Can Mixed-Metal Surfaces Provide an Additional Enhancement to SERS?

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Supplementary Raman Spectra

We plot the comparison between the experimental and theoretical Raman spectrum of BPE in Figure 1. We show the comparison in Figure 2 between experimental and calculated spectra of SERS and mixed-metal SERS with clusters of up to 18 metal atoms and BPE (*i.e.,* $Ag_{14}M_4$·BPE, where M={Ag, Pd, Pt}. In the case of pyridine, Figure 3 shows the Raman spectrum of the three layouts: Ag_6M·Py, where M={Ag, Pd, Pt}.

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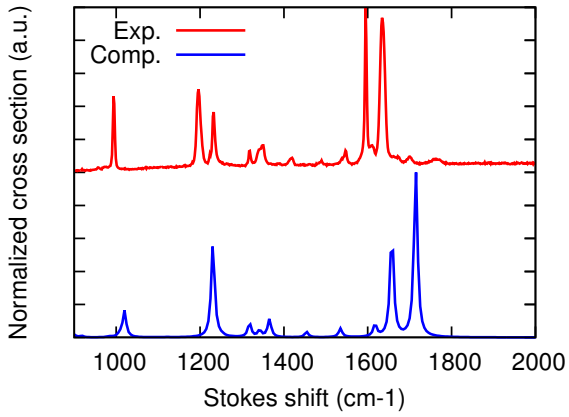

Figure 1: Experimental and computed spectra for BPE at 633 nm.

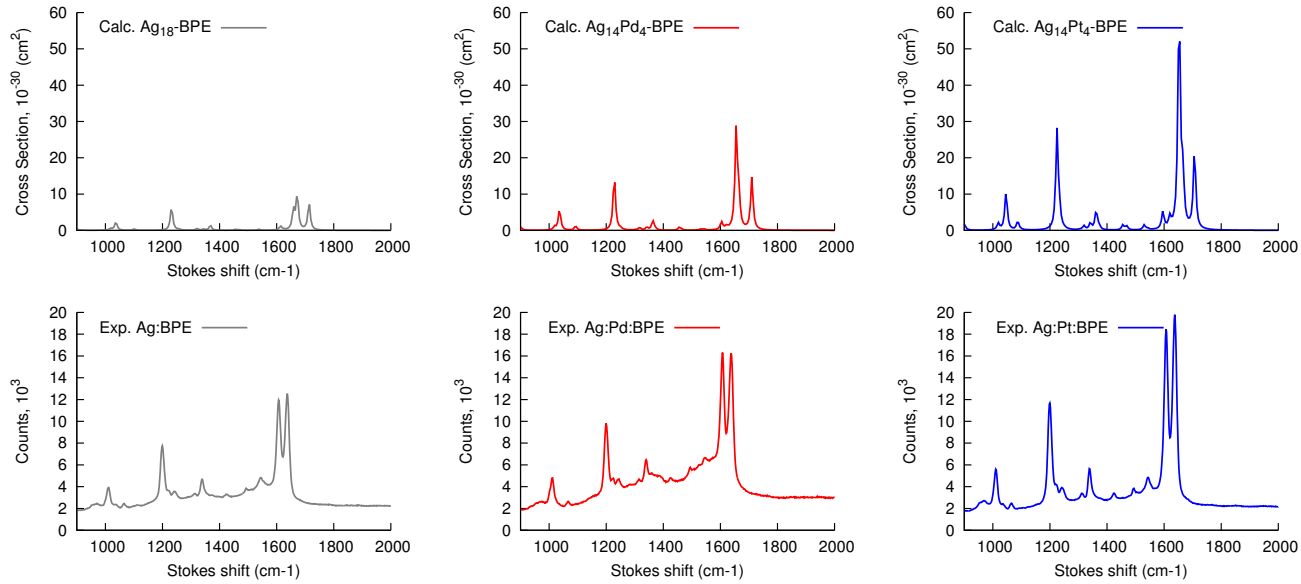

Figure 2: Calculated and experimental SERS spectra. **Top** Raman scattering simulations at 633 nm incident wavelength of BPE bound to $Ag_{14}M_4$ where M is: **left** Ag; **Center** Pd; **Right** Pt. **Bottom** Experimental Raman scattering cross-sections at 633 nm incident wavelength of BPE attached to: **Left** 80 nm Ag substrate; **Center** 80 nm Ag substrate with 1nm Pd layer; **Right** 80 nm Ag substrate with 1nm Pt layer.

