

Supporting information

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1. Synthesis

The reactions were done in an inert gas atmosphere performing standard Schlenk techniques. THF and Cyclopentane were pre-dried with sodium. $^i\text{Pr}_2^n\text{BuP}$ and $\text{Au}_{32}(\text{}^n\text{Bu}_3\text{P})_{12}\text{Cl}_8$ were synthesized as described earlier by our group.[1][2]

1.1 Synthesis of $^i\text{Pr}_2^n\text{BuPAuCl}$ 1

321 mg (1mmol) (THT)AuCl is solved in 20 ml THF. 0,2 ml (1 mmol) $^i\text{Pr}_2^n\text{BuP}$ is added. The solution becomes colourless. The solvent is removed after one hour.

1.2 Synthesis of $\text{Au}_{30}(\text{}^i\text{Pr}_2^n\text{BuP})_{12}\text{Cl}_6$ 2

406 mg (1 mmol) $^i\text{Pr}_2^n\text{BuPAuCl}$ is suspended in 20 ml ethanol. 38 mg (1mmol) NaBH_4 is suspended in ethanol and added quickly to the suspension, which turns black immediately. The ethanol is removed after one hour and the black solid is extracted with 20 ml cyclopentane. The extract is stored at 6 °C. If there is oil, the extract is filtered again. After a few weeks, the $\text{Au}_{30}(\text{}^i\text{Pr}_2^n\text{BuP})_{12}\text{Cl}_6$ cluster crystallizes in form of black rhombus.

2. NMR Data

Devices: Bruker Avancell+400 ($\text{Au}_{30}(\text{}^i\text{Pr}_2^n\text{BuP})_{12}\text{Cl}_6$)

Bruker AVIIIHD-300 ($^i\text{Pr}_2^n\text{BuPAuCl}$)

The chemical shifts are given in ppm against the external standards SiMe_4 (1 H, 13 C,) and 85% phosphoric acid (31 P). C_6D_6 and CDCl_3 was dried with 3 Å molecular sieves.

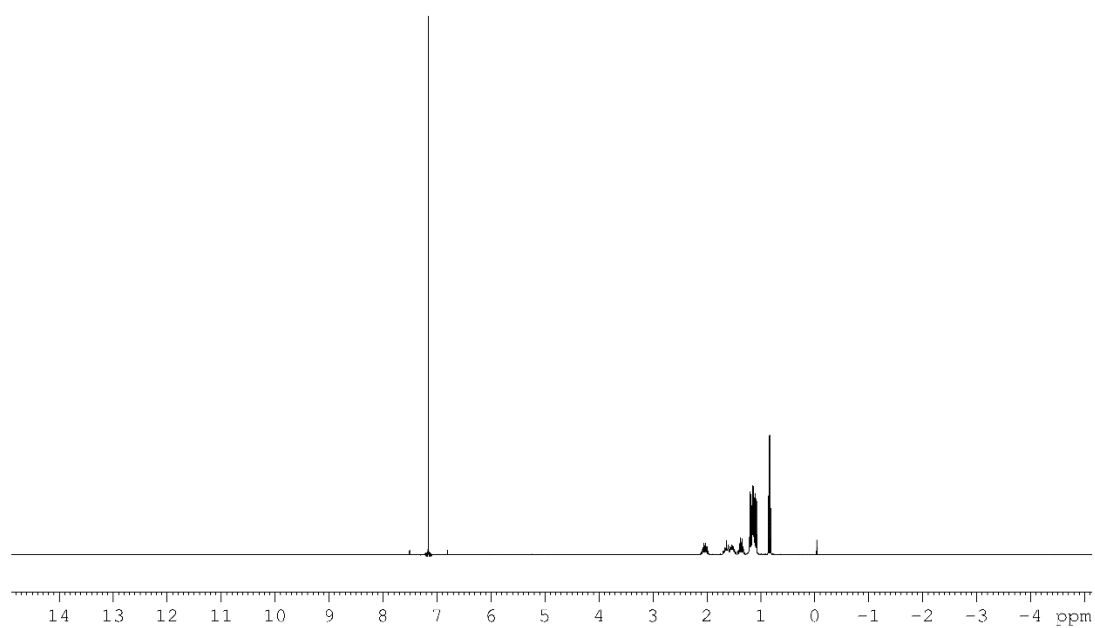


Figure S1: ^1H NMR-spectrum of **1** at RT in CDCl_3

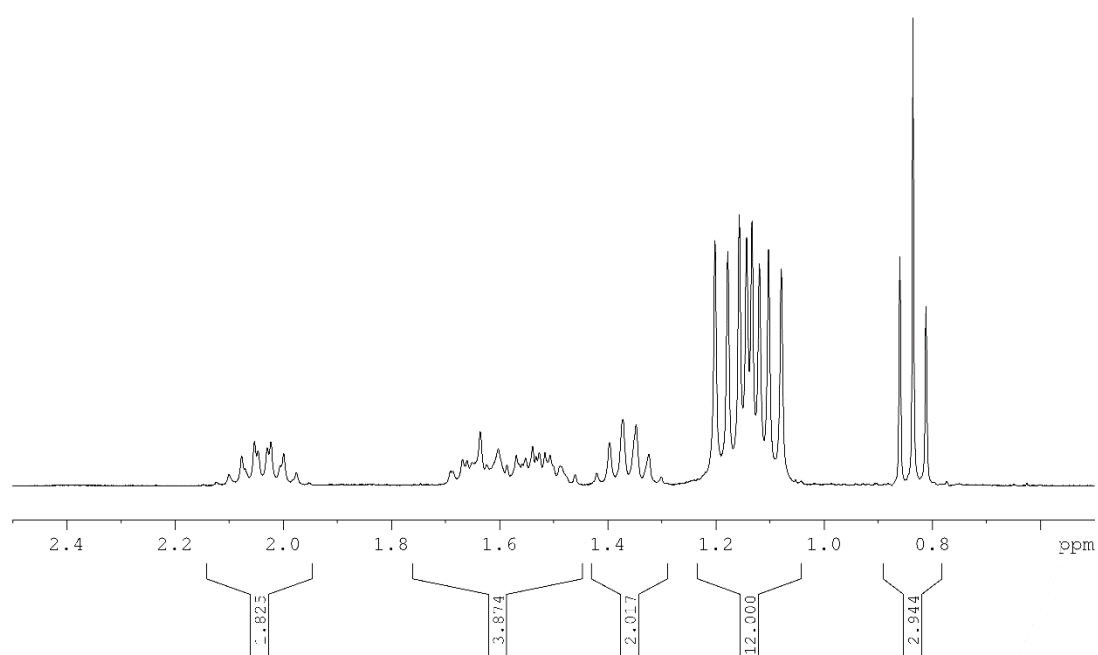


Figure S2: ^1H NMR-spectrum of **1** at RT in CDCl_3 , the section between 0.5 and 2.5 ppm is enlarged

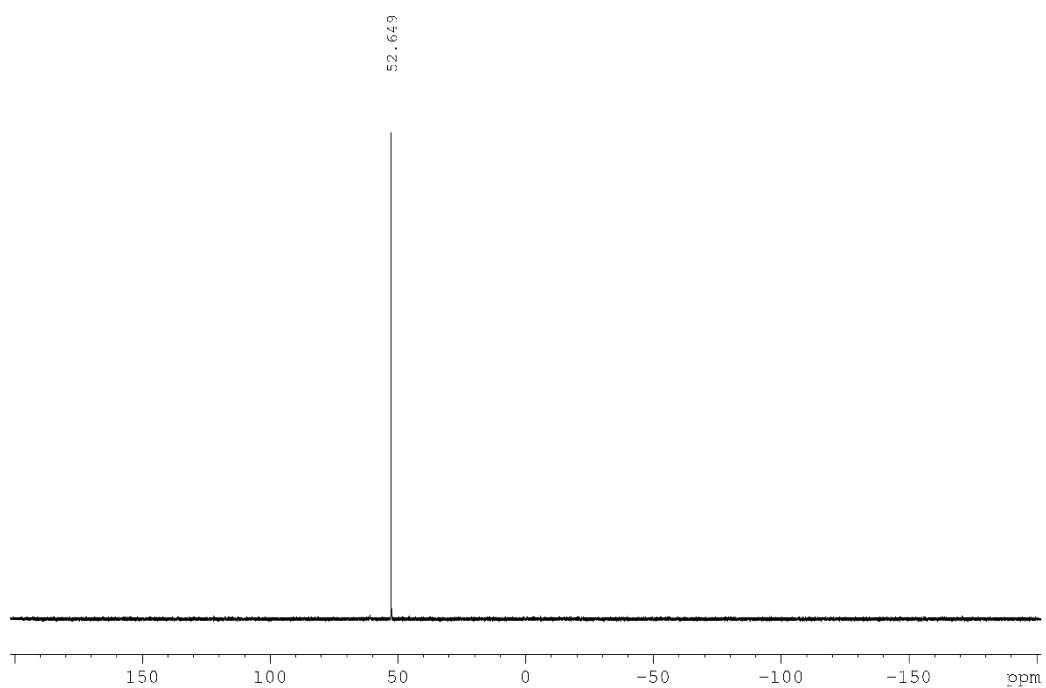


Figure S3: ³¹P NMR spectrum of **1** at RT in CDCl₃

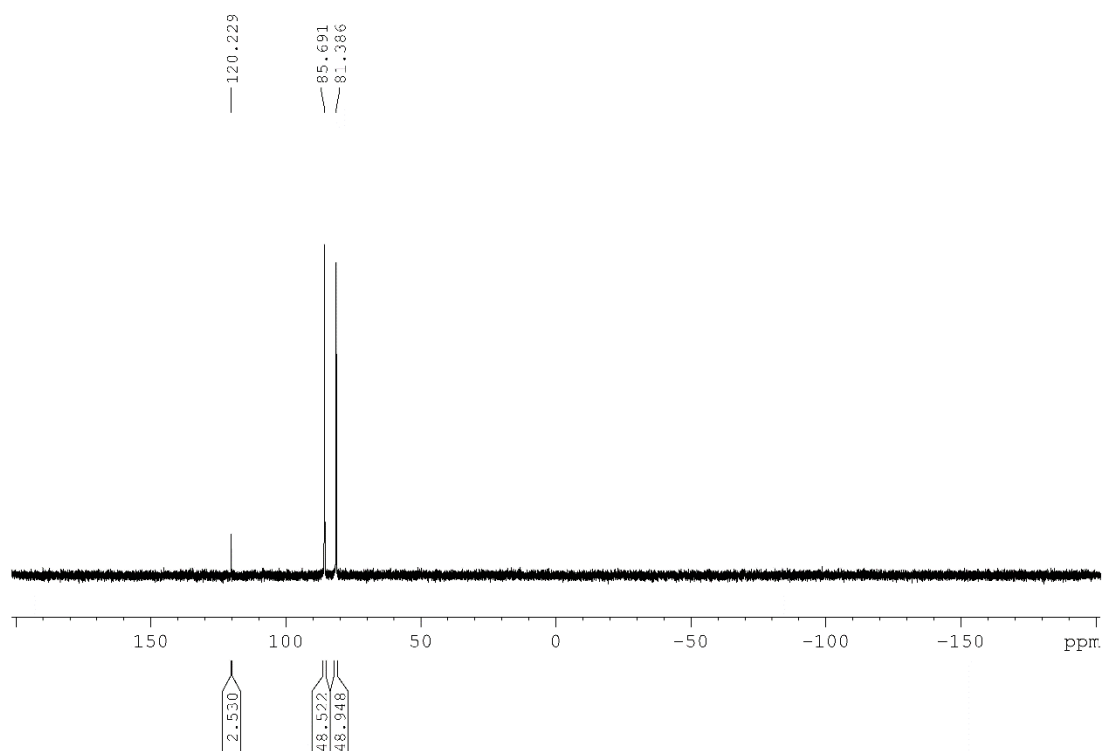


Figure S4: ³¹P NMR spectrum of **1** at RT in C₆D₆

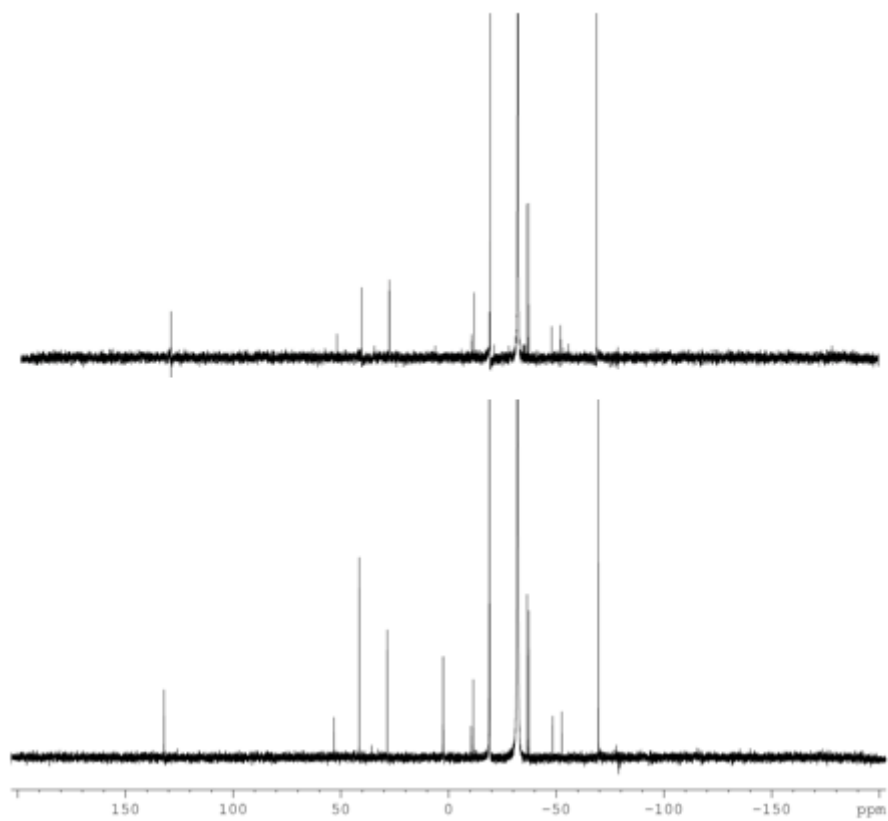


Figure S5: ^{31}P NMR spectrum of PBu_3 (up) and $\text{PBu}_3 + \mathbf{1}$ (bottom) in C_6D_6 .

