Quantum Dot (Au_n/Ag_n, n = 3-8) Capped Single Lipids: Interactions and Physicochemical Properties

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Supplementary Table ST1: DMPC- Au/Ag clusters interactions energy (in Kcal/mol) (For different sites).

Cluster		Au			Ag	
	Choline	Carboxylate	Phosphate	Choline	Carboxylate	Phosphate
QD3	4.83	-16.06	-28.74	8.97	-8.91	-20.14
QD4-a	-2.07	-16.38	-29.87	-1.69	-10.48	-27.23
QD4-b	-1.63	-14.37	-11.61	-0.88	-9.29	-9.35
QD5-a	-5.84	NS	-28.36	0.50	NS	-16.82
QD5-b	5.40	-17.88	-32.57	11.73	-9.48	-21.77
QD5-c	-2.26	-8.72	-21.08	-0.69	-5.84	-10.60
Qd5-d	NS	NS	-28.55	NS	NS	-23.59
QD6-a	-2.38	-8.78	-21.34	-1.07	-2.38	-16.32
QD7-a	-2.45	-3.14	-17.13	-0.63	-2.57	-15.12
QD7-b	-2.20	-4.96	-18.01	-1.32	-3.76	-16.13
QD7-c	-1.94	-6.53	-17.26	-0.25	-5.02	-13.74
QD8-a	-2.32	-5.65	-21.46	-1.00	-3.07	-18.26
QD8-b	-1.57	-2.45	-9.79	-1.19	-2.13	-13.62

Supplementary Table ST2: DMPE- Au/Ag clusters interactions energy (in Kcal/mol) (for different sites).

Cluster	Au			Ag		
	Ethanolamine	Carboxylate	Phosphate	Ethanolamine	Carboxylate	Phosphate
QD3	-0.63	-13.80	-20.33	-0.06	-7.84	-13.99
QD4-a	-3.01	-15.56	-21.71	-2.45	-10.54	-15.50
QD4-b	-0.19	-11.73	-6.90	-0.63	-9.91	-5.71
QD5-a	-1.94	NS	-18.70	-1.00	NS	-11.55
QD5-b	3.20	-16.88	-24.97	-3.07	-11.55	-14.24
QD5-c	-1.07	-1.26	-12.68	-2.51	-5.27	-9.73
Qd5-d	NS	NS	-21.08	NS	NS	-16.38
QD6-a	-2.32	-2.20	-13.36	-1.32	-4.52	-10.54
QD7-a	-1.57	-1.26	-12.61	0.19	-5.08	-10.48
QD7-b	-2.57	-6.02	-9.22	-1.32	-2.95	-7.09
QD7-c	-1.69	-5.52	-10.10	-0.25	-5.02	-9.10
QD8-a	-1.44	-4.83	-8.60	-1.00	-2.38	-7.72
QD8-b	-2.51	-2.89	-5.65	-2.07	-4.89	-11.11

Supplementary Table ST3: DMPG- Au/Ag clusters interactions energy (in Kcal/mol) (for different sites).

Cluster	Au			Ag		
	Glycerol	Carboxylate	Phosphate	Glycerol	Carboxylate	Phosphate
QD3	5.33	-14.50	-34.58	7.09	-10.04	-23.53
QD4-a	-22.34	-15.31	-40.35	-9.98	-10.79	-30.62
QD4-b	-3.70	-12.05	-9.41	-9.91	-11.11	0.75
QD5-a	1.76	NS	-27.42	1.63	NS	-16.75
QD5-b	3.26	-18.51	-43.42	10.98	-11.86	-31.38
QD5-c	-4.27	-9.54	-17.38	-2.45	-6.71	-10.92
Qd5-d	NS	NS	NS	NS	NS	-26.67
QD6-a	-1.69	-2.32	-22.90	-4.64	-2.76	-15.37
QD7-a	-3.32	-2.51	-10.73	-1.94	-1.51	-8.34
QD7-b	-2.26	NS	NS	-5.52	-1.38	-16.75
QD7-c	-0.88	-6.59	-8.66	-5.08	-5.71	-17.38
QD8-a	-3.01	-5.52	-15.37	-1.07	-4.02	-11.36
QD8-b	-7.40	-2.89	-22.72	-6.53	-4.77	-16.69

