

Supporting information

Table S1. B3LYP optimized cartesian coordinates of all investigated species and relative zero point corrected energies.

Watson-Crick	AT				
	$E_{ZPE}=-999.632307$ a.u.				
	H	-4.27391200	0.03403900	-4.73427200	
	N	-5.29781500	0.03314100	-4.94657100	
	C	-5.62505300	0.04770200	-6.28704200	
	N	-6.99904900	0.04422900	-6.54863600	
	C	-7.39654500	0.05897200	-7.95564900	
	C	-7.92205400	0.02654300	-5.52584800	
	C	-7.59055800	0.01187700	-4.21161000	
	C	-8.59697000	-0.00753600	-3.09697700	
	C	-6.17127200	0.01493600	-3.86703400	
	O	-5.74903600	0.00244100	-2.70493500	
	O	-4.79768200	0.06273300	-7.18852000	
	H	-7.00456500	0.95133500	-8.45063800	
	H	-6.99839200	-0.81898900	-8.47110200	
	H	-8.48654200	0.05579800	-8.01159700	
	H	-8.95871900	0.02507400	-5.84876200	
	H	-9.62048100	-0.00821100	-3.48558700	
	H	-8.46427100	-0.89321200	-2.46493400	
	H	-8.47387900	0.86336100	-2.44282400	
	N	0.19370300	-0.01818100	-1.78057500	
	C	1.41300000	-0.01675000	-2.26677900	
	N	1.46803200	0.00405000	-3.64697400	
	C	2.64290300	0.01140200	-4.50326700	
	C	0.15699900	0.01676500	-4.07481200	
	N	-0.29336400	0.03793400	-5.33963000	
	C	-1.62458000	0.04480100	-5.37886400	
	N	-2.48750100	0.03358000	-4.34452000	
	C	-2.01351700	0.01231800	-3.07668900	
	N	-2.87978000	0.00100200	-2.04949900	
	C	-0.60909900	0.00289100	-2.90601100	
	H	2.31872400	-0.03016100	-1.67306800	
	H	3.25508200	0.89941500	-4.31612800	
	H	3.24826300	-0.88601500	-4.34048100	
	H	2.29381700	0.02688900	-5.53730100	
	H	-2.09282200	0.06104300	-6.36069900	
	H	-3.88893200	0.00895900	-2.21782900	
	H	-2.51874900	-0.01545000	-1.10802700	
		AT-Cu			
		$E_{ZPE}=-1196.345883$ a.u.			
		N	-5.17146600	0.03363200	-5.36573800
		C	-5.81662800	0.05020800	-6.57647100
		N	-7.22274400	0.05034100	-6.53445700
		C	-7.92257100	0.06815400	-7.81571700
		C	-7.89517100	0.03448400	-5.33622200
		C	-7.26672600	0.01789300	-4.13482300
		C	-7.99208000	0.00041500	-2.81949000
	C	-5.80652100	0.01723700	-4.14392600	
	O	-5.14030300	0.00225400	-3.08322500	
	O	-5.23505900	0.06437400	-7.66145500	
	H	-7.64867800	0.95999600	-8.38604900	
	H	-7.65077700	-0.80882800	-8.40962000	
	H	-8.99881100	0.06696100	-7.62946500	
	H	-8.97863800	0.03608900	-5.41496800	

H	-9.07795200	0.00269000	-2.96473700
H	-7.72276100	-0.88586400	-2.23281700
H	-7.72223500	0.87045100	-2.20922100
N	0.61218600	-0.02510400	-1.60069000
C	1.90531200	-0.02229800	-1.82810700
N	2.23878300	-0.00220900	-3.16876100
C	3.56671400	0.00668300	-3.76601400
C	1.04387500	0.00871700	-3.84963600
N	0.85295000	0.02895900	-5.18165300
C	-0.42957600	0.03425700	-5.49647300
N	-1.49610200	0.02199500	-4.64903600
C	-1.28979600	0.00153700	-3.29426400
N	-2.32161000	-0.01052000	-2.44593700
C	0.05724800	-0.00582100	-2.86346200
H	2.67067900	-0.03431200	-1.06242200
H	4.12328700	0.89568200	-3.45448800
H	4.12390200	-0.89037600	-3.47972900
H	3.44136200	0.02197900	-4.84985200
H	-0.68463600	0.05028200	-6.55148200
H	-3.30979000	-0.00463000	-2.75089400
H	-2.11506300	-0.02542400	-1.45666500
Cu	-3.30410900	0.03122800	-5.24034700
AT-Ag			
$E_{ZPE}=-1146.013948$ a.u.			
N	-5.33349000	0.03599500	-5.58261500
C	-6.08663300	0.04965900	-6.72594000
N	-7.48428600	0.04565800	-6.55169100
C	-8.30210900	0.05971500	-7.76079100
C	-8.03979000	0.02918900	-5.29519900
C	-7.29991400	0.01565000	-4.15918300
C	-7.89697900	-0.00249300	-2.78083600
C	-5.84569000	0.01900800	-4.30657000
O	-5.08525900	0.00703600	-3.31131200
O	-5.61219500	0.06455900	-7.86200000
H	-8.08794100	0.95275100	-8.35434500
H	-8.08286400	-0.81584400	-8.37798900
H	-9.35605000	0.05290700	-7.47390100
H	-9.12585400	0.02768400	-5.27049800
H	-8.99178600	-0.00360500	-2.82173000
H	-7.57020600	-0.88719400	-2.22158600
H	-7.57286800	0.86889000	-2.19953700
N	0.59875100	-0.01784600	-1.58013500
C	1.90667600	-0.01788400	-1.69549500
N	2.35432600	-0.00120100	-3.00261700
C	3.72841400	0.00388200	-3.48412200
C	1.22206100	0.01036300	-3.78344400
N	1.14526500	0.02807500	-5.12690200
C	-0.10723100	0.03532100	-5.54721400
N	-1.24081700	0.02709400	-4.79586500
C	-1.15175800	0.00885100	-3.43059300
N	-2.24412300	-0.00009500	-2.66057500
C	0.15476800	0.00006900	-2.88595000
H	2.60342200	-0.02968500	-0.86682100
H	4.25771000	0.89358900	-3.12998700
H	4.25790200	-0.89244900	-3.14748400
H	3.69605700	0.01461600	-4.57477700
H	-0.26935300	0.04956500	-6.62071200
H	-3.21163300	0.00467000	-3.01983400
H	-2.10546100	-0.01370500	-1.65934100
Ag	-3.23679500	0.03785000	-5.60282200

AT-Au

$E_{ZPE} = -1134.90676$ a.u.

N	-5.33618500	0.03308600	-5.45727600
C	-6.01091300	0.04678200	-6.65502700
N	-7.41457500	0.04545200	-6.56420400
C	-8.15284100	0.05993600	-7.82400900
C	-8.05121100	0.03088400	-5.34657100
C	-7.38919500	0.01712400	-4.16437900
C	-8.07666400	0.00105800	-2.82895100
C	-5.92857700	0.01786600	-4.20515200
O	-5.23723500	0.00602200	-3.16741300
O	-5.46691800	0.05999800	-7.75563400
H	-7.89752100	0.95099900	-8.40397500
H	-7.89788300	-0.81778300	-8.42414200
H	-9.22277500	0.05768600	-7.60467700
H	-9.13636500	0.03109200	-5.39381500
H	-9.16617000	0.00182100	-2.94315600
H	-7.78915500	-0.88380200	-2.24887800
H	-7.79009300	0.87232100	-2.22819900
N	0.70839900	-0.02043300	-1.57174600
C	2.00836800	-0.01812800	-1.75715600
N	2.38575200	0.00072000	-3.08597200
C	3.73275500	0.00890200	-3.63990000
C	1.21402600	0.01118800	-3.80542300
N	1.06639200	0.03020400	-5.14262600
C	-0.20303500	0.03510600	-5.50180900
N	-1.29238200	0.02339400	-4.68413900
C	-1.13659100	0.00424100	-3.32387800
N	-2.19086500	-0.00699500	-2.50049500
C	0.19586500	-0.00253600	-2.85174800
H	2.74815900	-0.02946600	-0.96672400
H	4.27851400	0.89833000	-3.31128400
H	4.27986800	-0.88788100	-3.33435600
H	3.64270700	0.02290000	-4.72722800
H	-0.42999300	0.04992100	-6.56230400
H	-3.16410000	-0.00100800	-2.82997000
H	-2.01038200	-0.02043600	-1.50610300
Au	-3.28491300	0.03208200	-5.35209400

GC

$E_{ZPE} = -1015.703609$ a.u.

