

Supplementary Materials

Core-Size Conversion of $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$ to $\text{Au}_{30}(\text{S-}t\text{Bu})_{18}$ Nanomolecules

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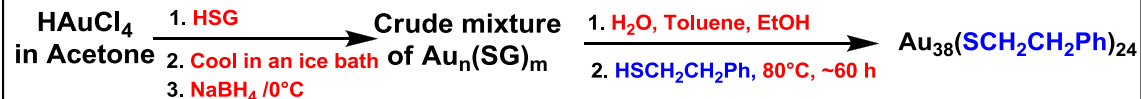
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Step 1



Scheme S1. The protocol for the synthesis of $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$.

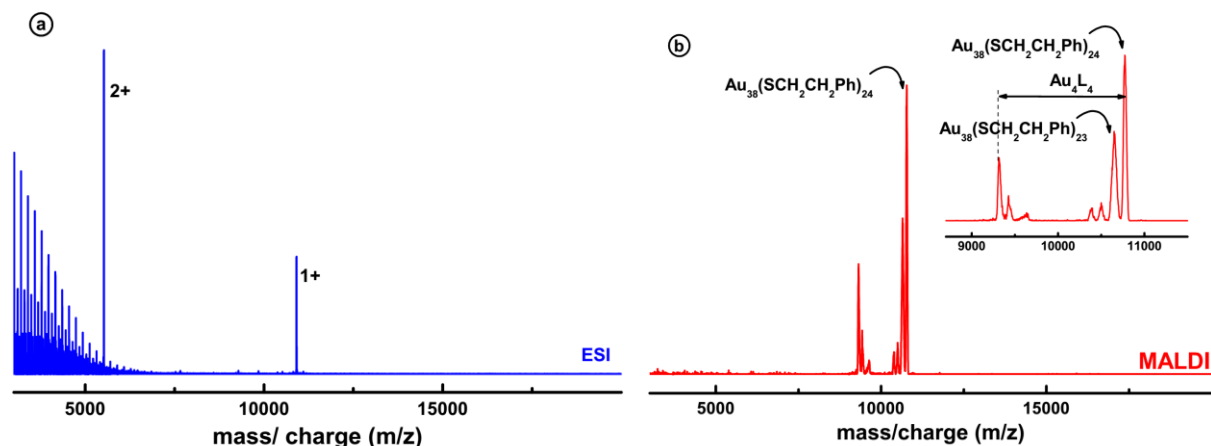


Figure S1. (a) ESI mass spectrum showing $\text{Au}_{38}(\text{PET})_{24}$ peaks in the 1+ and 2+ charges states. The inset shows the expansion of the 10,900 to 10,920 m/z region, showing the $\text{Au}_{38}(\text{PET})_{24}$ with 1+ charge state overlap with theoretical spectrum. (b) MALDI mass spectrum of $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$. Inset shows the expansion of the 9,000 to 11,000 m/z region, showing completely exchanged $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$, a partial $\text{SCH}_2\text{CH}_2\text{Ph}$ exchange ($\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{23}$) and a fragment of m/z difference of four gold and four ligands.