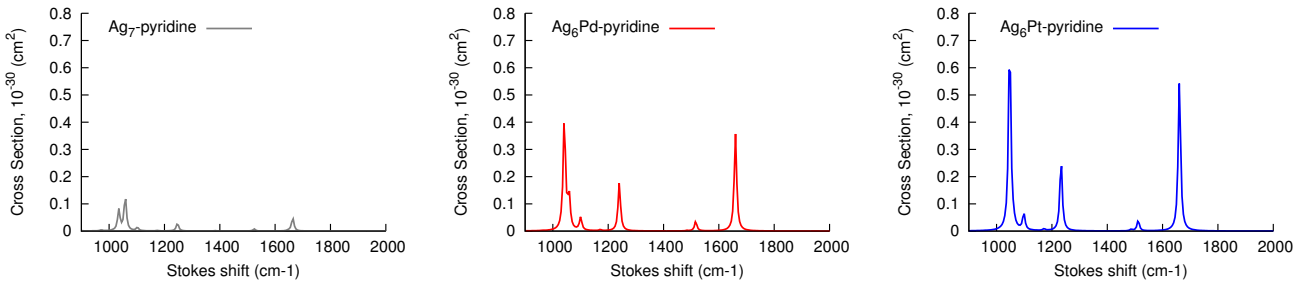

Figure 3: Calculated Raman spectra at 633 nm excitation wavelength for gold-containing clusters: $Ag_6M{\cdot}Py$. M is: **Left** Ag; **Center** Pd; and **right** Pt. There is an overall enhancement of the Raman spectra, as we modify the substrate from bare Ag to Pd, and Pt (*i. e.*, from left to right).

System geometries

Metal clusters

Following, we present the geometries of the metal clusters used to obtain the binding energy.

Table 1: Ag_7.

Atom	x	y	z
Ag	-0.0000377	0.9854162	2.1864651
Ag	0.0000282	-1.7748765	1.6129021
Ag	-1.4814373	0.0000642	0.0000306
Ag	-0.0000153	0.4878173	-2.3481398
Ag	0.0000287	2.3838829	-0.2616382
Ag	-0.0000064	-2.0823769	-1.1896511
Ag	1.4814397	0.0000729	0.0000312

Table 2: Ag_6Pd.

Atom	x	y	z
Ag	-0.0331693	-1.4431260	1.9838790
Ag	-0.0333483	-2.3329779	-0.7591728
Pd	-1.2447453	-0.0000648	0.0000403
Ag	-0.0333226	2.3336869	-0.7564394
Ag	-0.0331600	1.4409508	1.9856049
Ag	-0.0333371	0.0016354	-2.4534673
Ag	1.3941198	-0.0001053	-0.0004442

Table 3: Ag_6Pt.

Atom	x	y	z
Ag	0.0432406	0.7207105	2.3832266
Ag	0.0430201	-2.0438965	1.4218547
Pt	-1.0018777	0.0001079	-0.0000226
Ag	0.0432152	0.8177114	-2.3517255
Ag	0.0432435	2.4893768	0.0510291
Ag	0.0431627	-1.9838477	-1.5044045
Ag	1.5959869	-0.0002497	0.0000604

Table 4: Au_7.

Atom	x	y	z
Au	-0.0028539	1.6515915	1.7221441
Au	-0.0015080	-1.1277486	2.1028645
Au	-1.5392736	-0.0003518	0.0002373
Au	-0.0069224	-0.3231396	-2.3640922
Au	0.0059561	2.1483539	-1.0382623
Au	0.0051831	-2.3484526	-0.4231924
Au	1.5394187	-0.0002527	0.0003010

Table 5: Au_6Pd.

