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A Theoretical Study of M-M' Polar-Covalent Bonding in Heterobimetallic Multinuclear Organometallic Complexes of Monovalent Group 10 Metal Centres

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Dedicated to Roald Hoffmann, Professor Emeritus at Cornell University (USA).

Converged Copper complex at DFT level: TPSS/def2TZVP

Complex 1 and 1a

C	-6.06644800	0.18031400	-0.07102700
C	-5.32638100	0.26112500	-1.25435800
C	-3.92921400	0.22789700	-1.25220600
C	-3.21046500	0.11179000	-0.02535600
C	-3.97287500	0.03697300	1.17843000
C	-5.36911500	0.07213500	1.13614600
Cu	-1.66083600	-1.15866200	-0.14062700
C	-1.00517900	-3.04495300	-0.41483200
C	-1.46751000	-3.95969900	0.57863000
C	-1.93214300	-5.22594100	0.21518700
C	-1.95626600	-5.64606200	-1.11871300
C	-1.49956600	-4.75854800	-2.09709500
C	-1.02822700	-3.48309400	-1.77192200
Cu	0.61310800	-1.99558700	0.11869900
C	2.50717600	-1.86554800	0.77152500
C	3.45039700	-2.60691100	-0.00101600
C	4.45756000	-3.34345800	0.62775200
C	4.57736600	-3.38551000	2.02062500
C	3.65952000	-2.65817000	2.78451400
C	2.64018300	-1.90808700	2.19087600
Cu	2.08157900	-0.06298100	-0.00323800
C	2.61096200	1.70674700	-0.78974100
C	2.72503300	1.73732800	-2.21021300
C	3.78030200	2.42257600	-2.82136600
C	4.75179400	3.09360900	-2.07418100

C	4.64919800	3.06431800	-0.67863400
C	3.60893600	2.39260300	-0.03336800
Cu	0.73928200	1.95925000	-0.10819000
C	-0.80106000	3.10321200	0.46065600
C	-1.20172100	4.07148800	-0.50827500
C	-1.58594400	5.35474400	-0.11146500
C	-1.59104800	5.73831700	1.23340400
C	-1.18585600	4.80044800	2.18755000
C	-0.79514900	3.50706800	1.82872900
C	1.71586500	1.02815800	-3.08719000
C	3.56522800	2.40357400	1.47992200
C	5.87400400	3.84439200	-2.75013800
C	3.38715300	-2.60794600	-1.51352200
C	1.69054900	-1.13837200	3.08329500
C	5.65194300	-4.21549900	2.68097500
Cu	-1.58380200	1.27330800	0.13912700
C	-1.19926000	3.74194300	-1.98555500
C	-0.35502600	2.55685200	2.92129400
C	-2.04474300	7.11840400	1.64426900
C	-1.45456400	-3.58859100	2.04591900
C	-0.54265100	-2.58660400	-2.89029100
C	-2.43727100	-7.02904000	-1.48678000
C	-3.20416300	0.31341900	-2.57811100
C	-3.29430800	-0.06369700	2.52771600
C	-7.57594100	0.18334300	-0.09746700
H	3.84925700	2.43413300	-3.90929200
H	5.40156200	3.57958600	-0.08096100

H	5.16985200	-3.89994100	0.01820600
H	3.74415700	-2.67599800	3.87132300
H	-1.88760500	6.07799700	-0.86939100
H	-1.17317400	5.08747000	3.23926300
H	-2.28753800	-5.90479300	0.99074300
H	-1.51515600	-5.06954700	-3.14191100
H	-5.85474500	0.35287700	-2.20356400
H	-5.93094100	0.01795700	2.06889300
H	-1.16049200	-2.54147400	2.17719700
H	-2.44176600	-3.72959800	2.50253800
H	-0.74404000	-4.21174900	2.60395100
H	-1.32874000	-2.41453900	-3.63567300
H	-0.22544800	-1.61612200	-2.49381800
H	0.30931600	-3.03579100	-3.41607800
H	-2.77118600	-7.06976100	-2.52833200
H	-1.63248300	-7.76679600	-1.36880300
H	-3.26591400	-7.34630800	-0.84487700
H	4.29727800	-2.17702100	-1.94926000
H	3.28604300	-3.62706900	-1.90689400
H	2.53151100	-2.01944800	-1.86370700
H	0.90554900	-0.66275100	2.48438600
H	1.21387600	-1.79523300	3.82123700
H	2.21693600	-0.35313400	3.64089800
H	5.31691100	-5.25270200	2.81494400
H	6.56295600	-4.24316600	2.07410500
H	5.90662900	-3.82246900	3.67038700
H	2.18604500	0.21968300	-3.66153400

H	0.91796300	0.59268100	-2.47493900
H	1.26114200	1.71645700	-3.81031600
H	3.51181400	3.42801300	1.86901200
H	2.68959300	1.85393600	1.84374300
H	4.46167100	1.93675800	1.90671400
H	5.73591700	4.92884800	-2.65171000
H	6.84309500	3.60027000	-2.30018200
H	5.92199400	3.60910600	-3.81763400
H	-0.43086500	4.31845400	-2.51651800
H	-0.99109600	2.67797800	-2.14360100
H	-2.16437500	3.97817900	-2.44982800
H	-0.12515900	1.57110400	2.50306000
H	0.54337300	2.92860800	3.43023700
H	-1.13284900	2.43593900	3.68503300
H	-1.79559900	7.86315800	0.88122900
H	-3.13360800	7.14536800	1.78436200
H	-1.58468600	7.42364200	2.58953100
H	-3.64561600	-0.93917600	3.08729400
H	-2.20815900	-0.14445400	2.40883700
H	-3.50424600	0.82097500	3.14201900
H	-3.46158900	1.23531400	-3.11403600
H	-2.11918200	0.29676300	-2.42665000
H	-3.47127200	-0.52720300	-3.23055400
H	-7.98918400	0.63486500	0.81034700
H	-7.95772900	0.73421800	-0.96305800
H	-7.96704700	-0.84085000	-0.16133700

AuCu complex

Complex 2 and 2a

C	-5.91245800	-0.22208400	1.81565200
C	-5.71454600	-0.09849300	0.43505900
C	-4.43605000	-0.02624700	-0.11988300
C	-3.28070500	-0.08030500	0.71761100
C	-3.48882800	-0.20510700	2.12194100
C	-4.78668300	-0.27285700	2.64060300
Cu	-1.80814700	-1.23175400	0.00352500
C	-1.18361700	-3.00515900	-0.78192000
C	-1.76978800	-4.05679300	-0.01584000
C	-2.56480400	-5.02147200	-0.63981800
C	-2.80942700	-4.99795600	-2.01663300
C	-2.22499500	-3.97742200	-2.77268700
C	-1.42302100	-2.99306300	-2.18816300
Au	0.62211900	-2.10978200	-0.04681700
C	2.64557700	-1.89265300	0.65029700
C	3.68811300	-2.36631600	-0.20105800
C	4.89478600	-2.81077100	0.34542500
C	5.12454700	-2.81197100	1.72458300
C	4.10029400	-2.36165500	2.56330400
C	2.87799600	-1.91082000	2.05824000
Cu	2.11081300	-0.01451500	0.08429000
C	2.74456900	1.84891500	-0.36869900

C	3.28562600	1.87962100	-1.68933700
C	4.56899900	2.38582300	-1.91119500
C	5.35993100	2.87649600	-0.86808000
C	4.83017600	2.85581400	0.42588800
C	3.55247900	2.35817000	0.69227000
Au	0.60705900	2.07274600	-0.18493600
C	-1.27034800	3.10298100	-0.17971400
C	-1.82463100	3.49238400	-1.43663500
C	-2.69708400	4.58071700	-1.51258900
C	-3.05193400	5.32370100	-0.38184900
C	-2.49794400	4.95594300	0.84735400
C	-1.62145600	3.87371500	0.96849900
C	2.48653300	1.39672700	-2.88062800
C	3.04843100	2.39351400	2.11861500
C	6.75860700	3.38246200	-1.12557400
C	3.50753200	-2.43127600	-1.70198700
C	1.80696000	-1.47644600	3.03466900
C	6.45237800	-3.25506700	2.28952500
Cu	-1.80865900	1.17831900	0.19479100
C	-1.45457500	2.77129100	-2.71406500
C	-1.03884900	3.56738000	2.33090000
C	-4.03028600	6.46882300	-0.48161100
C	-1.51894300	-4.17486900	1.47173700
C	-0.79522100	-1.94435400	-3.08003500
C	-3.70622700	-6.02654900	-2.66204700
C	-4.30236100	0.12057700	-1.62015200
C	-2.32166900	-0.26499700	3.08399900

