

Electronic Supplementary Information (ESI) to

On Au_nAt clusters as potential astatine carriers

by Sławomir Ostrowski, Agnieszka Majkowska-Pilip, Aleksander Bilewicz*, and Jan Cz. Dobrowolski*

The ESI contains Cartesian XYZ coordinates (in ångströms) of all studied systems calculated using the rLC-ωPBE and uLC-ωPBE functionals (for the closed-shell Au₁₂, Au₁₄ and Au₁₃X systems and for the open-shell Au₁₃ and Au₁₂X systems in doublet and quartet states, respectively) combined with the Stuttgart/Cologne Group (SDD) basis sets with quasi-relativistic pseudopotential as implemented in Gaussian 09 suite of programs. Additionally, the D3 Grimme dispersion correction was applied.

Table 1SI. Total energies (hartrees) of the open-shell clusters considered in the doublet and quartet spin states. The Au₁₂F-4 system in the quartet state (*italic*) was not fully optimized and exhibited one imaginary frequency

System	Au ₁₃	Au ₁₂ F	Au ₁₂ Cl	Au ₁₂ Br	Au ₁₂ I	Au ₁₂ At
Doublets						
1	-1765.181138	-1729.210549	-2089.492925	-1642.854844	-1640.904791	-1640.537986
2	-1765.181041	-1729.200718	-2089.484937	-1642.849794	-1640.902175	-1640.536150
3	-1765.153717	-1729.205957	-2089.486221	-1642.856825	-1640.904165	-1640.535338
4	-1765.129280	-1729.161360	-2089.441376	-1642.802743	-1640.850717	-1640.482439
Quartets						
1	-1765.142858	-1729.102422	-2089.383442	-1642.744318	-1640.794308	-1640.426959
2	-1765.155336	-1729.164903	-2089.449762	-1642.811766	-1640.854088	-1640.486052
3	-1765.138992	-1729.171417	-2089.452541	-1642.814035	-1640.863222	-1640.495527
4	-1765.092734	<i>-1729.112613</i>	-2089.364433	-1642.716449	-1640.765310	-1640.397783

Note on calculations and on performing optimizations

Interaction energy of the AuX molecules was calculated using the counterpoise method. The clusters with even number of atoms, Au₁₂, Au₁₄, and Au₁₃X were considered as close-shell systems, while those of odd number of atoms, Au₁₃ and Au₁₂X, as open-shell species in the doublet state and calculated within the unrestricted DFT approach. We checked that the spin contamination from higher spin states was small as the deviations in the expectation value of the spin-squared expectation value $\langle S^2 \rangle$ from the exact values 0.75 for a doublet,¹⁶ were between 0.7521 to 0.7574 for Au₁₃ clusters and from 0.7511 to 0.7520 for Au₁₂X systems. For quartets the exact expectation value is 3.75 and the obtained values for Au₁₃ and Au₁₂X systems were between 3.7516 and 3.7778. So, no results were discarded because of large spin contamination.

Optimizations with symmetry constraints yielded not-fully optimized clusters (displaying some imaginary frequencies) whereas when constraints were released the optimized clusters in local minima were slightly distorted from their initial symmetries, except for the planar structures which remained planar. In this moment it is difficult to judge whether the decreased symmetry is a physical effect or an artefact introduced by theory level. Remark that high symmetry reported for the clusters in early studies may be due to the fact that optimization control by frequency calculations for the Au clusters of similar size was very difficult more than a decade ago.^{20,21} Also, use of specific basis set with quasi-relativistic pseudopotential, necessary to model Au and At properties and interactions, could eventually introduce a distortion. However, the aim of this study has not required to carefully consider symmetry condition but to qualitatively evaluate difference between halogen-Au cluster interaction.

The optimization of the Au₁₃X clusters, where X=F, Cl, Br, I, or At replaced one of the shell Au atoms, always yielded a distorted system, too (Fig. 2). Therefore, except the Au₁₃X clusters derived from a direct optimization of the Au₁₃-3 structure with the halogen atom, several other Au₁₃X as well as Au₁₂X systems were considered (Fig. 2).

Au₁₂ (Singlet state)

Au ₁₂ -1				Au ₁₂ -3			
Au	3.63465200	-1.94130900	0.08624400	Au	-1.35235100	3.93331000	0.00000000
Au	0.24692400	1.02811800	-1.39743100	Au	-2.74936300	1.58665600	0.00000000
Au	1.30513900	-1.48733300	-1.36580200	Au	-1.35413600	-0.78037700	0.00000000
Au	1.34268000	-1.15374000	1.48527300	Au	0.00000000	1.56279100	0.00000000
Au	2.84320400	0.62606100	-0.13436400	Au	-4.08517400	-0.79528100	0.00000000
Au	1.56653200	2.92763400	0.12872900	Au	1.35338200	-0.78151800	0.00000000
Au	-3.63470800	-1.94061800	-0.08640100	Au	0.00065600	-3.17255600	0.00000000
Au	-1.30575600	-1.48753400	1.36572900	Au	-2.72959600	-3.13823800	0.00000000
Au	-0.24664100	1.02722400	1.39735500	Au	1.35432000	3.93449400	0.00000000
Au	-1.56500200	2.92727500	-0.12776800	Au	2.74831900	1.58646000	0.00000000
Au	-1.34289400	-1.15280500	-1.48530700	Au	4.08313700	-0.79536900	0.00000000
Au	-2.84413000	0.62702700	0.13374300	Au	2.73080500	-3.14037300	0.00000000
Au ₁₂ -2							
Au	0.75206800	1.40177000	-1.25249600				
Au	2.69476500	2.38134900	0.40930700				
Au	1.51262300	0.00140500	1.39760700				
Au	0.75154700	-1.40472400	-1.25197900				
Au	2.69322800	-2.38179200	0.41164200				
Au	3.26507200	-0.00104900	-0.74816300				
Au	-2.69492300	-2.38131600	-0.40926900				
Au	-0.75211100	-1.40179500	1.25244800				
Au	-0.75150600	1.40469600	1.25204000				
Au	-1.51262200	-0.00149400	-1.39760300				
Au	-3.26508600	0.00113600	0.74815900				
Au	-2.69305500	2.38181400	-0.41169200				

Au₁₄ (Singlet state)

Au ₁₄ -1				Au ₁₄ -2			
Au	1.34116900	0.88209400	-1.50406200	Au	0.72405900	-4.08802500	0.00000000
Au	2.74436600	2.72229400	0.09148500	Au	2.63331200	-2.12485300	0.00000000
Au	1.35840000	0.57738200	1.34058300	Au	1.95823000	0.51475400	0.00000000
Au	0.29181600	-1.55521800	-1.49669400	Au	0.00000000	-1.43958300	0.00000000
Au	2.21090200	-2.16785500	0.38871400	Au	4.57887800	-0.20876300	0.00000000
Au	3.64444500	0.04501400	-0.13008100	Au	-0.70889100	1.25382200	0.00000000
Au	-2.21649200	-2.16429900	-0.38879600	Au	1.24607600	3.14495500	0.00000000
Au	-0.29650400	-1.55318500	1.49578400	Au	3.88339300	2.43268600	0.00000000
Au	-1.33845500	0.88721000	1.50465700	Au	-1.94420900	-3.30892600	0.00000000
Au	-1.35675200	0.58006900	-1.34017600	Au	-2.59925400	-0.68326700	0.00000000
Au	-3.64298200	0.05265000	0.13137500	Au	-3.32206800	1.92409300	0.00000000
Au	-2.73877200	2.72838200	-0.09219100	Au	-1.38228600	3.91590500	0.00000000
Au	-0.00424400	-3.89724900	0.00073700	Au	-1.14579600	-5.93953500	0.00000000
Au	0.00310300	2.86271200	-0.00133300	Au	-3.92144400	4.60673700	0.00000000

Au₁₃ (Doublet state)

