

Isolation of atomically precise mixed ligand shell PdAu₂₄ clusters

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Supporting Information

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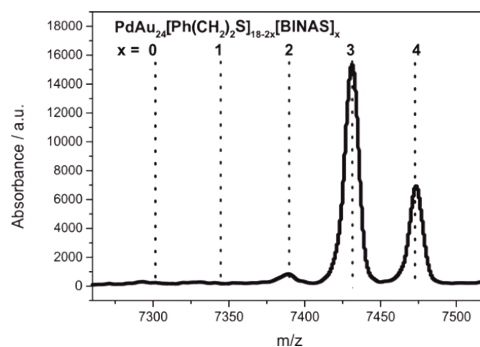


Figure S1. MALDI-TOF mass spectra of the crude exchanged product after 72h reaction. The original $\text{PdAu}_{24}(\text{2-PET})_{18}$ and $\text{PdAu}_{24}(\text{2-PET})_{16}(\text{R-BINAS})_1$ are no longer observed, resulting in a higher amount of exchanged BINAS.

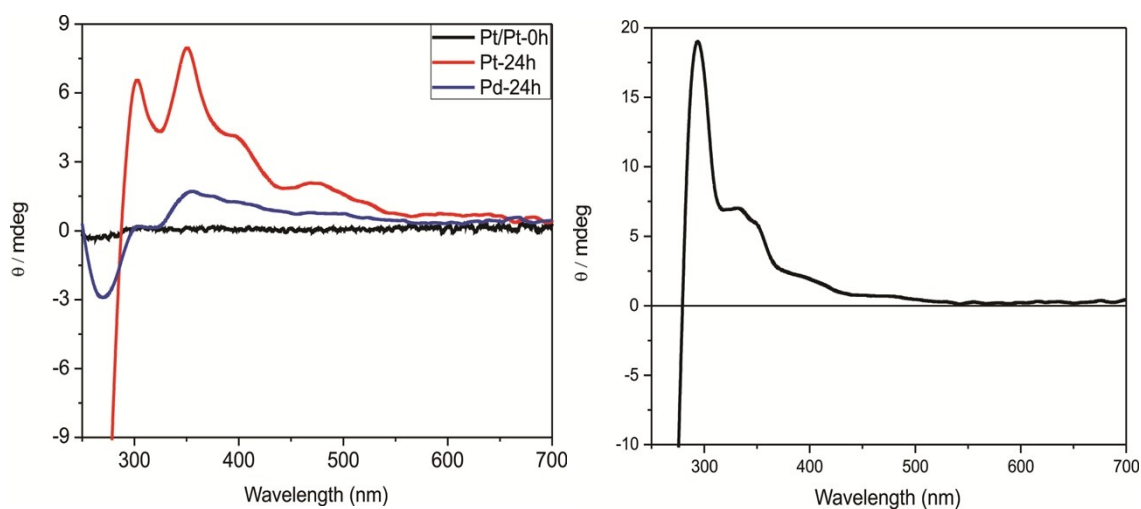
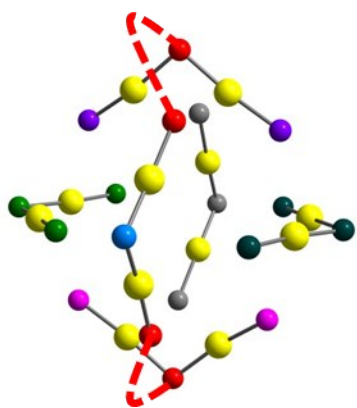


Figure S2. CD spectra of $\text{PdAu}_{24}(\text{2-PET})_{18-2x}(\text{R-BINAS})_x$ and $\text{PtAu}_{24}(\text{2-PET})_{18-2x}(\text{R-BINAS})_x$ after 24h exchange reaction (left) and CD spectra of pure R-BINAS (right). The CD signal confirms the induced secondary level of chirality.

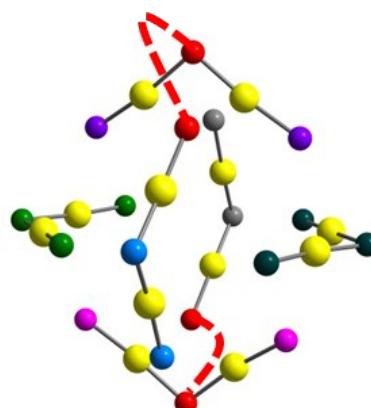
All possible exchange isomers of PdAu₂₄(2-PET)₁₄(R-BINAS)₂

PdAu₂₄(2-PET)₁₈ consists of six dimeric staples, containing one apex and two core sulphurs. Assuming an interstaple binding mode of dithiol ligands, BINAS binds from the apex S-atom in one staple to a core S-atom in another staple. Statistically, after one BINAS ligand is exchanged, five apex sulphurs remain available for the 2nd BINAS, resulting in ten possible isomers of PdAu₂₄(2-PET)₁₄(R-BINAS)₂. However, repetition of isomers can occur considering the high symmetry of the cluster. Herein all ten configurations are identified and after rotation, matched to identical isomers. Isomers I3/I5 and I4/I6 are enantiomers concerning their adsorption pattern.

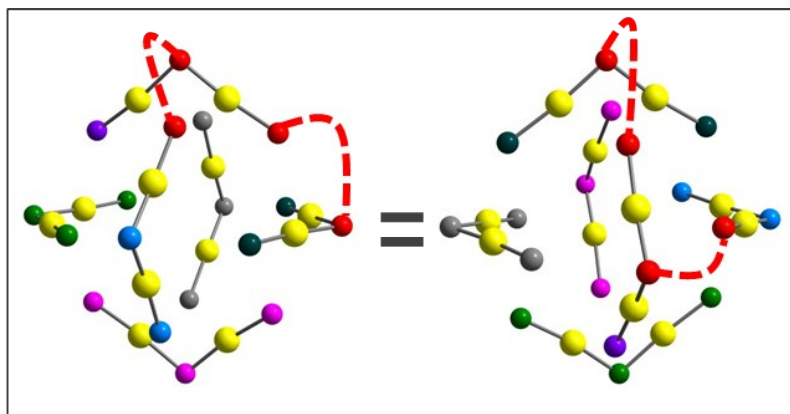
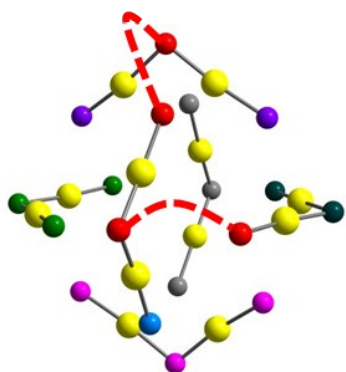
Structure I1



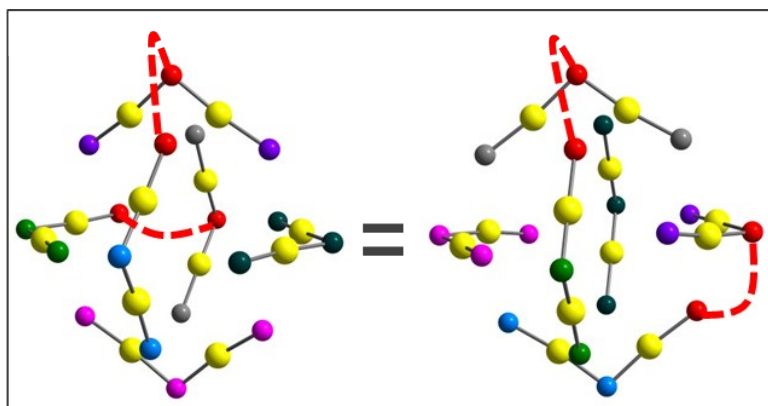
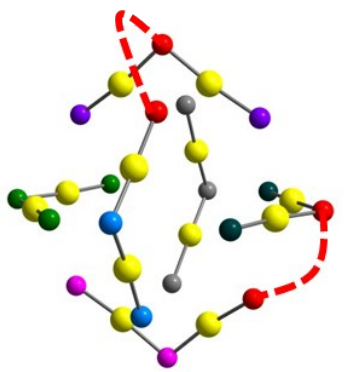
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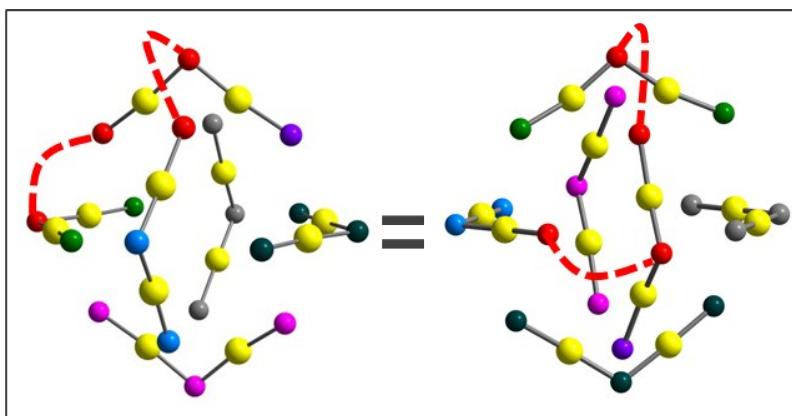
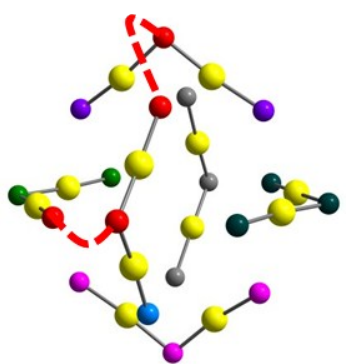
Structure I3



Structure I4



Structure I5



Structure I6

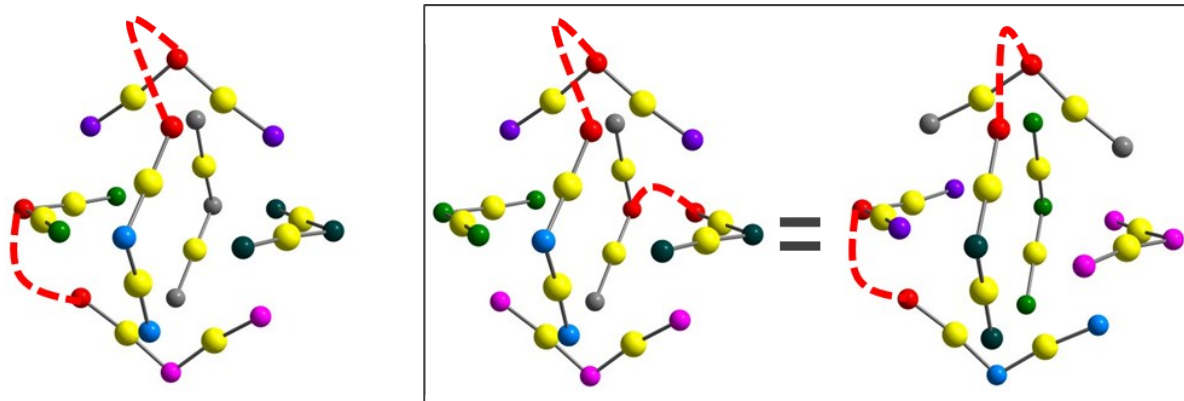
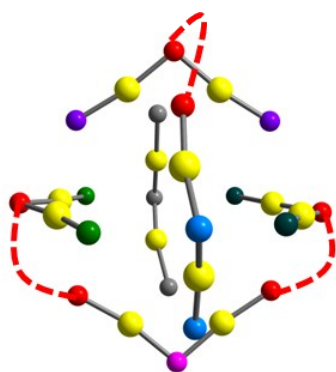
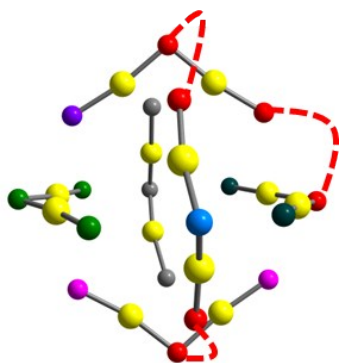