H	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.92312000
C	1.21349000	0.00000000	2.53129400
N	1.25437500	0.01754600	3.95031600
C	2.57186200	0.01956700	4.58380800
C	0.09963700	0.03076000	4.67169500
C	-1.11806900	0.02695900	4.06939500
C	-1.13570600	0.00843200	2.63071400
N	-2.29235500	0.00137700	1.95638100
O	2.29206900	-0.01477700	1.92450700
H	3.12900900	-0.87506700	4.29479500
H	3.14192400	0.89369400	4.25983300
H	2.44298100	0.04180600	5.66810400
H	0.21274500	0.04374700	5.75098800
H	-2.03104200	0.03669300	4.65205300
H	-3.16952000	-0.00819900	2.45364700

H	-2.30091500	-0.04052400	0.92107200
N	-0.03314500	-0.04281600	-1.03145300
C	1.15118000	-0.02722200	-1.73064000
N	2.28395200	0.10500900	-1.00167500
N	1.21861400	-0.11142100	-3.05121000
C	-0.00018800	-0.20388500	-3.62502400
N	-0.24264900	-0.30219700	-4.97471200
C	0.76215000	-0.32227400	-6.02234700
C	-1.62214000	-0.37297800	-5.10880600
N	-2.26277600	-0.32867800	-3.96993500
C	-1.26198300	-0.22191800	-3.02059200
C	-1.32407300	-0.13811200	-1.59318000
O	-2.32168900	-0.14221400	-0.85688300
H	2.28941800	0.04071300	0.01977300
H	3.15149800	0.00783600	-1.50577400
H	1.74033300	-0.25096100	-5.54366700
H	0.63291700	0.52544700	-6.70373800
H	0.70939900	-1.25396600	-6.59573200
H	-2.08271300	-0.45654700	-6.08542400

GC-Cu

$E_{ZPE} = -1212.443491$ a.u.

Cu	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	1.90598500
C	1.22558200	0.00000000	2.53795900
N	1.22052900	0.02166700	3.95321000
C	2.52632000	0.02831800	4.61503900
C	0.05119500	0.03515600	4.64886300
C	-1.15570300	0.02614900	4.02513600
C	-1.16455700	0.00441600	2.59047600
N	-2.30945200	-0.01014200	1.90542300
O	2.29233400	-0.01700900	1.93728300
H	3.09327900	-0.86116500	4.33051000
H	3.09563900	0.90916000	4.30887100
H	2.37257200	0.04177700	5.69580700
H	0.14112700	0.05196000	5.72999500
H	-2.07837900	0.03456400	4.59121100
H	-3.18829900	-0.01100000	2.40174600
H	-2.33186800	-0.04752000	0.86514000
N	-0.42980800	-0.01590100	-1.83259700
C	0.37303200	0.04507400	-2.93045700
N	1.72633800	0.18532700	-2.69712100
N	-0.02502500	0.02320000	-4.19868700
C	-1.36600500	-0.04897900	-4.30296000
N	-2.08974700	-0.08007300	-5.47257800
C	-1.54278400	-0.04636000	-6.81620500
C	-3.42114300	-0.15708900	-5.08931300
N	-3.59529000	-0.17543800	-3.79314600
C	-2.31186100	-0.10831800	-3.27556800
C	-1.82573600	-0.09234900	-1.93147900
O	-2.51540100	-0.14061100	-0.88350500
H	2.06849700	-0.14218400	-1.80309800
H	2.30857400	-0.03966200	-3.49234600
H	-0.46496700	0.10380500	-6.73095400
H	-1.73199600	-0.98823700	-7.34332000
H	-1.97681700	0.77842000	-7.39109500
H	-4.21140200	-0.19422600	-5.82910800

GC-Ag

E _{ZPE} =-1162.077363 a.u.			
Ag	0.00000000	0.00000000	0.00000000
N	0.00000000	0.00000000	2.16170300
C	1.22748000	0.00000000	2.78252800
N	1.23405400	0.01124700	4.19900100
C	2.54380900	0.01651100	4.85228700
C	0.06892700	0.01378200	4.90185300
C	-1.14180600	0.00790300	4.28604500
C	-1.15778600	0.00148200	2.84949200
N	-2.31256600	-0.00273400	2.17871000
O	2.29033900	-0.00869300	2.17411700
H	3.11282400	0.89521300	4.53979100
H	3.10775700	-0.87478200	4.56700000
H	2.39742400	0.03367000	5.93408800
H	0.16553700	0.02048500	5.98260000
H	-2.06058100	0.00971000	4.85853700
H	-3.18347900	0.00028700	2.68866800
H	-2.36392000	-0.00986500	1.14291600
N	-0.83465400	-0.01431600	-1.95295000
C	-0.26452600	0.00942800	-3.18507500
N	1.11831400	0.05092000	-3.22703000
N	-0.90202800	0.03718700	-4.35266800
C	-2.23912200	0.05637200	-4.19101700
N	-3.18015900	0.09252600	-5.19446600
C	-2.90800100	0.12647000	-6.61925500
C	-4.41143300	0.09291700	-4.55477500
N	-4.32663700	0.05976900	-3.24986900
C	-2.96444300	0.03628200	-2.99745100
C	-2.22452800	-0.00372000	-1.77343300
O	-2.70561700	-0.02575100	-0.61548000
H	1.59582300	-0.37161500	-2.44174600
H	1.49979800	-0.19321300	-4.13157900
H	-1.82420600	0.11530900	-6.74885800
H	-3.33855700	-0.74677300	-7.12147100
H	-3.31390000	1.03651400	-7.07434900
H	-5.33319100	0.11899800	-5.12317600
GC-Au			
E _{ZPE} =-1150.985942 a.u.			
N	-3.67708400	-0.89706800	-0.02855700
C	-3.95152600	-2.33480700	-0.07313600
H	-4.46332500	-2.58783200	-1.00455500
H	-4.59903500	-2.61666100	0.76035600
H	-3.00503200	-2.87496600	-0.00943500
C	-2.41619700	-0.40011300	0.07612300
C	-2.17117000	0.93541700	0.11694000
C	-3.29429700	1.82469100	0.04326900
N	-4.54283200	1.31950700	-0.06342400
C	-4.80130800	-0.03817100	-0.10043400
N	-3.11546900	3.14891600	0.07919400
O	-5.92082100	-0.51490800	-0.18973800
O	-5.04779500	5.33971400	-0.02702000
C	-6.27246100	5.55893300	-0.13083900
N	-7.18191300	4.48312100	-0.23639200
C	-8.52876500	4.65789800	-0.35449700
N	-9.29172600	3.52186300	-0.51390200
N	-9.16117900	5.82550500	-0.36886900
C	-8.30885600	6.86477900	-0.27201000
C	-6.91749300	6.83629900	-0.15628500