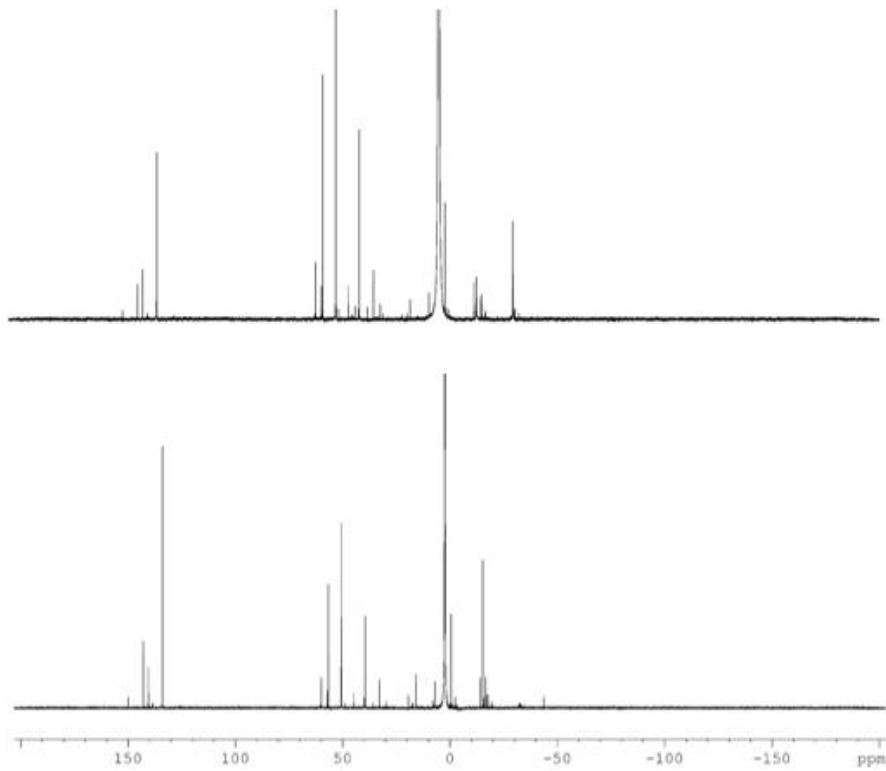


Figure S6: ^{31}P NMR spectrum of $\mathbf{2} + \text{P}^i\text{Pr}_2^n\text{Bu}$ (up) and $\text{P}^i\text{Pr}_2^n\text{Bu}$ (bottom) in C_6D_6 .

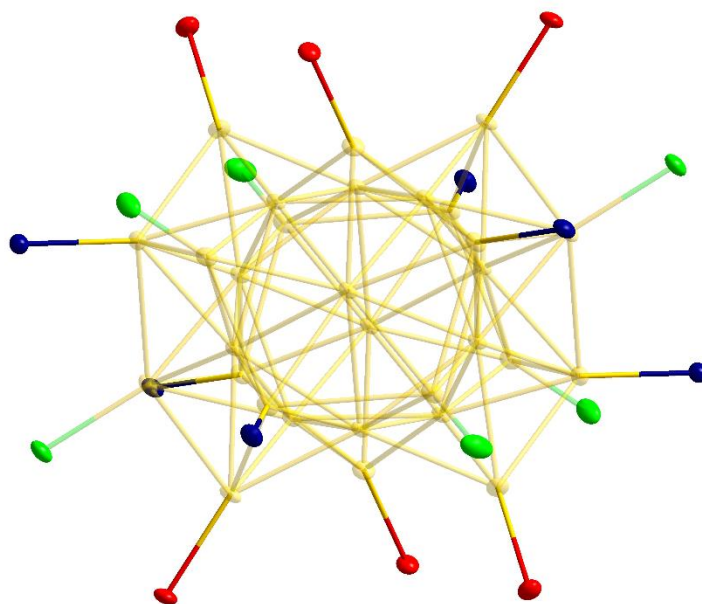


Figure S7: Core of **1** based on the crystal structure (gold: yellow; chlorine: green; phosphorus: blue, red (based on the chemical surrounding))

3. UV/Vis

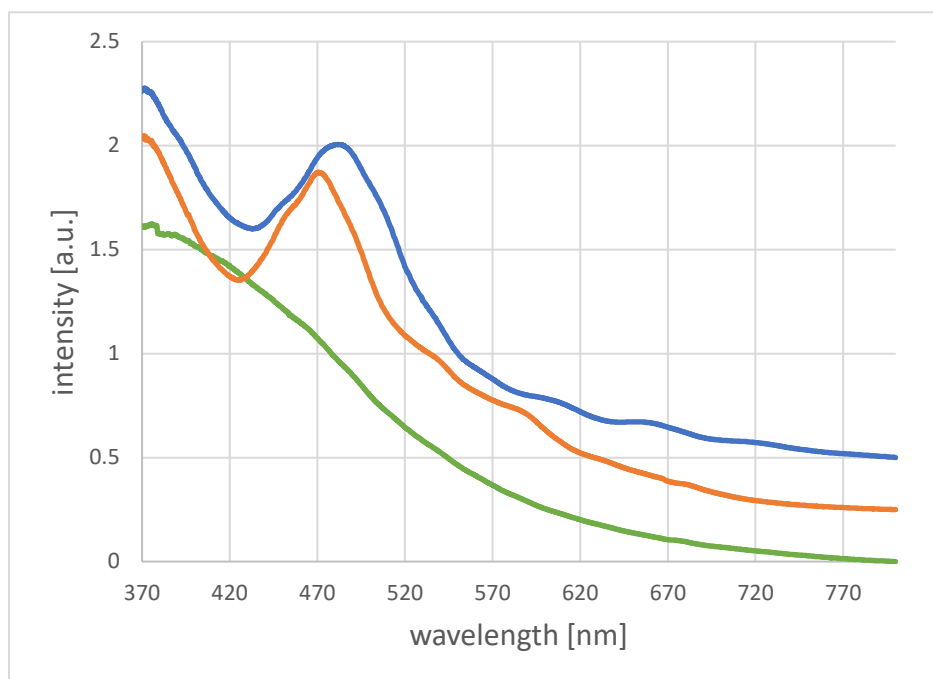


Figure S8: UV/Vis spectra of **1** (orange), **3** (blue) and **3** + $i\text{Pr}_2n\text{BuP}$ (green) in benzene.

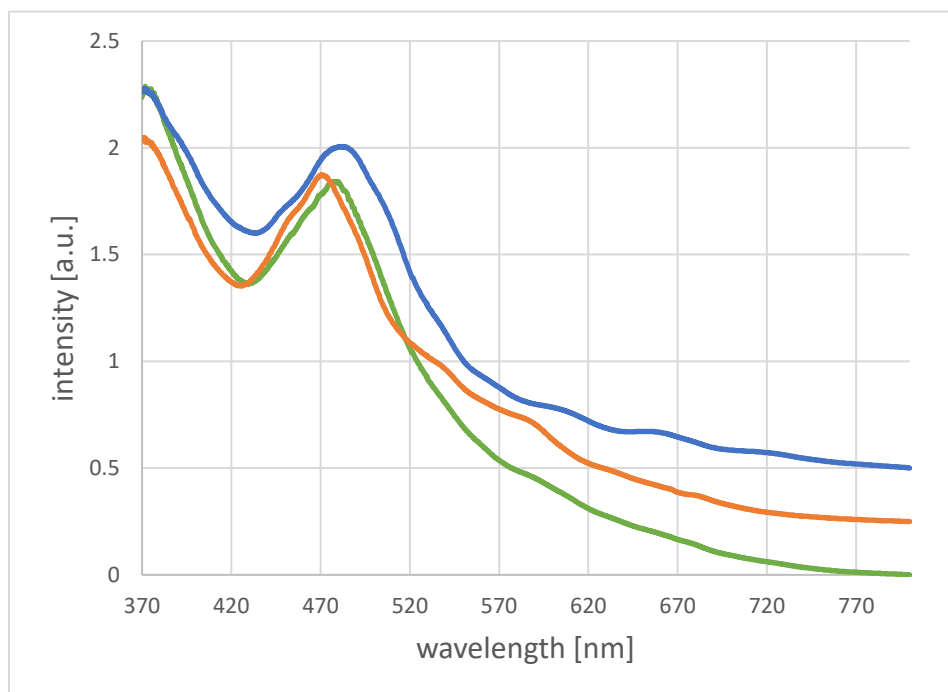


Figure S9: UV/Vis spectra of **1** (orange), **3** (blue) and **1** + $n\text{Bu}_3\text{P}$ (green) in benzene.

4. Crystallographic data

Crystals were mounted on the diffractometer at 100 K. The data were collected on a Bruker APEX II DUO diffractometer equipped with an μ S microfocus sealed tube and QUAZAR optics for monochromated MoK α radiation ($\lambda = 0.71073$ Å) and equipped with an Oxford Cryosystems cryostat. A semiempirical absorption correction was applied using the program SADABS. The structure was solved by direct methods and refined against F² for all observed reflections. Programs used: SHELXS and SHELXL[3] within the Olex2 program package. [4]

*i*Pr₂ⁿBuPAuCl **1**

CCDC Number:	
Empirical formula	C ₁₀ H ₂₃ AuClP
Formula weight	406.67
Temperature/K	100
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	9.6698(3)
b/Å	8.4076(3)
c/Å	16.4655(5)
α /°	90
β /°	91.9380(10)
γ /°	90
Volume/Å ³	1337.88(8)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	2.019
μ/mm^{-1}	11.277
F(000)	776.0
Crystal size/mm ³	0.461 × 0.194 × 0.056
Radiation	MoK α ($\lambda = 0.71073$)
2 θ range for data collection/°	4.95 to 59.998
Index ranges	-13 ≤ h ≤ 13, -11 ≤ k ≤ 11, -21 ≤ l ≤ 23
Reflections collected	20898
Independent reflections	3892 [R _{int} = 0.0363, R _{sigma} = 0.0304]
Data/restraints/parameters	3892/0/123
Goodness-of-fit on F ₂	1.041
Final R indexes [$I \geq 2\sigma(I)$]	R ₁ = 0.0182, wR ₂ = 0.0422
Final R indexes [all data]	R ₁ = 0.0207, wR ₂ = 0.0437
Largest diff. peak/hole / eÅ ⁻³	1.03/-2.56

Au₃₀(PⁱPr₂ⁿBu)₁₂Cl₆ 2

CCDC Number	
Empirical formula	C ₁₂₀ H ₂₇₆ Au _{30.06} Cl ₆ P ₁₂
Formula weight	8224.54
Temperature/K	100
Crystal system	monoclinic
Space group	P2 ₁ /n
a/Å	18.5234(9)
b/Å	19.3804(8)
c/Å	24.5820(11)
α/°	90
β/°	96.1050(10)
γ/°	90
Volume/Å ³	8774.7(7)
Z	2
ρ _{calc} /cm ³	3.113
μ/mm ⁻¹	25.248
F(000)	7305.0
Crystal size/mm ³	0.286 × 0.177 × 0.028
Radiation	MoKα (λ = 0.71073)
2θ range for data collection/°	3.586 to 49.426
Index ranges	-21 ≤ h ≤ 21, -22 ≤ k ≤ 22, -28 ≤ l ≤ 28
Reflections collected	109202
Independent reflections	14950 [R _{int} = 0.0428, R _{sigma} = 0.0235]
Data/restraints/parameters	14950/18/762
Goodness-of-fit on F ₂	1.054
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0292, wR ₂ = 0.0785
Final R indexes [all data]	R ₁ = 0.0346, wR ₂ = 0.0836
Largest diff. peak/hole / eÅ ⁻³	2.71/-2.38

5. Quantum chemical calculations:

All quantum chemical calculations have been done on a DFT level with the B-P86 functional (exchange: LDA + Becke (B88); correlation: LDA (VWN) + Perdew (P86)). The def-SV(P) basis set and additional for the gold atoms, def-ecp was used.

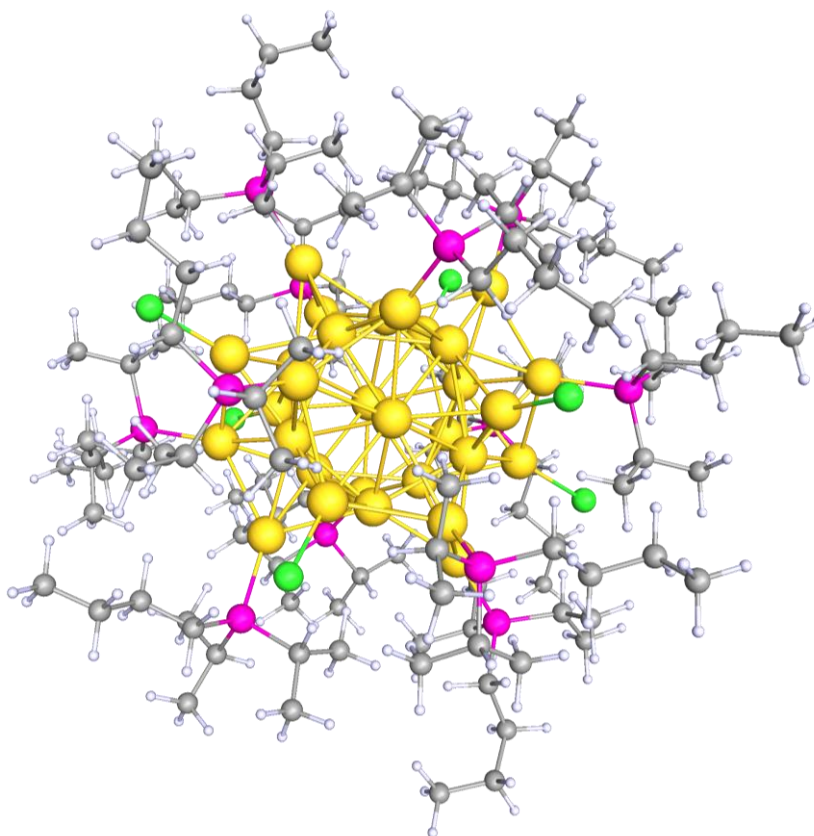


Figure S10: Geometry optimized structure of **2**

Point group: C_1

Energy: -15669.96961061505 H

HOMO-LUMO-Gap: 0.869 eV

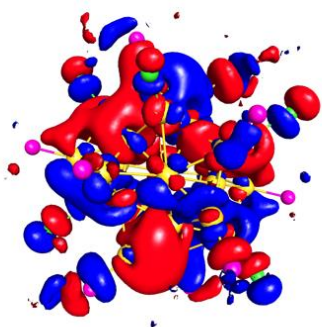
Atomic coordinates:

1 au	3.31597561173539	36.86894301019531	4.17861777406424	2 au	-2.15699388452618	36.32463717495765	5.01109412255903
3 au	0.88642086853421	32.09903277073298	3.13907892400418	4 au	-0.07400038794539	41.05972971141510	2.39325419208094
5 au	4.12170171232049	39.65414427929019	-0.77728339134599	6 au	4.79964705676733	34.19450802639857	-0.60693953830403
7 au	8.42647455088144	37.42219381681051	1.67472040696308	8 au	0.80786047599077	39.87919008347568	7.84255069473764
9 au	1.26115160515792	34.16336351479666	8.47242797002129	10 au	4.97881550669558	41.87549853028280	4.17623817322864
11 au	6.31673763518837	32.37528006252408	4.09531221783939	12 au	-4.13711868452662	32.89677542755150	0.83596714187726
13 au	-4.82841278993814	38.36116098293484	0.69025843390446	14 au	-7.52781276278237	34.97159218470762	4.21533193826681
15 au	-4.58897384041868	41.27219897021203	5.17455990693119	16 au	0.05430802738412	31.49532426204032	-2.33268045122360
17 au	3.81119724407742	28.62967829321482	0.20914208503837	18 au	-1.74949666455577	27.84502992717249	1.38670604773024
19 h	-0.58982847751183	28.82295103283428	7.58005564202422	20 au	-0.91147440317564	40.46389924962403	-3.07350951650906
21 au	-3.82939068391066	43.93389890174657	-0.14560357609056	22 au	1.72883264058269	44.71566339480822	-1.32639210062942
23 au	2.12224632070599	36.23529839714933	-4.93717938204746	24 au	7.50147193860853	37.49931696901680	-4.15040870166590
25 h	7.84524413371321	43.62576139340917	-1.85977207853159	26 au	4.57566518140911	31.31634800894177	-5.10981648880744
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29 h	-1.37065916649981	45.61131667225113	6.40427529679382	30 p	2.45773955869323	31.15927849163177	11.66937129740472
31 h	-1.67566135373128	34.55201241849461	13.34867323672865	32 cl	7.78900669300666	45.27557043689794	5.73540270517064

