Supplementary Information (SI)

This section includes the optimized geometries of the gold complexes [(μ-1, *n*-$C_2B_{10}H_{10}$){Au(PPh_3)}$_2$], with *n* = {2, 7, 12}. The computational method consists in the B3LYP Hartree-Fock/DFT hybrid method as implemented in the suite of programmes Gaussian03 [1], with the 6-31G* basis set for all atoms except Au, where LANL2DZ pseudopotentials are used for. Also included in this SI are the frontier orbitals in complexes [(μ-1, *n*-$C_2B_{10}H_{10}$){Au(PPh_3)}$_2$], with *n* = {2, 7}.

Figure S1a. Optimized geometry for complex [(μ-1,2-$C_2B_{10}H_{10}$){Au(PPh_3)}$_2$], C_1 symmetry. B3LYP calculations – 6-31G* basis set for all atoms except Au; LANL2DZ pseudopotential for Au atoms.

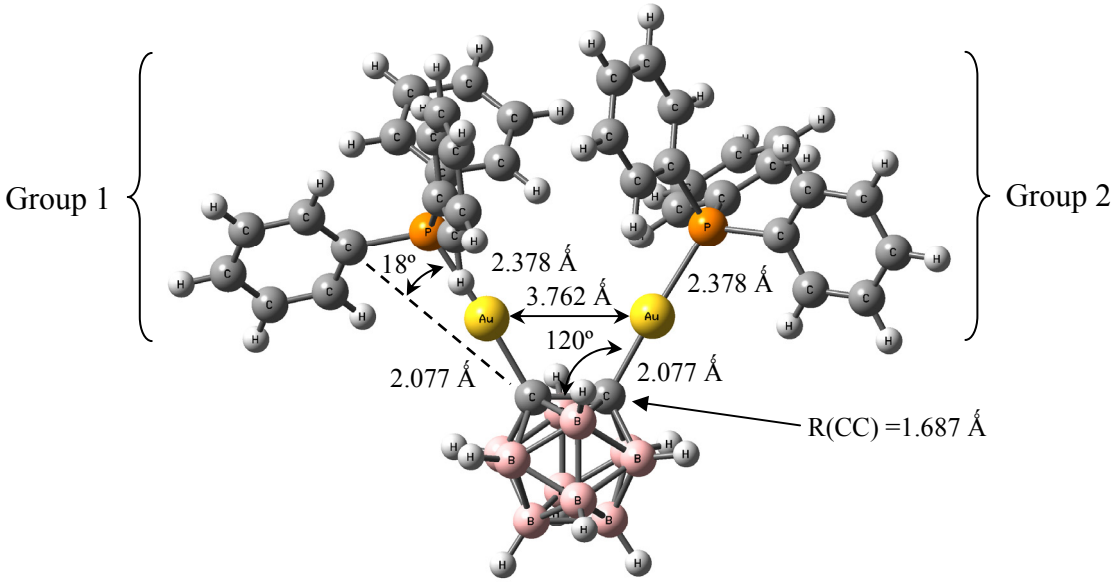
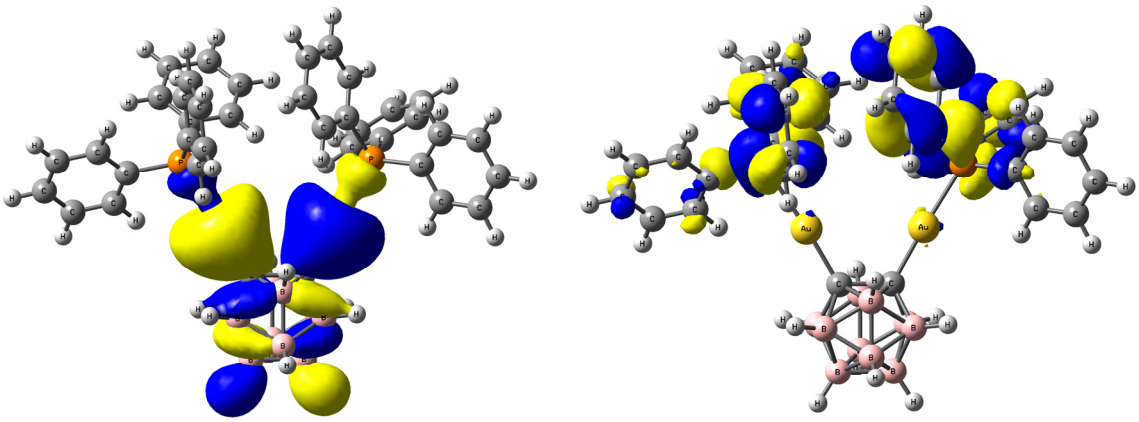


Figure S1b. (a) HOMO and (b) LUMO of [(μ-1,2-$C_2B_{10}H_{10}$){Au(PPh_3)}$_2$] (orbital function isovalue = 0.02). Calculations with the optimized geometry at the B3LYP level – 6-31G* for all atoms, except Au; LANL2DZ pseudopotential for Au.