Figure S3. Isomers of $\text{PdAu}_{24}(\text{2-PET})_{14}(\text{R-BINAS})_2$

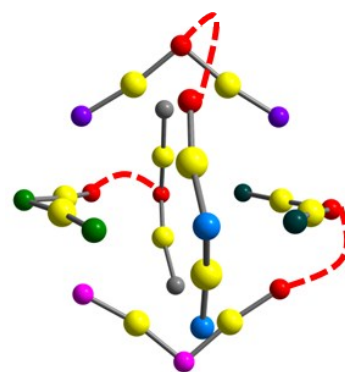
All possible exchange isomers of PdAu₂₄(2-PET)₁₂(R-BINAS)₃

Statistically, 15 configurations of PdAu₂₄(2-PET)₁₂(R-BINAS)₃ are possible. However, due to the high relative energy of I5, eight structures can be excluded. Below the seven remaining isomers are shown.

Structure 1

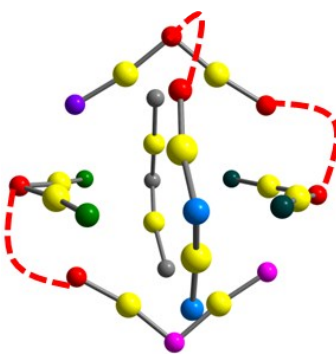
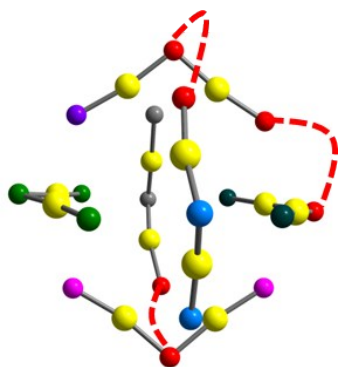


Structure 5

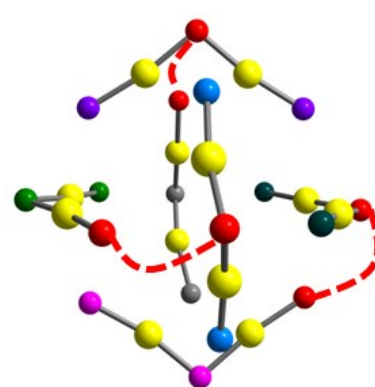


Structure 6

Structure 4



Structure 3



Structure 2

Structure 7

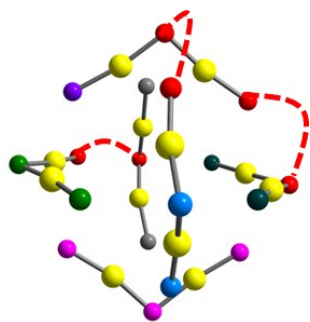


Figure S3. Isomers of $\text{PdAu}_{24}(\text{2-PET})_{12}(\text{R-BINAS})_3$

Coordinates of all optimized structures

Coordinates of PdAu₂₄(CH₃)₁₈

Au	11.19999982194495	12.800000021179429	12.800000012011285
Au	12.015295196649351	13.695768958929241	15.300889560533506
Au	11.006520280827029	15.577864643252681	13.194906445992613
Au	9.187017000794432	13.678281091330090	14.487833631156821
Au	13.608207857889232	14.107593552972219	13.082676013121310
Au	13.193165713463292	11.309807061730316	14.066196934760084
Au	15.109578074577261	13.389821865797057	15.507437315366531
Au	9.806710888497575	13.006810128726903	17.398333559050972
Au	13.390539095573537	16.406512903399438	15.187507166981939
Au	7.405408862405634	11.390224048418151	15.376741079055849
Au	10.394937272331864	11.218685091650356	14.974565609402056
Au	10.392115262625024	16.988055569418709	10.593952587455654
Au	8.122744502103329	16.410997371353883	13.320154127601782
S	7.624936364278374	12.290913634568762	17.475225202130378
S	15.425990631921985	15.629650651635393	15.897384550547285
S	10.269881973758654	9.310886263248648	16.374290944421496
S	15.118335871235715	11.084512300020339	15.413570213146700
S	8.695217091328763	18.007819570335432	11.768529335608418
S	15.515602803448786	15.228638258410639	12.228025164462053
S	11.938597183100155	13.877937707606806	17.655714392349580
S	11.430467009421106	17.447849198400700	14.563075621312764
S	7.455341663286251	15.154247839369310	15.142955753006762

C	11.022909501469016	9.849323574355415	17.930389139059340
H	12.070661245922413	10.140468546404955	17.789401885411198
H	10.465562187252155	10.739140451345529	18.288348798990473
C	11.627868603926991	15.621892836116444	18.024887542506026
H	12.517300983946100	16.203386410497490	17.722941068957525
H	10.766433274413117	15.998968162100111	17.455938119511778
C	11.904507468190005	18.828782200052110	13.494320588549982
H	12.695892240191688	18.529326091539101	12.793661792682604
H	11.011310384380231	19.127194251237245	12.922705994856290
C	15.307567524243956	15.715444169050800	17.700544128481244
H	15.192800507817502	16.768652917547609	17.996012602486363
H	14.452598534455468	15.125798377271698	18.065975115717109
C	14.428098562564971	10.644483854488259	17.025361087873765
H	13.641315222466435	11.356167450354377	17.318825531039888
H	13.991764304638931	9.631099249064551	16.941004257982726
C	7.329066346076852	18.037892063465442	10.590257762643166
H	7.639772436429983	18.620935207414576	9.712257326309491
H	7.051376497567215	17.010683846204099	10.295338411210400
C	8.190107729157740	16.106848248582338	16.494530914221066
H	8.316170247191375	15.431955926386337	17.357214243711734
H	9.167446604800160	16.513478127771720	16.193630524537106
C	7.678186011332620	10.816302436196866	18.518083271148736
H	8.339660344969857	10.054516149832843	18.075226299780624
H	8.040646751144681	11.098405718713710	19.517259063633830
C	14.855205664740128	16.903014811382711	12.052409893937032

H	13.842224612859964	16.882136152154999	11.617962694382266
H	14.800368791489090	17.336933929588891	13.067160839680939
Au	10.384704826109447	11.904231027413205	10.299110486744274
Au	11.393479720381295	10.022135362957718	12.405093581335759
Au	13.212983027890436	11.921718905301685	11.112166389154469
Au	8.791792164050849	11.492406473189865	12.517323970013424
Au	9.206834296115648	14.290192923479919	11.533803094993260
Au	7.290421889089885	12.210178066152455	10.092562675614802
Au	12.593289119713194	12.593189855508610	8.201666450265652
Au	9.009460900710458	9.193487097038897	10.412492823715317
Au	14.994591103149190	14.209775948748263	10.223258898965014
Au	12.005062733700759	14.381314877307702	10.625434408679034
Au	12.007884728185768	8.611944417159393	15.006047372159173
Au	14.277255496856679	9.189002618031685	12.279845916645161
S	14.775063652472367	13.309086377570981	8.124774817800015
S	6.974009341685496	9.970349308874995	9.702615426560513
S	12.130118017033752	16.289113698586029	9.225709039306293
S	7.281664081957887	14.515487652355050	10.186429829844167
S	13.704782890458299	7.592180395497378	13.831470625593994
S	6.884397184923349	10.371361756309007	13.371974812374660
S	10.461402832453368	11.722062291814183	7.944285606985877
S	10.969533005266989	8.152150847700833	11.036924382575037
S	14.944658419218147	10.445752162685769	10.457044233440556
C	11.377090108123957	15.750676398575521	7.669610975488085
H	10.329338945878025	15.459531460637077	7.810598076676489

H	11.934437856862806	14.860859440885521	7.311651135826145
C	10.772131306197844	9.978107176828905	7.575112429038801
H	9.882699069937305	9.396613632704565	7.877058906453816
H	11.633566794141979	9.601031830775801	8.144061839793546
C	10.495492455501523	6.771217837490368	12.105679378330199
H	9.704107729641219	7.070673917404829	12.806338158841651
H	11.388689577697596	6.472805736199865	12.677293985025313
C	7.092432537709764	9.884555842963401	7.899455855022800
H	7.207199522327235	8.831347014872808	7.603987381498648
H	7.947401420384158	10.474201573820835	7.534024870181314
C	7.971901242292827	14.955516130546121	8.574638926836791
H	8.758684734433421	14.243832460384269	8.281174490163075
H	8.408235653947816	15.968900700766495	8.658995827416739
C	15.070933581349378	7.562107857761962	15.009742319815034
H	14.760227490426130	6.979064765459387	15.887742640786172
H	15.348623490386382	8.589316133517448	15.304661614485639
C	14.209892277583757	9.493151641189542	9.105469173753207
H	14.083829822664589	10.168044074535077	8.242785683081189
H	13.232553432307093	9.086521940552322	9.406369461101592
C	14.721814009973979	14.783697608342280	7.081916800407835
H	14.060339646221854	15.545483812560201	7.524773662554308
H	14.359353226725599	14.501594239020550	6.082740862452535
C	7.544794213365659	8.696985167274587	13.547589974003211
H	8.557775457692097	8.717863884127087	13.982037306217112
H	7.599631194939017	8.263066125974479	12.532839200101547

H	12.250994138774312	19.665459687295453	14.119279154181291
H	6.466484870931358	18.515021517600093	11.077467280133845
H	7.168575274228280	14.945106095937154	7.824701548054957
H	11.447859192292112	16.567387052621935	6.936969764044152
H	15.741011698699024	15.188874423588267	7.015149678396215
H	14.884602057664274	8.664686932241336	8.844879327776550
H	10.960150833056327	9.870061001812635	6.497460623238969
H	6.161802865698291	10.291161561154025	7.478082128412663
H	10.149005822993663	5.934540386748417	11.480720784455711
H	15.933515189941810	7.084978409108186	14.522532737978720
H	6.873588429114913	8.103547909145020	14.185610430016633
H	10.952140751693314	9.032612965100878	18.663030207816480
H	6.658988263366622	10.411125561330511	18.584850320817200
H	15.231424702658002	10.654893903585313	17.775298566507949
H	16.238197116852216	15.308838376320136	18.121917853336086
H	11.439849141323270	15.729939061802009	19.102539342600746
H	7.515397886261578	16.935313073989004	16.755120763884534
H	15.526411568096941	17.496452134762340	11.414389520655805