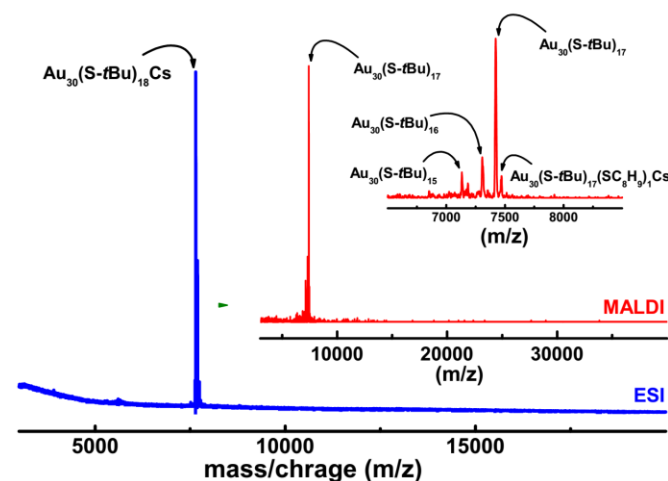


Figure S2. ESI and MALDI mass spectra of $\text{Au}_{30}(\text{S-tBu})_{18}$ nanomolecules. Extend spectra shows purity of the final product the expanded MALDI spectrum in the inset (red) shows fragmentation of $\text{Au}_{30}(\text{S-tBu})_{18}$ at low laser. It should be noted that all ligand shell intact molecular peak of $\text{Au}_{30}(\text{S-tBu})_{18}$ was not the dominating peak in the MALDI mass spectrum and instead $\text{Au}_{30}(\text{S-tBu})_{17}$ was the base peak.

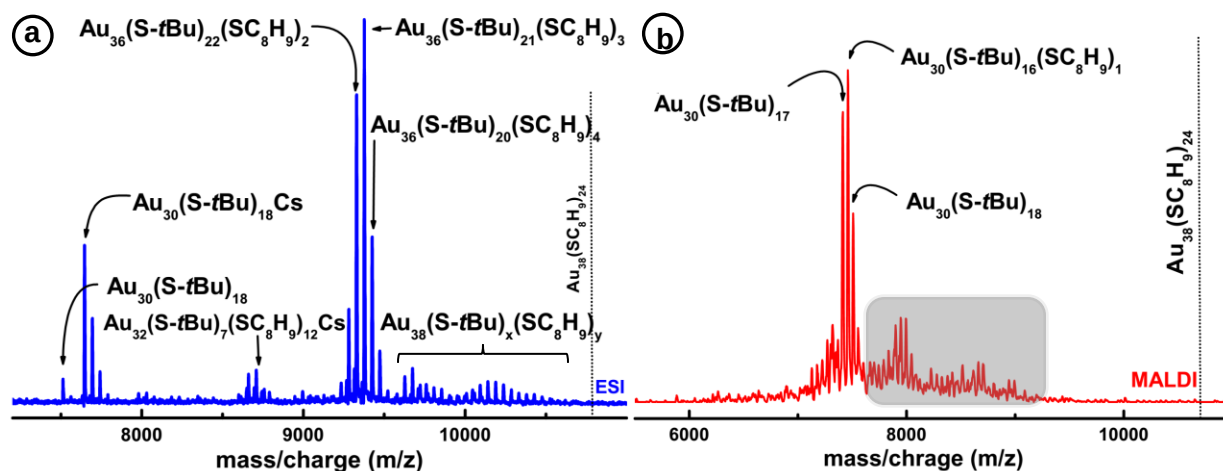


Figure S3. Mass spectra of the 5 min sample during the transformation of the $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$ to $\text{Au}_{30}(\text{S-tBu})_{18}$. (a) ESI-MS illustrating intermediates of the reaction. Well known $\text{Au}_{36}(\text{SR})_{24}$ species (where R represents combination of both phenylethanethiol and *tert*-butylthiol) was observed as an intermediate species along with other unstable clusters of species. x and y represents a combination of ligands adding upto 24. (b) MALDI-MS showing fragments of the remaining Au_{38} and Au_{36} species (the gray area) and incomplete transformation of $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$ to $\text{Au}_{30}(\text{S-tBu})_{18}$.

Table S1. Absolute electronic energy values for the $\text{Au}_N(\text{SR})_M$ systems.