Au ₁₃ -1				Au ₁₃ -3			
Au	0.29264600	-2.55292000	0.00000000	Au	2.56133800	1.18011200	0.04456100
Au	0.48338200	0.00086400	1.40601200	Au	-0.88865400	1.49331000	-2.25707000
Au	2.69151900	-1.35553800	0.00000000	Au	-2.30016100	1.62365200	0.15594400
Au	0.48338200	0.00086400	-1.40601200	Au	0.91778600	1.45577400	2.26777100
Au	-1.92048300	-1.32286100	-1.42343300	Au	-1.64928200	0.00562100	2.31737000
Au	-2.13540600	-3.71051100	0.00000000	Au	0.25490300	2.80353000	-0.09114500
Au	2.69152300	1.35149700	0.00000000	Au	0.88872800	-1.49072300	2.25643900
Au	0.29550800	2.55385300	0.00000000	Au	-2.56082400	-1.17982700	-0.04474200
Au	-1.92048300	1.32420000	-1.42263300	Au	-0.91882200	-1.45522800	-2.26867200
Au	-1.92048300	-1.32286100	1.42343300	Au	2.29930700	-1.62381200	-0.15414300
Au	-1.92048300	1.32420000	1.42263300	Au	-0.25408400	-2.80410800	0.09121100
Au	-2.13314400	3.71207200	0.00000000	Au	1.64992200	-0.00898700	-2.31776900
Au	5.01252200	-0.00285700	0.00000000	Au	-0.00015700	0.00068500	0.00024700
Au ₁₃ -2				Au ₁₃ -4			
Au	0.80221200	-1.68854500	1.22391800	Au	1.35121200	3.49891200	0.00000000
Au	2.82000200	-2.64966600	-0.35341200	Au	2.71779300	1.18923000	0.00000000
Au	1.53156800	-0.39539300	-1.42481000	Au	1.39547200	-1.25941300	0.00000000
Au	0.70664600	1.05614000	1.36242300	Au	0.00000000	1.08083600	0.00000000
Au	2.48934000	2.16899100	-0.43486800	Au	4.08512700	-1.19761800	0.00000000
Au	3.28679200	-0.18154400	0.70462000	Au	-1.33331700	-1.26826700	0.00000000
Au	-2.48877600	2.16832500	0.43680200	Au	0.09622500	-3.65778200	0.00000000
Au	-0.70665600	1.05669500	-1.36312500	Au	2.81020700	-3.62161200	0.00000000
Au	-0.80267800	-1.68762000	-1.22311200	Au	-1.44946400	3.40238000	0.00000000
Au	-1.53169000	-0.39608700	1.42504600	Au	-2.76184900	1.05352700	0.00000000
Au	-3.28577600	-0.18034000	-0.70645900	Au	-4.10759400	-1.33980900	0.00000000
Au	-2.82101800	-2.64885100	0.35293700	Au	-2.63220800	-3.61317100	0.00000000
Au	0.00003300	3.37789600	0.00004100	Au	-0.17160200	5.73278900	0.00000000

Au₁₃ (Quartet state)

Au ₁₃ -1				Au ₁₃ -3			
Au	3.12920000	-0.32012300	0.20163100	Au	-2.15062500	-2.12394200	-0.00012700
Au	-0.00465700	-0.82562200	-2.52940000	Au	-2.14988600	2.12379200	-0.00038500
Au	1.37992000	-2.26062100	-0.59895200	Au	0.00035500	1.96719200	-1.87479100
Au	0.01289500	-0.76870500	1.44606100	Au	-0.00004100	-1.96670500	-1.87372400
Au	1.31536400	1.59935400	1.49296700	Au	2.13857500	-0.00064600	-1.77130200
Au	3.47511800	2.38549800	-0.00125900	Au	-2.13877400	-0.00016500	-1.77012000
Au	-1.35336300	-2.27604700	-0.58456600	Au	2.15038400	-2.12327100	0.00020800
Au	-3.12969800	-0.35360400	0.19708500	Au	2.15053800	2.12246400	-0.00008400
Au	-1.33515900	1.57363000	1.49733900	Au	0.00006300	1.96734200	1.87500900
Au	1.32953900	1.19588400	-1.30896200	Au	-0.00033500	-1.96678100	1.87385000
Au	-1.34692300	1.18847000	-1.30589600	Au	2.13871400	-0.00040400	1.77128200
Au	-3.50405600	2.34886000	0.01006100	Au	-2.13926400	0.00007200	1.76993400
Au	0.03181900	-3.48697500	1.48388900	Au	0.00029600	0.00105000	0.00025000
Au ₁₃ -2				Au ₁₃ -4 not-fully-optimized system			
Au	-1.19990100	-1.55819300	-0.62803500	Au	3.48544000	1.42365300	0.00007700
Au	-3.49422100	-1.22773600	0.85655300	Au	1.15506500	2.74247300	-0.15099600
Au	-1.03461100	-1.13524700	2.22013000	Au	-1.22702300	1.35511100	0.29424300
Au	-0.61793000	1.03434600	-1.74153900	Au	1.11956800	-0.00036200	-0.00289700
Au	-1.91328500	1.12982500	0.75745100	Au	-1.36499900	3.94200200	-0.39327100
Au	-3.25107700	0.20508900	-1.52493600	Au	-1.22633400	-1.35521900	-0.30870500
Au	1.91264900	1.14927100	-0.72885700	Au	-3.62730200	-0.00118000	-0.00275700
Au	0.61722300	0.99165400	1.76635300	Au	-3.66457500	2.59760700	0.61583000
Au	1.20121500	-1.57340400	0.58960300	Au	3.48363900	-1.42694700	-0.00081500
Au	1.03569800	-1.07846200	-2.24839400	Au	1.15180400	-2.74251200	0.15789100
Au	3.25034100	0.16714400	1.53014900	Au	-1.37054100	-3.93202800	0.41648300
Au	3.49488500	-1.20464300	-0.88628900	Au	-3.66426900	-2.59954600	-0.62201400
Au	-0.00098800	3.10035500	0.03781200	Au	5.74952800	-0.00305200	-0.00306900

Au₁₂-At (Doublet state)

Au ₁₂ -At-1				Au ₁₂ -At-3			
Au	0.27606100	-0.00097700	2.64150100	Au	-0.23450500	2.58928300	0.00000000
Au	2.81039900	-0.00520200	1.50379000	Au	-0.47655300	-0.00018600	1.40043100
Au	1.46504100	-0.00361500	-1.93084600	Au	-2.62282200	1.40952200	0.00000000
Au	-1.84437800	1.32926200	1.13113700	Au	-0.47655300	-0.00018600	-1.40043100
Au	-0.84747700	3.61392500	-0.07841400	Au	1.92619700	1.32250900	-1.42990500
Au	0.87093300	1.56479000	0.42240100	Au	2.21459300	3.70030500	0.00000000
Au	-3.40276400	0.00664700	-0.78461200	Au	-2.62299600	-1.40868700	0.00000000
Au	-0.97083800	1.31985500	-1.62837400	Au	-0.23511200	-2.58926500	0.00000000
Au	0.86305500	-1.56557800	0.42211500	Au	1.92619700	-1.32289700	-1.42985700
Au	-1.85288900	-1.32713500	1.13105500	Au	1.92619700	1.32250900	1.42990500
Au	-0.97737000	-1.31541400	-1.62857200	Au	1.92619700	-1.32289700	1.42985700
Au	-0.85937400	-3.61142000	-0.08058100	Au	2.21384800	-3.70069800	0.00000000
At	4.15410100	-0.00477500	-1.04149900	At	-5.07894300	0.00064200	0.00000000
Au ₁₂ -At-2				Au ₁₂ -At-4			
Au	-1.10177500	-1.35207800	-1.86515400	Au	1.48582400	3.40485000	0.00000000
Au	-2.22731200	-2.47987200	0.44977800	Au	2.74606300	1.07260400	0.00000000
Au	-1.22740200	0.00046100	1.34902000	Au	1.36333800	-1.29355200	0.00000000
Au	-1.10118600	1.35044100	-1.86544400	Au	0.00000000	1.06480000	0.00000000
Au	-2.22738000	2.48023000	0.44803200	Au	4.10241700	-1.31814000	0.00000000
Au	-3.25172500	-0.00017000	-0.39665700	Au	-1.36250100	-1.29409200	0.00000000
Au	2.98934600	1.93843800	-0.77362600	Au	0.00054000	-3.69584100	0.00000000
Au	0.49184600	2.20514600	0.26020000	Au	2.71085000	-3.64923200	0.00000000
Au	0.49185400	-2.20448600	0.26121500	Au	-1.48722100	3.40376000	0.00000000
Au	1.22990100	-0.00118400	-1.67586300	Au	-2.74624200	1.07088300	0.00000000
Au	2.18746800	0.00070900	0.98408800	Au	-4.10225700	-1.31961300	0.00000000
Au	2.99008700	-1.93894100	-0.77128200	Au	-2.70951500	-3.64997900	0.00000000
At	0.70289300	0.00121300	3.34188000	At	-0.00120300	5.76565600	0.00000000

