

Supporting Information

Pd₂Au₃₆(SR)₂₄ cluster: structure studies

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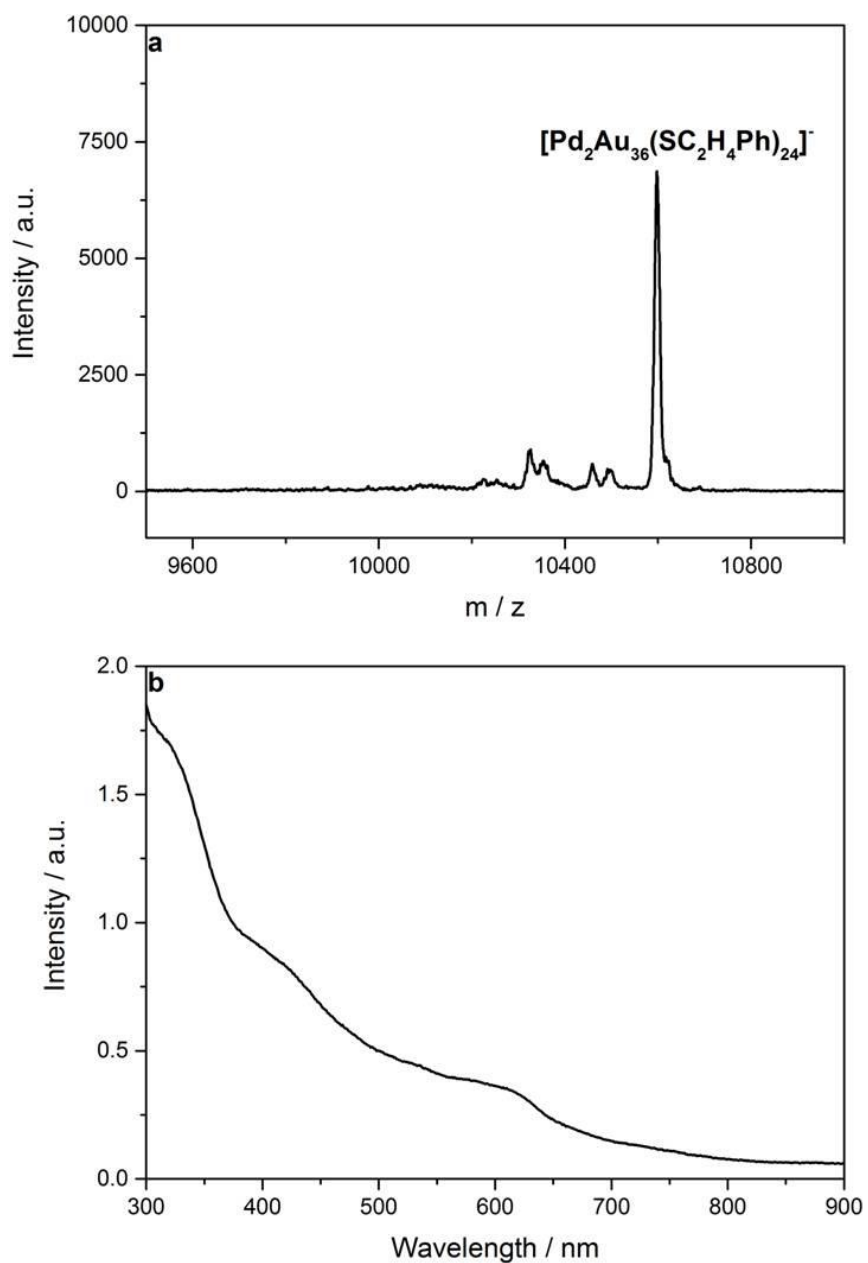
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Experimental Methods

All chemicals were purchased from standard suppliers and used as received. Nanopure water (>18 M Ω) was used.

Synthesis and Isolation of Pd₂Au₃₆(SCH₂CH₂Ph)₂₄ (enantiomer 2). Pd₂Au₃₆(SC₂H₄Ph)₂₄ enantiomer 2 is synthesized and separated according to previous method reported by our group.¹



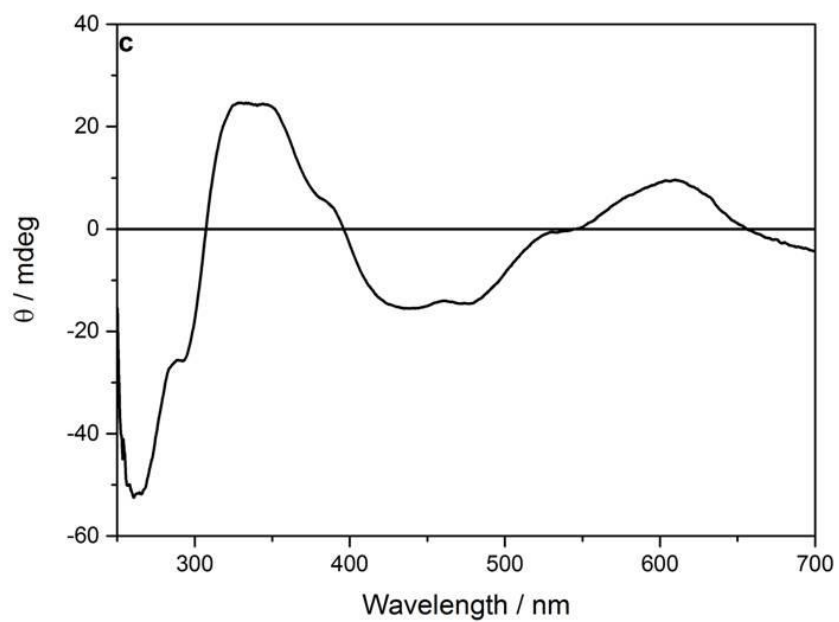


Figure S1. (a) MALDI, (b) UV-vis and (c) CD spectra of $\text{Pd}_2\text{Au}_{36}(\text{SC}_2\text{H}_4\text{Ph})_{24}$ enantiomer 2.

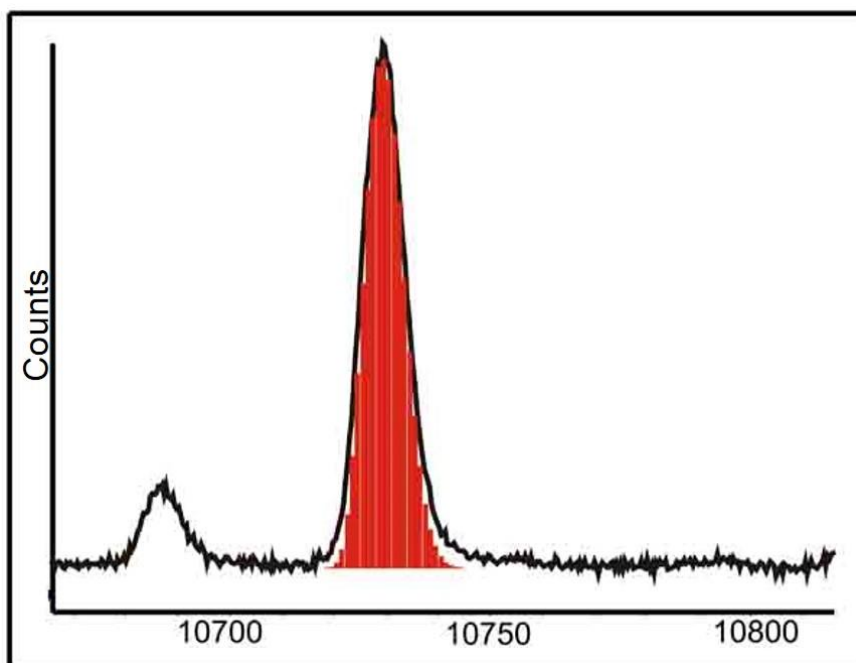
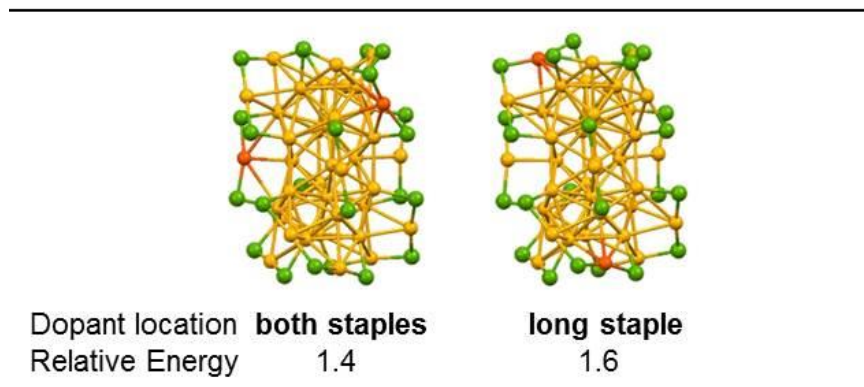


Figure S2. Positive polarization ESI-MS spectrum of $[\text{Pd}_2\text{Au}_{36}(\text{SC}_2\text{H}_4\text{Ph})_{24} + \text{Cs}]^+$. black: experimental, red: theoretical isotropic distribution



Scheme S1. Optimized structures for two staples doped $\text{Pd}_2\text{Au}_{36}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$ models. R group is omitted for the sake of simplicity. Key: red = Pd; yellow = Au; green = S

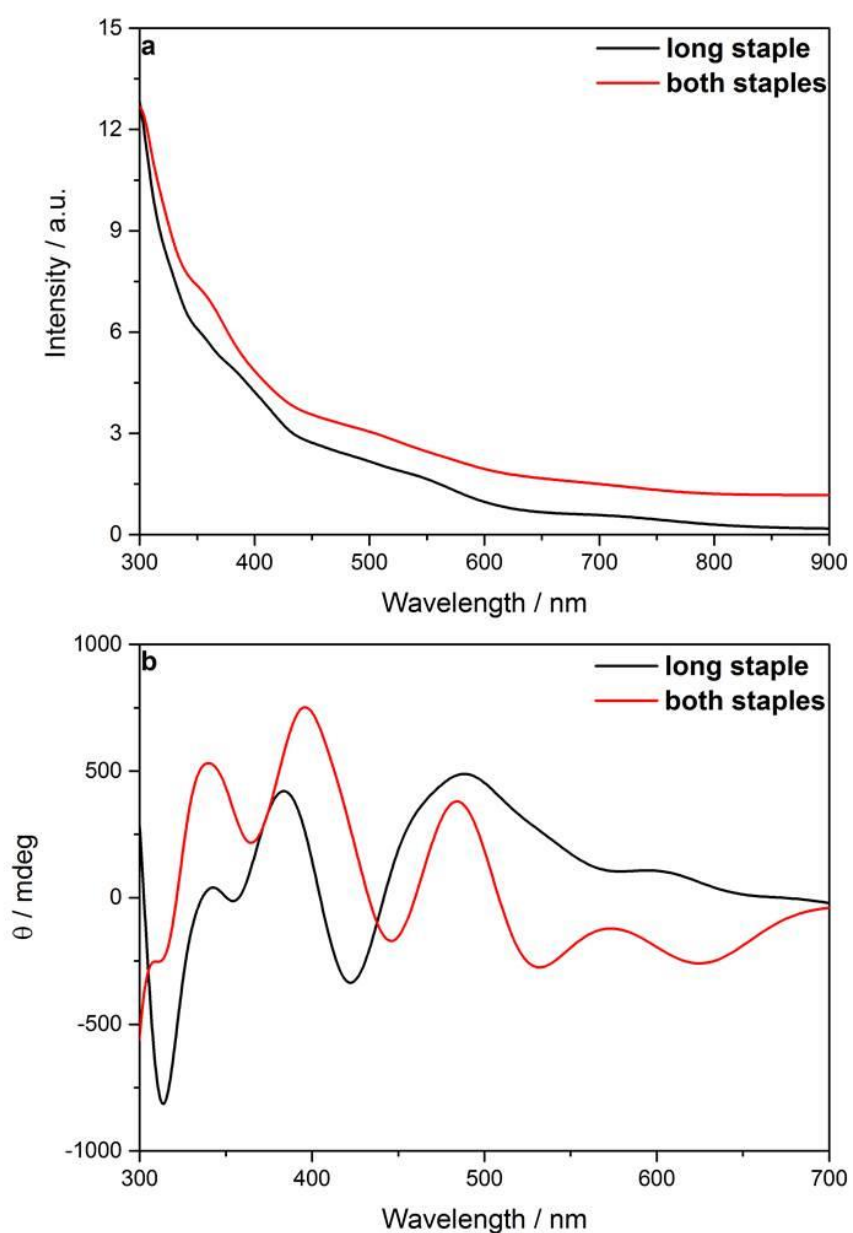


Figure S3. Theoretical (a) optical absorption and (b) CD spectra of two staple doped models