System : $\text{Au}_N(\text{SR})_M$	N,M=30,18,R=tBu	N,M=36,24,R=tBu	N,M=38,24,R=EtPh
$\text{Au}_N(\text{SR})_M$	1687.98201666	2117.67843145	2730.59465752
Au_N	996.60577862	1195.83837315	1262.35730340
$(\text{SR})_M^{\text{crown}}$	689.039641560	918.874554633	1465.20378111
SR_relaxed	38.27338148	38.27338148	61.00837653
HSR_relaxed	38.91610700	38.91610700	61.65151849
Au_atom	33.1443376704	33.1443376704	33.1443376704
$\text{Au}_N(\text{SR})_M_{\text{anion-adiab}}$	1688.04648476	2117.74821839	2730.67891792
$\text{Au}_N(\text{SR})_M_{\text{cation-adiab}}$	1687.79592159	2117.49365427	2730.42134317

Note: The nomenclature is the following: $\text{Au}_N(\text{SR})_M$ = full nanomolecule; Au_N = gold cluster in the interacting configuration; $(\text{SR})_M$ = crown or shell of ligands in the interacting configuration; SR_relaxed = fully relaxed SR thiol; fully relaxed HSR thiol; Au_atom = isolated Au atom; $\text{Au}_N(\text{SR})_M_{\text{anion-adiab}}$ = total energy of $\text{Au}_N(\text{SR})_M$ anion in the geometry of the neutral species; $\text{Au}_N(\text{SR})_M_{\text{cation-adiab}}$ = total energy of $\text{Au}_N(\text{SR})_M$ cation in the geometry of the neutral species. All energies are in atomic units.

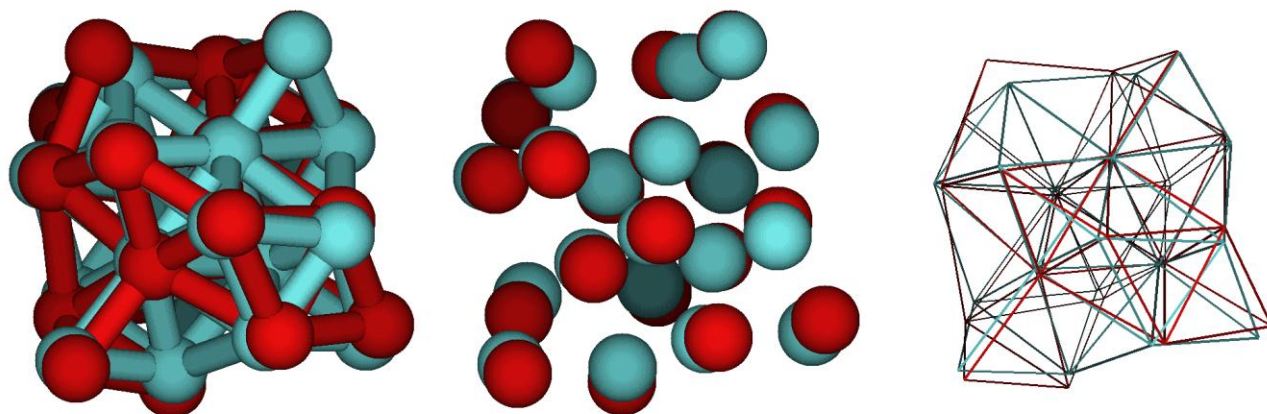


Figure S4. Schematic pictures according to different view formats comparing the Au_{20} core skeleton of $\text{Au}_{36}(\text{SR})_{24}$ nanomolecules derived from the crystallographic data for $\text{Au}_{36}(\text{SPh})_{24}$ in Ref. ¹ and from simulation data for $\text{Au}_{36}(\text{S-}t\text{Bu})_{24}$ from the present simulations. See main text for more details.