Au₁₂-At (Quartet state)

Au ₁₂ -At-1				Au ₁₂ -At-3			
Au	-0.15166300	-0.00016600	2.73252500	Au	2.78531600	-2.25575800	-0.61027100
Au	2.41720500	-0.00002800	1.84664800	Au	-0.75230700	-0.69543000	1.31096900
Au	2.03539800	0.00079800	-1.65595900	Au	0.90829000	-2.87415000	1.33609900
Au	-2.24060300	1.34939200	1.20303400	Au	1.96138000	0.29952800	-1.36106900
Au	-1.20119000	3.32587800	-0.39084600	Au	0.11650100	-1.96938900	-1.26058600
Au	0.53678400	1.45678100	0.46835700	Au	-2.47799400	-1.40143300	-0.92700400
Au	-2.62630700	0.00025100	-1.03007000	Au	2.78648000	2.25384000	0.61245900
Au	-0.29264300	1.36416900	-2.14714900	Au	0.91228000	2.87370900	-1.33595500
Au	0.53707600	-1.45703400	0.46839800	Au	-0.74956000	0.69585400	-1.30966400
Au	-2.24042200	-1.35043300	1.20224900	Au	-2.47811100	1.40347900	0.92515900
Au	-0.29223600	-1.36363200	-2.14710800	Au	1.95875700	-0.30063900	1.36042300
Au	-1.20023900	-3.32621000	-0.39192000	Au	0.11678000	1.96956800	1.26008500
At	4.38574500	0.00021800	-0.14699400	At	-4.72867200	0.00076400	-0.00059900
Au ₁₂ -At-2				Au ₁₂ -At-4			
Au	-2.79147600	0.57554700	-1.35182600	Au	3.40807000	-1.41089400	0.02141900
Au	-1.60949700	-1.51000600	-2.77785600	Au	1.03729900	-2.81067700	0.01172900
Au	1.03269600	-2.16194400	-0.00358500	Au	-1.30399500	-1.31938100	0.10363100
Au	-2.78348200	0.57537900	1.36162300	Au	1.06746400	-0.00001900	0.09761200
Au	-1.59713500	-1.51081200	2.78146100	Au	-1.32695200	-4.06138400	-0.23374800
Au	-1.57006500	-1.56943700	0.00152200	Au	-1.30403000	1.31932500	0.10330300
Au	1.50903300	2.46890200	1.37535800	Au	-3.74342500	0.00001500	0.61142200
Au	0.18185200	0.09873100	1.51209200	Au	-3.62372700	-2.66392200	-0.24671900
Au	0.17490800	0.09891600	-1.51588900	Au	3.40802400	1.41092700	0.02142500
Au	-0.99651200	2.21255800	-0.00020200	Au	1.03723200	2.81064200	0.01197400
Au	2.84099200	0.51215600	-0.00072800	Au	-1.32701100	4.06139600	-0.23365000
Au	1.50819300	2.46567300	-1.37972400	Au	-3.62373900	2.66389900	-0.24696900
At	3.81104700	-2.09644000	-0.00208900	At	5.85045200	0.00006900	-0.01991500

Au₁₂-X-1 (F,Cl,Br,I) (Doublet state)

Au ₁₂ -F-1				Au ₁₂ -Br-1			
Au	-0.00003000	1.31467000	-2.19640500	Au	-0.89571000	0.00263900	-2.45171600
Au	-0.00019700	3.32463900	-0.28529500	Au	-3.18951000	0.00936100	-0.89903000
Au	-0.00024500	1.25581900	2.29145100	Au	-1.38105000	0.00426100	2.16976100
Au	1.32750900	-1.14580500	-1.43100200	Au	1.44267500	1.32439100	-1.31743400
Au	3.65365600	-0.65855600	-0.00365700	Au	0.70202700	3.62630700	0.03420800
Au	1.75529800	1.26583500	-0.04721400	Au	-1.12852300	1.63769400	-0.21536900
Au	0.00038400	-3.15579700	0.00540500	Au	3.26221700	-0.00949000	0.34747600
Au	1.31861000	-1.02705500	1.45770800	Au	0.98788500	1.31475600	1.54021400
Au	-1.75536900	1.26555500	-0.04712500	Au	-1.13844700	-1.63125900	-0.21512700
Au	-1.32670400	-1.14586200	-1.43075200	Au	1.43428800	-1.33148000	-1.31707900
Au	-1.31927100	-1.02733600	1.45802000	Au	0.97983700	-1.32157600	1.54063100
Au	-3.65360100	-0.65904400	-0.00462500	Au	0.68088600	-3.63030500	0.03280900
F	-0.00034700	3.44913100	2.04952500	Br	-3.96483800	0.01061400	1.69433300
Au ₁₂ -Cl-1				Au ₁₂ -I-1			
Au	-0.00176600	1.19327400	-2.30506600	Au	0.63271200	0.00014200	2.55518800
Au	-0.00405700	3.32200800	-0.53321100	Au	3.05013700	0.00117000	1.19297400
Au	-0.00135000	1.24856100	2.31537700	Au	1.44934500	0.00069000	-2.06510000
Au	1.33071800	-1.23342500	-1.40751800	Au	-1.62045600	1.32708100	1.23437200
Au	3.63575100	-0.62685300	0.00448300	Au	-0.74537000	3.61851500	-0.05537700
Au	1.65737900	1.22566400	-0.07583100	Au	1.02796900	1.59322600	0.31643100
Au	0.00396100	-3.20548800	0.08147800	Au	-3.31570900	-0.00120200	-0.55894600
Au	1.31967800	-1.04309600	1.47599500	Au	-0.95969700	1.31689600	-1.58633600
Au	-1.66105400	1.22226700	-0.07538300	Au	1.02944000	-1.59261400	0.31623400
Au	-1.32616800	-1.23588400	-1.40676900	Au	-1.61910600	-1.32773100	1.23417400
Au	-1.31812500	-1.04593100	1.47654900	Au	-0.95859000	-1.31797300	-1.58644200
Au	-3.63415100	-0.63597700	0.00322900	Au	-0.74267700	-3.61906300	-0.05492500
Cl	-0.00379400	3.78678800	2.07569400	I	4.13185000	0.00128800	-1.40448300

Au₁₂-X-1 (F,Cl,Br,I) (Quartet state)