Coordinates of PdAu₂₄(CH₃)₁₆(S-BINAS)₁

Au	15.410494831081191	11.906298202770394	14.276849354246698
Au	16.209398687000096	12.783862015902168	16.776160280824929
Au	15.201970602909968	14.659038237706222	14.674436323056481
Au	13.320869103968038	12.791220660373986	15.910534584095277
Au	17.886243339091120	13.128194428893631	14.590881834148714
Au	17.454878383158906	10.401254800181457	15.487810155278993
Au	19.292062975959535	12.394690685121910	17.083471256517392
Au	13.808870845426677	12.210583481676450	18.797700731754496
Au	17.690423095318778	15.504047974374078	16.410078671433148
Au	11.414066792121154	10.592764984714741	16.787626986319502
Au	14.526924280845499	10.335556664118764	16.396110444638946
Au	14.410502991857022	15.995313167744575	11.812134683170651
Au	12.229042155714314	15.486735547403395	14.688482888322152
S	11.739534735322289	11.227674246230453	18.967815149607230
S	19.507275935321019	14.635242522782773	17.526680644942630
S	14.772995710524365	8.544966583350131	17.907418258922142
S	19.435523584462796	10.117356227269285	16.758924389844847
S	12.770195147169199	17.009140681709685	13.038237880628895
S	19.996845295603109	13.877135685966657	13.821070992537383
S	15.835059411318760	13.314743488552777	19.038441027738013
S	15.954321003032710	16.728536974163990	15.500735436067433
S	11.470490311012286	14.178273862247595	16.421984880131880

Au	14.599092475749449	11.096315679653232	11.730544428039231
Au	15.602521012731376	9.192863671329050	13.812667162642596
Au	17.453430415682906	11.009496001882644	12.538023616895872
Au	12.990598745870168	10.596846472430853	13.985480912241545
Au	13.401560570142578	13.396200241573549	12.997183046549319
Au	11.605901711103446	11.408881801792575	11.408355203595390
Au	16.999229272107819	11.606208615758488	9.612994543881381
Au	13.200665300372709	8.290571610884951	12.092792283036898
Au	19.396306283453473	13.107034575094559	11.733487445977639
Au	16.297981518013387	13.497505086740896	12.191078148337816
Au	16.472277861883388	7.802451636866107	16.519204844470547
Au	18.495523556936433	8.213180354596476	13.674998172157292
S	19.142903173895533	12.440067004350025	9.552047188676648
S	11.359700364793646	9.158064746070883	11.026134321312860
S	16.355782292787886	15.352872170370713	10.735462211665935
S	11.395225411097648	13.695541069329781	11.685061997328880
S	18.015965151965492	6.635911643134872	15.271827432542526
S	10.830028008058481	9.905796192026983	14.664223554901703
S	14.910538974030500	10.631474488474282	9.434758009106604
S	14.913216987910678	7.059585459828704	13.047952990850026
S	19.236583174137877	9.564060779978382	11.964418560643377
C	11.228529143300362	17.105702956435056	12.188339656896405
C	10.954009790359054	16.596262056953051	10.938588698447933
C	10.244670601629020	17.817632912444573	12.909095105066534
C	9.654849877015213	16.812278041573528	10.381675417589777

C	9.010639573577588	18.035097954285192	12.385469513385935
H	10.506933017050750	18.181825162472617	13.906625628648571
C	8.679655634024201	17.543904871276698	11.109471479522220
H	8.255631498580417	18.590357393868889	12.950598818947325
C	11.970746851196223	14.442669187155820	10.200819691490647
C	11.865672132228115	15.821946749248792	10.074627907467473
C	12.455538734166725	13.672228178486103	9.123126819153812
C	12.375433541495392	16.454182016736922	8.910913594052182
C	12.841910103785318	14.266207580660586	7.956794596926683
H	12.497975254385642	12.581213798732250	9.250907587178350
C	12.862375776900647	15.667730613547135	7.832621896039670
H	13.196481603801702	13.656189147737923	7.118575339739001
C	7.410836502143575	17.758406172522800	10.548646139566065
C	9.292326366023573	16.307128476539368	9.117003649230861
C	8.046138199798790	16.532762208589190	8.594499586033756
C	7.094761759998571	17.269582205370671	9.309776832183042
H	6.678411463611145	18.327570387098437	11.131062217022116
H	10.023105792225870	15.725256476233376	8.547173917343727
H	7.793370792425287	16.130184896660438	7.608846858059659
H	6.103313024832355	17.445909466966818	8.883319446125798
C	13.349026978223771	16.309970527003731	6.682074695673523
C	12.392124588741709	17.855682879993036	8.785170652751214
C	13.364466616994816	17.676455195748478	6.592119877508005
C	12.884258701917679	18.452982655714393	7.655926924439023
H	12.024326077566947	18.457015154549467	9.622836057896469

H	12.908606916489713	19.542687275148747	7.581893060810190
H	13.752410571989028	18.163199979373807	5.693254085972565
H	13.725156673758541	15.691156299788869	5.859439060602734
C	16.671636814716475	17.556003930411343	14.064310988220369
H	15.841723244360120	17.957428468230695	13.461521237531505
H	17.325869305374216	18.370522680580844	14.407913997409691
H	17.242320739374758	16.850903286653299	13.443596433764119
C	19.845731549112326	15.672024853241084	13.663311161187385
H	19.647630549620672	16.087891153968034	14.667617907927800
H	20.789120804871576	16.071408592346582	13.264818586869632
H	19.018992115442515	15.939026717613588	12.990636168604331
C	19.069287774458253	14.023579058973951	8.685643945240990
H	18.700425098886733	13.860151727215539	7.662787353976245
H	18.414130735465960	14.730865898850151	9.217746693759494
H	20.088200831758947	14.433536381112823	8.657682215449286
C	15.780435860418708	14.711345905435611	9.153578104932006
H	15.687738822116625	15.539977412165813	8.435762961051077
H	16.499822575670240	13.953091086019672	8.791130751107687
H	14.808203298982345	14.221696815193926	9.268638729060610
C	11.736977083535397	8.994350977638094	9.270267154196940
H	12.657934188273467	9.544683202814429	9.017826932037725
H	11.856390063015324	7.927774748593857	9.033011284371732
H	10.897656540215300	9.414210892037266	8.699132415063099
C	15.282885447582750	8.861742090547262	9.453805930980790
H	14.338687191974397	8.314032282660959	9.624263191309419

H	15.734379032329972	8.569582147386921	8.494773000332239
H	15.962582331191367	8.625547833652494	10.283453268300290
C	18.737218723456028	8.680637391844520	10.466208645981812
H	18.518170698897777	9.430124684449540	9.683841156377637
H	19.565733640210436	8.032136728386375	10.147806723040375
H	17.843410069952064	8.070984810982928	10.646665057721222
C	14.126846248995205	6.302185316254102	14.492304894835701
H	13.454585974351952	5.497979587553982	14.159550388592375
H	14.924487830352847	5.895876929006255	15.136751634649571
H	13.562380160102437	7.051101658767868	15.066751419609888
C	19.507205520156536	6.638690665437790	16.290217886221569
H	19.301122036026158	6.107276404407571	17.231118500801955
H	20.298992080808002	6.119741568046272	15.732300976767197
H	19.833124817704011	7.671850006566339	16.496616338379201
C	18.930363363877696	9.428484124920224	18.352017930317217
H	18.369044422106125	8.490434858403930	18.166360628378232
H	19.834156694104148	9.231910326820564	18.947081378403080
H	18.281537984419266	10.126949555673649	18.893515453866875
C	15.602114745885283	9.337445063300335	19.304074715974959
H	14.836453757075279	9.875382324176451	19.890777553225181
H	16.096780933699396	8.573786262412062	19.922348403788646
H	16.334314916004388	10.075263418197252	18.947603611609857
C	10.878731215984219	8.099653940298099	14.737106898503040
H	9.917696366731752	7.736941430725436	15.129446078718688
H	11.038513873881136	7.724292293167061	13.711660159605355

H	11.695970414153246	7.744773833552959	15.377559445565410
C	12.068026866259773	9.682208716780282	19.841989506656571
H	12.809929838752817	9.072628605638409	19.296519262965678
H	12.437698240402209	9.921239546495020	20.849756603040824
H	11.123530237125616	9.124765356249499	19.911121554526751
C	11.913379866880899	15.094874035023265	17.914766628953675
H	11.090892609650950	15.779692215308485	18.161538219190028
H	12.062541946852392	14.362801034686420	18.727636126613792
H	12.839683206567125	15.664942545415782	17.773335543590591
C	15.398500871819822	15.065740034892659	18.928380296649706
H	14.842858421241043	15.364920945353857	19.828660975024505
H	16.335032339350455	15.644234388490494	18.841398637073187
H	14.798414972465919	15.257176859059628	18.026812041558895
C	19.057840864362991	14.801075308013752	19.265560542564224
H	18.943848639108960	15.870967487260346	19.491319010878186
H	18.119510484521129	14.262866626771245	19.486381677354483
H	19.870648582660838	14.376443933675155	19.872744856451540

Coordinates of PdAu₂₄(CH₃)₁₄(S-BINAS)₂ (Isomer 1)

Au	15.110313298098257	16.690052034286900	14.596012814249326
Au	15.985070741728110	17.498733318178623	17.112710331302996
Au	14.994928009088024	19.402042170013122	14.993424287961105
Au	13.105940343835204	17.616332455887168	16.303624624207032
Au	17.601115138673762	17.887972974563585	14.903395420559699
Au	17.013314458427640	15.097416724045388	15.897339344779576
Au	18.991473349735241	17.002708579909001	17.400495817976047
Au	13.603575535500994	16.992410872813355	19.190053795322765
Au	17.409594561236847	20.196352712785728	16.805412636464002
Au	11.106215490402514	15.595856577256839	17.099453801947849
Au	14.187039423612275	15.116866359213377	16.698367937111463
Au	14.282788577947771	20.795262213059740	12.138275314975338
Au	12.121030889878766	20.325629732428027	15.006474443150248
S	11.494173825035924	16.100366357049069	19.304316529192349
S	19.245666577531743	19.248562735808179	17.832585987512253
S	14.200310516586919	13.198113065106613	18.060428230642977
S	19.044784989571777	14.724957277072740	17.043541005787777
S	12.648211060441167	21.848229994849230	13.347365081057616
S	19.751079016618501	18.656078032050040	14.270828838480137
S	15.660744577231767	18.012757143734383	19.398287716226847
S	15.697726482177142	21.460566318555728	15.898733683144741
S	11.310071431690028	19.095545000542831	16.779745208797305
Au	14.306527570412133	15.818580051547764	12.093185400145561