N	-6.40416400	8.12038100	-0.07893900
C	-7.45781000	8.89248800	-0.14661400
N	-8.65230700	8.19687400	-0.26573700
C	-9.99799600	8.73188300	-0.35950800
H	-3.89137400	3.83455400	0.03103900
H	-2.17847200	3.51696900	0.15577400
H	-1.16173100	1.31660100	0.20110800
H	-1.61800700	-1.13331900	0.12561700
Au	-6.12238600	2.71063500	-0.17913900
H	-8.89418600	2.65501900	-0.17591900
H	-10.27687900	3.65509100	-0.33168600
H	-10.27786800	9.25818200	0.55986300
H	-10.08418200	9.42094900	-1.20627800
H	-10.67833800	7.89172300	-0.51039500
H	-7.44523500	9.97518600	-0.11815500
AU			
$E_{ZPE} = -960.354436$ a.u.			
H	-0.00220000	-0.04423400	-0.00964100
N	1.04375600	-0.03613400	-0.01006700
C	1.64297600	-1.27794100	-0.01808600
N	3.04710000	-1.25474900	-0.01835800
C	3.72162800	-2.55226900	-0.02715000
C	3.73681300	-0.06716500	-0.01094900
C	1.67351400	1.20700600	-0.00233600
O	1.01800100	2.25279000	0.00461300
O	1.02415100	-2.33241000	-0.02478200
H	3.43644000	-3.13290700	0.85389200
H	3.43755300	-3.12047200	-0.91664400
H	4.80035100	-2.38580100	-0.02532400
H	4.81775100	-0.16367000	-0.01187900
N	-4.98142900	1.92762600	0.01338700
C	-6.07530100	1.20206100	0.01233100
N	-5.84637600	-0.16028800	0.00307300
C	-6.82107500	-1.23896800	-0.00067800
C	-4.47550100	-0.31053800	-0.00176400
N	-3.77524000	-1.45629800	-0.01089600
C	-2.46432400	-1.22173200	-0.01360500
N	-1.83132000	-0.03258100	-0.00864300
C	-2.55545900	1.11147600	0.00047200
N	-1.91907200	2.29464900	0.00553000
C	-3.96509300	0.99040700	0.00439100
H	-7.08345900	1.59773400	0.01780300
H	-7.44930000	-1.19877900	0.89493800
H	-7.45651700	-1.18597000	-0.89050800
H	-6.26787800	-2.17982300	-0.00964400
H	-1.80520300	-2.08718800	-0.02076100
H	-0.89674600	2.33823100	0.00155100
H	-2.46623500	3.14178200	0.01243800
C	3.12459400	1.14009200	-0.00299800
H	3.68736300	2.06365400	0.00283600
AU-Cu			
$E_{ZPE} = -1157.103002$ a.u.			
N	0.76350700	-0.42518700	-0.01127800
C	1.66146700	-1.46114000	-0.01777000
N	3.03050700	-1.11196400	-0.01823500
C	3.99228300	-2.21075000	-0.02530100
C	3.42079300	0.20124100	-0.01297000

C	1.11048900	0.91133700	-0.00576700
O	0.22487400	1.79459300	0.00005700
O	1.33955200	-2.64825400	-0.02264000
H	3.85259400	-2.84281800	0.85575600
H	3.85121800	-2.83281400	-0.91326200
H	5.00213200	-1.79445100	-0.02374300
H	4.49366800	0.36786300	-0.01397700
N	-5.70850400	1.98639700	0.01362300
C	-6.91988200	1.47995000	0.01264800
N	-6.95006500	0.09858200	0.00486500
C	-8.11393800	-0.77633900	0.00216900
C	-5.63457000	-0.30260800	0.00031500
N	-5.15508500	-1.56009400	-0.00779400
C	-3.83472100	-1.58483400	-0.01050300
N	-2.98092500	-0.52331600	-0.00613100
C	-3.48042200	0.75303500	0.00165200
N	-2.66086400	1.80768400	0.00494900
C	-4.88928500	0.87659600	0.00547300
H	-7.83500000	2.05852500	0.01761200
H	-8.71987200	-0.61385000	0.89856400
H	-8.72561600	-0.60049300	-0.88776200
H	-7.75295400	-1.80602300	-0.00664600
H	-3.35324800	-2.55770000	-0.01669800
H	-1.62988300	1.72706200	0.00269800
H	-3.08008200	2.72728400	0.01189400
C	2.52900200	1.22036400	-0.00676300
H	2.84545300	2.25507300	-0.00249100
Cu	-1.08732000	-0.70374300	-0.01001400
AU-Ag			
E_{ZPE} = -1106.736641 a.u.			
N	0.95742300	-0.59066800	-0.01371500
C	1.94571900	-1.53665200	-0.02054800
N	3.27731700	-1.05948100	-0.02037900
C	4.33859300	-2.06196900	-0.02781000
C	3.54055200	0.28489600	-0.01373300
C	1.17148000	0.77143100	-0.00695000
O	0.20805700	1.56896800	-0.00002600
O	1.73966200	-2.74951600	-0.02670600
H	4.25969400	-2.70504500	0.85287700
H	4.25711600	-2.69474800	-0.91570500
H	5.30482600	-1.55239100	-0.02626100
H	4.59263100	0.55353000	-0.01420500
N	-5.71770300	2.00505800	0.01329000
C	-6.96761000	1.60295600	0.01326400
N	-7.11458800	0.22905700	0.00645100
C	-8.34767800	-0.54514700	0.00497700
C	-5.83745000	-0.28167300	0.00165400
N	-5.46490400	-1.57494300	-0.00567600
C	-4.15043000	-1.70736600	-0.00866200
N	-3.21153600	-0.72360000	-0.00515300
C	-3.60084000	0.58818300	0.00259200
N	-2.70624900	1.58093800	0.00684900
C	-4.99553100	0.82992900	0.00607000
H	-7.83056200	2.25685500	0.01799900
H	-8.93751100	-0.33234900	0.90161400
H	-8.94332700	-0.31939100	-0.88460100
H	-8.07405700	-1.60142400	-0.00353700
H	-3.75394300	-2.71814500	-0.01464000
H	-1.68318400	1.44484700	0.00345800
H	-3.06294600	2.52679700	0.01167400

	C	2.55565100	1.21418400	-0.00701700
	H	2.77247600	2.27426000	-0.00174700
	Ag	-1.08583000	-1.06574300	-0.01211500
	AU-Au			
	E _{ZPE} =-1095.646754 a.u.			
	N	0.96023000	-0.47804000	-0.01215000
	C	1.88018800	-1.49777000	-0.01942300
	N	3.23729600	-1.10598700	-0.01937800
	C	4.22860900	-2.17848500	-0.02733600
	C	3.59251900	0.21732300	-0.01268900
	C	1.26221900	0.87814900	-0.00510000
	O	0.35885800	1.73469000	0.00104800
	O	1.59342800	-2.69061000	-0.02575500
	H	4.10642500	-2.81482100	0.85319800
	H	4.10464700	-2.80347800	-0.91573400
	H	5.22647100	-1.73431100	-0.02549000
	H	4.66062500	0.41169200	-0.01341600
	N	-5.79345300	2.00014800	0.01276800
	C	-7.02081000	1.53341000	0.01313200
	N	-7.09667500	0.15398900	0.00599400
	C	-8.28876000	-0.68276400	0.00456300
	C	-5.79540000	-0.29023900	0.00061900
	N	-5.35741700	-1.56246000	-0.00719900
	C	-4.04006600	-1.63368500	-0.01034200
	N	-3.15740700	-0.59624500	-0.00670100
	C	-3.60830900	0.69660100	0.00115100
	N	-2.76120100	1.73190200	0.00452000
	C	-5.01198200	0.86414100	0.00513900
	H	-7.91632000	2.14188500	0.01837300
	H	-8.88830500	-0.49962000	0.90115300
	H	-8.89443900	-0.48759900	-0.88533200
	H	-7.96147200	-1.72362400	-0.00354700
	H	-3.58445500	-2.61791200	-0.01665600
	H	-1.73945400	1.62530900	0.00282000
	H	-3.15647200	2.66210400	0.01112800
	C	2.67601300	1.21296000	-0.00564800
	H	2.96701200	2.25499200	-0.00038500
	Au	-1.06685100	-0.81400600	-0.01090000
Wobble	GU			
	E _{ZPE} =-1035.58731 a.u.			
	H	-2.71278400	0.00612900	-7.19802000
	N	-3.57056100	0.03525800	-7.78220300
	C	-4.76357900	0.04197800	-7.11407500
	N	-5.90757500	0.08210400	-7.90578600
	C	-7.19726300	0.08663500	-7.21564700
	C	-5.81571900	0.11498800	-9.28334500
	C	-4.63511800	0.10897800	-9.93503800
	C	-3.38289900	0.06680900	-9.18644500
	O	-2.26558400	0.05818500	-9.66979400
	O	-4.86967800	0.01412000	-5.87974900
	H	-7.29757300	-0.80503700	-6.59171800
	H	-7.28518900	0.96842100	-6.57539800
	H	-7.99107200	0.09959800	-7.96430500
	H	-6.76717800	0.14558800	-9.80352100
	N	1.08759500	-0.00560000	-3.99569000