Au ₁₂ -F-1				Au ₁₂ -Br-1			
Au	0.00000200	1.05165400	-2.13817700	Au	0.17337300	-0.00002500	2.73210900
Au	0.00004000	2.93773100	-0.25407100	Au	2.69016200	0.00006600	1.71396500
Au	0.00002200	1.57902800	2.30015200	Au	2.24238600	0.00047400	-1.67096400
Au	1.29577400	-1.27913600	-1.24565200	Au	-1.99031000	1.35019700	1.25849900
Au	3.64080500	-0.96710500	0.06973000	Au	-1.00759400	3.31824700	-0.39813100
Au	2.25468000	1.36095000	-0.53008900	Au	0.74644900	1.46876900	0.45216700
Au	-0.00005800	-3.04396800	0.44865700	Au	-2.40277900	0.00013000	-0.97036500
Au	1.29971300	-0.59007100	1.42118600	Au	-0.08043500	1.36566500	-2.15951600
Au	-2.25460800	1.36100600	-0.53007500	Au	0.74662800	-1.46884100	0.45229500
Au	-1.29580300	-1.27909800	-1.24566000	Au	-1.99021400	-1.35097800	1.25793300
Au	-1.29974600	-0.59003000	1.42121000	Au	-0.08024100	-1.36527600	-2.15936300
Au	-3.64083000	-0.96701900	0.06970900	Au	-1.00685200	-3.31852700	-0.39881600
F	0.00007300	3.73985500	1.87036800	Br	4.42270700	0.00022500	-0.24786500
Au ₁₂ -Cl-1				Au ₁₂ -I-1			
Au	0.00003400	0.86307300	-2.21064900	Au	-0.04067800	-0.00047200	2.73245800
Au	0.00012400	2.88570300	-0.46942100	Au	-2.58660400	0.00054500	1.78517900
Au	0.00006200	1.69630700	2.18812300	Au	-2.16546400	-0.00217900	-1.67368000
Au	1.29656100	-1.40910100	-1.17477000	Au	2.08628300	-1.34935700	1.23000200
Au	3.64113500	-0.99725900	0.11760900	Au	1.07264800	-3.32337900	-0.38996100
Au	2.25352000	1.28630100	-0.63716900	Au	-0.67268700	-1.46002600	0.45902200
Au	-0.00013200	-3.04976400	0.64355500	Au	2.49068800	0.00131000	-0.99935800
Au	1.29642200	-0.52778600	1.42899700	Au	0.16384300	-1.36468900	-2.15145600
Au	-2.25340300	1.28647500	-0.63712800	Au	-0.67309300	1.46073900	0.45965500
Au	-1.29670400	-1.40903300	-1.17478100	Au	2.08589400	1.35049400	1.23050600
Au	-1.29645300	-0.52769600	1.42898500	Au	0.16165900	1.36370600	-2.15190100
Au	-3.64121600	-0.99699900	0.11760500	Au	1.07205500	3.32291200	-0.39205600
Cl	0.00022500	4.18132800	1.76143000	I	-4.46356200	0.00058600	-0.20630900

Au₁₂-X-2 (F,Cl,Br,I) (Doublet state)

Au ₁₂ -F-2				Au ₁₂ -Br-2			
Au	0.98693800	-1.34938100	1.70172500	Au	-0.99746100	-1.35064000	-1.76153400
Au	2.17963100	-2.48578400	-0.59443100	Au	-2.20551100	-2.48392900	0.51932700
Au	1.20961200	0.00002000	-1.56803700	Au	-1.23012500	0.00005000	1.47828400
Au	0.98676000	1.34933100	1.70161300	Au	-0.99727900	1.35041900	-1.76143200
Au	2.17943800	2.48592300	-0.59438400	Au	-2.20552700	2.48398600	0.51911800
Au	3.13960600	0.00009400	0.25793600	Au	-3.17313400	-0.00001800	-0.34585100
Au	-3.11007500	1.86463600	0.23783100	Au	3.07028900	1.90281500	-0.41110000
Au	-0.53161000	2.28463800	-0.45192800	Au	0.51154500	2.24541600	0.41119300
Au	-0.53141400	-2.28452100	-0.45196800	Au	0.51154300	-2.24524300	0.41121800
Au	-1.33077700	-0.00017100	1.30211400	Au	1.32184400	-0.00024200	-1.42728300
Au	-2.01651800	0.00006600	-1.43572600	Au	2.08687500	0.00017300	1.28995900
Au	-3.11000400	-1.86486000	0.23752600	Au	3.07047200	-1.90285200	-0.41061500
F	-0.45281900	0.00007700	-3.00437600	Br	0.53374400	0.00014200	3.36024400
Au ₁₂ -Cl-2				Au ₁₂ -I-2			
Au	-0.97393200	-1.35056900	-1.71772800	Au	-1.02942500	-1.35017000	-1.80362500
Au	-2.20029900	-2.48082300	0.56438800	Au	-2.21324000	-2.48310500	0.48103500
Au	-1.22956000	0.00003200	1.53524000	Au	-1.23970200	0.00005600	1.42746300
Au	-0.97376500	1.35040500	-1.71760500	Au	-1.02926700	1.34994100	-1.80356200
Au	-2.20026400	2.48089900	0.56424500	Au	-2.21329100	2.48314200	0.48080500
Au	-3.14921300	0.00001200	-0.31693500	Au	-3.20621200	-0.00003900	-0.37511000
Au	3.08406300	1.90244800	-0.30715400	Au	3.05037100	1.91177000	-0.53795300
Au	0.51454400	2.24715000	0.47131500	Au	0.50756300	2.23164200	0.35104300
Au	0.51449800	-2.24699500	0.47133100	Au	0.50759500	-2.23149200	0.35107600
Au	1.34094900	-0.00021100	-1.34209700	Au	1.29558700	-0.00022100	-1.51509400
Au	2.08022700	0.00014200	1.38029700	Au	2.12612300	0.00016500	1.18768900
Au	3.08417900	-1.90252000	-0.30672000	Au	3.05057700	-1.91177700	-0.53750700
Cl	0.50454700	0.00014600	3.35249800	I	0.58627000	0.00013100	3.41897300

Au₁₂-X-2 (F,Cl,Br,I) (Quartet state)

Au ₁₂ -F-2				Au ₁₂ -Br-2			
Au	-0.89347400	2.22024600	-0.88722500	Au	-0.61261100	-2.10459500	1.37937000
Au	-2.12889300	0.26821900	-2.44161800	Au	-2.21502400	-0.28945600	2.69976300
Au	-1.32775800	-1.95935400	-0.71177700	Au	-1.39460300	2.52981900	0.01525100
Au	-1.01577800	2.15035900	1.84280700	Au	-0.61254800	-2.09838200	-1.35790700
Au	-2.26390100	-1.84714000	1.89553600	Au	-2.22877700	-0.31536300	-2.69756200
Au	-2.43914200	0.32504300	0.31770300	Au	-2.25696600	-0.02827400	0.00084700
Au	2.84487300	-0.36312300	1.55209100	Au	2.65958700	-0.24423600	-1.36834700
Au	0.09098200	-0.48471100	1.34766400	Au	0.08580200	0.60816600	-1.49797700
Au	0.56519500	0.05888300	-1.75350500	Au	0.10451300	0.59481500	1.47965100
Au	1.49480400	1.80874400	0.48060300	Au	1.69629000	-2.47635300	0.00791600
Au	1.80088900	-2.05117700	-0.44481300	Au	1.87955800	2.12498600	-0.01238900
Au	3.24704900	0.26781000	-1.05662200	Au	2.68530000	-0.23316800	1.35061500
F	0.22079200	-3.45668700	-1.23629400	Br	0.47282600	4.36089600	0.00173300
Au ₁₂ -Cl-2				Au ₁₂ -I-2			
Au	0.52031300	-2.03938500	-1.31211300	Au	-2.50310200	-1.06289100	1.34113000
Au	2.22633300	-0.39135400	-2.69694600	Au	-1.80629500	1.22457000	2.77863200
Au	1.47843600	2.55153600	0.07450300	Au	0.70511200	2.38750600	0.01387200
Au	0.52402100	-2.06607400	1.42504800	Au	-2.49256600	-1.04627900	-1.36743800
Au	2.17823700	-0.25075200	2.69664200	Au	-1.78577800	1.25942200	-2.77108400
Au	2.25065100	-0.03360300	-0.00210500	Au	-1.73761900	1.30507900	0.00434200
Au	-2.75178300	0.00632900	1.31878100	Au	2.10932100	-1.98113600	-1.37950400
Au	-0.11903400	0.64542800	1.44618400	Au	0.28688700	0.02418600	-1.52141200
Au	-0.03018400	0.70168900	-1.53405100	Au	0.27675500	0.00899100	1.52713900
Au	-1.80710300	-2.29705500	0.04734900	Au	-0.40176500	-2.29407400	-0.01216900
Au	-1.77404600	2.28914200	-0.06325600	Au	2.98521100	0.21379800	0.00556300
Au	-2.63428400	-0.06088400	-1.40046600	Au	2.10378400	-1.99077600	1.37003100
Cl	-0.28606300	4.39139200	0.00199500	I	3.36876100	2.90899500	0.01624300

Au₁₂-X-3 (F,Cl,Br,I) (Doublet state)

