

## Theoretical Exploration of the Forces Governing the interaction between Gold-Phthalocyanine and Gold Surface Clusters

Pablo Castro-Latorre,<sup>\*a</sup> Sebastián Miranda-Rojas<sup>\*b</sup> and Fernando Mendizabal<sup>\*a</sup>

<sup>a</sup>Departamento de Química, Facultad de Ciencias, Universidad de Chile, Casilla 653, Santiago, Chile. E-mail: pablo.castro@ug.uchile.cl, hagua@uchile.cl

<sup>b</sup>Departamento de Ciencias Químicas, Facultad de Ciencias Exactas, Universidad Andres Bello, Avenida República 275, Santiago, Chile.

**Table S1.** Interaction energies ( $\Delta E_{\text{int}}$ ) between AuPc, H<sub>2</sub>Pc with Au<sub>n</sub> (n=26, 58) optimized without dispersion correction. The energies are corrected for BSSE (in Kcal/mol). Au<sub>26</sub> is model 1 and Au<sub>58</sub> is model 2.

System	Method	$\Delta E_{\text{int}}$
Au <sub>26</sub> -AuPc	PBE	4.4
	TPSS	4.0
	TPSS-D3	-76.2
Au <sub>26</sub> -H <sub>2</sub> Pc	PBE	0.8
	TPSS	7.1
	TPSS-D3	-63.0
Au <sub>58</sub> -AuPc	PBE	-6.3
	TPSS	2.9
	TPSS-D3	-109.2
Au <sub>58</sub> -H <sub>2</sub> Pc	PBE	1.28
	TPSS	10.68
	TPSS-D3	-92.0

**Table S2.** Interaction energies ( $\Delta E_{\text{int}}$ ) and energy decomposition analysis for the complexes formed between AuPc and H<sub>2</sub>Pc with Au<sub>n</sub> (n=26, 58). The energies are corrected for BSSE (in Kcal/mol). Au<sub>26</sub> is model 1 and Au<sub>58</sub> is model 2.

System	Method	$\Delta E_{\text{TOT}}$	$\Delta E_{\text{ELECT}}$	$\Delta E_{\text{POL}}$	$\Delta E_{\text{DISP}}$
Au <sub>26</sub> -AuPc	PBE-D3	-55.3	78.5	-72.8	-60.9
	TPSS-D3	-76.2	92.7	-79.7	-89.1
Au <sub>26</sub> -H <sub>2</sub> Pc	PBE-D3	-45.5	68.8	-60.1	-54.2
	TPSS-D3	-63.0	91.2	-75.4	-78.9

**Table S3.** Adsorption Energies ( $\Delta E_{\text{int}}$ ) in kcal/mol between MPc and Au<sub>n</sub> (M= Fe, Co, Cu; n = 26, 58) with counterpoise correction (CP). Denoting the two closed M-Au distances in angstroms. Au<sub>26</sub> is model 1 and Au<sub>58</sub> is model 2.

System	Method	M-Au	M-Au	$\Delta E_{\text{int}}$
FePc-Au <sub>26</sub>	PBE	3.23	3.62	-3.9
	PBE-D3	3.23	3.34	-63.5
	TPSS	3.18	3.41	-0.2
	TPSS-D3	3.21	3.25	-86.8
CoPc-Au <sub>26</sub>	PBE	3.35	3.62	-3.6
	PBE-D3	3.25	3.40	-61.7
	TPSS	3.22	3.42	0.1
CuPc-Au <sub>26</sub>	PBE	3.74	3.79	-31.8
	PBE-D3	3.27	3.42	-85.1
	TPSS	3.37	3.42	-25.0
	TPSS-D3	3.12	3.20	-109.0
CoPc-Au <sub>58</sub>	PBE	3.40	3.50	-3.7
	PBE-D3	3.25	3.26	-88.4
	TPSS	3.22	3.27	-1.3

	TPSS-D3	3.15	3.23	-120.8
CuPc-Au <sub>58</sub>	PBE	3.63	3.96	-42.1
	PBE-D3	3.25	3.36	-119.9
	TPSS	3.30	3.56	-33.1
	TPSS-D3	3.08	3.16	-153.4

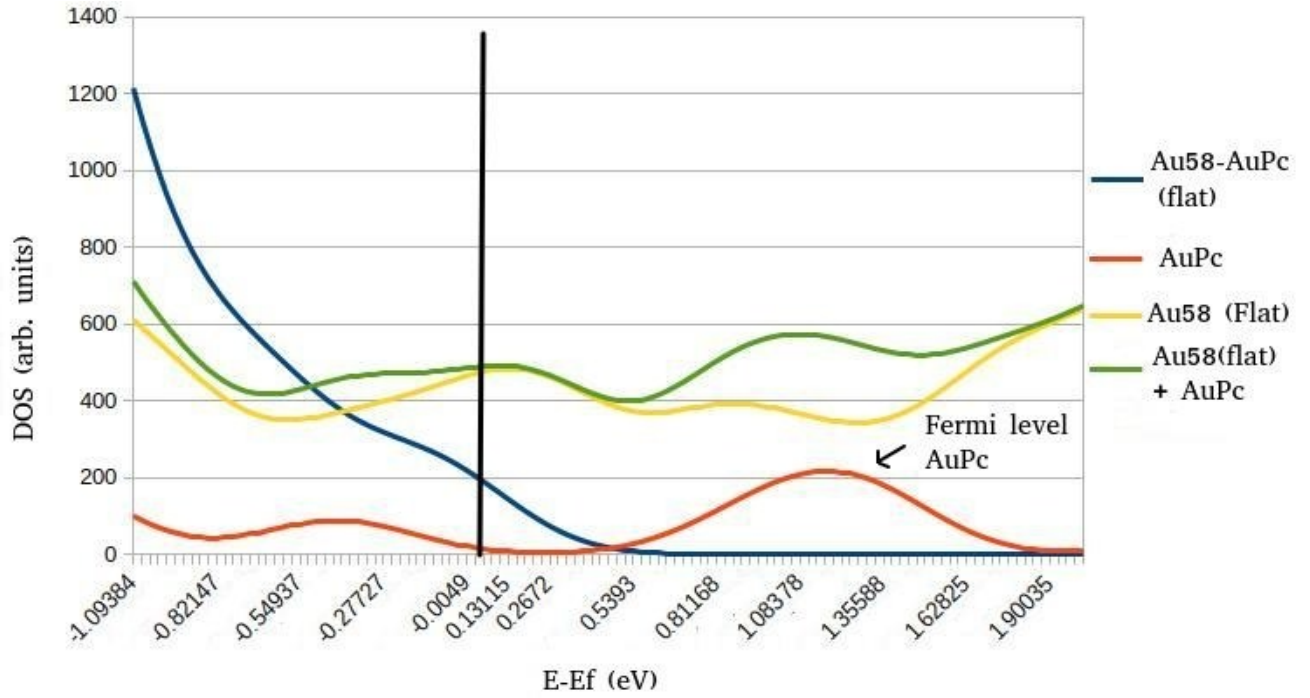
**Table S4.** Natural Population Atomic (NPA) analysis of the substrate (Au-cluster) and the ligands (AuPc or H<sub>2</sub>Pc). Au<sub>26</sub> is model 1 and Au<sub>58</sub> is model 2.

System	Method	Au-cluster	Au	Pc
AuPc	PBE-D3		1.21	-1.21
	TPSS-D3		1.24	-1.24
Au <sub>26</sub> -AuPc	PBE-D3	-0.14	1.24	-1.10
	TPSS-D3	-0.07	1.28	-1.21
Au <sub>26</sub> -H <sub>2</sub> Pc	PBE-D3	-0.06		0.06
	TPSS-D3	0.00		0.00