C	-7.30617000	-0.30171500	2.39117500
H	4.96521400	2.39662200	-2.92657600
H	5.43299500	3.23452300	1.25125100
H	5.68067700	-3.16186900	-0.32315000
H	4.26053700	-2.35942700	3.64139900
H	-3.11365300	4.85754700	-2.48097800
H	-2.75946400	5.52636500	1.73844100
H	-3.00962800	-5.81187900	-0.03553400
H	-2.40225600	-3.94625500	-3.84764100
H	-6.58255900	-0.05927200	-0.22359100
H	-4.92489400	-0.37037600	3.71753200
H	-1.27136800	-3.20114700	1.90779200
H	-2.39347500	-4.58189300	1.99100300
H	-0.67254600	-4.84572300	1.66981300
H	-1.45789200	-1.68132700	-3.91211600
H	-0.55976300	-1.03797600	-2.51214600
H	0.14456800	-2.31362500	-3.51164300
H	-3.46051500	-6.16054400	-3.72028400
H	-3.62350000	-6.99689900	-2.16152900
H	-4.75855800	-5.71782000	-2.60452500
H	4.43632400	-2.17709400	-2.22483900
H	3.21794400	-3.44321000	-2.01467100
H	2.71856900	-1.74811700	-2.03307100
H	1.10071900	-0.78695200	2.56075100
H	1.23077500	-2.34088600	3.39036000
H	2.24388900	-0.98845400	3.91300900
H	6.91556300	-4.02323100	1.66177400

H	7.15328500	-2.41146300	2.34586700
H	6.34033900	-3.65611600	3.30198400
H	3.11339300	0.82138000	-3.57148600
H	1.64621700	0.77142900	-2.56234800
H	2.07402300	2.24467800	-3.44267500
H	2.73188800	3.40761100	2.39548400
H	2.18566700	1.73218300	2.24666000
H	3.83164400	2.08985600	2.82244700
H	7.03071200	4.17583400	-0.42180600
H	7.49344300	2.57473600	-1.00855200
H	6.85954400	3.77261700	-2.14338500
H	-0.61430200	3.27312200	-3.21135300
H	-1.14407100	1.74159300	-2.50939400
H	-2.29295600	2.75563200	-3.41913100
H	-0.65673200	2.54257300	2.37395200
H	-0.20035600	4.24019500	2.55382600
H	-1.78629800	3.70065500	3.12103900
H	-3.96261000	6.96677600	-1.45435000
H	-5.06223700	6.11089100	-0.36756700
H	-3.85309400	7.21281000	0.30158900
H	-2.34490800	-1.18396600	3.68304700
H	-1.37210900	-0.23503100	2.53799100
H	-2.34126500	0.57850500	3.78560400
H	-4.88177600	-0.64539400	-2.14926100
H	-4.66759200	1.10010000	-1.95455000
H	-3.25387800	0.02987900	-1.92533800
H	-7.28002500	-0.38348800	3.48188700

H	-7.89332700	0.58737300	2.13070900
H	-7.84703300	-1.17146800	1.99829900

CuAg complex

Complex 3 and 3a

Cu	1.64406700	1.51492300	0.17450200
Cu	2.09724600	-0.85771100	-0.15298600
Cu	-2.37786100	-0.49889900	0.20551600
C	-2.28350200	-2.39369900	0.78937700
C	-2.27037100	-2.60949000	2.19727600
C	-3.01167300	-3.31732000	-0.01488200
C	-2.97924000	-3.67802800	2.75490200
C	-3.70657100	-4.37544900	0.57819000
C	-3.70723400	-4.57069400	1.96269700
H	-2.96050800	-3.82327000	3.83524700
H	-4.26059300	-5.06918000	-0.05451100
C	1.66775600	-2.60367100	-0.99659900
C	2.22263400	-3.73958000	-0.33960500
C	1.62920400	-2.61314200	-2.41989900
C	2.72918200	-4.80769200	-1.08548500
C	2.14543700	-3.70063000	-3.13196700
C	2.70312500	-4.80631000	-2.48370700
H	3.15258600	-5.66665900	-0.56451600
H	2.10974300	-3.68868500	-4.22152500
C	-3.16536300	1.25094800	-0.26888000
C	-3.90593100	1.89863000	0.76173400

C	-3.62295200	1.40526800	-1.60853800
C	-5.04778200	2.64192800	0.45098900
C	-4.77235000	2.15429300	-1.88077000
C	-5.49693800	2.78480200	-0.86568200
H	-5.60429300	3.12328600	1.25544100
H	-5.11137300	2.25275700	-2.91225700
C	3.32301400	0.51250700	0.64748700
C	4.44235800	0.84632700	-0.17278300
C	3.55307200	0.36711200	2.04734800
C	5.70767600	1.02082100	0.39227700
C	4.83398500	0.55098200	2.57717300
C	5.92544400	0.87594500	1.76670800
H	6.54801500	1.27839700	-0.25278700
H	4.98753500	0.43902200	3.65070500
C	0.65196200	3.20696000	-0.11647400
C	0.60187500	4.06841900	1.01661200
C	0.79167900	3.80715000	-1.40041900
C	0.70908200	5.45287600	0.85502200
C	0.89895500	5.19605400	-1.52141100
C	0.86231700	6.03731000	-0.40564700
H	0.66873000	6.09527500	1.73487500
H	1.00557700	5.63631900	-2.51306300
C	4.28400100	1.02406200	-1.66789600
H	3.25721400	0.79784900	-1.97732200
H	4.51093100	2.05391500	-1.97143200
H	4.96173100	0.36268300	-2.22142200
C	2.42333900	0.01104400	2.98971300

H	2.28259600	0.78494500	3.75452000
H	1.48369200	-0.10210600	2.43737500
H	2.62678600	-0.92998900	3.51629000
C	7.30713900	1.04084500	2.35270700
H	7.26079000	1.26482400	3.42299700
H	7.89495100	0.12121000	2.23214900
H	7.85766500	1.84580300	1.85418100
C	2.28075300	-3.82174600	1.17116000
H	1.67423300	-4.65608500	1.54542400
H	3.30800800	-3.97990200	1.52166500
H	1.90213600	-2.89879300	1.62448100
C	1.03892200	-1.45604000	-3.19727700
H	0.68392900	-0.67562200	-2.51494200
H	1.77959600	-1.01169600	-3.87402800
H	0.19200600	-1.78251200	-3.81401900
C	3.28252100	-5.95743400	-3.27057300
H	4.36386500	-5.82844800	-3.41178400
H	3.13326100	-6.90994100	-2.75138300
H	2.82773200	-6.02938900	-4.26361900
C	-1.49192500	-1.69929600	3.12334700
H	-0.67899900	-2.24329400	3.62106600
H	-1.04911500	-0.86773600	2.56430200
H	-2.13448700	-1.28543100	3.91011600
C	-3.05878700	-3.17964100	-1.52200400
H	-2.48021700	-2.30950700	-1.85100400
H	-2.64351500	-4.06829900	-2.01335100
H	-4.08948600	-3.06026000	-1.87853900

C	-4.49086600	-5.70076000	2.58604300
H	-5.52370200	-5.39076900	2.79366400
H	-4.53809900	-6.56787800	1.91922200
H	-4.04663600	-6.01724300	3.53519700
C	-3.49935700	1.77636900	2.21503700
H	-4.22451600	1.17550200	2.77892000
H	-2.51981800	1.29468600	2.30559400
H	-3.44538300	2.75962200	2.69758100
C	-2.89205300	0.76399700	-2.76946500
H	-2.01050700	0.21657700	-2.41809400
H	-3.54024900	0.06179700	-3.30856900
H	-2.55879000	1.51812300	-3.49333200
C	-6.71247900	3.62219300	-1.18344800
H	-7.45245600	3.57164700	-0.37791200
H	-6.43718400	4.67782000	-1.30887400
H	-7.18931100	3.29459300	-2.11274500
C	0.82147500	2.97143300	-2.66232600
H	1.73637500	3.15322900	-3.23956700
H	0.77348900	1.90410000	-2.42125100
H	-0.02733800	3.21123400	-3.31512000
C	0.45436300	3.51643000	2.41859700
H	-0.37361500	3.99942900	2.95157300
H	0.26442900	2.43792400	2.39365500
H	1.36475900	3.68692600	3.00742200
C	1.00587400	7.53280500	-0.55583100
H	0.59793600	7.87813200	-1.51137100
H	0.49335200	8.06484400	0.25207200

H	2.06309000	7.82830700	-0.52477100
Ag	-0.92986400	1.61072600	-0.09335000
Ag	-0.25092800	-1.91626900	-0.06161900

Cu5-D3 1a

C	-5.90771800	0.17736100	0.08632200
C	-5.17564600	0.07297300	1.27307700
C	-3.78096800	0.01550900	1.26889800
C	-3.06746700	0.05999400	0.03841300
C	-3.81643700	0.16185300	-1.16789600
C	-5.21034600	0.21688700	-1.12520200
Cu	-1.46351400	1.22319100	0.15901200
C	-0.78155300	3.09213200	0.42286500
C	-1.30338900	3.98455300	-0.55733100
C	-1.82513200	5.22121800	-0.17642400
C	-1.84875800	5.62401300	1.16305700
C	-1.33110200	4.75565000	2.12846100
C	-0.80090700	3.51102200	1.78280500
Cu	0.77180300	2.01374300	-0.15149300
C	2.55707000	1.62394100	-0.90987800
C	3.64841400	2.24749800	-0.24113300
C	4.71142100	2.77551100	-0.97573300
C	4.73710500	2.71210400	-2.37271400
C	3.67047400	2.09423000	-3.03373900
C	2.59337300	1.55186400	-2.33085400
Cu	1.97627300	-0.05549100	-0.00278200