Au ₁₂ -F-3				Au ₁₂ -Br-3			
Au	-3.58303100	-1.97252500	0.09678600	Au	-3.69556400	-1.95746900	0.00061100
Au	0.02911900	0.96737300	1.40265400	Au	0.00230800	0.74194200	1.40512100
Au	-1.20516800	-1.51023000	1.34145900	Au	-1.31470200	-1.65992800	1.42687800
Au	-1.47848800	-1.37474300	-1.56555600	Au	-1.32392700	-1.65464800	-1.43325900
Au	-2.59124600	0.63909200	0.11325300	Au	-2.60189200	0.49775700	0.01408600
Au	-1.48535200	2.99119900	0.06622400	Au	-1.41774200	2.87342000	-0.00963700
Au	3.58248700	-1.97460100	-0.09183800	Au	3.70673300	-1.93663100	-0.00255700
Au	1.20458800	-1.51694600	-1.33863300	Au	1.32422500	-1.65121300	-1.42927900
Au	-0.03003500	0.96032200	-1.39937300	Au	-0.00470500	0.74174600	-1.40017700
Au	1.48647900	2.99053900	-0.07135700	Au	1.39950300	2.88060800	0.00518200
Au	1.47852700	-1.36647400	1.56630900	Au	1.33356700	-1.64800400	1.43116500
Au	2.59204200	0.63863600	-0.11978200	Au	2.59883500	0.51141900	-0.00763600
F	0.00069100	4.63780800	-0.00129700	Br	-0.01498400	5.10340500	-0.00112500
Au ₁₂ -Cl-3				Au ₁₂ -I-3			
Au	-3.57567700	-2.02989500	0.09481300	Au	2.03823500	-3.70476400	-0.00440000
Au	0.02991100	0.92778500	1.39839800	Au	-0.63836400	-0.00053400	1.40089900
Au	-1.19897300	-1.56066900	1.33917400	Au	1.75928300	-1.32748700	1.43037400
Au	-1.47894100	-1.41372500	-1.57091200	Au	1.75349900	-1.32516900	-1.42921300
Au	-2.58083700	0.58237100	0.11934700	Au	-0.40901000	-2.59089100	0.00472500
Au	-1.50736800	2.95608100	0.07522700	Au	-2.78922800	-1.40348400	-0.00126100
Au	3.57748700	-2.02789300	-0.09334400	Au	2.05243100	3.69744100	0.00158900
Au	1.19966400	-1.56293100	-1.33842000	Au	1.75911300	1.32169600	-1.43348900
Au	-0.03094100	0.92642900	-1.39783700	Au	-0.64278300	0.00184700	-1.40076100
Au	1.50701400	2.95716900	-0.07593800	Au	-2.78370800	1.41371700	0.00536800
Au	1.47995100	-1.41232400	1.57087300	Au	1.76288100	1.31922400	1.42756300
Au	2.57888300	0.58314100	-0.12140400	Au	-0.39838700	2.59167600	0.00010500
Cl	-0.00081100	4.99308700	0.00011300	I	-5.16326300	0.01002600	-0.00223500

Au₁₂-X-3 (F,Cl,Br,I) (Quartet state)

Au ₁₂ -F-3				Au ₁₂ -Br-3			
Au	2.36823300	-2.26686000	-0.75839800	Au	-2.49067800	2.28697100	-0.69574500
Au	-0.76702900	1.04286600	-1.33009500	Au	0.95498500	0.72696800	1.31385400
Au	-0.26947600	-1.63674600	-1.35052400	Au	-0.71523100	2.89354200	1.33040700
Au	2.90943400	-0.54984900	1.32789600	Au	-1.75391300	-0.31502000	-1.35849100
Au	1.95066900	0.39653000	-1.23939400	Au	0.18288900	1.96048500	-1.24983200
Au	1.16667400	2.92835600	-0.87061000	Au	2.75405400	1.29810500	-0.90643300
Au	-2.25789200	-2.37230700	0.75709400	Au	-2.49487800	-2.28528600	0.69570700
Au	0.34858400	-1.62901200	1.36069300	Au	-0.71427400	-2.89435000	-1.32358600
Au	0.71272100	1.07109200	1.32696300	Au	0.94910000	-0.72397200	-1.31324400
Au	-1.29905000	2.87441000	0.87597600	Au	2.75122400	-1.30306900	0.90418800
Au	-2.87971600	-0.68711600	-1.33430900	Au	-1.74779300	0.31428300	1.35070300
Au	-1.97209200	0.30884400	1.23381400	Au	0.17823900	-1.95586900	1.25401000
F	-0.09709900	4.56263200	0.00783100	Br	4.84445200	-0.00629000	-0.00347300
Au ₁₂ -Cl-3				Au ₁₂ -I-3			
Au	-2.43698200	2.24497200	0.71606500	Au	-2.60969600	2.27081600	-0.64912200
Au	1.05845100	-0.70545600	1.31394800	Au	0.88464400	0.70963100	1.30975900
Au	-1.65027200	-0.34628800	1.35382100	Au	-0.77986000	2.88432800	1.33405000
Au	-0.70096300	2.87885600	-1.33248700	Au	-1.82781900	-0.30820800	-1.35795000
Au	0.24342000	1.96806800	1.24418800	Au	0.06136100	1.96358000	-1.25457100
Au	2.82312500	1.35082900	0.89442000	Au	2.64702400	1.35587900	-0.92536500
Au	-2.34229400	-2.34529100	-0.70173900	Au	-2.61004900	-2.26967700	0.65100800
Au	-1.67970000	0.27845200	-1.35656800	Au	-0.78243000	-2.88410100	-1.33333100
Au	1.01293300	0.74704900	-1.31018600	Au	0.88154300	-0.70937500	-1.30732400
Au	2.87148000	-1.22845300	-0.90996400	Au	2.64733000	-1.35729600	0.92279400
Au	-0.56595600	-2.90582800	1.33441800	Au	-1.82468600	0.30865700	1.35588700
Au	0.32021900	-1.95723000	-1.24557800	Au	0.06147600	-1.96356600	1.25532500
Cl	4.86333700	0.09442400	-0.00156600	I	4.84607100	-0.00099800	-0.00172600

Au₁₂-X-4 (F,Cl,Br,I) (Doublet state)

Au ₁₂ -F-4				Au ₁₂ -Br-4			
Au	1.46754900	3.83999400	0.00000000	Au	1.48038000	3.69366100	0.00000000
Au	2.75656500	1.54581300	0.00000000	Au	2.74891600	1.37774900	0.00000000
Au	1.37048000	-0.82676500	0.00000000	Au	1.36577700	-0.99104400	0.00000000
Au	0.00000000	1.51542100	0.00000000	Au	0.00000000	1.36124200	0.00000000
Au	4.10826000	-0.84196500	0.00000000	Au	4.10486400	-1.01168500	0.00000000
Au	-1.37045900	-0.82676900	0.00000000	Au	-1.36575300	-0.99102700	0.00000000
Au	0.00007900	-3.22069900	0.00000000	Au	0.00007800	-3.39003500	0.00000000
Au	2.71564800	-3.17660000	0.00000000	Au	2.71212500	-3.34372700	0.00000000
Au	-1.46764800	3.83985800	0.00000000	Au	-1.48044800	3.69355400	0.00000000
Au	-2.75663000	1.54566700	0.00000000	Au	-2.74897300	1.37763600	0.00000000
Au	-4.10833000	-0.84210800	0.00000000	Au	-4.10493600	-1.01178700	0.00000000
Au	-2.71549700	-3.17659200	0.00000000	Au	-2.71197300	-3.34368100	0.00000000
F	-0.00015800	5.48385700	0.00000000	Br	-0.00012700	5.82149900	0.00000000
Au ₁₂ -Cl-4				Au ₁₂ -I-4			
Au	1.48243600	3.79895200	0.00000000	Au	1.48483900	3.58894100	0.00000000
Au	2.74984900	1.48705800	0.00000000	Au	2.74629000	1.26296500	0.00000000
Au	1.36677100	-0.88017000	0.00000000	Au	1.36400400	-1.10551400	0.00000000
Au	0.00000000	1.47244900	0.00000000	Au	0.00000000	1.25082500	0.00000000
Au	4.10675300	-0.89942800	0.00000000	Au	4.10249300	-1.12743000	0.00000000
Au	-1.36676300	-0.88014900	0.00000000	Au	-1.36388500	-1.10553800	0.00000000
Au	0.00005400	-3.27748100	0.00000000	Au	0.00019100	-3.50624300	0.00000000
Au	2.71294900	-3.23186000	0.00000000	Au	2.71123900	-3.45974400	0.00000000
Au	-1.48248000	3.79887700	0.00000000	Au	-1.48507200	3.58870000	0.00000000
Au	-2.74989500	1.48698500	0.00000000	Au	-2.74638700	1.26264500	0.00000000
Au	-4.10681800	-0.89949100	0.00000000	Au	-4.10257700	-1.12773500	0.00000000
Au	-2.71284100	-3.23181300	0.00000000	Au	-2.71088900	-3.45972500	0.00000000
Cl	-0.00007900	5.83704300	0.00000000	I	-0.00036400	5.86962900	0.00000000