Au	15.201058150149668	13.975260918279881	14.185490415174577
Au	17.180211054792416	15.723053283634474	12.941247851187729
Au	12.607273980436229	15.478146002547124	14.293022141904229
Au	13.135524849270935	18.198322312849566	13.313864493435270
Au	11.290943269328363	16.297742292755103	11.793170485897919
Au	16.720705197728471	16.405394752051944	10.083558415034982
Au	12.922011944677708	13.192391052893008	12.322062016572104
Au	19.196717795770841	17.804370687244827	12.204748592785768
Au	16.065641626736870	18.205527481106849	12.475695877531614
Au	15.807049758496028	12.292310585504003	16.676676669760585
Au	18.194054290361493	12.999956934919455	14.190720773571293
S	18.917080387605424	17.100283364640340	10.034279122634040
S	11.021250556618195	14.053945995339578	11.362369650070219
S	16.227040763791209	20.119149357573257	11.102722174449378
S	11.128032108793809	18.591093687651131	12.032932467243375
S	17.622997597004410	11.311486784135013	15.670742624296246
S	10.382500844790936	15.062321020763997	14.982837592631686
S	14.624415422628889	15.473529391211445	9.774921166431429
S	14.730518656597400	11.920213217245646	13.068806588425458
S	18.977669300290721	14.272697921824490	12.431171590538678
C	11.090681207812274	21.975200862969167	12.524425961204404
C	10.776713747112272	21.466675991685058	11.282223046815972
C	10.133287038282136	22.703629848825731	13.266214510951656
C	9.464994816994830	21.692271695266186	10.761968722462337
C	8.888712484999527	22.937476748585873	12.771798355777278

H	10.424764274799927	23.068905580893851	14.256259716898143
C	8.517779512509540	22.443582814526636	11.507825158793429
H	8.153328886537093	23.501580723418016	13.354651213714305
C	11.762411634426586	19.298913108974137	10.557528955354757
C	11.663189900602484	20.674328670067318	10.407002058632500
C	12.295828495957190	18.506392033273031	9.519469852994735
C	12.187599532802180	21.283939248733805	9.239463876088051
C	12.726047234626632	19.077803066665183	8.357865017132610
H	12.342683175475829	17.420770631277126	9.675912650899745
C	12.725629918532690	20.476847599111647	8.199631792003382
H	13.127773751024625	18.453107011601428	7.551730206725981
C	7.236214271079678	22.662480407445635	10.978912641284046
C	9.058341491020689	21.163729128938236	9.522485902282227
C	7.796974176358156	21.384555598425489	9.035742897476485
C	6.876368493379156	22.147683407496309	9.762742909198783
H	6.527156678036768	23.254737175599082	11.567528728196789
H	9.766010347229853	20.563434863868356	8.943168640176664
H	7.508344360966513	20.957593355641503	8.071001424467282
H	5.874043259596522	22.323749008003514	9.362219792888446
C	13.254276415231354	21.096678591537160	7.056233111618212
C	12.177203731358766	22.679337427896368	9.069558975598142
C	13.251208896717653	22.461060198016078	6.927704992898876
C	12.702234738340922	23.255541462691156	7.943902169810744
H	11.751828538831631	23.295361783141256	9.867062641133375
H	12.699658058748563	24.343280948731245	7.843100224083654

H	13.675440235901203	22.930341117603717	6.036039476578946
H	13.674545652965977	20.460048127787758	6.269440915894621
C	16.455059846421850	22.324216173202640	14.503009263397139
H	15.640735814670583	22.715270780361450	13.871952726794387
H	17.080284818046319	23.147777779263837	14.877724861820065
H	17.063606338822790	21.636908333966090	13.899694785606920
C	19.522515110962892	20.436508017941410	14.047721752425714
H	19.254393328702470	20.870549749441519	15.029519209192204
H	20.464584177565243	20.868868765638382	13.683156217490351
H	18.719331407029507	20.642874595898814	13.326380571669272
C	18.954315682621434	18.661343697239808	9.125270079039803
H	18.560063036104562	18.499088393263474	8.111906791789211
H	18.365288046488804	19.433324209150587	9.645620166013144
H	20.003546758476897	18.983938181342559	9.071708565037824
C	15.688861765319610	19.590607308621667	9.466568157940918
H	15.554596536475881	20.476645432631027	8.827184519023167
H	16.452456814362076	18.914452494038191	9.047706647612236
H	14.741380279146812	19.044348765133922	9.527903026767243
C	11.355466511037985	13.958399437151346	9.590557142727310
H	12.286024000129766	14.496799756068093	9.342235727645480
H	11.440288946008957	12.901681585123189	9.301682819223499
H	10.514716150912259	14.430913963338600	9.063563981630228
C	15.007485681550222	13.708931915610592	9.668279146794994
H	14.071256489486226	13.142937006109968	9.816216541497461
H	15.442443551875456	13.484775147033890	8.683253715590215

H	15.710284529436560	13.419641992981710	10.461812495784558
C	18.457458139879332	13.322629244404252	10.981815789039443
H	18.304403244940350	14.028281744833924	10.146961860424522
H	19.253598080160085	12.606046971309267	10.734219561693685
H	17.525464541164474	12.774995673976537	11.177651929272432
C	18.613686979069097	13.969917575431102	18.629444911647113
H	18.032276308932023	13.053882618146622	18.429206222328229
H	19.544786631424273	13.717378477534156	19.156426908011351
H	18.018244552201331	14.653153011061226	19.248677534597665
C	15.140657119471689	13.813255307435702	19.477345820771866
H	14.475292164137269	14.481442321738719	20.053692410415131
H	15.476626434440378	12.969868656600728	20.097585090047264
H	16.001829058948996	14.402785055931252	19.134414594668719
C	10.078910833042032	13.281091714086783	15.058106318487223
H	9.065063695142035	13.124907252807095	15.453224280246801
H	10.145002756920212	12.876514854974475	14.035355965679354
H	10.804962910526545	12.774270320731855	15.707063363173045
C	11.697168807170215	14.494284360369534	20.099503406136598
H	12.366820238455258	13.844387213174969	19.510677100821542
H	12.101030348919153	14.647722036971050	21.109759398083451
H	10.706721568895043	14.023646810536333	20.160764609716907
C	11.755343857623854	20.050708704406706	18.249930716783652
H	10.926160777854301	20.731236371934497	18.489736544974878
H	11.919691810344776	19.340480301219998	19.078028595242102
H	12.669065086114303	20.636694182585032	18.085538925347564

C	15.235889449516941	19.769170659046594	19.336213070525755
H	14.774158646984574	20.068212717401810	20.287784549984320
H	16.165081473924118	20.338503017366378	19.152223810860573
H	14.546121261208690	19.966657114449834	18.503882741776422
C	18.886314281721443	19.398126762944344	19.594389302080153
H	18.847190511857775	20.464758680901202	19.856972360514860
H	17.928304670468791	18.907677584359462	19.841665694368984
H	19.695830767424233	18.906442255952506	20.152845109178184
C	14.091019509855897	10.921569623678149	14.367499476978677
C	14.825961190243271	9.829031617465864	14.786086475623652
C	12.837005486879276	11.199471923839587	14.942186839191955
C	14.270329988701921	8.936957468505589	15.737955736409443
C	12.297582763547727	10.362968508037172	15.870968878483890
H	12.310328245234860	12.097562185341472	14.598342682479869
C	14.930666290891443	7.758086189077805	16.131312797805887
C	12.981054435793640	9.201896247891373	16.278041582354280
H	11.308283563691671	10.569053927410385	16.295289761430020
C	14.344816092795769	6.882098752577869	17.006618624578316
H	15.920472378326460	7.549503341126799	15.712384791910482
C	12.413259225054757	8.289246223655679	17.179010882369472
C	13.075967386192731	7.146318993389775	17.537824492794485
H	14.870852867894733	5.966646904887331	17.292847986355195
H	11.417519899271202	8.509962257670781	17.577609652960046
H	12.620521982083396	6.443606751726457	18.240976446055061
C	16.097595913025813	9.493540731927125	14.127353434942179

C	16.040322026098504	8.534350373096402	13.074961681944187
C	17.313818199231843	10.058650884485871	14.452840397425309
C	14.814508807772157	7.988867233960553	12.648375549571453
C	17.224443334218002	8.138293010745141	12.401422239901095
C	18.490762020927836	9.638384103138961	13.791253719491042
C	14.760792000178524	7.101330738502865	11.605891053152712
H	13.897229023476651	8.299628527327112	13.156935745677574
C	17.140128500055908	7.216175815101115	11.345555455975227
C	18.450349502754090	8.701465579908929	12.805121378599084
H	19.437703617204765	10.101325918538503	14.084867127317372
C	15.931595047905814	6.706801776384607	10.948485643531370
H	13.794549969058908	6.704653214241951	11.283120351414407
H	18.066560771160542	6.922376300260955	10.839889594344903
H	19.370542992077766	8.387184354308905	12.300818761372891
H	15.877743352646108	5.999501487712146	10.117370519124675

Coordinates of PdAu₂₄(CH₃)₁₄(S-BINAS)₂ (Isomer 2)

Au	15.138648675729037	14.844926327709093	14.625154539459130
Au	15.897682717510488	15.678514101256932	17.179852370123239
Au	15.004461751409650	17.604011214248239	15.017859112349980
Au	13.089463981126510	15.793874250848480	16.288435479238352
Au	17.610069136005244	15.998689581285271	15.000976266019627
Au	17.011952112617593	13.280929565517718	15.894850996060219
Au	18.794249134681415	14.828824903557241	17.598458545293241
Au	13.504549217963646	15.196214920309304	19.130959235416121
Au	17.503462555527960	18.203518804921288	16.914694945480406
Au	11.194303979447866	13.517056770835620	17.066817955410460
Au	14.181535013505984	13.282526621275121	16.729936000440084
Au	14.306093086004346	19.007444262057010	12.291719789249482
Au	12.124693609563465	18.590986762057970	15.086067077576486
S	11.440284212101623	14.192088637572780	19.243077471897553
S	19.228033166324483	17.072227721552931	17.957423999589938
S	14.498666820609714	11.507411186921209	18.289672966084350
S	18.768758586824500	12.503955935429882	17.428754432774262
S	12.639951143741769	20.096490196097129	13.416793404593941
S	19.794301094594168	16.729407923707079	14.429732903524162
S	15.541582018096882	16.242504096433553	19.450786604925792
S	15.860629533944790	19.560867207321390	16.014019229797238
S	11.301767217920203	17.264797896455093	16.773615334689218
Au	14.384886504533446	14.085933582232103	12.093593682541528