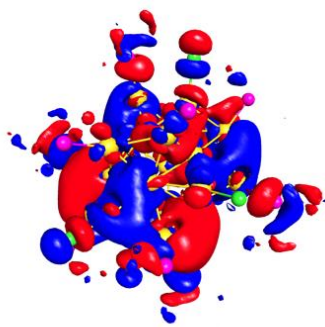
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37 au	-4.99915117776784	30.67885709817854	-4.11831994058442	38 h	-7.87293110452964	28.93747669780362	1.90065951148981
39 au	-6.34879234967270	40.17951526268079	-4.00985838551638	40 p	-10.26586628560157	35.03687509716986	7.79809236636910
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45 p	-4.45732226179301	24.26805831297048	1.904811301933587	46 c	0.05729355081582	27.29840618397302	8.87649504296946
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113 h	-3.88372008050770	43.44727251978340	10.93772907503497	114 c	-2.77972921596364	41.30858899953266	13.24778700143542
115 c	-2.98115023360592	45.22983324615999	14.56246529380385	116 c	2.18750669956278	48.38005549392080	11.31625443122396
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123 h	6.97677679736364	31.17915083981232	11.48637301669657	124 c	6.22276704570332	33.99561004426611	14.43624159410342
125 h	-1.44015159549065	29.79313890884832	13.54625855867366	126 c	1.10946397272158	29.57394516850333	16.75092876451758
127 h	-2.54057740221749	33.34784496135111	16.42446191562546	128 h	0.49535671326266	34.7776609512413	15.9418681104975
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139 c	-14.19417371166674	32.26097423236240	5.5110956568959	140 h	-11.11717163455658	30.61771518356074	7.58922284501087
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143 h	-13.37881769677097	37.92017027220993	6.14410598110106	144 c	-13.76599026272263	38.66105709731662	10.21276985917730
145 c	-3.05679266795130	29.83426213441643	-13.49003077080786	146 c	2.44728438080492	29.31588626680256	-12.43149052461345
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153 h	7.70864532794867	24.75168522854330	5.46750460956134	154 h	5.94625372568828	21.90273356259771	6.08982760935632
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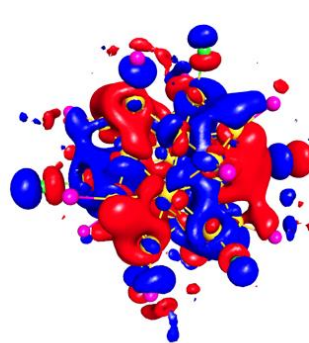
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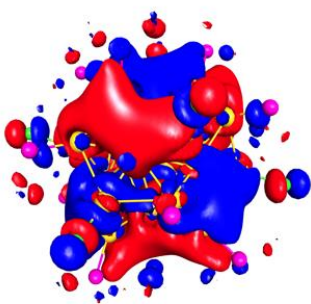
HOMO



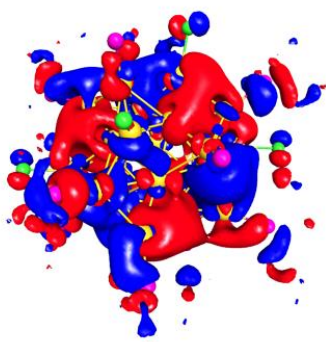
HOMO - 1



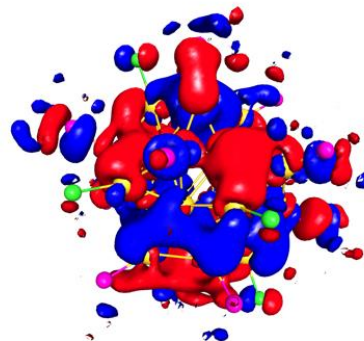
HOMO - 2



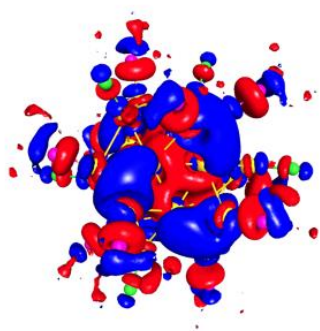
LUMO



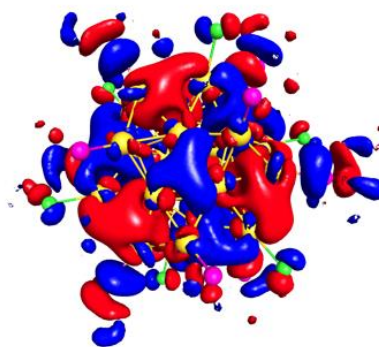
LUMO + 1



LUMO + 2



LUMO +3



LUMO +4

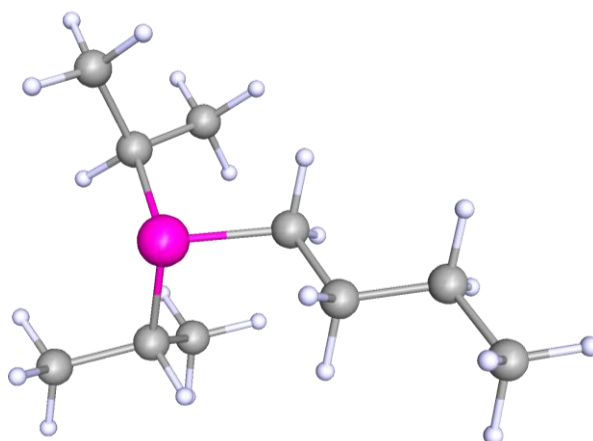


Figure S11: Geometry optimized structure of $(\text{Pr}_2)\text{BuP}$

Point group: C_1

Energy: -735.87633553543 H

HOMO-LUMO-Gap: 5.571 eV

1 p	0.11709545658854	0.09893755093767	-0.36154297421865	2 c	-1.59373885260306	1.84357203162367	-3.02554088141821
3 c	-1.33739743580592	1.46647222534433	2.63564235416048	4 c	-1.34113384275355	-3.14335527742134	-0.49591757045569
5 c	-4.23070305022030	1.62544080243955	2.81773080735606	6 h	-0.66415098463353	0.11119183515303	4.10570489949933
7 c	-0.09361899380344	4.03786378282669	3.19892740889408	8 h	-4.81305055724419	2.22501734992729	4.75261740621893
9 h	-5.01243335190364	3.04340310933186	1.47579385020224	10 h	-5.16595391220879	-0.21693001836069	2.43309678713797
11 h	-0.69284474958636	4.76248055108012	5.08342802121485	12 h	2.00327171883752	3.90020737650377	3.18938455740978
13 h	-0.64290906076145	5.49068177020070	1.77673306863508	14 c	0.20570208012788	2.01577746963504	-5.31091044528337
15 h	-1.84444501739771	3.79240397023167	-2.26059163844355	16 c	-4.19777651404623	0.83736994398349	-3.83576036212072
17 h	-4.04979888963780	-1.07636113976710	-4.69377643285238	18 h	-5.04348181392601	2.10086654701301	-5.29528853617998
19 h	-5.55680121305985	0.71812522237679	-2.24272388155593	20 h	2.04599237686377	2.88192504075105	-4.78607615100524
21 h	0.61372248692464	0.10903813163822	-6.10654456590394	22 h	-0.64739422768175	3.16906120836513	-6.85430771468136
23 h	-1.01588549979581	-3.83586215929491	-2.45969289385655	24 h	-3.42906678460234	-3.08564607077327	-0.22689289734091
25 c	-0.13242891734768	-5.00660853176777	1.38235942104148	26 h	1.95909384241360	-5.00087129202240	1.12082568676432
27 h	-0.46443189979385	-4.34968604836388	3.35862884747461	28 c	-1.13344817811793	-7.72486868013517	1.11825166988254
29 h	-0.79136145355114	-8.39523606060934	-0.85129887075026	30 h	-3.22717653042901	-7.72089954563605	1.36683025561873
31 c	0.06268264092922	-9.58240288270495	2.99657182728609	32 h	-0.30733151512621	-9.00475460548516	4.98620619047341
33 h	-0.69950343668362	-11.52605817996574	2.74896107818547	34 h	2.15004635859753	-9.68231244798381	2.74971655229163

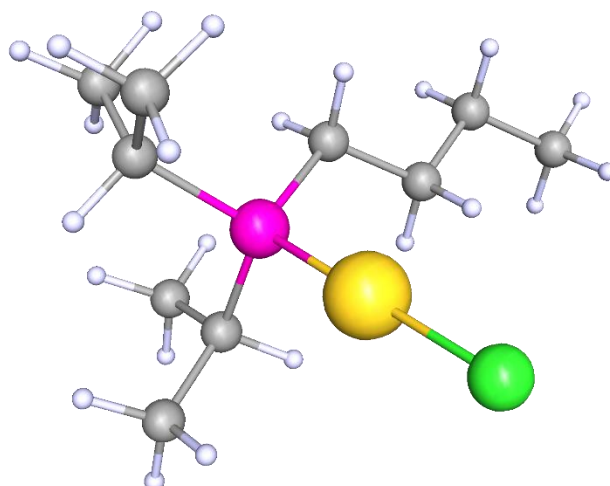


Figure S12: Geometry optimized structure of **1**

Point group: C_1

Energy: -1331.97716043729 H

HOMO-LUMO-Gap: 4.676 eV

1 au	4.36504672798423	-0.05777069010105	-0.24847276666808	2 p	0.03693093003921	-0.01104715359815	-0.29951582367987
3 cl	8.74857843274661	-0.14834827420561	-0.15097830323336	4 c	-1.35635597943654	1.83360038660153	-3.02171036947938
5 c	-1.22868742118166	1.36742820726181	2.73106822925131	6 c	-1.30291429121852	-3.25262350275089	-0.54697970714613
7 c	-4.11777244665515	1.33786556073965	3.04140423157467	8 h	-0.38977540514159	0.06641853102138	4.16096824564868
9 c	-0.11217372568904	4.01479129649957	3.19181217008204	10 h	-4.61879385917849	1.88971808894176	5.00928114991559
11 h	-5.05281973232939	2.71742865378713	1.76155951429052	12 h	-4.95884394272820	-0.55587982729388	2.69611281943271
13 h	-0.63174178646528	4.68405852445019	5.11714114062321	14 h	1.98396765999744	4.00752919369615	3.04805542862451
15 h	-0.85590543040733	5.42626800031184	1.82034625376253	16 c	0.41311364660543	1.73400838045194	-5.33172491847061
17 h	-1.37822141660167	3.81378365276984	-2.30308756577706	18 c	-4.07033363769289	1.06847795158887	-3.74372400762882
19 h	-4.12779560184807	-0.85892205843363	-4.57909831929008	20 h	-4.80728168382352	2.39438135161106	-5.20194007021732
21 h	-5.40161567555404	1.11377100764388	-2.12378573370347	22 h	2.33648439611675	2.43890464167283	-4.87310937082931
23 h	0.61545058383357	-0.22630920415697	-6.06726918162513	24 h	-0.37369468103073	2.91607306948204	-6.88500034329605
25 h	-0.76607180883078	-3.93208817526619	-2.46654406322036	26 h	-3.40357081728940	-3.14908083364587	-0.50421805966556
27 c	-0.31598329643194	-5.10524919353124	1.46588868055992	28 h	1.79046460439098	-5.07303056616779	1.46336540124992
29 h	-0.90828800428950	-4.46340741963483	3.38380272903405	30 c	-1.25222257755626	-7.82712681857165	1.04547187423851
31 h	-0.64218884855401	-8.47477832695816	-0.86508149042273	32 h	-3.36054088709888	-7.84469276446631	1.01727488357473
33 c	-0.28997104871103	-9.68451878667470	3.05305389897609	34 h	-0.92801792181249	-9.13037539386404	4.97999800009214
35 h	-0.99025198445125	-11.63207988731196	2.68836116735908	36 h	1.81173715781854	-9.75767865339673	3.08055111609635

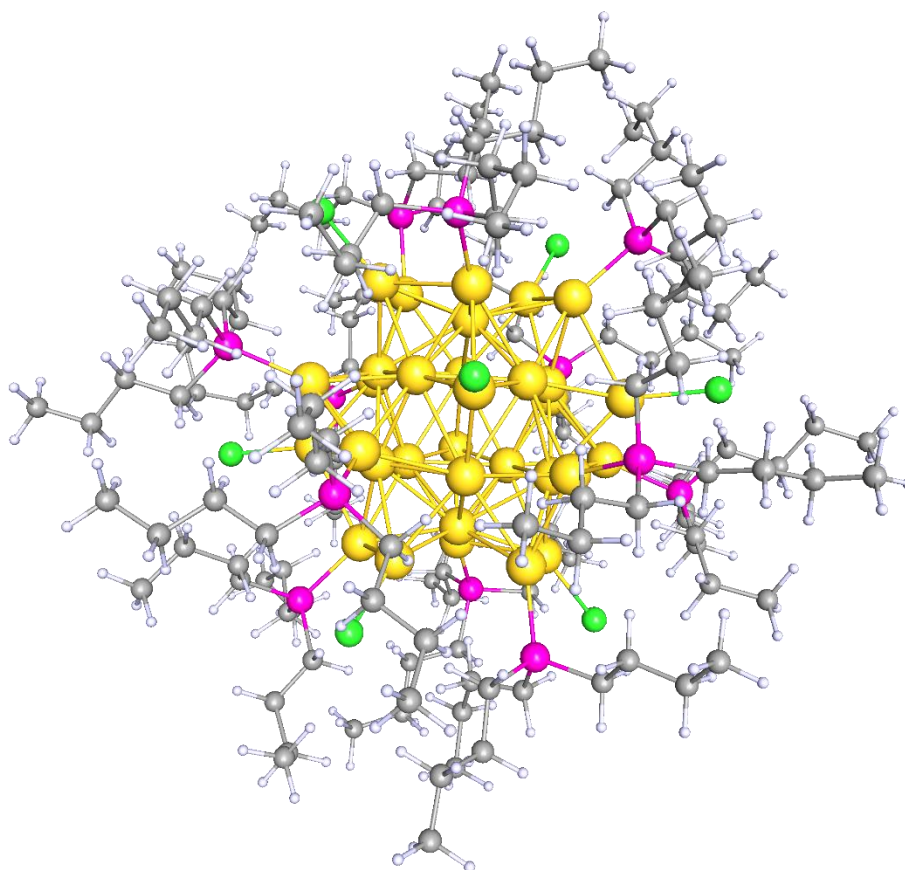


Figure S13: Geometry optimized structure of $\text{Au}_{32}(\mu^3\text{Bu}_3\text{P})_{12}\text{Cl}_8$