C	1.54796200	0.00647400	-2.77144600
N	0.55485100	-0.01442900	-1.80371200
C	0.71224300	-0.01062300	-0.35939100
C	-0.63461900	-0.04331100	-2.48901100
N	-1.86815600	-0.06379200	-1.92641400
C	-2.82540400	-0.09591100	-2.82911900
C	-1.33956900	-0.05740500	-4.81521500
C	-0.28468900	-0.03803800	-3.84320600
H	2.59468300	0.02995400	-2.49508400
H	1.27663700	-0.88846600	-0.02835400
H	1.22970200	0.89545400	-0.02752800
H	-0.28432800	-0.03741400	0.08437000
H	-4.58328800	0.13472900	-11.01528300
O	-1.27895400	-0.04374500	-6.04790800
N	-4.13710800	-0.18019200	-2.43273800
H	-4.29991500	0.06005400	-1.46488500
H	-4.84736000	0.11706900	-3.08894400
N	-2.60395700	-0.09495600	-4.17927100
H	-3.41080200	-0.10752400	-4.81728200

GU-Cu

$E_{ZPE} = -1232.316328$ a.u.

H	-3.19218400	0.10184800	-7.15554600
N	-3.90142000	0.09507100	-7.92009000
C	-5.20571300	0.04833700	-7.55624000
N	-6.14935200	0.03401500	-8.55920100
C	-7.56405800	-0.01863800	-8.17397900
C	-5.75748000	0.06710200	-9.88702300
C	-4.46400700	0.11500200	-10.26067700
C	-3.40540900	0.13357900	-9.25595600
O	-2.21278000	0.17683800	-9.47633700
O	-5.61026000	0.01709400	-6.36192400
H	-7.76482100	-0.91995500	-7.59023800
H	-7.82656900	0.85446300	-7.57193800
H	-8.16536900	-0.02997600	-9.08398200
H	-6.57284700	0.05146300	-10.60134700
N	0.69869900	0.00845700	-4.28282600
C	1.41107300	-0.04420200	-3.18764100
N	0.65040600	-0.07691700	-2.02728700
C	1.11322000	-0.13213100	-0.65260900
C	-0.66050900	-0.03927600	-2.43994800
N	-1.74677400	-0.04646800	-1.64166100
C	-2.87663700	-0.01316400	-2.33811100
C	-1.85765900	0.05500900	-4.53377400
C	-0.61205400	0.01289400	-3.83685000
H	2.49306600	-0.06436200	-3.14399600
H	1.75780900	-1.00319100	-0.49522700
H	1.66647200	0.77542600	-0.38696800
H	0.23471400	-0.21534400	-0.01021900
H	-4.17591500	0.14037000	-11.30321700
O	-2.03904300	0.10089300	-5.77509500
N	-4.06248400	-0.07607300	-1.62839200
H	-3.95655500	0.15136900	-0.64830300
H	-4.86287500	0.35141300	-2.07571200
N	-2.98069200	0.03691400	-3.69310100
Cu	-4.42733800	0.02622400	-4.88626600

GU-Ag

$E_{ZPE} = -1181.951984$ a.u.

H	-3.30188400	0.10140500	-6.86970400
N	-3.93823000	0.10255500	-7.69046500
C	-5.27680800	0.03460400	-7.46503300
N	-6.10161200	0.02675800	-8.57283700
C	-7.54826600	-0.04953600	-8.34588000
C	-5.56941500	0.08905100	-9.84886900
C	-4.24423800	0.15971500	-10.07960400
C	-3.30228100	0.17238100	-8.96550400
O	-2.09365000	0.23497300	-9.05539900
O	-5.81179900	-0.02084800	-6.33011400
H	-7.80013600	-0.96459000	-7.80477500
H	-7.88694100	0.80765400	-7.75921300
H	-8.04706200	-0.04910500	-9.31602500
H	-6.30214600	0.07690600	-10.64797900
N	0.69197100	-0.00719100	-4.17170300
C	1.49955200	-0.05630700	-3.14460400
N	0.84589600	-0.08281200	-1.92051300
C	1.42921400	-0.14050300	-0.59280900
C	-0.49685900	-0.04723300	-2.21469500
N	-1.50780400	-0.04836300	-1.32313300
C	-2.69460700	-0.01571800	-1.92068600
C	-1.87632100	0.04057000	-4.19694300
C	-0.57357200	-0.00017700	-3.61006900
H	2.58121500	-0.07598100	-3.19776600
H	2.02039900	-1.05365200	-0.46443400
H	2.06972000	0.72888500	-0.40913900
H	0.61047200	-0.14076100	0.12902500
H	-3.84447700	0.20819600	-11.08366300
O	-2.15754800	0.07817400	-5.41884300
N	-3.81375700	-0.07258100	-1.10542200
H	-3.61009500	0.15314800	-0.14011400
H	-4.63775300	0.38604000	-1.47158900
N	-2.91817800	0.02778900	-3.25814100
Ag	-4.63962300	-0.01193400	-4.49688500

GU-Au

$E_{ZPE} = -1170.854559$ a.u.

H	-3.38800200	0.06522200	-7.08926600
N	-4.05802800	0.07220200	-7.88304500
C	-5.38917200	0.04903300	-7.61565900
N	-6.25190400	0.05531600	-8.68836700
C	-7.69326500	0.02856800	-8.41141900
C	-5.76336200	0.08441400	-9.98365200
C	-4.44600600	0.10830400	-10.26227800
C	-3.46398900	0.10441500	-9.18391600
O	-2.25892100	0.12418800	-9.31367200
O	-5.90004400	0.02251000	-6.46065500
H	-7.95514200	-0.87225200	-7.85183500
H	-7.98300400	0.90290100	-7.82418600
H	-8.22302300	0.03513200	-9.36479200
H	-6.52484200	0.08637900	-10.75518400
N	0.78777500	0.00421000	-4.21859700
C	1.50240400	-0.02413100	-3.12378200
N	0.74313200	-0.05192800	-1.96273000
C	1.20677300	-0.09110500	-0.58770600
C	-0.56817100	-0.04043700	-2.37519700
N	-1.65229400	-0.05411800	-1.57209600
C	-2.78618900	-0.04427600	-2.25824600
C	-1.76273000	0.01532400	-4.48394700