Atom	x	y	z
Au	-0.1094141	-0.9877790	2.2362752
Au	-0.1087515	-2.4321631	-0.2481716
Pd	-1.3937139	0.0000939	0.0000599
Au	-0.1092229	2.1133890	-1.2287393
Au	-0.1085127	1.8217261	1.6308597
Au	-0.1090349	-0.5151002	-2.3901690
Au	1.2977976	-0.0001236	-0.0000873

Table 6: Au_6Pt.

Atom	x	y	z
Au	-0.0616127	0.6456741	2.3937232
Au	-0.0604815	-2.0765803	1.3547722
Pt	-1.1746187	-0.0001335	-0.0023203
Au	-0.0595032	0.8839566	-2.3178806
Au	-0.0592394	2.4758709	0.1256846
Au	-0.0582807	-1.9293728	-1.5577357
Au	1.4624653	0.0005838	0.0037343

BPE clusters

We provide the geometries of BPE and BPE attached with metal clusters.

Table 7: BPE.

Atom	x	y	z
C	-0.1920659	1.9210033	0.0109416
C	-0.4585209	0.4879194	0.0148347
C	0.4573152	-0.4877191	0.0122478
C	0.1914327	-1.9208602	0.0096643
C	1.0109379	-4.1771248	-0.1231533
C	1.2559476	-2.8135478	-0.1129178
C	-1.0815515	-2.4837106	0.1256654
C	-1.2178804	-3.8592491	0.1055578
N	-0.2004739	-4.7088696	-0.0169428
H	-1.5125428	0.2239617	0.0035216
H	1.5111611	-0.2232855	-0.0048914
H	1.8364136	-4.8771922	-0.2209701
H	2.2716967	-2.4444607	-0.2036699
H	-1.9633368	-1.8653297	0.2399800
H	-2.2042712	-4.3062664	0.1956077
C	1.0812219	2.4831357	0.1267513
C	-1.2560458	2.8141527	-0.1129859
C	-1.0102507	4.1775869	-0.1237688
N	0.2014797	4.7086690	-0.0177968
C	1.2183435	3.8586138	0.1058873
H	1.9625475	1.8641193	0.2412522
H	-2.2719810	2.4455763	-0.2036218
H	-1.8352600	4.8781046	-0.2222895
H	2.2048997	4.3051727	0.1963755

Pyridine clusters

We provide the geometries of pyridine attached with metal clusters.

Table 8: Ag_7·BPE.

Atom	x	y	z
C	-8.8332529	-0.1996544	-0.0030354
C	-7.3848795	-0.3626033	-0.0066235
C	-6.4756388	0.6194832	-0.0106573
C	-5.0290833	0.4507041	-0.0130224
C	-2.8351554	1.4361021	0.0302225
C	-4.2097592	1.5794821	0.0300632
C	-4.3813890	-0.7867757	-0.0576841
C	-3.0031150	-0.8350069	-0.0543092
N	-2.2309786	0.2518172	-0.0109507
H	-7.0481373	-1.3957269	-0.0005069
H	-6.8108230	1.6527333	-0.0063891
H	-2.1853640	2.3046581	0.0645633
H	-4.6450417	2.5715926	0.0647896
H	-4.9372169	-1.7147874	-0.0983538
H	-2.4829149	-1.7867634	-0.0886888
C	-9.4844810	1.0350694	-0.0416883
C	-9.6459342	-1.3319312	0.0404332
C	-11.0239693	-1.1868244	0.0456998
N	-11.6399196	-0.0120235	0.0101545
C	-10.8664989	1.0703754	-0.0329453
H	-8.9311872	1.9652333	-0.0811013
H	-9.2047165	-2.3221479	0.0709319
H	-11.6635259	-2.0646221	0.0801294
H	-11.3836801	2.0254669	-0.0631312
Ag	1.8209288	2.2458146	-0.6629222
Ag	1.7666938	1.3038228	1.9634939
Ag	0.1212219	0.0780705	-0.0044318
Ag	1.5075265	-2.2589872	-0.8010367
Ag	1.7082504	0.0406037	-2.3718815
Ag	1.5731050	-1.4807791	1.8782619
Ag	3.2120690	-0.1369614	0.0073489

Table 9: Ag_6Pd·BPE.