Point group: C_1

Energy: -17788.91558969258 H

HOMO-LUMO-Gap: 0.488 eV

1 au	24.84359628604379	26.15887918462396	34.37098876549325	2 au	22.90741216584299	27.30086487213529	29.21809111963159
3 au	30.43211561043692	27.33379746065258	34.45174462797550	4 au	26.87814965104154	30.60134050077204	31.67760664384629
5 au	28.69004438665984	22.11744341911229	33.70558821492658	6 au	24.20961365186486	22.10225353555652	30.69615769484829
7 au	28.25191950132082	24.77134225294482	38.46777043494478	8 au	26.39609028194443	30.49667878465694	37.07106788050838
9 au	21.89619390425361	30.58408612619165	33.71503936750112	10 au	19.83153040374952	24.72351841899555	32.61680699058364
11 au	24.02606885574130	20.88430978792290	36.00941108084707	12 au	25.51628046341471	23.70710340191784	25.52392444659026
13 au	27.23680708646400	28.94289769265489	26.28131997165319	14 au	23.32391368699229	32.35899242744523	27.83587583936986
15 au	22.59323794249609	28.14249276283117	23.79285699811080	16 au	20.31602851329224	22.95475409658700	27.11136284555461
17 au	33.02866173852411	23.73568234861131	30.72382519583113	18 au	31.70351485549106	28.93995004322366	29.27335858020576
19 au	33.32464628430920	22.99518038029780	36.22378590758296	20 au	35.62362643120551	28.11177586842968	32.81997913371470
21 au	31.73783069214887	32.34600402410069	33.50030545730390	22 au	29.48207612718574	33.63719902523896	27.75321482268981
23 au	29.06590196124812	20.42969591748129	28.37197903123621	24 au	32.63452591457634	18.71890895186223	32.23089009433284
25 au	26.44370457083098	17.41318286001344	32.25327899452071	26 au	24.19656659193159	18.70292792196424	26.47568585432756
27 cl	27.71897594692039	24.18549443573717	43.02194572948429	28 h	30.66212276984475	18.18037950666137	38.51164628887115
29 p	27.60398711754203	32.51720358238017	40.85442759402095	30 p	17.91453409884424	32.57857287183317	33.72468005550137
31 cl	15.60517695045670	23.93849147314990	34.40972651216255	32 p	21.51889183347637	20.02740441410788	39.59210867633257
33 au	31.06802079174985	24.83793894803787	25.57579177783750	34 au	27.68391622210336	26.27104924338629	21.51558974577372
35 au	29.44611107900882	20.37908892691611	23.01804377180042	36 au	31.88826206031484	30.16938418681492	23.96688789891065
37 cl	21.21432767387487	36.49256953281525	27.35522069658342	38 p	20.61868553753359	30.16849909449699	20.35971968509672
39 p	16.41810718119904	21.13631441748317	26.07491396499517	40 au	33.97772893161076	20.30423341088843	26.27614042708151
41 au	36.04751941494447	26.32898400433491	27.28891716875439	42 p	35.39034555818842	20.99451690917530	39.61598212254933
43 p	39.57658026748975	29.90343372187238	33.70014460374691	44 cl	33.33987517536425	36.46134125771924	34.98951933014622
45 p	29.14599928784045	38.04867112723255	28.39423844662974	46 cl	34.81225324892696	14.71651107182054	33.24724928937770
47 p	26.75497921855875	12.99722839616626	31.64043938817599	48 cl	22.46910041964256	14.58814954203908	25.10384407756767
49 c	31.22718500361474	17.47609417191100	40.41583518346196	50 c	28.38891956974360	35.89192192828344	40.29374871747289
51 c	30.37181926378399	31.13747833858790	42.49106042922037	52 c	25.24508744499771	32.46600136353719	43.45914219746565
53 c	15.74626499135082	31.04616586353036	36.01794367483126	54 c	18.10131704719860	35.97428743241208	34.58895961340652
55 c	16.26856030267309	32.50593932433110	30.61332028039833	56 h	15.86353188771755	28.98513924762376	35.58387079830221
57 c	22.88335836633757	17.70937543353568	41.84781651648906	58 c	20.95816492371438	22.76048344879147	41.69923589646994
59 c	18.36550737818798	18.8189832141603	38.65469739486685	60 cl	28.04102147723050	26.89252439368226	16.94468185921367
61 h	25.47800867807077	32.77894052768756	21.49584270724170	62 p	28.40188757579645	18.28244295170218	19.23064267309219
63 p	34.36705098525212	31.02886624997692	20.35788947887599	64 c	23.04959023559669	31.71610379201433	18.35110203736200

65 c	18.2526932393849	32.56448853782730	21.36819934447016	66 c	18.97787990296106	28.23325032358685	17.92784932721822
67 c	13.76029837091269	23.27816588284947	25.25081421360205	68 c	16.69387603464125	18.88889217950718	23.39386370846117
69 c	15.15260531447918	19.31656450295003	28.78159860819956	70 p	38.06343909634889	18.55604234430562	25.96372262558812
71 cl	40.27297126161003	27.14010470575180	25.47670034765162	72 c	33.01277323086813	19.40746803899631	41.65887688495654
73 c	37.80250313471957	18.65961409816731	38.58935013896277	74 c	37.00742291008228	22.99804190058000	42.00935824128469
75 c	42.20934666632738	27.73222062360920	34.53282822719756	76 c	39.43518005765544	32.26108637992164	36.29494040398811
77 c	40.80966262244625	31.61494502234599	30.91254110350193	78 c	32.17792076376156	39.80350027949840	28.57029761210301
79 c	27.26984965697547	39.54381271401916	25.83810680193858	80 c	27.42729706703821	38.74110025094112	31.38552324056963
81 c	23.72222213882472	11.23481083882175	31.62273052694727	82 c	28.75602450525148	11.53177425537011	34.11602096768284
83 c	28.29161965215469	12.28633848322148	28.55321096596805	84 h	29.45411096826848	17.46386562792626	41.55475837360327
85 c	32.20572041449127	14.74774689091039	40.19279799339620	86 h	29.71079846671766	35.90930903548335	38.65163619819373
87 h	26.61322337210152	36.78765331041902	39.60024860458524	88 c	29.51553881878372	37.39459286397300	42.50472036513987
89 h	30.59557522254964	32.22431663344920	44.28087357698844	90 h	29.80562719835580	29.17513509377381	43.01590701791762
91 c	32.83273066577953	31.10272314015952	40.96290681020970	92 h	24.99756829924559	30.42944101190105	43.93588090782083
93 h	26.15188410679932	33.37543454823369	45.13055613970513	94 c	22.69062236798316	33.70543091177906	42.89295671405397
95 h	16.65635852376132	31.29324974834500	37.89815792725480	96 c	12.96756709929520	31.88671173591075	36.05812584479705
97 h	16.14698220359217	36.74910704698521	34.61818155974154	98 c	19.47343535150083	36.47160462963523	37.09409470728930
99 h	17.79537301068826	32.43607665378934	29.16958717125948	100 h	15.27622816183171	30.64881857350727	30.54520369889821
101 c	14.48113985809044	34.71941386723343	30.02612021409106	102 h	24.65394873789207	18.61346480058255	42.54406388122604
103 h	21.57383141922553	17.58840186054571	43.49496697705160	104 c	23.41886192775653	15.07017428023999	40.78117732226659
105 h	19.79689893547359	22.04671456699119	43.30471122448996	106 h	22.85657340857690	23.26835423224699	42.46678084613621
107 c	19.73295055253927	25.06262137341918	40.43846431743533	108 h	17.61538334845011	20.23049526657483	37.27898076593932
109 h	18.72156827928345	17.06880759868375	37.53996318723463	110 c	16.42935486269166	18.33171691957965	40.75844040779656
111 c	24.89353049862618	33.56489256466637	19.62976172184842	112 c	27.20719027759097	15.03189277692059	19.7969942922758
113 c	25.97131119515857	19.87266190125091	17.28596022661702	114 c	31.04947293051774	17.91792636653735	16.94962944869635
115 c	33.05784164360335	33.44729735312735	18.17345576453814	116 c	34.76867569980478	28.32402001505701	18.17845986689630
117 c	37.58046147279425	32.11018465368466	21.24110553655422	118 h	24.15105994750647	30.08419491855372	17.59371788067927
119 h	22.06910828556264	32.60149135000085	16.71149928050654	120 h	16.82879702967350	31.51004468934551	22.50818555414390
121 h	19.25025992190831	33.80353167095976	22.74529588022157	122 c	16.95081754512813	34.07774647529362	19.25821719298822
123 h	18.46719597556571	29.54452745926803	16.35931107912486	124 h	20.43718613447061	26.92402572534517	17.16784627443597
125 c	16.64628724847004	26.75216846688427	18.79762605942892	126 h	14.11528983147803	23.96163390544551	23.29451659340711
127 h	12.01633861598045	22.09539525710174	25.18148756373640	128 c	13.40663176654730	25.49683961217465	27.09279843758948
129 h	17.47553813672507	20.01556847349470	21.79414485576476	130 h	18.22875560222222	17.55574008138975	23.94733583484372
131 c	14.28834871502486	17.48597263420740	22.56853813413739	132 h	14.68166054039890	20.73739642824487	30.26565910424159
133 h	13.35149930190676	18.42904365511306	28.14575394895185	134 c	16.99034812856748	17.36419781080657	29.88684459046963
135 c	39.97275278793951	20.37860157791950	23.65859442630114	136 c	38.16297800138058	15.21908774505960	24.86695152528929
137 c	39.65825013654793	18.57376712017266	29.08834726690743	138 h	40.04756618970514	22.33948848375518	24.43260166100686
139 h	31.86481632172874	21.01755674715937	42.39163556447973	140 h	34.02446156096529	18.5815456774923	43.31065631092254
141 h	39.14651073790213	19.73758823280961	37.37649576626224	142 h	36.80688178639713	17.35427119338126	37.27090456611430
143 c	39.23658630079230	17.24588113647882	40.68229100699364	144 h	37.55584263758579	21.72199701821149	43.59427814636274
145 h	35.30317253353237	24.29315260315772	42.76106367056237	146 c	39.30552126656710	24.50207533047048	41.08959770247251
147 h	41.91719972338512	27.16252566123990	36.53558138950337	148 h	43.98596912376210	28.86530281491396	34.46856265796379
149 c	42.42291376842869	25.40986099947094	32.79963881674804	150 h	38.73487081259631	31.20739936730842	37.97762403030465
151 h	37.87629660256709	33.57618623933804	35.76882645056790	152 c	41.88393843464398	33.68522342794671	36.93639444089308
153 h	41.18860448488508	30.15794062535750	29.43677552388953	154 h	42.65616831099540	32.45549519702087	31.47711793455053
155 c	39.00077175980619	33.60971705995103	29.83520930303489	156 h	33.21620843422884	38.98440182115544	30.20994695551446
157 h	31.73861605314041	41.80382204271621	29.05563449693960	158 c	33.76596800458023	39.68707355501308	26.14721341199159
159 h	25.49110884687457	38.41636005255414	25.77415573203880	160 h	28.30443472652786	39.13802168527355	24.05071643777508
161 c	26.63214111627894	42.36598879864446	26.04011310093719	162 h	27.86688869641367	37.14237444762243	32.67698855091496
163 h	25.39021835551784	38.56300765016650	30.87687242961044	164 c	28.00617278023791	41.25789875124114	37.12132150692509
165 h	22.64083830420109	19.98478565086982	29.97805356148989	166 h	24.15382968774398	9.21589715337053	31.2119167904769
167 c	22.18856351155556	11.45337575907853	34.07316650793341	168 h	30.49194304329719	12.72572514269566	34.17441218709936
169 h	27.74790288387201	11.86113511914900	35.93481830927266	170 c	29.50436003104932	8.74282700928327	33.84126996206540
171 h	27.17281906219667	13.85370091744692	27.27418343917565	172 h	30.35616395695810	12.51479728867400	28.90640027308123
173 c	27.67063380996752	9.73991933288124	27.30302097650941	174 c	32.67414810902893	13.40439887636040	42.71651615205308
175 h	30.77938414716899	13.65318015559478	39.10166565929144	176 h	33.93932846297248	14.68481505197690	39.00688170584041
177 h	28.20062686217117	37.39338471842107	44.15471456414453	178 h	31.28910086333608	36.46714256762181	43.16032652402341
179 c	30.12986893865768	40.13739494087395	41.76693918552930	180 h	32.60894901189529	29.75590465919642	39.35886825816205
181 h	33.20951999890100	32.97821060359453	40.08176255281016	182 c	35.12420551771134	30.33255514589092	42.57767534710971
183 h	22.97027580251474	35.68469916862642	42.22667012717162	184 h	21.76308843838868	32.681925577773149	41.30500346346559
185 c	20.93656826598534	33.73977154330876	45.20886972641493	186 h	12.13422276596896	31.57640540472657	34.15243175551814
187 h	12.81745846719530	33.95370749571129	36.44879092691301	188 c	11.36060270869462	30.42335379580456	37.99824428618184
189 c	19.61773959190971	39.28528921887850	37.81982022373221	190 h	21.42146747895334	35.68348251578103	36.95698614723317
191 h	18.53001252376977	35.41814652772193	38.65616594566335	192 c	13.02393635930320	34.3510662329087	27.54540830147222
193 h	13.09893136944622	35.01282738062910	31.58748464093932	194 h	15.61940955213974	36.48106582336250	29.87717748708454
195 h	21.64910553046576	14.23591917827621	39.99741310681264	196 h	24.75609544379528	15.23150759058553	39.15975554052886
197 c	24.50217901111712	13.26879022538927	42.78668295003754	198 h	17.92625745299652	24.53747571910684	39.49361482002821
199 h	20.9923883576060	25.74558627475694	38.89936437314581	200 c	19.24920056908581	27.23918513661076	42.30234132114537
201 h	17.16537098137595	16.91036835559251	42.13160529162901	202 h	16.10693832712082	20.10130267895620	41.85439714556468
203 c	13.87917226283731	17.41733697453428	39.70621420744694	204 h	26.64667431720776	33.58178556587315	18.46069051510749
205 c	23.98175116439430	36.30408684984961	19.96768425897562	206 h	25.84537856704344	15.16460318441754	21.40027024241556
207 h	28.85067645765315	13.94922860185868	20.5453359136078	208 c	25.98525996309582	13.64610961067368	17.55973139690492
209 h	25.76090020586610	18.74040381069339	15.52349529240014	210 h	26.77088493619639	21.74938568101379	16.75087629266753
211 c	23.43328806187561	20.23082050378425	18.64204438789818	212 h	31.51482878459107	19.86554311779043	16.30302958385402
213 h	30.30844565757083	16.87656597560498	15.27351746092125	214 c	33.41657869806215	16.61594058942834	18.00032694948764
215 h	31.23218839807226	32.64210905035000	17.49999110345605	216 h	34.33547295920217	33.53498883301749	16.49944078538742
217 c	32.67033478194067	36.09184229391621	19.28987028491280	218 h	35.98113133280065	28.99913991102521	16.59421512119365
219 h	32.84380133841852	27.95864936253692	17.39532166231465	220 c	35.82067282684841	25.90426755735203	19.37426252951179
221 h	38.31336687479515	30.66060720524596	22.58613229613112	222 h	37.30837710134577	33.85823610870231	22.38217844339837
223 c	39.48683664412049	32.55730199640928	19.10139773158816	224 h	15.85440176443202	32.76248477065098	18.03331546496480