Au	15.207312941670338	12.105959572794768	14.112338786092755
Au	17.189946418008716	13.927057638190531	12.936122548249845
Au	12.692109013801625	13.597027107300697	14.279561273554645
Au	13.185584741299477	16.400795645038798	13.384680552202207
Au	11.407949550239110	14.473056325216744	11.734417972972413
Au	16.808193867758217	14.714539440060342	10.100856060705048
Au	12.899434267674648	11.226048674682257	12.293566529189530
Au	19.204634801526584	16.092513231903883	12.298450969406707
Au	16.106180322130307	16.475840133053875	12.580508731046825
Au	15.983638158772298	10.715986769796819	16.706245261441868
Au	18.274333332431546	11.272842274063134	13.986092225513856
S	18.967510596706020	15.520036421212273	10.085420896210806
S	11.124623050761523	12.241207049339073	11.244044608178895
S	16.256791218727319	18.393577961273898	11.206961680234189
S	11.205899019697656	16.759615481620763	12.064407148513236
S	17.441993497259325	9.601723263105255	15.302068591148398
S	10.550134718326250	12.853005586861775	14.949411617256427
S	14.753408942854097	13.696527896352940	9.794288473872674
S	14.589047828122935	9.981595623236691	13.255087764345898
S	19.129972162073081	12.676760626313444	12.375278004967754
C	11.088077098726567	20.173975792855209	12.571808048768295
C	10.795045383229350	19.655783809648465	11.326672661288342
C	10.112504357558647	20.897466106233395	13.296526849299898
C	9.483565815583185	19.864416526660481	10.791386623437003
C	8.871536530678814	21.110958051416794	12.788482858131136

H	10.386811182331348	21.277234560551292	14.284332332886400
C	8.518940709589833	20.604717180436680	11.524356942566735
H	8.123374958971771	21.672008724650183	13.357746950038106
C	11.818920475491375	17.502708804970649	10.594944070275746
C	11.694663808196893	18.876856896660613	10.450856688086269
C	12.344663280919777	16.720566798621824	9.545456831852073
C	12.186781014815367	19.494458907555515	9.270275475388738
C	12.732432002398197	17.297578038448385	8.372479185894534
H	12.420178780561320	15.635238306011599	9.698455747783584
C	12.701788705186686	18.694172869896011	8.213630621777236
H	13.118175212828206	16.678034451813101	7.555384741776230
C	7.238974359719071	20.807234581598212	10.983164271923137
C	9.096100776589999	19.330922419062443	9.546539678707777
C	7.839422101446370	19.543728864848198	9.043899885484645
C	6.901508992682230	20.295592041564305	9.759204105928768
H	6.514847624642297	21.381921715723120	11.569919461417932
H	9.814196889132974	18.734021078134582	8.977280587232132
H	7.566495306139985	19.118095427773934	8.074173660008247
H	5.903335608231659	20.462097787952079	9.345340587761152
C	13.169015370399975	19.317911821668424	7.045844503850434
C	12.152630703010566	20.890585340714704	9.096580749594493
C	13.142905616978041	20.680657287279395	6.912956626663092
C	12.631040555816510	21.470806621004318	7.951346878736402
H	11.750920792407086	21.504448049798917	9.908864757718192
H	12.618806594420906	22.558882124292762	7.848747332649769

H	13.523413167918530	21.150511973623143	6.002193555002397
H	13.564062832369061	18.681622949811167	6.246514626602288
C	16.629089390419754	20.417377650475281	14.620717849114023
H	15.826574185789612	20.918552918676436	14.057608004640887
H	17.351056555328711	21.154711920733124	14.999784754200856
H	17.131027375031820	19.707108425710540	13.947647027020103
C	19.726079865107952	18.534424706148858	14.353278755184883
H	19.493333806206302	18.908650544102620	15.366605577656467
H	20.704761435739378	18.910820216547304	14.023187737074579
H	18.947085392940913	18.870698600215281	13.656334604795216
C	18.938712779983980	17.103690050369956	9.221180885119214
H	18.541562617761031	16.950082160277958	8.207833285801708
H	18.323143641402460	17.839025902972754	9.764157560745231
H	19.972211865544445	17.472857909436669	9.161714723590192
C	15.666163830980897	17.866076174805237	9.587944903237135
H	15.533599066695949	18.748176965077629	8.942826671117839
H	16.396619270804521	17.162272451115093	9.150749460932900
H	14.708771021278110	17.343258769677185	9.684380197808078
C	11.524000101281484	12.150633531010619	9.485609862633908
H	12.482613639709074	12.653451513325624	9.272750371402035
H	11.574121654273910	11.094408187795532	9.185246647004238
H	10.720102781386066	12.656409578651848	8.932252837769163
C	15.192487112022178	11.941383493960993	9.804631282615629
H	14.263528250098942	11.357036731013006	9.936562743402858
H	15.685417878272331	11.677802075587151	8.858160210148133

H	15.854017132552622	11.719671471238428	10.655627298033895
C	18.806418194466321	11.800650440769775	10.825397332314260
H	18.724723017641708	12.550201364076727	10.021487012815488
H	19.651829171528568	11.124698452661452	10.632542196520005
H	17.873843117401922	11.225219874850980	10.875909934063463
C	13.773994470823837	9.132123686696657	14.628502711833146
H	13.119117861463689	8.341026131282140	14.235664232889539
H	14.564105072021203	8.700699253686510	15.263763111057303
H	13.190391811667366	9.840121919802462	15.232599897341418
C	15.557942044748675	12.344301466072235	19.490456833981114
H	14.921176750253466	13.033772018525685	20.076257691836787
H	16.031525440915424	11.599213609614134	20.144540240031287
H	16.328967723918275	12.939116293591228	18.976523604733448
C	10.678060475374069	11.050056167201159	14.995257879760150
H	9.718671646713297	10.640482325052313	15.342270936087088
H	10.902715578410817	10.695284611978011	13.972617803991584
H	11.483173603457370	10.730834937034489	15.668311366270768
C	11.762340710379908	12.669775904287464	20.154959223124344
H	12.549063166302837	12.072742675102198	19.660900955116901
H	12.072695587297607	12.932511756002359	21.175607791632732
H	10.830786628123185	12.086630019406028	20.182599161370131
C	11.718433164211259	18.126288694866872	18.307717541090817
H	10.893829110432414	18.808169674289751	18.560279127596861
H	11.844753381504308	17.364485113674544	19.097556515158541
H	12.650467387979857	18.696004533465750	18.209630812700045

C	15.169945615387910	18.008327367937301	19.386191266800878
H	14.645678535406116	18.309288901705433	20.304392525011814
H	16.127842685715560	18.549558192006181	19.290054950751752
H	14.555618188420830	18.246348243099305	18.506194103106186
C	18.882761251654557	17.315709975460145	19.709282038567913
H	18.934666787558058	18.391319813815446	19.928880689553111
H	17.880151077201702	16.925737851584675	19.957364878570740
H	19.641621524909706	16.772761216198248	20.289792983034218
C	18.609035734051766	9.075304601376491	16.519029277667141
C	19.834242466357992	9.654916248977335	16.787449863495574
C	18.189554775184597	7.910813782741026	17.198974381539177
C	20.666084997401040	9.043351158258261	17.775077188094521
C	18.992811899527769	7.300884927883515	18.109404263244095
H	17.205209199933098	7.502247998957713	16.951939711342046
C	21.920705353592602	9.575926744968523	18.124605195112750
C	20.251875062295294	7.844582556482374	18.419450685891380
H	18.676521197500815	6.376517952260225	18.604919024129888
C	22.731526047917406	8.943865694172954	19.030677320090778
H	22.244627585601098	10.509046681159788	17.652754171686357
C	21.106460779341830	7.216264841167556	19.337427864318620
C	22.331183286913841	7.746940044435982	19.636595990515161
H	23.705162905738884	9.376499510576510	19.278944978287846
H	20.764419853075523	6.285579768698160	19.804310841876127
H	22.992908889560187	7.244758253774488	20.346372353492928
C	20.403745071416910	10.799899907535981	16.045770486328625

C	21.456124106394046	10.521775205936567	15.125823523562159
C	20.062894286736341	12.123953305736887	16.294478044849011
C	21.850610670728933	9.204431150294127	14.824943599231737
C	22.139346683015308	11.587352919744490	14.482531860125372
C	20.740099671343479	13.169670737917670	15.629468610376531
C	22.885954033786035	8.954524325039813	13.962562877544464
H	21.311945944151006	8.373738354550417	15.292294751341499
C	23.200160156690924	11.301323251897557	13.609021320203778
C	21.744716766306972	12.910147710053316	14.751691378435035
H	20.435605270081560	14.204325538976653	15.842498014820922
C	23.580487208209384	10.009519309473207	13.358989170323962
H	23.169325498167602	7.921539660340547	13.744976064993066
H	23.715139719277598	12.141039892980572	13.131787571188914
H	22.257906151347882	13.733777935911249	14.244119621947688
H	24.418251614270769	9.802407767758201	12.686257737894437

Coordinates of PdAu₂₄(CH₃)₁₄(S-BINAS)₂ (Isomer 3)

Au	16.950119491549209	15.853005662212425	14.585838331530118
Au	17.793534023376097	16.692400295868858	17.096159792810990
Au	16.805884913472191	18.594582850561814	14.993960617090938
Au	14.923901431252544	16.787542834566679	16.290625356164153
Au	19.396331761603928	17.115034492074482	14.884107224434816
Au	18.896719762976531	14.302367166571388	15.803713610628538
Au	20.797417791151311	16.283456109154113	17.320246287063586
Au	15.408456792933620	16.202448971520827	19.196203170515560
Au	19.266218174511273	19.481331355098025	16.792662987951637
Au	13.111602037277255	14.531445901405892	17.210082629367950
Au	16.012581737074509	14.286611942774698	16.705262271575688
Au	16.103231829723935	19.902915493301808	12.186713302048535
Au	13.985393489028365	19.503678165088559	15.072119010794623
S	13.349095117494466	15.206660575964037	19.394199760222293
S	21.097680195965971	18.515643695440314	17.792540589321305
S	16.298490569798346	12.517490133098134	18.272905880094459
S	20.925478488507810	13.994557796882090	16.999103654642997
S	14.454165783474414	20.978002775602750	13.351203216813007
S	21.392431204725987	18.171349016528129	14.154406684328015
S	17.473963793966870	17.219337116485267	19.376415846339917
S	17.409792835696823	20.622962424992615	16.030790060357624
S	13.127886777608145	18.233345912721848	16.794634451199862
Au	16.109855887282563	14.994040695180720	12.077945432516303