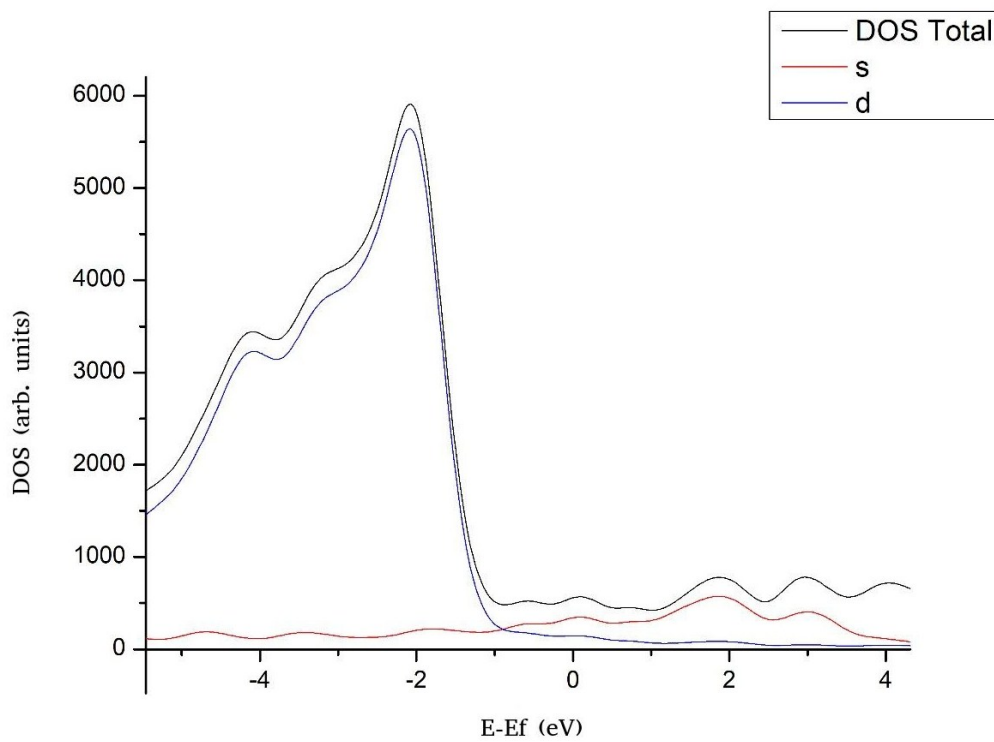
**Table S5.** Fragmental electronic chemical potential ( $\mu$ ) of the ligand (AuPc or H<sub>2</sub>Pc) and the gold substrate (Au<sub>26</sub> or Au<sub>58</sub>). The  $\Delta\mu$  was calculated from the difference between the  $\mu$  of the substrate and the ligand. Au<sub>26</sub> is model 1 and Au<sub>58</sub> is model 2.

System	Method	$\mu_{\text{Au-substrate}}$	$\mu_{\text{AuPc}}$	$\Delta\mu$
Au <sub>26</sub> -AuPc	PBE-D3	-4.82	-4.13	-0.69
	TPSS-D3	-4.69	-4.06	-0.63
Au <sub>26</sub> -H <sub>2</sub> Pc	PBE-D3	-4.82	-4.71	-0.11
	TPSS-D3	-4.70	-4.65	-0.05

**Figure S1:** DOS diagram of Au<sub>58</sub>(flat)-AuPc



**Figure S2.** DOS diagram of Au<sub>58</sub> clusters



## Systems coordinates (xyz coord)

### Au<sub>26</sub>-AuPc (PBE)

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
Au	3.7169670	-3.2770260	-1.8513200
Au	3.7629750	-0.3934560	-1.8563520
Au	3.6271390	-7.6064830	-4.3411260
Au	3.6730900	-4.7228400	-4.3461980
Au	3.7190390	-1.8393400	-4.3512700
Au	3.7649900	1.0443020	-4.3563420
Au	3.6292110	-6.1687260	-6.8411990
Au	3.6752190	-3.2851550	-6.8462310
Au	3.7211110	-0.4015830	-6.8513430
Au	3.6313400	-4.7310410	-9.3412310
Au	3.6772910	-1.8473980	-9.3463040
Au	1.3466120	-4.6798690	-0.9965850
Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860
Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
Au	7.2939966	-3.3923570	-4.3008439

C	7.1030460	-5.8043438	-6.1129049
C	6.8591125	-6.1383890	-7.4960890
C	6.8742961	-4.9210151	-8.2275327
C	7.1149239	-3.8601578	-7.2827750
N	7.2289908	-4.4417974	-6.0435775
C	7.2727850	-5.2092514	-1.8795218
C	7.2607744	-6.6285177	-1.5331530
C	7.2533448	-7.3548731	-2.7410133
C	7.2466927	-6.3832207	-3.8315213
N	7.2894529	-5.1351928	-3.2545769
C	7.2599890	-0.9755045	-2.4852708
C	7.0690621	-0.6320161	-1.0961090
C	7.0356077	-1.8498019	-0.3669424
C	7.2107664	-2.9192487	-1.3166634
N	7.3230583	-2.3426629	-2.5577431
C	7.2815514	-1.5742334	-6.7224982
C	7.3140832	-0.1552377	-7.0689492
C	7.3624121	0.5703671	-5.8611072
C	7.3504331	-0.4012783	-4.7700494
N	7.3229958	-1.6497519	-5.3479067
N	7.1878981	-2.5677434	-7.5495801
N	7.1614273	-6.6494241	-5.0983659
N	7.2339481	-4.2134511	-1.0505499
N	7.3229707	-0.1333047	-3.5013546
C	6.7761485	-1.8522452	1.0149708
C	7.3821571	1.9676387	-5.8603164
C	7.2801290	0.5016062	-8.3021378
C	6.5923306	-4.9081334	-9.6050415
C	6.5941743	-7.3613283	-8.1385360
C	7.2230610	-8.7516902	-2.7413542
C	7.2361335	-7.2836664	-0.2989299

C	6.8799412	0.6004779	-0.4474026
C	6.6336990	0.5933597	0.9238452
H	6.4784420	1.5463338	1.4557456
C	6.5712526	-0.6219444	1.6483639
C	7.3532666	2.6246748	-7.0948015
C	7.3017069	1.9001544	-8.3013352
H	7.2763434	2.4455480	-9.2591879
C	6.3144330	-6.1282978	-10.2323957
C	6.3265292	-7.3440534	-9.5058563
H	6.1145145	-8.2887667	-10.0328661
C	7.2088018	-8.6819441	-0.2992411
H	7.1895833	-9.2263428	0.6593213
C	7.2032035	-9.4074984	-1.5061943
H	6.9215099	1.5398524	-1.0235949
H	6.7668204	-2.8020497	1.5756497
H	7.4198084	2.5212685	-4.9073187
H	7.2351710	-0.0791272	-9.2386205
H	6.6279642	-3.9605713	-10.1686916
H	6.6027530	-8.3014258	-7.5618683
H	7.3691960	3.7266556	-7.1256688
H	6.3843747	-0.5938736	2.7350514
H	6.1144627	-6.1494929	-11.3169957
H	7.2155444	-9.3064031	-3.6943706

### **Au<sub>26</sub>-AuPc (PBE-D3)**

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
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Au	1.3466120	-4.6798690	-0.9965850
Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860
Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
Au	7.0349805	-3.4078158	-4.3108346
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C	6.6724392	-6.1247435	-7.5409462
C	6.6998722	-4.9007613	-8.2619865
C	6.9014741	-3.8469544	-7.3030424
N	6.9981692	-4.4396515	-6.0658708
C	6.9572022	-5.2471907	-1.9080281
C	6.8244826	-6.6647885	-1.5799586
C	6.8437535	-7.3804905	-2.7950582
C	6.9518597	-6.4014124	-3.8719048
N	7.0300075	-5.1620066	-3.2817526



C	7.0410480	-1.0101529	-2.4693431
C	6.8868582	-0.6784652	-1.0727453
C	6.8545536	-1.9035775	-0.3548200
C	6.9836563	-2.9647155	-1.3184471
N	7.0867660	-2.3763437	-2.5565289
C	6.9909968	-1.5651309	-6.7138527
C	6.9269536	-0.1429398	-7.0406475
C	6.9790956	0.5706081	-5.8247598
C	7.0610116	-0.4124713	-4.7479874
N	7.0631121	-1.6542959	-5.3404490
N	6.9305799	-2.5493789	-7.5536390
N	6.8977161	-6.6567020	-5.1425902
N	6.9511737	-4.2616241	-1.0674947
N	7.0658524	-0.1564922	-3.4772425
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C	6.8786690	1.9642560	-5.8014190
C	6.7718795	0.5228632	-8.2602535
C	6.4096654	-4.8739411	-9.6388384
C	6.4007849	-7.3422583	-8.1914757
C	6.6765717	-8.7673508	-2.8178849
C	6.6354935	-7.3218808	-0.3599808
C	6.6991975	0.5492859	-0.4140657
C	6.4569996	0.5308773	0.9579072
H	6.2985975	1.4785416	1.4976735
C	6.3935656	-0.6908923	1.6726947
C	6.7251369	2.6303575	-7.0226289
C	6.6718316	1.9183794	-8.2365935
H	6.5423574	2.4699277	-9.1822257
C	6.1271912	-6.0917404	-10.2760228
C	6.1355138	-7.3138365	-9.5592553
H	5.9143603	-8.2524656	-10.0925883

C	6.4676809	-8.7105913	-0.3833310
H	6.3088511	-9.2551227	0.5620805
C	6.4899304	-9.4248799	-1.5970180
H	6.7320935	1.4915295	-0.9858109
H	6.5842636	-2.8742589	1.5796626
H	6.9176325	2.5064264	-4.8418032
H	6.7186226	-0.0515548	-9.2002755
H	6.4579187	-3.9227405	-10.1954385
H	6.3967461	-8.2832970	-7.6166317
H	6.6385933	3.7292683	-7.0361682
H	6.2091265	-0.6716806	2.7599120
H	5.9285690	-6.1032280	-11.3607660