(a) (b)

Figure S2a. Optimized geometry for complex [(μ-1,7-$C_2B_{10}H_{10}$){Au(PPh_3)}$_2$], C_2 symmetry. B3LYP calculations – 6-31G* basis set for all atoms, except Au; LANL2DZ pseudopotential for Au atoms.

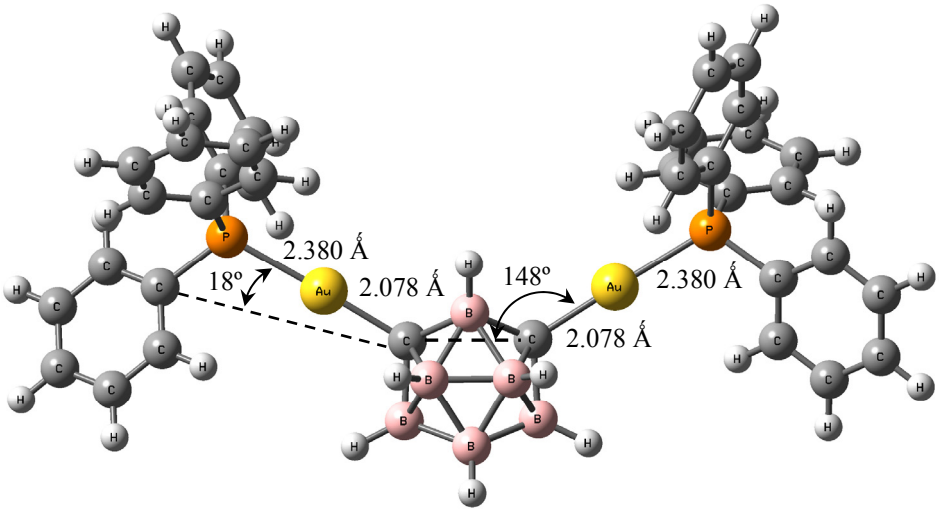
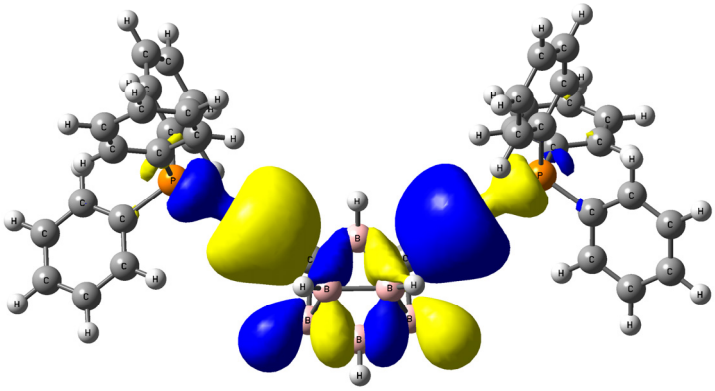


Figure S2b. (a) HOMO and (b) LUMO of [(μ-1,7-$C_2B_{10}H_{10}$){Au(PPh_3)}$_2$] (orbital function isovalue = 0.02). Calculations with the optimized geometry at the B3LYP level – 6-31G* for all atoms, except Au; LANL2DZ pseudopotential for Au.

(a)



(b)

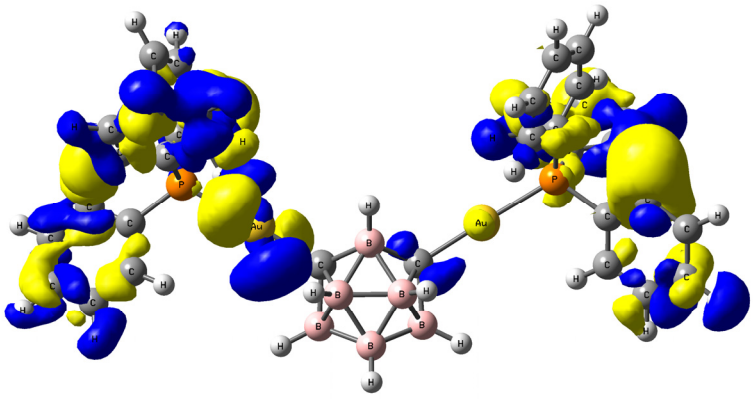


Table S1, Table S2 and Table S3 include the cartesian coordinates (in Å) of the optimized geometries for gold complexes [(μ-1,*n*-$C_2B_{10}H_{10}$){$Au(PPh_3)$}$_2$], with *n* = {2, 7, 12} respectively; B3LYP calculations – 6-31G* basis set for all atoms, except Au; LANL2DZ pseudopotentials are used for Au atoms.

