22831416920198
C	5.99173484662845	-7.00490153834396	-0.61035498336140
H	9.91907203533824	-1.51816464405044	6.68298866524608
C	7.59541775604814	-4.65342414415475	3.93597459426129
C	4.56220111294055	-7.49094475177137	1.41380661743806
C	3.23858518621670	-7.94133849818636	3.51563075713527
C	6.17997699012836	-5.05320514236786	5.98619629021008

H	2.23249395125578	-8.25401775866512	3.79451501244427
N	6.98474657389462	-5.80557218896608	3.34401407407839
N	5.64959302242339	-7.05754275791208	2.23867206751146
H	6.00817280460979	-4.60024764728492	6.96242148337459
H	9.23593996584200	-5.39954159073101	1.76879954006121
H	6.85784709640971	-7.55024195061262	-0.22704859559391
H	3.94925505659525	-8.63023175988228	3.98040934786297
H	6.48441770043754	-6.09194344043026	6.14018713469077
C	7.44147595679434	-7.09755454231870	3.49231268093056
C	6.59891472298714	-7.88779168968907	2.79366163512790
H	8.31619818441267	-7.33219535809121	4.07531488222588
H	6.58793969818111	-8.95391322631825	2.64086156741629

[AuCl₂]⁻

Coordinates from ORCA-job

Au	-3.54983844504653	2.02446446148997	0.00009821713191
Cl	-5.82566256341151	1.97858524426328	0.00334243047787
Cl	-1.27397899154194	2.07001029424675	-0.00344064760978

DMSO

Coordinates from ORCA-job

S	-4.12771042281068	-0.93306982428853	4.50591855907150
C	-5.51578965962075	-0.34369576089182	5.46907880904772
H	-5.14627710787574	0.16414891159649	6.36162325182897
H	-6.11303002008043	-1.21446843271472	5.73944323494394
H	-6.10734404534004	0.33345987951150	4.85053165318950
C	-3.30818476651967	0.64365567684580	4.29976033795382
H	-2.37429958000512	0.45202953408370	3.77140529954227
H	-3.11347048183938	1.08016879910753	5.28090925657881
H	-3.94644108388519	1.29537522727939	3.70088780444738
O	-3.26949283202299	-1.74707401052934	5.42940179339606

Cys

Coordinates from ORCA-job

H	2.21694735285129	-3.03584660448594	9.47349953449256
S	0.31730812362329	-1.33141562721508	10.26669999356017
N	1.92639254164557	-3.69395703087810	8.75068371091014
O	2.17389473037938	-1.56094968735916	7.02328544085301
C	1.07962961060709	-2.04062673599307	7.18914793989680
H	1.67047664171776	-4.54309555300504	9.24396028680115
O	0.01050088794122	-1.63514050327707	6.49195226890945
H	0.29315242524699	-0.92180204233323	5.89969103244154
C	0.72323955233431	-3.14652167287016	8.15649227276115
C	-0.31618635732042	-2.64622881449330	9.17576575459020
H	-0.61704376486442	-3.51724127764487	9.76700684405944
H	-1.20265687363601	-2.30273654251983	8.63702964567619
H	0.24884512947391	-3.93013790792513	7.55208527504808

[Cu(IMes)Cl] - DMSO AR

Coordinates from ORCA-job

Cl	6.14805107145322	-2.22933317443538	1.67601267466069
Cu	4.40995831276490	-1.03917620937599	1.27432248547241
H	4.23094863863888	0.60737718391501	-1.66323155085264
C	4.13814578929822	1.69322878139051	-1.75590618093761
C	2.87690872149408	0.03279712440163	0.96122996302228
H	2.39905569797629	-1.24263183323171	3.63012626684712
H	4.71845417791024	2.01256739125796	-2.62153436864853
C	4.62192611249666	2.38345538913079	-0.51778398040332
H	2.04888139870337	-1.45290596475517	-1.60298760970200
C	5.73557077107052	3.21328297191959	-0.55574310150053
C	3.97726065361672	2.21429517000147	0.70921919495163
H	3.08415895677734	1.90817377563386	-1.94953459783587
C	1.15871532958363	-1.71897537226485	1.06111706740820
C	1.33088661974968	-1.47146571132693	3.56817172276964
H	3.68271928400538	1.59841119384795	3.46163020620726
C	1.02449763694283	-2.26747843100838	2.33700102332028
H	6.24544844021248	3.35829724392548	-1.50360453510583
N	1.58527159990995	-0.36002534982503	0.92839965971707
N	2.82459486180787	1.36870223415903	0.77074011890849
C	0.88294985112206	-2.44900544279420	-0.09509951790784
H	1.04956082593840	-2.02883192230824	4.46171028860572
C	0.60297480865089	-3.58925966719401	2.43273654706184
H	0.76740519735324	-6.44056446430509	1.52896390801728
C	1.03850365556295	-1.84436818576245	-1.45677493915854
C	4.41308457660591	2.84786600697928	1.87153895740794

C	0.46310096720909	-3.76662433306938	0.05405097279828
C	0.31989914318586	-4.35498003308139	1.30597687552765
C	6.20924725337424	3.86085704818581	0.58198869029504
H	8.32930584830093	4.12729198288394	0.38413130526733
H	0.48922300025747	-4.02905911040318	3.41901814763383
C	3.70789069899111	2.65430187455596	3.17861189137642
C	5.53417970075464	3.66805642844476	1.78151381327876
C	-0.10531621300371	-5.78589737835711	1.43845187093967
H	0.24235743328379	-4.34752240475197	-0.83631802977852
H	0.84320432811741	-2.58884477426827	-2.22852156669628
C	7.42661523828999	4.73250329293315	0.51158819389427
H	0.79937458404509	-0.51665948707654	3.57369376187985
H	4.21243854472382	3.20967595183490	3.96919118110611
H	7.37494846422504	5.41497194205177	-0.34003943391856
C	0.74013949051268	0.71037449350551	0.72477605534941
H	5.88682063660821	4.16891443380105	2.67791326099140
C	1.52438992638507	1.80466458212546	0.62558932463444
H	0.34830785769672	-1.00984571850261	-1.60682894011193
H	-0.67323004498143	-6.11282924798060	0.56596344036266
H	2.67080437475111	2.99669903764922	3.12908119100827
H	-0.71641612939563	-5.93652546569404	2.33053628088322
H	7.54501035046231	5.32215248608213	1.42155759808515
H	-0.32961279288119	0.59696917639466	0.66921956237645
H	1.27915404040171	2.84136574860889	0.46616271144224
H	4.53178262156981	-7.08249021813343	-0.09485284285887
H	6.12024612577768	-7.60598606899571	1.74147415032140
O	3.37852080680218	-7.50395211996761	2.45735404170583
C	4.18958855943989	-6.14009240351504	0.33677733164163
C	5.89909837976542	-6.71286053648459	2.32859511251734

H	3.16957218739989	-5.91948560344296	0.02144286493690
S	4.17645814613041	-6.27825078501342	2.11996913226009
H	4.84963216097035	-5.31774000721140	0.05517608438175
H	6.51313907257683	-5.86956579718110	2.00790261700720
H	6.05541224860612	-6.90169972390154	3.39072364713607

[Cu(IMes)Cl] - DMSO TS

Coordinates from ORCA-job

H	6.99777600522715	1.73787142439472	-0.97171859075513
C	6.39559543569404	1.75371075370441	-0.06828907445622
Cl	3.35659845274039	-1.48558948137300	5.82182521980160
C	4.51794335022989	0.77786526698342	-1.41823029465659
C	5.08765901135289	1.28979149807167	-0.13083498481428
Cu	3.69558128656380	-1.78209546205184	2.04842103112512
H	-0.88661392892013	-4.09020951677730	-0.53023950334140
C	-0.69720688315930	-3.43832226220357	0.31724664501712
C	8.37161538770589	2.70214005746637	1.15705248924029
C	6.94819347422248	2.23570369874332	1.11479706668510
C	-1.31918112012055	-3.69927771676623	1.53373054642038
C	-2.27380226482559	-4.84558977107155	1.67750247919021
C	0.16274401924755	-2.35886696280262	0.14945737252256
C	0.81251983056215	-2.09897042905241	-1.17495952003521
C	-1.05738638832952	-2.85241231139156	2.60541281581441
C	0.39612812256448	-1.53456019382525	1.25135675000591
C	2.58193235410442	-0.38911589183958	1.32885442068667
C	4.32894297619925	1.32019661426639	1.04148464270347
C	-0.20525193122950	-1.75888692469486	2.48974951957862
C	6.15353180761378	2.25776381372955	2.25515325713145
H	-1.53383861081909	-3.04114307385865	3.56274517801757
N	1.25447279027072	-0.40024538326695	1.08499397590806
N	2.97547224390247	0.85681375145242	0.98983522419228
C	4.83694764309273	1.80616455733979	2.24524454128010
C	0.05531336121041	-0.86907631626320	3.66527641887542

C	0.82502154931959	0.81816342866154	0.60430891801881
C	1.91381494484609	1.61369482142681	0.54465079367878
H	6.56376952703064	2.64438093626888	3.18306210618675
H	-0.20582032316728	1.00496559648952	0.35388314131406
H	2.02872251685934	2.63811387492322	0.23206728511931
C	4.00882699656153	1.84320131828974	3.49246950363263
H	1.05528732221102	-1.03974052189695	4.07683342259162
H	-0.66866275012028	-1.06568572336324	4.45653471046658
H	-0.00750989049367	0.18714723964436	3.39433147408432
H	-3.30181077749742	-4.51410158814214	1.49904183366371
H	-2.23850297227582	-5.26796430598277	2.68330700175696
H	-2.05531088157250	-5.63656551124660	0.95804540135649
H	0.50962212865686	-2.85328792705872	-1.90094783648416
H	1.90272853050736	-2.11787303985007	-1.09416034766764
H	0.53832006432995	-1.11688272662014	-1.56925021085059
H	3.02291934666790	2.27650227167796	3.30926633009624
H	4.50792048194910	2.43302473754346	4.26150706265237
H	3.84949324219074	0.83655785273739	3.89113059816384
H	8.63285004906779	3.25745518705010	0.25380506765397
H	9.05472302659140	1.84938310188484	1.22109613593311
H	8.55446172530651	3.33848885029218	2.02407395565672
H	5.27978153337854	0.77776737503620	-2.19767687160096
H	3.68304291565720	1.39570412767724	-1.76025420918784
H	4.13747325386111	-0.24124563727089	-1.30844829644034
H	3.45262433669174	-5.00086565126457	3.23192250537966
S	5.06967642106715	-3.37162584437235	2.77617664954376
C	4.20206459468319	-4.49487543493084	3.83973979901320
H	3.73130020841047	-3.89853078620682	4.62583279392298
O	5.79409742811402	-4.14255327827641	1.73872201147762

H	5.67773350645695	-2.21480820216951	4.72309410993105
C	6.24353412846561	-2.69884443455083	3.92242773803905
H	6.84930687501929	-1.97546458033437	3.37767326110264
H	4.92401881248458	-5.20567173799388	4.24509432414525
H	6.85534570362541	-3.52142352703489	4.29687221148048