#### **Au<sub>26</sub>-AuPc (TPSS)**

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
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Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860

Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
Au	7.1448663	-3.4010408	-4.3028854
C	6.9500859	-5.8202070	-6.1038333
C	6.6960858	-6.1580610	-7.4841709
C	6.7280943	-4.9441703	-8.2226452
C	6.9788359	-3.8821734	-7.2842863
N	7.0871431	-4.4586299	-6.0411354
C	7.1634544	-5.2093760	-1.8734431
C	7.1844820	-6.6273813	-1.5218501
C	7.1668022	-7.3585859	-2.7271068
C	7.1213961	-6.3911968	-3.8205969
N	7.1565291	-5.1401507	-3.2496202
C	7.1195360	-0.9767601	-2.4973574
C	6.9264174	-0.6287956	-1.1094956
C	6.9047592	-1.8445084	-0.3749669
C	7.0838646	-2.9156822	-1.3198343
N	7.1892522	-2.3437932	-2.5646023
C	7.1679513	-1.5935136	-6.7339752
C	7.2307648	-0.1770135	-7.0866186
C	7.2701980	0.5542241	-5.8814785
C	7.2261955	-0.4115988	-4.7857326
N	7.1883344	-1.6630449	-5.3578607
N	7.0711379	-2.5898445	-7.5589360

N	7.0200426	-6.6646999	-5.0862456
N	7.1239574	-4.2105210	-1.0465597
N	7.1910028	-0.1361636	-3.5175042
C	6.6469428	-1.8443764	1.0098673
C	7.3212637	1.9518002	-5.8875593
C	7.2378951	0.4733709	-8.3248127
C	6.4408311	-4.9342819	-9.6019177
C	6.4145088	-7.3834937	-8.1205575
C	7.1736989	-8.7567560	-2.7224646
C	7.2069854	-7.2784016	-0.2842173
C	6.7326514	0.6069783	-0.4634528
C	6.4894926	0.6029279	0.9084779
H	6.3319804	1.5520985	1.4361227
C	6.4352920	-0.6110406	1.6388900
C	7.3324540	2.6019114	-7.1264226
C	7.2905058	1.8714190	-8.3305501
H	7.2985407	2.4098538	-9.2869248
C	6.1446032	-6.1568143	-10.2217630
C	6.1437294	-7.3698562	-9.4875757
H	5.9211640	-8.3100059	-10.0077549
C	7.2162918	-8.6772261	-0.2798647
H	7.2360409	-9.2164406	0.6758821
C	7.2007348	-9.4078072	-1.4845472
H	6.7704656	1.5418790	-1.0370880
H	6.6570241	-2.7849900	1.5758436
H	7.3532040	2.5102069	-4.9433073
H	7.2026746	-0.1065241	-9.2558949
H	6.5045633	-3.9994995	-10.1741567
H	6.4176346	-8.3180513	-7.5447892
H	7.3736616	3.6980637	-7.1632875
H	6.2576951	-0.5783148	2.7220057

H 5.9517624 -6.1836045 -11.3025213

**Au<sub>26</sub>-AuPc (TPSS-D3)**

Au 3.7148940 -4.7147830 0.6487530  
Au 3.7608460 -1.8311410 0.6436810  
Au 3.6710750 -6.1605980 -1.8462070  
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Au 3.7190390 -1.8393400 -4.3512700  
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Au 3.6292110 -6.1687260 -6.8411990  
Au 3.6752190 -3.2851550 -6.8462310  
Au 3.7211110 -0.4015830 -6.8513430  
Au 3.6313400 -4.7310410 -9.3412310  
Au 3.6772910 -1.8473980 -9.3463040  
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Au 1.3487420 -3.2421840 -3.4966180  
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Au 1.3507570 -1.8044260 -5.9966090  
Au 1.3068780 -3.2503120 -8.4916100  
Au -0.9777930 -3.1992120 -0.1469230  
Au -1.0216720 -4.6450970 -2.6419240  
Au -0.9757210 -1.7614550 -2.6469960  
Au -1.0196000 -3.2073410 -5.1419970  
Au 6.8856820 -3.3931638 -4.2736811  
C 6.7559894 -5.7905466 -6.1094026

C	6.5634010	-6.1177734	-7.5023208
C	6.6037694	-4.8950039	-8.2269309
C	6.7812898	-3.8388983	-7.2688529
N	6.8660301	-4.4285151	-6.0273796
C	6.8233728	-5.2286320	-1.8654269
C	6.6961810	-6.6463367	-1.5359688
C	6.7274919	-7.3644440	-2.7503070
C	6.8276703	-6.3865566	-3.8284228
N	6.8965952	-5.1454739	-3.2405384
C	6.9007448	-0.9921811	-2.4365944
C	6.7508251	-0.6575687	-1.0402089
C	6.7275751	-1.8822245	-0.3192985
C	6.8511722	-2.9438077	-1.2795891
N	6.9494843	-2.3582407	-2.5212401
C	6.8528764	-1.5543755	-6.6831528
C	6.7707172	-0.1334981	-7.0103005
C	6.8278022	0.5821852	-5.7948353
C	6.9210801	-0.3986765	-4.7177590
N	6.9254387	-1.6419338	-5.3084184
N	6.8022534	-2.5393384	-7.5242664
N	6.7725346	-6.6468290	-5.0998005
N	6.8167181	-4.2426088	-1.0239613
N	6.9252329	-0.1374570	-3.4468471
C	6.4577705	-1.8980779	1.0648252
C	6.7003652	1.9748746	-5.7693871
C	6.5821135	0.5293153	-8.2291045
C	6.3301966	-4.8693394	-9.6093173
C	6.2942592	-7.3385226	-8.1530036
C	6.5668346	-8.7529625	-2.7722820
C	6.5043568	-7.3020993	-0.3141565
C	6.5584270	0.5730672	-0.3837067

C	6.3114871	0.5557750	0.9875038
H	6.1474295	1.4986330	1.5234364
C	6.2490573	-0.6663105	1.7054442
C	6.5114196	2.6367102	-6.9886582
C	6.4519887	1.9230660	-8.2021742
H	6.2934003	2.4696349	-9.1403370
C	6.0478454	-6.0901090	-10.2452433
C	6.0429882	-7.3114795	-9.5239703
H	5.8229010	-8.2450953	-10.0560577
C	6.3418559	-8.6917567	-0.3375690
H	6.1806978	-9.2340084	0.6027792
C	6.3740412	-9.4081566	-1.5508210
H	6.5890141	1.5101911	-0.9536757
H	6.4681858	-2.8453454	1.6198598
H	6.7445410	2.5170013	-4.8159524
H	6.5239528	-0.0414754	-9.1647318
H	6.3993100	-3.9270320	-10.1687283
H	6.2821272	-8.2749523	-7.5807545
H	6.4013938	3.7283862	-7.0011571
H	6.0647215	-0.6444555	2.7873821
H	5.8663080	-6.1055897	-11.3279630

### **Au<sub>26</sub>-H<sub>2</sub>Pc (PBE)**

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
Au	3.7169670	-3.2770260	-1.8513200
Au	3.7629750	-0.3934560	-1.8563520
Au	3.6271390	-7.6064830	-4.3411260
Au	3.6730900	-4.7228400	-4.3461980
Au	3.7190390	-1.8393400	-4.3512700

Au	3.7649900	1.0443020	-4.3563420
Au	3.6292110	-6.1687260	-6.8411990
Au	3.6752190	-3.2851550	-6.8462310
Au	3.7211110	-0.4015830	-6.8513430
Au	3.6313400	-4.7310410	-9.3412310
Au	3.6772910	-1.8473980	-9.3463040
Au	1.3466120	-4.6798690	-0.9965850
Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860
Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
N	7.3413594	-2.0432519	-5.8250922
N	7.3990241	-2.0785400	-2.9707049
N	7.3064196	-0.1523093	-4.3744169
N	7.2783562	-3.5076906	-7.7064284
N	7.3946043	-3.4847498	-1.0425195
N	7.2697132	-4.9132190	-5.7781258
N	7.3210507	-4.9486182	-2.9232371
N	7.1306355	-6.8334011	-4.3693653
C	7.2790257	-0.0315757	-6.8503054
C	7.2548923	-0.0354051	-1.9149829
C	7.2918327	-1.0369788	-7.8463323
C	7.3015563	-1.0312129	-0.9207398
C	7.3159874	-0.7014082	-5.5566421