C	2.45741200	-1.76015700	0.91988200
C	2.46276300	-1.67354800	2.34051800
C	3.49921200	-2.25345400	3.07483900
C	4.55239800	-2.92586400	2.44686900
C	4.55609000	-3.00558800	1.05015500
C	3.53583700	-2.43867500	0.28516000
Cu	0.67250000	-2.07202800	0.12659900
C	-0.92800400	-3.06163500	-0.48145800
C	-1.50450400	-3.95160300	0.47017000
C	-2.10426000	-5.13919900	0.04954600
C	-2.15625200	-5.49323800	-1.30277500
C	-1.57675000	-4.63218100	-2.23935200
C	-0.97066400	-3.43490800	-1.85387300
C	1.35437200	-0.94555200	3.06506500
C	3.59025100	-2.53704100	-1.22297100
C	5.64715400	-3.57416800	3.25778800
C	3.67111900	2.32972600	1.26860100
C	1.47054500	0.87716900	-3.08427300
C	5.87742300	3.32158700	-3.15037700
Cu	-1.52944800	-1.17532400	-0.14536700
C	-1.45219500	-3.62917200	1.94611900
C	-0.34234100	-2.54849900	-2.90371700
C	-2.84659400	-6.76070900	-1.74190000
C	-1.28645500	3.60580100	-2.02067000
C	-0.23946200	2.61720400	2.86399300
C	-2.39892100	6.97376500	1.55223500
C	-3.03992500	-0.08306200	2.58278800

C	-3.11467900	0.18449100	-2.50671600
C	-7.41313300	0.27232400	0.11333600
H	3.49294100	-2.18013500	4.16221800
H	5.37708100	-3.52095500	0.55204200
H	5.54317200	3.24751800	-0.45312400
H	3.68660800	2.03403600	-4.12181600
H	-2.54527100	-5.80759600	0.78875400
H	-1.60265600	-4.90396300	-3.29444900
H	-2.23115100	5.88802600	-0.93686500
H	-1.34989400	5.05766800	3.17545500
H	-5.70977500	0.03617400	2.22234100
H	-5.77191800	0.28767300	-2.05653700
H	-1.01820700	2.54966500	-2.13757900
H	-2.26368700	3.76930000	-2.48934800
H	-0.54967800	4.20190900	-2.57390700
H	-0.95450400	2.47348000	3.68231000
H	0.01436600	1.63673100	2.44763800
H	0.67258900	3.04664100	3.29776600
H	-2.72195800	6.98398400	2.59775800
H	-1.63587300	7.75424700	1.43377300
H	-3.25057200	7.25203900	0.92286600
H	4.50373600	1.74982100	1.68530800
H	3.78328800	3.36511000	1.61208200
H	2.73916300	1.92790300	1.68423900
H	0.67587200	0.58577800	-2.38633500
H	1.04065700	1.53723500	-3.84695900
H	1.82175400	-0.02830700	-3.59460500

H	5.66858500	4.37324400	-3.38692800
H	6.80906700	3.29365000	-2.57639800
H	6.03718100	2.79772300	-4.09811600
H	1.73302000	-0.05134200	3.57555500
H	0.58399500	-0.62685700	2.35176400
H	0.88400800	-1.58164700	3.82429400
H	3.66107800	-3.57988600	-1.55471400
H	2.68835500	-2.09568700	-1.66395600
H	4.45931300	-2.00161200	-1.62453300
H	5.42201900	-4.63343900	3.43863800
H	6.60830200	-3.52919500	2.73542700
H	5.75879800	-3.08998900	4.23291300
H	-0.72718700	-4.27047500	2.46349300
H	-1.14390300	-2.58844400	2.09891700
H	-2.42672900	-3.77680700	2.42519700
H	-0.03516500	-1.59722600	-2.45708400
H	0.54831100	-3.02061900	-3.33778800
H	-1.03590100	-2.33991100	-3.72651300
H	-2.73777300	-7.55251400	-0.99372900
H	-3.92175600	-6.58852800	-1.88292600
H	-2.44368600	-7.12336400	-2.69267900
H	-3.41682900	1.05255300	-3.10436200
H	-2.02808500	0.22472200	-2.36636500
H	-3.34777000	-0.71510500	-3.08953200
H	-3.36299300	-0.95730900	3.16039600
H	-1.96145900	-0.16761600	2.40597600
H	-3.21402600	0.80466500	3.20291900

H	-7.85419300	-0.15431800	-0.79313600
H	-7.82872300	-0.25010000	0.98080400
H	-7.73591600	1.32001600	0.17447500

Cu-Au D3 3a

Cu	1.57179200	-0.88204300	-0.18081800
Cu	1.85635100	1.43360100	-0.13668800
Cu	-2.18449400	-0.06088200	-0.00364800
C	-2.53607600	1.56998400	-1.09761600
C	-2.52448800	1.12227800	-2.44943800
C	-3.71656500	2.20170500	-0.60559800
C	-3.65315300	1.30406100	-3.25550600
C	-4.81801700	2.36872500	-1.44380000
C	-4.80795800	1.92254500	-2.77199300
H	-3.63368700	0.94634500	-4.28448600
H	-5.71623800	2.84487700	-1.05167400
C	1.00507100	3.01281800	0.75999600
C	1.52715400	4.18585200	0.14226500
C	1.25815900	2.81142500	2.14842100
C	2.26800900	5.09995800	0.89451300
C	2.00739000	3.74865500	2.86462100
C	2.52290400	4.89682000	2.25541200
H	2.66703100	5.98924800	0.40757000
H	2.20025900	3.57738000	3.92326400
C	-2.80696400	-1.78294400	0.81239100
C	-3.73549700	-2.40519100	-0.07696700
C	-3.22608200	-1.53716700	2.15123300
C	-5.00696800	-2.75652500	0.37291000

C	-4.51108500	-1.90366800	2.56300900
C	-5.41500800	-2.51479800	1.69125300
H	-5.70787300	-3.21802000	-0.32221400
H	-4.81993100	-1.69643200	3.58726400
C	3.24788900	0.15166200	-0.69145900
C	4.29160700	-0.07404600	0.25322600
C	3.55336300	-0.00556500	-2.07056300
C	5.56090000	-0.45668800	-0.17918100
C	4.83684500	-0.39244400	-2.46757200
C	5.85307500	-0.62695600	-1.53800700
H	6.34210200	-0.64016100	0.55823400
H	5.04733500	-0.52713200	-3.52870500
C	1.23899700	-2.84849900	0.21446300
C	1.71730000	-3.31743700	-1.04755300
C	2.08182700	-3.02016400	1.35384000
C	2.99221500	-3.88169300	-1.14770100
C	3.34753400	-3.59310700	1.20877100
C	3.83192600	-4.00383700	-0.03714400
H	3.35339600	-4.20329500	-2.12357900
H	3.98728800	-3.69231000	2.08482600
C	4.03045600	0.12263800	1.72933100
H	3.00971200	-0.18442100	1.98401700
H	4.73016800	-0.45187000	2.34523400
H	4.12160900	1.18212200	2.00218400
C	2.49497100	0.22851700	-3.12448200
H	2.36678100	-0.64967000	-3.76830600
H	1.53336200	0.44922000	-2.64989100

H	2.75767300	1.07568500	-3.77065900
C	7.23689500	-1.03052400	-1.98794500
H	7.19746300	-1.65513700	-2.88669100
H	7.84232100	-0.14685300	-2.22969900
H	7.76501600	-1.58493200	-1.20517600
C	1.26144200	4.46509600	-1.32113700
H	0.26976800	4.91598000	-1.45367200
H	2.00512400	5.15089700	-1.73962600
H	1.27093200	3.53721100	-1.90546400
C	0.69638200	1.60427700	2.86500200
H	0.62107600	0.74679700	2.18241300
H	1.31542500	1.32031100	3.72231800
H	-0.31651500	1.81254700	3.23189400
C	3.36934800	5.87370700	3.03523700
H	4.43574600	5.63528300	2.92671700
H	3.22583100	6.89872100	2.67788700
H	3.13189400	5.84291100	4.10332200
C	-1.29144100	0.47427500	-3.03933700
H	-0.63054900	1.23199800	-3.47919900
H	-0.71438700	-0.04666300	-2.26389300
H	-1.55018600	-0.24212100	-3.82639300
C	-3.77834000	2.70302400	0.82069600
H	-3.31480800	1.98391300	1.50673400
H	-3.22788300	3.64650500	0.92498700
H	-4.81153800	2.87288400	1.13996300
C	-6.03092600	2.08052000	-3.64269300
H	-6.82341900	1.38796900	-3.33076500

H	-6.44058300	3.09446500	-3.57105100
H	-5.80166700	1.87580500	-4.69282600
C	-3.34620200	-2.70249400	-1.50895200
H	-4.22891500	-2.85505000	-2.13817700
H	-2.75453100	-1.88349700	-1.93361900
H	-2.72811100	-3.60758200	-1.56220100
C	-2.28722000	-0.89932300	3.15180600
H	-1.55784900	-0.25774500	2.64725900
H	-2.83422700	-0.29930200	3.88714900
H	-1.72309600	-1.66601300	3.69870000
C	-6.79446500	-2.91602300	2.15405600
H	-7.55220300	-2.67451200	1.40036900
H	-6.84608300	-3.99831500	2.33119100
H	-7.06377800	-2.41314200	3.08795600
C	1.60820800	-2.60267200	2.72851700
H	2.44586900	-2.49741300	3.42533100
H	1.06581700	-1.65147200	2.68396600
H	0.91433200	-3.34750900	3.13802000
C	0.84980200	-3.22555200	-2.28454900
H	0.11327900	-4.03875100	-2.29825700
H	0.28735100	-2.28538100	-2.30389900
H	1.45053200	-3.29445300	-3.19698700
C	5.24670900	-4.50069100	-0.19299200
H	5.62512100	-4.93525100	0.73771000
H	5.32357900	-5.25292800	-0.98491000
H	5.90668600	-3.66599000	-0.46479600
Au	-0.65929600	1.99829100	-0.14335400