Supplementary Table ST4: (a) Relative Energies (in kcal/mol) for DMPC/DMPE/DMPG lipid with different conformer of Au cluster

Cluster	Cluster-Shape	DMPC			DMPE			DMPG		
		Ch	Ca	Ph	Ch	Ca	Ph	Ch	Ca	Ph
Au4a	Pendate	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Au4b	Planar	1.6943	3.2630	19.5155	4.0788	5.0828	16.0642	19.8920	4.5181	32.1912
Au5a	Linear	15.6250	NS	11.9227	18.3233	NS	13.1777	25.2259	NS	15.2485
Au5b	Pendate	27.6104	10.7932	8.4714	24.2218	4.3298	7.6556	27.4849	10.9814	0.0
Au5c	Planar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	6.0868
Au5d	TBP	NS	NS	14.9347	NS	NS	13.9934	NS	NS	NS
Au7a	Planar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
Au7b	PBP	17.3820	15.3112	16.2525	16.1270	12.3619	20.5195	18.1978	NS	NS
Au7c	Bicapped-TBP	16.3152	12.4247	15.6877	15.6877	11.5462	18.3233	18.2605	11.7344	17.8840
Au8a	Planar	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.3805
Au8b	Bicapped-Oh	6.7143	9.1616	17.6330	4.8946	7.9066	0.0142	1.5688	8.5969	0.0

(b) **Relative Energies (in kcal/mol) for DMPG with different conformers of Au cluster (single point calculation, 6-311G** for C, H, O, P, Na; RECP19|SD for Au)**

DMPG-Au cluster	Relative Energy (Kcal/mol)
DMPG-Au4a-Ca	0.0
DMPG-Au4b-Ca	4.4553
DMPG-Au8a-Ch	0.0
DMPG-Au8b-Ch	0.8157

Supplementary Table ST5: Bond lengths (in Å) for DMPC, DMPE and DMPG with Au Qds (for different sites of interaction).

Gold-Cluster	DMPC			DMPE			DMPG		
	Choline	Carboxylate	Phosphate	Choline	Carboxylate	Phosphate	Choline	Carboxylate	Phosphate
Au3	2.257	2.283	2.217	2.359	2.323	2.265	2.381	2.311	2.176
Au4a	3.479	2.264	2.201	2.756	2.284	2.258	2.362	2.279	2.163
Au4b	2.743	2.296	2.348	2.348	2.322	2.428	2.412	2.319	2.35
Au5a	2.992		2.207	2.684		2.274	2.35		2.181
Au5b	2.35	2.257	2.204	2.35	2.273	2.249	2.745	2.265	2.155
Au5c	3.229	2.414	2.275	2.43	3.037	2.358	2.579	2.426	2.233
Au5d			2.226			2.259			
Au6a	3.424	2.424	2.257	3.141	2.898	2.348	3.613	2.912	2.238
Au7a	3.083	2.79	2.47	2.436	2.752	2.337	3.059	2.884	2.368
Au7b	3.003	2.497	2.325	2.386	NS	2.378	2.699		
Au7c	3.432	2.531	2.297	2.41	2.511	2.409	2.422	2.5	2.354
Au8a	3.228	2.595	2.418	2.426	2.628	2.444	2.984	2.612	2.335
Au8b	3.152	2.757	2.353	2.503	2.966	2.356	2.649	2.93	2.247