[Cu(IMes)Cl] - DMSO AP

Coordinates from ORCA-job

Cl	7.12223803948805	-0.18851171185885	4.33431245868705
Cu	3.57683385456903	-1.26643259345337	1.28349710480933
H	3.73704779026024	0.69692929284831	-1.76950419429975
C	3.98979361170100	1.76053171737858	-1.78998997887099
C	2.36415650780935	0.17645536812310	0.92053318640311
H	1.52155256781583	-0.84957881403463	3.57708381271105
H	4.67799640613237	1.93343934958267	-2.61726855784419
C	4.60613882595677	2.19888126289507	-0.49689253902750
H	1.28528766847686	-1.10519922903517	-1.64727172326501
C	5.87779403816366	2.76492452249573	-0.47022672421358
C	3.93554974726092	2.05562458669735	0.71625110733501
H	3.06427626305737	2.30450098206208	-1.99728230514282
C	0.29475490241315	-1.14448306629160	0.98107712934969
C	0.43147105247393	-0.86290983948561	3.48718999038454
H	3.58724497861637	1.23858340075586	3.44833105870716
C	0.00008399095898	-1.61038916419033	2.26299289256983
H	6.41624884566349	2.88189606378841	-1.40570935824951
N	1.02074922745711	0.08079183009790	0.83869077078812
N	2.62321449059974	1.48351407568034	0.71672136171482
C	-0.10391637144172	-1.82501664383164	-0.16955334618777
H	0.02157073175449	-1.33032962213672	4.38243262335126
C	-0.71104249745455	-2.80029320742104	2.37065540251502
H	-1.16339343694327	-5.64385596766351	1.49994031874604
C	0.21627644212377	-1.30515671727235	-1.53740719455123
C	4.49183578610461	2.46246690825664	1.93064150739494

C	-0.81490349319168	-3.00926608464754	-0.00788351940146
C	-1.12450140349689	-3.51449974011924	1.25038487048851
C	6.47163314268035	3.18046933564264	0.71550663489662
H	8.50944171786869	3.23425007302016	1.38928578514803
H	-0.95178207607135	-3.17500928788848	3.36090394450580
C	3.75441430748608	2.29566096861750	3.22335440215749
C	5.76232898006746	3.02286597044889	1.90318036965255
C	-1.86446891303564	-4.80954832551428	1.39642456004047
H	-1.13403455686602	-3.55010886517107	-0.89364223333891
H	-0.07978688088339	-2.02778505176681	-2.29775362400013
C	7.84203725975104	3.78740123640429	0.72309146918678
H	0.10067494425321	0.17837393941306	3.45860354123308
H	4.32290402606564	2.73180867400524	4.04451788975764
H	8.27924027764354	3.79041284911249	-0.27607666158196
C	0.44722308575375	1.30796851319089	0.58761246785083
H	6.21153778272308	3.34034669118035	2.83931244291874
C	1.46159858754808	2.19606122939438	0.51027298656583
H	-0.30697044030375	-0.36660479485336	-1.74088569705486
H	-2.48650811974889	-5.01118178715705	0.52283335217703
H	2.77279202218270	2.77546672545344	3.19047550224377
H	-2.49891163700065	-4.80581651659955	2.28471937951368
H	7.81071375057906	4.81893359427072	1.08477347599478
H	-0.61776264007748	1.43672066159815	0.48973379405384
H	1.46328369871942	3.25837250414630	0.33174908735453
H	5.32360466758848	-5.06907513719788	0.61634893046545
H	7.06097525863966	-3.64608714037165	1.85709587910197
O	4.45238598502369	-3.76966463215267	2.99291973568929
C	4.67146380243800	-4.22355470255796	0.39073559544713
C	6.52129601126632	-2.70865226500393	1.71053589016198

H	3.63040233101252	-4.53819080854684	0.32474933574330
S	4.78646118282748	-3.06738932938079	1.73319250970950
H	4.97712187084749	-3.72074259260254	-0.52782700751051
H	6.76366860119799	-2.26008718702174	0.74552217829993
H	6.71595340349258	-2.00108150133216	2.52268792871393

[Cu(IMes)Cl] - Cys- AR

Coordinates from ORCA-job

H	5.84361000240826	3.37691479910648	-2.52943390860282
C	5.62236032718091	3.23201508688157	-1.47627508173802
Cl	5.81809653622911	-2.47770385077117	0.30492800003533
C	3.56597631256682	1.97217408370946	-2.17847493477910
C	4.47465597006462	2.52880045695025	-1.12600150014254
Cu	4.29291232886384	-0.98330060639084	0.54622294506573
H	-0.38373946651860	-3.74865403619692	-0.20039518541261
C	0.02045258665558	-3.16035347015493	0.61796974170057
C	7.72768696614590	4.48896309554194	-0.92349828232726
C	6.48438493505797	3.75610759818109	-0.51859253151056
C	-0.02121657696093	-3.67004249870100	1.91198650117678
C	-0.64853100607841	-5.00217515079566	2.19048544908621
C	0.56856126267046	-1.91456396404048	0.33666459795488
C	0.60353154360999	-1.39270914247077	-1.06675583334920
C	0.51430393226678	-2.90553052476045	2.94316342716146
C	1.08903623226505	-1.17780136009373	1.40171112492281
C	2.93213015469476	0.32411147806752	0.77546219144425
C	4.20491618053441	2.35994715338170	0.23219039766442
C	1.07478497423514	-1.65299229171381	2.71268073488874
C	6.17565702676612	3.56610202947362	0.82448538805785
H	0.49745350450830	-3.29425805259634	3.95790622022509
N	1.64791479867427	0.11280288195034	1.13803046690868
N	3.01666127974414	1.66340374088821	0.61935247282562
C	5.03990885247280	2.87108159927265	1.22592278556450
C	1.64385485374100	-0.85022719208094	3.84235302508214

C	0.94326666128338	1.29576549225978	1.20788621517394
C	1.80959343267928	2.27724555089286	0.87958774982429
H	6.83368794099994	3.97339814622763	1.58615716828070
H	-0.09843118014394	1.32971269102018	1.48023956696069
H	1.67946532393071	3.34407563300024	0.80652312780484
C	4.73106030280118	2.68225893457267	2.67934676233240
H	2.68149009896732	-0.56741640215227	3.64661355169853
H	1.61166845240756	-1.42311792343476	4.76918708510298
H	1.08328949236108	0.07634102886205	3.99504050386477
H	-0.45918741613509	-5.70638112272893	1.37772339540700
H	-1.73449029430174	-4.90370866398072	2.28832592024420
H	-0.27184613039571	-5.42808036799549	3.12232918525024
H	0.11872750600146	-2.09419668238251	-1.74562737692341
H	1.63215315283833	-1.24177606144057	-1.40601905520220
H	0.09517060676484	-0.42840887373762	-1.14908324204468
H	3.77613353966541	3.14127764012326	2.94917515692627
H	5.51011604669117	3.13092240966400	3.29558537508922
H	4.65855238639504	1.62138137394534	2.93388802801910
H	7.60079902578696	4.98045322181308	-1.88968728675286
H	8.57068114699974	3.79690480641342	-1.01615601806504
H	8.00301787970399	5.24083376461774	-0.18182477667922
H	3.91444229099468	2.25635478589406	-3.17139428395988
H	2.54124352422093	2.33301510969075	-2.05733218507547
H	3.52783189843773	0.88040980627449	-2.12732982529765
S	0.85479089227809	-5.40562116603039	6.05410981656964
O	-2.45010180594005	-7.14500933747018	6.13843357930793
H	0.23443787128708	-8.00289731035288	5.72943180231113
C	-1.81987368611404	-6.86950423082786	7.12947876115698
C	0.55761454591349	-6.27292216626463	7.62843727456184

N	-0.07648950895974	-8.46679401835343	6.58245073508145
H	-3.14583588032915	-5.69362298579087	7.75356886486118
O	-2.28285131296863	-6.01765457031441	8.05302501750177
C	-0.46216945015624	-7.41849622133753	7.50696010327942
H	0.21421577326905	-5.57103994955703	8.39236734094897
H	1.48712477931764	-6.71941593197350	7.99659616662846
H	0.74832431694138	-8.92329499623229	6.95872252630435
H	-0.58546573529296	-7.86442327555067	8.50233505760361

[Cu(IMes)Cl] - Cys⁻ TS

Coordinates from ORCA-job

H	5.68278443264738	3.52872448470655	-2.68264485655540
C	5.51627627786885	3.42831466534058	-1.61430906751996
Cl	6.05162839753118	-2.27084107481627	-0.37481197226136
C	3.60128809342098	1.89667196763396	-2.15454367729025
C	4.47457141393759	2.61880283679632	-1.17502467151273
Cu	4.64989124370652	-0.83154703672764	0.43401313342907
H	0.24997299535771	-3.98981083125438	0.08418118229149
C	0.61932761670772	-3.35013986047046	0.88003650551817
C	7.46766408676064	4.96445688538793	-1.22596060622454
C	6.33696089181061	4.11664268521481	-0.72645803834397
C	0.62798297703955	-3.82302789842068	2.18727587915812
C	0.10682555259860	-5.18946947525570	2.51542964035959
C	1.06850163655545	-2.07377628249268	0.55619968474992
C	1.04199379626785	-1.59237197071394	-0.86168598382099
C	1.10948777643164	-2.98663206156663	3.19001840788947
C	1.54210556193343	-1.26859316881849	1.59189249480717
C	3.22199739173013	0.36906632709776	0.83369875935159
C	4.27052956487797	2.50948023228792	0.20120055918265
C	1.56872711154381	-1.70309632347432	2.91834735009250
C	6.09394583716902	3.98446965380961	0.63648279413574
H	1.13085562645941	-3.34087930169284	4.21629894262588
N	1.98730251492851	0.05669651726500	1.28971667864463
N	3.18346023381069	1.71176197383890	0.67794498904772
C	5.06521986644758	3.18673526380066	1.12641397495048
C	2.07265825767449	-0.82168051586630	4.01957910414888

C	1.19499356689679	1.17898411163725	1.41355273942361
C	1.95175821983306	2.22604150062626	1.02656207141185
H	6.71935073113577	4.52049619940769	1.34396654056579
H	0.17610336165854	1.12869663307740	1.75962755857235
H	1.72932693872329	3.27822705553261	0.96450633494097
C	4.82530044537908	3.06716269328941	2.60002566382856
H	3.08742750828117	-0.46955616130396	3.81531154425918
H	2.08129683907932	-1.36264246305755	4.96581674781899
H	1.44319776254425	0.06436752714356	4.13989668325637
H	0.08860494939055	-5.82966490523253	1.63212137280749
H	-0.91529815942489	-5.12988257046519	2.90262797213148
H	0.71545138497493	-5.67119677923913	3.28336734034158
H	0.56114980925025	-2.32916973681962	-1.50516263151862
H	2.05468490470096	-1.41772965173236	-1.23608582632084
H	0.49988848817340	-0.64768583491808	-0.95426634552784
H	3.84100384181903	3.45325209888213	2.87866644962884
H	5.57841674145063	3.62747348605536	3.15418416926298
H	4.86792123136930	2.02304292598961	2.92229539587821
H	7.22708876131459	5.41820440657813	-2.18921280144403
H	8.36985363577662	4.36065138701039	-1.36621669327361
H	7.71111633184262	5.75731095903179	-0.51672767359886
H	3.85582710993005	2.18308585200648	-3.17505578256145
H	2.54378858680565	2.11719754018807	-1.98750660187107
H	3.71966020377832	0.81326697409064	-2.06208466237118
S	6.57294035065046	-0.36874822050409	3.38750927499072
O	5.39639097605408	-2.73599553246619	6.02286979135535
H	4.86603559839620	-2.49576632978802	3.31687451659855
C	6.45151490472032	-2.88685571570968	5.45726461370560
C	7.44591341804512	-1.96556701333941	3.35793250687079

N	5.36563215364444	-3.38322085365227	3.34694325531786
H	7.43655155768433	-2.68276746285815	7.04510652653506
O	7.62015670240902	-2.85829147938971	6.10953353368999
C	6.64451228227114	-3.12542795867597	3.97849916009518
H	8.40418074102815	-1.88311987828236	3.87664298845449
H	7.66025705431663	-2.25305005069877	2.32395789849830
H	5.54170620633005	-3.61778508658223	2.37431885056164
H	7.25975570454674	-4.03020535744101	3.89528631083079