Atom	x	y	z
C	-8.4382946	-0.1708251	-0.0045432
C	-6.9920354	-0.3441112	-0.0048278
C	-6.0754587	0.6325156	-0.0009541
C	-4.6322956	0.4571052	-0.0003273
C	-2.4301190	1.4324052	0.0229646
C	-3.8025691	1.5785497	0.0215709
C	-3.9868648	-0.7822971	-0.0204590
C	-2.6111331	-0.8426020	-0.0177167
N	-1.8219446	0.2417512	0.0030653
H	-6.6618057	-1.3793462	-0.0050890
H	-6.4053181	1.6676697	0.0050823
H	-1.7781037	2.2959693	0.0411670
H	-4.2283694	2.5752079	0.0382437
H	-4.5443972	-1.7099474	-0.0395852
H	-2.0981701	-1.7953456	-0.0322987
C	-9.0816025	1.0689119	-0.0274346
C	-9.2607599	-1.2971550	0.0194841
C	-10.6374375	-1.1419319	0.0215750
N	-11.2456249	0.0375471	0.0008101
C	-10.4631904	1.1142286	-0.0234528
H	-8.5216310	1.9956517	-0.0501616
H	-8.8271448	-2.2910624	0.0373080
H	-11.2832412	-2.0157284	0.0408380
H	-10.9728040	2.0737920	-0.0413742
Ag	1.7551237	2.2656813	-0.7876201
Ag	1.6674000	1.4236421	1.9514484
Pd	0.2849934	0.0696262	-0.0005752
Ag	1.3857259	-2.3542233	-0.7212534
Ag	1.5443666	-0.0663678	-2.4362761
Ag	1.4380537	-1.4316698	1.9921581
Ag	2.9664195	-0.1450719	0.0032345

Table 10: Ag_6Pt·BPE.

Atom	x	y	z
C	-8.3960658	-0.1721206	-0.0063984
C	-6.9508730	-0.3481609	-0.0086484
C	-6.0318635	0.6276001	-0.0058371
C	-4.5911722	0.4516654	-0.0065735
C	-2.3869872	1.4291168	0.0143981
C	-3.7572864	1.5709983	0.0135686
C	-3.9439948	-0.7879115	-0.0259917
C	-2.5711927	-0.8550295	-0.0241337
N	-1.7779630	0.2329979	-0.0046724
H	-6.6224918	-1.3840071	-0.0093134
H	-6.3610057	1.6630090	0.0004886
H	-1.7310972	2.2880973	0.0315695
H	-4.1797729	2.5690196	0.0296603
H	-4.5008805	-1.7159303	-0.0437505
H	-2.0554803	-1.8048007	-0.0378334
C	-9.0373899	1.0689626	-0.0285030
C	-9.2213832	-1.2967281	0.0188346
C	-10.5975969	-1.1386168	0.0228410
N	-11.2036844	0.0420970	0.0028459
C	-10.4187939	1.1170432	-0.0225874
H	-8.4758455	1.9947281	-0.0521530
H	-8.7899164	-2.2915918	0.0360983
H	-11.2451180	-2.0111473	0.0430717
H	-10.9263794	2.0777131	-0.0398829
Ag	1.7144689	2.2662333	-0.7938508
Ag	1.6173396	1.4269161	1.9554559
Pt	0.2577820	0.0642282	-0.0029437
Ag	1.3347190	-2.3707616	-0.7179060
Ag	1.5015554	-0.0780060	-2.4413605
Ag	1.3800755	-1.4379496	2.0018349
Ag	2.9521745	-0.1568480	0.0083530

Table 11: Ag_{18}·BPE .