	C	-0.52165500	-0.00574800	-3.77094700
	H	2.58460300	-0.02701200	-3.08112200
	H	1.80603300	-0.98912700	-0.40326800
	H	1.80697400	0.79436500	-0.35234900
	H	0.32719000	-0.10953800	0.05828500
	H	-4.08147200	0.13070700	-11.28056200
	O	-1.93525500	0.04995900	-5.71651300
	N	-3.96585700	-0.11942800	-1.54797300
	H	-3.86830800	0.12019600	-0.57048800
	H	-4.78781500	0.25231000	-2.00585100
	N	-2.88413000	-0.00710500	-3.61773900
	Au	-4.56054200	0.00300600	-4.78921400
Hoogsten	AT			
	$E_{ZPE} = -999.632583$ a.u.			
	N	1.23287500	-4.87146400	0.01766800
	C	2.42497300	-4.17820400	0.02598100
	C	2.51137800	-2.82561800	0.03632300
	C	1.26505800	-2.06321700	0.03857000
	N	0.10539900	-2.82725600	0.03019700
	C	0.00626700	-4.20224600	0.01927000
	O	1.21337300	-0.82915800	0.04756700
	O	-1.06011700	-4.80617000	0.01133000
	C	1.18335300	-6.33272500	0.00552500
	N	-2.44307500	-1.55779600	0.02621900
	C	-2.92806600	-0.26243700	0.03118300
	C	-4.32489900	-0.27025800	0.02302200
	N	-4.68651200	-1.60645500	0.01292900
	C	-3.51358300	-2.32157000	0.01544200
	C	-2.30529000	1.00988000	0.04232300
	N	-3.10150500	2.10209900	0.04427600
	C	-4.43100200	1.93250700	0.03567800
	N	-5.13589800	0.79515900	0.02475800
	N	-0.97060500	1.18236500	0.05116900
	C	-6.04921400	-2.11517600	0.00134500
	H	-5.01524500	2.85109200	0.03783500
	H	-3.48579800	-3.40383300	0.00907200
	H	-6.24112000	-2.72960800	0.88643400
	H	-6.23390100	-2.70936200	-0.89901900
	H	-6.71852100	-1.25313000	0.00827600
	H	-0.30371600	0.41021400	0.04821600
	H	-0.62698700	2.13135600	0.05737500
	H	3.31322700	-4.80246000	0.02326300
	H	-0.80412000	-2.31678000	0.03086500
	H	2.20460000	-6.71764700	0.00801600
	H	0.65875800	-6.68696300	-0.88576400
	H	0.64908900	-6.70103600	0.88523500
	C	3.81080600	-2.07291200	0.04553300
	H	3.88444400	-1.42959200	0.93003900
	H	4.66624000	-2.75602500	0.04050700
	H	3.88706600	-1.41320100	-0.82651200
	AT-Cu			
	$E_{ZPE} = -1196.383341$ a.u.			
	N	3.21396700	-3.73267700	-0.21357700
	C	4.02881700	-2.62496300	-0.20872100
	C	3.55272200	-1.35658600	-0.16768900
	C	2.10194200	-1.18565500	-0.12786800
	N	1.32313300	-2.32156000	-0.13351500

C	1.81580600	-3.60129600	-0.17496600
O	1.57035000	-0.05533700	-0.09027000
Cu	-0.52263600	-2.03874100	-0.08607700
N	-2.33791100	-1.54654600	-0.03577500
C	-2.84450600	-0.24886700	0.00086400
C	-4.23901200	-0.30517500	0.03044300
N	-4.56810300	-1.65094400	0.01104400
C	-3.39685500	-2.34272600	-0.02811500
C	-2.26203100	1.04924200	0.01327600
N	-3.11284300	2.10225200	0.05216000
C	-4.43148000	1.88649900	0.07688000
N	-5.09275900	0.72159600	0.06910000
N	-0.94703700	1.30622800	-0.01058100
C	-5.92006500	-2.19119600	0.03251500
O	1.10247000	-4.60635500	-0.17976200
C	3.75156400	-5.08958000	-0.25798700
H	-5.04918900	2.78177500	0.10758500
H	-3.35565300	-3.42231700	-0.05032700
H	-5.86680200	-3.28055000	-0.01395600
H	-6.48372600	-1.81363900	-0.82415500
H	-6.42881000	-1.88676100	0.95071900
H	-0.18962200	0.61298100	-0.03956000
H	-0.68381800	2.28229800	0.00275000
H	5.09392400	-2.83576300	-0.24052700
H	4.84203500	-5.03541000	-0.28602600
H	3.38622400	-5.61438100	-1.14496400
H	3.43386000	-5.65377600	0.62318500
C	4.43297100	-0.13934700	-0.16247400
H	4.25910700	0.46763300	0.73385100
H	5.49269700	-0.41509200	-0.19444500
H	4.21622700	0.50620300	-1.02174600
AT-Ag			
$E_{ZPE} = -1146.016851$ a.u.			
N	3.47947900	-3.77151200	-0.21979000
C	4.20514800	-2.60394900	-0.21192400
C	3.63138800	-1.37646800	-0.17138800
C	2.17076300	-1.31959900	-0.13472800
N	1.48681200	-2.51250100	-0.14342800
C	2.07275100	-3.74952900	-0.18450300
O	1.55334600	-0.23324400	-0.09645000
Ag	-0.58797000	-2.29225400	-0.09141500
N	-2.59903800	-1.62012100	-0.03189700
C	-2.99640100	-0.28598300	0.00398900
C	-4.39232500	-0.22834100	0.03614400
N	-4.82985700	-1.54254800	0.01916700
C	-3.71712800	-2.32581000	-0.02128300
C	-2.31380600	0.96386800	0.01389900
N	-3.08071900	2.07992600	0.05288300
C	-4.41154900	1.97079100	0.08007100
N	-5.16274500	0.86194400	0.07489000
N	-0.98370500	1.13181300	-0.01197500
C	-6.22140600	-1.97043200	0.04364800
O	1.44260000	-4.80801100	-0.19201800
C	4.12050100	-5.08228100	-0.26506800
H	-4.95597000	2.91256100	0.11066300
H	-3.76629800	-3.40524700	-0.04222700
H	-6.25753100	-3.06068000	0.00113500
H	-6.75347800	-1.55108300	-0.81379900
H	-6.70259300	-1.62205000	0.96106700

H	-0.26477000	0.40191100	-0.04173100
H	-0.66059300	2.08982100	-0.00001800
H	5.28359100	-2.73086600	-0.24148300
H	5.20369000	-4.94428500	-0.29120100
H	3.79834000	-5.63293000	-1.15315600
H	3.84596100	-5.67096800	0.61462800
C	4.41417200	-0.09456800	-0.16237400
H	4.19316400	0.49555600	0.73504800
H	5.49231300	-0.28611200	-0.19389100
H	4.14882200	0.53465000	-1.02019600
AT-Au			
E_{ZPE}=-1134.930465 a.u.			
N	3.41415200	-3.76071100	-0.21983900
C	4.18519300	-2.62253900	-0.21093300
C	3.66115400	-1.37409900	-0.16874700
C	2.20531900	-1.25005300	-0.13167600
N	1.47505800	-2.42566800	-0.14178300
C	2.01155600	-3.69179700	-0.18493000
O	1.63573800	-0.14367100	-0.09280900
Au	-0.55849300	-2.16734700	-0.09091300
N	-2.55466900	-1.59557500	-0.03349700
C	-2.98031000	-0.27143900	0.00408900
C	-4.37638100	-0.25317100	0.03420300
N	-4.77970200	-1.57889100	0.01405700
C	-3.65037900	-2.33652100	-0.02608000
C	-2.32752800	0.99396600	0.01705300
N	-3.12266600	2.08938500	0.05654300
C	-4.45056200	1.94537200	0.08146900
N	-5.17337300	0.81758700	0.07355200
N	-1.00119900	1.19064000	-0.00634700
C	-6.16047600	-2.04170700	0.03750500
O	1.34390800	-4.72304800	-0.19408700
C	4.00463700	-5.09569700	-0.26648200
H	-5.01916800	2.87262100	0.11249200
H	-3.66356700	-3.41618200	-0.04938100
H	-6.16973200	-3.13165700	-0.02091200
H	-6.70499400	-1.62281800	-0.81216100
H	-6.64639800	-1.71853300	0.96162600
H	-0.27855000	0.46630100	-0.03654100
H	-0.69325900	2.15345800	0.00706600
H	5.25755100	-2.79213500	-0.24052900
H	5.09209700	-4.99805300	-0.28977300
H	3.66370100	-5.63129800	-1.15663800
H	3.70562900	-5.67474400	0.61147700
C	4.49409400	-0.12419700	-0.15906900
H	4.29542200	0.47362100	0.73820200
H	5.56348200	-0.35941600	-0.18943600
H	4.25442400	0.51443800	-1.01738000
AU			
E_{ZPE}=-960.355675 a.u.			
C	-4.32394300	-0.27042100	0.02224600
C	-2.92715800	-0.25840500	0.03134600
C	-2.30830700	1.01602400	0.04308300
N	-3.10816700	2.10565500	0.04485800
C	-4.43701400	1.93192300	0.03551600
N	-5.13831400	0.79233300	0.02374800