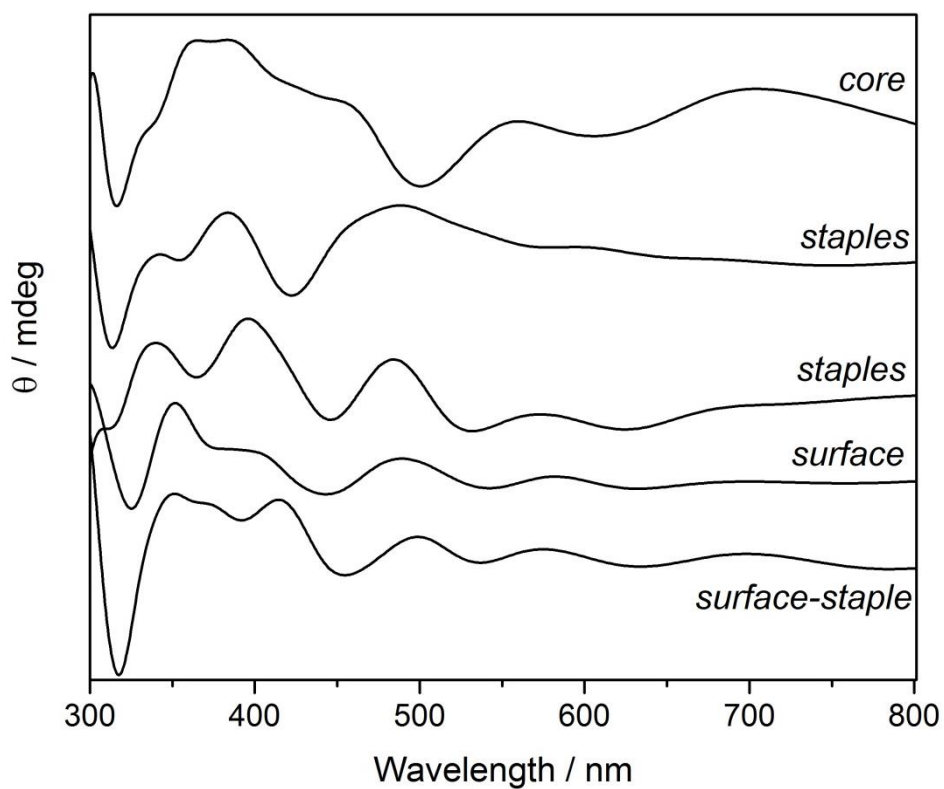


Figure S4. Theoretical CD spectra of different doped Pd atoms locations in $\text{Pd}_2\text{Au}_{36}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$

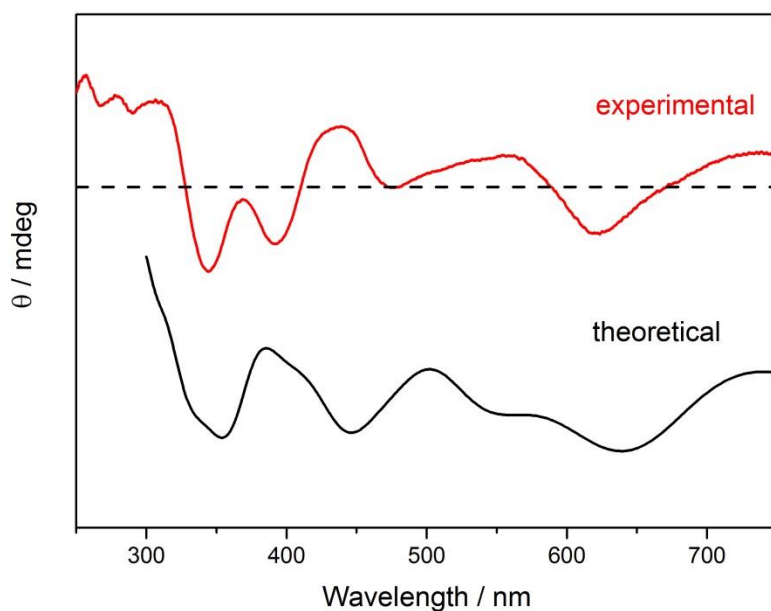
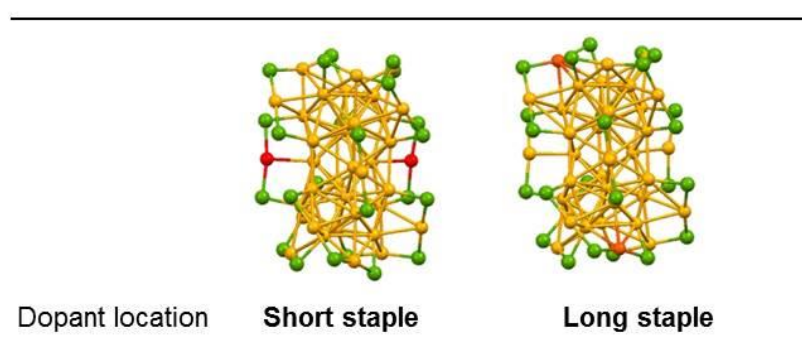


Figure S5. Theoretical and Experimental CD spectra of $\text{Au}_{38}(\text{SCH}_2\text{CH}_2\text{Ph})_{24}$

Table S1. Pd K-edge EXAFS Analysis for the Pd₂Au₃₆(SC₂H₄Ph)₂₄ staple and core doped mixture

	Pd-S	Pd-Au
theoretical CN _{staple}	2	0
theoretical CN _{surface}	1	9
theoretical CN _{core}	0	12
experimental CN _{mixture}	1.1(2)	5.5*
σ^2	0.003(3)	0.009(4)
E0	2.9(4.5)	-2.4(2.6)
R	2.35(5)	2.8(1)
R factor (%)	1.3	
*fixed		



Scheme S2. Optimized staples doped Pd₂Au₃₆(SCH₂CH₂Ph)₂₄ models for EXAFS fitting. R group is omitted for the sake of simplicity. Key: red = Pd; yellow = Au; green = S

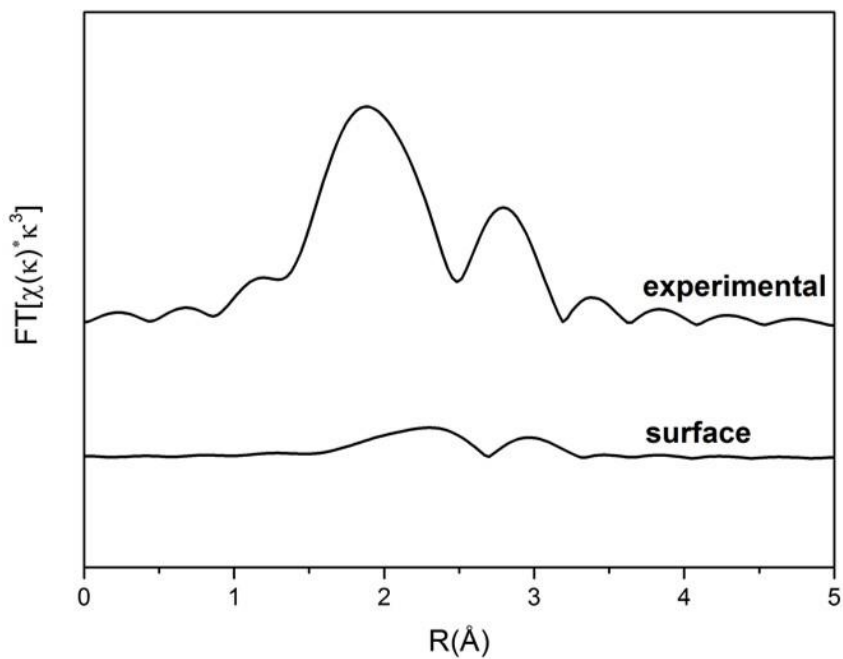


Figure S6. EXAFS spectra of $\text{Pd}_2\text{Au}_{36}(\text{SC}_2\text{H}_4\text{Ph})_{24}$ in R space: experimental and theoretical surface doped model

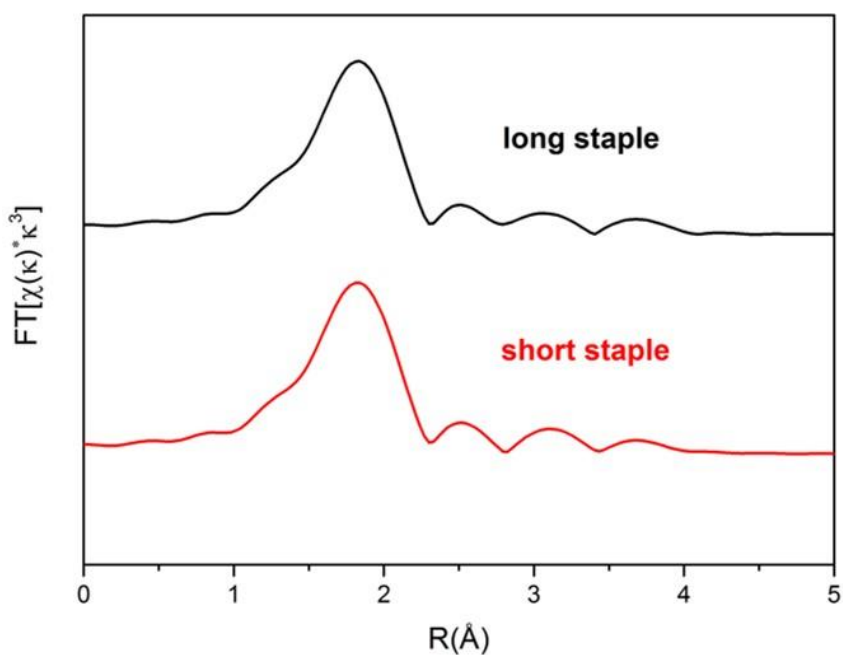


Figure S7. Simulated Pd K-edge EXAFS spectra in R space for two staple doped $\text{Pd}_2\text{Au}_{36}(\text{SC}_2\text{H}_4)_{24}$ models.

References

- (1) Barrabes, N.; Zhang, B.; Burgi, T. *J Am Chem Soc* **2014**, *136*, 14361.

Optimized Coordination for core doped Pd₂Au₃₆(SC₂H₄Ph)₂₄⁽⁻²⁾

1	C	17.7431	8.6452	20.649
2	Pd	17.7277	17.6183	18.5598
3	Au	18.4019	19.1951	16.3862
4	Au	17.284	21.6858	17.0116
5	Au	19.618	21.344	15.1233
6	Au	22.3338	20.4084	18.873
7	Au	15.7943	19.2003	17.4181
8	Pd	19.791	21.0233	17.9235
9	Au	17.5447	20.2652	19.4068
10	Au	15.7703	18.4082	20.3935
11	Au	16.8063	16.9756	15.9966
12	Au	21.1864	19.2184	16.4003
13	Au	20.3342	18.4805	18.9756
14	Au	20.0841	20.7091	20.6133
15	Au	21.131	22.9993	19.2813
16	Au	19.6594	16.721	16.8576
17	Au	19.7019	15.8839	19.6104
18	Au	19.4179	23.4955	16.8669
19	Au	18.0861	18.8039	13.4756
20	Au	15.189	16.597	18.4019
21	Au	21.9938	21.9999	16.6086
22	Au	18.5161	18.2104	21.099
23	Au	15.0814	14.487	16.0132
24	Au	18.3922	22.884	19.5145
25	Au	17.5935	23.6839	14.5229
26	Au	17.0929	15.8022	20.5135
27	Au	18.4068	14.5036	14.9147
28	Au	13.0066	18.6094	18.994
29	Au	21.0826	23.8527	14.2121
30	Au	17.6042	14.9899	17.79
31	Au	18.5927	13.0935	20.1127
32	Au	15.8968	21.6714	21.4007
33	Au	19.5909	25.598	19.1975
34	Au	20.0914	23.5908	22.0776
35	Au	24.2748	19.8752	16.6004
36	Au	19.2094	15.4104	22.5899
37	Au	14.0067	16.1066	21.282
38	Au	24.1885	22.8715	18.4838
39	Au	22.8569	17.2734	19.9923
40	S	20.5427	15.332	15.1431
41	S	16.3736	13.5922	14.3337

42	S	19.1422	17.6081	23.3054
43	S	16.637	17.0183	13.6291
44	S	20.2988	21.43	22.8579
45	S	15.7625	22.6079	15.4272
46	S	16.6255	23.7798	20.8387
47	S	19.3856	20.6103	12.8764
48	S	23.1717	23.1408	14.9069
49	S	13.5682	20.013	17.2453
50	S	25.6929	21.3496	17.6557
51	S	12.2286	17.4956	20.8424
52	S	13.557	15.059	17.6545
53	S	14.7892	19.7737	22.0759
54	S	15.6064	14.5454	21.833
55	S	20.1006	25.8003	21.4432
56	S	18.995	25.8158	16.9773
57	S	19.194	24.7974	13.3004
58	S	19.6278	13.1883	22.1723
59	S	24.071	19.2248	19.9786
60	S	17.4801	12.6446	18.1458
61	S	21.9059	15.1887	20.1963
62	S	23.1165	18.2311	15.4741
63	C	15.4003	24.2389	19.5783
64	H	15.4796	23.5267	18.7378
65	H	14.3953	24.1394	20.0239
66	C	15.7658	12.419	18.7058
67	H	15.4275	13.3693	19.1532
68	H	15.1681	12.2652	17.7855
69	C	15.6394	25.651	19.0988
70	H	16.6787	25.7331	18.7227
71	H	15.5404	26.3525	19.9475
72	C	14.6602	25.9765	18.0282
73	C	16.5487	11.8413	14.7809
74	H	16.7179	11.7641	15.8705
75	H	15.595	11.3445	14.536
76	C	21.9087	21.1074	11.9879
77	H	21.9457	21.8545	12.813
78	H	21.4534	21.6266	11.1244
79	C	14.9388	14.4777	24.5073
80	H	14.0292	15.0786	24.323
81	H	15.2718	14.6877	25.5402
82	C	20.4665	26.6006	16.2754
83	H	21.3318	25.9439	16.4678
84	H	20.3225	26.6426	15.1796
85	C	26.4006	22.2762	16.2707
86	H	25.5719	22.6719	15.6561
87	H	26.9466	23.127	16.7141