Atom	x	y	z
Ag	-0.1934921	-2.8144949	-0.4942414
Ag	-1.4887110	-0.4640262	-1.2623737
Ag	1.2979576	-0.6063242	-1.3357114
Ag	-0.0308425	-0.5936136	1.1756115
Ag	-2.7740990	1.9054651	-2.1684266
Ag	0.0162002	1.9990901	-2.1933944
Ag	2.7800771	1.6159062	-2.3091850
Ag	-1.3474572	1.8493565	0.3250891
Ag	1.4825832	1.7040701	0.2540065
Ag	0.1270947	1.7311607	2.7597745
Ag	3.7023323	-0.0292234	-0.0956758
Ag	2.5614965	0.3447042	2.4846982
Ag	-2.4461596	0.5962655	2.6080831
Ag	-3.7543786	0.3616750	0.0930080
Ag	1.4547071	3.2308207	-4.1678697
Ag	-1.3848040	3.3784841	-4.0969475
Ag	1.5661614	1.0802576	4.9948569
Ag	-1.2580264	1.2211091	5.0634825
C	0.6380342	-7.2021774	-1.1389962
C	0.6758990	-5.8269183	-1.0642939
N	-0.3338878	-5.0888504	-0.5941499
C	-1.4257105	-5.7310243	-0.1801645
C	-1.5480207	-7.1056499	-0.2186834
C	-0.5009058	-7.8883902	-0.7078570
C	-0.6481341	-9.3358087	-0.7404153
C	0.2626798	-10.2091023	-1.1871424
C	0.1256807	-11.6593791	-1.2239820
C	-1.0196493	-13.7323329	-0.8573338
C	-0.9994430	-12.3525237	-0.7733729
C	1.1699642	-12.4275422	-1.7367710
C	1.0489817	-13.8074516	-1.7765098
N	-0.0215279	-14.4633949	-1.3476932
H	1.4992990	-7.7260069	-1.5325039
H	1.5542639	-5.2831692	-1.3943020
H	-2.2344675	-5.1149449	0.1975158
H	-2.4618016	-7.5698508	0.1329571
H	-1.5965902	-9.7040766	-0.3607161
H	1.2097518	-9.8376226	-1.5690472
H	-1.8890412	-14.2833852	-0.5097751
H	-1.8554179	-11.8346322	-0.3588327
H	2.0726264	-11.9512565	-2.1033014
H	1.8578018	-14.4138531	-2.1746765

Table 12: $Ag_{14}Pd_4$·BPE.

Atom	x	y	z
Pd	-0.0789862	-1.4128522	1.2309374
Pd	0.8957397	-1.1292430	-1.3416993
Pd	-0.4087719	1.1603560	2.0585550
Pd	-0.9535000	0.7194897	-0.5750261
Ag	3.4935288	-0.6037001	-1.7160428
Ag	1.8257297	0.8046523	0.4378419
Ag	1.7082665	2.5666852	2.9120917
Ag	1.1200767	1.5438447	-2.1991575
Ag	0.2547188	3.1522789	0.1177705
Ag	-1.5008008	2.8057701	-2.1925278
Ag	-0.8208312	3.8095018	2.6799333
Ag	-2.5186642	2.5397457	0.7323446
Ag	-1.1122748	-0.0394629	-3.1592345
Ag	1.5683235	-0.7453154	-3.8908398
Ag	1.8241261	-0.2391483	2.9931514
Ag	2.7031337	-1.8166269	0.6943072
Ag	-2.6507399	-0.3014438	1.2300465
Ag	-3.4741389	0.9369675	-1.4959270
C	-0.6148193	-5.6798627	1.8963237
C	-0.3688074	-4.3290024	1.9991095
N	-0.2849837	-3.5093022	0.9423627
C	-0.4493434	-4.0545022	-0.2680895
C	-0.6941204	-5.4000818	-0.4563416
C	-0.7861565	-6.2622755	0.6367363
C	-1.0451455	-7.6757087	0.4139762
C	-1.1806259	-8.6144762	1.3594397
C	-1.4413765	-10.0306993	1.1392438
C	-1.8195049	-11.9761203	-0.2108748
C	-1.5712177	-10.6191841	-0.1208109
C	-1.5742587	-10.8788250	2.2384947
C	-1.8231173	-12.2270086	2.0387515
N	-1.9467515	-12.7830549	0.8400757
H	-0.6643926	-6.2683434	2.8035400
H	-0.2277913	-3.8666535	2.9691963
H	-0.3793991	-3.3717798	-1.1100759
H	-0.8141526	-5.7783674	-1.4649644
H	-1.1348480	-7.9594078	-0.6308038
H	-1.0973968	-8.3288068	2.4045620
H	-1.9219406	-12.4435763	-1.1864142
H	-1.4801444	-10.0362468	-1.0289874
H	-1.4841770	-10.4875997	3.2459749
H	-1.9280217	-12.8929546	2.8910352