Table S1. Gold Complex [(μ-1,2-$C_2B_{10}H_{10}$){$Au(PPh_3)$}$_2$]

Atom	X	Y	Z
Au	1.895786	1.151363	0.004496
Au	-1.866561	1.134238	0.022353
P	3.181546	-0.847752	0.002975
P	-3.169351	-0.855725	0.000273
C	0.852453	2.946259	0.001102
C	-0.834554	2.936512	0.008681
B	0.013241	3.391655	1.425462
B	1.439326	4.296180	0.876556
B	1.431004	4.288155	-0.891553
B	-0.000289	3.378953	-1.419464
B	-1.427397	4.280578	0.889175
B	0.003509	5.171380	1.441342
B	0.882902	5.731765	-0.011565
B	-0.009767	5.158238	-1.451356
B	-1.436060	4.272674	-0.878531
B	-0.895221	5.722227	-0.003402
C	4.930968	-2.045248	1.904445
C	5.293244	-2.424679	3.198280
C	4.464731	-2.114778	4.278802
C	3.273278	-1.417708	4.066141
C	2.908666	-1.033154	2.775278
C	3.730407	-1.353235	1.681708
H	5.588282	-2.276885	1.071531
H	6.227198	-2.955442	3.361536
H	4.752912	-2.405003	5.285438
H	2.634007	-1.157768	4.905106
H	1.994939	-0.466110	2.617174
C	2.443137	-3.596307	-0.191135
C	1.730677	-4.656567	-0.755912
C	0.842740	-4.424027	-1.807591
C	0.664286	-3.127594	-2.296828
C	1.372354	-2.065475	-1.734206
C	2.272629	-2.291789	-0.679182
H	3.125620	-3.784982	0.632120
H	1.867749	-5.662799	-0.369148
H	0.283962	-5.249196	-2.240467
H	-0.037069	-2.939008	-3.104176
H	1.218186	-1.056030	-2.106816
C	5.244861	-1.783732	-1.721765
C	6.420745	-1.623669	-2.457306
C	7.070825	-0.388281	-2.481292

C	6.541622	0.692128	-1.771556
C	5.364883	0.538892	-1.038673
C	4.711203	-0.703950	-1.001900
H	4.739200	-2.744719	-1.718022
H	6.824434	-2.463835	-3.015765
H	7.982821	-0.265084	-3.058901
H	7.036507	1.658720	-1.796596
H	4.946590	1.387429	-0.503493
C	-3.254213	-3.139915	-1.698062
C	-3.233715	-3.768277	-2.944916
C	-3.066739	-3.013659	-4.108651
C	-2.915308	-1.627069	-4.024101
C	-2.934352	-0.995481	-2.779665
C	-3.112805	-1.746825	-1.606561
H	-3.371539	-3.734657	-0.797061
H	-3.347510	-4.847361	-3.005921
H	-3.051762	-3.504526	-5.078044
H	-2.777931	-1.035625	-4.924902
H	-2.802930	0.081660	-2.716887
C	-3.600119	-2.856182	1.984736
C	-3.162321	-3.783043	2.933502
C	-1.797393	-3.953406	3.170845
C	-0.866004	-3.192790	2.459457
C	-1.298585	-2.262218	1.515350
C	-2.670191	-2.091558	1.265060
H	-4.663838	-2.723140	1.813141
H	-3.890336	-4.366799	3.490220
H	-1.460350	-4.671358	3.913674
H	0.197525	-3.313022	2.645652
H	-0.571574	-1.662980	0.973897
C	-5.976926	-1.266002	-0.264390
C	-7.310809	-0.968113	0.020427
C	-7.626504	0.086035	0.879899
C	-6.605812	0.848002	1.452641
C	-5.271619	0.557510	1.167554
C	-4.945961	-0.508428	0.312344
H	-5.741559	-2.080236	-0.942989
H	-8.102391	-1.556880	-0.435005
H	-8.665631	0.319235	1.095320
H	-6.845644	1.677553	2.111556
H	-4.481839	1.166729	1.599125
H	0.000559	2.643712	-2.351054
H	0.021233	2.664395	2.363058
H	-2.436932	4.145245	1.503413
H	-2.451083	4.131844	-1.481802
H	2.441639	4.158242	-1.504859
H	2.455794	4.171814	1.481157
H	1.526656	6.734149	-0.019315
H	-0.017445	5.740046	-2.490296
H	-1.549854	6.717556	-0.004942
H	0.004745	5.762679	2.474911