88	S	22.8764	24.5952	19.2739
89	C	21.9658	28.5401	16.3386
90	C	20.7018	27.9696	16.867
91	H	19.8468	28.631	16.6458
92	H	20.7479	27.8521	17.9671
93	C	27.9665	22.2866	14.3995
94	C	27.3092	21.4236	15.4169
95	H	26.7089	20.6241	14.9425
96	H	28.0595	20.9205	16.0538
97	C	27.3613	22.5394	13.1722
98	H	26.4281	22.019	12.9186
99	C	29.7291	23.8263	13.8064
100	H	30.6664	24.3286	14.0629
101	C	29.1126	24.0789	12.5916
102	H	29.5563	24.7865	11.8858
103	C	27.9295	23.4302	12.276
104	H	27.4384	23.6241	11.3176
105	C	24.8777	25.2611	14.5464
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109	C	23.9413	24.6529	15.5662
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111	H	24.4796	24.3607	16.4936
112	C	23.3191	26.73	13.2563
113	H	23.1445	27.3042	14.1744
114	C	23.7241	25.266	10.9442
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116	C	18.5992	26.6275	22.0384
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118	H	18.6461	26.6514	23.1384
119	C	13.3277	18.8358	24.6612
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122	C	15.5814	19.1805	23.6038
123	H	16.5517	18.7122	23.3611
124	H	15.7804	20.0583	24.2425
125	C	12.1275	18.1844	24.4052
126	H	12.1533	17.2222	23.8794
127	C	14.6287	18.2142	24.2623
128	H	14.4229	17.3777	23.5558
129	H	15.1236	17.761	25.1444
130	C	10.7539	14.1287	16.4303
131	C	11.1313	12.7968	16.3087
132	H	12.0258	12.5541	15.7233
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134	H	11.675	16.5051	17.5387
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137	H	12.2465	14.7859	15.0485
138	H	10.8655	15.8944	15.2205
139	C	16.021	14.9426	23.5569
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141	H	16.2008	16.0257	23.65
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143	H	17.5542	11.3556	12.9419
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145	C	17.8654	9.7743	14.3424
146	C	20.6945	16.4062	13.6881
147	H	19.9013	17.1843	13.731
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149	C	21.9464	16.9343	10.7272
150	H	22.8532	16.5297	11.1918
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152	C	22.051	17.8412	9.6859
153	H	23.0396	18.1543	9.3339
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155	H	21.412	14.8762	12.3604
156	H	19.6455	15.0867	12.3795
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162	C	10.8831	19.9982	25.3661
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164	C	10.9156	18.7561	24.7549
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220	H	24.1789	26.8985	20.4328
221	H	24.8613	26.2384	21.9355
222	C	25.786	25.5175	20.1515
223	C	23.4872	24.9384	20.9493
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243	H	18.5538	22.9271	24.6951
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247	H	18.1112	24.3562	11.2344
248	C	20.2341	24.1632	10.826
249	H	21.12	23.7728	11.3715
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251	C	25.9249	16.8273	16.3977
252	C	28.2175	18.2852	17.0345
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254	C	23.4056	16.7293	16.4488
255	H	23.3553	16.9753	17.5301
256	H	22.5438	16.0721	16.232
257	C	9.5527	20.4246	20.2697
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259	C	24.6962	16.0548	16.0619
260	H	24.6827	15.8376	14.9785
261	H	24.719	15.0705	16.5723
262	C	26.1505	17.2633	17.6993
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264	C	18.9061	10.8533	23.4863
265	H	19.9137	10.8329	23.9374
266	H	18.2075	10.413	24.2227
267	C	18.4942	12.2969	23.2873
268	H	18.5306	12.8353	24.2507
269	H	17.4659	12.3672	22.8923
270	C	18.9016	10.0319	22.2432
271	C	18.8946	8.5322	19.8879

272	H	18.8855	7.947	18.9631
273	C	17.7435	9.3946	21.8135
274	H	16.8239	9.5004	22.4046
275	C	20.0526	9.9102	21.4704
276	H	20.9628	10.4279	21.7933
277	C	20.0518	9.1716	20.2992
278	H	20.96	9.1061	19.6941
279	C	18.1536	7.0601	14.9488
280	H	18.2748	5.9993	15.1831
281	C	18.3477	9.3699	15.5846
282	H	18.6107	10.1303	16.3325
283	C	18.493	8.0272	15.883
284	H	18.8872	7.7334	16.8615
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302	C	16.0532	20.3586	11.0671
303	H	17.0721	20.6954	11.2988
304	C	15.2132	21.9182	12.8314
305	H	14.3467	22.5999	12.9046
306	H	16.0893	22.5463	12.5747
307	C	22.4304	14.2398	18.7355
308	H	22.0421	14.7284	17.8253
309	H	23.533	14.2567	18.698
310	C	15.7169	29.9112	23.0593
311	H	15.4624	30.3275	24.039
312	C	14.8385	30.0495	21.995
313	H	13.8902	30.5774	22.1296
314	C	21.4154	20.7532	27.8625
315	H	22.1591	20.4704	28.6132
316	C	21.6238	21.8565	27.0506
317	H	22.5482	22.4365	27.1383

318	C	20.2571	20.0081	27.7141
319	H	20.0879	19.1283	28.3431
320	C	19.3139	20.3669	26.7652
321	H	18.4084	19.7609	26.6399
322	C	13.6987	20.4542	11.4758
323	H	12.8484	20.8584	12.0379
324	C	13.4852	19.4925	10.5034
325	H	12.468	19.1389	10.3091
326	C	14.5593	18.9601	9.8083
327	H	14.3969	18.1934	9.0458
328	C	15.8443	19.3953	10.0943
329	H	16.7006	18.9741	9.5567
330	C	10.1901	18.5642	12.4351
331	H	9.2537	19.0446	12.1396
332	C	10.6673	17.4718	11.7294
333	H	10.1073	17.08	10.8744
334	C	10.9083	19.0435	13.5201
335	H	10.5383	19.9009	14.0893
336	C	11.8623	16.8786	12.1
337	H	12.2542	16.0274	11.5326
338	C	12.7458	26.3812	16.0414
339	H	11.9911	26.5293	15.2639
340	C	14.949	25.6942	16.6987
341	H	15.9401	25.2999	16.4326
342	C	12.4489	26.6741	17.3631
343	H	11.4613	27.0581	17.6341
344	C	13.9999	25.892	15.7121
345	H	14.2504	25.6418	14.6767
346	C	17.5236	8.7957	13.4173
347	H	17.1377	9.1059	12.4401
348	C	17.6647	7.4502	13.7137
349	H	17.3903	6.6982	12.968
350	C	14.6299	13.0294	24.3458
351	C	13.3348	11.2806	23.3016
352	H	12.5224	10.974	22.6335
353	C	15.4485	12.0568	24.9093
354	H	16.2943	12.3657	25.5349
355	C	13.5701	12.6216	23.5434
356	H	12.9398	13.3859	23.0729
357	H	16.8265	8.1417	20.3227
358	C	19.6286	22.2025	9.3668
359	H	19.3158	21.6476	10.2631
360	C	19.5371	21.5986	8.1239
361	H	19.1454	20.5785	8.0519
362	C	20.1143	23.5025	9.4948
363	C	20.5062	24.1723	8.3399

364	H	20.8856	25.1967	8.4317
365	C	21.9011	12.8298	18.8577
366	H	20.7963	12.8698	18.9805
367	H	22.2887	12.3788	19.7912
368	C	22.8678	26.354	10.9282
369	H	22.3443	26.6294	10.007
370	C	24.3836	24.9205	12.1129
371	H	25.053	24.0523	12.1329
372	C	22.662	27.0814	12.0903
373	H	21.9671	27.9273	12.0965
374	C	19.6606	18.0017	9.6085
375	H	18.7499	18.4297	9.1717
376	C	20.9031	18.3732	9.1187
377	H	20.9759	19.1015	8.3047
378	C	25.1219	20.643	10.0492
379	H	25.5334	20.9265	9.0753
380	C	25.3446	19.5372	12.1599
381	H	25.9279	18.9463	12.876
382	C	25.8789	19.8835	10.9275
383	H	26.888	19.5631	10.6552
384	C	23.8393	21.0375	10.3965
385	H	23.2358	21.63	9.6976
386	C	24.0672	19.9404	12.5047
387	H	23.6662	19.658	13.4856
388	C	11.634	9.9281	20.4369
389	H	10.6149	9.5728	20.6253
390	C	14.0018	9.5551	20.4464
391	H	14.8618	8.9057	20.6524
392	C	12.7191	9.1046	20.6982
393	H	12.5608	8.0983	21.0974
394	C	13.1384	11.6435	19.6729
395	H	13.283	12.6472	19.2515
396	C	11.8504	11.1961	19.9226
397	H	11.0013	11.845	19.6817
398	C	20.4227	23.5691	7.097
399	H	20.736	24.1183	6.204
400	C	19.9334	22.2777	6.9833
401	H	19.8617	21.8005	6.0017
402	C	21.0198	19.9633	12.4149
403	H	21.438	19.4196	13.2805
404	H	20.8643	19.2482	11.5899
405	C	27.9953	17.8733	15.7311
406	H	28.7105	18.1291	14.943
407	C	27.2894	17.9802	18.0179
408	H	27.4356	18.3278	19.0448
409	C	26.8569	17.1481	15.4195

410	H	26.6701	16.8307	14.3867
411	C	22.2483	11.9798	17.6854
412	C	22.9064	10.411	15.4717
413	H	23.1644	9.7978	14.6028
414	C	23.5752	11.678	17.396
415	H	24.3632	12.0643	18.053
416	C	21.581	10.701	15.75
417	H	20.7835	10.3096	15.1086
418	C	23.9047	10.9026	16.2987
419	H	24.9545	10.6797	16.0855
420	C	21.2579	11.4834	16.8468
421	H	20.2093	11.7245	17.0664
422	C	24.0067	19.821	21.6901
423	H	22.9819	19.7267	22.0887
424	H	24.6723	19.1667	22.2782
425	C	24.4801	21.2607	21.7421
426	H	23.642	21.9211	21.4519
427	H	25.2639	21.4064	20.9702
428	C	25.0235	21.6183	23.08
429	C	26.0843	22.2073	25.594
430	H	26.5019	22.4414	26.5778
431	C	26.214	21.0355	23.508
432	H	26.7283	20.3338	22.8414
433	C	24.8967	22.7879	25.1832
434	H	24.3686	23.4793	25.847
435	C	26.7412	21.3224	24.7514
436	H	27.6757	20.8509	25.0707
437	C	24.3668	22.4933	23.9356
438	H	23.4137	22.9352	23.62
439	C	21.1667	16.1827	25.2043
440	C	21.086	14.7964	25.2662
441	H	21.4634	14.2062	24.4227
442	C	21.7404	16.8575	24.0035
443	H	21.8698	16.1089	23.1981
444	H	22.7492	17.2508	24.2369
445	C	19.9918	14.9128	27.4001
446	H	19.5206	14.4208	28.2564
447	C	20.509	14.1632	26.3552
448	H	20.4525	13.0704	26.3779
449	C	20.0712	16.2954	27.3482
450	H	19.6588	16.8982	28.1646
451	C	20.654	16.923	26.2616
452	H	20.6904	18.0181	26.2258
453	C	20.9161	18.0063	23.4693
454	H	21.2876	18.315	22.4758
455	H	20.9552	18.8954	24.1249

456	C	9.4698	13.2696	21.3981
457	H	10.4572	12.8625	21.6469
458	C	8.4014	12.4134	21.1875
459	H	8.5515	11.3319	21.2679
460	C	9.3169	14.6463	21.2961
461	C	8.0586	15.1474	20.9763
462	H	7.9202	16.2319	20.897
463	C	7.1526	12.9239	20.8753
464	H	6.3062	12.2516	20.7094
465	C	6.9852	14.2972	20.7708
466	H	6.0018	14.7104	20.5262
467	H	14.0989	15.8549	12.9193
468	H	13.9601	16.4401	14.581
469	H	15.0362	18.1076	12.2335
470	H	14.8975	18.6509	13.9277