[Cu(IMes)Cl] - Cys- AP

Coordinates from ORCA-job

H	5.78966515583344	0.40029980369061	-2.11309962966950
H	4.95137461912785	-0.54174235031385	-0.87455194123906
C	5.04049876665707	0.45256002654063	-1.32284888262416
H	7.39719511833017	1.74262050729301	-1.09098967749017
H	1.92247709729227	-1.91457408666880	-0.71915338601974
H	0.60359385300354	-3.03854484055452	-1.08044114141941
C	0.84820329181208	-2.08298940204828	-0.61642928707912
H	4.07459544282880	0.68528019557547	-1.77716071475965
Cu	4.19983097089261	-0.95197034623459	2.29562779425014
H	-0.66601960275783	-3.90799825407028	0.66399447037370
C	6.70100536405102	2.04244030800614	-0.31356279167379
C	5.43149682163373	1.47207586310207	-0.29765121761935
C	-0.37010163142215	-3.10139613186074	1.32784376595007
C	0.42562172549913	-2.07760409244617	0.82048338542311
H	8.94420017332186	3.44524925902087	-0.36978724690153
H	-1.75355869833620	-5.02934010697877	2.44625048401890
H	0.34266524994144	-1.29469284577341	-1.18172938235193
H	-1.24766252056176	-4.64076008841330	4.09857659475434
C	-1.65635510714041	-4.22350276103136	3.17497289954989
C	2.93239825425331	0.15434677440385	1.37534944015148
C	-0.78945070396760	-3.11854281467213	2.65206209404978
C	8.47966607841895	3.56079664624021	0.61061229925937
C	7.09690691370841	2.98280478416131	0.63040661642785
C	0.80475778314251	-1.05678026529651	1.69050868845848
C	4.55130867239927	1.87593281318453	0.70542078208791

H	9.11906499758517	3.05642166421709	1.34189706557263
N	1.60001406376359	0.02081890345046	1.18787456811189
N	3.23705191994586	1.31255700975442	0.74745136829049
C	-0.39262308596183	-2.07591042835662	3.48509772975880
C	0.40238270256925	-1.03256080607757	3.02805569760000
C	6.18295816004941	3.36390944325125	1.60854976638812
C	4.90373762088301	2.82460600799744	1.66737989452456
H	-2.66011243119204	-3.85446181896012	3.40583350610295
C	2.12192011557565	1.89115233115464	0.18031902996268
H	8.46873310397555	4.62172814166703	0.86892564513350
C	1.08572523607620	1.07302812430009	0.45851383571657
H	-0.71146898562816	-2.07068715123774	4.52320709883820
H	1.88763969070123	0.08278874515377	4.10910963210171
C	0.80603628980543	0.07897986768413	3.94698900544676
H	6.47138308642329	4.10320522649369	2.34977688994760
H	0.04018027704473	1.14180173821668	0.20861222909042
H	2.16679633320701	2.82079445657897	-0.36203735943376
C	3.94111624899044	3.25027866498414	2.73336896293825
H	3.58626665206205	2.39318144174835	3.31192593937018
H	0.31467604730998	-0.02944867318451	4.91394573865096
H	0.54241763784846	1.05552915612704	3.53223133235703
H	3.05850271729942	3.73470511470006	2.30679051746723
H	4.41682907778070	3.95351247324000	3.41679166769656
O	3.68758875960219	-3.50028219309012	5.93191942162664
N	3.06605022234858	-3.94880618899010	3.30104189161621
H	3.03625249675794	-4.06044191456180	2.29261729234883
H	2.95170745537319	-2.95448227941995	3.48155195798579
C	4.45170673663816	-4.15915512403896	5.27125126954386
C	4.36120640058327	-4.37932434908370	3.77961039589996

H	4.43913208298753	-5.46248723763766	3.62259497368491
H	5.53467258098729	-4.58342647402971	6.74816739370384
O	5.50829990974363	-4.78288517091062	5.79955000544386
C	5.58077510974861	-3.75746819453117	3.07796094943933
S	5.80557625120333	-1.96750547003047	3.34636451900162
H	5.48497308514671	-3.96450727510310	2.00985556015399
H	6.48588850554126	-4.25175742615330	3.43669962376876
Cl	4.58946983926182	-4.14336893017793	-0.76340903175900

[Cu(IMes)Cl] - Ligand Scrambling AR

Coordinates from ORCA-job

H	6.77497832305940	1.88778057666741	-2.79410561032674
C	6.40028467919135	2.22804097650468	-1.83330638658371
Cl	5.77977599803246	-1.85657772609351	2.44190998863525
C	4.28887136366012	0.95548577344454	-2.31129200201043
C	5.12790794132530	1.83524688077104	-1.43639865412333
Cu	4.35689264880478	-0.43584827265348	1.69364826786154
H	-0.27827275979925	-3.24499268785489	1.61421904102553
C	0.00933219200120	-2.30368490149921	2.07272928939074
C	8.58058533297961	3.42350543815707	-1.47815214551419
C	7.20105452721468	3.04026159668305	-1.03552039966507
C	-0.31043663882157	-2.06718919308835	3.40456715896936
C	-1.01242650271049	-3.10527987523537	4.22667910478644
C	0.69189561034565	-1.36632399096286	1.30270424149920
C	1.03152321169671	-1.65257891857675	-0.12777209873755
C	0.05569132045674	-0.84818293309522	3.96856213321310
C	1.05052649466627	-0.16442010889800	1.91109536059324
C	3.10651939971512	0.81247328578226	0.99773369736000
C	4.66407925060998	2.28512937335582	-0.19910161796138
C	0.73670161312696	0.12001310064944	3.24113116826362
C	6.69727361706737	3.47036431104987	0.18671023743260
H	-0.19075762301254	-0.64316601559462	5.00623980526569
N	1.76472063204870	0.81347484098746	1.14937966282078
N	3.35625805535328	1.89472104737346	0.22944764188358
C	5.42886356883707	3.10613400097840	0.62822571708670
C	1.12264292841411	1.42226304381771	3.87333295349471

C	1.18521389973150	1.87692259351422	0.49023262137940
C	2.19266759092710	2.56068080205302	-0.09325384471717
H	7.30481009260924	4.11150313564029	0.81817549108494
H	0.12169898142542	2.04801088422870	0.49611277340258
H	2.18793050762318	3.45029893571006	-0.70067322436329
C	4.91166658129196	3.58231527930155	1.95067724049718
H	2.20297306479228	1.58327744544779	3.82250837818079
H	0.82086105678549	1.44053927519833	4.92056022555683
H	0.65016938047492	2.26844779974843	3.36725869504689
H	-1.46040041500496	-3.87469905053638	3.59627562738885
H	-1.79607923384607	-2.65919072491832	4.84292436258442
H	-0.30900995670735	-3.59753125136626	4.90581187772452
H	0.59082486571268	-2.59874297171594	-0.44184112711881
H	2.11425892725114	-1.71514031408840	-0.27012792146438
H	0.66728517848061	-0.86500083940492	-0.79243235282068
H	3.95923468958937	4.10774051908649	1.84272076303505
H	5.62653323463152	4.25963130090005	2.41785980790418
H	4.73835186472589	2.74349806188780	2.63065081454998
H	8.60344107506979	3.65581534207825	-2.54493909383723
H	9.28222893178794	2.60023930837722	-1.31149433754179
H	8.94751079630290	4.28883912000019	-0.92435003274159
H	4.83636272057278	0.68161265701871	-3.21309103581405
H	3.36392466267503	1.45516790760932	-2.61166625831630
H	4.00146718212603	0.03818038138435	-1.79037175902093
Cl	-0.37544243024349	0.06377440441124	7.79350112268415
Cu	1.06391129409785	-1.36514589174605	8.48866243812767
H	-3.55896850058921	-6.19308314559942	9.04284251856234
H	5.65947754353774	3.13421372887579	7.44867882389918
H	6.98266776947101	2.19525107707104	6.76005583974371

C	-2.99745253610996	-6.30975047856038	9.97277283163082
C	6.38730554894214	2.34498033378072	7.66220520844032
C	5.69196615345700	1.08150433655574	8.07099627956554
C	-1.65124816500130	-5.65778352567490	9.87520979253320
C	5.38625023155096	0.09946346423677	7.13490248547217
H	5.67628192367505	0.24167923136780	6.09818558279375
H	-3.58466867373844	-5.88359211259958	10.78710706909806
C	-0.82126005688084	-5.90478930372384	8.78477721352559
H	3.32104077980519	-2.21553253466792	6.32859946562720
H	-2.89751662934458	-7.38377207964558	10.15513759696863
H	-1.16185706866942	-6.56628553183565	7.99376131706216
C	-1.19675581536739	-4.80179574589341	10.87097235556945
C	5.31902701702464	0.87264910411454	9.39506866173887
H	1.57846444253841	-4.67226048947805	6.97081790560888
C	2.34836985390280	-2.60807416533930	9.12571528683895
H	4.83635976774646	-1.84232470920579	5.49444683488241
C	4.72155049546212	-1.07096962396785	7.48743784348484
H	-1.83122181282777	-4.59700026250784	11.72792454008936
H	0.60910873558662	-2.24581114446248	11.51879332752067
H	5.55356880186440	1.62679660470127	10.14031871658860
C	4.40228746420149	-2.11061811256470	6.45779553603080
C	0.43553260662998	-5.32335544471165	8.67245312998427
H	3.18547131821738	-0.64975939956204	11.32656032048567
H	0.78642654127160	-6.24399736674471	6.77481873548386
C	0.05418215679025	-4.19458691307063	10.80531041209665
C	4.65219700597592	-0.27890483913066	9.79765214098705
C	1.30469334541867	-5.59839466850615	7.48368908286113
H	7.04018988206591	2.71221062820004	8.45620982988023
C	4.36321288982860	-1.23708900067957	8.82519155876100

C	0.85155230338611	-4.46905948944769	9.69572064131583
C	0.51228962236838	-3.27003750595076	11.89061449592875
C	4.26030552168976	-0.47448370340229	11.22999389082658
H	-0.20043651931660	-3.26791966250851	12.71538935901971
N	3.68453013400753	-2.43473585023459	9.21664066956433
N	2.14023900068348	-3.85492851702255	9.60090402725442
H	4.51929028758159	0.40549308717192	11.81869420349191
H	4.78617056789092	-3.09234907509185	6.74705370118543
H	2.23695328365878	-6.09020761706548	7.77397553650926
H	1.49059420923399	-3.56232386427657	12.28048428527159
H	4.76611270410454	-1.33861870049156	11.66923415946633
C	4.30141029573697	-3.55165232315279	9.73930118330952
C	3.32395888527531	-4.45057127897325	9.98238331715409
H	5.36686282145411	-3.60421928315308	9.88885873926537
H	3.36191413865965	-5.44779785966080	10.38785574056303

[Cu(IMes)Cl] - Ligand Scrambling TS

Coordinates from ORCA-job

H	6.76484302294333	2.48302867944691	3.03642451796479
C	5.70822226098522	2.61098607223965	3.25149707434884
Cl	0.63284281927047	0.72461305658116	6.57626015025591
C	5.27626141706476	0.55458767361654	1.88013171023386
C	4.80702708725344	1.67202462060757	2.75857390033459
Cu	2.23221255053860	-0.49034053718738	5.14311278411820
H	0.36505164609348	-5.23881700886098	1.96118538111894
C	0.00966879485015	-4.26660426101117	2.28895491981309
C	6.27881762843316	4.68892476488935	4.54779509226566
C	5.29013991721277	3.70805088703426	3.99488370966244
C	-1.26687939278196	-4.15084456231047	2.82633582295232
C	-2.13991344211624	-5.35602080881803	2.99911629804993
C	0.84825625572525	-3.16632529496646	2.14570245881925
C	2.20078213153815	-3.31775939423961	1.52082972457424
C	-1.70665688358190	-2.89171837573422	3.22126443229984
C	0.37600083698617	-1.92548632685706	2.57262516587353
C	2.00763735677992	-0.16651007219307	3.25183574492994
C	3.45656448831067	1.84170276825793	3.06080132306899
C	-0.90576546454237	-1.76197072069441	3.10115881190403
C	3.92649049303680	3.87521220081686	4.21591868529149
H	-2.70716632546545	-2.77951178622282	3.62827314129201
N	1.18744096212255	-0.76712962750699	2.35405724298462
N	2.51692785311949	0.88547721485642	2.55981182221620
C	2.98817247174607	2.96019158399118	3.75357060255610
C	-1.42078204816273	-0.41397063300305	3.49965639293151