Au₁₂-X-4 (F,Cl,Br,I) (Quartet state)

Au ₁₂ -F-4 not-fully-optimized system				Au ₁₂ -Br-4			
Au	3.89132600	-1.36488600	0.00243500	Au	-3.70505900	1.40819700	0.01881500
Au	1.59272900	-2.73206100	0.00090900	Au	-1.34656200	2.80824600	0.00530400
Au	-0.82671600	-1.38811000	-0.00053900	Au	0.99889700	1.32037300	0.11300800
Au	1.53306300	0.03947600	0.00030600	Au	-1.37004400	-0.00008300	0.09499500
Au	-0.65903800	-4.18365400	-0.00182700	Au	1.01649600	4.05550900	-0.24820200
Au	-0.89816100	1.34341800	0.00020800	Au	0.99904700	-1.32030400	0.11278600
Au	-3.28166800	-0.08543100	0.00222700	Au	3.43114900	0.00013100	0.65394800
Au	-3.11128800	-2.80764300	-0.00153800	Au	3.31742000	2.65260400	-0.25988000
Au	3.81354900	1.56455600	-0.00178400	Au	-3.70500700	-1.40839400	0.01871100
Au	1.44886700	2.80899200	0.00276700	Au	-1.34641200	-2.80829500	0.00500300
Au	-0.87719500	4.14409800	-0.00245400	Au	1.01667100	-4.05542000	-0.24821900
Au	-3.25282700	2.64485100	-0.00062700	Au	3.31769400	-2.65251200	-0.25935600
F	5.50682300	0.14391500	-0.00072900	Br	-5.92340000	-0.00011600	-0.01560600
Au ₁₂ -Cl-4				Au ₁₂ -I-4			
Au	-3.83279600	-1.42376700	-0.00081700	Au	-3.59588700	1.40970800	0.01805200
Au	-1.54269400	-2.78438800	0.00086500	Au	-1.23086600	2.80828800	0.01023600
Au	0.87304700	-1.35059600	-0.00011400	Au	1.11484700	1.31994200	0.10611000
Au	-1.47961500	-0.00002500	0.00026900	Au	-1.25571800	0.00000000	0.09440600
Au	0.93161200	-4.03068100	0.00051600	Au	1.13113900	4.06164400	-0.23067100
Au	0.87287500	1.35063400	-0.00024800	Au	1.11486400	-1.31993400	0.10614600
Au	3.33690300	0.00014800	0.00000300	Au	3.55310700	0.00001200	0.61080200
Au	3.28138300	-2.73120100	-0.00037400	Au	3.43136900	2.66614200	-0.24848800
Au	-3.83291300	1.42336500	-0.00056500	Au	-3.59587600	-1.40974200	0.01803000
Au	-1.54298200	2.78436500	0.00159300	Au	-1.23083000	-2.80829000	0.01019800
Au	0.93126600	4.03074400	0.00042700	Au	1.13116800	-4.06163400	-0.23067800
Au	3.28110600	2.73145600	-0.00105000	Au	3.43140500	-2.66612000	-0.24844300
Cl	-5.93518900	-0.00024800	-0.00234000	I	-5.96036000	-0.00002300	-0.02340300

Au₁₃-At (Singlet state)

Au ₁₃ -At-1				Au ₁₃ -At-3			
Au	-2.38653800	1.64305000	0.07893300	Au	-1.07049900	-1.44838000	1.45272300
Au	0.22679800	0.00135600	1.53554300	Au	-2.75205800	-2.72290300	-0.28050100
Au	-2.39405400	-1.63950800	0.07714500	Au	-0.56166900	-1.25334400	-1.32365700
Au	-0.24937200	-1.33453200	-1.73583400	Au	1.31566600	-0.52237800	2.11948000
Au	-0.24473800	1.33578500	-1.73638500	Au	2.07779800	-1.69993400	-0.36536400
Au	-1.46350600	3.74609400	-1.25046600	Au	0.16496600	-3.55454300	-0.04618700
Au	0.17334200	-2.63689900	0.79214800	Au	2.07630700	1.70021600	0.36474100
Au	2.53542100	-1.49016600	1.07411400	Au	1.31636800	0.52157200	-2.12110000
Au	2.03564100	-0.00327000	-1.29498000	Au	-1.06857000	1.44901400	-1.45193300
Au	0.18282000	2.63960700	0.78954100	Au	-0.56267900	1.25349300	1.32483400
Au	2.54040300	1.48420600	1.07340000	Au	0.16350800	3.55550500	0.04830600
Au	4.52634600	-0.00682500	-0.08622300	Au	-2.75336200	2.72132700	0.27958300
Au	-1.47150700	-3.74318300	-1.25071700	Au	-2.98738400	-0.00062800	-0.00173300
At	-3.72792400	0.00398000	1.79727800	At	4.31396600	0.00091300	0.00075100
Au ₁₃ -At-2				Au ₁₃ -At-4			
Au	1.65997200	0.65149200	1.37407500	Au	-0.25511000	-0.77266300	-2.62727600
Au	0.93139400	0.83499200	-1.47660100	Au	1.99070800	-1.72480200	0.55044100
Au	-0.91186800	1.22387800	1.54152800	Au	-0.26447900	-1.88988700	1.98153700
Au	-0.60939100	3.06514000	-0.50725300	Au	-2.56752800	-1.87067400	-1.71799000
Au	2.02020600	3.00376900	-0.21948900	Au	-2.58149100	-0.55684400	2.46272200
Au	-2.93793500	-0.52261800	0.74182200	Au	-0.23701300	-2.68155800	-0.58038700
Au	-1.78768600	0.61459400	-1.49613100	Au	-2.57050000	2.42376300	-0.75611200
Au	-0.28673600	-1.58045100	-1.54635100	Au	-0.25333700	0.83853300	2.60605100
Au	-0.21095000	-1.37861400	1.27897400	Au	1.98681900	1.32921000	1.22788200
Au	-2.16910200	-2.98430500	0.07376200	Au	-0.24164700	1.84234900	-2.03022500
Au	0.56897400	-3.77517100	-0.08374000	Au	-0.25583400	2.66682500	0.64382500
Au	-3.15706300	2.34035200	0.25290600	Au	1.99248900	0.39483600	-1.76233200
Au	2.25526200	-1.64232600	-0.33383000	Au	-1.29087700	0.00012800	-0.00393400
At	4.30775300	0.13873200	0.37206900	At	4.22678000	0.00072700	0.00539000
Au ₁₃ -At-5							
Au	0.76969900	4.02635000	0.00000000				
Au	2.62780600	2.04344700	0.00000000				
Au	1.96033400	-0.61621500	0.00000000				
Au	0.00000000	1.39117900	0.00000000				
Au	4.53937700	0.09782400	0.00000000				
Au	-0.70209500	-1.29466500	0.00000000				
Au	1.25898800	-3.22119200	0.00000000				
Au	3.90316500	-2.57493300	0.00000000				
Au	-1.95066600	3.30937300	0.00000000				
Au	-2.58773200	0.69431400	0.00000000				
Au	-3.31798400	-1.90520300	0.00000000				
Au	-1.35616200	-3.94202400	0.00000000				
Au	-3.92316600	-4.54359600	0.00000000				
At	-1.13533600	6.07402200	0.00000000				

Au₁₃-X-1 (F,Cl,Br,I) (Singlet state)