Table S2. Gold Complex [(μ-1,7-$C_2B_{10}H_{10}$){$Au(PPh_3)$}$_2$]

Atom	X	Y	Z
Au	-3.109215	-0.679975	0.001046
Au	3.109237	-0.680032	-0.000420
P	-5.164292	0.520445	0.002376
P	5.164276	0.520454	-0.002351
C	-6.607863	-0.548095	-0.384240
C	-6.580706	-1.882053	0.054551
H	-5.709469	-2.260211	0.582865
C	-7.661309	-2.727274	-0.197229
H	-7.627592	-3.758215	0.143367
C	-8.773123	-2.253507	-0.897407
H	-9.610416	-2.915518	-1.100792
C	-8.802820	-0.931477	-1.345530
H	-9.662070	-0.561668	-1.898456
C	-7.725664	-0.080128	-1.091852
H	-7.752226	0.943630	-1.452971
C	-5.545581	1.303222	1.620296
C	-4.476463	1.789235	2.390582
H	-3.456600	1.671038	2.034020
C	-4.717431	2.408596	3.616847
H	-3.882635	2.777523	4.206064
C	-6.024694	2.538567	4.091374
H	-6.210420	3.012765	5.051254
C	-7.091665	2.048099	3.336195
H	-8.109414	2.138744	3.705953
C	-6.855758	1.432307	2.105485
H	-7.690109	1.044407	1.528976
C	-5.211741	1.880417	-1.232029
C	-4.561080	1.679453	-2.460655
H	-4.029501	0.749474	-2.644857
C	-4.584780	2.672061	-3.439972
H	-4.076843	2.506092	-4.385832
C	-5.246790	3.878414	-3.199215
H	-5.257453	4.654434	-3.959761
C	-5.886648	4.089328	-1.976552
H	-6.396132	5.029234	-1.782019
C	-5.871124	3.095850	-0.995246
H	-6.364665	3.271418	-0.044175
C	6.608083	-0.548122	0.383284
C	6.580826	-1.881914	-0.056017
H	5.709391	-2.259919	-0.584115
C	7.661585	-2.727162	0.194982
H	7.627797	-3.757970	-0.146004
C	8.773659	-2.253596	0.894889
H	9.611077	-2.915633	1.097667
C	8.803456	-0.931744	1.343522
H	9.662909	-0.562098	1.896240
C	7.726140	-0.080361	1.090619
H	7.752785	0.943260	1.452117

C	5.544693	1.303513	-1.620339
C	6.854661	1.433061	-2.105988
H	7.689335	1.045313	-1.529844
C	7.089941	2.049105	-3.336688
H	8.107529	2.140109	-3.706802
C	6.022548	2.539367	-4.091410
H	6.207785	3.013764	-5.051285
C	4.715498	2.408934	-3.616431
H	3.880377	2.777696	-4.205288
C	4.475157	1.789323	-2.390165
H	3.455461	1.670781	-2.033243
C	5.212365	1.880186	1.232281
C	4.562484	1.678882	2.461269
H	4.031132	0.748800	2.645605
C	4.586675	2.671277	3.440786
H	4.079344	2.505046	4.386925
C	5.248396	3.877761	3.199876
H	5.259435	4.653620	3.960580
C	5.887474	4.089010	1.976866
H	6.396732	5.029015	1.782221
C	5.871460	3.095741	0.995353
H	6.364405	3.271566	0.044021
C	-1.341898	-1.773556	0.000181
B	-0.000106	-1.190775	0.881088
H	-0.000041	-0.142685	1.436690
B	-0.887335	-2.610328	1.434553
H	-1.562024	-2.535373	2.410111
B	-1.431194	-3.495937	-0.000017
H	-2.494737	-4.028628	-0.000169
B	-0.887352	-2.609785	-1.434307
H	-1.562136	-2.534969	-2.409935
B	0.000126	-1.190492	-0.880486
H	0.000065	-0.142236	-1.435776
C	1.341899	-1.773578	0.000237
B	0.887340	-2.610262	1.434463
H	1.562140	-2.535763	2.410102
B	0.000024	-4.054957	0.892916
H	0.000012	-5.058185	1.534008
B	-0.000071	-4.054673	-0.893214
H	-0.000087	-5.057696	-1.534627
B	0.887319	-2.609892	-1.434403
H	1.562002	-2.534663	-2.409945
B	1.431158	-3.495970	-0.000120
H	2.494690	-4.028682	-0.000145