Optimized Coordination for surface doped Pd₂Au₃₆(SC₂H₄Ph)₂₄⁽⁻²⁾

1	C	17.6091	8.657	20.6496
2	Au	17.7052	17.6129	18.4943
3	Au	18.3237	19.1913	16.2717
4	Au	17.1799	21.6753	17.0682
5	Au	19.6047	21.3311	15.1057
6	Au	22.2915	20.4067	18.8701
7	Au	15.7109	19.19	17.4817
8	Au	19.6902	21.0052	17.9393
9	Au	17.4035	20.289	19.4804
10	Pd	15.6751	18.3894	20.3718
11	Au	16.7926	16.9227	15.9273
12	Pd	21.1201	19.245	16.4345
13	Au	20.3265	18.4777	18.9954
14	Au	20.0095	20.6823	20.6663
15	Au	21.062	22.9928	19.3271
16	Au	19.7794	16.794	16.8037
17	Au	19.6851	15.8863	19.5986
18	Au	19.3859	23.4763	16.8602
19	Au	17.9975	18.7986	13.4087
20	Au	15.1075	16.5829	18.4661
21	Au	21.9837	21.9786	16.593
22	Au	18.3971	18.2806	21.1008
23	Au	15.0754	14.5024	16.0021
24	Au	18.3039	22.9075	19.6041
25	Au	17.5032	23.6741	14.5907
26	Au	17.0737	15.811	20.4976
27	Au	18.3949	14.5003	14.8769
28	Au	13.0112	18.6672	19.064
29	Au	20.9999	23.7992	14.2041
30	Au	17.7017	14.9751	17.6812
31	Au	18.5881	13.1124	20.0992
32	Au	15.7911	21.5994	21.4006
33	Au	19.4913	25.5948	19.2665
34	Au	19.9243	23.6012	22.0857
35	Au	24.0841	19.8663	16.5929
36	Au	19.1982	15.4768	22.521
37	Au	14.0108	16.1271	21.2706
38	Au	24.1072	22.8092	18.4746
39	Au	22.7443	17.2573	20.0114
40	S	20.5202	15.3464	15.0441
41	S	16.3489	13.6021	14.3086

42 S	19.0675	17.6488	23.2832
43 S	16.5259	17.0296	13.5728
44 S	20.1467	21.4524	22.8862
45 S	15.6699	22.5933	15.4765
46 S	16.4473	23.7495	20.855
47 S	19.3506	20.5771	12.8697
48 S	23.1207	23.1422	14.862
49 S	13.4994	20.0058	17.2483
50 S	25.5994	21.2907	17.6097
51 S	12.2401	17.546	20.9077
52 S	13.524	15.0598	17.6143
53 S	14.7692	19.6576	22.0546
54 S	15.5927	14.5434	21.8085
55 S	19.9616	25.8279	21.5102
56 S	18.9734	25.7802	17.0255
57 S	19.0945	24.7596	13.3294
58 S	19.6253	13.239	22.1559
59 S	23.9723	19.202	20.0266
60 S	17.4662	12.6546	18.1401
61 S	21.862	15.1413	20.2065
62 S	22.9083	18.2086	15.5054
63 C	15.2919	24.1878	19.5243
64 H	15.4388	23.4852	18.6833
65 H	14.2639	24.0621	19.907
66 C	15.7416	12.4826	18.6897
67 H	15.4217	13.4465	19.1242
68 H	15.1502	12.3316	17.7642
69 C	15.5219	25.6117	19.0698
70 H	16.5651	25.7062	18.7071
71 H	15.4106	26.2955	19.9312
72 C	14.5544	25.9583	17.9936
73 C	16.5002	11.8484	14.7518
74 H	16.6832	11.7683	15.8395
75 H	15.5342	11.3689	14.5224
76 C	21.8698	21.0447	11.9751
77 H	21.9051	21.8168	12.7772
78 H	21.4107	21.5343	11.0969
79 C	14.9094	14.4946	24.4804
80 H	14.0027	15.0987	24.2917
81 H	15.244	14.7058	25.5116
82 C	20.4744	26.531	16.3459
83 H	21.3323	25.9053	16.6436
84 H	20.387	26.4787	15.2451
85 C	26.2946	22.227	16.2228
86 H	25.462	22.6362	15.6217
87 H	26.8571	23.0696	16.663

88	S	22.8033	24.5672	19.2141
89	C	21.9259	28.5176	16.3095
90	C	20.657	27.9482	16.8324
91	H	19.793	28.5632	16.5266
92	H	20.6626	27.9211	17.9393
93	C	27.8231	22.2394	14.317
94	C	27.1819	21.3749	15.3447
95	H	26.5696	20.5776	14.8814
96	H	27.9448	20.8683	15.9622
97	C	27.2094	22.4702	13.0906
98	H	26.2782	21.9395	12.8524
99	C	29.5717	23.7825	13.6886
100	H	30.5056	24.2981	13.9328
101	C	28.951	24.004	12.4694
102	H	29.3922	24.6952	11.7457
103	C	27.7697	23.3436	12.1727
104	H	27.2724	23.5111	11.2123
105	C	24.8187	25.2604	14.4792
106	H	25.2852	26.1546	14.9377
107	H	25.6323	24.5458	14.2486
108	C	24.1166	25.6511	13.2238
109	C	23.8936	24.6573	15.5118
110	H	23.1074	25.369	15.8114
111	H	24.4396	24.3658	16.4339
112	C	23.2567	26.7438	13.2123
113	H	23.1191	27.332	14.1283
114	C	23.5809	25.2538	10.904
115	H	23.698	24.6488	9.9991
116	C	18.4324	26.6353	22.0659
117	H	17.5727	26.0225	21.7383
118	H	18.4457	26.6574	23.1669
119	C	13.243	18.781	24.6399
120	C	13.1358	20.0506	25.1984
121	H	14.0427	20.6388	25.3781
122	C	15.5221	19.1451	23.636
123	H	16.5057	18.6838	23.4451
124	H	15.6839	20.0476	24.2501
125	C	12.073	18.0779	24.3846
126	H	12.1473	17.0976	23.8983
127	C	14.5698	18.183	24.2995
128	H	14.3997	17.324	23.6127
129	H	15.048	17.7675	25.2096
130	C	10.711	14.2172	16.3988
131	C	11.074	12.8873	16.2264
132	H	11.9476	12.6573	15.6071
133	C	12.3189	16.1045	16.7422

134	H	11.6925	16.5636	17.5308
135	H	12.8557	16.9311	16.249
136	C	11.4883	15.3146	15.7579
137	H	12.1541	14.8979	14.9796
138	H	10.8063	16.0232	15.2504
139	C	15.997	14.9552	23.5325
140	H	16.9649	14.465	23.7457
141	H	16.1636	16.0411	23.6118
142	C	17.6326	11.2114	13.9803
143	H	17.4691	11.3486	12.8974
144	H	18.5565	11.7716	14.2322
145	C	17.7939	9.7666	14.296
146	C	20.6306	16.4219	13.5867
147	H	19.8559	17.2163	13.6619
148	H	21.6125	16.9262	13.6625
149	C	21.8838	16.9456	10.6531
150	H	22.7707	16.4883	11.1046
151	C	20.6256	16.5899	11.1282
152	C	22.0296	17.89	9.6511
153	H	23.0312	18.1827	9.3193
154	C	20.4887	15.6623	12.2863
155	H	21.2543	14.867	12.2429
156	H	19.5015	15.1628	12.2784
157	C	19.5072	17.1968	10.5648
158	H	18.5119	16.9411	10.948
159	C	23.2528	20.6211	11.6245
160	C	11.8998	20.5947	25.4999
161	H	11.8415	21.6014	25.9234
162	C	10.7397	19.8792	25.2453
163	H	9.7608	20.3158	25.4651
164	C	10.8333	18.6167	24.6845
165	H	9.9245	18.0491	24.4569
166	C	12.0201	21.3671	20.7028
167	H	13.0403	21.7434	20.8787
168	C	11.3511	20.7342	21.7337
169	H	11.8438	20.6143	22.7056
170	C	13.5305	21.6469	18.0336
171	H	14.1553	21.571	18.9429
172	H	14.0601	22.3024	17.3203
173	C	11.4363	21.4959	19.4456
174	C	12.155	22.1851	18.3363
175	H	12.2835	23.2572	18.5898
176	H	11.5368	22.1595	17.4219
177	C	10.1662	20.9701	19.2494
178	H	9.7096	21.0541	18.2569
179	C	10.0817	20.2182	21.5253

180	H	9.5618	19.7108	22.3448
181	C	13.2942	26.4592	18.3064
182	H	13.0555	26.6737	19.3544
183	C	17.0826	28.7113	21.6684
184	C	18.3898	28.0283	21.4724
185	H	18.5926	27.9285	20.3877
186	H	19.2125	28.6316	21.8967
187	C	14.9426	29.3996	20.7865
188	H	14.2419	29.4407	19.946
189	C	16.7408	29.2918	22.8846
190	H	17.4592	29.2568	23.7114
191	C	16.1658	28.7724	20.6253
192	H	16.432	28.3225	19.6619
193	C	24.3383	28.5217	16.2803
194	H	25.2879	28.1378	16.6686
195	C	24.3338	29.4791	15.2764
196	H	25.277	29.8506	14.8672
197	C	21.9339	29.4722	15.2996
198	H	20.9774	29.8381	14.9106
199	C	23.1444	28.0438	16.7895
200	H	23.1415	27.2732	17.5736
201	C	23.128	29.9497	14.7844
202	H	23.1172	30.6918	13.981
203	C	9.277	12.1724	17.648
204	H	8.7209	11.371	18.1458
205	C	9.6252	14.5053	17.2189
206	H	9.3331	15.5514	17.3681
207	C	8.913	13.4955	17.8425
208	H	8.0741	13.7427	18.5017
209	C	10.3607	11.871	16.8398
210	H	10.6723	10.8313	16.707
211	C	10.9088	16.4296	20.3763
212	H	10.0918	17.074	20.0067
213	H	11.2522	15.7851	19.5481
214	C	10.4713	15.6064	21.5672
215	H	11.3387	15.0104	21.9087
216	H	10.2298	16.3018	22.3956
217	C	29.0099	22.9071	14.6014
218	H	29.4975	22.73	15.5675
219	C	24.5014	25.9763	20.8304
220	H	24.1208	26.8943	20.349
221	H	24.7733	26.2431	21.8678
222	C	25.699	25.4829	20.0948
223	C	23.3846	24.9547	20.8889
224	H	22.517	25.349	21.4457
225	H	23.7136	24.0253	21.3813

226	C	26.517	24.5087	20.6562
227	H	26.291	24.1323	21.662
228	C	27.0478	25.4062	18.0939
229	H	27.2412	25.7451	17.0708
230	C	25.9761	25.9201	18.8052
231	H	25.3152	26.6649	18.3445
232	C	27.8601	24.4422	18.6677
233	H	28.7019	24.0295	18.1024
234	C	27.5906	23.9937	19.9509
235	H	28.2191	23.2218	20.4049
236	C	19.3018	21.5416	25.9346
237	C	18.5229	21.1047	23.6155
238	H	17.7313	21.3141	22.8642
239	H	18.5076	20.0141	23.8058
240	C	20.4892	22.2578	26.0486
241	H	20.65	23.1165	25.3869
242	C	18.2982	21.8867	24.8914
243	H	18.3321	22.9651	24.6569
244	H	17.2793	21.6566	25.2541
245	C	18.8979	23.9273	11.7237
246	H	18.7364	22.8527	11.9187
247	H	17.9843	24.3394	11.2637
248	C	20.1089	24.1345	10.8524
249	H	20.9895	23.7373	11.4037
250	H	20.3184	25.2119	10.7319
251	C	25.8558	16.8841	16.3525
252	C	28.1492	18.3311	17.0169
253	H	29.0459	18.9019	17.2755
254	C	23.3333	16.7114	16.4472
255	H	23.3125	16.9464	17.5313
256	H	22.5016	16.0117	16.255
257	C	9.4906	20.3351	20.2792
258	H	8.4919	19.9249	20.1002
259	C	24.638	16.1002	16.0055
260	H	24.6092	15.9282	14.9147
261	H	24.7018	15.096	16.4708
262	C	26.0665	17.3256	17.6552
263	H	25.3127	17.1243	18.4293
264	C	18.8496	10.8957	23.4302
265	H	19.8609	10.8419	23.8719
266	H	18.1444	10.4684	24.1684
267	C	18.4764	12.3539	23.2595
268	H	18.5313	12.8696	24.2352
269	H	17.448	12.4618	22.8723
270	C	18.8064	10.0796	22.1826
271	C	18.7287	8.5646	19.8409