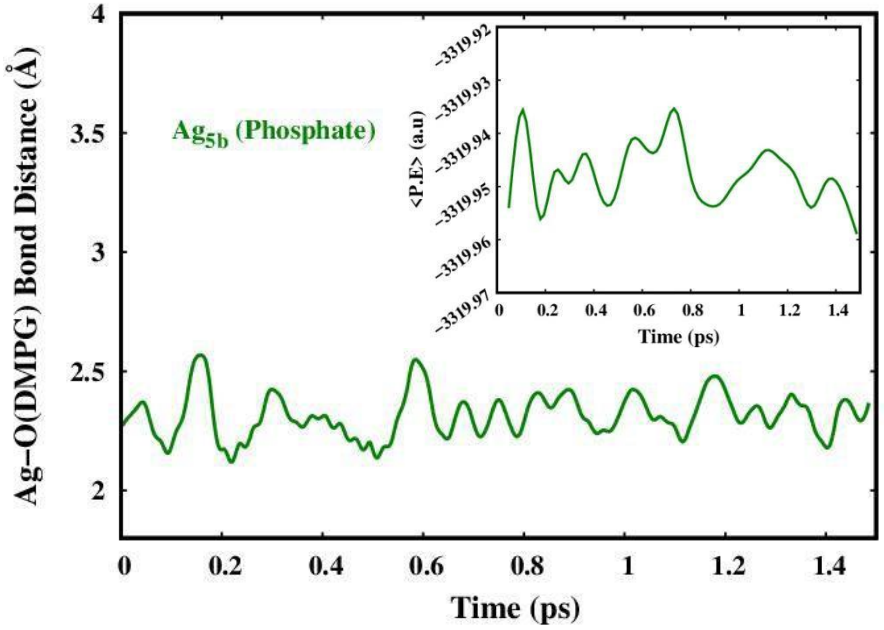
Supplementary Table ST6: DMPC - Au/Ag charge transfer.

Cluster	Au			Ag		
	Choline	Carboxylate	Phosphate	Choline	Carboxylate	Phosphate
Qd3	-0.1727	-0.3131	-0.422	-0.159	-0.3586	-0.4687
Qd4-a	-0.1833		-0.4653	-0.1717		-0.507
Qd4-b	-0.0547	-0.369	-0.4766	-0.0576	-0.4214	-0.6031
Qd4-c	-0.1203	-0.3431	-0.4547	-0.0801	-0.3858	-0.501
Qd5-a	-0.1022		-0.4755	-0.1104		-0.5108
Qd5-b	-0.0463	-0.4006	-0.4847	-0.1398	-0.4408	-0.5435
Qd5-c	-0.1032	-0.107	-0.4756	-0.0849	-0.1131	-0.5145
Qd5-d			-0.5311			-0.5892
Qd6-c	-0.0832	-0.3121	-0.432	-0.0801	-0.3426	-0.475
Qd6-e	-0.195	-0.3885	-0.4729	-0.1889	-0.4368	-0.5128
Qd7-c	-0.0857	-0.3225	-0.4308	-0.0958	-0.422	-0.48
Qd7-d	-0.082	-0.2641	-0.4616	-0.0816	-0.3644	-0.4926
Qd7-f	-0.061	-0.3394	-0.453	-0.0626	-0.3812	-0.501
Qd8-c	-0.0719	-0.3532	-0.4649	-0.0489	-0.3883	-0.5169
Qd8-f	-0.0969	-0.3753	-0.4493	-0.0829	-0.3784	-0.4932