Au	17.010913089423624	13.111550376586742	14.126026026488184
Au	18.983884580650013	14.910404983183595	12.902309859988309
Au	14.480596108764573	14.598368822895450	14.295821873350057
Au	14.987958318067463	17.336855891927410	13.315777278075181
Au	13.200286895370130	15.406658461024705	11.786497997499147
Au	18.494125411776583	15.520497283199282	10.009894406039956
Au	14.322639832859453	12.274580718960443	12.404489334494018
Au	20.888606769651396	17.087334760519866	12.190288348955880
Au	17.810791212392100	17.384308514806577	12.419755956373399
Au	17.885377601657957	11.716257627585096	16.798595696322998
Au	19.891105820067171	12.185148429152340	13.912768025526864
S	20.697277157537474	16.195269861506812	10.077926308847792
S	18.039572137588085	19.298582289365772	11.064604890623462
S	12.968644878272633	17.707021442188655	12.063291659813553
S	19.364341603834937	10.570994286577470	15.462481811431546
S	12.320511354516844	14.010129935216870	15.119993821827725
S	16.345765987869395	14.717173656090077	9.748368180564361
S	16.262698428469857	11.186193647683149	13.004303678070611
S	20.713185991052981	13.452285274210963	12.170597198700026
C	12.876838596412352	21.065106525467669	12.554898401854832
C	12.533075204586304	20.573969387656174	11.311364368464549
C	11.931797158776149	21.768256640066912	13.335710540941998
C	11.202619773966035	20.796858104450365	10.834075228789970
C	10.672089362858559	21.997883540212523	12.882128974250561
H	12.246176646085559	22.116710654101418	14.324541905302921

C	10.270312396877875	21.523192519053570	11.621360818959353
H	9.948821073777248	22.544534470899098	13.496739300409079
C	13.560033699057461	18.431624653963272	10.575517578730709
C	13.402159610573552	19.799004506954716	10.404948330995342
C	14.113232188206773	17.644849331466915	9.545084065551389
C	13.858508261159521	20.403268429836078	9.205336114834537
C	14.489323299343528	18.207909136601167	8.362717564138340
H	14.221231709880380	16.563559703352677	9.713849201038350
C	14.401198394949221	19.598177540429791	8.164973701543872
H	14.897872030013643	17.579883175574967	7.563016304540888
C	8.971191610922725	21.742945746093184	11.135591470071573
C	10.762064490909603	20.297010204917648	9.591563385431176
C	9.485390956764535	20.521838733900758	9.145799038979506
C	8.579260799918528	21.257627313611447	9.917059032290215
H	8.274839185736425	22.310892130386481	11.762763604530280
H	11.458888979897010	19.718659555192403	8.977775609230495
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H	7.564153667224923	21.436524826010153	9.551102958107480
C	14.837146006157473	20.208232709855384	6.978030821320821
C	13.765364028030044	21.792067639905497	8.995912750072939
C	14.746245654101406	21.563845731826003	6.809401807838085
C	14.203042911134768	22.358615427053589	7.829288370328393
H	13.344481196695401	22.412366814062814	9.793681337504035
H	14.131750236588040	23.441867578015721	7.692045160530721
H	15.093552420717316	22.031489895585466	5.883420749440592

H	15.254812795878562	19.570836248145330	6.189798137523002
C	17.899575309398990	21.742762842224344	14.700595039963199
H	16.973857229037922	22.100378967120520	14.222042057810091
H	18.455945826589179	22.590062808903546	15.126794536705281
H	18.509984252747614	21.231034432200570	13.943691691568137
C	20.847036158018536	19.856337095738517	13.785103998950385
H	20.610033910519508	20.349773528817060	14.747578501420788
H	21.661424139895733	20.387752928730347	13.272768157559225
H	19.949693540181347	19.850431949909058	13.146681774904607
C	20.830823293509358	17.678379417465869	9.055431332538175
H	20.487767598945481	17.454123068750945	8.035667397871832
H	20.236939133203958	18.501135736042102	9.482451110143669
H	21.889540389424521	17.972282800240496	9.041999510010216
C	17.518276116876862	18.777301213842058	9.419376120604941
H	17.475316015621171	19.656094842775538	8.758092091086102
H	18.245957137808823	18.035914575674450	9.045111503480205
H	16.532913779516253	18.299830735556988	9.457080817117598
C	16.512594995646367	12.929988385975930	9.529171268334538
H	15.515296888372568	12.483933653559559	9.669719253817158
H	16.886878496155120	12.718891499127773	8.517831902290419
H	17.190326510677568	12.498524275927487	10.279581822796741
C	20.080383143134362	12.573321451617238	10.720683027960398
H	19.926479998308849	13.315877367015384	9.916370081190262
H	20.826754444725818	11.827650053803213	10.412289450648423
H	19.127339069950999	12.074067616628767	10.941092184052229

C	15.879538477665225	9.975770161859028	14.289503558093751
H	15.157827321349869	9.235970643325063	13.909923926912855
H	16.829031725477783	9.486245021889445	14.558758770015883
H	15.462304805550890	10.468582933173858	15.176901732487957
C	20.874759387719550	10.464409745609291	16.447919598946516
H	20.664043899825661	9.891324550188170	17.361392475530540
H	21.634582299256998	9.944745148979710	15.846703384463853
H	21.242480204943597	11.472480750725865	16.699829062024101
C	20.526397475575852	13.259198052513073	18.605507382729222
H	19.892362396956297	12.366309788623290	18.438696379699046
H	21.467292662856885	12.967771578295636	19.095377072311674
H	19.981466989682517	13.961807256395952	19.246965546021713
C	17.242239959232084	13.379737919813222	19.549324378738199
H	16.522379489023617	13.947823696370454	20.165948354553919
H	17.793482896769863	12.658185547639107	20.169678263676996
H	17.936631668501949	14.095341164808083	19.084844546864812
C	13.684071195378658	13.686900575570025	20.306334687953687
H	14.423752622004507	13.063560965424694	19.773413014151444
H	14.052408294373029	13.946473072451719	21.309202349719985
H	12.739178193464786	13.132159871288859	20.391441077687087
C	13.577619255655556	19.109430979952212	18.310360150207668
H	12.749374419862393	19.780321196610927	18.581280380851208
H	13.738189379721542	18.357534434610436	19.103252074507655
H	14.497520952568259	19.692250316164234	18.172763750372958
C	17.099485599859925	18.985532822325382	19.347751301548904

H	16.579331257357769	19.263663439353788	20.275737239530013
H	18.054502111952701	19.532508966242940	19.256833422269640
H	16.480983104944670	19.240234349325608	18.475207374792287
C	20.710709787085484	18.641029449734958	19.552658788607058
H	20.650333337447808	19.704708983634820	19.823394186415889
H	19.756444475622850	18.135019247767911	19.780902508793332
H	21.520192757730246	18.156749598583978	20.117214845946133
C	12.299943614399705	12.262090907158507	14.962822498885306
C	12.935346811849378	11.390098159015027	15.812536379529773
C	11.528105419741781	11.770620202226578	13.877420745914161
C	12.857335339881448	10.003705419780983	15.607111735533733
H	13.518649678571254	11.786329474908603	16.655545570242595
C	11.469639644714043	10.421227700547361	13.652846522644564
C	13.503747377889248	9.088258311448895	16.459814056103788
C	12.137652869803340	9.505119990147101	14.485648325672072
H	10.866031751883867	10.044751336453803	12.819457167232272
C	13.454465002022662	7.743508845371925	16.210750217417448
H	14.065483129350749	9.479968102782994	17.314874154006965
C	12.105704972723521	8.118781944850449	14.257018321421347
C	12.753831728625372	7.252745952539954	15.097580170694927
H	13.968834127478859	7.046972289778918	16.878816638466994
H	11.555761488092795	7.745014070155787	13.386656345349040
H	12.730082197444824	6.176268045874104	14.904124020897482
C	10.672392738609547	12.710331354920244	13.131590890025521
C	9.418616413485376	13.038362339378534	13.724792163942457

C	11.034263990264243	13.328910920912399	11.956622797993433
C	9.050657584048126	12.544603186255008	14.989239119794263
C	8.541523956941013	13.950197339272162	13.080024001327761
C	10.131866505736250	14.192624114208208	11.293727168464216
C	7.890853373251431	12.951064238204333	15.595415499753082
H	9.724963718018065	11.851942574590915	15.503001089045400
C	7.348835455546662	14.329122676314825	13.713439618358199
C	8.920633485705046	14.488895753595042	11.836149729459720
H	10.455417476841708	14.656225698206564	10.356145449847647
C	7.028037420448642	13.848587343371308	14.955305998370429
H	7.646653028882284	12.584031240433847	16.596224779255234
H	6.697505917377574	15.048220540174480	13.204372529915327
H	8.246320024032698	15.190201108346338	11.333781214825295
H	6.110721614677067	14.175217313817299	15.453790268216938
S	12.627594869759129	13.232226057323176	11.182872604733745

Coordinates of PdAu₂₄(CH₃)₁₄(*S*-BINAS)₂ (Isomer 4)

Au	14.849645865253027	12.543973253130897	12.993947877992978
Au	12.785912872748725	10.711131609550982	13.062438269659014
Au	15.404845895408958	10.078438383207969	11.878818985399711
Au	15.193851009815061	10.405211494698825	14.794090360103647
Au	13.381364207047717	12.044298894654792	10.676757645735496
Au	12.285861161405970	13.610000193216001	12.899076818506297
Au	10.491482942955336	11.685136330435949	11.225348312314921
Au	12.687536386878232	9.470157541134901	15.963548348784482
Au	12.811294611272237	9.081577079191483	10.467970026619993
Au	14.782242174108982	11.469190888318220	17.864114858130769
Au	13.396598849483103	12.404851340452284	15.396975266066011
Au	18.276573234664340	10.220876705188767	10.491529139846849
Au	17.411957772264273	8.600923198804695	13.598729338040354
S	10.640501397276211	9.718518196659982	10.045156490335055
S	9.977266203326328	13.629876864288436	12.363908111033112
S	18.730894783814644	8.348973703800457	11.716175888277586
S	12.772711609169759	12.259523098600244	8.394058670792008
S	11.530071468837544	8.961042042017549	14.032368674576674
S	14.897809119463316	8.100948504546301	10.702701666161428
S	16.348144842207276	8.537298881145940	15.647389547257543
Au	16.989245600298954	14.315516051811480	12.906720338546265
Au	14.318497111420511	15.007299702907536	14.124627556326253
Au	14.517522233927243	14.696461668686039	11.209721034673704
Au	16.215044113096305	13.115871416796343	15.327215157153510

Au	17.420953984992043	11.494369337484656	13.126285877231709
Au	19.192561833838177	13.385864425619747	14.799800937298880
Au	17.092431637186735	15.578589577826390	9.920185877712061
Au	16.999309881825997	16.015429161004160	15.396174595569194
Au	14.398453508195756	13.889841697145405	8.319231752387934
Au	16.211819091928700	12.609317193144520	10.590181216644449
Au	11.612324754356282	14.915173514579315	15.516289289526219
Au	12.322388073176649	16.600811265379864	12.494608037227305
S	15.962203952834386	15.524926381011170	7.919883085649375
S	19.121312776219327	15.361567310861332	15.959257466409444
S	17.676218895287359	11.812807151968924	8.923217288149003
S	19.715832480117562	11.332708559813685	13.871178780092967
S	11.217302839546047	16.927830728884850	14.480104752853956
S	16.697737286134700	12.705114050597469	17.601286622997264
S	18.364565853606553	15.908618611551253	11.824669249033832
S	14.994455165091146	17.095477620745548	15.000347027213504
S	13.410415021950270	16.648144569486988	10.463627643751838
C	20.345487760320950	8.305179779623161	12.430765435134127
C	21.316463572679371	9.283070383167198	12.355613669554188
C	20.604806069685758	7.080385101468625	13.086055833608961
C	22.592200575094893	9.022772883849266	12.951783288802824
C	21.817475555891811	6.820205709740431	13.639670620907525
H	19.795831963201074	6.344561605760145	13.132035283295794
C	22.846377998902348	7.777986895896397	13.586582109173831
H	22.011685177033879	5.864397192088409	14.136876907672677