Au	-0.70142800	-2.07915900	0.43197500

Cu-Ag D3 3b

Cu	1.40550200	1.48633900	0.04320600
Cu	-0.77292600	2.18781700	0.78182500
Cu	-0.70876300	-2.45879300	-0.77114800
C	-2.33681300	-1.63997200	-1.50043600
C	-2.30078300	-1.05224600	-2.79588500
C	-3.61613100	-1.90298700	-0.92898300
C	-3.48817300	-0.76795300	-3.47909400
C	-4.78151600	-1.61085800	-1.63919000
C	-4.73829900	-1.03946100	-2.91701900
H	-3.43965000	-0.31585200	-4.46963500
H	-5.74988000	-1.81756700	-1.18348800
C	-2.33262000	1.28889500	1.55430500
C	-3.64707800	1.51507200	1.05553900
C	-2.20184900	0.69627300	2.84062700
C	-4.76043500	1.17576500	1.82689500
C	-3.33829400	0.36605700	3.58559000
C	-4.62667000	0.59702100	3.09461800
H	-5.75912600	1.35107600	1.42713500
H	-3.21915200	-0.09002000	4.56822400
C	0.87955600	-3.33950900	-0.01668300
C	1.77144200	-4.00710800	-0.90523300
C	0.83087300	-3.78766300	1.33422600
C	2.55052300	-5.07486800	-0.45574400
C	1.62540400	-4.86024100	1.75029400

C	2.49453300	-5.51331600	0.87173800
H	3.22199100	-5.57786200	-1.15181600
H	1.57144600	-5.19437800	2.78655600
C	0.62972800	3.34375600	-0.03424600
C	1.27708900	4.25190100	0.85512200
C	0.28799500	3.81323200	-1.33319300
C	1.53046300	5.56443900	0.46183800
C	0.55920900	5.13716300	-1.69577800
C	1.17155900	6.02800400	-0.81144700
H	2.02050200	6.24701800	1.15603200
H	0.28662800	5.48441600	-2.69234700
C	3.03712800	0.37087700	-0.04554400
C	3.71412100	0.49604200	-1.28764600
C	3.81384900	0.33410200	1.14756100
C	5.10828900	0.61428100	-1.31432000
C	5.20139800	0.45733900	1.08080600
C	5.86799000	0.60234800	-0.14294000
H	5.61445800	0.72452900	-2.27316800
H	5.78276600	0.43937000	2.00247000
C	1.73909300	3.77186300	2.21374900
H	1.09497300	2.96239700	2.57910500
H	2.75780800	3.36664100	2.14949900
H	1.74362800	4.57880400	2.95412600
C	-0.35593900	2.89294300	-2.34818300
H	0.29624600	2.75117200	-3.21885500
H	-0.54861300	1.90689500	-1.90807000
H	-1.30874300	3.29551800	-2.71221300

C	1.42817100	7.46270900	-1.20479300
H	1.33407100	7.60271800	-2.28595900
H	0.70978500	8.13413100	-0.71669100
H	2.43052200	7.78460700	-0.90087600
C	-3.85719300	2.08092800	-0.33392200
H	-3.95826100	1.27237300	-1.07028000
H	-4.76492800	2.69240800	-0.38472100
H	-3.00398600	2.69787700	-0.63745800
C	-0.83192100	0.45302400	3.43556800
H	-0.08964000	0.30392400	2.64166500
H	-0.50774900	1.31645400	4.03150000
H	-0.82268800	-0.42444600	4.09078000
C	-5.84539700	0.24663800	3.91372900
H	-6.24454900	1.13641800	4.41823400
H	-6.64564900	-0.15610900	3.28328400
H	-5.60791100	-0.49276100	4.68499500
C	-0.97893300	-0.76045400	-3.47367600
H	-1.03581500	0.13348500	-4.10419400
H	-0.18719600	-0.61114500	-2.72979000
H	-0.67511000	-1.59977000	-4.11297900
C	-3.73204500	-2.45969100	0.47567100
H	-2.84342700	-3.04277200	0.74223500
H	-3.82403500	-1.64667400	1.20822100
H	-4.61316700	-3.10244800	0.58055300
C	-6.01279000	-0.73622000	-3.66710300
H	-6.45257200	-1.65515800	-4.07621800
H	-6.76257900	-0.28330100	-3.00873400

H	-5.83047600	-0.05369300	-4.50291900
C	1.87021200	-3.59283800	-2.35915300
H	1.42054200	-4.34937700	-3.01469500
H	1.34469100	-2.64671000	-2.53272900
H	2.91441700	-3.46723500	-2.66851300
C	-0.08955300	-3.13455100	2.34450700
H	-0.57303300	-2.24738400	1.92046100
H	-0.87892500	-3.82655300	2.66403300
H	0.45953200	-2.82666600	3.24231600
C	3.37784200	-6.64063700	1.34938500
H	3.51544700	-7.39663200	0.56910400
H	4.37353900	-6.26489100	1.61972500
H	2.95781200	-7.12881200	2.23444800
C	3.14714000	0.13126900	2.49064400
H	3.74941900	0.54207500	3.30770700
H	2.16027800	0.60646600	2.51097900
H	2.99555000	-0.93811000	2.68986400
C	2.95497700	0.50296200	-2.59737100
H	3.08585400	-0.44689800	-3.13153900
H	1.88125900	0.64023300	-2.42621000
H	3.30444000	1.30504100	-3.25722300
C	7.36814300	0.76629300	-0.18549500
H	7.86310200	0.07589700	0.50645900
H	7.76030200	0.58660000	-1.19116900
H	7.65690700	1.78388000	0.10843800
Ag	1.37150400	-1.09702000	-0.05388700
Ag	-1.39144900	-0.12869300	-0.01280000

Cu4L4 DFT-D

Cu	1.392499	1.218027	0.005598
Cu	-0.983372	1.162197	0.067481
Cu	-0.926976	-1.217219	0.059696
C	0.174534	2.765522	0.379683
C	0.127437	3.757929	-0.641349
C	0.207131	3.206039	1.732457
C	0.114993	5.112314	-0.309231
C	0.192354	4.570831	2.031371
C	0.145389	5.537966	1.024135
H	0.082602	5.858820	-1.102840
H	0.220687	4.893161	3.072000
C	2.986880	0.069190	-0.376789
C	4.001729	0.084628	0.619668
C	3.396177	0.062772	-1.742206
C	5.350184	0.091402	0.254416
C	4.750910	0.070442	-2.073232
C	5.743569	0.085533	-1.086361
H	6.116454	0.099978	1.029177
H	5.046754	0.062357	-3.122325
C	0.309571	-2.763891	0.371914
C	0.293702	-3.754645	-0.650504
C	0.341674	-3.206738	1.724973
C	0.305196	-5.110485	-0.320268
C	0.352672	-4.571016	2.021587
C	0.331096	-5.537654	1.011597

H	0.296095	-5.856483	-1.114816
H	0.381103	-4.894061	3.062091
C	3.632621	0.098654	2.085659
H	2.545185	0.036761	2.203568
H	4.085775	-0.744697	2.620524
H	3.976012	1.019602	2.573014
C	2.364092	0.047490	-2.847947
H	2.447646	0.936419	-3.484859
H	2.480696	-0.831671	-3.492964
H	1.354648	0.027182	-2.420261
C	7.203245	0.105397	-1.466811
H	7.437564	-0.694388	-2.178675
H	7.469882	1.054929	-1.947566
H	7.842845	-0.018579	-0.588156
C	0.085761	3.350968	-2.097086
H	-0.852882	3.664414	-2.570665
H	0.907524	3.805383	-2.663395
H	0.165079	2.262176	-2.189035
C	0.260960	2.203064	2.863094
H	0.276352	1.183195	2.460598
H	1.157503	2.342111	3.479225
H	-0.609740	2.297281	3.523272
C	0.116970	7.008179	1.360944
H	0.877578	7.558574	0.795524
H	-0.855734	7.448958	1.108886
H	0.295017	7.173322	2.427531
C	0.371774	-2.203983	2.856873