Table 13: $Ag_{14}Pt_4$·BPE.

Atom	x	y	z
Pt	0.6394475	-1.5432638	1.1351692
Pt	1.0685767	-0.0958891	-1.1274877
Pt	0.5273117	1.0611911	1.2996897
Pt	-1.3971877	-0.3460276	-0.0224343
Ag	3.4085448	0.5083400	-2.3601756
Ag	3.0796450	1.1936415	0.3533106
Ag	2.3449512	1.9471527	3.0430751
Ag	-1.2154984	1.1345371	-2.3622363
Ag	-1.0187524	2.8839474	-0.0326060
Ag	-3.4067844	1.3992121	-0.4467443
Ag	-0.3111708	3.1228924	2.9304199
Ag	-2.1035537	1.0963256	2.2269538
Ag	-0.6987235	-1.7254515	-2.4079236
Ag	1.0626320	0.0290100	-3.8295142
Ag	1.5527720	3.6799051	0.8600645
Ag	1.3181666	2.5296025	-1.6815328
Ag	-3.7910278	-0.9432231	1.1317225
Ag	-3.3608301	-1.1907394	-1.7137352
C	1.7143400	-5.6863908	1.3330709
C	1.6955349	-4.3122629	1.3283601
N	0.5902564	-3.5910469	1.0708539
C	-0.5359662	-4.2647385	0.7928351
C	-0.5896935	-5.6420461	0.7742989
C	0.5469672	-6.4047362	1.0512748
C	0.4621900	-7.8540464	1.0289831
C	1.4588475	-8.7113404	1.2898832
C	1.3743647	-10.1647968	1.2698929
C	0.2585013	-12.2629437	0.9451231
C	0.2247851	-10.8812021	0.9278076
C	2.4980535	-10.9189628	1.6086389
C	2.4262102	-12.3023451	1.5946349
N	1.3318712	-12.9798982	1.2706804
H	2.6481117	-6.1883506	1.5513807
H	2.5938572	-3.7413894	1.5307734
H	-1.4033068	-3.6534092	0.5783771
H	-1.5304708	-6.1277920	0.5419454
H	-0.5190950	-8.2461694	0.7764915
H	2.4386794	-8.3203084	1.5503238
H	-0.6305679	-12.8287900	0.6803373
H	-0.6918942	-10.3777577	0.6464985
H	3.4247462	-10.4270141	1.8832100
H	3.2981820	-12.8948145	1.8583911

Table 14: Au_7·BPE.