C	20.633769721467150	11.680658751547806	12.416158397237025
C	21.187436409878572	10.612812612331609	11.723659279692043
C	20.867215550672928	13.002323836429502	11.982139338520970
C	21.883752802078416	10.860594587064387	10.512423590090275
C	21.618591491221046	13.252325592629699	10.871673804346857
H	20.434185744564608	13.824420600278630	12.569258415810989
C	22.106563640623737	12.195697997975220	10.079557783508202
H	21.804164721440074	14.283234288697468	10.552664575411878
C	24.106080262088611	7.527240184306196	14.152326490639929
C	23.629298335046908	9.977424271287987	12.945252098682376
C	24.850676034535617	9.705818813784218	13.504993344034109
C	25.098465374467061	8.469414682350754	14.109876886542070
H	24.270901309524263	6.558436820045489	14.637003078152862
H	23.449285630531826	10.951499091710119	12.483490045246880
H	25.635576423773848	10.467487694740853	13.483138371717310
H	26.076858125448201	8.264133043579154	14.552784790333437
C	22.785713222129534	12.421627391885751	8.871223759710832
C	22.372041954579998	9.807549394584681	9.717762878344093
C	23.227567656346267	11.375224880398854	8.105431113887221
C	23.017649716225520	10.058109115913997	8.536821521711948
H	22.201573144458493	8.779801826144430	10.055553944026080
H	23.363531628980333	9.224741420431313	7.919765150537644
H	23.739793624347364	11.560805466999332	7.156957157819434
H	22.942442268940052	13.456789270857229	8.547643855022018
C	15.704060198859276	8.292080115559799	9.098464502462644

H	16.784979860488743	8.137894267587685	9.248435147587093
H	15.303254685454675	7.539377710140475	8.404131085718863
H	15.549600917006179	9.299912267974264	8.690571299725139
C	13.575157101209538	10.863986623300351	7.566591089752412
H	13.135534718241638	9.931641648975036	7.966367630266071
H	13.387906660611691	10.940563638879926	6.486150597939965
H	14.658757368152177	10.865384988574808	7.753257249988239
C	17.058291659363892	14.711656226485086	6.733459007723363
H	17.992469325656945	15.285662942680425	6.654096537271148
H	17.274636075206800	13.676973181404602	7.042142201585648
H	16.543284734011429	14.697175145066955	5.762383095413516
C	19.055255856283104	12.974481249658821	8.925387455616359
H	19.854249238620444	12.595816067735004	8.269424892293657
H	18.688477646272968	13.954499411312943	8.571692750557878
H	19.450183631887182	13.106103476950549	9.939167150731052
C	20.164253783642216	16.419841758489852	14.928646499039699
H	19.879045698792886	16.324969644956411	13.867534288465936
H	20.053252248679268	17.461948866825857	15.259171511596982
H	21.207054508535936	16.095098152679792	15.053249548975993
C	17.766394649206017	17.502918509059519	12.431008403051704
H	18.139870277961855	17.644469683438889	13.460137641212601
H	18.133647396147914	18.302113369221694	11.770833224285361
H	16.668632773864445	17.518375004794411	12.465798427042273
C	14.568990944494715	18.023803880001687	10.675608426738291
H	15.458140459979473	17.823835475051911	10.052097301966700

H	14.074335116830705	18.947932962908936	10.344423784650855
H	14.874573618688100	18.128557869487022	11.725579764120498
C	14.305970148014971	17.306197385130659	16.658829534385788
H	14.696705699674608	18.244056770458840	17.078639929864000
H	13.208200460079039	17.351646893353863	16.575825364896541
H	14.591398651914085	16.467694212276186	17.307049219729539
C	9.466933050397049	16.788996865027034	14.050151436790360
H	8.882682570537638	16.696212098620030	14.975808567872264
H	9.174561511782349	17.699500579168067	13.508689826408323
H	9.301093413444420	15.910441350001484	13.404162665706947
C	9.213276694655340	13.048037912463172	13.897243458225855
H	9.321272152149728	13.848978292040405	14.652637481931800
H	8.148735157710371	12.841123974232879	13.713696628846106
H	9.714172985388673	12.146732627964278	14.275366765767629
C	16.456025050012212	14.268714819147155	18.471247731900842
H	16.519516624483860	14.088841162558300	19.554664661684182
H	17.257702302178636	14.951086720260129	18.146820601138288
H	15.476847439179707	14.707559317093716	18.236263815694798
C	15.230183519257329	7.120239398771830	15.540504762170716
H	15.756238005990525	6.236852417075313	15.927837331986858
H	14.338605708998307	7.337296435726694	16.154435576956640
H	14.915103731608475	6.934852903483331	14.506744005762410
C	12.336112421935740	7.482357055913301	13.383174155686238
H	12.113569667648756	6.626387015659605	14.036489519101220
H	11.946821065802675	7.308546723107041	12.364092473752903

H	13.423631935602042	7.632454290007679	13.310381555469519
C	9.695179570127587	8.574533407747298	11.073359062975364
H	9.839943246476230	7.554463328748758	10.688856348264386
H	10.027222639349723	8.636607269162607	12.124680552739887
H	8.633819487922292	8.853249621193292	11.015952120920787
C	12.218170077278540	13.371676542537593	18.384526198008579
C	12.030788673771477	12.435765490910201	19.383679745811225
C	12.884546917446313	14.577877862907652	18.667557318603922
C	12.545921881173951	12.669735026728096	20.678476968089264
C	13.364351746667385	14.829982860912354	19.919308244061067
H	12.982434668681309	15.306848870796655	17.854206358111302
C	12.395632357956821	11.725378717583677	21.710839427186649
C	13.225343191874346	13.886652967843219	20.954918087712258
H	13.876922428613231	15.774079090465113	20.134742595133197
C	12.886867776148030	11.973838479545378	22.963770309061331
H	11.888843965402167	10.781122102613518	21.484121825015649
C	13.712046233246749	14.113516760395571	22.253244743140854
C	13.546249079875478	13.179363658186753	23.241659116692166
H	12.764220352120727	11.226842069846102	23.753075816489535
H	14.226963238335522	15.057936009325381	22.458016092726893
H	13.927270320077668	13.366606388116036	24.249393520067457
C	11.171121951439755	11.267419446302489	19.155380931133429
C	9.791327610815340	11.405422094028566	19.479106936336738
C	11.632265096342783	10.065534778494385	18.671215271664895
C	9.261570236955507	12.625797316879208	19.936122041761919

C	8.909206340017937	10.304249663424800	19.316580295145542
C	10.749176172597528	8.968849362623057	18.531690310067553
C	7.926291267777976	12.751110265180246	20.219290355651555
H	9.936482563382155	13.479561663232417	20.052661899090438
C	7.549524846268299	10.460366544401499	19.624786408549806
C	9.431897557106307	9.084802450580014	18.848255292164744
H	11.150330284006072	8.029761484800819	18.140067177410749
C	7.062134295225415	11.661156403141549	20.068347351363226
H	7.532099088136846	13.711904541315723	20.560995827489535
H	6.887870476123078	9.597544133498953	19.500216999322951
H	8.753220612121751	8.234661035230092	18.722490354462273
H	5.998254937126580	11.771256477765299	20.299166860807819
S	13.303011996193790	9.723493116992636	18.182902394781436
S	11.547377167840807	12.997733738672284	16.804233118138285

Coordinates of PdAu₂₄(CH₃)₁₄(S-BINAS)₂ (Isomer 5)

Au	12.334800	13.254800	14.770800
Au	10.240300	11.714900	13.786800
Au	13.120500	10.863200	13.583600
Au	11.947000	10.912700	16.247700
Au	11.839900	13.060100	12.037500
Au	10.025600	14.611400	13.883300
Au	8.935100	13.026000	11.375900
Au	9.135400	10.032400	16.358000
Au	11.316200	10.307300	11.094800
Au	10.944500	11.437000	18.986600
Au	10.196500	13.026000	16.496800
Au	16.545600	11.334800	13.283600
Au	14.524600	9.134300	15.459900
S	9.294400	9.875300	18.641300
S	9.426900	11.172600	10.098900
S	8.042900	13.584600	17.318300
S	8.197800	14.954300	12.406100
S	16.375500	9.175000	14.072800
S	12.031800	13.666800	9.744200
S	8.707800	9.964700	14.087300
S	13.131500	9.161900	11.945600
S	12.802200	8.823400	16.958700
Au	14.331800	14.945600	15.700200

Au	11.516200	15.628900	15.978600
Au	12.727800	15.640400	13.367200
Au	12.853800	13.438500	17.505400
Au	14.658800	12.027200	15.651500
Au	15.834900	13.550600	17.973300
Au	15.703500	16.505500	13.406000
Au	13.528000	16.233600	18.356800
Au	13.550500	15.154500	10.659600
Au	14.458900	13.447500	13.049800
Au	8.435400	15.558100	16.178800
Au	10.376400	17.573800	13.975300
S	15.347500	15.295100	19.393100
S	16.643200	11.618400	16.984700
S	8.587800	17.725700	15.410500
S	12.631800	12.801900	19.784000
S	16.168700	16.335400	15.393400
S	11.731100	17.403700	17.520500
S	12.018500	17.683600	12.376300
C	17.607500	8.783000	15.276600
C	18.555000	9.659600	15.760600
C	17.558200	7.448700	15.736100
C	19.477000	9.194500	16.745200
C	18.434500	6.994500	16.671900
H	16.786400	6.792000	15.323000
C	19.415400	7.851300	17.206700

H	18.384300	5.960600	17.028500
C	17.974100	12.078800	15.929300
C	18.708700	11.062700	15.330100
C	18.315200	13.424900	15.707300
C	19.782000	11.394800	14.458700
C	19.336500	13.753600	14.865700
H	17.737300	14.195200	16.236600
C	20.075800	12.760600	14.201200
H	19.597400	14.801500	14.686300
C	20.325800	7.412000	18.180200
C	20.456900	10.040200	17.296000
C	21.333000	9.584000	18.246200
C	21.272000	8.259800	18.693900
H	20.259600	6.373200	18.521200
H	20.508000	11.077300	16.950900
H	22.081500	10.265800	18.661700
H	21.978000	7.905800	19.451600
C	21.104800	13.090400	13.304300
C	20.575700	10.411500	13.838200
C	21.849300	12.112100	12.702500
C	21.587100	10.764100	12.983100
H	20.363300	9.358300	14.043100
H	22.188500	9.985400	12.505500
H	22.645300	12.377500	12.002400
H	21.290100	14.148800	13.092000