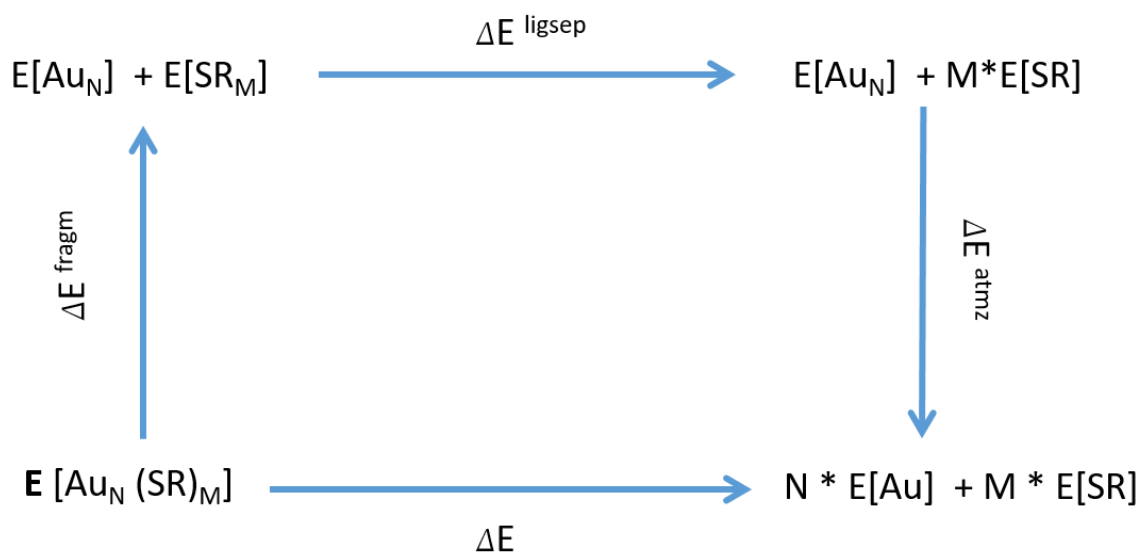


Figure S5. Born-Haber cycle for monolayer-protected clusters

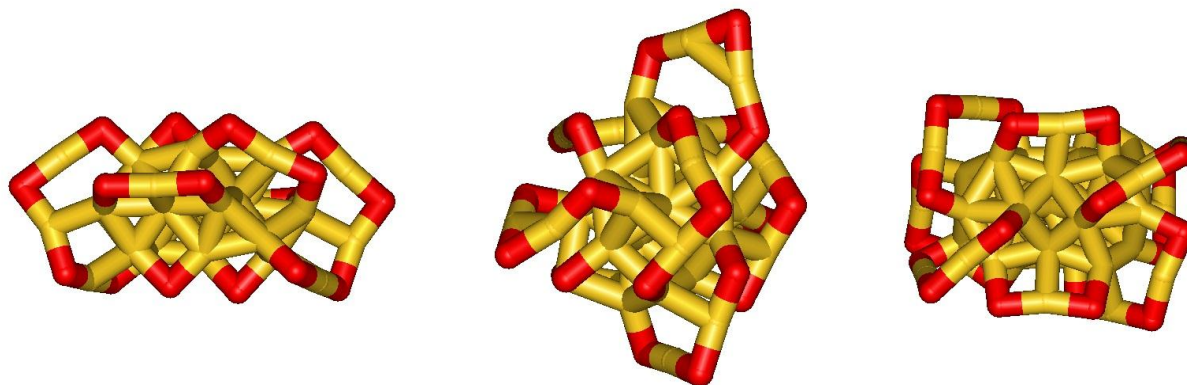


Figure S6. Schematic pictures of the $Au_N(S)_M$ skeletal framework of $Au_{30}(S^iBu)_{18}$, $Au_{36}(S^iBu)_{24}$ and $Au_{38}(SCH_2CH_2Ph)_{24}$, respectively, from left to right

Table S2. Energy differences for the reactions considered in the main text.