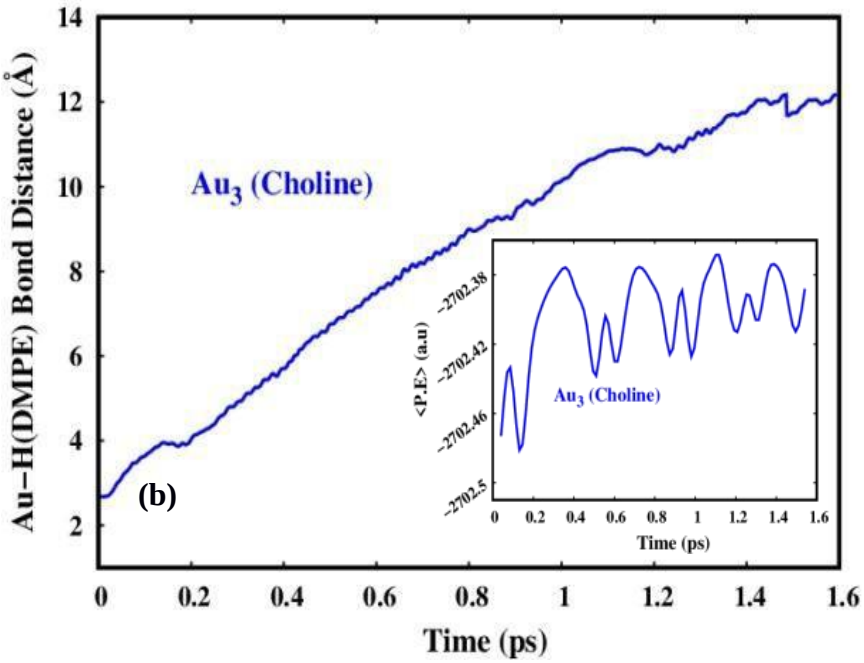
Supplementary Table ST7: PO_2^- stretching frequencies for Qd-Lipid complexes.

Au_n	**PO_2^- Stretching Frequency (cm^{-1})**			**Ag_n**	**PO_2^- Stretching Frequency (cm^{-1})**		
	DMPC	**DMPE**	**DMPG**		**DMPC**	**DMPE**	**DMPG**
Au_3	1008.8	952.4	979.1	Ag_3	1031.2	943.2	1013.7
Au_{4b}	985.2	965.5	968.2	Ag_{4b}	1012.8	944.2	1012.6
Au_{4c}	1018.0	937.2	996.2	Ag_{4c}	1024.2	937.9	987.6
Au_{5a}	990.3	950.3	965.8	Ag_{5a}	1018.8	941.0	1004.2
Au_{5b}	1010.2	966.7	973.2	Ag_{5b}	1029.3	945.0	1015.0
Au_{5c}	999.6	946.6	999.5	Ag_{5c}	1026.6	941.7	1012.4
Au_{5d}	995.6	956.7		Ag_{5d}	1028.8	950.5	1011.9
Au_{6c}	1003.8	951.1	975.8	Ag_{6c}	1021.3	946.2	1009.0
Au_{7c}	987.9	951.8	1013.4	Ag_{7c}	1025.5	939.3	1020.1
Au_{7d}	1002.8	940.8		Ag_{7d}	1023.7	933.5	1010.3
Au_{7f}	998.9	941.0	1009.2	Ag_{7f}	1020.5	938.4	1008.7
Au_{8c}	991.7	938.2	992.7	Ag_{8c}	1001.2	938.2	1011.1
Au_{8d}	1016.9	946.2	980.0	Ag_{8d}	1024.3	936.2	1013.9

Supplementary Figure SF1: Bond length fluctuations and short-time averaged potential energies for $Ag_{(5b)}$-DMPG (ph).



Supplementary Figure SF2: Bond length fluctuations and short time averaged potential energies as a function of steps for Au_3-DMPE (ch).



Cartesian coordinates of selected Qd-Lipid complexes:

1) Phosphate site

a) Au_{5b}-DMPG

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C	-1.739546	-3.315406	-31.053960
C	-2.103940	-3.250030	-29.553571
C	-3.627493	-3.287258	-29.290733
C	-4.001125	-3.230015	-27.790801
C	-5.526705	-3.272206	-27.534927
C	-5.908959	-3.224062	-26.036464
C	-7.435768	-3.261593	-25.789971
C	-7.826087	-3.218827	-24.292549
C	-9.356932	-3.222972	-24.059557
C	-9.769377	-3.180358	-22.567126
C	-11.304085	-3.136667	-22.364250
C	-11.735513	-3.134876	-20.878607
C	-13.278210	-3.075161	-20.719343
C	-13.739122	-3.208006	-19.268080
O	-13.197284	-2.679728	-18.295865
O	-14.860602	-4.007670	-19.195987
C	-15.347582	-4.416841	-17.871660
C	-15.085261	-5.934971	-17.717657
O	-13.691177	-6.228977	-18.030538
C	-13.455198	-6.932958	-19.201079
O	-14.340720	-7.399114	-19.913226
C	-16.860717	-4.155616	-17.793456
O	-17.209364	-2.778780	-17.446991
P	-17.351908	-2.344829	-15.862503
O	-18.213752	-1.095483	-15.807880
O	-15.805624	-2.050817	-15.360903
C	-15.081286	-0.911101	-15.936038
C	-14.547557	0.000553	-14.808605
O	-13.571680	0.924399	-15.352618
C	-15.593440	0.930382	-14.146036
O	-16.578080	0.241557	-13.321176
O	-17.732216	-3.624995	-15.056861
C	-11.956621	-7.048469	-19.461856
C	-11.616955	-7.103317	-20.969899
C	-10.095410	-7.154245	-21.229882
C	-9.740128	-7.175446	-22.734863
C	-8.217595	-7.170162	-23.000849
C	-7.850720	-7.197082	-24.502149
C	-6.326078	-7.160544	-24.757311
C	-5.948688	-7.205014	-26.255653
C	-4.424082	-7.161825	-26.508304
C	-4.048656	-7.214283	-28.007273
C	-2.525362	-7.161755	-28.268715
C	-2.155166	-7.209811	-29.769958

C	-0.633632	-7.128382	-30.029883
Na	-18.825198	0.022741	-13.980687
H	-15.053562	1.685578	-13.547354
H	-0.646316	-3.288748	-31.202324
H	-0.408443	-7.171740	-31.109676
H	-14.803034	-3.850922	-17.104902
H	-15.734063	-6.527364	-18.378848
H	-15.242823	-6.224084	-16.667788
H	-13.768511	-3.860764	-21.314424
H	-11.446281	-6.208490	-18.964059
H	-17.313292	-4.332994	-18.780082
H	-15.721061	-0.336911	-16.626629
H	-14.089120	-0.644385	-14.028706
H	-12.112383	-7.978011	-21.422470
H	-17.309524	-4.840158	-17.056909
H	-11.282022	-2.281303	-20.347659
H	-2.175957	-2.465248	-31.607541
H	-0.100399	-7.962778	-29.540197
H	-2.118639	-4.244486	-31.514724
H	-0.213311	-6.185659	-29.636640
H	-14.233677	-1.332190	-16.502884
H	-12.044483	-6.215203	-21.468943
H	-11.352512	-4.046154	-20.385447
H	-11.608231	-7.971082	-18.960441
H	-13.653189	-2.104671	-21.093745
H	-2.554728	-8.141349	-30.213053
H	-1.682077	-2.327811	-29.111928
H	-1.624968	-4.094014	-29.023804
H	-2.659935	-6.376653	-30.293209
H	-5.434132	-4.074859	-25.513008
H	-6.427664	-6.354902	-26.776536
H	-5.942987	-4.192629	-27.987123
H	-10.194688	-8.067314	-23.206026
H	-4.006702	-6.240467	-26.059139
H	-9.357080	-4.067104	-22.049754
H	-9.793563	-4.125783	-24.529118
H	-8.326660	-6.336250	-25.008954
H	-4.536021	-6.370670	-28.531679
H	-3.518876	-4.075481	-27.264728
H	-7.373033	-4.084420	-23.772601
H	-10.198735	-6.297158	-23.227381
H	-8.278548	-8.105820	-24.967084
H	-6.367975	-8.122343	-26.710880
H	-7.772532	-6.270832	-22.533015
H	-7.855871	-4.176232	-26.250450
H	-5.487720	-2.307194	-25.581689
H	-9.309842	-2.298123	-22.082479
H	-4.049333	-4.208417	-29.736701
H	-7.755034	-8.040285	-22.496628
H	-9.804064	-2.355785	-24.582684
H	-2.110733	-6.237250	-27.821987
H	-5.904739	-6.243473	-24.302036