C	1.18800429857790	-0.10858523941795	1.14155514961214
C	2.02765771505044	0.93524690024693	1.27221187364764
H	3.57717790821777	4.74707360135841	4.76080771392282
H	0.59163925055589	-0.44288156130515	0.30923198298710
H	2.31917382966555	1.70462836967882	0.57705312868033
C	1.52561528215097	3.19299395069829	3.96809541523438
H	-0.81589123154161	0.02251941784715	4.29891910984853
H	-2.45066317854423	-0.48936448993467	3.84936583750125
H	-1.39613283843880	0.28433687098090	2.65823314779738
H	-1.85074202974157	-6.15620597172456	2.31601836406756
H	-3.19050927951444	-5.11233129572521	2.82927284242108
H	-2.05821884168943	-5.74690122118601	4.01867331780440
H	2.42648166925969	-4.37079934677736	1.35264369716194
H	2.98439996274410	-2.89198235018913	2.15015305271334
H	2.25080386198839	-2.80251053566045	0.55735056152329
H	0.97328005819270	3.12471910477960	3.02726550793256
H	1.35852549747520	4.18316174563450	4.39318134241360
H	1.10218772456652	2.45110210410664	4.65060799663983
H	6.41512775953746	4.53324129149579	5.62258397037343
H	5.93440187340686	5.71666907645166	4.41300817710624
H	7.25362513163415	4.58226982980021	4.06986190994727
H	6.36120704238460	0.46573626461044	1.91971059680785
H	4.99171579907403	0.73960611665020	0.83966106138041
H	4.83733829967435	-0.40228313998445	2.16538988210236
Cl	3.76807834367704	2.32610456448297	8.00623115675862
Cu	3.05501629059332	0.41303249838275	7.21050120065422
H	-2.67023451374910	-2.70041636074634	10.58281098163232
H	9.09496441157143	1.28286949565859	4.03603123625235
H	9.78990008089138	-0.31068401907629	3.75397414505868

C	-2.64676133076771	-2.49475645691945	9.51041811310645
C	9.33832596309745	0.32877491209520	4.51469691977239
C	8.10688738930248	-0.29938180316400	5.09139573539420
C	-1.24257023958925	-2.49883887719031	8.98755030001255
C	7.29288857313560	-1.11414124680755	4.31241006892297
H	7.57506419981299	-1.32596382245559	3.28605661947948
H	-3.26167439527619	-3.23735387758601	8.99999254118007
C	-0.93292995092134	-3.10012603252171	7.77343505094660
H	5.31635502973659	-3.61301257059658	4.34723405600229
H	-3.11293647104876	-1.51613981348151	9.35940780859870
H	-1.71605087636066	-3.59604200449501	7.20809968561861
C	-0.21434470512013	-1.89907755707668	9.70709386813415
C	7.74822938019754	-0.08145537881638	6.41686664089113
H	1.14295811394133	-3.11310222005677	5.25591565986838
C	3.38750700146227	-1.48818151971994	6.87725862916603
H	4.24147539563681	-2.27174959247155	3.97168425207386
C	6.12446106100344	-1.67592870574600	4.81235295529928
H	-0.43011795027129	-1.45205994335959	10.67297887600410
H	2.44091332709968	-0.24433771756593	9.66185043398456
H	8.39435315089939	0.51647787021553	7.05235543035447
C	5.28843140917297	-2.58681814166863	3.96954633414158
C	0.36010318554399	-3.09806133086559	7.26138051142815
H	5.39492649446608	0.14829691219742	8.57193118252987
H	-0.24509775006297	-4.17205158428682	5.51758754190425
C	1.09292808976310	-1.86581918732624	9.23623396869305
C	6.59800006392742	-0.63423085940049	6.97007158546900
C	0.66770775284231	-3.79021006935328	5.97140690086816
H	10.08043177779277	0.53050179016236	5.28890192221151
C	5.77835708951426	-1.39433379499920	6.13375960072705

C	1.35103429309489	-2.44880089108684	7.99524758312927
C	2.17158366718530	-1.22993310765851	10.05627206488120
C	6.29552499025211	-0.45359172814040	8.42475210497196
H	1.83414076583314	-1.09262713769934	11.08400747007296
N	4.62281005195090	-2.03478121569552	6.68821854762212
N	2.69829233404781	-2.48711974039667	7.50516167351216
H	7.12533007724459	0.04883924359940	8.92226931755608
H	5.64884235558163	-2.59747464816494	2.94117140915773
H	1.35050649724282	-4.63093152155335	6.12174008679555
H	3.08344654429842	-1.83063480168217	10.06727343506850
H	6.13147043923579	-1.41522351223308	8.91819134680982
C	4.69081310218351	-3.31615135793740	7.17194920030652
C	3.47750448401162	-3.60132211699673	7.68703883248763
H	5.59270433626234	-3.90208646413013	7.11263190627792
H	3.10135866777338	-4.48769416086774	8.16989055812193

[Cu(IMes)Cl] - Ligand Scrambling TS - D3BJ

Coordinates from ORCA-job

H	6.87092114163588	2.03850617531057	2.63203544962888
C	5.85643633779199	2.22125931261898	2.97009855822669
Cl	0.49758646478629	0.56185293855528	6.63057343163038
C	5.12951514611230	0.31885313885801	1.50769598235499
C	4.83897279897730	1.39626937522703	2.50511499603232
Cu	2.04591843337529	-0.47309882210103	5.15762084729484
H	0.23306353388047	-5.27174593656130	2.19634596264756
C	-0.11850199351995	-4.28256599119716	2.47278762820541
C	6.73082106290064	4.08957999381325	4.40106249837627
C	5.60872383555219	3.26018033554357	3.85790628442534
C	-1.38882396198511	-4.13529244806587	3.01829556199059
C	-2.25859942516723	-5.32848597289062	3.26775462805868
C	0.72349549887789	-3.19412688552690	2.27840625155722
C	2.09448440039697	-3.37407034948619	1.70618532401623
C	-1.81851070230084	-2.85916760527364	3.36727214180145
C	0.25245966489085	-1.93322977634214	2.63860580402947
C	1.93996684387423	-0.22315688644713	3.23661409432953
C	3.54580809742590	1.63329473847209	2.96761974164596
C	-1.01668817885915	-1.73891551275374	3.18090415457748
C	4.29440815361600	3.49975455812313	4.24664285031544
H	-2.80992004233293	-2.72627313852122	3.78940696387807
N	1.07485033034745	-0.79759329167314	2.36827910062827
N	2.49852149343474	0.77728627609151	2.51096502699954
C	3.24245164299032	2.70556090776656	3.80717046341133
C	-1.50641945268365	-0.37069835160751	3.53549866917787

C	1.09007060812170	-0.17227450334167	1.13767007516089
C	1.99108574202109	0.82543228951917	1.22926476921615
H	4.07689373943663	4.33145796531522	4.90950359469345
H	0.46268528960318	-0.49587786553391	0.32424671292278
H	2.31792706593181	1.55809016650351	0.51086143257055
C	1.83310933772960	3.01596757261062	4.19854432715817
H	-0.89158281012632	0.07312802757326	4.32333644656262
H	-2.53720089753789	-0.41506657681415	3.88743110124998
H	-1.46480062203152	0.30174238518601	2.67435793099304
H	-1.97734319496356	-6.16513467007356	2.62646001349211
H	-3.31154095093054	-5.09443657439357	3.09960122105648
H	-2.16135934819128	-5.66081905085394	4.30676523580265
H	2.28117145673612	-4.42467427408001	1.48497995595602
H	2.85850071665601	-3.02814512805460	2.40684874691731
H	2.22446897521303	-2.79910922516145	0.78574725019922
H	1.17817915412218	3.04053991789632	3.32353336605205
H	1.78415604484877	3.98458716492439	4.69664545152552
H	1.43122834197896	2.26184311438685	4.87990723877926
H	6.43248740775184	5.13294235592001	4.52158701013290
H	7.60655853960358	4.04650126022530	3.75193485432855
H	7.03270858981992	3.72132727727469	5.38705740121311
H	6.18972154704644	0.06694176894868	1.51476559656233
H	4.87368687682587	0.65075503356022	0.49680940523565
H	4.55278381685264	-0.58540848519522	1.70361707271251
Cl	3.59433417290252	2.40606001433666	8.00255641414445
Cu	2.97617800850436	0.43189338237474	7.24666892355584
H	-3.17016608264022	-3.48962104805365	8.97311242204636
H	9.36687210639083	1.84957215687010	5.36956528356827
H	8.95593312670827	1.35545236825507	3.71814280353983

C	-2.65866486180510	-2.56324232774011	9.24192166251789
C	9.12939363208396	0.99531909721862	4.73395827318975
C	7.94090232068992	0.24605461340386	5.25251223397460
C	-1.22879981818765	-2.58080183563061	8.79618059810186
C	7.21349195363276	-0.59460144253181	4.41552163758412
H	7.50473647358424	-0.69351273191994	3.37508214342424
H	-3.19986710019797	-1.74236306490628	8.76081589157583
C	-0.86953047335968	-3.16420813380648	7.58430548564162
H	5.32228000982640	-3.23543731294403	4.34008049170448
H	-2.73572749157487	-2.42090483586016	10.32089483226429
H	-1.63042778401385	-3.63676271340908	6.97040742384839
C	-0.23381721114457	-1.99873588881390	9.57196575636458
C	7.56032095922398	0.34857366066801	6.58479690697529
H	1.33673324273069	-3.09077811706403	5.17517593940191
C	3.40680454997621	-1.45034590891773	6.93678667993565
H	4.29108949324655	-1.87776019816399	3.90924325307479
C	6.11429537052968	-1.30710516751609	4.87374852288003
H	-0.49381827882185	-1.55880817687794	10.52991799819577
H	2.35902903744007	-0.30064520908978	9.65912374581233
H	8.12950133268882	0.98575762423226	7.25461418519052
C	5.33309642229150	-2.20704286525069	3.97043534935514
C	0.44306025644819	-3.15560829734664	7.13180634448636
H	5.25959307827691	0.35551362150715	8.70949894774502
H	-0.07958864713098	-4.13088314029570	5.30685135804125
C	1.09363046399771	-1.96072679590470	9.15809718036554
C	6.47982321386161	-0.36280972302788	7.09805299325780
C	0.81119741947026	-3.79210089723570	5.83050397582545
H	10.01113757255612	0.34770874652174	4.70264989702042
C	5.75684559232445	-1.16002653371653	6.21336619735622

C	1.40161522185404	-2.53019661614759	7.92670957521620
C	2.13621890498061	-1.31324807377244	10.01356037989770
C	6.13358701524860	-0.28294040862277	8.55165807176510
H	1.78635808951557	-1.23182539119319	11.04306937731621
N	4.65754244590247	-1.92513796674078	6.70914122357449
N	2.75607158298288	-2.51802414964208	7.47139104459187
H	6.96649544212367	0.13807770247350	9.11546072519786
H	5.75736123469781	-2.20984180292314	2.96786785804350
H	1.47265179422531	-4.65045984869250	5.97463497705866
H	3.07631219869710	-1.86801212806420	10.00418521843277
H	5.89750161515986	-1.26729090552463	8.96174092202369
C	4.78085804539682	-3.24048102871559	7.08670848981990
C	3.57670056245169	-3.61600278885451	7.56790219044545
H	5.70764489672513	-3.78016369688183	6.98778991076755
H	3.23198233914886	-4.55231254437190	7.97334965754156