C	7.3267889	-0.7507956	-3.1973048
C	7.3168830	-2.3230389	-7.1654444
C	7.3809568	-2.3082668	-1.6411558
C	7.0543060	-5.9531838	-7.8225765
C	7.2965002	-5.9534936	-0.9008785
C	6.9803041	-6.9450289	-6.8250371
C	7.2027744	-6.9563331	-1.8950033
C	7.2235755	-4.6823213	-7.1071564
C	7.3574770	-4.6691495	-1.5834959
C	7.1353390	-6.2350138	-5.5468646
C	7.2191035	-6.2871541	-3.1891345
C	7.2238666	1.3233885	-7.1988900
C	7.1489779	1.3152020	-1.5765842
C	7.2471756	-0.7045149	-9.2050804
C	7.2432556	-0.7014024	0.4344421
C	7.1827854	1.6511331	-8.5558084
C	7.0918210	1.6493337	-0.2169991
C	7.1950112	0.6484789	-9.5479890
C	7.1393602	0.6538987	0.7760962
C	6.9413246	-6.2810113	-9.1751270
C	7.2903517	-6.2853411	0.4586035
C	6.7920007	-8.2885940	-7.1579935
C	7.1043801	-8.3078079	-1.5443137
C	6.7552380	-7.6288740	-9.5106959
C	7.1923713	-7.6349452	0.8037784
C	6.6802818	-8.6198487	-8.5146818
C	7.1004079	-8.6349534	-0.1868751
H	7.3295465	-2.7671615	-5.0900248
H	7.2160729	2.0972355	-6.4131658
H	7.1147649	2.0858037	-2.3650698
H	7.2585983	-1.4992975	-9.9694959

H	7.2878273	-1.4920573	1.2023251
H	7.1398980	2.7103142	-8.8590944
H	7.0100691	2.7077710	0.0812001
H	7.1618800	0.9400233	-10.6108201
H	7.0956823	0.9467217	1.8383327
H	7.0077955	-5.4946333	-9.9459324
H	7.3651411	-5.4929606	1.2219124
H	6.7398996	-9.0564371	-6.3676690
H	7.0325531	-9.0796447	-2.3285880
H	6.6664598	-7.9196015	-10.5706345
H	7.1863173	-7.9261162	1.8671245
H	6.5336603	-9.6725714	-8.8082556

#### **Au<sub>26</sub>-H<sub>2</sub>Pc (PBE-D3)**

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
Au	3.7169670	-3.2770260	-1.8513200
Au	3.7629750	-0.3934560	-1.8563520
Au	3.6271390	-7.6064830	-4.3411260
Au	3.6730900	-4.7228400	-4.3461980
Au	3.7190390	-1.8393400	-4.3512700
Au	3.7649900	1.0443020	-4.3563420
Au	3.6292110	-6.1687260	-6.8411990
Au	3.6752190	-3.2851550	-6.8462310
Au	3.7211110	-0.4015830	-6.8513430
Au	3.6313400	-4.7310410	-9.3412310
Au	3.6772910	-1.8473980	-9.3463040
Au	1.3466120	-4.6798690	-0.9965850
Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860

Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
N	7.0811717	-2.0178481	-5.8253492
N	7.1353709	-2.0435987	-2.9848496
N	6.9271893	-0.1243088	-4.3862632
N	7.0646479	-3.4898029	-7.7049622
N	7.1351008	-3.4518790	-1.0552399
N	7.0379509	-4.8960201	-5.7754479
N	7.0646513	-4.9232084	-2.9321486
N	6.7855373	-6.8050697	-4.3677218
C	6.8541875	-0.0235511	-6.8628192
C	6.8607295	-0.0159460	-1.9249316
C	6.9460888	-1.0320117	-7.8525979
C	6.9709553	-1.0103985	-0.9325344
C	6.9659424	-0.6790531	-5.5651848
C	6.9898215	-0.7215998	-3.2098040
C	7.0647148	-2.3051704	-7.1645870
C	7.1160961	-2.2774766	-1.6549742
C	6.7853002	-5.9208064	-7.8232829
C	6.9270038	-5.9050366	-0.9024519
C	6.6370009	-6.9072483	-6.8265635
C	6.7844436	-6.9088085	-1.8913148
C	7.0055692	-4.6621398	-7.1053478
C	7.0816819	-4.6359188	-1.5931016

C	6.8355595	-6.2090587	-5.5452885
C	6.8881102	-6.2551298	-3.1900753
C	6.6411809	1.3144832	-7.2219392
C	6.6219299	1.3179197	-1.5811231
C	6.8182854	-0.7251794	-9.2121422
C	6.8426489	-0.6997597	0.4225415
C	6.5229465	1.6186398	-8.5808820
C	6.4960212	1.6335979	-0.2209572
C	6.6107978	0.6114920	-9.5644282
C	6.6064160	0.6387184	0.7680273
C	6.6233541	-6.2277914	-9.1757778
C	6.8180597	-6.2119842	0.4587614
C	6.3237306	-8.2277396	-7.1640834
C	6.5364946	-8.2392967	-1.5315147
C	6.3160750	-7.5532630	-9.5144818
C	6.5722213	-7.5411326	0.8121533
C	6.1651464	-8.5388947	-8.5217337
C	6.4319311	-8.5421245	-0.1719745
H	7.0975963	-2.7343788	-5.0828334
H	6.5686342	2.0914905	-6.4426594
H	6.5296883	2.0863662	-2.3670392
H	6.8905697	-1.5262640	-9.9665973
H	6.9334805	-1.4931161	1.1838778
H	6.3521847	2.6626145	-8.8909130
H	6.3017633	2.6763872	0.0795941
H	6.5074083	0.8838550	-10.6276529
H	6.4993456	0.9163498	1.8296547
H	6.7445434	-5.4428931	-9.9414455
H	6.9250261	-5.4159696	1.2145803
H	6.2045331	-8.9905637	-6.3759968
H	6.4162269	-9.0093808	-2.3114606

H	6.1844882	-7.8276541	-10.5741292
H	6.4781742	-7.8126220	1.8765794

**Au<sub>26</sub>-H<sub>2</sub>Pc (TPSS)**

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
Au	3.7169670	-3.2770260	-1.8513200
Au	3.7629750	-0.3934560	-1.8563520
Au	3.6271390	-7.6064830	-4.3411260
Au	3.6730900	-4.7228400	-4.3461980
Au	3.7190390	-1.8393400	-4.3512700
Au	3.7649900	1.0443020	-4.3563420
Au	3.6292110	-6.1687260	-6.8411990
Au	3.6752190	-3.2851550	-6.8462310
Au	3.7211110	-0.4015830	-6.8513430
Au	3.6313400	-4.7310410	-9.3412310
Au	3.6772910	-1.8473980	-9.3463040
Au	1.3466120	-4.6798690	-0.9965850
Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860
Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
N	7.2356328	-2.0297008	-5.8234638

N	7.3042208	-2.0632012	-2.9708796
N	7.2195086	-0.1341715	-4.3731808
N	7.1858457	-3.4907422	-7.7116316
N	7.3305626	-3.4684787	-1.0407119
N	7.1504025	-4.8933833	-5.7801668
N	7.2178726	-4.9271870	-2.9266478
N	7.0152030	-6.8157020	-4.3714589
C	7.2278744	-0.0159437	-6.8482122
C	7.1788022	-0.0184159	-1.9128939
C	7.2411160	-1.0207039	-7.8448437
C	7.2361275	-1.0143334	-0.9189957
C	7.2299885	-0.6868912	-5.5551272
C	7.2351927	-0.7344479	-3.1952946
C	7.2299561	-2.3071679	-7.1655045
C	7.3025457	-2.2910237	-1.6401677
C	6.9437462	-5.9354959	-7.8258251
C	7.2597150	-5.9381018	-0.9065778
C	6.8546897	-6.9257035	-6.8270158
C	7.1468957	-6.9393321	-1.9005819
C	7.1138951	-4.6653992	-7.1106826
C	7.2870066	-4.6518538	-1.5866313
C	7.0101206	-6.2150627	-5.5495469
C	7.1212941	-6.2668223	-3.1923084
C	7.2145514	1.3415717	-7.1958478
C	7.0910695	1.3346332	-1.5740424
C	7.2384582	-0.6863758	-9.2050159
C	7.2073556	-0.6835115	0.4380238
C	7.2145051	1.6706155	-8.5531941
C	7.0637475	1.6693639	-0.2133705
C	7.2265496	0.6679836	-9.5467182
C	7.1222252	0.6734182	0.7797744

C	6.8488996	-6.2660436	-9.1805265
C	7.3078008	-6.2742455	0.4521656
C	6.6680459	-8.2711905	-7.1596799
C	7.0822551	-8.2946397	-1.5516311
C	6.6632193	-7.6147211	-9.5148961
C	7.2435620	-7.6265695	0.7952174
C	6.5720031	-8.6039378	-8.5173756
C	7.1316972	-8.6254523	-0.1958055
H	7.2024804	-2.7525797	-5.0918103
H	7.2078924	2.1134547	-6.4155650
H	7.0497193	2.1038137	-2.3561828
H	7.2529134	-1.4744540	-9.9685471
H	7.2613871	-1.4675633	1.2044535
H	7.2066244	2.7256682	-8.8555544
H	6.9990588	2.7237800	0.0851293
H	7.2272793	0.9601861	-10.6046945
H	7.1036150	0.9664586	1.8375059
H	6.9331681	-5.4887880	-9.9512058
H	7.3984062	-5.4893096	1.2136804
H	6.6078077	-9.0367914	-6.3750583
H	6.9974135	-9.0638219	-2.3298384
H	6.5900251	-7.9075246	-10.5702313
H	7.2812608	-7.9204958	1.8520255
H	6.4281376	-9.6521745	-8.8097084