H	1.286625	-2.302973	3.453723
H	0.333796	-1.183835	2.456480
H	-0.479485	-2.338593	3.534915
C	0.272246	-3.346941	-2.106363
H	-0.599095	-3.763960	-2.625686
H	0.234152	-2.255557	-2.193835
H	1.168090	-3.700325	-2.631671
C	0.309988	-7.007586	1.349609
H	0.760093	-7.196282	2.329143
H	-0.720855	-7.384192	1.381563
H	0.849390	-7.595465	0.599924
Cu	1.449796	-1.160053	0.004145
C	-2.539068	-0.065458	-0.237629
C	-3.489537	-0.084147	0.818113
C	-3.004589	-0.057845	-1.580641
C	-4.865639	-0.082128	0.541342
C	-4.380181	-0.055083	-1.859530
C	-5.304752	-0.047285	-0.796793
C	-1.990683	-0.047123	-2.705771
H	-0.979844	-0.011096	-2.281374
H	-2.060088	-0.945501	-3.332105
H	-2.113347	0.821616	-3.363949
C	-4.883742	-0.059622	-3.286572
H	-5.318518	0.910734	-3.563080
H	-4.081853	-0.271925	-3.995261
H	-5.665473	-0.813646	-3.431624
C	-6.785223	-0.011238	-1.099330

H	-6.992274	0.538357	-2.021217
H	-7.190855	-1.024959	-1.229039
H	-7.349900	0.462393	-0.292930
C	-5.882283	-0.116890	1.662077
H	-6.399428	0.846654	1.766766
H	-6.651217	-0.876042	1.480418
H	-5.414346	-0.342061	2.621528
C	-2.989856	-0.102099	2.247214
H	-1.894947	-0.058652	2.250452
H	-3.364677	0.751241	2.825690
H	-3.290870	-1.015089	2.776762

Cu4L4-DFT

Cu	1.425027	1.187862	0.008378
Cu	-0.969190	1.185647	0.059147
Cu	-0.962456	-1.213029	0.044074
C	0.232316	2.795260	0.297589
C	0.210207	3.739134	-0.774530
C	0.265755	3.318295	1.624379
C	0.220022	5.110989	-0.516305
C	0.275059	4.699393	1.846245
C	0.252162	5.613082	0.789933
H	0.203363	5.810472	-1.352648
H	0.301557	5.075458	2.869148
C	3.032806	-0.004288	-0.289307
C	3.994178	0.006356	0.763637
C	3.532017	0.011907	-1.628259

C	5.363248	0.032444	0.478404
C	4.905645	0.037599	-1.876342
C	5.840243	0.049190	-0.834454
H	6.079382	0.040398	1.300273
H	5.260734	0.049213	-2.907277
C	0.245653	-2.819648	0.281068
C	0.218416	-3.759482	-0.793597
C	0.273789	-3.347310	1.606780
C	0.216704	-5.132878	-0.539234
C	0.270923	-4.728405	1.824590
C	0.239406	-5.638967	0.764851
H	0.200057	-5.830243	-1.377255
H	0.296978	-5.107421	2.846500
C	3.561530	-0.014044	2.213902
H	2.469104	-0.010243	2.290277
H	3.936857	-0.908149	2.727590
H	3.946609	0.858223	2.756715
C	2.586117	-0.001751	-2.810943
H	2.738987	0.873500	-3.454375
H	2.738665	-0.892854	-3.432606
H	1.544729	0.001695	-2.469192
C	7.321209	0.083511	-1.126225
H	7.618917	-0.758857	-1.762156
H	7.597103	1.002404	-1.658302
H	7.907782	0.037826	-0.203870
C	0.175214	3.276720	-2.215679
H	-0.728901	3.632368	-2.725703

H	1.036860	3.658984	-2.777091
H	0.189419	2.183126	-2.270016
C	0.291379	2.397434	2.826062
H	0.294780	1.349221	2.506192
H	1.182143	2.571222	3.442503
H	-0.583956	2.556212	3.468271
C	0.261196	7.101234	1.044852
H	1.121786	7.579812	0.561878
H	-0.640867	7.576590	0.640332
H	0.307918	7.319354	2.115902
C	0.313519	-2.429631	2.810594
H	1.219630	-2.594377	3.406949
H	0.298559	-1.380554	2.493912
H	-0.545547	-2.600766	3.471160
C	0.194606	-3.293295	-2.233661
H	-0.708805	-3.641987	-2.749730
H	0.216366	-2.199646	-2.285464
H	1.056959	-3.680008	-2.790987
C	0.208376	-7.126986	1.018192
H	0.575555	-7.367269	2.020783
H	-0.815561	-7.515438	0.938208
H	0.818646	-7.668205	0.287122
Cu	1.433860	-1.208066	-0.002306
C	-2.580547	-0.017517	-0.180961
C	-3.487052	-0.016665	0.917893
C	-3.117434	-0.000020	-1.500901
C	-4.877195	0.015582	0.708044

C	-4.506545	0.031854	-1.712363
C	-5.380815	0.060328	-0.607378
C	-2.171113	-0.010693	-2.685580
H	-1.135030	0.003234	-2.326990
H	-2.299095	-0.906436	-3.307193
H	-2.316494	0.859824	-3.337471
C	-5.083926	0.039610	-3.113242
H	-5.495691	1.024768	-3.374129
H	-4.331612	-0.207788	-3.863920
H	-5.901819	-0.683327	-3.211492
C	-6.873206	0.132253	-0.848338
H	-7.106740	0.758200	-1.714814
H	-7.295036	-0.863233	-1.049855
H	-7.405395	0.542503	0.012407
C	-5.839922	0.002697	1.879395
H	-6.336202	0.974898	2.005254
H	-6.629103	-0.744908	1.740348
H	-5.331762	-0.226327	2.817291
C	-2.933607	-0.047150	2.328822
H	-1.838852	-0.028975	2.294372
H	-3.267980	0.813481	2.921824
H	-3.236974	-0.952828	2.870259

Cuau4-D

Cu	0.68822000	1.66881000	-0.06549300
Cu	1.45523000	-0.56120100	-0.06546700
Au	-0.90809800	-1.60022800	0.07999100

C	2.54061500	1.06166800	-0.47779100
C	3.52986500	1.36718300	0.49907400
C	2.90474500	1.14345900	-1.84996100
C	4.81583100	1.73430200	0.10369000
C	4.20401100	1.50902600	-2.21032800
C	5.17281900	1.80663600	-1.24814900
H	5.56349200	1.96724100	0.86191600
H	4.47204500	1.56573900	-3.26506300
C	-0.90851500	2.87855300	0.32535500
C	-0.81859600	3.79334400	-0.76294800
C	-0.49828900	3.32772300	1.61678100
C	-0.34262700	5.09058100	-0.54950900
C	-0.02646300	4.63246100	1.78613600
C	0.06211300	5.52682400	0.71493700
H	-0.27806000	5.77683800	-1.39280900
H	0.28692800	4.95752200	2.77756500
C	-2.96123200	-0.85095000	-0.17395500
C	-3.82450600	-1.16586400	0.91510200
C	-3.46383900	-1.01154700	-1.49778200
C	-5.12258800	-1.61456000	0.67129600
C	-4.76717700	-1.46568500	-1.70093200
C	-5.61051200	-1.77449300	-0.62944100
H	-5.77550600	-1.84403900	1.51296900
H	-5.14181100	-1.57802600	-2.71801900
C	-1.28396900	3.38907600	-2.14192600
H	-1.08617400	2.32789800	-2.32551600
H	-2.36799100	3.53286600	-2.23488100

H	-0.79557800	3.98476400	-2.91985700
C	-0.61460000	2.41998900	2.81965000
H	0.11375800	2.68631100	3.59236000
H	-1.61745500	2.49418400	3.25929200
H	-0.46558100	1.37299600	2.53299200
C	0.62180300	6.91334900	0.91318300
H	0.28115900	7.34838400	1.85862100
H	1.71898900	6.88846800	0.94133300
H	0.32586700	7.58019800	0.09794400
C	3.19460800	1.29266900	1.97120100
H	3.82413200	0.55667000	2.48650400
H	3.34531100	2.26036800	2.46476800
H	2.14722800	0.99969400	2.10597200
C	1.88552100	0.85530200	-2.92989000
H	0.97984000	0.41815100	-2.49161100
H	1.59477900	1.77445100	-3.45433100
H	2.27923100	0.16017600	-3.68045800
C	6.57733400	2.18149600	-1.65196900
H	6.91365000	3.08270300	-1.12694700
H	7.28402400	1.37940700	-1.40368000
H	6.64374200	2.36568400	-2.72824800
C	-2.60925600	-0.68492800	-2.70125100
H	-3.05094100	0.13111100	-3.28613600
H	-1.60573500	-0.37888400	-2.39066200
H	-2.51732100	-1.55274900	-3.36539000
C	-3.35277500	-1.03686200	2.34514200
H	-3.18904600	-2.02521000	2.79260900

H	-2.41007000	-0.48385300	2.39303700
H	-4.09540300	-0.51545100	2.95972100
C	-7.00657700	-2.29173500	-0.87066700
H	-7.40798900	-1.92437800	-1.82027900
H	-7.01107900	-3.38886800	-0.91322900
H	-7.68560400	-1.99235500	-0.06601700
Au	-1.79143700	0.98927700	0.09182900
C	0.97988200	-2.50829400	0.28955300
C	1.64401400	-3.08582800	-0.83059500
C	1.59583300	-2.58861100	1.57330800
C	2.88601000	-3.72596400	-0.66754000
C	2.83787500	-3.23330700	1.72588400
C	3.49312500	-3.76852600	0.60167300
C	0.89586800	-2.00021000	2.77984100
H	0.04118600	-1.39746200	2.45629100
H	0.51377600	-2.78968600	3.44079600
H	1.56274600	-1.36713100	3.37491700
C	3.47648600	-3.34130600	3.09366700
H	4.22782700	-2.55452300	3.25188900
H	2.73423300	-3.24690600	3.88837000
H	3.98140800	-4.30287600	3.22431000
C	4.86848500	-4.37942700	0.75262300
H	5.42014700	-3.92096200	1.57663500
H	4.81347200	-5.45850500	0.95533200
H	5.46189600	-4.24950100	-0.15567700
C	3.57983100	-4.35666700	-1.85497800
H	4.35367200	-3.69389500	-2.26739000