N	-4.68175700	-1.60763600	0.01153200
C	-3.50689400	-2.31935000	0.01491500
N	-2.43844300	-1.55256900	0.02644900
N	-0.97443200	1.19290800	0.05272500
H	-5.02416500	2.84865000	0.03737800
C	-6.04312000	-2.11993400	-0.00030400
H	-3.47660100	-3.40151800	0.00832700
H	-6.23317300	-2.73510900	0.88466500
H	-6.22612100	-2.71434800	-0.90081900
H	-6.71481100	-1.25971100	0.00710300
H	-0.30481100	0.42309300	0.05018500
H	-0.63373900	2.14297300	0.05945900
O	1.21561000	-0.80585100	0.05198700
C	1.27481800	-2.03726000	0.04207300
C	2.50407300	-2.81231600	0.03943700
N	0.11554400	-2.81068200	0.03231400
C	2.44007900	-4.16420300	0.02780700
C	0.02255900	-4.18487200	0.01991900
N	1.25347800	-4.85798400	0.01833000
H	3.33223000	-4.78200000	0.02532200
O	-1.03908900	-4.79503600	0.01091000
H	-0.79740700	-2.30552000	0.03284800
C	1.20172700	-6.31944100	0.00492100
H	2.22255200	-6.70559400	0.00796700
H	0.67730200	-6.67151800	-0.88714200
H	0.66608300	-6.68704700	0.88389400
H	3.44997800	-2.28794300	0.04679500
AU-Cu			
E_{ZPE} = -1157.105957 a.u.			
C	-4.23242100	-0.29990300	0.03003100
C	-2.83797600	-0.24213800	0.00107000
C	-2.25691200	1.05667700	0.01395500
N	-3.10900000	2.10872300	0.05247500
C	-4.42733800	1.89151300	0.07652000
N	-5.08736500	0.72584100	0.06839300
N	-4.56017800	-1.64602600	0.01033100
C	-3.38831000	-2.33661000	-0.02842900
N	-2.33007300	-1.53939800	-0.03554900
N	-0.94231300	1.31484700	-0.00919000
H	-5.04608300	2.78608200	0.10699200
C	-5.91164000	-2.18753400	0.03128800
H	-3.34616800	-3.41615600	-0.05077900
H	-5.85741000	-3.27681000	-0.01595300
H	-6.47552400	-1.80983800	-0.82516700
H	-6.42077300	-1.88418800	0.94964000
H	-0.18467800	0.62182500	-0.03710800
H	-0.67957700	2.29103900	0.00456700
O	1.56881500	-0.05294400	-0.08472600
C	2.10575500	-1.17856700	-0.12366700
C	3.54588600	-1.36676300	-0.16267400
N	1.33000100	-2.32117500	-0.13222200
C	4.04170700	-2.62566200	-0.20605900
C	1.82701900	-3.59803600	-0.17559100
N	3.23110900	-3.73137400	-0.21375200
H	5.10751000	-2.83007000	-0.23729600
O	1.12067100	-4.60665800	-0.18338800
Cu	-0.51499900	-2.03240900	-0.08536500
C	3.76627600	-5.08935700	-0.26049100
H	4.85690500	-5.03671600	-0.28722700
H	3.40062100	-5.61112500	-1.14896100

H	3.44623200	-5.65431700	0.61916200
H	4.19253500	-0.49922100	-0.15728000
AU-Ag			
$E_{ZPE}=-1106.739498$ a.u.			
C	-4.39398900	-0.22488400	0.03606100
C	-2.99788800	-0.27843500	0.00431400
C	-2.31901000	0.97359900	0.01507900
N	-3.08941700	2.08728600	0.05429000
C	-4.41988400	1.97414900	0.08090700
N	-5.16775700	0.86301600	0.07507300
N	-4.82771600	-1.54032000	0.01828200
C	-3.71277300	-2.32037400	-0.02226000
N	-2.59669700	-1.61138000	-0.03217500
N	-0.98953200	1.14538000	-0.01029000
H	-4.96708600	2.91426100	0.11191300
C	-6.21802200	-1.97226700	0.04212200
H	-3.75886800	-3.39991800	-0.04382300
H	-6.25099900	-3.06257500	-0.00143000
H	-6.75114600	-1.55361200	-0.81500700
H	-6.70040000	-1.62611500	0.95976200
H	-0.26887100	0.41718600	-0.03987200
H	-0.66890300	2.10420700	0.00229300
O	1.54144800	-0.22219700	-0.09249200
C	2.16740800	-1.30139400	-0.13205700
C	3.61893700	-1.37169100	-0.16789800
N	1.49058200	-2.50287600	-0.14271100
C	4.21523300	-2.58641200	-0.21005400
C	2.08442200	-3.73484200	-0.18490600
N	3.49738800	-3.75393800	-0.21953000
H	5.29430700	-2.70337700	-0.23858400
O	1.46484500	-4.79833000	-0.19403200
Ag	-0.58452500	-2.28047200	-0.09129200
C	4.14018500	-5.06398700	-0.26558300
H	5.22323200	-4.92420400	-0.29055800
H	3.81917900	-5.61355300	-1.15457900
H	3.86520700	-5.65354900	0.61320500
H	4.19341600	-0.45483300	-0.16061700
AU-Au			
$E_{ZPE}=-1095.653310$ a.u.			
C	-4.37717300	-0.25108400	0.03385400
C	-2.98107400	-0.26582300	0.00468700
C	-2.33144300	1.00134400	0.01836600
N	-3.12956600	2.09465100	0.05755000
C	-4.45704200	1.94727300	0.08159000
N	-5.17699500	0.81760100	0.07290600
N	-4.77714700	-1.57778200	0.01311900
C	-3.64598900	-2.33263000	-0.02641500
N	-2.55210500	-1.58884100	-0.03291600
N	-1.00577000	1.20121700	-0.00407300
H	-5.02801500	2.87304400	0.11232000
C	-6.15682600	-2.04392200	0.03554700
H	-3.65655700	-3.41229400	-0.04994900
H	-6.16343600	-3.13386900	-0.02331900
H	-6.70182200	-1.62597200	-0.81427000
H	-6.64408700	-1.72227000	0.95949000
H	-0.28092700	0.47887400	-0.03407100
H	-0.70019000	2.16480800	0.00968700

O	1.62723200	-0.12754600	-0.08888700
C	2.20365700	-1.22799500	-0.12845000
C	3.64971500	-1.36762900	-0.16544500
N	1.47894900	-2.41203700	-0.14004000
C	4.19550000	-2.60468800	-0.20908600
C	2.02218500	-3.67394600	-0.18441600
N	3.43074700	-3.74225900	-0.21924700
H	5.26866300	-2.76574400	-0.23842400
O	1.36320900	-4.70964100	-0.19508800
Au	-0.55531400	-2.15774700	-0.08958300
C	4.02127400	-5.07741700	-0.26739100
H	5.10879400	-4.97935900	-0.28869200
H	3.68154500	-5.61100300	-1.15906000
H	3.72045100	-5.65747600	0.60907200
H	4.26066300	-0.47484800	-0.15780600

DT

$E_{ZPE} = -983.570270$ a.u.