**Au<sub>26</sub>-H<sub>2</sub>Pc (TPSS-D3)**

Au	3.7148940	-4.7147830	0.6487530
Au	3.7608460	-1.8311410	0.6436810
Au	3.6710750	-6.1605980	-1.8462070
Au	3.7169670	-3.2770260	-1.8513200
Au	3.7629750	-0.3934560	-1.8563520

Au	3.6271390	-7.6064830	-4.3411260
Au	3.6730900	-4.7228400	-4.3461980
Au	3.7190390	-1.8393400	-4.3512700
Au	3.7649900	1.0443020	-4.3563420
Au	3.6292110	-6.1687260	-6.8411990
Au	3.6752190	-3.2851550	-6.8462310
Au	3.7211110	-0.4015830	-6.8513430
Au	3.6313400	-4.7310410	-9.3412310
Au	3.6772910	-1.8473980	-9.3463040
Au	1.3466120	-4.6798690	-0.9965850
Au	1.3925610	-1.7963690	-1.0016570
Au	1.3027330	-6.1257550	-3.4915860
Au	1.3487420	-3.2421840	-3.4966180
Au	1.3946340	-0.3586120	-3.5017300
Au	1.3048050	-4.6880680	-5.9915370
Au	1.3507570	-1.8044260	-5.9966090
Au	1.3068780	-3.2503120	-8.4916100
Au	-0.9777930	-3.1992120	-0.1469230
Au	-1.0216720	-4.6450970	-2.6419240
Au	-0.9757210	-1.7614550	-2.6469960
Au	-1.0196000	-3.2073410	-5.1419970
N	6.9562209	-1.5793131	-5.1696079
N	7.0178707	-2.2874902	-2.3922995
N	6.9349938	-0.0813553	-3.3087214
N	6.8570867	-2.5336998	-7.3563418
N	6.8684894	-4.1081737	-0.8494817
N	6.9177575	-4.3597070	-5.8116436
N	6.9261345	-5.0690759	-3.0362687
N	6.7650749	-6.5612345	-4.8954380
C	6.8346812	0.6225389	-5.6707132
C	6.7074242	-0.5524041	-0.9063887



C	6.7899578	-0.1113549	-6.8812061
C	6.7099189	-1.7559638	-0.1730202
C	6.9395222	-0.3396782	-4.5846215
C	6.9137810	-0.9454238	-2.3089700
C	6.8898913	-1.5219302	-6.5382185
C	6.8998505	-2.8217010	-1.1560052
C	6.6385372	-4.8822370	-8.0374347
C	6.7374210	-6.5292324	-1.3200766
C	6.5578929	-6.0807284	-7.2988757
C	6.7343068	-7.2643247	-2.5297189
C	6.8349663	-3.8203355	-7.0492745
C	6.8677992	-5.1214287	-1.6676848
C	6.7706276	-5.6971953	-5.8962999
C	6.8325227	-6.3050725	-3.6189477
C	6.6871517	2.0158446	-5.6660997
C	6.4555575	0.6776373	-0.2863072
C	6.5904674	0.5354241	-8.1093650
C	6.3898959	-1.7705135	1.1932708
C	6.4921454	2.6566793	-6.8933765
C	6.1686119	0.6753397	1.0846178
C	6.4427268	1.9257248	-8.0993676
C	6.1201030	-0.5308626	1.8142160
C	6.3959918	-4.8644507	-9.4154199
C	6.5611300	-7.1691812	-0.0863216
C	6.2559730	-7.3005518	-7.9216244
C	6.5561061	-8.6525230	-2.5280921
C	6.0935112	-6.0920280	-10.0446526
C	6.3819857	-8.5545986	-0.0896349
C	6.0361122	-7.2928408	-9.3069148
C	6.3808364	-9.2874662	-1.2960529
H	6.9572347	-2.4615386	-4.6397437

H	6.7240158	2.5725578	-4.7207551
H	6.4681595	1.6053588	-0.8725217
H	6.5419852	-0.0476917	-9.0379157
H	6.4177668	-2.7092013	1.7626978
H	6.3681903	3.7466110	-6.9214468
H	5.9591832	1.6212836	1.5990752
H	6.2774962	2.4588978	-9.0440996
H	5.8984995	-0.5021526	2.8889668
H	6.4870977	-3.9290891	-9.9833800
H	6.5507919	-6.5839360	0.8418492
H	6.2105916	-8.2266280	-7.3338958
H	6.5437902	-9.2094929	-3.4736030
H	5.9415215	-6.1203942	-11.1318441
H	6.2322353	-9.0839140	0.8598624
H	5.8006889	-8.2302570	-9.8256476

#### **Au<sub>58</sub>-AuPc (PBE)**

Au	-0.5558531	-0.2116859	-5.0905861
N	-2.1981274	0.9806187	-5.1747236
C	-2.1579467	2.3496089	-5.1976167
C	-3.4914260	0.5157078	-5.1734302
C	-3.5317724	2.8198248	-5.2337545
C	-4.3631960	1.6760752	-5.2187772
N	1.0882753	-1.4040197	-5.0580674
C	1.0481307	-2.7737979	-5.0093220
C	2.4235981	-3.2412652	-4.9833308
C	3.2524548	-2.0956243	-5.0100393
N	0.6355464	1.4329125	-5.1263693
C	2.0095232	1.3925494	-5.0922595
C	0.1710884	2.7228405	-5.1567497
C	2.4777413	2.7697090	-5.1018949

C	1.3335885	3.5978356	-5.1414841
N	-1.7469750	-1.8570190	-5.0943417
C	-3.1199128	-1.8131938	-5.0793200
C	-1.2818572	-3.1444479	-5.0081561
C	-3.5885260	-3.1849266	-4.9711106
C	-2.4448663	-4.0135599	-4.9246182
N	-0.0295955	-3.5173650	-4.9873180
N	2.7481484	0.3176566	-5.0618157
N	-1.0802507	3.0943489	-5.1918246
N	-3.8601420	-0.7384081	-5.1288003
C	-5.4669673	4.2273961	-5.2925028
H	-5.9264600	5.2290037	-5.3176055
C	-6.2968128	3.0874509	-5.2787324
H	-7.3915114	3.2168118	-5.2947379
C	5.1914984	-3.4975902	-4.9152709
H	6.2867860	-3.6207491	-4.8831344
C	-4.9916055	-5.1124070	-4.7261485
H	-5.9924015	-5.5686102	-4.6482225
C	-3.8501561	-5.9388821	-4.6770761
H	-3.9760024	-7.0279263	-4.5603455
C	2.7379869	5.5364544	-5.1276646
H	2.8633619	6.6317338	-5.1339003
C	3.8789105	4.7103315	-5.0905745
H	4.8798171	5.1716778	-5.0646287
C	-5.7569031	1.7992627	-5.2398773
C	-4.0752355	4.1081571	-5.2683589
C	-2.5628648	-5.3999793	-4.7735329
C	-4.8753003	-3.7260911	-4.8714655
C	1.4508074	4.9908717	-5.1539441
C	3.7637824	3.3173143	-5.0753596
C	2.9722931	-4.5272630	-4.9308970

C	4.6465300	-2.2122249	-4.9721519
H	2.3169545	-5.4138085	-4.9168525
H	-1.6629525	-6.0366691	-4.7382478
H	-5.7607340	-3.0695434	-4.9074284
H	-6.3972305	0.9018967	-5.2238394
H	-3.4157357	4.9916645	-5.2713361
H	0.5515690	5.6283407	-5.1785143
H	4.6508531	2.6634988	-5.0380407
H	5.2842106	-1.3128867	-4.9865167
C	4.3650904	-4.6410050	-4.8971063
H	4.8276017	-5.6410960	-4.8573411
C	2.3797825	-0.9381285	-5.0528767
Au	5.2595290	1.6764350	-1.3620180
Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470
Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710
Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300
Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360

Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280
Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380

Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160

### **Au<sub>58</sub>-AuPc (PBE-D3)**

Au	5.2595290	1.6764350	-1.3620180
Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470
Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710
Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300
Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360
Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280

Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380
Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830

Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
Au	-0.5502326	0.1318521	-4.6966060
C	2.2350261	-1.0515344	-4.6902677
C	3.6308982	-0.6426126	-4.6368672
C	3.6541456	0.7702459	-4.6372691
C	2.2710271	1.2242169	-4.6890979
N	1.4810651	0.0984819	-4.7060740
C	-1.7317434	-2.6513726	-4.7288759
C	-1.3318681	-4.0418320	-4.6870888
C	0.0868276	-4.0681623	-4.6742656
C	0.5389311	-2.6903889	-4.7048515
N	-0.5800979	-1.9006945	-4.7378272
C	-3.3355752	1.3149073	-4.8054857
C	-4.7343847	0.9084584	-4.8349054
C	-4.7588881	-0.5050099	-4.8367090
C	-3.3736577	-0.9586753	-4.7958108
N	-2.5826375	0.1660063	-4.7763499
C	0.6313548	2.9177862	-4.7152743
C	0.2267333	4.3098114	-4.7387980
C	-1.1917828	4.3316867	-4.7558974
C	-1.6396870	2.9541058	-4.7425002
N	-0.5145842	2.1637592	-4.7224893
N	1.8620283	2.4598506	-4.7034242
N	1.7852668	-2.2737556	-4.6896235
N	-2.9620651	-2.1930211	-4.7759759
N	-2.8832797	2.5356020	-4.7876305
C	-5.9663072	-1.2072669	-4.8628792
C	-1.8936849	5.5414424	-4.8028447



C	0.9663988	5.4976774	-4.7745751
C	4.8596999	1.4762274	-4.5584556
C	4.8124573	-1.3836592	-4.5286764
C	0.7826629	-5.2835357	-4.6411720
C	-2.0770990	-5.2271736	-4.6502378
C	-5.9188805	1.6497367	-4.8253143
C	-7.1292037	0.9442151	-4.8380243
H	-8.0799339	1.5028913	-4.8321414
C	-7.1519806	-0.4647578	-4.8688964
C	-1.1504671	6.7241494	-4.8468016
C	0.2606235	6.7024306	-4.8338658
H	0.8165482	7.6537451	-4.8708194
C	6.0425703	0.7342718	-4.4686506
C	6.0188050	-0.6763359	-4.4433933
H	6.9677744	-1.2309010	-4.3525288
C	-1.3768881	-6.4365593	-4.6153583
H	-1.9353436	-7.3867180	-4.5915219
C	0.0355479	-6.4643131	-4.6135196
H	-5.8900159	2.7516551	-4.7999283
H	-5.9688368	-2.3098796	-4.8639133
H	-2.9962172	5.5441282	-4.8093974
H	2.0685117	5.4692511	-4.7540696
H	4.8635487	2.5795739	-4.5597105
H	4.7831716	-2.4861527	-4.5097935
H	-1.6743821	7.6930720	-4.8881869
H	-8.1216348	-0.9892603	-4.8850887
H	7.0093677	1.2598747	-4.3970844
H	1.8853161	-5.2923926	-4.6311508

**Au<sub>58</sub>-AuPc (TPSS)**

Au	5.2595290	1.6764350	-1.3620180
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Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470
Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710
Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300
Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360
Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280
Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020

Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380
Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
Au	0.1110942	-0.1263538	-4.9212584
C	2.6399430	-1.7883769	-4.9662102
C	4.0878580	-1.6384758	-4.9896374
C	4.3627860	-0.2536922	-4.9871123
C	3.0826026	0.4388539	-4.9694418

N	2.1026449	-0.5221008	-4.9546124
C	-1.5492682	-2.6522087	-4.9322521
C	-1.4035444	-4.0942179	-4.8783011
C	-0.0152608	-4.3729652	-4.8846649
C	0.6750377	-3.0977566	-4.9320754
N	-0.2865936	-2.1180576	-4.9508175
C	-2.4169533	1.5359632	-5.0000425
C	-3.8642212	1.3862966	-5.0399351
C	-4.1397557	0.0012731	-5.0549043
C	-2.8606355	-0.6911583	-5.0036623
N	-1.8804865	0.2698813	-4.9735798
C	1.7723968	2.4018655	-4.9637429
C	1.6263118	3.8451668	-4.9916680
C	0.2380467	4.1231852	-4.9924822
C	-0.4523653	2.8471327	-4.9685625
N	0.5105929	1.8654501	-4.9504360
N	2.9009258	1.7318559	-4.9789880
N	1.9733017	-2.9100999	-4.9580888
N	-2.6788428	-1.9836602	-4.9806106
N	-1.7497129	2.6570687	-4.9951443
C	-5.4544752	-0.4742382	-5.0981149
C	-0.2333835	5.4414155	-5.0441113
C	2.5706251	4.8779924	-5.0399112
C	5.6774838	0.2238958	-4.9862052
C	5.1229399	-2.5794750	-5.0000603
C	0.4542342	-5.6930893	-4.8554007
C	-2.3487434	-5.1271700	-4.8233698
C	-4.8986417	2.3291292	-5.0517522
C	-6.2132054	1.8513677	-5.0974511
H	-7.0462297	2.5655756	-5.1102660
C	-6.4873960	0.4690684	-5.1245460

C	0.7122002	6.4684596	-5.0976791
C	2.0960491	6.1910657	-5.0941438
H	2.8099530	7.0232818	-5.1367610
C	6.7110419	-0.7182168	-4.9931053
C	6.4370523	-2.1009548	-5.0031042
H	7.2721697	-2.8127564	-5.0059433
C	-1.8752201	-6.4420095	-4.7848536
H	-2.5899250	-7.2740392	-4.7478142
C	-0.4907249	-6.7211233	-4.8061523
H	-4.6775483	3.4037983	-5.0306114
H	-5.6590914	-1.5521149	-5.1115553
H	-1.3104256	5.6497626	-5.0458593
H	3.6445483	4.6531271	-5.0382994
H	5.8813694	1.3018511	-4.9758275
H	4.9010420	-3.6537480	-5.0016025
H	0.3746463	7.5115696	-5.1432886
H	-7.5301147	0.1288013	-5.1658206
H	7.7540393	-0.3776284	-4.9865427
H	1.5313994	-5.9012276	-4.8713409

### **Au<sub>58</sub>-AuPc (TPSS-D3)**

Au	5.2595290	1.6764350	-1.3620180
Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470
Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710

Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300
Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360
Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280
Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870

Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380
Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
Au	0.1906369	0.2064020	-4.5232471
C	1.5933479	-2.4807715	-4.5035559
C	2.9290980	-3.0471049	-4.4724188
C	3.8446342	-1.9615187	-4.4835285
C	3.0600268	-0.7441423	-4.5242828
N	1.7389535	-1.1122135	-4.5552366
C	-2.4880378	-1.1986452	-4.6233929
C	-3.0638390	-2.5283442	-4.5664286
C	-1.9855990	-3.4492050	-4.5095776
C	-0.7579357	-2.6732070	-4.5426429
N	-1.1220693	-1.3484164	-4.6126320
C	-1.2106978	2.8927137	-4.5630880
C	-2.5470512	3.4609250	-4.5865799
C	-3.4625313	2.3770030	-4.6192494

C	-2.6790287	1.1565609	-4.6123705
N	-1.3548699	1.5260113	-4.6044868
C	2.8708041	1.6119032	-4.5477195
C	3.4470731	2.9443627	-4.5708747
C	2.3693909	3.8655516	-4.5790411
C	1.1416951	3.0885815	-4.5561772
N	1.5049238	1.7614785	-4.5592123
N	3.5286278	0.4825464	-4.5119937
N	0.4622980	-3.1460285	-4.5015549
N	-3.1478581	-0.0686979	-4.6199983
N	-0.0794399	3.5583211	-4.5454220
C	-4.8452706	2.5971081	-4.6701766
C	2.6010089	5.2448695	-4.6169599
C	4.7747525	3.3819726	-4.5954434
C	5.2282005	-2.1792485	-4.4501614
C	3.3829209	-4.3726578	-4.4555407
C	-2.2166459	-4.8275502	-4.4041121
C	-4.3937325	-2.9681147	-4.5236840
C	-2.9985877	4.7860777	-4.6105495
C	-4.3805312	5.0023063	-4.6606258
H	-4.7648284	6.0297358	-4.6859798
C	-5.2908348	3.9223470	-4.6973024
C	3.9318088	5.6803405	-4.6570822
C	5.0035423	4.7626459	-4.6420326
H	6.0345151	5.1378380	-4.6700838
C	5.6767433	-3.5040743	-4.4145369
C	4.7659097	-4.5871972	-4.4171636
H	5.1530900	-5.6141832	-4.4076152
C	-4.6231548	-4.3455426	-4.4193055
H	-5.6540851	-4.7233088	-4.4010678
C	-3.5479176	-5.2638307	-4.3596109



H	-2.2831281	5.6172789	-4.5871170
H	-5.5456458	1.7519530	-4.6964964
H	1.7605301	5.9505012	-4.6196013
H	5.6015440	2.6606667	-4.5714139
H	5.9294252	-1.3344618	-4.4558540
H	2.6672637	-5.2042528	-4.4750016
H	4.1468747	6.7556078	-4.6936368
H	-6.3675212	4.1288088	-4.7385625
H	6.7548921	-3.7071557	-4.3908172
H	-1.3742269	-5.5309314	-4.3688814