Atom	x	y	z
C	-9.4360356	-0.1496203	-0.0038725
C	-7.9878594	-0.3126048	-0.0078771
C	-7.0779340	0.6692687	-0.0165683
C	-5.6328724	0.4966494	-0.0183449
C	-3.4366717	1.4806588	0.0234131
C	-4.8094506	1.6231115	0.0211688
C	-4.9882632	-0.7430758	-0.0582844
C	-3.6122318	-0.8004961	-0.0535798
N	-2.8405863	0.2895665	-0.0126682
H	-7.6515987	-1.3458782	0.0024189
H	-7.4113401	1.7029044	-0.0162253
H	-2.7820227	2.3438478	0.0549841
H	-5.2403053	2.6170079	0.0517799
H	-5.5455664	-1.6700173	-0.0964128
H	-3.0920144	-1.7507518	-0.0842242
C	-10.0864777	1.0850623	-0.0527823
C	-10.2478227	-1.2819146	0.0512186
C	-11.6259448	-1.1366346	0.0579779
N	-12.2411689	0.0380759	0.0129485
C	-11.4685004	1.1203967	-0.0417062
H	-9.5333608	2.0148302	-0.1023536
H	-9.8064658	-2.2717581	0.0898331
H	-12.2657497	-2.0137539	0.1017172
H	-11.9860785	2.0749044	-0.0798332
Au	1.0897920	2.2592973	-0.6497059
Au	1.1342956	1.2881974	1.9430607
Au	-0.6265708	0.1148861	-0.0017312
Au	0.7133290	-2.2339640	-0.8126533
Au	1.1214091	0.0523753	-2.3275671
Au	0.8930423	-1.4737365	1.8453181
Au	2.6457604	-0.1641179	0.0097109

Table 15: Au_6Pd·BPE.

Atom	x	y	z
C	-9.0846325	-0.0926870	-0.0261631
C	-7.6387335	-0.2728291	-0.0272064
C	-6.7173914	0.6986415	-0.0349363
C	-5.2746369	0.5128147	-0.0345682
C	-3.0668587	1.4747387	-0.0240892
C	-4.4384437	1.6295193	-0.0256621
C	-4.6392812	-0.7316777	-0.0424799
C	-3.2639207	-0.8023943	-0.0403623
N	-2.4717322	0.2785315	-0.0315320
H	-7.3140127	-1.3097868	-0.0175264
H	-7.0404135	1.7357876	-0.0392809
H	-2.4079489	2.3331642	-0.0157600
H	-4.8578964	2.6288572	-0.0192638
H	-5.2036537	-1.6552018	-0.0514541
H	-2.7566334	-1.7582257	-0.0453975
C	-9.7212660	1.1499479	-0.0603839
C	-9.9113584	-1.2152099	0.0105934
C	-11.2874845	-1.0535237	0.0134309
N	-11.8894450	0.1287068	-0.0181685
C	-11.1027107	1.2017828	-0.0545285
H	-9.1569227	2.0737199	-0.0932995
H	-9.4822361	-2.2108422	0.0375791
H	-11.9375338	-1.9238124	0.0425141
H	-11.6081594	2.1632670	-0.0811486
Au	1.1284483	2.2719198	-0.8128337
Au	1.0027870	1.4617001	1.9405191
Pd	-0.3813848	0.0936211	-0.0166427
Au	0.7221472	-2.3531693	-0.6952618
Au	0.9323295	-0.0840262	-2.4362175
Au	0.7495833	-1.3962840	2.0123879
Au	2.3124000	-0.1426961	0.0264995

Table 16: Au_6Pt·BPE.

Atom	x	y	z
C	-8.9714821	-0.0942366	-0.0114380
C	-7.5263912	-0.2773531	-0.0110380
C	-6.6028196	0.6928436	-0.0106559
C	-5.1619809	0.5049264	-0.0093135
C	-2.9523092	1.4671879	0.0133897
C	-4.3217949	1.6190316	0.0109287
C	-4.5266944	-0.7401344	-0.0266490
C	-3.1540973	-0.8184048	-0.0231731
N	-2.3589053	0.2655195	-0.0043315
H	-7.2039301	-1.3150810	-0.0076689
H	-6.9243939	1.7304378	-0.0084415
H	-2.2884449	2.3201006	0.0307240
H	-4.7373804	2.6197277	0.0257117
H	-5.0911067	-1.6633762	-0.0441175
H	-2.6441611	-1.7714065	-0.0350718
C	-9.6055612	1.1499855	-0.0390301
C	-9.8005821	-1.2153979	0.0168128
C	-11.1763379	-1.0509134	0.0182612
N	-11.7757883	0.1327729	-0.0070252
C	-10.9868721	1.2045086	-0.0353144
H	-9.0394882	2.0729085	-0.0652451
H	-9.3734465	-2.2120134	0.0383561
H	-11.8282289	-1.9200073	0.0408006
H	-11.4903994	2.1671212	-0.0568962
Au	1.1197379	2.2913144	-0.8000731
Au	1.0163072	1.4486474	1.9663025
Pt	-0.3295940	0.0842613	-0.0017764
Au	0.7141748	-2.3660355	-0.7252844
Au	0.8982397	-0.0630720	-2.4541331
Au	0.7624646	-1.4317393	2.0113423
Au	2.3523032	-0.1501856	0.0113697