Table S3. Gold Complex $[(\mu\text{-}1,12\text{-}C_2B_{10}H_{10})\{Au(PPh_3)\}_2]$

Atom	X	Y	Z
Au	-3.657607	-0.037497	-0.010171
B	-0.740018	-0.504667	-1.427900
H	-1.328249	-0.849612	-2.401232
B	-0.731575	-1.517665	0.025816
H	-1.314246	-2.553430	0.043193
B	-0.753376	-0.449003	1.439042
H	-1.350959	-0.756386	2.419144
B	-0.775216	1.224972	0.858531
H	-1.388396	2.058868	1.442763
B	-0.767120	1.190562	-0.913193
H	-1.374354	2.001142	-1.535151
C	-1.579406	-0.023586	-0.006981
C	-6.799378	-1.561310	-0.614754
C	-8.002876	-1.585983	-1.335390
H	-8.518059	-0.658582	-1.566605
C	-8.537959	-2.801115	-1.767503
H	-9.468229	-2.809664	-2.329064
C	-7.877922	-3.998592	-1.485718
H	-8.293638	-4.942272	-1.828318
C	-6.676858	-3.981158	-0.772806
H	-6.153228	-4.908918	-0.560350
C	-6.136020	-2.769507	-0.343238
H	-5.191468	-2.758788	0.194418
C	-6.738307	1.336411	-1.049704
C	-6.037186	1.707023	-2.208753
H	-5.095270	1.220873	-2.448886
C	-6.537524	2.705692	-3.044545
H	-5.984829	2.986530	-3.936569
C	-7.734724	3.350579	-2.726592
H	-8.118992	4.134578	-3.373468
C	-8.431968	2.994778	-1.570177
H	-9.359169	3.500479	-1.314515
C	-7.937638	1.992879	-0.733226
H	-8.479415	1.731037	0.170798
C	-6.744801	0.265622	1.672065
C	-7.935741	-0.340731	2.098464
H	-8.471412	-1.013991	1.436019
C	-8.431344	-0.091003	3.379997
H	-9.352156	-0.569297	3.702818
C	-7.744031	0.763021	4.244153
H	-8.129040	0.951890	5.242540
C	-6.554377	1.365599	3.827787
H	-6.009178	2.021854	4.500240
C	-6.052380	1.114840	2.551155
H	-5.115639	1.569119	2.238720
P	-6.041353	-0.003310	-0.003527
Au	3.657607	0.037491	0.010157

B	0.740024	0.504652	1.427881
H	1.328250	0.849595	2.401215
B	0.731575	1.517653	-0.025833
H	1.314245	2.553419	-0.043211
B	0.753378	0.448992	-1.439057
H	1.350960	0.756372	-2.419160
B	0.775221	-1.224983	-0.858544
H	1.388396	-2.058879	-1.442779
B	0.767116	-1.190577	0.913177
H	1.374334	-2.001166	1.535133
C	1.579406	0.023576	0.006965
C	6.799364	1.561376	0.614605
C	8.002856	1.586130	1.335248
H	8.518039	0.658752	1.566557
C	8.537927	2.801310	1.767244
H	9.468192	2.809922	2.328812
C	7.877884	3.998750	1.485333
H	8.293585	4.942469	1.827843
C	6.676823	3.981237	0.772409
H	6.153201	4.908982	0.559864
C	6.135999	2.769542	0.342960
H	5.191452	2.758760	-0.194705
C	6.738316	-1.336298	1.049851
C	6.037204	-1.706774	2.208948
H	5.095302	-1.220582	2.449051
C	6.537541	-2.705359	3.044841
H	5.984853	-2.986094	3.936903
C	7.734727	-3.350299	2.726941
H	8.118991	-4.134234	3.373898
C	8.431960	-2.994631	1.570480
H	9.359149	-3.500374	1.314857
C	7.937627	-1.992818	0.733423
H	8.479404	-1.731083	-0.170631
C	6.744815	-0.265785	-1.672032
C	7.935767	0.340511	-2.098476
H	8.471444	1.013823	-1.436089
C	8.431378	0.090657	-3.379982
H	9.352200	0.568907	-3.702839
C	7.744059	-0.763436	-4.244065
H	8.129075	-0.952402	-5.242431
C	6.554392	-1.365957	-3.827655
H	6.009189	-2.022266	-4.500052
C	6.052388	-1.115073	-2.551051
H	5.115636	-1.569309	-2.238583
P	6.041354	0.003312	0.003529

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