247 h	40.29482558582790	18.63077570737185	41.86337387298769	248 h	37.87380871184813	16.29106474438979	41.97415222445949
249 c	41.121196515482538	15.26275090992028	39.67933950234204	250 h	40.65577290214873	23.23510477199429	40.0838506033418
251 h	38.67190917557097	25.92429028670158	39.67090907415688	252 c	40.70596252680595	25.81450761037132	43.27294555312665
253 c	44.89405093183050	23.91668237082482	33.15460689522314	254 h	42.28099058734126	25.99372530711462	30.78301027231866
255 h	40.76406654057813	24.15527672311379	33.13882173884907	256 h	43.37656986825009	32.30655249843891	37.48851453703271
257 h	42.60480172115052	34.68706467500253	35.22900315256089	258 c	41.56504850811000	35.62467299717783	39.08770362921783
259 h	38.41079164956836	34.98182762501469	31.32124083753412	260 h	37.23793233056367	32.63867308851813	29.21637311985353
261 c	40.13900166550310	35.04881202034970	27.58096783705930	262 h	32.63846421723177	40.38277773168731	24.50825047436021
263 h	34.23753504754472	37.67771826730703	25.71783199204480	264 c	36.20321955335017	41.25819749196187	26.32570301593547
265 h	25.54745263217730	42.71435898210964	27.81047443904579	266 h	28.38888977608001	43.52415898408695	26.17746327648027
267 c	25.04120533753233	43.29104552120927	23.79124854971226	268 h	29.98297333299679	41.20791188789239	33.43029661556837
269 h	27.88526175921896	42.87088570083748	31.36447225866355	270 c	26.20703238297161	41.76755637937939	34.93168304189513
271 h	23.36269678613135	10.86483491647688	35.72108702540852	272 h	21.69380079849379	13.47528265239776	34.40545707750088
273 c	19.77640544512481	9.83455337768118	34.02903026188317	274 h	30.58487493258157	8.48337419166330	32.05282397591345
275 h	27.79754040649596	7.51341993024162	33.69399257886877	276 c	31.15962769417702	7.83726373637616	36.05205231371050
277 h	25.61922994764893	9.69300470505057	26.84238155444589	278 h	28.04078013424104	8.14070244202621	28.62138564545223
279 c	29.17009972939399	9.31024797889074	24.85473098472563	280 h	33.28012638662559	11.41455627158415	42.40673043949172
281 h	30.93259001776999	13.36218575289533	43.89978499585364	282 h	34.17895671746711	14.33230213060271	43.85834045910286
283 h	31.39253611173100	40.11094445139791	40.08141430528082	284 h	28.360989179091145	41.10261390965523	41.15024512690434
285 c	31.36651133563768	41.64773995919361	43.90359475035420	286 h	36.71736371173346	29.87137897822837	41.28239422181668
287 h	34.67317827679329	28.54683330317088	43.60150767393265	288 c	36.013613151613740	32.34211181218286	44.46648182931097
289 h	21.88047732293229	34.79868241746006	46.76836977006764	290 h	20.69363299054741	31.77059430874673	45.91625052719422
291 c	18.33822646411905	34.90367326831232	44.68703384957019	292 h	9.33410766153213	30.87534330501422	37.64606610289057
293 h	11.57727005214502	28.36101038142613	37.62761288877275	294 c	11.98130338053846	30.99810906422704	30.76792976926027
295 h	20.54344245066926	40.35110213442653	36.25647738193607	296 h	20.90544367196712	39.46666549225558	39.47797961669645
297 c	17.07429415369510	40.51116113567890	38.46823544952757	298 h	14.40642153025019	34.01056528530365	25.99357512242614
299 h	11.84981281783532	32.60763856315227	27.68017078282884	300 c	11.33881938035609	36.60523656468009	26.87041277654370
301 h	26.8009118800754	14.09421282533936	43.56089944632488	302 h	23.16275508654705	13.16467197751538	44.41114451997851
303 c	25.02388566034094	10.59886621796952	41.79984699453519	304 h	21.06782385471662	27.76344902356124	43.22828521069895
305 h	18.65811479971195	28.92499883909481	41.18655681066994	306 c	17.24492024624262	26.69684893763636	42.32393192321969
307 h	13.17413874314616	18.84347851375953	38.32605345147028	308 h	14.18244212351558	15.64469852895573	38.6049626712008
309 c	11.88990074838058	16.96055713883338	41.75797527040376	310 c	23.52176285347659	37.75675231426845	17.50360793083357
311 h	25.44441161827665	37.32218685865176	21.08173351201038	312 h	22.25955163177769	36.36363308459415	21.17171412895688
313 h	27.31281711625940	13.53737891513770	15.92424156128925	314 h	24.31195108205102	14.73377167767442	16.88771658240303
315 c	25.11346655926599	10.96555477283473	18.26877414576590	316 h	23.72308449879410	21.55110869684707	20.25802135589193
317 h	22.77100773837116	18.42010960579071	19.49262904129745	318 c	21.36016486375473	21.28293514948517	16.89897946722336
319 h	32.91655081413008	14.72071758631438	18.77593410239839	320 h	34.14678732974411	17.73481904031503	19.63032531991352
321 c	35.49651528277432	16.29282986117940	15.99823694124648	322 h	34.48682796340638	36.81972506212846	20.07289834813053
323 h	31.33913172309541	35.97349390911941	20.91990845562365	324 c	31.66968983845178	37.98018168703521	17.32135759951428
325 h	37.68118529161821	26.26062568053759	20.29479337663081	326 h	34.52376475594580	25.29848201492593	20.92081000559169
327 c	36.07602377687616	23.7356446772304	17.45440178895626	328 h	38.76375637282398	34.0041020923135	17.47491895193212
329 h	39.74057776787470	30.78492613288088	17.99196644587894	330 c	42.08108273292994	33.39894953241291	20.10584434395410
331 h	14.06310276791607	36.88196560301066	18.56753025660999	332 h	13.72169780600288	35.28804528286995	21.50552760937831
333 c	16.44550930726776	38.7625513481451	21.55365011991670	334 h	16.61987614010219	24.31655210618632	15.48584738228597
335 h	14.61517340715941	27.00214846091437	15.24377757643128	336 c	12.990662702849907	23.87712985387249	17.35703169209997
337 h	10.76050476642188	28.39313608805870	28.21758686504534	338 h	9.29608727160999	25.62599453476274	27.00725018754294
339 c	10.63060524456069	28.23117619427454	24.12107880571754	340 h	12.85291887846843	15.03950274839104	19.61790868255527
341 h	15.66757290767591	16.67666501453123	18.77888404739938	342 c	16.27952588232852	13.28555880230332	21.03939152294546
343 h	15.21924500173444	17.32776411137916	33.58785575861669	344 h	17.43508655915979	14.85274903186638	33.06509440143303
345 c	13.72436346030059	14.09838509341549	31.51040733433971	346 h	43.83690166807084	19.30984356727918	24.64882699363537
347 h	42.55662527243576	17.54742885974379	22.07826637690307	348 c	43.91070455881353	21.29674434437390	21.06266758680307
349 h	37.92644425642877	13.45412718538386	28.58432921945393	350 h	34.97433738073877	13.86234915677303	27.08608327181643
351 c	37.10771688469355	10.57945323128225	25.78312235359032	352 c	42.81193200201875	16.61728370218894	32.16443168810967
353 h	43.76423295647599	18.44445645603756	28.60157748536843	354 h	42.2689608899467	15.44840917439960	28.28374437884889
355 h	42.34675774089277	14.65965577885768	41.28288139324387	356 h	42.40783930816474	16.18620557902548	38.28652072160385
357 c	39.90353152719307	12.92266860829668	38.48243609963620	358 h	39.34260633521762	26.99993338619660	44.35491521105520
359 h	41.38338598247378	24.26335853483868	44.62154609524259	360 c	42.94231553687521	27.46087668914019	42.42881647783032
361 h	44.90924307396272	22.34632037174459	31.75156946988053	362 h	46.52444183253102	25.15157053958936	32.64277027464717
363 c	45.3182548060388	22.82947496758046	35.80640444311607	364 h	43.48275918702106	36.26415753123282	39.67954969947322
365 h	40.73938622211082	34.653406474356195	40.7683192123241	366 c	39.95942350498467	37.93735708226786	38.40455779986466
367 h	40.78931250582186	33.65485092510434	26.14400674385316	368 h	38.59260736748580	36.14631368435523	26.66950616757481
369 c	42.30145205462244	36.85673884507175	28.25049304676345	370 h	35.70559536387017	43.24076765834709	26.84021604021330
371 h	37.38073828335317	40.53237683841049	27.91422041418641	372 c	37.75285019366425	41.26414370685092	23.87994932955837
373 h	23.29134599418653	42.12352272207531	23.68350876859060	374 h	26.09516658400555	42.92846703052522	22.00088081412511
375 c	24.34381098564334	46.09504006280201	32.95713598146429	376 h	26.30084572450835	40.14639148717688	36.27455203800947
377 h	24.22502750189676	41.81290201122253	34.21633697258522	378 c	26.79172899125870	44.23011855810598	36.33495090822140
379 h	20.30466907350628	7.82809010226766	33.65773251893290	380 h	18.57518604829008	10.42180105162848	32.40031747970357
381 c	18.23963873098008	9.98424974444725	36.47794883453603	382 h	32.84769372344446	0.90907823399598	36.17829867562899
383 h	30.10340213449503	8.09520947570013	37.85930247174534	384 c	31.99771710170999	5.07872876358839	35.79896521724068
385 h	28.76729479993721	10.89895822685552	23.53413255008749	386 h	31.23318500389829	9.39850324875139	25.26983779274604
387 c	28.54497772603640	6.79358733102222	23.56922665425944	388 h	31.77933874801924	43.62051436345114	43.30716571218053
389 h	30.12435168070505	41.74388413910066	45.60016905827392	390 h	33.18479570286992	40.77401005625705	44.50272211230389
391 h	37.70044991179309	31.68802710639999	45.53954271750036	392 h	36.53953398147203	34.12480482495506	43.47843159104804
393 h	34.53080897562118	32.81683767081851	45.88062454360794	394 h	17.15249675267822	34.93748375782853	46.42219741946357
395 h	18.50631713061897	36.88382179340644	43.99363571395139	396 h	17.28685729644448	33.81173912195175	43.22748457399122
397 h	10.69047402457746	29.96075951293536	42.06252047837407	398 h	13.94132552201521	30.43527672952584	41.27831263525501
399 h	11.88076821501672	33.05207397336876	41.18609179280335	400 h	17.32555656977824	42.51219367660209	39.06088140794670
401 h	15.75451700660327	40.51257181983642	36.83121435642936	402 h	16.12296148475182	39.49608323430790	40.04875625609524
403 h	10.28754498730892	36.27124236206392	25.08042306346342	404 h	9.91951380838858	36.98021234970171	28.37863653832427
405 h	12.4775363635097	38.35623918899891	26.62076262492160	406 h	25.78871131287266	9.35721904654029	4

429 c	31.28887281904056	40.65671394640441	18.35301664075292	430 h	34.21425041779195	23.45119192214884	16.50874671187869
431 h	36.46546835329502	21.96254078879514	18.52132673576708	432 c	38.14430455656489	24.10358088872007	15.45865258563471
433 h	42.77176621240444	31.95253270835277	21.47191234167016	434 h	41.84884111031221	35.17821299357628	21.21340548939680
435 c	44.04286722251816	33.80196482876371	18.01659687086921	436 h	15.03432587247264	39.82633729208116	22.12458399791549
437 h	17.48008556994696	37.78976191381242	23.28817772309458	438 h	17.83438752754727	39.31382116849266	20.27937347664106
439 h	12.00980713623386	23.07482758529040	15.6805500068189	440 h	13.58155514542241	22.26300597973862	18.57093148407243
441 h	11.57841381848806	24.99990654035880	18.44033388633906	442 h	8.85617007243164	29.35373120810385	24.02130489647798
443 h	12.23271046662523	29.54666372956576	23.75107156773986	444 h	10.57742260606189	26.83960394746672	22.54480935740967
445 h	16.51853015344255	12.03583809756340	19.36495195256493	446 h	18.19699569772903	13.75824977142595	21.76165454142220
447 h	15.31404135906415	12.15928307295206	22.53293147364852	448 h	13.08002417756802	13.05391827366312	33.21861619357491
449 h	12.04332132364600	15.08963614511154	30.72520998477661	450 h	14.34055030535742	12.67265870219155	30.08862301498413
451 h	43.92714661953224	23.22586589217991	21.90675437232663	452 h	42.72639569829912	21.44253352375492	19.32403871233105
453 c	46.59848343179261	20.50089441360862	20.34323624707502	454 h	35.92037110923987	10.36583200455505	24.05292130829485
455 h	39.08093002439083	10.13785508802643	25.18345069089885	456 c	36.27504530245346	8.66990463077276	27.79572640796621
457 h	41.30275203313212	15.34975204255574	32.90546211142640	458 h	42.68653670924390	18.38192831965027	33.30761159766137
459 c	45.40782214240308	15.39735375534374	32.54569297549849	460 h	41.37364708748752	11.56475230700248	37.83732647121440
461 h	38.70741822892719	13.39918037759593	36.82009515300869	462 h	38.68094164538731	11.91762989638529	39.87070184219144
463 h	43.93524135435960	28.29219588699623	44.07647880003879	464 h	42.31687765994378	29.02976754318137	41.19213671194311
465 h	44.35375242011533	26.31900687030553	41.34870488022374	466 h	47.04232729666766	21.63818472524600	35.87625844850786
467 h	43.69061729122375	21.62383495799693	36.40112686067327	468 h	45.53363262498866	24.33966611652670	37.25347515384954
469 h	39.84755464733816	39.27476562980423	40.02309723527490	470 h	37.99220105378357	37.42888204332159	37.86286034567268
471 h	40.80155199308130	38.98180415020720	36.78216478506918	472 h	42.96336151660228	37.90903631429163	26.55401311410165
473 h	43.96982148658581	35.84479555777723	29.03623093993689	474 h	41.69117376460016	38.27712952200520	29.68041939440276
475 h	39.50377294747592	42.40908454919098	24.08234210768306	476 h	36.64855879862464	42.06625404562948	22.27741820185387
477 h	38.33174247855116	39.31622457489144	23.32991118651646	478 h	23.19029068662036	46.69920483138819	22.30711604432070
479 h	26.05958030190565	47.31270454044464	24.01301403987192	480 h	23.22665282093680	46.50110749041503	25.69334328699848
481 h	25.45817673884133	44.54127506074206	37.93063447855059	482 h	26.64889086467979	45.89452813812472	35.05459642609716
483 h	28.73985696355578	44.20874347049820	37.12823117926730	484 h	16.52004790882455	8.77969493434052	36.38032161235254
485 h	19.37279886222004	9.34393105000878	38.13236222834256	486 h	17.60935803381707	11.95418871655970	36.87166359387721
487 h	33.19050263818252	4.48604219456122	37.42505530811944	488 h	30.34664045050990	3.77610253200475	35.71374865538736
489 h	33.12476662713965	4.78354785808225	34.04655851956590	490 h	29.64914779553413	6.53745606972099	21.79830985267014
491 h	28.97719692700067	5.16219737053231	24.82699624710405	492 h	26.50514697944885	6.68245656575068	23.06709509389934
493 h	23.12208789722484	7.68142071234550	16.69598401546985	494 h	24.90397678419508	9.44236595934625	14.40607230709751
495 h	21.96626289538456	10.66918262859278	15.58081326310238	496 h	18.86651751226990	20.29419306154523	13.72955276641290
497 h	19.62147985916567	17.68808303685574	15.77089491337621	498 h	21.91709506212652	18.84650772716193	13.55478837210436
499 h	39.33627767088591	14.79564030436831	15.49795880004644	500 h	37.51679017436047	13.17792687424197	17.86242248418412
501 h	38.80005836257398	16.24993848481294	18.51401040112296	502 h	30.58754231781560	41.96098869552489	16.86168504923037
503 h	33.08751967521635	41.45260379062626	19.10172045919101	504 h	29.88728219104168	40.68138726574607	19.92277347481213
505 h	38.27717826172196	22.43650565745518	14.18226729470972	506 h	40.02838622934876	24.36472246489913	16.36165287856909
507 h	37.78584073151395	25.78165217461530	14.24274969480211	508 h	43.42289650523674	35.28042626259212	16.65279328522331
509 h	45.89429876305712	34.40521088942680	18.80792438501107	510 h	44.36753305568781	32.03374696777272	16.92301074906478
511 h	47.46345344085569	21.85612543214284	18.98934369754122	512 h	46.62438867047163	18.59889567040927	19.44197876251340
513 h	47.84781201241884	20.41219144376341	22.03434504763711	514 h	36.31846788601767	6.70207061614311	27.05762896228509
515 h	34.32156134135870	9.06644182990198	28.46743099050356	516 h	37.52554045784719	8.75819454450311	29.48401816146198
517 h	45.74798470877845	14.94062470099102	34.56980899159586	518 h	46.95920631189659	16.67130910668475	31.91184411264431
519 h	45.57986708351157	13.60544692749720	31.45569900795296	520 h	19.11850895576428	36.89704311853740	32.99191412467516