Table 17: Ag_7·Py.

Atom	x	y	z
Ag	0.5229397	0.5995725	2.2976440
Ag	0.4845818	-2.0011371	1.2809694
Ag	-1.0522591	0.0076908	-0.0004484
Ag	0.5235558	0.8630565	-2.2117439
Ag	0.4983766	2.3696729	0.1385572
Ag	0.4899878	-1.8384947	-1.5048650
Ag	2.0441986	-0.0101649	0.0005370
C	-5.4829420	-1.1776694	0.0003480
C	-6.1879632	0.0147301	0.0001304
C	-5.4806318	1.2057446	-0.0007570
C	-4.0969725	1.1558352	-0.0020500
N	-3.4159511	0.0120549	-0.0018420
C	-4.0991982	-1.1304570	-0.0011141
H	-5.9915723	-2.1337329	0.0024210
H	-7.2719995	0.0157839	0.0003739
H	-5.9873229	2.1628276	-0.0000565
H	-3.5036463	2.0645966	-0.0038516
H	-3.5075179	-2.0402754	-0.0018672

Table 18: Ag_6Pd·Py.

Atom	x	y	z
Ag	3.0446536	0.6323971	2.3451708
Ag	3.0197869	-2.0553953	1.3574998
Pd	1.7699688	-0.0125670	-0.0008391
Ag	3.0491769	0.8093868	-2.2886711
Ag	3.0962435	2.4027376	0.0930536
Ag	3.0194971	-1.9459549	-1.5091445
Ag	4.4587477	-0.0540478	-0.0004895
C	-2.4393769	-1.1643940	0.0013197
C	-3.1410210	0.0295673	0.0019408
C	-2.4209644	1.2124266	0.0005050
C	-1.0387420	1.1574503	-0.0011930
N	-0.3548967	0.0079379	-0.0014528
C	-1.0565403	-1.1309547	-0.0004367
H	-2.9496959	-2.1194526	0.0022073
H	-4.2248050	0.0379878	0.0034068
H	-2.9162861	2.1753377	0.0007335
H	-0.4421237	2.0603605	-0.0025155
H	-0.4736225	-2.0428234	-0.0010951

Table 19: $Ag_6Pt{\cdot}Py$.

Atom	x	y	z
Ag	0.4946916	0.6614903	2.3532508
Ag	0.4750086	-2.0366055	1.3634058
Pt	-0.7536857	0.0116220	0.0004102
Ag	0.4971701	0.8377680	-2.2961662
Ag	0.5483040	2.4384464	0.0926846
Ag	0.4731269	-1.9270745	-1.5140292
Ag	1.9464474	-0.0268621	-0.0005319
C	-4.8918847	-1.1380881	0.0011665
C	-5.5950171	0.0551682	0.0015829
C	-4.8720486	1.2364226	0.0012507
C	-3.4917526	1.1861093	0.0005121
N	-2.8066453	0.0318819	0.0003566
C	-3.5110096	-1.1108674	0.0004895
H	-5.4006176	-2.0938654	0.0012158
H	-6.6784276	0.0642469	0.0021758
H	-5.3646587	2.2006041	0.0013160
H	-2.8912153	2.0847585	-0.0002176
H	-2.9252934	-2.0193161	-0.0001151