[Cu(IMes)Cl] - Ligand Scrambling AP

Coordinates from ORCA-job

H	7.39479669920115	-2.27491897624643	-2.42317933433622
C	7.12573632624597	-1.82771028731482	-1.47106216492297
C	4.82073661568278	-2.77388504333126	-1.78677337319310
C	5.82580126488266	-1.98903871500322	-1.00138315578305
H	-0.32803793209759	-5.91654965799365	2.24430335025507
C	0.19994004527862	-5.09312368816310	2.71560805751745
C	9.48337846406420	-0.97599715565615	-1.26916733361897
C	8.08077998745243	-1.11103766358418	-0.75849326723337
C	0.08915332477081	-4.90840810030206	4.08849412748955
C	-0.75245443928427	-5.82165905790441	4.92738190623009
C	0.97632630508292	-4.25432310138137	1.92088009205408
C	1.08935435163468	-4.48494466660784	0.44541691083257
C	0.77534432481848	-3.84672479696678	4.67244505212280
C	1.65164354450323	-3.20859614881266	2.54770574353688
C	3.77205047682073	-2.60662127909441	1.47941146436295
C	5.49944278265737	-1.40355779333284	0.22154479381647
C	1.56440793298289	-2.98305700020472	3.92301872540368
C	7.71058238219556	-0.54054591454163	0.45530019147331
H	0.70511829569311	-3.69109378769490	5.74494755900541
N	2.47721165545076	-2.34674847360315	1.75755105858225
N	4.17079353478532	-1.55616004157796	0.73146604897873
C	6.42525960678362	-0.67311678457462	0.96798373974880
C	2.30426403143094	-1.85805717966561	4.57958202277041
C	2.07111832191717	-1.15635016631601	1.19356605786504
C	3.14375008471672	-0.65570655498804	0.54303192010337

H	8.44193611672729	0.02624015109455	1.02350879676993
H	1.06803575109096	-0.77915284694427	1.30305639272634
H	3.26766285599899	0.24795397312170	-0.03008108235204
C	6.05971016797174	-0.05736301582175	2.28336611005917
H	3.38159075128183	-1.94065130643370	4.41077860916455
H	2.12490444122467	-1.86161703763760	5.65474530837615
H	1.99234765628736	-0.88800616623117	4.18344652082999
H	-1.64822837837678	-5.30599750563034	5.28599006838176
H	-0.20178191727360	-6.15959608110918	5.80919787001524
H	-1.07227384741202	-6.69759822559395	4.36144900518023
H	0.43462787440292	-5.29932492674421	0.13509510036971
H	2.11436462232519	-4.74575123824286	0.16631873110997
H	0.82078255882313	-3.59072323678809	-0.12272636169785
H	5.22621786220081	0.64280542369533	2.18367438437955
H	6.91016925955576	0.48284447790225	2.69921688957737
H	5.75234096703039	-0.81967534377752	3.00494878093652
H	9.52682469559010	-1.10931095080251	-2.35123951479002
H	10.13197317997516	-1.73306333982876	-0.81677331568991
H	9.90257980382507	0.00064695018467	-1.01971553928327
H	5.25230465707810	-3.11043597730684	-2.72941772318064
H	3.93054150683865	-2.17933010893263	-2.00847435644421
H	4.48672167062320	-3.65367651154494	-1.22948042793128
Cu	4.78326126724579	-4.14927314490503	2.00587775943365
H	0.82389427224106	-7.86411689928847	-1.63943346879909
H	8.37769245221810	-0.40180060528089	6.08338694874448
H	9.91029010454432	-0.71762672845426	5.25787157463656
C	1.48246956252475	-8.70511452574511	-1.39927832760521
C	9.13644114977360	-1.16356243506438	5.88370501551741
C	8.52939261025201	-2.36405592776846	5.22306709096867

C	2.56384191910039	-8.27458136463381	-0.45526446726822
C	8.93699631226885	-2.76815540222330	3.95774402200029
H	9.70805606574872	-2.20461957441531	3.44120518281589
H	0.86340041644805	-9.48980786379204	-0.96108103630657
C	3.77010173871205	-7.77447580966005	-0.93454358809220
H	8.02763608560698	-4.18078377154971	1.23036347820956
H	1.89951009084555	-9.07127423223804	-2.33906905400503
H	3.93825727493896	-7.72307252829230	-2.00604450723211
C	2.37740318943103	-8.34393834178023	0.92128322205031
C	7.53949903456906	-3.10182078867021	5.86724871713751
H	6.18494628001528	-5.74551433593328	-0.38471469883912
C	5.77021971550935	-5.70091916572246	2.54856630774632
H	9.66893076105490	-3.65783805165600	1.63077848615314
C	8.38649687746335	-3.88068698962119	3.32736957939330
H	1.44473414667840	-8.73697449756427	1.31451403362891
H	3.22322217782897	-7.02782763729888	3.77139812464882
H	7.20655130590416	-2.80064421467235	6.85606993337493
C	8.83834774549996	-4.28363574099932	1.95763718967859
C	4.77785182541732	-7.34092757800634	-0.07964804641869
H	4.96173110401673	-5.00552341540014	5.41416815148516
H	6.09146414533527	-6.91274853574433	-1.71109836797665
C	3.35361841431190	-7.92269035754259	1.81798054322123
C	6.95917924097349	-4.21962055776806	5.28119602289689
C	6.06517490527174	-6.80540434212975	-0.62668131109304
H	9.58356931986031	-1.43000738398630	6.84515201812977
C	7.40117951289673	-4.59175228458429	4.00974148998001
C	4.54550119375739	-7.42154479176225	1.29393190348258
C	3.12118853130655	-8.00681339608819	3.29501047937912
C	5.88982753620884	-4.98995700370873	5.99234109484770

H	2.11976124795162	-8.38441694628638	3.50184577168518
N	6.82625524777724	-5.74555696114856	3.38781532206355
N	5.57001159268133	-6.98841248717330	2.19466140941893
H	5.67979062321726	-4.54259109057808	6.96380193483023
H	9.16148239911201	-5.32736912785022	1.93097548863902
H	6.92839435113644	-7.32845363566412	-0.20719265991784
H	3.84112563941121	-8.67270114367427	3.77824477851052
H	6.18294171863714	-6.03103459703928	6.15177413917199
C	7.28008558600022	-7.03646084087086	3.55672441635656
C	6.48462901466965	-7.82338277334154	2.80080528712163
H	8.11777096649600	-7.27419897741093	4.19091238139643
H	6.48722471040846	-8.88858299144479	2.64031184404091
Cu	2.23566754471918	-5.83918309534894	8.14448624069398
Cl	1.54554536529669	-3.93558689805676	8.83766368134857
Cl	2.92914546324045	-7.73933333192249	7.44703402914420

[Au(IMes)Cl] - DMSO AR

Coordinates from ORCA-job

Cl	5.52522672680379	-2.83543818472929	1.43491382330220
Au	3.90228461767618	-1.23057800901718	1.15546408846199
H	3.89381476954088	0.71442178298664	-1.72525934396742
C	4.05182081377904	1.79579970716941	-1.76186030885979
C	2.50277238518357	0.14968572980172	0.90890209086792
H	1.55832392548675	-0.82075886543388	3.65011220923147
H	4.72610758989010	2.01626497557601	-2.58929985759705
C	4.62086566549928	2.30400445714439	-0.47369001376054
H	1.69851773184437	-1.40937510852162	-1.56363179832559
C	5.84494602921945	2.96174751884223	-0.44525162963191
C	3.94687817282526	2.13690902029858	0.73595684752396
H	3.08316083684912	2.25416455071011	-1.97879439229580
C	0.51561784148513	-1.30237403473456	1.01418512593876
C	0.47755083546559	-0.90947116054669	3.50715433138298
H	3.59964732048944	1.36415951431682	3.47278192167795
C	0.16115947181939	-1.72846319943017	2.29429352209354
H	6.38268717797026	3.10268644489231	-1.37796969818029
N	1.16841243323571	-0.03716077818391	0.86478285821467
N	2.67728264276841	1.47525622317312	0.73571006550123
C	0.23316161356983	-2.05066321844172	-0.12726044258425
H	0.05283162497631	-1.37024197896843	4.39874698814315
C	-0.49226583629965	-2.94961260922849	2.41009199155411
H	-0.74825176615246	-5.83858881676260	1.69697851723117
C	0.61910221811457	-1.56956348431702	-1.49147045644452
C	4.45251896986472	2.61190136457234	1.94499293295646

C	-0.42247295618293	-3.26543958106264	0.04182984018648
C	-0.79074262035482	-3.73196052530061	1.29882890133439
C	6.39186228949806	3.44542604103905	0.73918283383310
H	8.53547411547239	3.39164575833396	0.77353337503255
H	-0.77858231902281	-3.29536824477330	3.39867264589074
C	3.70903764665978	2.42534580865041	3.23122325500341
C	5.68025817409112	3.26489697673930	1.91996684257742
C	-1.47471438694523	-5.05574375766819	1.45704874621752
H	-0.65340100129125	-3.85959420580768	-0.83694360634904
H	0.32876155716796	-2.29806518257711	-2.24838759324094
C	7.72606137370259	4.12791356270637	0.74250612903226
H	0.08194261469682	0.10577131815757	3.42334407966080
H	4.24011878543484	2.90885237013192	4.05081205123034
H	7.86683048587219	4.72603072529441	-0.15988786786942
C	0.51338003761346	1.15903024129948	0.66373888697038
H	6.08731359074602	3.64493881013037	2.85184428404694
C	1.46443384197177	2.11230265565592	0.58248442186357
H	0.13726570565951	-0.61762276354490	-1.73105037705624
H	-1.98501409165196	-5.35029890386750	0.53882056564789
H	2.70192701375237	2.84692128190042	3.17931837046403
H	-2.20341076824741	-5.03006931370089	2.26963769493201
H	7.83691543551572	4.77614884289414	1.61310703278098
H	-0.55999595056068	1.21865224302105	0.59750827468353
H	1.39276074179679	3.17639552913553	0.43239386004777
H	6.80976701195429	-8.47049716915331	0.26092423435129
H	8.40934072629432	-7.19363938054339	1.68555390725638
O	6.18259407287595	-8.29706642403921	3.01732699551067
C	5.96407320299087	-7.80206335211210	0.42915885258767
C	7.69500670776107	-6.41046852763286	1.94475018626893

H	5.02181199078275	-8.34616170319161	0.36236265972751
S	6.06259019811171	-7.12890710061495	2.08334190182715
H	5.96748812163299	-6.97672490022077	-0.28455347542307
H	7.67133138564401	-5.63149368631666	1.18076036255470
H	7.93701345465114	-5.97151928412976	2.91289235598346