C	14.535700	9.624900	10.906000
H	15.448200	9.258900	11.402100
H	14.426000	9.159400	9.916300
H	14.609000	10.716900	10.810000
C	13.104700	12.400700	9.020700
H	12.595600	11.421600	9.103500
H	13.269700	12.653100	7.962900
H	14.070000	12.354700	9.542900
C	16.661400	16.498600	19.091100
H	16.760900	16.704800	18.015000
H	16.411900	17.423500	19.629300
H	17.602600	16.083600	19.476900
C	15.563000	17.875600	14.700600
H	14.976200	18.395400	15.473000
H	16.428600	18.484300	14.395400
H	14.932900	17.657000	13.825800
C	13.026700	19.101600	12.864000
H	13.964100	19.061900	12.285000
H	12.467300	20.012400	12.609200
H	13.250400	19.100200	13.937300
C	10.414300	17.128100	18.727800
H	10.603300	17.749600	19.615200
H	9.460700	17.410100	18.254400
H	10.363300	16.070600	19.022300
C	7.196700	17.890600	14.271800

H	6.259500	17.750600	14.828800
H	7.231200	18.900300	13.840200
H	7.274400	17.150500	13.458500
C	6.714800	14.436200	13.305000
H	6.682400	14.980300	14.268500
H	5.833200	14.683500	12.696000
H	6.729700	13.358700	13.507400
C	6.989400	12.578800	16.253400
H	6.991100	11.549700	16.658000
H	5.968300	12.986000	16.245700
H	7.394300	12.541000	15.231800
C	11.750300	14.155700	20.593100
H	11.508200	13.860200	21.624200
H	12.411400	15.039600	20.593000
H	10.824100	14.398000	20.055300
C	7.803200	10.697000	19.239600
H	7.744900	11.730700	18.856100
H	6.925800	10.119500	18.915100
H	7.848300	10.723600	20.336700
C	11.783200	7.523200	16.222000
H	12.142700	6.553900	16.596000
H	10.735800	7.687900	16.529800
H	11.845100	7.538100	15.126900
C	9.642400	8.533000	13.502100
H	9.156800	7.609100	13.848000

H	9.665200	8.570300	12.399100
H	10.678500	8.576700	13.864600
C	8.136000	9.988100	10.535800
H	8.398800	9.009300	10.109700
H	8.029400	9.909700	11.630700
H	7.188400	10.341400	10.106100
S	16.602300	13.222400	11.959700
S	15.239300	16.678700	11.262500
C	16.249400	15.955100	9.948500
C	17.515500	15.501300	10.273500
C	15.801300	15.855100	8.610600
C	18.335800	14.911100	9.274100
C	16.582000	15.314100	7.637300
H	14.797100	16.236400	8.390100
C	19.616400	14.394700	9.557100
C	17.864000	14.818800	7.936700
H	16.225500	15.260200	6.602600
C	20.391200	13.841000	8.571600
H	19.989300	14.453100	10.583900
C	18.683900	14.254900	6.947700
C	19.930400	13.778600	7.250100
H	21.380800	13.446200	8.818100
H	18.295300	14.205300	5.924200
H	20.559400	13.344300	6.467500
C	18.093900	15.657200	11.618400

C	18.889500	16.824100	11.839800
C	17.971300	14.737800	12.639400
C	18.914500	17.881800	10.909200
C	19.647200	16.961700	13.034000
C	18.784800	14.844700	13.781100
C	19.636200	19.020100	11.152000
H	18.326400	17.783100	9.991900
C	20.393100	18.134900	13.247500
C	19.619600	15.913900	13.966000
H	18.714500	14.084000	14.563600
C	20.384100	19.149300	12.330300
H	19.625600	19.834700	10.421100
H	20.971000	18.225100	14.173400
H	20.251700	15.974500	14.859100
H	20.956700	20.061200	12.514800

Coordinates of PdAu₂₄(CH₃)₁₄(S-BINAS)₂ (Isomer 6)

Au	12.926842104531575	13.818804334439831	16.903445935644093
Au	12.926842	13.818804	16.903446
Au	10.478445	13.001367	15.900117
Au	12.412121	11.118413	17.118945
Au	11.054510	13.085969	18.815182
Au	12.807972	12.492230	14.478387
Au	11.886953	15.309480	14.780364
Au	10.409563	13.293405	12.876742
Au	8.213412	13.781975	17.999524
Au	10.801345	10.197693	14.601938
Au	10.123796	15.399337	20.504331
Au	10.787221	15.508327	17.523468
Au	15.101984	9.712247	18.194752
Au	12.085342	10.395305	20.072981
S	7.959649	14.791491	20.041646
S	9.943729	11.054985	12.648072
S	9.346422	17.342462	17.076836
S	10.827952	15.549669	12.670000
S	13.725064	8.796686	19.779260
S	13.521713	11.628220	12.387127
S	8.142500	12.633621	15.991596
S	11.540912	9.037281	16.460149
S	10.328117	11.770214	20.641703

Au	15.397055	14.600914	17.980905
Au	13.414876	16.530266	16.699476
Au	14.789240	14.614259	14.996675
Au	13.068873	15.203731	19.325134
Au	13.918921	12.401074	19.085502
Au	15.402660	14.387244	20.991152
Au	17.509546	13.886421	15.610552
Au	15.008449	17.415280	19.202242
Au	15.597319	12.392314	13.008363
Au	15.087965	12.197086	16.300604
Au	10.911178	17.997518	15.507725
Au	14.002575	17.393540	13.824852
S	15.970584	16.607034	21.131948
S	16.229544	10.147225	16.229422
S	14.971089	12.118256	21.231629
S	12.400624	19.019934	14.079210
S	12.169552	16.039306	21.352119
S	17.672036	15.099934	17.570694
S	14.278246	18.625075	17.369852
C	14.366095	8.740396	21.423427
C	15.582667	9.234511	21.848280
C	13.503716	8.071469	22.320371
C	15.950814	9.050750	23.215086
C	13.850347	7.885355	23.621706
H	12.545920	7.706359	21.935446

C	15.080374	8.366743	24.107103
H	13.175876	7.360988	24.307722
C	16.434810	11.291562	20.719791
C	16.556133	9.937331	20.988690
C	17.476442	11.987156	20.069674
C	17.732312	9.253943	20.579444
C	18.624813	11.348913	19.714552
H	17.331357	13.057410	19.869002
C	18.783697	9.969335	19.943986
H	19.438636	11.905138	19.235606
C	15.457047	8.190988	25.448154
C	17.166445	9.540571	23.727969
C	17.509917	9.353016	25.041750
C	16.652633	8.670081	25.912175
H	14.765300	7.664223	26.114221
H	17.840147	10.081223	23.055438
H	18.460755	9.745133	25.413641
H	16.934673	8.527267	26.958011
C	19.949455	9.288188	19.562625
C	17.906429	7.877130	20.804264
C	20.092160	7.945980	19.799828
C	19.057565	7.237553	20.424200
H	17.094833	7.321404	21.284007
H	19.165491	6.164645	20.606190
H	21.009897	7.430449	19.501776

H	20.745326	9.859902	19.073463
C	12.972306	8.096425	15.885995
H	13.509264	7.731677	16.775909
H	12.628104	7.251433	15.273262
H	13.658686	8.728032	15.304269
C	13.683230	9.848630	12.670752
H	12.674970	9.443751	12.872107
H	14.109797	9.385990	11.768753
H	14.334666	9.649288	13.533315
C	17.974384	10.445620	16.583180
H	18.431772	9.524060	16.973366
H	18.451490	10.738850	15.635722
H	18.095869	11.253719	17.315920
C	17.730575	16.618074	20.732646
H	17.924774	16.061519	19.798066
H	18.056004	17.660960	20.622112
H	18.274061	16.138461	21.558902
C	17.558173	16.808556	16.983586
H	17.328941	17.449977	17.854564
H	18.513980	17.100573	16.527895
H	16.740778	16.912919	16.252419
C	12.825683	19.530257	17.948606
H	13.141028	20.331602	18.632243
H	12.323974	19.952779	17.062789
H	12.120254	18.858628	18.457721

C	11.568846	19.042352	12.477292
H	10.669796	19.670039	12.553155
H	12.264753	19.469002	11.741560
H	11.297313	18.019561	12.166762
C	9.229450	16.356392	12.918029
H	9.398610	17.299023	13.473496
H	8.786676	16.562130	11.932929
H	8.549059	15.719887	13.496691
C	8.031174	16.530828	16.141677
H	7.347537	16.057875	16.869742
H	7.491373	17.270326	15.532700
H	8.448486	15.738558	15.503773
C	12.193027	17.837902	21.180301
H	11.709788	18.282447	22.061637
H	13.247632	18.159015	21.115886
H	11.667177	18.154794	20.270748
C	7.139276	16.356253	19.676752
H	7.725001	16.944847	18.950004
H	6.137339	16.144410	19.277479
H	7.057586	16.920640	20.616813
C	8.850591	10.893931	20.081731
H	8.500576	10.239477	20.892612
H	8.082049	11.648339	19.840334
H	9.060200	10.291347	19.188056
C	8.048255	10.901428	16.497564

H	7.037817	10.679439	16.868160
H	8.286817	10.277273	15.617954
H	8.793180	10.686707	17.276192
C	8.155962	10.960514	12.867463
H	7.865803	9.904680	12.963538
H	7.844114	11.529285	13.759512
H	7.682289	11.397711	11.976872
C	15.483884	15.210990	11.921675
C	16.517042	14.623156	11.207663
C	14.151760	15.119699	11.467735
C	16.221550	13.989675	9.967453
C	13.857175	14.488517	10.299286
H	13.359513	15.567282	12.082049
C	17.226726	13.433655	9.154520
C	14.876793	13.926045	9.508826
H	12.816524	14.420456	9.964324
C	16.923288	12.864145	7.945463
H	18.263074	13.470353	9.503773
C	14.595300	13.319961	8.274951
C	15.597508	12.802572	7.498355
H	17.724071	12.451030	7.326577
H	13.551009	13.276835	7.947243
H	15.363927	12.339448	6.535945
C	17.924255	14.772210	11.631024
C	18.711028	15.744905	10.943782

C	18.524133	14.036368	12.636693
C	18.156371	16.561052	9.940812
C	20.080158	15.931292	11.275626
C	19.886389	14.228742	12.954650
C	18.912729	17.505342	9.297463
H	17.099734	16.436599	9.688368
C	20.833554	16.901663	10.595129
C	20.645551	15.140627	12.291949
H	20.315318	13.620658	13.756958
C	20.264163	17.679206	9.622302
H	18.455535	18.131887	8.526907
H	21.886232	17.027987	10.870055
H	21.701907	15.276776	12.546324
H	20.859678	18.436153	9.104081
S	15.862542	16.079077	13.406033
S	17.767021	12.764360	13.604559