H	4.06972300	-5.29537600	-1.57939100
H	2.87476500	-4.57421500	-2.65925600
C	0.99693000	-3.02294100	-2.19707600
H	0.11293900	-2.37865600	-2.15919400
H	1.68092500	-2.63210600	-2.95863800
H	0.66915200	-4.01735700	-2.52779300

Cu2Au2-DFT

Cu	0.02565400	1.87824100	0.00059500
Cu	1.63607500	0.09877400	0.00020400
Au	-0.16079000	-1.73673500	0.00049700
C	2.02863500	2.07973700	-0.00234000
C	2.59294400	2.56520200	1.21649900
C	2.58673300	2.56306100	-1.22191700
C	3.65645400	3.46924800	1.19480200
C	3.65201500	3.46925000	-1.20446100
C	4.20354000	3.93280600	-0.00747400
H	4.07289600	3.82376100	2.13810500
H	4.06550600	3.82403400	-2.14866700
C	-1.98467000	2.41116400	0.00161400
C	-2.14526400	3.13286500	-1.21967500
C	-2.14243000	3.13168600	1.22384900
C	-2.41718500	4.50421500	-1.19580700
C	-2.41430500	4.50317100	1.20192400
C	-2.54888000	5.21047200	0.00358100
H	-2.53131700	5.03628000	-2.13996600
H	-2.52608900	5.03437700	2.14683500
C	-2.35843300	-1.89621100	-0.00073200

C	-2.92897900	-2.37246700	1.22016900
C	-2.92700600	-2.37052000	-1.22285700
C	-4.00828900	-3.25741600	1.19668200
C	-4.00689000	-3.25562900	-1.20200700
C	-4.56243800	-3.71371300	-0.00362300
H	-4.43598200	-3.59678400	2.14009900
H	-4.43356300	-3.59366000	-2.14631000
C	-2.08878000	2.42773600	-2.55648900
H	-1.40242600	1.57532900	-2.52581400
H	-3.07865800	2.03505400	-2.82330000
H	-1.77443300	3.10939900	-3.35411900
C	-2.08302200	2.42512900	2.55983000
H	-1.76893100	3.10645600	3.35785000
H	-3.07188700	2.03040200	2.82738500
H	-1.39518400	1.57396800	2.52738900
C	-2.79871300	6.69904900	0.00438300
H	-3.34885300	7.00974400	0.89839100
H	-1.85059800	7.25308300	-0.00720000
H	-3.36871900	7.00741200	-0.87798600
C	2.04382200	2.12416600	2.55674800
H	2.84063900	1.75689800	3.21482800
H	1.55149100	2.95685400	3.07539300
H	1.30634700	1.32409400	2.42752300
C	2.03597400	2.12097800	-2.56079700
H	1.28546400	1.33364300	-2.42849300
H	1.55987200	2.95763700	-3.08813500
H	2.82963100	1.73577900	-3.21261600

C	5.36474600	4.89787000	-0.00588200
H	5.15773000	5.76708700	0.62935000
H	6.27243100	4.42109300	0.38553600
H	5.58294300	5.25681400	-1.01613900
C	-2.37510800	-1.94964000	-2.56763000
H	-3.18341000	-1.70784100	-3.26746200
H	-1.72471500	-1.07579500	-2.46921500
H	-1.78560800	-2.75985800	-3.01597000
C	-2.37878700	-1.95258300	2.56602300
H	-1.79030200	-2.76325900	3.01484200
H	-1.72791100	-1.07896100	2.46892000
H	-3.18795600	-1.71068000	3.26481600
C	-5.71405900	-4.68906100	-0.00424900
H	-6.30769700	-4.60356200	-0.91988100
H	-5.34806500	-5.72277200	0.05556300
H	-6.37394700	-4.52677300	0.85429000
Au	-1.98945000	0.29449000	0.00029500
C	1.96370900	-1.94630400	0.00118700
C	2.64420100	-2.20282900	-1.22571300
C	2.64378200	-2.20326200	1.22812000
C	3.96814500	-2.67898200	-1.22158700
C	3.96787300	-2.67911400	1.22428800
C	4.63576700	-2.88500300	0.00144700
C	1.92904000	-1.98590900	2.54664900
H	0.96312900	-1.50145900	2.37394900
H	1.73384400	-2.93917600	3.05634000
H	2.51205900	-1.36271100	3.23469000

C	4.68416700	-2.97749100	2.52628700
H	5.38720600	-2.17617500	2.79495800
H	3.98357700	-3.08700600	3.35587900
H	5.26336800	-3.90425300	2.45913200
C	6.08154100	-3.33413600	0.00151200
H	6.61375200	-2.96995200	0.88394000
H	6.16506400	-4.43075200	0.00129500
H	6.61390900	-2.96960300	-0.88068100
C	4.68472500	-2.97791900	-2.52330100
H	5.38816800	-2.17700500	-2.79208400
H	5.26355500	-3.90488200	-2.45557200
H	3.98434000	-3.08755300	-3.35304700
C	1.92985600	-1.98521800	-2.54440400
H	0.96479100	-1.49891100	-2.37217900
H	2.51397400	-1.36373300	-3.23298600
H	1.73280800	-2.93862100	-3.05317500

CU2Ag2dft

Cu	-1.300162	1.397527	-0.012328
Cu	1.122861	1.147105	-0.045985
Ag	0.977319	-1.406727	-0.051134
C	0.068152	2.852706	-0.282760
C	0.193926	3.780228	0.796377
C	0.118818	3.381487	-1.606373
C	0.365033	5.142958	0.547002
C	0.291109	4.753495	-1.818622
C	0.417717	5.651344	-0.756225
H	0.460471	5.830204	1.388191

H	0.328304	5.134625	-2.839326
C	-3.118297	0.564224	0.250429
C	-4.024242	0.767073	-0.829985
C	-3.633521	0.699557	1.573559
C	-5.355940	1.116171	-0.583859
C	-4.969868	1.050165	1.782372
C	-5.847691	1.268299	0.715326
H	-6.030202	1.272946	-1.426004
H	-5.339961	1.154428	2.802620
C	-0.545558	-3.026428	-0.225141
C	-0.618330	-3.892877	0.902028
C	-0.629647	-3.617443	-1.517571
C	-0.766361	-5.272372	0.726719
C	-0.777275	-5.001198	-1.655633
C	-0.844742	-5.847362	-0.545006
H	-0.825260	-5.917369	1.603700
H	-0.844834	-5.432606	-2.654590
C	-3.578659	0.604617	-2.267926
H	-2.498614	0.431985	-2.322174
H	-4.081631	-0.247946	-2.742295
H	-3.817135	1.494435	-2.863105
C	-2.756427	0.458390	2.784805
H	-2.810731	1.295322	3.491239
H	-3.070294	-0.444077	3.325188
H	-1.710875	0.324669	2.485952
C	-7.279802	1.677344	0.962139
H	-7.701730	1.150274	1.824660

H	-7.347524	2.752790	1.173105
H	-7.907815	1.471519	0.089842
C	0.137421	3.310745	2.234392
H	1.036191	3.609859	2.787710
H	-0.725866	3.740708	2.757942
H	0.053357	2.219817	2.280594
C	-0.017153	2.478886	-2.814363
H	-0.116768	1.432734	-2.503460
H	-0.899660	2.743712	-3.410193
H	0.855885	2.559705	-3.473684
C	0.607296	7.129080	-1.001369
H	-0.191549	7.714012	-0.529481
H	1.556725	7.480929	-0.579314
H	0.607546	7.356080	-2.071628
C	-0.567463	-2.776651	-2.776517
H	-1.481654	-2.887795	-3.372928
H	-0.446880	-1.716347	-2.530459
H	0.273562	-3.078084	-3.413357
C	-0.541889	-3.357462	2.317185
H	0.315641	-3.781065	2.854865
H	-0.439308	-2.267310	2.316985
H	-1.442331	-3.616566	2.887966
C	-0.972980	-7.342055	-0.714484
H	-1.509012	-7.593783	-1.635247
H	0.016916	-7.813975	-0.771556
H	-1.502783	-7.794403	0.130034
Ag	-1.693840	-1.128948	-0.009379