[Au(IMes)Cl] - DMSO TS

Coordinates from ORCA-job

H	6.73655667251587	1.28072660345651	-1.44932141279569
C	6.14757458931067	1.38474677334407	-0.54312432644620
Cl	4.21271904295072	-2.81037005195628	3.98189299876919
C	4.21682946390757	0.37090143591164	-1.79017719792035
C	4.82324098807925	0.96191067872755	-0.55531039388182
Au	3.35960098854509	-2.03520535513573	1.71368620049541
H	-1.47600648049873	-4.14081376265273	-0.41866211234959
C	-1.18167739174671	-3.46452545541948	0.37835402576745
C	8.16955054790518	2.35661828746235	0.58804100613042
C	6.73121943618693	1.93661947387697	0.59221230625951
C	-1.67313151178069	-3.66774856644895	1.66494370260472
C	-2.61545291693919	-4.79711197467488	1.95104565486863
C	-0.31995696245089	-2.41683950264759	0.07970528565909
C	0.18441749184053	-2.21477023310554	-1.31574255284654
C	-1.28474694704369	-2.78847202347151	2.66821427835126
C	0.05016811474506	-1.56212075028812	1.11987897672663
C	2.27516732665588	-0.51729686523380	1.00740803741046
C	4.08301471296599	1.10882481907171	0.61758809290849
C	-0.42535737353245	-1.72235130744374	2.42015388433360
C	5.95428942262034	2.07068356067023	1.73818272523770
H	-1.66062207085883	-2.93081115810706	3.67672998850161
N	0.93674288615819	-0.47598464899375	0.83669162476399
N	2.71259980846802	0.69940803155367	0.62042853712599
C	4.62524265650854	1.66414147911722	1.77635912796141
C	-0.02938185233265	-0.78732651412537	3.52058571618840

C	0.54096641060172	0.75374969535785	0.34791338117798
C	1.65890931227002	1.49348786360358	0.21152590594657
H	6.39081076596730	2.50967697871920	2.63014514871296
H	-0.49212431674912	0.98288460632076	0.14761074795651
H	1.80543977595296	2.50319465023960	-0.13336943504104
C	3.81285000969049	1.81684982200208	3.02487475829108
H	1.04373664535160	-0.84727814592989	3.72294397656589
H	-0.56448598508893	-1.03165935497947	4.43813697953690
H	-0.24892506136155	0.25139225104550	3.26051645334251
H	-3.60274024471478	-4.59442927094079	1.52499866404525
H	-2.73860459725438	-4.94757418930312	3.02430125118914
H	-2.25934666194216	-5.72986455242639	1.50783861567839
H	-0.20952939710168	-2.98541569833414	-1.97832754458646
H	1.27640376101890	-2.24974633346078	-1.36242796557387
H	-0.11930788497686	-1.24103371601152	-1.70941449492990
H	2.88567765710384	2.36421105185935	2.83729406171911
H	4.38070677723091	2.35350142312934	3.78479747184865
H	3.53264407252804	0.84129626372064	3.43263793213272
H	8.49371739781412	2.65011171167153	-0.41184014112092
H	8.81216747347006	1.53191429928653	0.91223303678079
H	8.34048837393183	3.19085063505695	1.27067233452164
H	4.96373961921783	0.28665933051734	-2.57947299816029
H	3.39390834843041	0.98602642092154	-2.16457487702724
H	3.80848295851435	-0.62391870849799	-1.59311755277244
H	6.32037866110819	-4.12654883098227	2.37878734669925
H	6.69861337595346	-5.03834327991293	0.87228453252384
C	6.24314369624129	-4.14017886593829	1.29238637301620
H	6.68329339258718	-3.23633162171383	0.86893203175596
O	3.94186575258485	-5.45051919721238	1.36560338751405

S	4.50715126677221	-4.15597658970299	0.90518989642533
H	5.14562312321618	-5.11302484544614	-1.16152126082438
C	4.60595161205004	-4.20993277452754	-0.87140947286100
H	5.11891943905738	-3.31217417372144	-1.21856964292604
H	3.58429382848554	-4.22766982756430	-1.24967307434662

[Au(IMes)Cl] - DMSO AP

Coordinates from ORCA-job

H	6.73655667251587	1.28072660345651	-1.44932141279569
C	6.14757458931067	1.38474677334407	-0.54312432644620
Cl	4.21271904295072	-2.81037005195628	3.98189299876919
C	4.21682946390757	0.37090143591164	-1.79017719792035
C	4.82324098807925	0.96191067872755	-0.55531039388182
Au	3.35960098854509	-2.03520535513573	1.71368620049541
H	-1.47600648049873	-4.14081376265273	-0.41866211234959
C	-1.18167739174671	-3.46452545541948	0.37835402576745
C	8.16955054790518	2.35661828746235	0.58804100613042
C	6.73121943618693	1.93661947387697	0.59221230625951
C	-1.67313151178069	-3.66774856644895	1.66494370260472
C	-2.61545291693919	-4.79711197467488	1.95104565486863
C	-0.31995696245089	-2.41683950264759	0.07970528565909
C	0.18441749184053	-2.21477023310554	-1.31574255284654
C	-1.28474694704369	-2.78847202347151	2.66821427835126
C	0.05016811474506	-1.56212075028812	1.11987897672663
C	2.27516732665588	-0.51729686523380	1.00740803741046
C	4.08301471296599	1.10882481907171	0.61758809290849
C	-0.42535737353245	-1.72235130744374	2.42015388433360
C	5.95428942262034	2.07068356067023	1.73818272523770
H	-1.66062207085883	-2.93081115810706	3.67672998850161
N	0.93674288615819	-0.47598464899375	0.83669162476399
N	2.71259980846802	0.69940803155367	0.62042853712599
C	4.62524265650854	1.66414147911722	1.77635912796141
C	-0.02938185233265	-0.78732651412537	3.52058571618840

C	0.54096641060172	0.75374969535785	0.34791338117798
C	1.65890931227002	1.49348786360358	0.21152590594657
H	6.39081076596730	2.50967697871920	2.63014514871296
H	-0.49212431674912	0.98288460632076	0.14761074795651
H	1.80543977595296	2.50319465023960	-0.13336943504104
C	3.81285000969049	1.81684982200208	3.02487475829108
H	1.04373664535160	-0.84727814592989	3.72294397656589
H	-0.56448598508893	-1.03165935497947	4.43813697953690
H	-0.24892506136155	0.25139225104550	3.26051645334251
H	-3.60274024471478	-4.59442927094079	1.52499866404525
H	-2.73860459725438	-4.94757418930312	3.02430125118914
H	-2.25934666194216	-5.72986455242639	1.50783861567839
H	-0.20952939710168	-2.98541569833414	-1.97832754458646
H	1.27640376101890	-2.24974633346078	-1.36242796557387
H	-0.11930788497686	-1.24103371601152	-1.70941449492990
H	2.88567765710384	2.36421105185935	2.83729406171911
H	4.38070677723091	2.35350142312934	3.78479747184865
H	3.53264407252804	0.84129626372064	3.43263793213272
H	8.49371739781412	2.65011171167153	-0.41184014112092
H	8.81216747347006	1.53191429928653	0.91223303678079
H	8.34048837393183	3.19085063505695	1.27067233452164
H	4.96373961921783	0.28665933051734	-2.57947299816029
H	3.39390834843041	0.98602642092154	-2.16457487702724
H	3.80848295851435	-0.62391870849799	-1.59311755277244
H	6.32037866110819	-4.12654883098227	2.37878734669925
H	6.69861337595346	-5.03834327991293	0.87228453252384
C	6.24314369624129	-4.14017886593829	1.29238637301620
H	6.68329339258718	-3.23633162171383	0.86893203175596
O	3.94186575258485	-5.45051919721238	1.36560338751405

S	4.50715126677221	-4.15597658970299	0.90518989642533
H	5.14562312321618	-5.11302484544614	-1.16152126082438
C	4.60595161205004	-4.20993277452754	-0.87140947286100
H	5.11891943905738	-3.31217417372144	-1.21856964292604
H	3.58429382848554	-4.22766982756430	-1.24967307434662

[Au(IMes)Cl] - Cys⁻ AR

Coordinates from ORCA-job

Au	3.66829003440008	-0.09543531183774	3.09183645904352
H	5.30141989893133	-0.45396727838249	0.24777655941498
C	5.49921545259490	0.33915614291707	-0.47905287502568
C	2.67071512015203	0.36004857054494	1.44327618363916
H	0.28484232212697	1.01281914346297	3.20647180071621
H	6.50513866636876	0.19631377846280	-0.87333660066417
C	5.37243307951552	1.69082073266444	0.15221614174189
H	3.22487866018515	-2.49146022274510	0.68473599122401
C	6.47824900063946	2.52725029118928	0.27145388488038
C	4.15624919644051	2.15112347154918	0.65171358770684
H	4.78654617339760	0.20867866660873	-1.29737442002374
C	0.81980522870260	-1.26102248182997	1.59422787923501
C	-0.56930305507658	0.47350947213135	2.78810640851015
H	2.33366804552605	3.20816308804090	2.56762321801654
C	-0.21421233989240	-0.94667173288663	2.47358273347716
H	7.43466069329829	2.18434831965398	-0.11080827443167
N	1.53885230024936	-0.19431878747843	0.96556324789131
N	3.00408678790194	1.30851135436960	0.54473658060764
C	1.16131730708859	-2.57751496875866	1.28156276655273
H	-1.38470523326177	0.51027405692154	3.51034044339892
C	-0.91023441903258	-2.00134948117030	3.05631791044212
H	-0.72842789295687	-4.91913658251904	4.21217147101302
C	2.27171151525345	-2.89090726391310	0.32756335964779

C	4.01911678160275	3.40549791764065	1.24880347950207
C	0.43640234850173	-3.59462574977873	1.88956976349665
C	-0.59910686409886	-3.32752562919172	2.78050355013064
C	6.38951876125277	3.78105378958653	0.86387103537333
H	7.88550116773161	4.76125989585502	2.04889650662891
H	-1.71826583630283	-1.77496833524643	3.74514095998923
C	2.70193520504357	3.87557478169009	1.78325248142852
C	5.15186990235298	4.20342586812270	1.34196109018376
C	-1.34431043967440	-4.44803902408518	3.43995930103489
H	0.69069806328408	-4.62483273481704	1.65937408405948
H	2.37732661481000	-3.96884531597073	0.20703346976677
C	7.59710678632791	4.65785181194309	0.99868287783655
H	-0.88249766799539	1.01539156585243	1.89157568137344
H	2.79718028979355	4.87672698081048	2.20324631064366
H	8.44789286726827	4.24596208845977	0.45468213901270
C	1.16689613973453	0.40153071192665	-0.22115080033172
H	5.06331562159112	5.18187564094105	1.80458726492086
C	2.09008945390798	1.34893188687934	-0.48625730436008
H	2.08785871579668	-2.45247292404947	-0.65712989061983
H	-1.60651644087473	-5.22553019647769	2.71907453992351
H	1.93792491058566	3.90266944138394	1.00204204946081
H	-2.25902870447703	-4.09002637089332	3.91427276281687
H	7.39771002913596	5.66342992594521	0.62041276094469
H	0.28690473812299	0.09649366262394	-0.76183965430795
H	2.18294549147305	2.04168231433367	-1.30561722437178
H	5.50476216621523	-6.85433366978732	4.50619309555389
S	3.85389888619875	-4.69578785108238	4.31061850654407
N	5.05035814928299	-7.72326962917892	4.22973451240704
O	5.55352437376165	-6.76076111502936	1.70475337516230

C	4.40526024562197	-6.93119175616450	2.03232401263237
H	4.68670567350733	-8.12444503083416	5.08826146955452
O	3.38687510579793	-6.76387033547616	1.17879411549832
H	3.75307536317452	-6.47745688333257	0.32827336531261
C	3.92047054549458	-7.35908546792669	3.39800330165814
C	3.00440092025379	-6.27642330363792	3.99593652044918
H	2.60874136584511	-6.68462618569946	4.93164915438420
H	2.15379277016288	-6.12644331169608	3.32630995280179
H	3.31090046366837	-8.25671047257053	3.23333472343833
Cl	4.87146949356788	-0.58229996806334	4.98537220305269