Au_{38}		ΔE^{frag}	ΔE^{atmz}	ΔE^{ligsep}	$\Delta E^{hyrd-lig}$	$\Delta E^{H-ligsep}$	μ_{ligand}	IP/EA
	$(SCH_2CH_2Ph)_{24}$	3.440	3.257	1.137	4.847	1.109	1.692	4.72/2.29
	$(SPh)_{24}$	3.120	3.178	0.478	4.604	0.579	1.320	
	$(SCH_3)_{24}$	3.304	3.347	0.125	4.839	0.135	1.647	
Au_{36}								
	$(SPh)_{24}$	3.095	3.087	0.158	4.597	0.253	1.320	5.44/2.17
Au_{30}								
	$(StBu)_{18}$	3.532	3.440	0.179	4.861	0.178	1.681	
	$(SPh)_{18}$	3.037	3.522	0.300	4.613	0.409	1.320	5.06/1.75

Cartesian coordinates of the Au₃₈(SCH₂CH₂Ph)₂₄ structural model.

Au	19.5142016581	19.7735751436	20.8373717685
Au	19.2877131421	23.2477030939	22.1799950146
Au	18.9079447561	20.2542770805	18.1048550066
Au	19.6473338542	17.4956383716	19.1406857806
Au	18.9488701929	14.8188983150	19.7497403561
Au	18.9161608748	15.8010840510	16.8064870956
Au	18.7531823264	20.7784206018	15.2879143141
Au	18.7623609724	25.6328344120	19.5750357937
Au	18.3132082231	23.1135005704	17.2489474898
Au	18.6811410516	13.7823156938	22.8598602434
Au	20.1608582866	23.1799187812	14.2963344526
Au	20.3228160504	22.3466905700	19.3655670601
Au	20.2206557862	18.3428556876	16.4249219125
Au	18.1327422056	11.5357297387	20.3139213346
Au	17.7451028793	17.1867826788	21.4053523917
Au	17.1898830697	13.2903780376	14.6816684733
Au	17.3904616243	18.5151441988	16.3900210814
Au	17.5549376076	22.1938859258	19.9111259477
Au	17.3509632614	18.2236823178	13.4903855737
Au	21.2858411576	21.0466418654	16.8262955533
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Au	16.9352567445	16.7616212621	18.6319356518
Au	17.0393682322	13.8937134577	17.7475451685
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Au	22.1148076131	16.1537003271	20.2953100075
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Au	16.2276294223	14.8542033180	20.5106240840
Au	16.0382059251	15.9905519456	16.0174261805
Au	14.9125288474	21.0327693771	21.5059609974
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Au	23.5927047693	18.7471457704	16.7689129332
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C	14.0680273095	12.2331851488	24.7496827895
C	13.8691723229	18.6405071836	10.4646108995
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Cartesian coordinates of the Au₃₀(S-tBu)₂₄ structural model.

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Au	18.5859885824	20.0723528287	14.3721870297
Au	20.8087611882	18.2901432707	15.4177309339
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H	20.4948868847	26.2687341340	16.3867013095
H	21.5908568940	26.0805765628	17.7776799792
C	17.5183909483	26.0033574578	20.0025949412
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H	16.6993020133	26.1059484654	22.0291674859
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H	20.2007646344	26.3024915027	23.1862714560
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C	16.8286367680	12.5843548374	12.0057878867
C	17.2420615225	11.2119472208	11.4534645687
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H	14.9505525569	22.6506987341	19.7582000777
H	14.9198130527	24.0665444043	18.7041122285
H	13.9163613790	24.0379646573	20.1760926730
H	11.8328367294	24.5386588675	18.7297332321
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C	19.5690740323	21.9955986489	11.3634401957
C	20.2933016878	20.8813798806	10.6111662065
C	18.0650857581	21.9608053526	11.0928487064
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C	22.1340935157	16.5622509447	12.3635416086
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C	23.4957265366	21.7971318357	20.1088816987
C	24.1738999514	21.2936661285	18.8379506947
C	23.2022006544	23.2998396035	20.0158504423
C	24.3808680424	21.4853807552	21.3289991562
H	24.4042923285	20.2222216612	18.9006353007
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H	25.3473469418	21.9959193784	21.2129092603
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C	15.5629791943	26.2594443032	13.6298618584
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H	13.7493296245	22.6801396350	22.1957888363
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H	13.6917438284	22.5545114096	23.9683782071

Cartesian coordinates of the Au₃₆(S-tBu)₂₄ structural model.