### **Au<sub>58</sub>-H<sub>2</sub>Pc (PBE)**

Au	5.2595290	1.6764350	-1.3620180
Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470
Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710
Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300
Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360

Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280
Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380

Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
N	-1.3310957	1.0787158	-5.1099077
N	1.5276822	1.2043939	-5.0791893
N	0.0125726	3.0474962	-5.1059594
N	-3.1292103	-0.4867964	-5.0775084
N	3.5337273	-0.0854705	-5.0452264
N	-1.1236053	-1.7819010	-5.0765510
N	1.7364652	-1.6531231	-5.0665734
N	0.3924255	-3.6214440	-4.9690625
C	-2.4657991	3.0329167	-5.1452439
C	2.4599383	3.3127294	-5.0716437
C	-3.4066261	1.9738598	-5.1409647
C	3.5128863	2.3768520	-5.0560692
C	-1.1377406	2.4335712	-5.1208632
C	1.2229141	2.5196488	-5.0852391
C	-2.6558080	0.7263659	-5.1135189
C	2.8698172	1.0553675	-5.0599009
C	-3.1055966	-2.9394229	-4.8865884
C	3.8087056	-2.5461144	-4.9757411
C	-2.0538195	-3.8771941	-4.8491820
C	2.8693131	-3.6048116	-4.9616863
C	-2.4629545	-1.6260566	-5.0297268
C	3.0586831	-1.2989902	-5.0387197
C	-0.8182344	-3.0926335	-4.9759703

C	1.5417850	-3.0084983	-5.0088391
C	-2.8860086	4.3677412	-5.1644675
C	2.7133970	4.6847300	-5.0851556
C	-4.7821546	2.2331973	-5.1481772
C	4.8452743	2.7912391	-5.0524875
C	-4.2597580	4.6219265	-5.1767675
C	4.0509251	5.1033622	-5.0844198
C	-5.1960843	3.5677278	-5.1671033
C	5.1025518	4.1693864	-5.0669671
C	-4.4384368	-3.3445016	-4.7760223
C	5.1825725	-2.8020703	-4.9100383
C	-2.3102719	-5.2423560	-4.6925963
C	3.2885802	-4.9379218	-4.8882372
C	-4.6985973	-4.7138599	-4.6200970
C	5.5976036	-4.1336859	-4.8284109
C	-3.6469541	-5.6512276	-4.5783898
C	4.6614727	-5.1900144	-4.8213066
H	-0.5597872	0.3954893	-5.0650603
H	-2.1447273	5.1845091	-5.1673490
H	1.8800911	5.4073389	-5.0997379
H	-5.5060764	1.4005760	-5.1431116
H	5.6627259	2.0511207	-5.0438352
H	-4.6197785	5.6641990	-5.1930189
H	4.2835306	6.1810972	-5.0972568
H	-6.2737779	3.8023690	-5.1709101
H	6.1455665	4.5273207	-5.0698000
H	-5.2531506	-2.6012336	-4.8174704
H	5.9053444	-1.9696649	-4.9177744
H	-1.4794105	-5.9679281	-4.6739532
H	2.5462389	-5.7532599	-4.8891565
H	-5.7415174	-5.0668669	-4.5493555

H 6.6745680 -4.3638172 -4.7756665  
H -3.8818140 -6.7231734 -4.4681754

**Au<sub>58</sub>-H<sub>2</sub>Pc (PBE-D3)**

Au 5.2595290 1.6764350 -1.3620180  
Au 2.7826380 3.1718680 -1.3850780  
Au 2.7068820 0.3013020 -1.4063550  
Au 0.2672940 1.8085160 -1.4487060  
Au -2.2096280 3.3040890 -1.4716690  
Au -2.2853300 0.4336060 -1.4930470  
Au 2.6492610 -2.5815420 -1.4218810  
Au 0.1739110 -1.0865610 -1.4499360  
Au 0.0965830 -3.9565370 -1.4662210  
Au -2.3430580 -2.4494080 -1.5085710  
Au -4.8198970 -0.9538880 -1.5315320  
Au 0.3248850 4.6914960 -1.4332830  
Au -4.7485080 1.9418100 -1.5759660  
Au 5.1767570 -1.2184500 -1.3692300  
Au 7.7070890 0.1357210 -1.3040530  
Au 5.3381540 4.4788680 -1.4712660  
Au 2.9115150 6.0066420 -1.5139360  
Au -2.1203050 6.2307180 -1.4911920  
Au -4.6572730 4.8448560 -1.5296360  
Au -7.1930210 3.4806060 -1.6338590  
Au -4.9176690 -3.7456530 -1.4281100  
Au -2.4724700 -5.2850270 -1.3796000  
Au 2.5410960 -5.4953330 -1.4083280  
Au 5.0937750 -4.1203380 -1.3639880  
Au 7.6212700 -2.7572460 -1.3113370  
Au -7.3621820 -2.2068580 -1.4860030  
Au -7.2644100 0.5849070 -1.5894250  
Au 0.4670870 7.5453840 -1.5718270

Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380
Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
N	-1.2485199	1.6283759	-4.7407574

N	1.5969820	1.6132324	-4.6497524
N	0.1833657	3.5348797	-4.6896121
N	-3.1223978	0.1510438	-4.7725758
N	3.5331637	0.2174021	-4.6261045
N	-1.1856688	-1.2464646	-4.7602601
N	1.6613615	-1.2622655	-4.6981608
N	0.2282319	-3.1685118	-4.6786729
C	-2.2904940	3.6348843	-4.7603495
C	2.6422858	3.6673103	-4.6866666
C	-3.2806103	2.6202259	-4.7904517
C	3.6440725	2.6740623	-4.6577965
C	-0.9928593	2.9740561	-4.7230499
C	1.3640716	2.9441219	-4.6722176
C	-2.5884852	1.3390214	-4.7707815
C	2.9302609	1.3905271	-4.6395380
C	-3.2306598	-2.3017710	-4.6770441
C	3.6917523	-2.2514117	-4.6238541
C	-2.2295413	-3.2972225	-4.6425490
C	2.7029063	-3.2677539	-4.6530210
C	-2.5168412	-1.0214129	-4.7515842
C	2.9988827	-0.9709674	-4.6503085
C	-0.9515045	-2.5754249	-4.6988006
C	1.4053951	-2.6089209	-4.6857590
C	-2.6449813	4.9875091	-4.7784501
C	2.9707342	5.0220391	-4.7438535
C	-4.6409151	2.9419660	-4.8321225
C	4.9973276	3.0118959	-4.6740177
C	-4.0054701	5.3046655	-4.8223109
C	4.3305639	5.3642023	-4.7670744
C	-4.9907806	4.2952711	-4.8465579
C	5.3298092	4.3741031	-4.7253671

C	-4.5847633	-2.6373632	-4.6180082
C	5.0529686	-2.5706535	-4.5706684
C	-2.5599589	-4.6522290	-4.5594852
C	3.0604828	-4.6205564	-4.6386508
C	-4.9191781	-3.9973305	-4.5216181
C	5.4058281	-3.9237829	-4.5465107
C	-3.9197675	-4.9920777	-4.5021336
C	4.4214171	-4.9364062	-4.5864111
H	-0.5094524	0.9115493	-4.6776390
H	-1.8642856	5.7658914	-4.7510961
H	2.1773036	5.7873446	-4.7723905
H	-5.4030674	2.1447859	-4.8491600
H	5.7727655	2.2282969	-4.6439485
H	-4.3150688	6.3624148	-4.8338088
H	4.6230300	6.4260655	-4.8114238
H	-6.0560629	4.5784443	-4.8723941
H	6.3913736	4.6721638	-4.7410890
H	-5.3579235	-1.8503872	-4.6419821
H	5.8139306	-1.7725721	-4.5423134
H	-1.7669459	-5.4192942	-4.5504247
H	2.2802712	-5.3994526	-4.6699121
H	-5.9812756	-4.2944108	-4.4902252
H	6.4716102	-4.2043463	-4.505786

#### **Au<sub>58</sub>-H<sub>2</sub>Pc (TPSS)**

Au	5.2595290	1.6764350	-1.3620180
Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470



Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710
Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300
Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360
Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280
Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260

Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560
Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380
Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
N	-1.2459589	1.6031126	-4.9814071
N	1.6141639	1.5927079	-4.9185150
N	0.1925161	3.5091590	-4.9639961
N	-3.1253844	0.1310559	-4.9830638
N	3.5563473	0.2056188	-4.8964097
N	-1.1834378	-1.2579650	-4.9425509
N	1.6779152	-1.2688470	-4.9084625
N	0.2391779	-3.1739505	-4.8455068
C	-2.2811310	3.6119875	-5.0388716
C	2.6510279	3.6531439	-4.9316198