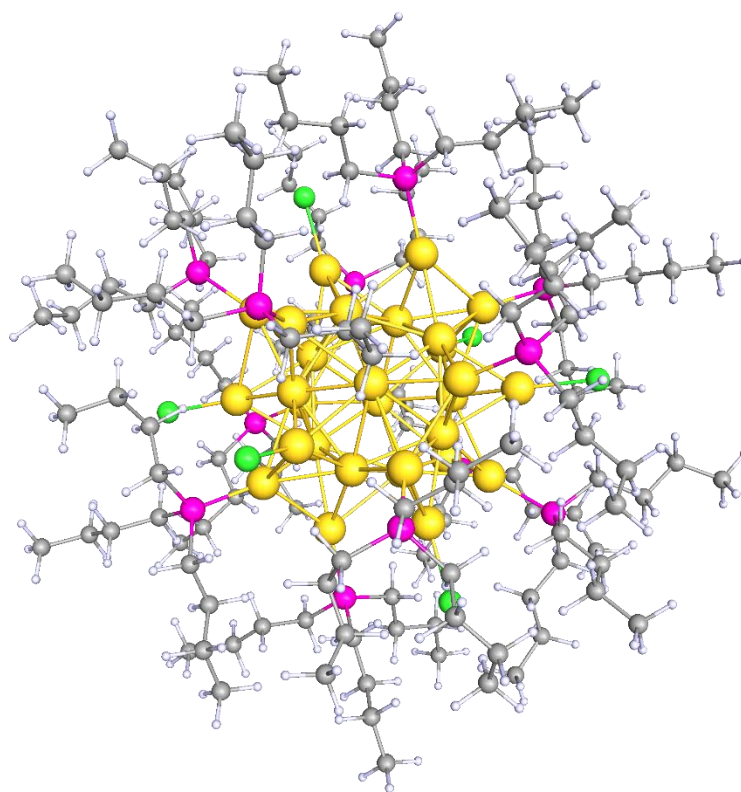


Figure S14: Geometry optimized structure of $\text{Au}_{30}(\mu^3\text{PBu}_3)_{12}\text{Cl}_6$

Point group: C_1

Energy: -16612.75788117461 H

HOMO-LUMO-Gap: 0.855 eV

1 au	25.10204023843793	26.23523233562979	34.24541789912931	2 au	23.02561295218068	27.14070751485702	29.10303838982716
3 au	30.47601903838007	27.41165212283811	34.43536878945745	4 au	27.05245918908325	30.65157472842295	31.51928740159018
5 au	28.67692421713901	21.91510128613939	33.75153900328131	6 au	24.02493532577913	21.97412012986226	30.54347782197746
7 au	27.99683160450979	24.38887140982436	38.37241206863840	8 au	26.65126989279637	30.84843318650414	36.79119440718751
9 au	21.98674610928589	30.51889488043957	33.46650004571170	10 au	20.11251895480966	24.89391607718420	33.06432883190524
11 au	23.89916583167928	20.96226130517021	35.87725948296443	12 au	25.55064736046667	23.76731960330700	25.46189719603053
13 au	27.39582879431847	29.21872372512416	26.24355287157598	14 au	23.24541210334522	32.26558965125505	27.80691049466736
15 au	22.45029999464159	28.01078047710579	23.86717173264374	16 au	20.40965117950301	23.19378389421769	26.36991786933935
17 au	33.01184624508553	23.98539619834166	30.82204197105172	18 au	32.02586129007004	29.10581507631615	29.31757355511655
19 au	33.59105443024276	23.35059497471024	36.13543156885796	20 au	35.62802362063299	28.02658900309748	33.48546457291818
21 au	30.07370216005901	33.7753746502063	27.95097796890287	22 au	28.98579669621929	20.46882319394610	28.54364710172060
23 au	32.89827003302732	18.93260255933919	32.29818673259710	24 au	25.95687070534881	17.32342467479716	32.01284181907708
25 cl	28.01856112582408	24.86727151590218	43.00284610806054	26 h	30.72087371843055	18.31780973135105	38.54462784570852
27 p	27.50259760536987	32.57072532592986	40.86063734311401	28 p	18.05500335446700	32.60150128334133	33.73217563661382
29 cl	15.68559348168943	23.80155339694732	34.19526253495334	30 p	21.44813795416568	19.95681443105544	39.4931069946959
31 au	30.91279605697379	24.78091121501382	25.63211335495917	32 au	27.99594427126458	26.75678200419949	21.57843654780187
33 au	29.26015565943242	20.04228458504218	23.30186808210569	34 au	32.17406268390782	30.12087499291562	24.03413709247572
35 cl	21.47697185253638	36.58971233351953	27.29221501524334	36 p	20.77323243125935	30.23285257123186	20.38419556484671
37 p	16.37278375716428	21.26716790694359	26.05007053216811	38 au	33.92798247110611	20.36148900100668	26.54324397125559
39 au	35.89797984522826	26.09638213738248	26.81670501013107	40 p	35.33702255365586	21.28017702031343	39.66914452481380
41 p	39.65512490406643	30.01191707571822	33.58311022372543	42 p	29.24858902340267	38.17990172928149	28.40344434709390
43 cl	34.93520314911225	14.83980964681814	33.36191755935776	44 p	26.72542982205064	12.90516391003252	31.66441443953273
45 c	31.23155004836028	17.70096417013323	40.49352140898561	46 c	27.85149927315774	36.08164709479185	40.66077879320795
47 c	30.46153159057717	31.43692438625359	42.36251666831310	48 c	25.24141813061406	32.01874525809609	43.50513403075430
49 c	15.82622466252029	30.88791044238398	35.84801718802890	50 c	18.18218544196625	35.91766888636960	34.89832813955836
51 c	16.44442960574269	32.83212230086183	30.60039280060707	52 h	15.97161346455390	28.86382889339008	35.27399531613609
53 c	22.87262668991135	17.63665623329949	41.67226353941544	54 c	20.91219433559221	22.64529984321936	41.62618216548042
55 c	18.26480897519305	18.72011174416194	38.61639466330983	56 cl	27.81542716399957	26.56935612265201	16.91867286496347

57 h	25.63776843650362	32.79376700552851	21.44069222773354	58 p	28.33926398301376	18.09578464278250	19.35179384979936
59 p	34.58617426107068	30.91713133948216	20.38165595914808	60 c	23.23510185971429	31.63506855430339	18.30123103205349
61 c	18.56458894733933	32.78954836814286	21.38616438258054	62 c	18.96465967767167	28.38978253085472	17.98789817682826
63 c	13.62691175282871	19.340566815385727	25.51792046145524	64 c	16.29023974539587	19.05680627844378	23.29575378592021
65 c	15.34507231586985	23.6465267166033	28.80866362359347	66 p	37.93449741466311	18.49189917269015	25.98019665268923
67 d	40.37817743670909	26.89978358302874	25.62764168679511	68 c	32.94483348221885	19.71239024724394	41.71727149929633
69 c	37.78262880780015	18.92540307688190	38.74003676052483	70 c	36.91812091348847	23.32515710647825	42.06502486852457
71 c	42.37894786665740	27.92578860956698	34.37313889921225	72 c	39.77762754775077	32.52713497947066	36.06013189944733
73 c	40.72485277577356	31.59102663975378	30.64523879153590	74 c	32.10017583834171	40.20322417190073	28.86097622492804
75 c	27.50268886825769	39.56911507626721	25.68949899911994	76 c	27.24009763295469	38.77066712689631	31.24790182457535
77 c	23.85504964238042	10.85794203335666	31.69650382264867	78 c	28.84884361967820	11.64117863989379	34.15746301950792
79 c	28.27614633988563	12.19376044262122	28.56521819880829	80 h	29.42037287570123	17.69448789339851	41.57060309237800
81 c	32.27103101903383	14.98273582056466	40.41986254187539	82 h	29.30587074623433	36.41829736185966	39.17684818504414
83 h	26.04901022100586	36.79920625718599	39.84338258519214	84 c	28.52135033066929	37.51631373532786	43.09673650822227
85 h	30.59775952710849	32.40554761542053	44.22731185844213	86 h	30.12576421642048	29.38912717649911	42.74751208938536
87 c	32.88533864754918	31.79614128560006	40.81318105778675	88 h	25.11482221329634	29.92431620925944	43.68684626964799
89 h	26.18546806192083	32.71430232506940	45.25661411694486	90 c	22.61821126352290	33.22675069309900	43.23814730044224
91 h	16.67350154675671	30.99696563135194	37.77061354135790	92 c	13.03525646811481	31.70659875277211	35.85664025454266
93 h	16.22622110517598	36.68738414320637	34.87507897698338	94 c	19.38983507415139	36.21300500577648	37.52022861952043
95 h	17.99175382502099	32.92121118920662	29.17979025319313	96 h	15.48762401636566	30.96683643730357	30.33025788779922
97 c	14.61995679624914	35.05113914816553	30.18901647993523	98 h	24.68766536933038	18.51147532293867	42.28279899400154
99 h	21.63051732662653	17.57420236674103	43.37386204426622	100 c	23.32282076027049	14.95515107988283	40.66559152512783
101 h	19.90250380584996	21.85942939839199	43.29886047564491	102 h	22.82676815777298	23.24433678807529	42.27648500803139
103 c	19.48334526749472	24.90134207749143	40.49562606093174	104 h	17.45874645887977	20.12135657685831	37.26117374476781
105 h	18.60352867522387	16.97182286745024	37.49368630920267	106 c	16.40569916802448	18.21233226609377	40.79029406400603
107 c	25.14257236273317	33.47297816572170	19.50845716175585	108 c	26.78883966792292	14.95804162164313	19.80382107525416
109 c	26.18652119213738	19.86808265308410	17.22861035900696	110 c	31.05188824932189	17.45917218450835	17.19456441168997
111 c	33.4030856129089	33.49525594343126	18.29476012424386	112 c	34.63777857105465	28.24926784312145	18.10725105620226
113 c	37.93935997281334	31.69599972413021	21.06845604756895	114 h	24.27638298217843	29.94714345692733	17.58350313087770
115 h	22.26656142789550	32.49966071125302	16.64326300497070	116 h	17.11672169868107	31.84829018078766	22.95153870351076
117 h	19.65955165005240	34.01117683553372	22.70456401827161	118 c	17.28638949418301	34.31428019780406	16.2693563857586
119 h	18.51456913156441	29.71256938111663	16.41057155763533	120 h	20.32207657268500	26.98095838578058	17.22090909073077
121 c	16.55163569814764	27.06837137009955	18.90659089496197	122 h	13.77479348752499	24.08696215210316	23.5333432929423
123 h	11.87819160323231	22.23448810681918	25.64098489059713	124 c	13.48049192957803	25.63646303108134	27.38002694190769
125 h	16.78611936846767	20.23012485783931	21.61774702285472	126 h	17.92022544657265	17.75890748581690	23.57792020355303
127 c	13.83159794845304	17.57839916948562	22.82282071265623	128 h	15.15155763470515	20.72112618989591	30.41350444916723
129 h	13.42508969007313	18.61929080442248	28.36832197531379	130 c	17.16923581050690	17.23835497318841	29.56717462322460
131 c	39.75111483402099	20.26986234103445	23.55221969899889	132 c	38.00002399000484	15.14533180457335	24.88975850302633
133 c	39.73952966724141	18.50534629460537	28.99926336023242	134 h	39.98426038683969	22.20619180492894	23.5637550542011
135 h	31.75536525340266	21.32421299947771	42.37649379834831	136 h	33.93636010011269	18.95801024645301	43.41509826237049
137 h	39.14315567489798	19.98532768367864	37.53075609892456	138 h	36.81947277926405	17.58795276254677	37.42932320747585
139 c	39.19137187478690	17.55621194121946	40.88425164141249	140 h	37.41674782675847	22.08766229244827	43.69643653875158
141 h	35.43288956696215	24.65008128100811	42.74740849766231	142 c	39.25720955337358	24.78402063308796	41.16053854356942
143 h	42.1559846303106	27.39613217932943	36.39672558737588	144 h	44.13173462617288	29.08806428225125	34.22604241757421
145 c	42.59921661790590	25.56218074475045	32.69094334665214	146 h	39.41838448539725	31.53528430592295	37.88239799835345
147 h	38.08557309466956	33.72879301812557	35.72614072456388	148 c	42.19442644081676	34.13477325746943	36.23594948548618
149 h	40.87573125020417	30.08738962282194	29.17292887949736	150 h	42.66879875999001	32.30895739414454	31.02122697721331
151 c	38.98060232592731	33.70001587518993	29.67915620698867	152 h	33.11576470359228	39.41052922005282	30.52637125526321
153 h	31.46947307326729	42.13763399861350	29.39617846995608	154 c	33.88016289888974	40.34191405485463	26.57176747149895
155 h	25.78597739552121	38.35937175939986	25.51331607004689	156 h	28.69057668490181	39.19130833339985	23.99253988335838
157 c	26.22237461496233	42.36575574610396	25.80775454320342	158 h	27.68547617305515	37.23005827576234	32.60827674877977
159 h	25.27842525530182	38.38518183028650	30.57771259706500	160 c	27.43647377919081	41.36460392716540	32.54993854544020
161 h	22.69044009944211	11.46303056392005	30.04982226808626	162 h	24.44411191689733	8.87129335607416	31.32916549508533
163 c	22.80723031142211	10.997633959410964	34.13148596362617	164 h	30.54344953632319	12.89765946438103	34.11421768626401
165 h	27.86990075591759	12.04043076974486	35.97901491216582	166 c	29.68441221098655	8.86108204984538	34.02409582726843
167 h	27.57671876482911	13.65949646179265	27.22953780337258	168 h	30.31188231297848	12.63958976928695	28.86963612676760
169 c	27.92236196448872	9.54028814331282	27.42427080154145	170 c	32.66959024365874	13.75837882005463	43.02047065532263
171 h	30.91130345781460	13.81125697084035	39.32270612035440	172 h	34.05145333178455	14.91106899116747	39.30586662438882
173 h	27.05452688583819	37.16344437368062	44.56711738115931	174 h	30.32977128740457	36.78196990044608	43.88787546920656
175 c	28.77258067615663	40.38706587999003	42.68899120049294	176 h	32.76099063199936	30.62297210413023	39.06722974331686
177 h	33.07685788115802	33.79783457640177	40.17426438546093	178 c	35.27378827161530	31.05598604008627	42.30594785815111
179 h	22.80041301661176	35.25894513989048	42.70923194052218	180 h	21.57835618109439	32.30384757122728	41.65957703689261
181 c	21.06145723121884	33.05232526101037	45.69068165309071	182 h	12.27356962064646	31.52959593775206	33.90500073617100
183 h	12.85003925750698	33.73894313586088	36.38868281544398	184 c	11.36345890538398	30.09503681763120	37.62404251998819
185 c	19.49198515519517	38.96666923139153	38.46919761874269	186 h	21.34049105146892	35.42237078212231	37.45282128005072
187 h	18.33978476021666	35.05234777985441	38.93116875754176	188 c	13.22578253078062	34.89626028051645	27.64427903273243
189 h	13.19798395598962	35.16585008028794	31.73693386109975	190 h	15.71786812769137	36.84386149527425	30.2376771352561
191 h	21.51712987246027	14.140626034726	39.94664938995175	192 h	24.63042007202716	15.03629846530566	39.01571742711313
193 c	24.40460351563316	13.19395944028156	42.71504275044079	194 h	17.67482153537895	24.28530764363798	39.61272324556594
195 h	20.62878037906887	25.71027095924265	38.92581808437657	196 c	18.93717693759332	26.97680561481251	42.46048551439807
197 h	17.20844403409043	16.806458076688701	42.14150982267889	198 h	16.09801396103571	19.98031435462236	41.89193905441717
199 c	13.82846724446468	17.25491321901691	39.83418439120279	200 h	26.92613012881149	33.32666424481902	18.39682423498629
201 c	24.35404850475497	36.27270199822986	19.62128135007073	202 h	25.12163606436719	15.32555321658804	21.03443645939401
203 h	28.11211537665300	13.81849771352504	20.97828470537087	204 c	26.00434122741297	13.49452644364625	17.41949905818579
205 h	26.10264292994566	18.81486469762356	15.40705630929880	206 h	27.11715654445615	21.72455485668316	16.85291869049480
207 c	23.53300754600519	20.33057314772189	18.30712683176501	208 h	31.95319895496416	19.33136726041375	16.86773115635268
209 h	30.26040932062056	16.83910042017743	15.34271570584749	210 c	33.01970986476247	15.54631481194426	18.13691948324221
211 h	31.46703341517524	32.89915273014735	17.72338408298066	212 h	34.58239288396970	33.47003884523937	16.54814108552605
213 c	33.35033270033364	36.16296302490228	19.43130583270275	214 h	35.75388767451560	28.89486087956368	16.44218574409281
215 h	32.64066994874803	28.00571589103772	17.47185347869005	216 c	35.64311599010068	25.73792721414288	19.15461608786226
217							