272	H	18.6949	7.9668	18.9242
273	C	17.6435	9.4158	21.808
274	H	16.7465	9.5096	22.4362
275	C	19.9247	9.9798	21.3601
276	H	20.8385	10.513	21.6455
277	C	19.8879	9.2358	20.1933
278	H	20.7699	9.186	19.547
279	C	18.1088	7.0597	14.9075
280	H	18.2419	6.0001	15.1428
281	C	18.2612	9.3698	15.5464
282	H	18.4997	10.1347	16.2976
283	C	18.4233	8.0294	15.847
284	H	18.8105	7.7383	16.8289
285	C	14.1827	10.895	19.8924
286	C	15.5866	11.3405	19.6574
287	H	16.0525	11.6441	20.6201
288	H	16.192	10.4793	19.3192
289	C	15.1716	10.7266	24.6416
290	H	15.8212	9.9687	25.0927
291	C	14.1243	10.3418	23.8189
292	H	13.9451	9.284	23.6049
293	C	12.4747	17.3501	13.168
294	C	11.984	18.4294	13.9003
295	H	12.556	18.8202	14.7536
296	C	14.9039	17.7753	13.2652
297	C	13.8054	16.7605	13.4801
298	C	14.8681	20.9149	11.8034
299	C	15.3858	21.2982	14.2321
300	H	16.2597	20.6146	14.1979
301	H	14.5193	20.7194	14.6029
302	C	15.9283	20.3796	11.0788
303	H	16.9524	20.7067	11.3012
304	C	15.1202	21.9184	12.876
305	H	14.2673	22.6161	12.9567
306	H	16.0054	22.5341	12.62
307	C	22.3575	14.2169	18.7205
308	H	21.9368	14.7155	17.8306
309	H	23.4585	14.2467	18.6519
310	C	15.5178	29.9182	23.0535
311	H	15.2684	30.3723	24.0166
312	C	14.6153	29.9752	22.003
313	H	13.6516	30.4753	22.1327
314	C	21.2636	20.7685	27.7661
315	H	22.0375	20.4598	28.4754
316	C	21.4628	21.8748	26.956
317	H	22.4	22.4373	27.0193

318	C	20.0829	20.0502	27.6645
319	H	19.9204	19.1681	28.2936
320	C	19.1139	20.434	26.7523
321	H	18.1891	19.8525	26.6542
322	C	13.5802	20.4771	11.5144
323	H	12.7355	20.8751	12.0877
324	C	13.3501	19.5308	10.5287
325	H	12.3303	19.1815	10.3394
326	C	14.4154	19.0096	9.8107
327	H	14.2434	18.2591	9.0343
328	C	15.7042	19.4375	10.0891
329	H	16.5527	19.0284	9.5306
330	C	10.0527	18.5645	12.4756
331	H	9.1098	19.0457	12.2011
332	C	10.5212	17.4805	11.7505
333	H	9.949	17.099	10.9004
334	C	10.787	19.0312	13.5553
335	H	10.4251	19.8819	14.1414
336	C	11.7222	16.8838	12.0975
337	H	12.1036	16.0382	11.5142
338	C	12.6562	26.3883	15.995
339	H	11.9072	26.5408	15.2132
340	C	14.8535	25.6899	16.6636
341	H	15.8461	25.2979	16.3981
342	C	12.3499	26.6751	17.3166
343	H	11.3603	27.0619	17.5779
344	C	13.9106	25.8969	15.6722
345	H	14.1615	25.6517	14.6359
346	C	17.4793	8.785	13.3639
347	H	17.1121	9.0892	12.3772
348	C	17.6295	7.4422	13.6662
349	H	17.3705	6.6847	12.9203
350	C	14.5962	13.0482	24.3153
351	C	13.3092	11.3059	23.2476
352	H	12.5055	11.0078	22.565
353	C	15.4074	12.0713	24.8816
354	H	16.251	12.3767	25.5125
355	C	13.5425	12.6459	23.5015
356	H	12.9196	13.4171	23.0309
357	H	16.6915	8.1321	20.3634
358	C	19.5532	22.1772	9.369
359	H	19.2549	21.6044	10.2592
360	C	19.4835	21.5856	8.1192
361	H	19.1185	20.556	8.0334
362	C	20.0052	23.4879	9.5135
363	C	20.3868	24.1794	8.3684

364	H	20.737	25.214	8.471
365	C	21.8441	12.801	18.8437
366	H	20.743	12.8325	18.9981
367	H	22.2634	12.3457	19.7608
368	C	22.7427	26.3564	10.8991
369	H	22.2116	26.6375	9.9838
370	C	24.2624	24.906	12.0596
371	H	24.9185	24.0284	12.0704
372	C	22.577	27.0964	12.0598
373	H	21.9035	27.9588	12.073
374	C	19.6484	18.1392	9.5576
375	H	18.7542	18.6178	9.1387
376	C	20.9079	18.4934	9.1009
377	H	21.0184	19.2616	8.3289
378	C	25.0755	20.539	10.0402
379	H	25.4791	20.7908	9.0545
380	C	25.325	19.5204	12.1917
381	H	25.9195	18.9622	12.9251
382	C	25.849	19.8304	10.9447
383	H	26.8663	19.5263	10.6813
384	C	23.7869	20.9237	10.3767
385	H	23.1649	21.4713	9.6574
386	C	24.0438	19.9191	12.529
387	H	23.6526	19.6657	13.5231
388	C	11.5701	10.0002	20.3555
389	H	10.5462	9.6514	20.5225
390	C	13.937	9.6155	20.387
391	H	14.7897	8.9562	20.5895
392	C	12.649	9.168	20.6185
393	H	12.484	8.1562	21.0021
394	C	13.0928	11.7182	19.634
395	H	13.2501	12.7261	19.2279
396	C	11.7991	11.2739	19.8612
397	H	10.9547	11.9284	19.6215
398	C	20.3287	23.5864	7.1183
399	H	20.6402	24.1491	6.2333
400	C	19.8731	22.285	6.9882
401	H	19.8199	21.8167	6.0013
402	C	20.9837	19.9107	12.4359
403	H	21.3928	19.3937	13.3229
404	H	20.8326	19.1692	11.6342
405	C	27.9455	17.9088	15.7135
406	H	28.6771	18.1498	14.9362
407	C	27.2014	18.0428	17.9857
408	H	27.3254	18.4057	19.0102
409	C	26.8052	17.1936	15.3874

410	H	26.6349	16.8708	14.3533
411	C	22.1658	11.963	17.6571
412	C	22.7913	10.3984	15.4303
413	H	23.0376	9.786	14.5573
414	C	23.4873	11.6545	17.3513
415	H	24.2856	12.0325	18.0007
416	C	21.4715	10.7015	15.7208
417	H	20.6646	10.3229	15.0829
418	C	23.8009	10.8791	16.25
419	H	24.8477	10.649	16.0292
420	C	21.1625	11.4798	16.825
421	H	20.1168	11.7268	17.056
422	C	23.8808	19.8264	21.7246
423	H	22.8525	19.7318	22.1131
424	H	24.5458	19.1929	22.3355
425	C	24.3374	21.2723	21.7491
426	H	23.4969	21.9131	21.423
427	H	25.1353	21.4057	20.99
428	C	24.8466	21.6695	23.0889
429	C	25.8174	22.3123	25.6274
430	H	26.1947	22.5594	26.6239
431	C	26.0657	21.1655	23.5362
432	H	26.6402	20.5047	22.8758
433	C	24.6067	22.8244	25.1906
434	H	24.0277	23.4862	25.8425
435	C	26.5462	21.4767	24.7945
436	H	27.5013	21.0625	25.1311
437	C	24.1199	22.4995	23.9332
438	H	23.1474	22.8817	23.5968
439	C	21.0872	16.237	25.1894
440	C	21.051	14.8493	25.2498
441	H	21.4571	14.2752	24.4093
442	C	21.6636	16.9245	23.9966
443	H	21.8002	16.1798	23.1884
444	H	22.6704	17.3188	24.2376
445	C	19.9276	14.9256	27.3693
446	H	19.4681	14.4159	28.2217
447	C	20.4798	14.1957	26.3297
448	H	20.46	13.1014	26.3511
449	C	19.9603	16.3099	27.3197
450	H	19.523	16.897	28.1345
451	C	20.5324	16.9585	26.2386
452	H	20.5329	18.0548	26.206
453	C	20.8344	18.0691	23.4637
454	H	21.2077	18.3846	22.4732
455	H	20.8613	18.9558	24.1231

456 C	9.4401	13.3355	21.3814
457 H	10.4191	12.9087	21.6301
458 C	8.3562	12.5027	21.1592
459 H	8.4848	11.4183	21.2325
460 C	9.3091	14.7151	21.2991
461 C	8.0629	15.2448	20.9767
462 H	7.9459	16.3318	20.9073
463 C	7.1183	13.0408	20.85
464 H	6.2617	12.3835	20.6761
465 C	6.975	14.4178	20.7578
466 H	6.0007	14.8521	20.5146
467 H	13.9839	15.8737	12.8464
468 H	13.8618	16.3956	14.529
469 H	14.9053	18.1388	12.2234
470 H	14.7708	18.6456	13.9284

Optimized Coordination for long staples doped Pd₂Au₃₆(SC₂H₄Ph)₂₄⁽⁻²⁾

1 C	17.7905	8.7971	20.6739
2 Au	17.7169	17.6739	18.5875
3 Au	18.2941	19.2008	16.2946
4 Au	17.193	21.6906	17.0973
5 Au	19.6067	21.4006	15.1823
6 Au	22.3264	20.5142	18.9858
7 Au	15.7198	19.1994	17.476
8 Au	19.7027	21.0355	18.0127
9 Au	17.4137	20.3086	19.5194
10 Au	15.6866	18.3995	20.4839
11 Au	16.7331	16.9265	16.0074
12 Au	21.1044	19.2792	16.4162
13 Au	20.4045	18.499	19.0731
14 Au	20.0144	20.7207	20.7146
15 Au	21.0779	23.0701	19.3984
16 Au	19.6885	16.7855	16.8878
17 Au	19.6941	15.8875	19.6047
18 Au	19.3873	23.5194	16.8904
19 Au	18.0836	18.8078	13.4802
20 Au	15.1201	16.5968	18.4861
21 Au	22.0005	22.0753	16.7018
22 Au	18.4842	18.2881	21.1752
23 Pd	15.1471	14.6492	16.2543
24 Au	18.301	22.9108	19.6027
25 Au	17.5058	23.6819	14.5955
26 Au	17.1071	15.7991	20.5213
27 Au	18.3902	14.532	14.9354
28 Au	12.9935	18.6742	19.096
29 Au	20.9947	23.8057	14.2109
30 Au	17.595	14.9435	17.7318
31 Au	18.6053	13.1921	20.2023
32 Au	15.8044	21.6906	21.4748
33 Au	19.4081	25.6077	19.2103
34 Au	19.9942	23.6799	22.0995
35 Au	24.1926	19.9124	16.7021
36 Au	19.2721	15.5143	22.6016
37 Au	14.0045	16.1132	21.3057
38 Pd	23.9262	22.8641	18.5363
39 Au	22.8061	17.2986	20.0812

40 S	20.5165	15.3829	15.1587
41 S	16.2861	13.6978	14.5544
42 S	19.1246	17.6863	23.3606
43 S	16.6398	17.0316	13.6266
44 S	20.2388	21.5336	22.9143
45 S	15.6904	22.5986	15.5024
46 S	16.505	23.806	20.8991
47 S	19.4037	20.6128	12.9469
48 S	23.0913	23.1495	14.8875
49 S	13.5204	20.0522	17.3242
50 S	25.5127	21.4527	17.7812
51 S	12.2339	17.5348	20.94
52 S	13.4862	15.0909	17.7514
53 S	14.749	19.7804	22.1782
54 S	15.6191	14.5712	21.8543
55 S	19.9357	25.8799	21.4421
56 S	18.9537	25.8296	16.9642
57 S	19.0908	24.7732	13.343
58 S	19.6864	13.2838	22.2414
59 S	24.0106	19.25	20.0967
60 S	17.5277	12.6293	18.262
61 S	21.8914	15.2011	20.2102
62 S	23.0482	18.2877	15.5369
63 C	15.3093	24.2613	19.6101
64 H	15.4051	23.5452	18.7743
65 H	14.2949	24.1649	20.0355
66 C	15.7955	12.4639	18.7711
67 H	15.4656	13.426	19.1993
68 H	15.2223	12.3298	17.8319
69 C	15.5571	25.6712	19.1263
70 H	16.6008	25.745	18.757
71 H	15.4598	26.3733	19.9741
72 C	14.5845	26.0015	18.0502
73 C	16.4789	11.944	14.9717
74 H	16.6675	11.8577	16.0584
75 H	15.5182	11.4515	14.745
76 C	21.9138	21.0981	12.0266
77 H	21.9441	21.9023	12.797
78 H	21.4359	21.5452	11.1347
79 C	14.9851	14.5228	24.528
80 H	14.0679	15.1128	24.3438
81 H	15.3227	14.743	25.5567
82 C	20.507	26.5536	16.3735
83 H	21.335	25.8988	16.6951
84 H	20.4729	26.5322	15.2681
85 C	26.237	22.3261	16.3662