C	-3.2733019	2.6018682	-5.0529276
C	3.6564658	2.6657874	-4.9102341
C	-0.9853890	2.9482184	-4.9889976
C	1.3768784	2.9223457	-4.9341381
C	-2.5875016	1.3186268	-5.0084764
C	2.9485550	1.3788764	-4.9044116
C	-3.2233106	-2.3236319	-4.8250510
C	3.7052910	-2.2655804	-4.8548472
C	-2.2178065	-3.3116806	-4.7829017
C	2.7136050	-3.2767427	-4.8451842
C	-2.5158394	-1.0409204	-4.9275786
C	3.0177804	-0.9828833	-4.8914410
C	-0.9443794	-2.5844660	-4.8594110
C	1.4176379	-2.6141686	-4.8699979
C	-2.6321061	4.9668431	-5.0814532
C	2.9726186	5.0115913	-4.9709767
C	-4.6338858	2.9287630	-5.1039492
C	5.0093255	3.0122040	-4.9223080
C	-3.9906223	5.2887013	-5.1338524
C	4.3301902	5.3619589	-4.9870898
C	-4.9794400	4.2820280	-5.1426562
C	5.3345498	4.3760118	-4.9594768
C	-4.5768634	-2.6683155	-4.7720520
C	5.0673905	-2.5911318	-4.8283397
C	-2.5405134	-4.6697841	-4.6968496
C	3.0670503	-4.6320727	-4.8191040
C	-4.9035844	-4.0296475	-4.6752046
C	5.4157727	-3.9441631	-4.7940895
C	-3.8980112	-5.0179888	-4.6441217
C	4.4270854	-4.9531185	-4.7941348
H	-0.5148445	0.8818410	-4.9239853

H	-1.8558239	5.7422554	-5.0769290
H	2.1820775	5.7724392	-4.9981114
H	-5.3959280	2.1393215	-5.1169553
H	5.7871144	2.2378705	-4.9097958
H	-4.2960801	6.3421592	-5.1702893
H	4.6164084	6.4210618	-5.0251938
H	-6.0380190	4.5687922	-5.1826404
H	6.3892855	4.6801773	-4.9772165
H	-5.3539103	-1.8941629	-4.8143951
H	5.8291590	-1.8012441	-4.8387135
H	-1.7503104	-5.4320555	-4.6912989
H	2.2906508	-5.4077305	-4.8288351
H	-5.9588284	-4.3336049	-4.6547607
H	6.4757609	-4.2292871	-4.7790007
H	-4.1859424	-6.0760988	-4.5927864

### **Au<sub>58</sub>-H<sub>2</sub>Pc (TPSS-D3)**

Au	5.2595290	1.6764350	-1.3620180
Au	2.7826380	3.1718680	-1.3850780
Au	2.7068820	0.3013020	-1.4063550
Au	0.2672940	1.8085160	-1.4487060
Au	-2.2096280	3.3040890	-1.4716690
Au	-2.2853300	0.4336060	-1.4930470
Au	2.6492610	-2.5815420	-1.4218810
Au	0.1739110	-1.0865610	-1.4499360
Au	0.0965830	-3.9565370	-1.4662210
Au	-2.3430580	-2.4494080	-1.5085710
Au	-4.8198970	-0.9538880	-1.5315320
Au	0.3248850	4.6914960	-1.4332830
Au	-4.7485080	1.9418100	-1.5759660
Au	5.1767570	-1.2184500	-1.3692300

Au	7.7070890	0.1357210	-1.3040530
Au	5.3381540	4.4788680	-1.4712660
Au	2.9115150	6.0066420	-1.5139360
Au	-2.1203050	6.2307180	-1.4911920
Au	-4.6572730	4.8448560	-1.5296360
Au	-7.1930210	3.4806060	-1.6338590
Au	-4.9176690	-3.7456530	-1.4281100
Au	-2.4724700	-5.2850270	-1.3796000
Au	2.5410960	-5.4953330	-1.4083280
Au	5.0937750	-4.1203380	-1.3639880
Au	7.6212700	-2.7572460	-1.3113370
Au	-7.3621820	-2.2068580	-1.4860030
Au	-7.2644100	0.5849070	-1.5894250
Au	0.4670870	7.5453840	-1.5718270
Au	7.7826670	2.9400730	-1.4133730
Au	-0.0279570	-6.8238220	-1.3217070
Au	-5.7202900	-2.2102450	0.8725870
Au	-3.2617370	-3.7342480	0.9455020
Au	-3.1510680	-0.8656090	0.8736410
Au	-0.7294540	-2.4011700	0.9264340
Au	1.7290990	-3.9251730	0.9993490
Au	1.8397150	-1.0566180	0.9274890
Au	-3.0585890	2.0156320	0.8069260
Au	-0.6000360	0.4916300	0.8798400
Au	-0.4893670	3.3602690	0.8079790
Au	1.9322470	1.8247070	0.8607720
Au	4.3908000	0.3007040	0.9336870
Au	-0.8219860	-5.2824950	0.9931510
Au	4.2860090	-2.5942790	0.9403620
Au	-5.6027050	0.6828580	0.8146660
Au	-4.9051860	-0.7978090	3.1392560

Au	-2.4647880	-2.3513730	3.1980300
Au	-2.3212280	0.5167320	3.2003290
Au	0.0823780	-1.0474290	3.2383630
Au	2.5226890	-2.6009380	3.2972350
Au	2.6662810	0.2670260	3.2994380
Au	-2.1955830	3.3975000	3.2077760
Au	0.2447280	1.8439920	3.2666480
Au	0.3883740	4.7120410	3.2688500
Au	2.7919780	3.1478810	3.3069830
Au	5.2322910	1.5943710	3.3657550
Au	-0.0432670	-3.9282010	3.2308160
Au	5.0949050	-1.2984980	3.2978380
Au	-4.7545370	2.0943060	3.1561060
N	-1.2396111	1.3277309	-4.5727489
N	1.6097440	1.4396560	-4.4972411
N	0.1094937	3.2997676	-4.5290259
N	-3.0616356	-0.2239908	-4.6119923
N	3.6119124	0.1333539	-4.5255112
N	-1.0592550	-1.5297309	-4.6002708
N	1.7929790	-1.4165905	-4.5706925
N	0.4419232	-3.3890933	-4.5360831
C	-2.3657546	3.2886149	-4.6108586
C	2.5602924	3.5405667	-4.5387764
C	-3.3127380	2.2330458	-4.6367295
C	3.6079205	2.5924712	-4.5279100
C	-1.0412458	2.6833749	-4.5637346
C	1.3167935	2.7605084	-4.5135503
C	-2.5710154	0.9841989	-4.6067146
C	2.9545000	1.2788753	-4.5081788
C	-3.0543823	-2.6793381	-4.5034417
C	3.8633791	-2.3250522	-4.5300693

C	-2.0061311	-3.6270549	-4.4750151
C	2.9148006	-3.3795105	-4.5371885
C	-2.4020471	-1.3676564	-4.5865740
C	3.1211844	-1.0747298	-4.5491376
C	-0.7647813	-2.8477580	-4.5433825
C	1.5921130	-2.7741132	-4.5540650
C	-2.7776788	4.6262923	-4.6454605
C	2.8247481	4.9096164	-4.6081191
C	-4.6886516	2.4941780	-4.6758100
C	4.9448632	2.9898261	-4.5703104
C	-4.1514912	4.8838216	-4.6972951
C	4.1682711	5.3114659	-4.6614644
C	-5.0937524	3.8323122	-4.7113939
C	5.2125836	4.3667047	-4.6331929
C	-4.3935821	-3.0776735	-4.4379049
C	5.2371880	-2.5889245	-4.4771310
C	-2.2705049	-4.9970881	-4.3687348
C	3.3224230	-4.7184984	-4.5094809
C	-4.6631486	-4.4520421	-4.3276697
C	5.6408953	-3.9278025	-4.4288411
C	-3.6146182	-5.3993507	-4.2951692
C	4.6958143	-4.9800366	-4.4510456
H	-0.4773919	0.6406849	-4.4967982
H	-2.0363708	5.4349791	-4.6240251
H	2.0017902	5.6357303	-4.6255047
H	-5.4133258	1.6694443	-4.6900316
H	5.7524669	2.2465826	-4.5534433
H	-4.5052046	5.9220529	-4.7277756
H	4.4114786	6.3799474	-4.7186517
H	-6.1643630	4.0708399	-4.7399633
H	6.2539145	4.7115524	-4.6731223

H	-5.1997176	-2.3324233	-4.4672143
H	5.9648574	-1.7673029	-4.4589028
H	-1.4473280	-5.7238366	-4.3622600
H	2.5776131	-5.5242632	-4.5346522
H	-5.7043793	-4.8008417	-4.3011701
H	6.7112207	-4.1662739	-4.3824558
H	-3.8585465	-6.4674170	-4.2288946