C	2.736883	-0.044600	0.164149
C	3.619088	-0.054716	-0.951838
C	3.295107	-0.048537	1.473207
C	5.012413	-0.030992	-0.765533
C	4.689192	-0.026486	1.660866
C	5.541989	0.006589	0.539821
C	2.372453	-0.063350	2.677065
H	1.329340	-0.018752	2.344247
H	2.493440	-0.975564	3.276247
H	2.552235	0.788628	3.344433
C	5.285572	-0.038733	3.054700
H	5.702085	0.941603	3.325339
H	4.541382	-0.294902	3.810429
H	6.100733	-0.766539	3.134211
C	7.041855	0.074751	0.731332
H	7.307930	0.528919	1.688511
H	7.496366	-0.926455	0.707746
H	7.518579	0.660875	-0.059534
C	5.957323	-0.042770	-1.950210
H	6.412601	0.944401	-2.112740
H	6.778545	-0.752265	-1.799190
H	5.446217	-0.320629	-2.873471
C	3.045802	-0.076657	-2.355190
H	1.952041	-0.042369	-2.309614
H	3.387184	0.778231	-2.952285
H	3.329568	-0.986758	-2.900094

CuAg4-dft-D3

Cu	-1.288007	1.411113	-0.006170
Cu	1.131020	1.139754	-0.037871
Ag	0.969575	-1.415321	-0.045905
C	0.093021	2.854352	-0.276026
C	0.224129	3.778444	0.804286
C	0.141376	3.386974	-1.599299
C	0.398108	5.142353	0.557288
C	0.316815	4.757824	-1.808903
C	0.451122	5.653044	-0.743777
H	0.492828	5.828719	1.399099
H	0.347170	5.141124	-2.829151
C	-3.112660	0.588396	0.247266
C	-4.014122	0.791949	-0.837841
C	-3.632156	0.727954	1.567541
C	-5.344749	1.146416	-0.597926
C	-4.968948	1.083889	1.770184
C	-5.840962	1.303415	0.699841
H	-6.015339	1.302936	-1.443124
H	-5.343590	1.191122	2.788391
C	-0.565315	-3.024089	-0.221109
C	-0.649905	-3.888741	0.906943
C	-0.657964	-3.613217	-1.513209
C	-0.818207	-5.265700	0.732081
C	-0.825517	-4.995341	-1.650598
C	-0.905361	-5.839590	-0.539963
H	-0.886379	-5.909822	1.609087
H	-0.899464	-5.426777	-2.649051

C	-3.563352	0.622237	-2.273265
H	-2.482375	0.454574	-2.323321
H	-4.060339	-0.236346	-2.743122
H	-3.804794	1.506551	-2.875311
C	-2.761534	0.487630	2.783400
H	-2.801567	1.335357	3.477922
H	-3.092846	-0.401053	3.336018
H	-1.718093	0.331024	2.488320
C	-7.271689	1.722695	0.937693
H	-7.645882	1.338474	1.892068
H	-7.356714	2.817154	0.968310
H	-7.929252	1.366062	0.138300
C	0.171205	3.306847	2.241702
H	1.087382	3.573991	2.782988
H	-0.669446	3.764023	2.778689
H	0.052490	2.219013	2.286222
C	-0.002997	2.487288	-2.808599
H	-0.110060	1.441471	-2.499307
H	-0.883939	2.759709	-3.403222
H	0.870128	2.562341	-3.468462
C	0.668929	7.126483	-0.989997
H	0.168666	7.734973	-0.229170
H	1.738158	7.374039	-0.955385
H	0.293493	7.425847	-1.973736
C	-0.583169	-2.774457	-2.772483
H	-1.496262	-2.877128	-3.372076
H	-0.452574	-1.715174	-2.527275

H	0.256997	-3.085068	-3.406094
C	-0.561489	-3.354020	2.321484
H	0.304959	-3.772507	2.848958
H	-0.465006	-2.263298	2.321276
H	-1.453509	-3.619423	2.902316
C	-1.057792	-7.332387	-0.707660
H	-1.514149	-7.579781	-1.671257
H	-0.080320	-7.830995	-0.667434
H	-1.675193	-7.761481	0.088518
Ag	-1.699004	-1.114046	-0.006348
C	2.737640	-0.064610	0.161217
C	3.613445	-0.081799	-0.959724
C	3.302981	-0.074968	1.467220
C	5.008339	-0.070571	-0.781443
C	4.698158	-0.064383	1.646596
C	5.545042	-0.037109	0.520954
C	2.387716	-0.082745	2.676589
H	1.342974	-0.027169	2.350631
H	2.503499	-0.997274	3.273314
H	2.580273	0.766041	3.344460
C	5.303279	-0.081924	3.036367
H	5.718085	0.898527	3.309622
H	4.564783	-0.344789	3.795478
H	6.121803	-0.806860	3.106585
C	7.045872	0.021269	0.709258
H	7.315619	0.513923	1.646609
H	7.488413	-0.985352	0.732139

H	7.530555	0.566682	-0.104932
C	5.945089	-0.092246	-1.972695
H	6.404638	0.891590	-2.143207
H	6.762949	-0.806188	-1.825093
H	5.425447	-0.371118	-2.890892
C	3.032239	-0.097329	-2.359779
H	1.939267	-0.050122	-2.308311
H	3.380507	0.753165	-2.959099
H	3.302097	-1.010988	-2.905875

Cu4HF-DFT

Cu	1.768817	1.087745	0.057156
Cu	-0.973759	1.559683	0.073180
Cu	-1.351805	-1.335445	0.077281
C	0.702971	2.842061	0.477971
C	0.818614	3.881273	-0.482003
C	0.663936	3.245107	1.818153
C	0.880071	5.203814	-0.107545
C	0.728600	4.591704	2.178970
C	0.834747	5.579042	1.232022
H	0.964955	5.968084	-0.860065
H	0.693304	4.859851	3.220635
C	3.173448	-0.431665	-0.427914
C	4.206807	-0.504455	0.517702
C	3.574179	-0.398844	-1.785108
C	5.545298	-0.527712	0.134783
C	4.905386	-0.420938	-2.145243
C	5.910827	-0.484885	-1.190415
H	6.308885	-0.575646	0.891460
H	5.175130	-0.386891	-3.186709
C	-0.029605	-3.003430	0.460695
C	-0.255178	-3.992771	-0.524360
C	-0.196913	-3.411651	1.794395
C	-0.629123	-5.278417	-0.185906
C	-0.570973	-4.711532	2.116512
C	-0.794681	-5.654931	1.138422
H	-0.796856	-6.005668	-0.961413
H	-0.689678	-4.986268	3.150086
C	3.925339	-0.585454	2.002910
H	2.895961	-0.350341	2.234928
H	4.125597	-1.585489	2.375291
H	4.558395	0.097028	2.558635
C	2.548956	-0.376150	-2.898651
H	2.949395	0.082324	-3.794430

H	2.244560	-1.384852	-3.160623
H	1.657838	0.167194	-2.615064
C	7.358603	-0.501090	-1.608513
H	7.565078	-1.347099	-2.255132
H	7.611865	0.398572	-2.159170
H	8.015314	-0.565608	-0.750889
C	0.911816	3.553128	-1.957385
H	0.789293	4.438553	-2.567775
H	1.879440	3.123601	-2.196036
H	0.157506	2.836495	-2.258779
C	0.576246	2.247945	2.953406
H	0.416752	1.241145	2.594611
H	1.492329	2.250019	3.535552
H	-0.233958	2.495283	3.630736
C	0.901143	7.034796	1.614115
H	1.823524	7.484124	1.261962
H	0.080310	7.588223	1.170912
H	0.853017	7.163646	2.687394
C	0.051857	-2.467165	2.951046
H	0.981653	-2.715335	3.453600
H	0.122370	-1.440484	2.621325
H	-0.739121	-2.530803	3.689920
C	-0.040771	-3.688494	-1.991742
H	-0.684775	-4.290910	-2.620830
H	-0.225878	-2.647221	-2.219439
H	0.984508	-3.905561	-2.276790
C	-1.231779	-7.054238	1.486711
H	-1.065060	-7.269754	2.534008
H	-2.289725	-7.186545	1.283885
H	-0.693278	-7.788606	0.899411
Cu	1.467298	-1.609437	0.006751
C	-2.643499	0.294142	-0.297596
C	-3.648287	0.454560	0.675525
C	-3.031594	0.349640	-1.647350
C	-4.978403	0.689460	0.320901
C	-4.356724	0.575224	-2.018713
C	-5.316778	0.783411	-1.031105
C	-1.986591	0.169889	-2.733043
H	-0.992798	0.138263	-2.310898
H	-2.134490	-0.755134	-3.282741
H	-2.011100	0.975900	-3.457203
C	-4.749520	0.603160	-3.482606
H	-4.688012	1.606040	-3.898221
H	-4.104053	-0.027900	-4.074704
H	-5.757842	0.251666	-3.635954
C	-6.734720	1.128776	-1.439248
H	-6.740400	1.779094	-2.302322
H	-7.303228	0.240439	-1.698820
H	-7.267712	1.637983	-0.655650
C	-6.054853	0.851732	1.377858
H	-6.320491	1.895617	1.519232
H	-6.957930	0.324546	1.105278

H	-5.744614	0.467974	2.333610
C	-3.269936	0.379176	2.143882
H	-2.205046	0.238810	2.257932
H	-3.540424	1.284487	2.678271
H	-3.759955	-0.447964	2.645141

Table S1: Selected interatomic distances and bond angles for the tetranuclear M_4L_4 and $M_2M_2'L_4$ complexes (L = Mesitylene) calculated at the TPSS/Def2TZVP level (versus the TPSS-D3(BJ)/Def2TZVP level in parentheses) compared to the HF/LANLD2DZ level of theory in the last column.