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Au	17.9016595080	20.2717017779	17.0502208945
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Au	18.7137591830	15.8385736801	19.3805075447
Au	16.8711846285	17.8512374174	18.6756922567
Au	19.8774926139	20.9620806400	18.9629290785
Au	15.9099917709	19.7448615765	15.0736572038
Au	21.3554273101	20.9358063921	16.4522109532
Au	18.5859885824	20.0723528287	14.3721870297
Au	20.8087611882	18.2901432707	15.4177309339
Au	17.1288025339	14.9590018562	16.8962113247
Au	15.0532528614	19.8839815437	17.9171084384
Au	17.7554340850	22.7752218554	18.1570575546
Au	18.9432526044	23.5451920389	15.6930851942
Au	17.2260624442	20.6439236865	19.9575420509
Au	22.2291686539	15.7906083457	18.5666719183
Au	19.7570189078	15.3160861355	16.1950291488
Au	14.7154766431	17.4187236326	16.5486151449
Au	15.5596349439	16.7458256983	13.1579256989
Au	15.7988536733	15.1823488044	20.2352377723
Au	18.9855036587	17.9050423170	12.4622621404
Au	19.0007705124	18.3405144872	20.7512997081
Au	14.1217511298	17.6435395478	19.3091666382
Au	15.8438190425	18.1142060423	21.8508858454
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Au	15.4771148888	22.9533552482	15.9983611259
Au	22.0365629733	21.5325162120	13.6364100633
Au	17.8552220188	15.2948687199	14.1591012309
Au	22.4205887248	18.5828006725	17.6658183380
Au	10.7492996326	18.4265893543	17.5915699026
Au	11.7312258529	19.5851725117	15.0546182021
Au	24.4114057261	19.7570137883	15.1361920503
Au	19.9797422631	21.3189076196	23.0401912541
Au	19.4060316795	23.6646075108	21.3263467875
Au	18.9604107497	12.3066932677	18.1605404244
Au	18.4813678490	12.0565896255	14.7429194381
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S	24.4044261920	21.6997254169	13.8259855452
S	24.5628300637	17.8689166608	16.5247840528
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C	16.6656652554	26.3873014012	15.8839228118
C	18.0802402272	26.3874238810	13.7941086152
H	15.4869852255	27.3574380613	13.5988752089
H	15.6336985608	25.9170830293	12.5902038334
H	14.6336455218	25.8852908170	14.0783474527
H	17.5093115992	26.0700522736	16.5068445389
H	16.6457045580	27.4897500419	15.8851362766
H	15.7312069545	26.0407487033	16.3407156015
H	18.9726100917	26.1158741584	14.3742660161
H	18.1945866371	26.0261741502	12.7645348627
H	18.0420757713	27.4878693190	13.7466421936
C	15.2094135665	21.2983535755	23.0606673931

C	15.3169378351	20.3366016366	24.2484644486
C	16.3165521640	22.3457052628	23.1041969306
C	13.8307828177	21.9824497230	23.0389152519
H	15.2085685781	20.9069292741	25.1837030402
H	14.5287584940	19.5724336168	24.2193712335
H	16.2940174633	19.8345540706	24.2570972085
H	17.3117595741	21.8810498288	23.0866132417
H	16.2576609470	23.0348774091	22.2535554080
H	16.2311348618	22.9324438360	24.0309071156
H	13.7493296245	22.6801396350	22.1957888363
H	13.0143470027	21.2532519492	22.9588400893
H	13.6917438284	22.5545114096	23.9683782071

13. References

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