[Au(IMes)Cl] - Cys: AP

Coordinates from ORCA-job

Au	4.55920693070653	-1.43652362727588	1.94463152017342
H	4.51675295943294	-0.16870754432945	-1.32895872779258
C	4.64459605792350	0.88233177238778	-1.60305554466065
C	3.15850540221994	-0.10171000618428	1.37264109875305
H	2.09702496804082	-0.39901232606924	4.20183378497236
H	5.27606890403264	0.93011686230881	-2.49012886478649
C	5.25838233182782	1.66248086756860	-0.48157787650967
H	2.43561874356164	-2.14921530370118	-0.72157532190870
C	6.48792738794196	2.28901942458909	-0.63907672620347
C	4.62218449855170	1.78143246555819	0.75579629483601
H	3.65532757456860	1.26679354756041	-1.86489745432220
C	1.16079946955226	-1.48956015965978	1.74622620944310
C	1.02541415983604	-0.59171596396483	4.09948431701141
H	4.39566643410643	1.62456146551551	3.61478202139810
C	0.76265316652333	-1.64907193206272	3.07231169866485
H	6.99633236713651	2.20548601462721	-1.59501143603487
N	1.82091759558600	-0.27865762941754	1.36331319034350
N	3.34475788740061	1.15936178700184	0.93247901064500
C	0.92220489999113	-2.46179426747953	0.77312068676875
H	0.63882412601573	-0.89939329531317	5.07090962555701
C	0.11364994628907	-2.83156309944778	3.41581529026500
H	-0.09317671861551	-5.92278550795363	2.95144096423399
C	1.35075325380107	-2.26656506462199	-0.64849025047231

C	5.17792670292146	2.49777133242074	1.81381947264997
C	0.27230600792088	-3.62514434790189	1.16673677147215
C	-0.13692861607336	-3.83000142347614	2.48157309742398
C	7.07961503759350	3.01588487384674	0.39099876806245
H	8.77173122771985	4.12830701348289	1.11297202137080
H	-0.20491630989366	-2.97159612695212	4.44430509485539
C	4.48568902466520	2.60494723078758	3.13779334804737
C	6.41243815966385	3.10796218138948	1.60665614368784
C	-0.81699307712956	-5.10523398111561	2.87881852894536
H	0.07824965857997	-4.39122508457927	0.42195420645826
H	1.05732351069106	-3.12280399633051	-1.25571124226287
C	8.40152508756836	3.69198508703676	0.18440612902126
H	0.55437344353445	0.35672017656364	3.82790674981607
H	5.04479800162519	3.25960726021845	3.80637061048478
H	9.14915688816695	2.98756443496616	-0.18877340076667
C	1.17667166794654	0.85939055452450	0.92395151055811
H	6.85943766016692	3.67485488923306	2.41928791946500
C	2.13779229624984	1.76582590980153	0.65142067754747
H	0.90200962617766	-1.36898371705062	-1.08227427389277
H	-1.56330317683895	-5.40155498160227	2.13841698600501
H	3.47336549597156	3.00363609595430	3.03284319788309
H	-1.30762116201303	-5.00731736244958	3.84815870932898
H	8.31799166434679	4.49268440487796	-0.55624969580486
H	0.10392637406981	0.91665381151135	0.84641861079840
H	2.07743916221338	2.77707463556587	0.28543447655556
H	3.98230724112006	-2.25782743319171	4.56040322884712
S	6.21604075055851	-2.91678407307408	2.54768530359060
N	3.75375503906120	-3.17806523609712	4.92627729123242
O	6.05719994241775	-2.42413280296323	6.19041627524082

C	6.02865210308542	-3.51223236463394	5.67267272032504
H	3.00857279711442	-3.54052585248956	4.34110738225914
O	7.01876725681293	-4.39968537750223	5.79584355764182
H	7.71979841928234	-4.00141777072546	6.33476234426346
C	4.90425129841875	-4.04502421955235	4.81341613188951
C	5.41335699309896	-4.32140868331662	3.38794219701760
H	4.57208963404839	-4.68562697514120	2.79621424192858
H	6.16246763933422	-5.11503512688052	3.42451649578645
H	4.63537878620044	-5.02297765659288	5.23219086340077
Cl	8.07134539716935	5.50862622180186	4.36025403849078

[Au(IMes)Cl] - Ligand Scrambling AR

Coordinates from ORCA-job

H	6.74041011531636	1.85363878010782	-3.02270581400573
C	6.37321296172896	2.21044729569819	-2.06513368532830
Cl	5.90916190958885	-1.98702795043303	2.33506201774057
C	4.26018538331555	0.92579389124233	-2.50157477943500
C	5.10558685355742	1.82185641039640	-1.65029791521345
Au	4.39324055864160	-0.47042602003741	1.51411619192668
H	-0.53675757044384	-3.06972820687208	1.44718240209029
C	-0.14938647105378	-2.17213418126306	1.91943597512222
C	8.55308871459237	3.41620447977851	-1.75038591769769
C	7.17849532860279	3.03878484549112	-1.28905236465938
C	-0.36116266326914	-1.96893757970980	3.27837115474775
C	-1.08640284292214	-2.98665074724910	4.10512882814890
C	0.54761794616715	-1.25527454290363	1.13927556403195
C	0.76593333152369	-1.49997568017274	-0.32184150772953
C	0.13433055220242	-0.80653571297762	3.86165616600496
C	1.03589235861983	-0.11086580687512	1.76754892595715
C	3.08955667631208	0.83940166670709	0.80358129504346
C	4.65373450838760	2.29325681776547	-0.41713889833882
C	0.83737108367930	0.13941630205346	3.12566543045953
C	6.68459511087389	3.49133805455244	-0.07103836916005
H	-0.03055399175299	-0.62801958351784	4.92018496997029
N	1.75470009201116	0.85237709316801	0.98947890752543
N	3.34827924020190	1.91266300956985	0.03023806200153

C	5.42160025699824	3.13229518383127	0.38836451826977
C	1.36482980347625	1.38084916921769	3.77631291258672
C	1.18154111402956	1.92409848850569	0.33853737256556
C	2.18581343155990	2.59198741473000	-0.26657059071612
H	7.29602505414297	4.14540545655778	0.54290950999824
H	0.12101808677023	2.10951455901475	0.36759755884309
H	2.18270739194524	3.48127183243151	-0.87410876075434
C	4.91393756659479	3.63213248927264	1.70532549364837
H	2.45278074424986	1.44311798894564	3.68514735539294
H	1.10926543699241	1.39321143694170	4.83567392964397
H	0.95274102178606	2.28158543561820	3.31361339796992
H	-1.70447497956048	-3.63574731037407	3.48309308556853
H	-1.72237534800646	-2.50841148616119	4.85273083057132
H	-0.37661847555083	-3.62247600374146	4.64398057112746
H	0.29346477069758	-2.43376514832946	-0.62616384757321
H	1.83206055097202	-1.56234873478180	-0.55743902885249
H	0.35063817928383	-0.69196309644831	-0.92992682944794
H	3.96868166143126	4.16933054407872	1.59200166129204
H	5.63860256203159	4.30642242383664	2.16138547571804
H	4.73156781005156	2.80533281972577	2.39755212425644
H	8.56534788941003	3.63333647642934	-2.82047238389896
H	9.25632714731821	2.59536843606231	-1.57902957940560
H	8.92486261748116	4.28928185384788	-1.21243905211556
H	4.79705197956431	0.64417132473209	-3.40726362535653
H	3.32816611012030	1.41630444295468	-2.79501170182280
H	3.98640573009817	0.01288711256463	-1.96574399192476
Cl	-0.48324958597839	0.19106822217746	7.81783712246076
Au	1.04010232462283	-1.32410023514017	8.62704554773561
H	-3.48055722911670	-6.34390893203233	8.90557020288416

H	5.80455187048360	3.01220979167562	7.53242476227861
H	7.29232322689240	2.09707390398254	7.31106409135821
C	-2.94762200932371	-6.47794395684223	9.84937301757640
C	6.48885404838974	2.30982397181357	8.01881370476958
C	5.76642830774327	1.05772959498245	8.41350248589998
C	-1.62622791358146	-5.77164056870852	9.83012032506565
C	5.58126818188962	0.02579321506386	7.49880282285022
H	5.98661609431877	0.12166780251886	6.49604365418356
H	-3.57955590513477	-6.11475012825844	10.66078929285041
C	-0.80719487897633	-5.83195242245330	8.70625755138500
H	3.64200504458840	-2.37451052383909	6.59868805848340
H	-2.80828939242390	-7.55402324740623	9.99123051764276
H	-1.14047109250837	-6.38134946529548	7.83097419426702
C	-1.18157585122181	-5.05706314253374	10.93633182615974
C	5.24850748378230	0.90805915571872	9.69538519563674
H	1.39673784959732	-4.29359276271278	6.97996305119975
C	2.35709731964858	-2.61905581170486	9.33990101759908
H	5.22100415530117	-1.98992778754269	5.89894050570997
C	4.89182256242568	-1.13436747106193	7.83137604361837
H	-1.81098418873528	-4.99329261967679	11.81856176641747
H	0.65589292884918	-2.58891917409556	11.90847870445172
H	5.39050174360181	1.70079389856838	10.42351711766208
C	4.70170212451487	-2.22868888627903	6.82705826243554
C	0.43325240796036	-5.20780314629423	8.66826904410160
H	2.92362868369558	-0.52649052469338	11.45161785116506
H	0.84967420940303	-5.95328546783732	6.70776364469598
C	0.05263600568457	-4.41469508158649	10.94865859083611
C	4.55212693050152	-0.23349029991072	10.07800495239634
C	1.29019204017427	-5.27934270229344	7.44234139392694

H	6.91276920639322	2.81369018673905	8.88883975875113
C	4.38350257363598	-1.23833088730710	9.12645498029771
C	0.84060659940108	-4.50426098255661	9.80284947224005
C	0.50315842064058	-3.64434880111261	12.15085825036595
C	4.00552675144093	-0.36914260080878	11.46555967880414
H	-0.24115910280717	-3.70806212692058	12.94437194375209
N	3.68271500573008	-2.43123240306134	9.49573246007257
N	2.12260540226026	-3.86678938619787	9.79316318789127
H	4.21334933606995	0.52970008997799	12.04583163928527
H	5.08323951041018	-3.18366993553389	7.19732713291743
H	2.29718175884788	-5.63455917300433	7.67487165396344
H	1.45162168578208	-4.02387096927130	12.53985804608638
H	4.44718957002810	-1.22251536584707	11.98737728950133
C	4.27368223650221	-3.54982163737662	10.04368833276751
C	3.29050259955982	-4.45440737406532	10.23128030603295
H	5.33066629519553	-3.59723426144035	10.24480762936327
H	3.31185735406776	-5.45446531449638	10.63047887340889

[Au(IMes)Cl] - Ligand Scrambling TS

Coordinates from ORCA-job

H	5.11935812704035	-1.88667442385712	-0.25239778272758
C	4.73833332818815	-0.95675071628363	0.15800292173535
Cl	7.71409700700373	-0.12104665814877	3.83739291212168
C	2.56976330226367	-2.14612575586228	0.59317923459111
C	3.43933849768687	-0.92986541742131	0.65579177247639
Au	2.34669866555020	-0.83125841057015	4.38627982840628
H	-3.19304137892254	-2.42177319560621	5.06174261881652
C	-2.58193645865881	-1.52454652042872	5.08313130509668
C	6.94183183253571	0.12378613774969	-0.38943969352721
C	5.54971528861068	0.17127581601989	0.16203062640519
C	-2.66920255788080	-0.66313615708602	6.17130381183654
C	-3.56801170779139	-0.97969169966468	7.32720638817108
C	-1.73433200206022	-1.26994185620746	4.01120725732493
C	-1.68754825610442	-2.19838998717903	2.83775556718777
C	-1.88936853107283	0.48851787878941	6.16864594813244
C	-0.95398106468789	-0.11478079942058	4.06197128888223
C	1.23397836120848	-0.07887070338230	2.91254894883905
C	2.97420925344592	0.27146814160530	1.18605387176805
C	-1.02411187769704	0.78910885403888	5.12243196281026
C	5.03404910516769	1.35668733769118	0.67836796828973
H	-1.95943319059291	1.18174366350198	7.00132063207041
N	-0.08930514030135	0.17403501495005	2.95747763012262
N	1.63558881428591	0.33147033439021	1.69299593043588
C	3.74597265260116	1.43529654661530	1.19157974178248
C	-0.21582237841610	2.04941250816543	5.13769878159798