239 h	36.94335614138332	15.10191171969057	23.06986570182095	240 h	38.39562282326555	17.68566513099752	30.40098956538379
241 h	39.9372237212871	20.53509726490841	29.51817600608860	242 c	42.29412681271855	17.11492633896228	29.13530369047995
243 h	40.18286725631333	18.97100621746185	42.08765012289498	244 h	37.81662585433602	16.57588798738856	42.14360252971841
245 c	41.15725325122109	15.61426766163589	39.94552585115710	246 h	40.60969329760425	23.47525393659443	40.21313215628138
247 h	38.67331231743994	26.18050771145608	39.69528358355392	248 c	40.63701077646919	26.12619458868341	43.34368268309358
249 c	45.11891603615451	24.139910277104341	33.02902180853819	250 h	42.39951924312255	26.08927281195730	30.66388889824131
251 h	40.98126492245962	24.27780973117764	33.10320552112729	252 h	43.86792597819422	32.87578860592197	36.44319958292777
253 h	42.47527263275508	35.19557748290006	34.43836051702370	254 c	42.19492655465256	36.02858138115502	38.45512594236588
255 h	38.61252412866720	35.12530897353319	31.19093711479289	256 h	37.11361608794975	32.85798766577253	29.18652811675531
257 c	40.07068562606857	35.05613992608424	27.34308343857261	258 h	32.84488906425376	41.12421964749356	24.91266696913816
259 h	34.47990252845079	38.39720805968068	26.02579369415900	260 c	36.22227868363728	41.99279450395531	27.07927667647232
261 h	25.39865031025740	42.64755369854745	27.41844965814492	262 h	28.39300718910998	43.59889275438719	26.17586482759828
263 c	25.40288261210074	43.25152920641255	23.36981472762841	264 h	29.35702870096315	41.60693432097792	33.38128144515034
265 h	27.20915034631156	42.91828451843990	31.14927029836820	266 c	25.45369659543335	41.71241249051098	34.64753057278439
267 h	23.46642815661563	10.45684340575581	35.78587939519762	268 h	21.68953637408239	12.99220309832897	34.46475635481978
269 c	19.94156077679161	9.26898408547357	34.04201892694893	270 h	30.78142176166045	8.54795863417519	32.25508023909144
271 h	28.01636737998554	7.57379917449648	33.93378593493438	272 c	31.35672023947600	8.10971187135876	36.28444454701175
273 h	25.87817632852400	9.19062985779253	27.05987920510018	274 h	28.53081049848468	8.06075565952600	28.79071575464141
275 c	29.3803691615237	9.17611744437262	24.93501380387739	276 h	33.32344419772791	11.76900097954834	28.788686161425
277 h	30.88582985311254	13.73598654380192	44.13984013048136	278 h	34.11049971014089	14.76858701142886	44.17449371991111
279 h	30.24287719854270	40.74904772966008	41.22275945665591	280 h	26.97051581915899	41.13341631073469	41.89095207012406
281 c	29.43762854948709	41.83721724999352	45.11040010940051	282 h	36.88958345284918	30.97129231620274	40.96072771438553
283 h	35.02907070236157	29.09764827218194	43.03883209185106	284 c	35.96140051081224	32.83836904348885	44.49026151326317
285 h	22.12460334862973	34.00159858275912	47.24482784623236	286 h	20.89302314628944	31.03297373930573	46.2627114082364
287 c	18.42000454290735	34.22545909044915	45.4727923283525	288 h	9.34698455928042	30.52387142489139	37.19032924280202
289 h	11.65041960837577	28.06336021578506	37.14987953443791	290 c	11.82117849356795	30.52343561341153	40.45501134172187
291 h	20.55579181771684	40.13376567957597	37.07546932227122	292 h	20.62969169172027	39.00439155995147	40.24253073311960
293 c	16.90991252391368	40.18457819415589	38.98859281106118	294 h	14.65233472092394	34.79318518168662	26.09949628678729
295 h	12.13054914208790	33.09820738349466	27.55730325798282	296 c	11.44631933424485	37.13856562986374	27.18393496971182
297 h	26.21962418073087	13.99843098724026	43.42095187958207	298 h	23.09862438062404	13.18626270436921	44.37019096340323
299 c	24.83649782007641	10.47047195108758	41.82547655508409	300 h	20.75219829432880	27.57027304385443	43.34856315328650
301 h	18.21054869754245	28.66687562616546	41.43449773855790	302 c	17.03521836003570	26.24223212573332	44.52614972051189
303 h	13.04833474182619	18.66223093628373	38.47573444086818	304 h	14.11708270521333	15.48189828452211	38.73027172095942
305 c	11.91756937689692	16.77404544381325	41.96102938894441	306 c	24.05470141112864	37.58160523833378	17.03672094871710
307 h	25.82118414815493	37.30443665970777	20.71904568739042	308 h	22.58751561613777	36.49120351052025	20.74061848990170
309 h	27.69418742760811	13.11070118671000	16.22106958649556	310 h	24.71288193264663	14.67385391909747	16.24654714373766
311 c	24.68207224206007	10.97222808322713	18.01998299902215	312 h	23.70784311206231	21.41879216013066	20.10315110377276
313 h	22.60123451155946	18.50230104394744	18.79893423486034	314 c	21.81825364310842	21.80665515402261	16.47593375346093
315 h	32.09844517080778	13.68745845549296	18.50797728633435	316 h	33.79959113445111	16.19344744468759	19.98442767338583
317 c	35.17892963866859	15.15673259443392	16.22352239546310	318 h	35.27019903785737	36.694339271728590	20.11962624911318
319 h	32.09568267305099	36.17724065746172	21.12419170551441	320 c	32.45536853107865	38.15257315406014	17.50464341130564
321 h	37.61393086421048	25.95782032300882	19.86471741750158	322 h	34.48483352740951	25.19270078356856	20.82744730871560
323 c	35.53737263928382	23.58718974953308	17.19385851348238	324 h	39.10813733486653	33.40570525610340	17.46976068132906
325 h	39.79387754343021	30.11571308480565	17.74111255934547	326 c	42.48055105657568	32.53825034857378	19.66928124171669
327 h	14.45398356086525	37.18116340592717	18.56273573269108	328 h	14.13140453302882	35.65915614572332	21.54201184353931
329 c	16.93075671372231	38.68118381697013	21.47355897176742	330 h	16.33101259883761	24.51725985981794	15.68443910243971
331 h	14.56768591133375	27.35380463915131	15.32105061509924	332 c	12.65962511778266	24.46997323794285	17.53750856809342
333 h	10.99426803426602	28.58270957109091	28.73072293583856	334 h	9.38679202407357	25.78814322966732	27.79678865815783
335 c	10.35506844258977	28.29837751652763	24.68464294976969	336 h	11.97657761730962	15.09836197887948	20.14641425840093
337 h	14.32478809114831	17.06630506050316	18.76350020190951	338 c	15.79941167665881	13.68086169301241	20.58712964817657
339 h	15.82021581975786	17.01739049253156	33.4325529942905	340 h	17.78126868943515	14.45136460337015	32.49490213617958
341 c	13.86965564010746	14.06294943876645	31.32360530078643	342 h	43.61086354265612	18.94713790513038	24.22558065180729
343 h	42.06102518339068	17.36910703489423	21.68615399740024	344 c	43.56188486427886	21.07805115527909	20.72049354174179
345 h	37.79472241916071	13.457675758645600	28.65490303838892	346 h	34.86664442433843	13.60959416041364	27.07255276290645
347 c	37.28658610627976	10.46431682436843	25.89530379319404	348 c	43.14589389392265	16.63229442661424	31.87539573906799
349 h	43.77896199593349	18.21855399000649	28.13142650418613	350 h	42.17896195154348	15.25914201652866	28.14669205706225
351 h	42.35492441553061	15.05085032470143	41.58533066931165	352 h	42.456882172343383	16.56401314702069	38.58307209576270
353 c	40.03408467551970	13.234515394868645	38.72607787312287	354 h	39.28851473818069	27.40599179118190	44.33355797244214
355 h	41.21415921600488	24.68664873359964	44.77170780078386	356 c	42.96786001691598	27.63364378014634	42.51009242211398
357 h	45.15901017708937	22.55345341421058	31.64557588286903	358 h	46.70781117013852	25.41268689987725	32.47785696833547
359 c	45.6022129483528	23.09514123849982	35.69110394772434	360 h	44.09775721681001	36.92703885143936	38.584498481954526
361 h	41.97271991074670	34.97189340847673	40.26577922181204	362 c	40.17698000426497	38.10609724964220	38.28967296050589
363 h	40.53861074229427	33.60858599701169	25.89057423542023	364 h	38.55175862263373	36.25235330554118	26.50857015550205
365 c	42.39858083577233	36.70976519231454	27.86019402537349	366 h	35.59496385590662	43.88745038853455	27.75940967299764
367 h	37.33002747518512	41.15033244555991	28.66207607034504	368 c	37.93338446121329	42.32317296797059	24.76260487605095
369 h	23.73573492397147	42.01463215445887	23.02013840671410	370 h	26.70099467575431	42.96093004732899	21.73423837973861
371 c	24.56350202303123	46.02514037527149	23.46315207195409	372 h	25.65083348116234	40.15319804437296	36.05105151805034
373 h	23.53339432708758	41.49344679943295	33.81046558141384	374 c	25.64729090831213	44.27229481600942	37.95479447488474
375 h	20.56358436623920	7.28524830596105	33.69120352263312	376 h	18.75343468165577	9.80007717736562	32.38424813185881
377 c	18.33316615363566	9.36391972862996	36.45162298158372	378 h	33.01149419117524	9.40828676788645	36.34959125376516
379 h	30.28663367403971	8.43267162454348	38.07201844861684	380 c	32.26165066685760	5.35757329918631	36.17875707983841
381 h	28.77474629404911	10.65686262371019	23.6398179143699	382 h	31.43019863748483	9.51229502841546	25.27494810120684
383 c	29.00403174209512	6.55080211306214	23.76402895423845	384 h	29.60443951972303	43.90082791405695	47.46988624207316
385 h	27.96682648489157	41.57111201733335	46.59158832702119	386 h	31.26824682008885	41.18442169315654	45.91697109027845
387 h	37.73621571629531	32.22871127751348	45.43944323418220	388 h	36.25673779076370	34.80682585008785	43.80374194169234
389 h	34.46667460805713	32.90041308401253	45.96813964818337	390 h	17.36490823880484	34.08051847958711	47.28522989255752
391 h	18.52453234126017	36.26483522351066	44.96131795914479	392 h	17.27377927505009	33.26249167581198	43.99500635912501
393 h	10.50608956436710	29.36548188166966	41.61675253709564	394 h	13.77348908726001	29.99803945843556	41.03111448378736
395 h	11.52186987626391	32.53996205934602	40.98226846643333	396 h	17.13074915859484	42.12291225729009	39.77283179538039
397 h	15.7477123695280	40.3527153609553	37.24457938496801	398 h	15.80362478947332	39.05971302254427	40.38209884134393
399 h	10.46779500210150	36.97635064692805	25				