C	-4.31699900	-0.25260100	0.01728700
C	-2.91471600	-0.20490100	0.08586700
C	-2.27870100	1.05796400	0.10857100
C	-3.17477100	2.14928900	0.04963400
C	-4.55883800	1.95151900	-0.01775800
N	-5.18186500	0.76192000	-0.03564300
N	-4.63437100	-1.60458200	0.00999100
C	-3.44667300	-2.28315800	0.07114400
N	-2.39826900	-1.49006200	0.11785200
N	-0.93137500	1.19538800	0.20522200
H	-2.78489800	3.16378900	0.06099700
H	-5.20912800	2.82380300	-0.06064100
C	-5.97587100	-2.15575000	-0.04756600
H	-3.38877500	-3.36448500	0.07587900
H	-5.90990100	-3.24554900	-0.07899800
H	-6.49301900	-1.79549800	-0.94146200
H	-6.55140400	-1.85107700	0.83171300
H	-0.29623400	0.40166100	0.12572100
H	-0.52443500	2.11125400	0.09377500
O	1.26436800	-0.81248400	0.01007800
C	1.29570000	-2.04704300	0.01221900
C	2.52880100	-2.82989800	-0.03630600
N	0.12404100	-2.79114000	0.06239900
C	2.42079300	-4.18072600	-0.03156100
C	3.83915300	-2.09813800	-0.08827700
C	0.00338900	-4.16385900	0.06039800
N	1.21811100	-4.85376900	0.01516900
H	3.29797300	-4.81961600	-0.06558700
O	-1.07111400	-4.75302600	0.09486800
H	-0.77706700	-2.26187100	0.09657400
C	1.14362700	-6.31379400	0.01196600
H	2.15794300	-6.71624100	-0.00947400
H	0.59030100	-6.66434000	-0.86345200
H	0.62593400	-6.66798700	0.90711900
H	4.68298700	-2.79499000	-0.11915900
H	3.89079000	-1.44985000	-0.97069900
H	3.95813700	-1.44599000	0.78469200

DT-Cu

$E_{ZPE} = -1180.320988$ a.u.

C	-4.24672000	-0.28503000	0.03053100
C	-2.84610300	-0.19428200	0.00213200
C	-2.24624500	1.09233400	0.01522600
C	-3.19169200	2.14675400	0.05686900
C	-4.56642200	1.90552800	0.08166600
N	-5.14736800	0.69376400	0.06986700
N	-4.53770100	-1.64482900	0.00867800
C	-3.35365500	-2.30547900	-0.03013800
N	-2.31351500	-1.48358800	-0.03579400
N	-0.91507500	1.31639000	-0.00923400
H	-2.83547300	3.17318800	0.06996000
H	-5.24700300	2.75404300	0.11341500
C	-5.87516700	-2.21604600	0.02807300
H	-3.28480800	-3.38376200	-0.05373700
H	-5.79729400	-3.30405300	-0.01922700
H	-6.44729400	-1.85020500	-0.82829800
H	-6.39287700	-1.92359700	0.94539100
H	-0.18104700	0.60084300	-0.03750200
H	-0.58504700	2.27012100	0.00405500
O	1.62543500	-0.02497700	-0.08798300
C	2.14005300	-1.16274400	-0.12679300
C	3.58853500	-1.35594900	-0.16554400
N	1.34387600	-2.28671600	-0.13273600
C	4.04567900	-2.63112300	-0.20675100
C	4.48687900	-0.15203500	-0.15932600
C	1.81731400	-3.57324100	-0.17423100
N	3.21391400	-3.72606700	-0.21234900
H	5.10752900	-2.85809900	-0.23805000
O	1.09012900	-4.56845100	-0.17986900
Cu	-0.49861300	-1.97567900	-0.08527600
C	3.73038500	-5.09093300	-0.25674800
H	4.82166500	-5.05380200	-0.28332700
H	3.35812500	-5.60982200	-1.14437500
H	3.40275600	-5.65067700	0.62365400
H	5.54251200	-0.44332600	-0.19079700
H	4.28024000	0.49703900	-1.01849900
H	4.32153700	0.45722200	0.73713300

DT-Ag

$E_{ZPE} = -1129.954449$ a.u.

C	-4.40619400	-0.20714200	0.03619600
C	-3.00130300	-0.22877000	0.00535500
C	-2.30437200	1.00953400	0.01480500
C	-3.16671800	2.13336300	0.05542500
C	-4.55547000	2.00117800	0.08277500
N	-5.22834300	0.83813700	0.07461900
N	-4.80490200	-1.53896600	0.01790100
C	-3.67584300	-2.29066000	-0.02139000
N	-2.57537300	-1.55611000	-0.03047000
N	-0.96043400	1.14514200	-0.01166700
H	-2.73145800	3.12883100	0.06567500
H	-5.16778700	2.90026500	0.11358900
C	-6.18408100	-2.00026300	0.04091200
H	-3.69576000	-3.37111900	-0.04280400
H	-6.19477900	-3.09118200	-0.00267700
H	-6.72619300	-1.59206600	-0.81585000
H	-6.67509100	-1.66357300	0.95772600
H	-0.26836300	0.39249000	-0.03954500
H	-0.57004100	2.07577700	-0.00051800
O	1.60475100	-0.20091100	-0.09081300

C	2.20713500	-1.29527700	-0.13035000
C	3.66722300	-1.37295800	-0.16762600
N	1.50641300	-2.47871400	-0.14051700
C	4.22399500	-2.60799800	-0.21055600
C	4.46792100	-0.10218300	-0.15737400
C	2.07511200	-3.72331700	-0.18391600
N	3.48191300	-3.76512900	-0.21976000
H	5.30062400	-2.74995500	-0.24033600
O	1.43137500	-4.77365500	-0.19295100
Ag	-0.56625000	-2.22771400	-0.08828300
C	4.10424200	-5.08458500	-0.26707000
H	5.18933700	-4.96189500	-0.29259000
H	3.77467300	-5.62920500	-1.15619800
H	3.82111600	-5.67109300	0.61139600
H	5.54337500	-0.30914200	-0.18654300
H	4.21353400	0.53054900	-1.01603900
H	4.25346100	0.49103300	0.73953100

DT-Au

$E_{ZPE} = -1118.868450$ a.u.

C	-4.38934600	-0.23265600	0.03397300
C	-2.98513300	-0.21343200	0.00641400
C	-2.31921300	1.04171900	0.01906200
C	-3.21174700	2.14143600	0.05904900
C	-4.59668500	1.97115300	0.08297500
N	-5.23836200	0.79061700	0.07189600
N	-4.75264100	-1.57508100	0.01282900
C	-3.60745200	-2.30006300	-0.02496900
N	-2.53057500	-1.53041100	-0.03028800
N	-0.97876700	1.20892800	-0.00380800
H	-2.80406900	3.14838800	0.07160300
H	-5.23304500	2.85331400	0.11339100
C	-6.11989000	-2.07188200	0.03371100
H	-3.59085900	-3.37974700	-0.04827500
H	-6.10271700	-3.16188500	-0.02489300
H	-6.67379800	-1.66554400	-0.81618800
H	-6.61629500	-1.76021800	0.95643700
H	-0.28197500	0.46198000	-0.03278500
H	-0.60623300	2.14669600	0.00746400
O	1.69026400	-0.11248600	-0.08742300
C	2.24328400	-1.22674600	-0.12761800
C	3.69763500	-1.37256800	-0.16593600
N	1.49563200	-2.39168100	-0.13811200
C	4.20355300	-2.62820500	-0.21013100
C	4.54875600	-0.13499000	-0.15541600
C	2.01371700	-3.66478600	-0.18357500
N	3.41564600	-3.75468600	-0.21966000
H	5.27332600	-2.81352600	-0.24078000
O	1.33224300	-4.68714400	-0.19384400
Au	-0.53598700	-2.10490700	-0.08588500
C	3.98602300	-5.09806700	-0.26874200
H	5.07494500	-5.01679900	-0.28933500
H	3.63919300	-5.62645400	-1.16101400
H	3.67630600	-5.67496900	0.60691400
H	5.61474400	-0.38552800	-0.18552000
H	4.31870600	0.50759700	-1.01347000
H	4.35826200	0.46534900	0.74200900