	Cu_4L_4	$Cu_2Au_2L_4$	$Cu_2Ag_2L_4$	Cu_4L_4 **(HF)**
M-M' (Å)		2.585 (2.571)	2.531 (2.434)	
M-M (Å)	2.398 (2.372)	2.399 (2.358)	2.562 (2.685)	2.851
M'-C (Å)		2.195 (2.135)	2.214 (2.223)	2.102
M-C (Å)	2.003 (1.978)	1.999 (2.042)	2.183 (2.010)	
M-C-M (°)	73.1 (72.8)	72.5 (73.9)	74.6 (73.12)	84.5
M-C-M' (°)		76.9 (75.6)	75.1 (74.2)	
E_{tot} (H)	-8040.19	-5030.67	-5053.09	-8023.22

Table S2: Selected interatomic distances and bond angles for the pentanuclear M_5L_5 and $M_3M_2'L_5$ complexes ($L = Me_3SiCH_2$) calculated at the TPSS/Def2TZVP level of theory.

	Cu_5L_5	$Cu_3Au_2L_5$	$Cu_3Ag_2L_5$
Si-CH_2 (Å)	1.891	1.886	1.875
M-M' (Å)		2.575	2.554
M-M (Å)	2.389	2. 384	2. 511
M'-C (Å)		2.214	2.114
M-C (Å)	2.031	2.110	2.041
M-C-M (°)	72.5	75.2	75.2
M-C-M' (°)		72.8	72.8
E_{tot} (H)	-10328.47	-7318.75	-7341.18

Table S3: Average NBO charge (*q*) on metal/ligand-donor atoms for models **1**, **2** and **3**, respectively, calculated at the TPSS-D3(BJ)/Def2TZVP level of theory. Metal charges are positive while bridging C-atoms (C_b) are negative.

q	**1**	**2**	**3**
Cu	0.47	0.52	0.49
C_b	-0.51	-0.46	-0.47
Cu	0.47	0.25	0.47
Cu	-	0.55	
C_b	-	-0.51	
Au	-	0.21	
Cu	-	-	0.49
C_b	-	-	-0.48
Ag	-	-	0.33

(Energy Decomposition Analysis (EDA))

The EDA* energies of the Cu3Au2 and Cu5 complexes were calculated including the Total Interaction energy and estimated energy differences:

* F.M. Bickehaupt, E.J. Baerends, Rev. in Comput. Chem. 15, 1, 2000.

a- Cu3Au2

```
-----------------------------------------------------
| * Total Interaction energy  =      -0.4001623458  |
 -----------------------------------------------------
: * Electrostatic Interaction =      -0.7258611268  :
:           Nuc---Nuc       =    7423.6642636188  :
:           1-electron      =  -14847.5953864686  :
:           2-electron      =    7423.2052617229  :
: * Exchange-Repulsion        =       1.0828034344  :
:           Exchange Int.   =      -0.4278451312  :
:           Repulsion       =       1.5106485656  :
: * Orbital Relaxation        =      -0.5777392934  :
: * Correlation Interaction   =      -0.1793653595  :
.....................................................
```

b- Cu5

```
-----------------------------------------------------
| * Total Interaction energy  =      -0.4089171623  |
 -----------------------------------------------------
: * Electrostatic Interaction =      -0.8577926097  :
:           Nuc---Nuc       =    8507.4350038762  :
:           1-electron      =  -17013.0105572402  :
:           2-electron      =    8504.7177607542  :
: * Exchange-Repulsion        =       1.0308395153  :
:           Exchange Int.   =      -0.4064157126  :
:           Repulsion       =       1.4372552278  :
: * Orbital Relaxation        =      -0.4151806718  :
: * Correlation Interaction   =      -0.1667833964  :
.....................................................
```

c- Cu3Ag2

At the TPSS/def2-TZVP level:

for Cu2Ag2 the total interaction energy is 238 kcal/mol

or 47 kcal/mol per each Cu-Ag bond with frozen fragments.

Thus, frozen fragments
E(Cu-Cu) = 51 kcal/mol
E(Cu-Ag) = 47 kcal/mol
E(Cu-Au) = 50 kcal/mol

For the relaxed fragments it is
E(Cu-Cu) = 40 kcal/mol
E(Cu-Ag) = 36 kcal/mol
E(Cu-Au) = 40 kcal/mol

EDA calculation on Cu3Ag2(Mes)5:

```
 -----------------------------------------------------
| * Total Interaction energy  =      -0.3791309617  |
 -----------------------------------------------------
: * Electrostatic Interaction =      -0.7348397626  :
:           Nuc---Nuc       =    7366.7922435028  :
:           1-electron      = -14731.6538595111  :
:           2-electron      =    7364.1267762457  :
: * Exchange-Repulsion        =       0.9511689056  :
:           Exchange Int.   =      -0.3880831047  :
:           Repulsion       =       1.3392520103  :
: * Orbital Relaxation        =      -0.4313479991  :
: * Correlation Interaction   =      -0.1641121054  :
```

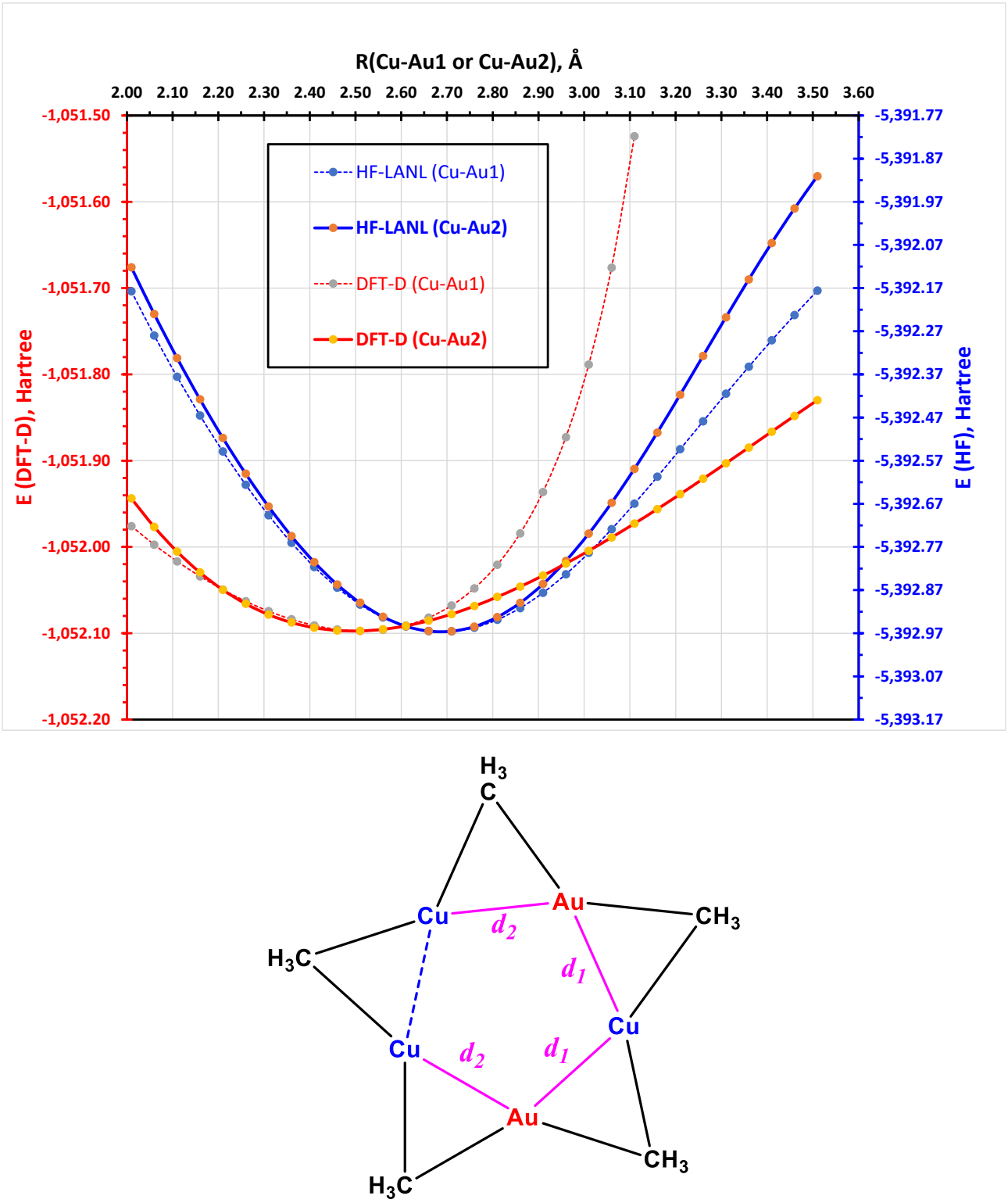

Figure S1. Potential energy surface (PES) plot upon varying only Cu-Au separations in [Cu_3Au_2(μ-Me_5)] at different levels of theory, HF/LANL2DZ and DFT-D (using TPSS-D3(BJ)/def2-TZVP). The Cu-Au1 and Cu-Au2 distances indicated in the PES figure (top) correspond to the d_1 and d_2, respectively, in the model shown (bottom) with each distance scanned while the other fixed.