86	H	25.4173	22.6355	15.6921
87	H	26.7125	23.2377	16.7699
88	S	22.7677	24.6796	19.2858
89	C	21.9793	28.5225	16.4029
90	C	20.7062	27.95	16.9118
91	H	19.8498	28.5876	16.6345
92	H	20.7162	27.8797	18.0176
93	C	27.8549	22.3208	14.5324
94	C	27.235	21.4893	15.598
95	H	26.711	20.6115	15.1741
96	H	28.0021	21.0952	16.2891
97	C	27.2531	22.446	13.2843
98	H	26.3526	21.8585	13.0644
99	C	29.5297	23.9183	13.842
100	H	30.4312	24.4962	14.0677
101	C	28.9207	24.0349	12.6016
102	H	29.3346	24.7097	11.847
103	C	27.7856	23.2903	12.3241
104	H	27.3031	23.3657	11.3442
105	C	24.83	25.2493	14.5753
106	H	25.2879	26.1357	15.0571
107	H	25.6457	24.5327	14.3631
108	C	24.1676	25.6553	13.302
109	C	23.8633	24.6492	15.5731
110	H	23.0742	25.3683	15.8434
111	H	24.3542	24.339	16.5223
112	C	23.3012	26.7429	13.2771
113	H	23.1349	27.3213	14.1952
114	C	23.7014	25.2801	10.963
115	H	23.8523	24.6848	10.0567
116	C	18.4565	26.7113	22.0784
117	H	17.5672	26.1217	21.795
118	H	18.5233	26.7341	23.1778
119	C	13.333	18.8173	24.7435
120	C	13.2208	20.0612	25.3553
121	H	14.124	20.6448	25.566
122	C	15.5778	19.2359	23.7012
123	H	16.5616	18.7974	23.4598
124	H	15.7484	20.1285	24.3265
125	C	12.1681	18.1184	24.4546
126	H	12.2515	17.1585	23.9307
127	C	14.6656	18.2463	24.3799
128	H	14.5046	17.3805	23.7014
129	H	15.1719	17.852	25.2824
130	C	10.7327	14.2698	16.4787
131	C	11.1107	12.9463	16.2844

132	H	11.9939	12.7393	15.6697
133	C	12.3056	16.171	16.8823
134	H	11.6548	16.6442	17.6463
135	H	12.8637	16.9851	16.3917
136	C	11.5068	15.3855	15.8683
137	H	12.2085	14.9832	15.1146
138	H	10.831	16.0871	15.3423
139	C	16.0557	14.9919	23.5658
140	H	17.0298	14.5036	23.7603
141	H	16.2269	16.0771	23.6454
142	C	17.6171	11.3222	14.1944
143	H	17.4576	11.4907	13.1153
144	H	18.5355	11.8878	14.4599
145	C	17.7925	9.871	14.4657
146	C	20.6929	16.4596	13.7105
147	H	19.8974	17.2379	13.7385
148	H	21.6609	16.9822	13.8287
149	C	21.9811	16.997	10.7611
150	H	22.8807	16.5353	11.1823
151	C	20.7362	16.6278	11.2597
152	C	22.0981	17.9561	9.7696
153	H	23.0897	18.2632	9.4241
154	C	20.6281	15.6886	12.4112
155	H	21.439	14.9392	12.3821
156	H	19.6707	15.136	12.3822
157	C	19.6012	17.2366	10.7322
158	H	18.6169	16.9684	11.1352
159	C	23.3	20.6884	11.6718
160	C	11.9819	20.5853	25.6783
161	H	11.9164	21.5693	26.15
162	C	10.8268	19.8751	25.3908
163	H	9.8483	20.2948	25.6383
164	C	10.9258	18.6393	24.7746
165	H	10.0222	18.0727	24.5273
166	C	12.0719	21.4814	20.8549
167	H	13.052	21.9398	21.0571
168	C	11.4148	20.8149	21.8721
169	H	11.8737	20.7414	22.8652
170	C	13.6202	21.6686	18.1505
171	H	14.2523	21.5588	19.0532
172	H	14.1589	22.3204	17.4411
173	C	11.5348	21.5415	19.5707
174	C	12.2645	22.2467	18.4781
175	H	12.4292	23.3062	18.7598
176	H	11.6464	22.2652	17.5627
177	C	10.3178	20.9138	19.3353

178	H	9.8979	20.9382	18.324
179	C	10.1984	20.1982	21.6234
180	H	9.6932	19.6616	22.433
181	C	13.3232	26.499	18.3648
182	H	13.0883	26.7209	19.413
183	C	17.1259	28.8059	21.7154
184	C	18.4192	28.1073	21.486
185	H	18.5982	28.0082	20.3976
186	H	19.2587	28.6971	21.8953
187	C	14.9502	29.4812	20.9138
188	H	14.2132	29.506	20.1051
189	C	16.8352	29.4013	22.9378
190	H	17.5857	29.3708	23.7359
191	C	16.1689	28.8587	20.7073
192	H	16.3968	28.4009	19.7377
193	C	24.3905	28.5184	16.3642
194	H	25.341	28.1313	16.748
195	C	24.386	29.4848	15.3687
196	H	25.3282	29.8536	14.9544
197	C	21.9869	29.4882	15.4048
198	H	21.0301	29.8612	15.0238
199	C	23.1973	28.0404	16.8772
200	H	23.1947	27.2675	17.6606
201	C	23.1799	29.9686	14.8907
202	H	23.1643	30.7206	14.0964
203	C	9.3116	12.1865	17.6786
204	H	8.7584	11.3719	18.1578
205	C	9.6408	14.5308	17.2991
206	H	9.3431	15.5713	17.4766
207	C	8.9346	13.502	17.8966
208	H	8.0909	13.7278	18.5566
209	C	10.4057	11.9116	16.8747
210	H	10.7322	10.8786	16.7271
211	C	10.9247	16.4003	20.4138
212	H	10.0999	17.0326	20.0406
213	H	11.2835	15.7576	19.5886
214	C	10.4956	15.5758	21.6085
215	H	11.3597	14.9667	21.935
216	H	10.2685	16.2668	22.4448
217	C	28.9999	23.065	14.7941
218	H	29.4782	22.966	15.7761
219	C	24.5354	25.9785	20.918
220	H	24.1803	26.9255	20.4742
221	H	24.84	26.1993	21.9572
222	C	25.7102	25.4768	20.1505
223	C	23.3817	24.9989	20.9692

224	H	22.5473	25.4091	21.5634
225	H	23.6979	24.0462	21.4268
226	C	26.5219	24.4767	20.6736
227	H	26.2933	24.0613	21.6638
228	C	27.0714	25.4832	18.1545
229	H	27.2716	25.8688	17.1491
230	C	25.9953	25.9647	18.8809
231	H	25.338	26.7324	18.4543
232	C	27.8799	24.4949	18.6922
233	H	28.7278	24.1061	18.1194
234	C	27.5972	23.9891	19.951
235	H	28.2202	23.1942	20.3712
236	C	19.4644	21.6047	25.9968
237	C	18.636	21.189	23.6868
238	H	17.8271	21.4059	22.9565
239	H	18.6238	20.0979	23.872
240	C	20.665	22.3008	26.0912
241	H	20.8349	23.153	25.4231
242	C	18.4481	21.9649	24.9705
243	H	18.4909	23.0456	24.7401
244	H	17.4335	21.7448	25.3506
245	C	18.9212	23.9516	11.7337
246	H	18.7495	22.8772	11.9206
247	H	18.0196	24.372	11.2584
248	C	20.1524	24.1632	10.8932
249	H	21.0199	23.7565	11.459
250	H	20.3657	25.2419	10.7902
251	C	25.8824	16.8999	16.4296
252	C	28.1593	18.3696	17.0942
253	H	29.0482	18.9537	17.3508
254	C	23.3574	16.7689	16.4781
255	H	23.3111	16.9972	17.5627
256	H	22.5095	16.099	16.2486
257	C	9.6506	20.2498	20.3515
258	H	8.6977	19.7533	20.1408
259	C	24.6604	16.1219	16.0775
260	H	24.6515	15.9217	14.9912
261	H	24.6925	15.1299	16.571
262	C	26.0968	17.3266	17.7354
263	H	25.349	17.1058	18.5103
264	C	18.946	10.9539	23.5494
265	H	19.9452	10.9208	24.0194
266	H	18.2314	10.5131	24.2688
267	C	18.5449	12.4034	23.3558
268	H	18.5754	12.9366	24.3218
269	H	17.5207	12.4799	22.9515

270	C	18.9481	10.1549	22.2928
271	C	18.9223	8.7645	19.8771
272	H	18.9051	8.2345	18.9199
273	C	17.801	9.4949	21.8704
274	H	16.8936	9.5504	22.4871
275	C	20.0834	10.1035	21.4903
276	H	20.9834	10.6385	21.8124
277	C	20.071	9.4216	20.2862
278	H	20.9599	9.4211	19.6482
279	C	18.1564	7.142	14.9604
280	H	18.3093	6.0774	15.1547
281	C	18.2398	9.427	15.708
282	H	18.4499	10.1617	16.4988
283	C	18.4236	8.0766	15.9491
284	H	18.7901	7.7464	16.9268
285	C	14.2093	10.8945	19.9453
286	C	15.6196	11.323	19.7321
287	H	16.0711	11.6222	20.7027
288	H	16.225	10.4589	19.4023
289	C	15.3149	10.7614	24.7009
290	H	15.9737	10.0182	25.1619
291	C	14.2883	10.3553	23.8634
292	H	14.1361	9.2941	23.6458
293	C	12.6026	17.3589	13.2388
294	C	12.1	18.4385	13.9626
295	H	12.651	18.8151	14.8369
296	C	15.0208	17.7695	13.2963
297	C	13.9236	16.7678	13.5753
298	C	14.9692	20.9076	11.8244
299	C	15.4152	21.2961	14.2663
300	H	16.2879	20.6116	14.2495
301	H	14.5413	20.7223	14.6273
302	C	16.0571	20.3912	11.1265
303	H	17.0706	20.7333	11.3741
304	C	15.1739	21.9129	12.9041
305	H	14.3065	22.5948	12.9632
306	H	16.0549	22.5456	12.6733
307	C	22.4177	14.2564	18.7516
308	H	22.0384	14.7488	17.84
309	H	23.5202	14.2611	18.7194
310	C	15.6198	30.029	23.1477
311	H	15.4094	30.4961	24.114
312	C	14.6716	30.0675	22.1374
313	H	13.7102	30.5593	22.3052
314	C	21.4339	20.819	27.817
315	H	22.2106	20.5071	28.5212

316	C	21.6408	21.9122	26.9931
317	H	22.5881	22.4569	27.0398
318	C	20.2432	20.1167	27.7309
319	H	20.0719	19.2471	28.3739
320	C	19.2703	20.5054	26.8251
321	H	18.3367	19.9365	26.7446
322	C	13.6958	20.454	11.5022
323	H	12.8342	20.8425	12.0569
324	C	13.5053	19.5079	10.5089
325	H	12.4949	19.1483	10.2942
326	C	14.5963	19.0028	9.8187
327	H	14.4539	18.2512	9.0377
328	C	15.8714	19.4479	10.1302
329	H	16.7391	19.0491	9.594
330	C	10.2123	18.5931	12.4824
331	H	9.2795	19.0798	12.1846
332	C	10.6937	17.5097	11.7654
333	H	10.1401	17.1346	10.8993
334	C	10.9177	19.0507	13.5855
335	H	10.5406	19.8991	14.1647
336	C	11.8805	16.9036	12.1424
337	H	12.2754	16.0592	11.5665
338	C	12.6755	26.4036	16.0579
339	H	11.9256	26.5522	15.2759
340	C	14.8775	25.7166	16.7219
341	H	15.8693	25.323	16.4577
342	C	12.3738	26.701	17.3775
343	H	11.3839	27.0853	17.6425
344	C	13.9292	25.9118	15.7329
345	H	14.1771	25.6598	14.6977
346	C	17.5188	8.9223	13.487
347	H	17.1608	9.2645	12.5102
348	C	17.6983	7.5704	13.7262
349	H	17.4816	6.8431	12.9378
350	C	14.6942	13.0711	24.3698
351	C	13.4579	11.303	23.2863
352	H	12.6672	10.9883	22.596
353	C	15.5178	12.1105	24.9448
354	H	16.3449	12.4376	25.5868
355	C	13.6566	12.6472	23.5468
356	H	13.0211	13.4036	23.07
357	H	16.8808	8.2818	20.3486
358	C	19.5998	22.2349	9.3759
359	H	19.266	21.6602	10.2511
360	C	19.546	21.6627	8.1167
361	H	19.1563	20.645	8.0052