DU

E _{ZPE} =-944.292314 a.u.			
C	0.00085300	-0.00096900	-0.00065400
C	1.40562900	-0.00140500	-0.00152600
C	2.08477500	1.23921200	-0.00148400
C	1.22439000	2.36049600	-0.00855500
C	-0.16716000	2.21022600	-0.00864400
N	-0.83054000	1.04248300	-0.00367300
N	-0.36281100	-1.34124300	-0.00068500
C	0.80231300	-2.06026400	-0.00289000
N	1.87855100	-1.30379000	-0.00353700
N	3.43881300	1.33098200	0.02946100
H	1.64862300	3.36114200	-0.00934000
H	-0.78862100	3.10428900	-0.01327100
C	-1.72380800	-1.84561800	0.00576700
H	0.82238100	-3.14290500	-0.00735500
H	-1.69747500	-2.93678900	-0.03533100
H	-2.27210200	-1.46100500	-0.85893300
H	-2.24374300	-1.52787400	0.91453600
H	4.04315300	0.51787700	-0.08608000
H	3.87053100	2.23386900	-0.09428600
O	5.55440400	-0.74073400	-0.28508200
C	5.54698700	-1.97339400	-0.29321400
N	4.35213400	-2.68313400	-0.19078600
C	6.59278700	-4.15916300	-0.40669600
C	4.18632900	-4.05013300	-0.19698700
N	5.37453200	-4.78825500	-0.30642000
H	7.44675000	-4.82375000	-0.48809900
O	3.09775300	-4.60559700	-0.11438500
H	3.47028800	-2.12639500	-0.10900900
C	5.24289700	-6.24455900	-0.31550400
H	6.23865300	-6.68577000	-0.38779600
H	4.63547300	-6.56550700	-1.16586800
H	4.75458300	-6.58517000	0.60097500
C	6.72844700	-2.81286700	-0.40543000
H	7.69735500	-2.33864300	-0.48573700
DU-Cu			
E _{ZPE} =-1141.043525 a.u.			
C	0.00027800	0.00082900	0.00042300
C	1.40409800	0.00239200	-0.00064100
C	2.08459500	1.24829400	0.00024800
C	1.20749400	2.36102100	0.00221600
C	-0.17994300	2.20787600	0.00305100
N	-0.83670700	1.03525900	0.00230100
N	-0.37603200	-1.33815000	-0.00120300
C	0.76418800	-2.07289200	-0.00281700
N	1.85427400	-1.31833600	-0.00279800
N	3.42762000	1.38707800	-0.00086700
H	1.62798000	3.36285200	0.00309700
H	-0.80566500	3.09816900	0.00450300
C	-1.74734800	-1.82284900	0.00190800
H	0.76523900	-3.15359300	-0.00436800
H	-1.73834200	-2.91438900	-0.02096100
H	-2.27796200	-1.44043100	-0.87373600
H	-2.26314700	-1.47770200	0.90181000
H	4.11472500	0.62595200	-0.00095100
H	3.81768800	2.31791200	0.00069300
O	5.87376100	-0.11843900	-0.00263000
C	6.31860600	-1.28373600	-0.00573500

N	5.45225700	-2.35977300	-0.00728200
C	8.13169100	-2.88548100	-0.00972400
C	5.84399200	-3.67277800	-0.01003400
N	7.23351300	-3.92134000	-0.01150400
H	9.17755000	-3.17710300	-0.01080000
O	5.05872600	-4.62156300	-0.01158700
Cu	3.63434800	-1.92606200	-0.00491200
C	7.65611500	-5.31899800	-0.01449900
H	8.74777900	-5.35678000	-0.01580600
H	7.26885200	-5.83104500	-0.89950500
H	7.27087100	-5.83429900	0.86951200
C	7.73953600	-1.58988800	-0.00677200
H	8.45450100	-0.77761900	-0.00527400
DU-Ag			
$E_{ZPE}=-1090.677082$ a.u.			
C	0.00023500	0.00116900	0.00068500
C	1.40565100	0.00119300	-0.00064000
C	2.08298800	1.25051000	0.00028500
C	1.20246700	2.36101300	0.00266900
C	-0.18427100	2.20724000	0.00377500
N	-0.83872800	1.03368800	0.00290600
N	-0.37752600	-1.33684300	-0.00117600
C	0.76341100	-2.07130200	-0.00306700
N	1.85252500	-1.31987700	-0.00301300
N	3.42468100	1.40726500	-0.00124900
H	1.62191800	3.36329900	0.00359500
H	-0.81097800	3.09689500	0.00548000
C	-1.74971400	-1.81905300	0.00183800
H	0.76024900	-3.15215300	-0.00477100
H	-1.74298500	-2.91064900	-0.02038000
H	-2.27955900	-1.43601300	-0.87401000
H	-2.26524500	-1.47224400	0.90125100
H	4.12947700	0.66579800	-0.00186800
H	3.79993200	2.34420900	0.00026600
O	6.00378300	0.09768700	-0.00318400
C	6.62799300	-0.98277700	-0.00672400
N	5.94892200	-2.18326200	-0.00863100
C	8.67519600	-2.27285800	-0.01220200
C	6.54123700	-3.41654400	-0.01251000
N	7.95468300	-3.43915000	-0.01429600
H	9.75433700	-2.39255700	-0.01373300
O	5.92040200	-4.47953800	-0.01398000
Ag	3.87210500	-1.96135600	-0.00588900
C	8.59512200	-4.75098900	-0.01823100
H	9.67887200	-4.61394800	-0.02034800
H	8.29403600	-5.31838600	-0.90303300
H	8.29799100	-5.32196700	0.86563500
C	8.08034300	-1.05701200	-0.00845200
H	8.65619100	-0.14082700	-0.00676900
DU-Au			
$E_{ZPE}=-1079.554510$ a.u.			
C	0.02864300	-0.02193100	0.00098600
C	1.43276000	0.01478100	-0.00058700
C	2.08258400	1.27853600	0.00064600
C	1.17543000	2.36712600	0.00345500
C	-0.20738400	2.17943800	0.00474100
N	-0.83386000	0.99066700	0.00365400

	N	-0.31749300	-1.36905100	-0.00123400
	C	0.83696900	-2.07998900	-0.00358900
	N	1.90422500	-1.29692700	-0.00339700
	N	3.42071500	1.46308900	-0.00081700
	H	1.57013700	3.37931700	0.00461500
	H	-0.85526700	3.05370000	0.00680100
	C	-1.67871100	-1.88256100	0.00157000
	H	0.86698400	-3.15962900	-0.00568100
	H	-1.64680500	-2.97359900	-0.01933800
	H	-2.21609500	-1.51244600	-0.87516000
	H	-2.20183700	-1.54622400	0.90047600
	H	4.12858000	0.72579400	-0.00235600
	H	3.78053600	2.40592000	0.00056400
	O	6.09706900	0.18103300	-0.00490500
	C	6.67093900	-0.92106600	-0.00784500
	N	5.94295600	-2.10351500	-0.00941600
	C	8.66076100	-2.30417900	-0.01251800
	C	6.48366200	-3.36677600	-0.01258600
	N	7.89293200	-3.43966000	-0.01414400
	H	9.73388200	-2.46851400	-0.01386500
	O	5.82329600	-4.40188500	-0.01373300
	C	8.48007600	-4.77691100	-0.01732900
	H	9.56817300	-4.68232300	-0.01894500
	H	8.15687900	-5.33163500	-0.90224000
	H	8.15980900	-5.33469500	0.86674300
	C	8.11752400	-1.06535700	-0.00943300
	H	8.73102300	-0.17422200	-0.00815400
	Au	3.90665000	-1.84564600	-0.00674800