Au ₁₃ -F-1				Au ₁₃ -Br-1			
Au	2.59160000	1.73120700	-0.62595100	Au	2.54130400	1.61762300	-0.45116900
Au	-0.32750000	-0.00929300	-1.67126500	Au	-0.28024700	-0.00002900	-1.61994700
Au	2.71413100	-1.55106100	-0.62225900	Au	2.54596600	-1.61413600	-0.45118300
Au	0.80874900	-1.30584300	1.45352800	Au	0.60015700	-1.33372700	1.57273200
Au	0.71165500	1.36419300	1.45630700	Au	0.59655300	1.33625100	1.57335500
Au	1.77301700	3.82652500	0.72173000	Au	1.76576200	3.74148600	0.92154900
Au	0.05869800	-2.60815100	-0.97713500	Au	-0.09483600	-2.62580600	-0.88962100
Au	-2.38644000	-1.60790100	-0.74638300	Au	-2.49109300	-1.50404600	-0.87370200
Au	-1.55800200	-0.05510100	1.48940600	Au	-1.71976600	-0.00178600	1.41431700
Au	-0.13093900	2.61060200	-0.97088100	Au	-0.10079900	2.62624900	-0.88939500
Au	-2.49740200	1.43514500	-0.74724900	Au	-2.49444700	1.49894500	-0.87362400
Au	-4.20398100	-0.15083000	0.69799500	Au	-4.32994500	-0.00467900	0.49680000
Au	2.03289200	-3.69382800	0.72516300	Au	1.77261800	-3.73790800	0.92248900
F	3.62980400	0.12583100	-1.60638300	Br	3.81180500	0.00352800	-1.92444400
Au ₁₃ -Cl-1				Au ₁₃ -I-1			
Au	2.60914900	1.65704300	-0.58511000	Au	2.48112100	1.63263200	-0.30699900
Au	-0.30197800	-0.00029400	-1.64961700	Au	-0.24099500	0.00053200	-1.58469100
Au	2.61284000	-1.65282200	-0.58535200	Au	2.48790800	-1.62844700	-0.30622000
Au	0.73049400	-1.33363300	1.49555700	Au	0.47096100	-1.33409100	1.64471900
Au	0.72734700	1.33592000	1.49595600	Au	0.46637100	1.33654900	1.64540600
Au	1.84561300	3.76343100	0.80416800	Au	1.65068500	3.74455600	1.06418300
Au	-0.06360500	-2.62056500	-0.93527100	Au	-0.12246400	-2.63431700	-0.84808500
Au	-2.46434300	-1.51190500	-0.79576000	Au	-2.50380400	-1.49433400	-0.95803700
Au	-1.59371600	-0.00157100	1.45162500	Au	-1.83925000	-0.00257400	1.36730900
Au	-0.06882600	2.62051600	-0.93540200	Au	-0.13102100	2.63578000	-0.84698000
Au	-2.46733300	1.50702300	-0.79582000	Au	-2.50856200	1.48799000	-0.95735200
Au	-4.24021500	-0.00419600	0.64668700	Au	-4.40819500	-0.00658600	0.33246500
Au	1.85263500	-3.75971400	0.80480000	Au	1.65915000	-3.74063100	1.06500000
Cl	3.81959600	0.00356900	-1.93531800	I	3.78319600	0.00438200	-1.95371000

Au₁₃-X-2 (F,Cl,Br,I) (Singlet state)

Au ₁₃ -F-2				Au ₁₃ -Br-2			
Au	0.36997000	2.08188200	-1.36283600	Au	0.47238700	1.88912600	-1.38313300
Au	0.83739600	1.35859300	1.40579200	Au	0.78728100	1.25623900	1.44673800
Au	1.35231500	-0.34993100	-1.43701300	Au	1.31237000	-0.59776300	-1.53318000
Au	3.17282000	-0.07710900	0.62603300	Au	3.11106200	-0.13683400	0.51706300
Au	2.90693200	2.49441200	-0.01474000	Au	2.85312400	2.46887700	0.11098800
Au	-0.19857700	-2.58097900	-0.86145900	Au	-0.24785800	-2.76159800	-0.73691000
Au	0.70284000	-1.37383300	1.49727600	Au	0.73528500	-1.47293200	1.51184600
Au	-1.52629800	0.09694200	1.53563600	Au	-1.54118800	-0.09412900	1.53989800
Au	-1.38517200	-0.07350700	-1.25932500	Au	-1.36466700	-0.17845600	-1.27471900
Au	-2.65898000	-2.18673500	0.10601200	Au	-2.74282200	-2.24173000	0.04159200
Au	-3.90077900	0.35310900	0.11074600	Au	-3.84636900	0.38342800	0.06436000
Au	2.60488800	-2.59635300	-0.25301100	Au	2.60198200	-2.73315800	-0.20107500
Au	-2.18797400	2.40630700	-0.00199100	Au	-1.97198400	2.32788700	0.13109800
F	-0.78456900	3.92544600	-0.79983900	Br	-0.35799100	4.26835500	-0.52944700
Au ₁₃ -Cl-2				Au ₁₃ -I-2			
Au	0.48602000	1.94235900	-1.40414700	Au	0.43319100	1.84643200	-1.38226000
Au	0.82459300	1.33788400	1.42592900	Au	0.72772300	1.17553800	1.45672600
Au	1.30593000	-0.54916600	-1.51724800	Au	1.32361900	-0.62973200	-1.53639200
Au	3.11862600	-0.11135100	0.52185800	Au	3.11138900	-0.12410000	0.51530600
Au	2.90423000	2.48943100	0.05073300	Au	2.76249400	2.47694300	0.16645100
Au	-0.29067300	-2.68233700	-0.73302200	Au	-0.17139700	-2.84639600	-0.73645600
Au	0.70065800	-1.38852600	1.51689200	Au	0.79862700	-1.55426800	1.50651100
Au	-1.53746000	0.05503700	1.53152200	Au	-1.54063200	-0.28838300	1.54142600
Au	-1.37633700	-0.10201600	-1.27465600	Au	-1.35160300	-0.26589000	-1.28017800
Au	-2.76563700	-2.13121200	0.09149800	Au	-2.69697000	-2.38551800	-0.02553600
Au	-3.85744600	0.48951400	0.05665800	Au	-3.83410700	0.22961900	0.07086200
Au	2.55800000	-2.69875200	-0.17600100	Au	2.68399400	-2.73403800	-0.23028900
Au	-1.99397000	2.43335400	0.04429300	Au	-1.95295900	2.18619500	0.25319500
Cl	-0.35566700	4.25568700	-0.62413400	I	-0.43728200	4.34290800	-0.47603400

Au₁₃-X-3 (F,Cl,Br,I) (Singlet state)

Au ₁₃ -F-3				Au ₁₃ -Br-3			
Au	1.37985600	0.10167900	-1.18723800	Au	-1.38386900	-0.51401900	-1.39815800
Au	2.73905200	2.36107400	-0.39468300	Au	-2.71085400	-2.50854900	-0.00079000
Au	1.35677300	0.94679200	1.51299000	Au	-1.38481400	-0.51325800	1.39694600
Au	-0.00666700	-1.88732400	-2.40162100	Au	0.00122600	1.47682400	-2.54578300
Au	1.54097400	-2.32352700	0.01080000	Au	-1.46677700	2.04144100	0.00212400
Au	3.56046200	-0.52454200	0.30570400	Au	-3.62425000	0.42020500	-0.00016500
Au	-1.50577900	-2.31542400	0.03492800	Au	1.46701200	2.04116400	0.00286200
Au	0.04372600	-1.24693800	2.25902900	Au	0.00044900	1.47652100	2.54719800
Au	-1.35856400	0.89764300	1.51574700	Au	1.38431400	-0.51399400	1.39631800
Au	-1.40825000	0.09913300	-1.19770400	Au	1.38481000	-0.51514600	-1.39855200
Au	-3.56584300	-0.55780200	0.32004900	Au	3.62425600	0.41986000	0.00036700
Au	-2.76196900	2.34268700	-0.36219300	Au	2.70924200	-2.51057300	0.00009500
Au	-0.01602300	2.50343800	-0.58336900	Au	-0.00088400	-2.67823600	0.00106100
F	0.01975700	-3.48380400	1.47081300	Br	0.00030900	4.23837300	-0.00794900
Au ₁₃ -Cl-3				Au ₁₃ -I-3			
Au	-1.38372000	-0.45570600	-1.41100800	Au	-1.38310600	-0.59554600	-1.40059200
Au	-2.71143200	-2.42937600	0.01067000	Au	-2.71261900	-2.58888100	-0.00172800
Au	-1.38729400	-0.41766400	1.38459300	Au	-1.38584200	-0.59195900	1.39454500
Au	-0.00002400	1.53254100	-2.55580700	Au	0.00397500	1.40657700	-2.52784900
Au	-1.47299500	2.11105400	0.01869600	Au	-1.45641100	1.96924600	0.00672400
Au	-3.62932700	0.49005100	-0.00695100	Au	-3.62020000	0.34982600	-0.00239500
Au	1.47175600	2.11161700	0.01851500	Au	1.46414000	1.96608600	0.00793700
Au	-0.00023200	1.55758300	2.56387100	Au	0.00099000	1.40423300	2.53660300
Au	1.38724900	-0.41730100	1.38458900	Au	1.38154800	-0.59532600	1.39362800
Au	1.38342900	-0.45565100	-1.41100500	Au	1.38300900	-0.60107900	-1.40025300
Au	3.62869500	0.49165700	-0.00707000	Au	3.62147800	0.33887900	-0.00106500
Au	2.71330200	-2.42795200	0.01097000	Au	2.70347500	-2.59822200	0.00109100
Au	0.00086500	-2.59718100	0.03308400	Au	-0.00490800	-2.76403500	0.00388300
Cl	-0.00125500	4.21175600	-0.15403600	I	0.00666800	4.32294100	-0.01569700