362 C	20.0753	23.5335	9.5465
363 C	20.496	24.2331	8.4208
364 H	20.8658	25.2575	8.548
365 C	21.8715	12.8521	18.8751
366 H	20.7717	12.9048	19.0281
367 H	22.2794	12.3857	19.7922
368 C	22.8498	26.3722	10.9481
369 H	22.3287	26.6528	10.0276
370 C	24.3545	24.9269	12.1329
371 H	25.0244	24.0589	12.1511
372 C	22.6479	27.0997	12.1105
373 H	21.9612	27.9522	12.1162
374 C	19.7147	18.1937	9.7353
375 H	18.8121	18.68	9.3457
376 C	20.9614	18.5603	9.255
377 H	21.0504	19.3415	8.4931
378 C	25.1375	20.6712	10.1026
379 H	25.5475	20.9604	9.1303
380 C	25.3631	19.5547	12.2075
381 H	25.9504	18.9671	12.9232
382 C	25.899	19.9155	10.98
383 H	26.9148	19.6146	10.7114
384 C	23.8507	21.0513	10.4478
385 H	23.2442	21.6406	9.7482
386 C	24.0802	19.9427	12.5497
387 H	23.6803	19.6516	13.528
388 C	11.5843	10.04	20.3945
389 H	10.5535	9.7078	20.5566
390 C	13.9443	9.6205	20.4427
391 H	14.7875	8.9521	20.6564
392 C	12.649	9.1922	20.6662
393 H	12.4664	8.1844	21.0531
394 C	13.134	11.732	19.6705
395 H	13.3037	12.7356	19.257
396 C	11.8339	11.3069	19.8932
397 H	10.9999	11.9706	19.6414
398 C	20.4498	23.6616	7.1609
399 H	20.7812	24.2359	6.2907
400 C	19.9721	22.3702	7.0037
401 H	19.9273	21.9154	6.0104
402 C	21.0524	19.9697	12.5391
403 H	21.4756	19.4975	13.4436
404 H	20.9112	19.1936	11.7704
405 C	27.9516	17.9631	15.7872
406 H	28.6716	18.2341	15.0086
407 C	27.2241	18.0557	18.067

408	H	27.3489	18.4134	19.0928
409	C	26.8197	17.2353	15.4607
410	H	26.6446	16.9224	14.425
411	C	22.1791	12.018	17.683
412	C	22.7809	10.4852	15.4307
413	H	23.018	9.8861	14.5466
414	C	23.4949	11.6792	17.384
415	H	24.2959	12.0233	18.0492
416	C	21.4665	10.8125	15.719
417	H	20.654	10.4635	15.0723
418	C	23.7971	10.9201	16.268
419	H	24.8388	10.6662	16.0486
420	C	21.1694	11.5776	16.8353
421	H	20.1293	11.849	17.0625
422	C	23.9895	19.8641	21.8037
423	H	22.9939	19.7208	22.2573
424	H	24.7206	19.2578	22.3642
425	C	24.3868	21.3269	21.8143
426	H	23.5249	21.934	21.4782
427	H	25.175	21.4879	21.0507
428	C	24.8833	21.7572	23.1495
429	C	25.8588	22.5033	25.6629
430	H	26.2402	22.7939	26.6463
431	C	26.1407	21.3439	23.5826
432	H	26.7475	20.7195	22.9166
433	C	24.6072	22.9233	25.2426
434	H	23.9983	23.561	25.8922
435	C	26.6244	21.7052	24.8264
436	H	27.6136	21.364	25.1466
437	C	24.1189	22.5463	24.0003
438	H	23.1186	22.8619	23.6776
439	C	21.1751	16.2985	25.2691
440	C	21.1008	14.91	25.295
441	H	21.475	14.3441	24.4348
442	C	21.7318	17.0064	24.0778
443	H	21.8775	16.2732	23.2616
444	H	22.7311	17.4243	24.312
445	C	20.027	14.9641	27.4427
446	H	19.5642	14.445	28.2869
447	C	20.5336	14.2464	26.3711
448	H	20.4797	13.1523	26.3632
449	C	20.1043	16.348	27.4299
450	H	19.705	16.9278	28.2687
451	C	20.6705	17.007	26.3518
452	H	20.7064	18.103	26.3485
453	C	20.8802	18.1407	23.5556

454 H	21.2544	18.4798	22.5723
455 H	20.8842	19.0171	24.2302
456 C	9.4491	13.3142	21.4243
457 H	10.4277	12.8823	21.6655
458 C	8.3637	12.4862	21.1921
459 H	8.4904	11.4007	21.2542
460 C	9.3252	14.6947	21.3441
461 C	8.0821	15.2296	21.0206
462 H	7.968	16.3172	20.9486
463 C	7.1287	13.0294	20.8806
464 H	6.2706	12.3767	20.6964
465 C	6.9926	14.4071	20.7947
466 H	6.024	14.8481	20.5419
467 H	14.0963	15.8512	12.9836
468 H	13.9922	16.4531	14.6428
469 H	15.0132	18.0887	12.2406
470 H	14.8988	18.6648	13.9266

Optimized Coordination for both long and short staple doped Pd₂Au₃₆(SC₂H₄Ph)₂₄⁽⁻²⁾

1 C	17.7591	8.8019	20.6333
2 Au	17.7272	17.6635	18.5562
3 Au	18.3444	19.2245	16.2862
4 Au	17.1998	21.6848	17.0878
5 Au	19.6451	21.3982	15.1241
6 Au	22.3317	20.4114	18.8988
7 Au	15.7264	19.2076	17.4877
8 Au	19.7203	20.9871	17.9474
9 Au	17.4077	20.3172	19.5254
10 Au	15.6832	18.4004	20.4913
11 Au	16.7901	16.98	16.0009
12 Au	21.1805	19.2071	16.3991
13 Au	20.3981	18.4778	19.0637
14 Au	20.0206	20.7047	20.6792
15 Au	21.0612	23.0091	19.3276
16 Au	19.725	16.7862	16.8614
17 Au	19.709	15.8822	19.6124
18 Au	19.403	23.5038	16.8775
19 Au	18.0885	18.8017	13.4757
20 Au	15.1249	16.6039	18.4878
21 Au	22.0176	21.9826	16.6011
22 Au	18.496	18.2198	21.1238
23 Au	15.0811	14.5057	16.009
24 Au	18.3064	22.911	19.6021
25 Au	17.5252	23.6864	14.5956
26 Au	17.0998	15.7993	20.5159
27 Au	18.4097	14.5146	14.8989
28 Au	12.9978	18.6768	19.0886
29 Au	21.0596	23.8117	14.2767
30 Au	17.6924	14.9926	17.7087
31 Au	18.5931	13.1877	20.1868
32 Pd	15.9226	21.5994	21.3726
33 Au	19.4128	25.5967	19.1988
34 Au	19.9887	23.6757	22.0782
35 Pd	24.0324	19.9722	16.6912
36 Au	19.2744	15.5146	22.602
37 Au	14.0073	16.0966	21.2962
38 Au	24.0998	22.8054	18.4897
39 Au	22.8088	17.2983	20.0827

40 S	20.5313	15.36	15.1246
41 S	16.3808	13.5775	14.3511
42 S	19.1144	17.6932	23.3485
43 S	16.6262	17.0291	13.6398
44 S	20.1519	21.5225	22.8784
45 S	15.6982	22.6148	15.4999
46 S	16.4788	23.7263	20.8512
47 S	19.4061	20.5983	12.9037
48 S	23.1889	23.1915	14.9069
49 S	13.5283	20.0524	17.3198
50 S	25.6036	21.2954	17.651
51 S	12.2512	17.5285	20.9263
52 S	13.5498	15.0774	17.635
53 S	14.8487	19.803	22.1827
54 S	15.6206	14.5381	21.8334
55 S	19.9653	25.8765	21.4262
56 S	18.9234	25.8193	16.9562
57 S	19.1551	24.7674	13.3796
58 S	19.6624	13.2799	22.2286
59 S	24.0186	19.2543	20.1247
60 S	17.5047	12.6927	18.2091
61 S	21.9021	15.1925	20.2069
62 S	23.1138	18.2539	15.5218
63 C	15.3202	24.2269	19.5479
64 H	15.4394	23.5408	18.6906
65 H	14.2972	24.0999	19.9458
66 C	15.7773	12.5049	18.7303
67 H	15.44	13.4663	19.1567
68 H	15.1979	12.3423	17.7996
69 C	15.5434	25.6567	19.1124
70 H	16.5876	25.7577	18.7522
71 H	15.4309	26.3249	19.9849
72 C	14.5742	26.0081	18.0414
73 C	16.5759	11.8493	14.8686
74 H	16.7308	11.8235	15.9626
75 H	15.6346	11.3273	14.6334
76 C	21.9198	21.1039	12.0267
77 H	21.9371	21.9187	12.7868
78 H	21.4425	21.534	11.127
79 C	15.0068	14.5243	24.5196
80 H	14.0911	15.1208	24.35
81 H	15.362	14.7438	25.542
82 C	20.4317	26.587	16.3061
83 H	21.2822	25.926	16.5429
84 H	20.3274	26.6108	15.2058
85 C	26.3078	22.2818	16.2983

86	H	25.4754	22.6348	15.6613
87	H	26.8102	23.1591	16.7428
88	S	22.8137	24.5739	19.2549
89	C	21.9354	28.5317	16.3693
90	C	20.6607	27.9645	16.8811
91	H	19.8115	28.6259	16.6372
92	H	20.688	27.8628	17.9833
93	C	27.8649	22.3387	14.4034
94	C	27.2752	21.4756	15.4615
95	H	26.733	20.6157	15.0255
96	H	28.0659	21.0552	16.1083
97	C	27.2294	22.4969	13.1759
98	H	26.3151	21.9255	12.967
99	C	29.5416	23.9258	13.6914
100	H	30.4569	24.4879	13.9007
101	C	28.901	24.0721	12.4715
102	H	29.3052	24.75	11.7137
103	C	27.746	23.3507	12.2162
104	H	27.2368	23.4508	11.2524
105	C	24.8664	25.3086	14.5495
106	H	25.3299	26.2053	15.0064
107	H	25.6787	24.5887	14.3363
108	C	24.1833	25.6893	13.28
109	C	23.9243	24.7152	15.5748
110	H	23.1301	25.4285	15.8487
111	H	24.458	24.4385	16.5075
112	C	23.3024	26.7648	13.2521
113	H	23.1291	27.3455	14.1666
114	C	23.71	25.2892	10.9474
115	H	23.8603	24.6868	10.0459
116	C	18.4485	26.6704	22.024
117	H	17.5887	26.0282	21.7516
118	H	18.5068	26.7346	23.1229
119	C	13.3513	18.7392	24.7042
120	C	13.2265	19.9962	25.2877
121	H	14.1253	20.5925	25.4799
122	C	15.6227	19.1682	23.7051
123	H	16.6035	18.7181	23.4739
124	H	15.8095	20.0402	24.357
125	C	12.1933	18.0212	24.4386
126	H	12.2844	17.0494	23.9379
127	C	14.688	18.1739	24.3467
128	H	14.5266	17.3328	23.6386
129	H	15.1685	17.7411	25.2477
130	C	10.7166	14.2839	16.4547
131	C	11.059	12.9488	16.278

132	H	11.9201	12.7068	15.6452
133	C	12.3483	16.1468	16.7914
134	H	11.7366	16.6051	17.5928
135	H	12.8894	16.9724	16.3002
136	C	11.5043	15.3712	15.8098
137	H	12.1657	14.945	15.0335
138	H	10.8334	16.0884	15.3004
139	C	16.065	14.9847	23.5388
140	H	17.0449	14.5102	23.7352
141	H	16.2243	16.0731	23.5973
142	C	17.7513	11.2164	14.1577
143	H	17.6548	11.3726	13.069
144	H	18.6646	11.7658	14.468
145	C	17.8774	9.7623	14.4483
146	C	20.6981	16.4545	13.6901
147	H	19.9102	17.2394	13.7385
148	H	21.6671	16.9725	13.8274
149	C	22.0175	17.034	10.7605
150	H	22.9034	16.5416	11.1763
151	C	20.7613	16.6802	11.2441
152	C	22.1633	18.0202	9.7999
153	H	23.1645	18.3139	9.4687
154	C	20.6262	15.7152	12.3716
155	H	21.4239	14.9522	12.3293
156	H	19.6588	15.1808	12.3212
157	C	19.6454	17.3295	10.7255
158	H	18.6505	17.0799	11.116
159	C	23.311	20.706	11.6821
160	C	11.9818	20.5184	25.593
161	H	11.906	21.516	26.0366
162	C	10.8336	19.7918	25.3194
163	H	9.8499	20.2167	25.5383
164	C	10.9452	18.5372	24.7431
165	H	10.0483	17.9541	24.5117
166	C	12.1123	21.4616	20.8447
167	H	13.106	21.8995	21.0322
168	C	11.4624	20.7993	21.8693
169	H	11.9354	20.7206	22.8546
170	C	13.6282	21.6711	18.1454
171	H	14.2635	21.5646	19.0486
172	H	14.1629	22.3214	17.4327
173	C	11.5526	21.5325	19.5706
174	C	12.2703	22.2419	18.4728
175	H	12.4347	23.3011	18.757
176	H	11.6467	22.261	17.5612
177	C	10.3279	20.9145	19.348