C	-0.51556401796218	0.73347668585413	1.77182266742614
C	0.56869806751670	0.83157741015063	0.97699079889500
H	5.65159962067196	2.24973419322930	0.68432494785315
H	-1.54450871744487	1.00578225391895	1.60776887455657
H	0.68305247411020	1.20744947766846	-0.02576469227650
C	3.20844957471168	2.73135113711139	1.71386340909280
H	0.85538577908544	1.83753598102984	5.19363399372495
H	-0.48565431119313	2.66237611296434	5.99762917748227
H	-0.37944083158174	2.63778079804891	4.23100101912701
H	-4.45333005482270	-1.52863445914018	7.00130912781107
H	-3.88721855191857	-0.07175379342378	7.84142331355617
H	-3.04694999960444	-1.60553604210507	8.05877465658065
H	-2.18141291054953	-3.13989593027716	3.07793115953918
H	-0.66171590378016	-2.41391660121427	2.53261623457388
H	-2.19696533225390	-1.76329792430253	1.97261203660877
H	2.83334248680381	2.62745654600728	2.73452053569588
H	2.38183557106062	3.09476721103142	1.09690519385690
H	3.98876516190850	3.49232386255396	1.71324209723663
H	7.66236283969914	0.51240324129103	0.33454264474094
H	7.02474872027438	0.73955101380893	-1.28967550505683
H	7.22988115892584	-0.89563922426455	-0.64863901458136
H	3.11528227153217	-2.98355424344224	0.15836119310633
H	1.68069836925136	-1.96227534904704	-0.01698463492622
H	2.22329228140183	-2.43987661052106	1.58599074004341
Cl	4.01256830799144	2.24937455640075	5.43589474193319
Au	4.05575824620512	0.14339228050776	6.33048618996522
H	0.73453524550920	-4.50266600717563	1.78183279668802
H	7.42130922648531	3.41436534801858	10.57766722541026
H	8.46856833764673	2.27866025578852	11.42301698600612

C	0.93958768460785	-5.18253903022162	2.61477933624179
C	7.42598604800150	2.51951015396589	11.20809993606753
C	6.73858527914494	1.38475207675606	10.51246778205638
C	1.64809513922001	-4.46323419805266	3.71907022366052
C	7.44066961557830	0.55749440370283	9.64189720347186
H	8.50275074977877	0.72207515234153	9.48885586019014
H	-0.01440075681013	-5.58797293473934	2.95388863283460
C	3.02256062731665	-4.24637317510840	3.65017106719884
H	7.19382483837039	-1.31117095384507	7.00715769201144
H	1.55095468100039	-5.99784841510448	2.22336261435600
H	3.57725761284142	-4.60985691419772	2.79118994227154
C	0.95213559462271	-3.98621241865382	4.82296005156932
C	5.38165221911208	1.14802059332920	10.70446865558345
H	5.58504819228659	-3.82632202349609	3.65364363152783
C	4.17710435860460	-1.58341150707284	7.28092359834089
H	8.64103181162762	-1.03714274466623	7.98532591936430
C	6.82122410003372	-0.48015546334015	8.95588542148090
H	-0.12007308671905	-4.13933167782553	4.88661191183348
H	1.18984237465584	-1.98145331133693	7.49957385105561
H	4.82220152329666	1.77669344217177	11.39028164133840
C	7.59898718526074	-1.35407056217884	8.02177538560328
C	3.72018501329582	-3.61482001293171	4.67011955475314
H	2.68138579770459	0.04440492417495	9.34477050607806
H	5.68442894592077	-4.07130135978500	5.40278105158201
C	1.59416279616810	-3.34282004426325	5.87652087077258
C	4.71397823707330	0.12345749068600	10.04281187682453
C	5.20849749011359	-3.47955824558979	4.61539462439329
H	6.92409113072588	2.77415870675598	12.14288460930496
C	5.45545717189264	-0.67058642702377	9.16832072970555

C	2.98511117860178	-3.17019572138577	5.78485935960089
C	0.83241414085498	-2.93074694819430	7.09735635226879
C	3.25170724200469	-0.10935805230049	10.26534380192505
H	-0.22836281371711	-2.83511842841521	6.86552746349576
N	4.79307655433312	-1.73222270283899	8.46855750329936
N	3.70161862520461	-2.79987248786865	6.96637637904090
H	2.86883776562157	0.57657258570910	11.02073646305436
H	7.57050846806108	-2.40076850564220	8.33605171278517
H	5.52345923982384	-2.44307679499625	4.75588205871466
H	0.93722892390221	-3.68036262490728	7.88786126537305
H	3.05488555064388	-1.13165520589196	10.59851983103707
C	4.70542138453450	-3.03718839164722	8.89980679146846
C	4.01897263910478	-3.71103910435551	7.95494747079422
H	5.13824328794393	-3.36199897343776	9.83102523920641
H	3.72876263105456	-4.74611627003273	7.88964672279147

[Au(IMes)Cl] - Ligand Scrambling AP

Coordinates from ORCA-job

H	7.35067055102705	-2.14034572127198	-2.45555889153903
C	7.06331714727947	-1.69259632385905	-1.50918927868681
C	4.79834117197100	-2.73246627123474	-1.81454832470204
C	5.77104508114064	-1.90008562450997	-1.03818399527966
H	-0.36087008777548	-5.91218167158879	2.21965805418262
C	0.15000916291019	-5.07342916812749	2.68243172502145
C	9.38284571494792	-0.74234980912600	-1.31939394178286
C	7.98769529477493	-0.92856730390801	-0.80531292176497
C	0.01138228125092	-4.85901425901599	4.04841838854686
C	-0.84256166374329	-5.75697217542318	4.89080002001168
C	0.93185689345588	-4.24399272352805	1.88390161091732
C	1.07523032889135	-4.50539148711391	0.41658565143882
C	0.67737664129785	-3.77933969739945	4.62166719694157
C	1.58491191225190	-3.17907722135916	2.50140444430670
C	3.70814243966311	-2.54157293182553	1.44274534162600
C	5.42276831878120	-1.31340681879150	0.17786893915545
C	1.47185352434654	-2.92407474252631	3.86908674985892
C	7.59534186910930	-0.35933799869301	0.40173156053035
H	0.58461153700016	-3.60104904003106	5.68855149222364
N	2.40591757442566	-2.31643178601737	1.70587826136737
N	4.09549997771378	-1.49851475968490	0.68275671553991
C	6.31662226592389	-0.53787878604914	0.91649261483808
C	2.18853125215885	-1.77843393690133	4.51439024440294
C	1.98058510744273	-1.14547816441372	1.11744941366086
C	3.04713452430116	-0.62931369937122	0.47071217678678

H	8.30294897604227	0.24383120716105	0.96230443479369
H	0.96750446101122	-0.79206801122100	1.21154166701337
H	3.15668105487777	0.26739262737011	-0.11574489046951
C	5.92549355027335	0.07856808461173	2.22385766353421
H	3.26899561432807	-1.85101037540964	4.36244302180144
H	1.99372133453484	-1.76472628631451	5.58673814805564
H	1.86998860891692	-0.81984909723946	4.09617322997192
H	-1.77092795673561	-5.25339309114636	5.17676304119244
H	-0.32803437902437	-6.03198984800742	5.81504173120803
H	-1.10792957086747	-6.66939418908686	4.35511672033436
H	0.42818895619878	-5.32743287131789	0.11056496876233
H	2.10608734454892	-4.77168564512036	0.16499967066886
H	0.81750325399521	-3.62421065960438	-0.17624824675744
H	5.08657517534359	0.76995897258526	2.10846313125200
H	6.76420627131362	0.62934764285935	2.64933127185157
H	5.61575555877104	-0.68371671175920	2.94421829821412
H	9.42251646215228	-0.84222824774033	-2.40525553801382
H	10.05306282657338	-1.49658683977873	-0.89480589787272
H	9.77861838922582	0.23657559593398	-1.04290552077040
H	5.24647673945194	-3.06846514831660	-2.74953275115584
H	3.88930832946692	-2.17296693066955	-2.05090565564078
H	4.49230949962874	-3.61474588490147	-1.24507292684576
Au	4.80093619189369	-4.14199493924374	2.01855723231988
H	0.87788509539751	-7.85699852717294	-1.63421446349766
H	8.60162834829787	-0.52987954108772	6.08832214889448
H	10.17186624540507	-0.96799552967010	5.40290295716524
C	1.48488711576097	-8.71880616626353	-1.33854769555084
C	9.32252927658694	-1.34446766073366	5.97397050982914
C	8.69281640200311	-2.52293738962441	5.29600942570320

C	2.57876206168724	-8.29700735419609	-0.40567135236695
C	9.12364972795296	-2.94283492831510	4.04360196519214
H	9.93241497558210	-2.41095188568314	3.55201663328522
H	0.81871942010960	-9.44241345533777	-0.86608026996860
C	3.79413815684193	-7.83357293079262	-0.89883862301085
H	8.22625114006619	-4.40888340758791	1.30299738775179
H	1.89042250333770	-9.15935054720288	-2.25114765638897
H	3.95830028613897	-7.80333564441183	-1.97169240476854
C	2.39587705773715	-8.33845090128749	0.97212108755324
C	7.65638923281491	-3.22099255315447	5.90996326698012
H	6.25295968404938	-5.85008077343682	-0.39027855971365
C	5.85319744665312	-5.77354250931344	2.58018241868968
H	9.84448440920086	-3.81830273484483	1.70859636724887
C	8.54794772079196	-4.03130150816531	3.39497031446003
H	1.45581610002235	-8.70242950319314	1.37524133047634
H	3.26931675571269	-6.99069680919367	3.79181268921270
H	7.30856960209667	-2.90915301503137	6.89019630105905
C	9.02931447710552	-4.45961292646886	2.04355578351902
C	4.81565888533322	-7.41098482071742	-0.05597433755601
H	5.01832812281671	-5.01293989444986	5.38841764979909
H	6.12966220872782	-7.03376610111098	-1.69896177605251
C	3.38575810338219	-7.92658054368356	1.85778686781433
C	7.04927830607302	-4.31378339238792	5.30481957256352
C	6.11110670745385	-6.91094658043523	-0.61614579665813
H	9.66997843922925	-1.60805012496720	6.97616637384487
C	7.51211863171046	-4.69825542982823	4.04521127176109
C	4.58625067380620	-7.46461514577747	1.31919227348751
C	3.15913889148311	-7.97896520605363	3.33675601966319
C	5.93462906354999	-5.04669050691937	5.98432613067616

H	2.15636183555173	-8.34552532547345	3.55587582262546
N	6.91495724490154	-5.83264588180511	3.40717727142293
N	5.62810955549287	-7.04990947612852	2.21014814159447
H	5.72517591740556	-4.60380485016637	6.95782433263921
H	9.38859448641818	-5.49209118217354	2.05500513090567
H	6.96571856208523	-7.44563927945712	-0.19395756337427
H	3.87709339478124	-8.63921519715730	3.83043067300584
H	6.17959379472738	-6.10156658346132	6.13382128100188
C	7.35151010260672	-7.13153806063297	3.55453670958924
C	6.53922813691331	-7.89993070465960	2.79852872706371
H	8.19230022066596	-7.38550060765127	4.17793829381893
H	6.52575337796197	-8.96295180788415	2.62579091497402
Au	2.20808595508384	-5.80119690714502	8.23762168563332
Cl	1.47741654704372	-3.77385232303073	8.96646532238174
Cl	2.94336408096893	-7.82805309654161	7.51230339456845

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