Au₁₃-X-4 (F,Cl,Br,I) (Singlet state)

Au ₁₃ -F-4				Au ₁₃ -Br-4			
Au	1.74925500	-1.16090100	-1.14854200	Au	-0.05162500	2.07665700	1.79703800
Au	-1.45317900	-2.74816500	0.70927800	Au	2.18619800	1.15246900	-1.36515700
Au	-2.91642300	-0.52440000	0.23981800	Au	-0.04417600	0.52031600	-2.69343400
Au	0.62507700	-0.63582700	-3.58255800	Au	-2.36584700	2.51336200	0.44975100
Au	-4.26944700	1.74259000	0.58747600	Au	-2.35461900	-0.87447400	-2.40481700
Au	-1.09520800	-1.41282800	-1.60750400	Au	-0.04411400	2.56529200	-0.95527200
Au	3.49361700	2.43624900	1.83091500	Au	-2.35927100	-1.65981700	1.94396000
Au	-1.63614700	2.03621800	0.28059300	Au	-0.03111500	-2.10825400	-1.73996300
Au	-0.13264000	-0.26890600	0.92745600	Au	2.19481700	-1.75617300	-0.30558600
Au	2.72690500	-0.02030700	1.14606200	Au	-0.04694400	-0.45321800	2.69328300
Au	1.07572000	2.27876500	0.71571500	Au	-0.03653900	-2.59684600	0.89876600
Au	1.59717000	-2.47506900	1.20285700	Au	2.18245500	0.61671200	1.68046600
Au	0.14305600	1.17445500	-1.59149200	Au	-1.09946700	-0.00094800	-0.00156300
F	0.08320200	-4.02923300	1.67033800	Br	4.22141900	0.01111200	0.00570600
Au ₁₃ -Cl-4				Au ₁₃ -I-4			
Au	2.63432300	-0.78420300	0.04142600	Au	-0.12179200	-0.43175800	2.70139300
Au	0.50140500	1.67504900	-2.29546300	Au	2.12127100	1.77404400	0.26754000
Au	-0.63613200	2.67013000	-0.09480000	Au	-0.11095900	2.55834800	-0.97864400
Au	2.44829300	0.69823200	2.30405200	Au	-2.44069600	0.94046300	2.36195000
Au	-1.82738700	1.88233800	2.21099100	Au	-2.43947300	1.58837700	-1.98611900
Au	1.94429300	1.92077300	-0.06375400	Au	-0.11860000	2.17003300	1.67437000
Au	-0.72726600	-2.40514200	2.33534200	Au	-2.44497100	-2.51495700	-0.37191200
Au	-2.63734600	0.72063700	-0.10298300	Au	-0.12601200	0.36616600	-2.71594800
Au	-1.70443400	-0.51761100	-2.27534800	Au	2.11248300	-0.65975800	-1.67124200
Au	0.69166800	-2.64001300	0.03524400	Au	-0.12512000	-2.53797300	1.04133800
Au	-1.99785400	-1.88691800	-0.00275500	Au	-0.12335300	-2.12650800	-1.72591600
Au	1.31081500	-1.33675500	-2.21018200	Au	2.11376700	-1.12113200	1.40517800
Au	-0.01549600	0.02754900	1.02147600	Au	-1.17014500	0.00012300	-0.00106400
Cl	0.07025400	-0.11184400	-4.19743400	I	4.28328900	-0.00815200	-0.00137800

Au₁₃-X-5 (F,Cl,Br,I) (Singlet state)

Au ₁₃ -F-5				Au ₁₃ -Br-5			
Au	-2.54368900	-3.70941300	0.00000000	Au	-2.02898700	-3.86314700	0.00000000
Au	0.13811900	-3.56328900	0.00000000	Au	0.63710800	-3.41413200	0.00000000
Au	1.48229300	-1.15120400	0.00000000	Au	1.71594200	-0.88329400	0.00000000
Au	-1.30762000	-1.27066000	0.00000000	Au	-1.05263200	-1.30158000	0.00000000
Au	2.86319400	-3.42838800	0.00000000	Au	3.33505900	-3.00692700	0.00000000
Au	0.00000000	1.15400200	0.00000000	Au	0.00000000	1.25758600	0.00000000
Au	2.76422400	1.21633600	0.00000000	Au	2.73312800	1.61225900	0.00000000
Au	4.25375000	-1.06234100	0.00000000	Au	4.45236400	-0.49892900	0.00000000
Au	-4.05001300	-1.34774100	0.00000000	Au	-3.76895500	-1.66505000	0.00000000
Au	-2.75893200	0.98546400	0.00000000	Au	-2.71386600	0.79832700	0.00000000
Au	-1.50523200	3.37232300	0.00000000	Au	-1.72660100	3.30937600	0.00000000
Au	1.34875500	3.51485300	0.00000000	Au	1.08065700	3.75703400	0.00000000
Au	-0.14362200	5.69119700	0.00000000	Au	-0.62246900	5.77069300	0.00000000
F	-4.75079200	-3.52109800	0.00000000	Br	-4.60626300	-4.22586100	0.00000000
Au ₁₃ -Cl-5				Au ₁₃ -I-5			
Au	-2.36810400	-3.78222400	0.00000000	Au	-1.70995300	-3.91248000	0.00000000
Au	0.31753400	-3.51869200	0.00000000	Au	0.92951700	-3.28881900	0.00000000
Au	1.56702200	-1.06454500	0.00000000	Au	1.84495300	-0.70001300	0.00000000
Au	-1.22294700	-1.29462300	0.00000000	Au	-0.89584600	-1.29135400	0.00000000
Au	3.03722000	-3.29099100	0.00000000	Au	3.59788700	-2.71819700	0.00000000
Au	0.00000000	1.18399400	0.00000000	Au	0.00000000	1.33375900	0.00000000
Au	2.75303300	1.35518200	0.00000000	Au	2.69995300	1.85812700	0.00000000
Au	4.32644600	-0.86751100	0.00000000	Au	4.54735200	-0.14020600	0.00000000
Au	-3.96074700	-1.46814200	0.00000000	Au	-3.58325900	-1.81624000	0.00000000
Au	-2.74209400	0.91276200	0.00000000	Au	-2.67325500	0.71139500	0.00000000
Au	-1.58567500	3.34799700	0.00000000	Au	-1.84599300	3.28195900	0.00000000
Au	1.24918100	3.60338000	0.00000000	Au	0.91811400	3.90021700	0.00000000
Au	-0.31795900	5.72536300	0.00000000	Au	-0.89595800	5.81335200	0.00000000
Cl	-4.89293300	-3.91258500	0.00000000	I	-4.37259300	-4.51865000	0.00000000