178	H	9.894	20.9443	18.3421
179	C	10.2363	20.1957	21.6364
180	H	9.7359	19.664	22.4524
181	C	13.311	26.501	18.356
182	H	13.0713	26.7087	19.4061
183	C	17.0725	28.7367	21.6667
184	C	18.3556	28.0415	21.3826
185	H	18.4696	27.9005	20.29
186	H	19.2141	28.6539	21.7154
187	C	14.8601	29.4012	20.9632
188	H	14.0855	29.4177	20.1901
189	C	16.8372	29.338	22.8979
190	H	17.625	29.3145	23.6598
191	C	16.0718	28.7851	20.7023
192	H	16.2564	28.3274	19.7242
193	C	24.3479	28.5226	16.3418
194	H	25.2956	28.134	16.7312
195	C	24.3503	29.4873	15.3452
196	H	25.2957	29.8559	14.9376
197	C	21.9507	29.4955	15.3684
198	H	20.9972	29.8725	14.9814
199	C	23.1503	28.0499	16.8506
200	H	23.1444	27.2792	17.6356
201	C	23.1476	29.9741	14.8619
202	H	23.1417	30.7289	14.0699
203	C	9.2758	12.262	17.727
204	H	8.7183	11.4741	18.2437
205	C	9.6461	14.5893	17.2882
206	H	9.3734	15.64	17.4485
207	C	8.931	13.5896	17.9227
208	H	8.1088	13.8487	18.5977
209	C	10.3416	11.9421	16.9027
210	H	10.6379	10.8983	16.7638
211	C	10.901	16.431	20.4175
212	H	10.0849	17.0843	20.0605
213	H	11.2197	15.7804	19.5839
214	C	10.4753	15.6141	21.6165
215	H	11.3459	15.0178	21.9495
216	H	10.241	16.3108	22.4457
217	C	29.0257	23.0661	14.6458
218	H	29.5333	22.9448	15.6109
219	C	24.5278	25.9201	20.9162
220	H	24.1491	26.8627	20.4847
221	H	24.8124	26.1316	21.9637
222	C	25.7212	25.4574	20.1548
223	C	23.4069	24.9033	20.9402

224	H	22.5436	25.2814	21.5155
225	H	23.7343	23.9567	21.3993
226	C	26.5466	24.4684	20.6778
227	H	26.3241	24.0511	21.6688
228	C	27.0726	25.4733	18.153
229	H	27.2631	25.8567	17.1448
230	C	25.996	25.9471	18.8841
231	H	25.3309	26.7087	18.4577
232	C	27.8924	24.4938	18.6895
233	H	28.7391	24.1089	18.1122
234	C	27.6224	23.9884	19.9515
235	H	28.2533	23.1979	20.368
236	C	19.272	21.5957	25.9118
237	C	18.5107	21.2007	23.5754
238	H	17.7254	21.4392	22.8137
239	H	18.4761	20.1068	23.7416
240	C	20.4783	22.2809	26.0131
241	H	20.6607	23.1246	25.3361
242	C	18.2786	21.9542	24.8654
243	H	18.3111	23.0392	24.6543
244	H	17.256	21.7156	25.2127
245	C	19.0024	23.957	11.7644
246	H	18.8394	22.88	11.944
247	H	18.0991	24.3703	11.2865
248	C	20.2311	24.173	10.9204
249	H	21.0998	23.7563	11.4757
250	H	20.452	25.2507	10.8255
251	C	25.9148	16.9448	16.4912
252	C	28.1517	18.4718	17.1709
253	H	29.0242	19.0758	17.4379
254	C	23.4007	16.7526	16.4978
255	H	23.3359	17.0072	17.5755
256	H	22.5695	16.0609	16.2718
257	C	9.6715	20.2508	20.373
258	H	8.7123	19.7614	20.1746
259	C	24.7227	16.1216	16.1404
260	H	24.7393	15.8895	15.0603
261	H	24.773	15.146	16.6664
262	C	26.0787	17.4334	17.7829
263	H	25.3085	17.238	18.5416
264	C	18.8948	10.9481	23.5267
265	H	19.8892	10.8979	24.005
266	H	18.1642	10.5127	24.2339
267	C	18.516	12.4051	23.3414
268	H	18.5623	12.9324	24.3107
269	H	17.4889	12.5001	22.9496

270	C	18.9003	10.162	22.2613
271	C	18.8787	8.8201	19.8183
272	H	18.8625	8.3058	18.852
273	C	17.7665	9.4769	21.843
274	H	16.865	9.4981	22.4696
275	C	20.0246	10.1575	21.4403
276	H	20.9156	10.7095	21.7585
277	C	20.0141	9.5022	20.2222
278	H	20.8902	9.5434	19.5668
279	C	18.1251	7.0278	14.9763
280	H	18.2401	5.9596	15.1806
281	C	18.2452	9.3139	15.7147
282	H	18.4401	10.0457	16.5109
283	C	18.3687	7.9601	15.9727
284	H	18.6702	7.6261	16.9703
285	C	14.2255	10.9236	19.9394
286	C	15.6274	11.3675	19.7008
287	H	16.0945	11.6725	20.6622
288	H	16.2349	10.5078	19.3613
289	C	15.2948	10.7592	24.7068
290	H	15.936	10.008	25.1797
291	C	14.2741	10.365	23.8565
292	H	14.1122	9.3044	23.6408
293	C	12.5914	17.3925	13.2042
294	C	12.0974	18.4753	13.9273
295	H	12.6585	18.8591	14.792
296	C	15.0198	17.7869	13.2979
297	C	13.9096	16.7935	13.5393
298	C	14.9738	20.917	11.8297
299	C	15.423	21.313	14.2659
300	H	16.2951	20.6271	14.2522
301	H	14.5473	20.7407	14.6259
302	C	16.0603	20.3838	11.1425
303	H	17.0747	20.7223	11.3913
304	C	15.1854	21.9274	12.9021
305	H	14.3236	22.6167	12.9593
306	H	16.071	22.5524	12.6687
307	C	22.4222	14.2514	18.7416
308	H	22.041	14.7495	17.8338
309	H	23.5247	14.2569	18.7045
310	C	15.6315	29.964	23.1609
311	H	15.4643	30.4385	24.132
312	C	14.6353	29.9907	22.1968
313	H	13.6782	30.4748	22.4099
314	C	21.2073	20.8132	27.7672
315	H	21.9669	20.5032	28.4911

316	C	21.4397	21.8928	26.9302
317	H	22.3934	22.4266	26.9753
318	C	20.0113	20.1195	27.6728
319	H	19.8245	19.2571	28.3217
320	C	19.0568	20.5047	26.7464
321	H	18.1206	19.9415	26.6544
322	C	13.6985	20.4681	11.5083
323	H	12.8369	20.868	12.0547
324	C	13.5061	19.513	10.5238
325	H	12.4947	19.1561	10.3069
326	C	14.5961	18.9921	9.8438
327	H	14.4509	18.2338	9.0695
328	C	15.8736	19.4291	10.1575
329	H	16.7425	19.0127	9.6364
330	C	10.1912	18.6171	12.4711
331	H	9.2552	19.1013	12.1787
332	C	10.6655	17.5302	11.7551
333	H	10.1018	17.1502	10.8979
334	C	10.909	19.0831	13.5628
335	H	10.5386	19.9333	14.1436
336	C	11.8569	16.9272	12.1215
337	H	12.2455	16.079	11.5474
338	C	12.6718	26.4331	16.0457
339	H	11.9236	26.5883	15.263
340	C	14.872	25.7412	16.7099
341	H	15.8651	25.3496	16.4463
342	C	12.3649	26.7139	17.3678
343	H	11.374	27.0944	17.6351
344	C	13.9278	25.9474	15.7198
345	H	14.1802	25.7094	14.6821
346	C	17.6237	8.817	13.4609
347	H	17.3315	9.1597	12.4631
348	C	17.7455	7.4619	13.7179
349	H	17.5467	6.7364	12.9236
350	C	14.7046	13.0748	24.3657
351	C	13.462	11.321	23.2671
352	H	12.6763	11.0179	22.5657
353	C	15.5098	12.1062	24.953
354	H	16.332	12.4228	25.6068
355	C	13.6745	12.6621	23.5282
356	H	13.0562	13.4276	23.0428
357	H	16.8602	8.2658	20.3106
358	C	19.6442	22.252	9.4105
359	H	19.3313	21.6734	10.2913
360	C	19.5545	21.6817	8.1529
361	H	19.1604	20.6647	8.0516

362 C	20.1287	23.549	9.5719
363 C	20.5218	24.2488	8.4358
364 H	20.8998	25.2711	8.5531
365 C	21.8736	12.8472	18.8607
366 H	20.7736	12.9034	19.0098
367 H	22.275	12.3813	19.7809
368 C	22.8514	26.3753	10.9269
369 H	22.3309	26.6473	10.0025
370 C	24.3699	24.9511	12.1179
371 H	25.0447	24.0871	12.142
372 C	22.6438	27.1079	12.0852
373 H	21.9502	27.9548	12.085
374 C	19.7872	18.3149	9.7611
375 H	18.8996	18.8393	9.386
376 C	21.0459	18.6686	9.2991
377 H	21.1526	19.4747	8.5654
378 C	25.1405	20.676	10.1034
379 H	25.5434	20.952	9.1239
380 C	25.3887	19.6092	12.232
381 H	25.9892	19.0502	12.9588
382 C	25.9133	19.9459	10.9929
383 H	26.932	19.6519	10.7261
384 C	23.8518	21.0498	10.4479
385 H	23.2333	21.6166	9.74
386 C	24.1026	19.9889	12.5736
387 H	23.7157	19.7198	13.5642
388 C	11.6166	10.0276	20.4076
389 H	10.593	9.6776	20.5773
390 C	13.984	9.6489	20.4464
391 H	14.8407	8.9979	20.6601
392 C	12.6969	9.2	20.6791
393 H	12.5332	8.1911	21.0711
394 C	13.1338	11.7421	19.6715
395 H	13.2861	12.7468	19.2559
396 C	11.842	11.297	19.9022
397 H	10.9957	11.9471	19.6553
398 C	20.438	23.6784	7.1768
399 H	20.7446	24.2527	6.2976
400 C	19.9518	22.3895	7.0306
401 H	19.8775	21.9357	6.0388
402 C	21.0714	19.97	12.5471
403 H	21.4823	19.5298	13.473
404 H	20.9632	19.1731	11.7954
405 C	27.9908	18.0125	15.8746
406 H	28.7338	18.2577	15.1098
407 C	27.1875	18.185	18.123

408	H	27.2733	18.5814	19.1381
409	C	26.8789	17.2557	15.5402
410	H	26.7424	16.9008	14.5128
411	C	22.1795	12.0039	17.6721
412	C	22.7737	10.45	15.4292
413	H	23.0073	9.8463	14.5473
414	C	23.4976	11.7051	17.34
415	H	24.3068	12.0897	17.9713
416	C	21.4573	10.7354	15.75
417	H	20.643	10.3438	15.1294
418	C	23.7959	10.9383	16.2282
419	H	24.8393	10.7204	15.9799
420	C	21.1634	11.5105	16.8606
421	H	20.1202	11.7486	17.1099
422	C	23.9049	19.9001	21.8192
423	H	22.9168	19.6763	22.2563
424	H	24.6735	19.375	22.4125
425	C	24.1564	21.3944	21.8061
426	H	23.2177	21.9033	21.5156
427	H	24.8867	21.6326	21.0022
428	C	24.6623	21.8927	23.1139
429	C	25.6501	22.7693	25.5738
430	H	26.0402	23.1171	26.5347
431	C	25.9577	21.5768	23.5175
432	H	26.5865	20.9708	22.8548
433	C	24.3593	23.0865	25.1859
434	H	23.7182	23.68	25.846
435	C	26.4502	22.0082	24.7348
436	H	27.4693	21.7485	25.0375
437	C	23.867	22.6505	23.9652
438	H	22.8369	22.8843	23.6629
439	C	21.2198	16.3549	25.2438
440	C	21.144	14.9672	25.2727
441	H	21.4894	14.4004	24.3998
442	C	21.7429	17.06	24.0372
443	H	21.8849	16.3235	23.2234
444	H	22.7409	17.4906	24.2497
445	C	20.139	15.0272	27.4521
446	H	19.708	14.5122	28.3151
447	C	20.6097	14.3055	26.3667
448	H	20.5468	13.213	26.3608
449	C	20.2158	16.4109	27.4332
450	H	19.8424	16.9914	28.2834
451	C	20.748	17.069	26.3379
452	H	20.7787	18.1648	26.3282
453	C	20.8631	18.1765	23.5297

454 H	21.2158	18.5304	22.5451
455 H	20.8555	19.0493	24.2088
456 C	9.4467	13.3412	21.4232
457 H	10.4277	12.9136	21.6633
458 C	8.3636	12.5093	21.1937
459 H	8.4939	11.4244	21.2572
460 C	9.3139	14.7217	21.3507
461 C	8.0677	15.251	21.0298
462 H	7.9501	16.3384	20.9608
463 C	7.1249	13.0477	20.8885
464 H	6.2685	12.3917	20.7093
465 C	6.981	14.4251	20.8038
466 H	6.0087	14.8597	20.5539
467 H	14.0808	15.8827	12.9387
468 H	13.9541	16.4674	14.6021
469 H	15.0327	18.1238	12.2478
470 H	14.8974	18.6735	13.9403