421 h	36.15695298964553	16.99607057701229	15.90723355809962	422 c	37.10867404812068	13.14917954609266	17.02881650500285
423 h	30.53133927919816	37.63119164702848	16.82125414991431	424 h	33.70643242506839	38.07543425386807	15.80941979819818
425 c	32.41357178642710	40.85828334831176	18.54067748087090	426 h	33.55372373735283	23.41254503656440	16.50618512297536
427 h	35.98325653183657	21.78156794168176	18.18423781635302	428 c	37.33284975013450	23.88457138761915	14.93309823828256
429 h	43.10401200060136	31.06730878764137	21.04079517045513	430 h	42.47765195508877	34.35761593099362	20.73406645267967
431 c	44.36400568886722	32.70373508588637	17.47127050263873	432 h	15.56519820461519	40.17039560291879	22.05663316652639
433 h	17.99738014521777	38.09703127076470	23.18935915189351	434 h	18.30180054438674	39.56955897542466	20.14627138711108
435 h	11.63149662631547	23.67372326307158	15.88530939121312	436 h	13.09540467173560	22.87222704270573	18.83624714784690
437 h	11.33805985967308	25.75905633571139	18.54595334611541	438 h	8.58326058891184	29.42706820836371	24.77272027820657
439 h	11.90019917600279	29.59001283634895	24.07248663086727	440 h	10.09881542698029	26.85890130303923	23.17244645383352
441 h	15.66810896853426	12.46902104059127	18.87452794598515	442 h	17.78771316039386	14.35173305858190	20.72244891547917
443 h	15.42772303161572	12.45653387879305	22.25856450125091	444 h	13.34092409195517	12.93309371354074	33.01641991481826
445 h	12.19159632151704	15.22312517234158	30.81298906169420	446 h	14.21104557588794	12.71181632625571	29.74416257450127
447 h	43.76211210828989	22.96182553407397	21.63885722719026	448 h	42.27003334751318	21.37476446258430	19.08110263219459
449 c	46.14091117472103	20.15479323412709	19.77096368062248	450 h	36.20354664091631	10.12848421138102	24.11681827867821
451 h	39.31335757301545	10.16795783578270	25.39198472310245	452 c	36.51936002650871	8.51807347716936	27.90389447951488
453 h	41.66374906251646	15.50485385096748	32.85760146069253	454 h	43.24639590630152	18.46879923913891	32.90196013962642
455 c	45.70210281458235	15.27650549161926	32.05554246483994	456 h	41.55653835834403	11.91676117251591	38.11798293491623
457 h	38.86221694486540	13.67497171901019	37.03668584714954	458 h	38.81075118836971	12.19668547978944	40.0889962293091
459 h	43.92899399989803	28.53114744501524	44.15038862958331	460 h	42.45007286571509	29.16772319831935	41.16601588413755
461 h	44.37586897652147	26.40129641428283	41.54725090227503	462 h	47.38616832819497	21.98486617984733	35.76174407309733
463 h	44.04000073813205	21.82369236456990	36.30476850288538	464 h	45.76582792134735	24.62697029383997	37.12327202738862
465 h	40.36643058527434	39.46881524469602	39.87905882632167	466 h	38.22664955939182	37.32474017141512	38.36987124417563
467 h	40.3507785185770	39.19628454169459	36.49739048299530	468 h	43.03892890892497	37.68773237078555	26.11224674313276
469 h	44.03004863211615	35.58534142881745	28.56516163948561	470 h	41.98274703774437	38.19302105796088	29.29651604219002
471 h	39.61238904772826	43.50516686790782	25.21222267647522	472 h	36.90588733695074	43.25367362598735	23.17985835122679
473 h	38.63394581387579	40.46967854446827	24.05693771606918	474 h	23.61891179408586	46.60099287133698	21.67546241245155
475 h	26.19939281137258	47.31629380881873	23.76053970423197	476 h	23.20237375489104	46.35842358475321	25.03288683441597
477 h	24.17850643510843	44.46725420870185	37.48627454943845	478 h	25.39583628441466	45.86890222951889	34.64693031355446
479 h	27.52349709450548	44.51574778064946	36.91637956385897	480 h	16.66807724024939	8.08867390946840	36.31209771107984
481 h	19.44454059162364	8.77529873044246	38.13834979368698	482 h	17.61515032937804	11.30793240905232	36.81592913518485
483 h	33.46137393450717	4.88260035092132	37.83847599669168	484 h	30.64278715562861	4.01170076914701	36.16048116571264
485 h	33.40472453793023	4.99471443956032	34.44979537787837	486 h	30.07949963301078	6.34770520592743	21.96917126846662
487 h	29.65611348914608	5.03214629120134	25.06636004495051	488 h	26.97639041171242	6.18435554991283	23.3353199904327
489 h	22.95227161272814	7.68681034861459	16.15174143125236	490 h	25.57663448839286	9.01691095688508	14.46204383453706
491 h	22.57775810841179	10.60136458194628	14.45434149112469	492 h	19.77210504355456	21.53428046739097	12.87434063862978
493 h	20.18191616770876	18.55746330919087	14.45097968727597	494 h	22.78772378108016	20.01282649360107	12.83001813512176
495 h	38.62197654134481	12.92212462005696	15.58768696301715	496 h	36.19720454498349	11.27070808632366	17.29260841374618
497 h	38.03719750604287	13.65711509284137	18.84625789232310	498 h	31.77801301891168	42.22877945630124	17.07885780896426
499 h	34.32149917207656	41.46082605733769	19.19191608367668	500 h	31.10419137014780	41.03034046216443	20.17894760161076
501 h	37.22724605030760	22.21851125228343	13.65313042079537	502 h	39.33210640813350	24.07120117225835	15.56752241126727
503 h	36.87400434302388	25.57837415672299	13.77429250737877	504 h	43.81735506686740	34.20235125705249	16.09756351203496
505 h	46.30256980909965	33.14653461976353	18.15425166547856	506 h	44.46608358685324	30.88753382474151	16.41317020572004
507 h	46.99155306563688	21.51799901394221	18.41502154936811	508 h	45.98392937172851	18.29875793102044	18.78993262654263
509 h	47.49999961818116	19.91308496900294	21.35972653372416	510 h	36.78290934867846	6.55034114270169	27.21090414345072
511 h	34.50334591448535	8.74078694545083	28.46102298663753	512 h	37.66134604667035	8.74760887300495	29.65409193176360
513 h	46.25304505464051	14.94149398691739	34.05656977900532	514 h	47.23697243612433	16.39967095856393	31.15367715824960
515 h	45.64494505325328	13.40475095641977	31.09437271393694	516 h	19.28598348666201	36.97510913200878	33.45034190754661

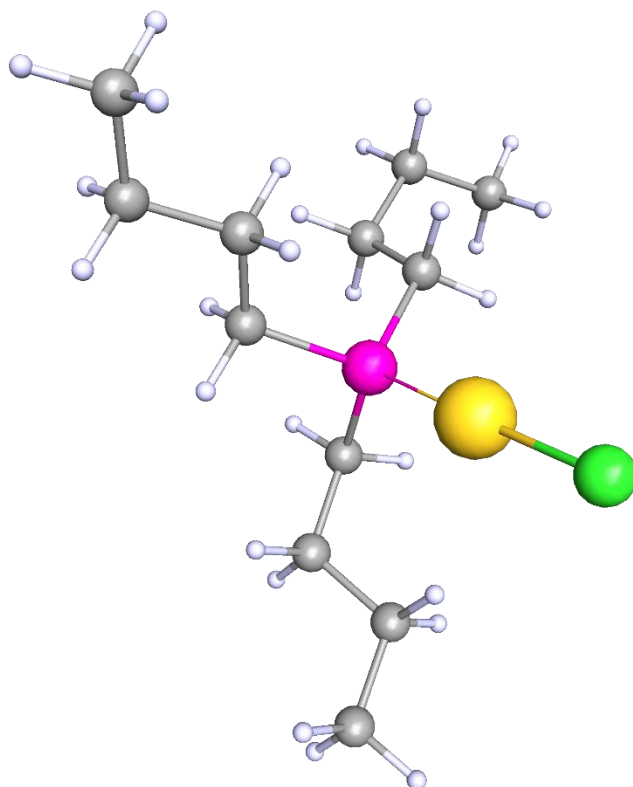


Figure S15: Geometry optimized structure of $n\text{Bu}_3\text{PAuCl}$

Point group: C_1

Energy: -1410.54298364668 H

HOMO-LUMO-Gap: 4.71 eV

1 au	5.35984158231412	-1.83224507267573	0.82343121059919	2 p	1.10581814270516	-1.12737340454558	0.65959337531162
3 cl	9.66870549872115	-2.60307867963926	1.06588549929142	4 c	-0.04590563174174	1.05776742941543	-1.85269118890492
5 c	-0.08524508189861	0.27622320686930	3.65869372500253	6 c	-0.74781371650270	-4.06600156814004	0.12944064528603
7 c	-2.94358297688180	0.76248326566431	3.88188996925634	8 h	1.01896894830676	2.05144783926536	3.89378061485741
9 c	-3.74782926116221	1.82899557517782	6.47588410044780	10 h	-3.56604351926293	2.09631007513263	2.37465912241984
11 h	-3.99054321415529	-1.03318933577499	3.55084057244724	12 c	0.97670362958723	0.56707725030365	-4.54233161430340
13 h	-2.14670015714342	0.93607142392666	-1.83214935258022	14 c	3.63518576606858	1.62529298024140	-5.04777536369226
15 h	0.94556562158437	-1.49800351289417	-4.96634927854234	16 h	-0.37278446582511	1.43785298093254	-5.90684680660247
17 h	-0.21548197014523	-4.73305423663239	-1.79516391698463	18 h	-2.79373139286210	-3.56987558745871	0.05753935462908
19 c	-0.24283268855072	-6.16076781463981	2.07962611788497	20 h	1.83147782042879	-6.51194308773053	2.19404006075200
21 h	-0.83171194799851	-5.51054612009673	3.99604902180147	22 c	-1.61967341822131	-8.64528957118756	1.45316682145091
23 h	-1.01499693280595	-9.30176626305522	-0.45605748678080	24 h	-3.69107908918385	-8.27861938075030	1.31015612015837
25 c	-1.13351935754004	-10.73899060716615	3.39891991019858	26 h	-1.78325988737946	-10.16975266720187	5.31756779916199
27 h	-2.14546715776392	-12.50774201004599	2.88528162131558	28 h	0.91538262427624	-11.19393591024921	3.53533802814735
29 h	0.57493203748089	-1.00646024718298	5.19161593130263	30 h	-5.85212170475547	1.87424630564404	6.53331183631381
31 h	-3.16008712120570	0.48096561115205	7.98591171345567	32 c	-2.72619789032769	4.47587498360566	7.07990173421691
33 h	-3.28986275718989	5.86777383662108	5.60488534830609	34 h	-0.62866075518592	4.50929749735664	7.21895251781839
35 h	-3.47583452414661	5.16672555891922	8.91746913740205	36 h	3.61671010321805	3.70419547761437	-4.69779634318574
37 c	4.57295430910861	1.09426903905527	-7.73755861261171	38 h	4.99446445478564	0.81250049442407	-3.65584541826366
39 h	3.28469869397423	1.91878848502491	-9.18429767628727	40 h	6.48445066044766	1.90881708566542	-8.04726451697936
41 h	4.70373239764347	-0.97293013039618	-8.10607909089020	42 h	0.45624049567508	3.00564301221397	-1.23021703739084

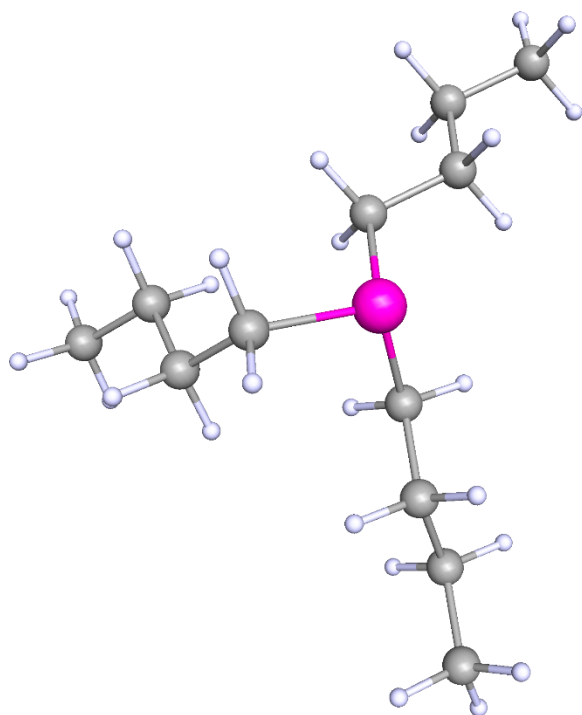


Figure S16: Geometry optimized structure of $n\text{Bu}_3\text{P}$

Point group: C_1

Energy: -814.44171774973

HOMO-LUMO-Gap: 5.571 eV

1 p	1.08324971646512	-0.71518109412445	0.06702941602759	2 c	-0.55728627093723	1.25887359692706	-2.40885273362709
3 c	0.05280047590567	0.75550067810789	3.15993621326821	4 c	-0.91078335749772	-3.65682810888719	-0.09006861510340
5 c	-2.69908294398483	0.70903184881696	4.11684011582322	6 h	0.76245048327801	2.74041281899702	3.08679044773232
7 h	-2.66324877369267	1.21733047796494	6.16563044226679	8 c	-4.56568846116949	2.49343136482490	2.78370320156902
9 h	-3.45066399592255	-1.25953890348683	4.05477174242161	10 c	0.56436981199425	0.83892779237710	-5.06017184415184
11 h	-2.62999116135323	0.88624112812252	-2.43622892232333	12 h	2.63412273508842	1.23219931629977	-5.00811610612770
13 h	0.38527182958256	-1.19380321317389	-5.59616557807705	14 c	-0.68417031827496	2.46946444404838	-7.11919267992828
15 h	-0.75552358624689	-4.34191796890885	-2.07746643941668	16 h	-2.94665355998844	-3.20457345991993	0.22193097099955
17 c	-0.03880053996891	-5.75177300189502	1.72510868068386	18 h	2.01296103453597	-6.12593986272509	1.41794938758057
19 h	-0.20765031137393	-5.08371366427262	3.71846226477267	20 c	-1.52791365810426	-8.23327408056112	1.43459053418307
21 h	-1.35387086274072	-8.91038548783955	-0.55458086584213	22 h	-3.57966315762766	-7.84969663905572	1.73234251470830
23 c	-0.65879660456568	-10.32127224970545	3.24960398013446	24 h	-0.87529161635240	-9.72961953586964	5.25764608903539
25 h	-1.77235417907994	-12.08483432565737	2.98518415301357	26 h	1.36859839319799	-10.79939884478572	2.95094788875951
27 h	-0.31402361292576	3.27504080599148	-1.84836979278312	28 h	1.27412932489275	-0.19807433872721	4.58673848482138
29 c	-7.17727171325515	2.54600576833424	4.04499312797988	30 h	-3.75859944071823	4.44107232376203	2.75648354018027
31 h	-4.78135252465184	1.93391226739803	0.76858809881370	32 h	-7.05002501193595	3.18669368535858	6.04576404220054
33 h	-8.06229718163879	0.63635957775034	4.05358708539524	34 h	-8.49081840509964	3.84725825834894	3.04437650533863
35 h	-2.75307451161616	2.06528724056312	-7.16452420441622	36 h	-0.50929353801616	4.50227874398275	-6.58702341388002
37 c	0.44269813912442	2.05735025721973	-9.75929369513301	38 h	-0.50173950498114	3.26551421359548	-11.19758629589952
39 h	2.49629712099271	2.51500599328194	-9.79461990823687	40 h	0.23503129436891	0.05607532274901	-10.37648485788198

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