H	-7.389081	-2.313522	-23.828732
H	-4.463951	-8.137885	-28.454253
H	-3.941527	-8.006186	-25.980013
H	-6.006864	-2.425347	-28.062195
H	-3.580572	-2.308197	-27.344760
H	-11.758259	-4.007876	-22.873951
H	-9.665441	-8.048076	-20.737839
H	-5.848322	-8.011907	-24.234904
H	-7.908853	-2.408978	-26.313873
H	-4.109146	-2.442080	-29.819254
H	-2.033402	-8.004583	-27.745128
H	-11.712252	-2.239153	-22.867043
H	-9.611636	-6.277767	-20.756069
H	-12.907820	0.408626	-15.853927
H	-16.170840	1.453671	-14.924414
H	-16.112580	-0.230815	-12.602668
Au	-19.293291	-3.752446	-13.576648
Au	-20.876789	-1.931349	-12.067815
Au	-21.049841	0.746422	-12.072680
Au	-21.087460	-4.644417	-11.805982
Au	-19.674873	2.964874	-12.687956

b) Au_{8b} - DMPE

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C	-1.569707	-3.566362	-31.201939
C	-1.933056	-3.482216	-29.701990
C	-3.458017	-3.479628	-29.445319
C	-3.838668	-3.411491	-27.948342
C	-5.365350	-3.414407	-27.702511
C	-5.753190	-3.357807	-26.206212
C	-7.282251	-3.362984	-25.972131
C	-7.686947	-3.306497	-24.480617
C	-9.217818	-3.294098	-24.259846
C	-9.625865	-3.236586	-22.769229
C	-11.157469	-3.212304	-22.553062
C	-11.561686	-3.221952	-21.061226
C	-13.098007	-3.213592	-20.871112
C	-13.519158	-3.354329	-19.410225
O	-12.876597	-2.948491	-18.442083
O	-14.731849	-4.007086	-19.322331
C	-15.234202	-4.380299	-17.991419
C	-15.254264	-5.923432	-17.923513
O	-13.895128	-6.405666	-18.153436
C	-13.634769	-6.978709	-19.388914
O	-14.502547	-7.273926	-20.204632
C	-16.640704	-3.790609	-17.814338
O	-16.597811	-2.362166	-17.491142
P	-16.531196	-1.925627	-15.912468
O	-16.939435	-0.387955	-16.033998
O	-14.946193	-1.955652	-15.481150

C	-13.997865	-0.981119	-16.054184
C	-13.708013	0.118369	-15.017218
N	-14.957222	0.872900	-14.633234
O	-17.303861	-2.846430	-14.992115
C	-12.131524	-7.169941	-19.577314
C	-11.726003	-7.184563	-21.068975
C	-10.196053	-7.221145	-21.277509
C	-9.803392	-7.236575	-22.773192
C	-8.276632	-7.233915	-23.015869
C	-7.897585	-7.269941	-24.515156
C	-6.372443	-7.262088	-24.769163
C	-5.994833	-7.320788	-26.268259
C	-4.468055	-7.314361	-26.518121
C	-4.085493	-7.377870	-28.015888
C	-2.558915	-7.364372	-28.267579
C	-2.175567	-7.425123	-29.765357
C	-0.649851	-7.397834	-30.013443
H	-16.291812	0.197955	-15.482420
H	-14.835300	1.881470	-14.780981
H	-15.158323	0.741333	-13.634771
H	-0.476343	-3.568123	-31.350208
H	-0.420595	-7.441610	-31.092244
H	-14.546809	-3.981359	-17.232644
H	-15.933706	-6.362933	-18.668571
H	-15.536430	-6.246306	-16.910355
H	-13.574327	-4.019247	-21.451871
H	-11.607997	-6.371696	-19.026078
H	-17.205611	-3.865915	-18.753617
H	-14.395283	-0.558816	-16.991057
H	-13.258008	-0.342869	-14.123009
H	-12.198309	-8.047681	-21.566936
H	-17.181735	-4.330361	-17.015552
H	-11.120602	-2.355828	-20.540136
H	-1.984735	-2.708945	-31.760848
H	-0.150637	-8.254570	-29.527008
H	-1.971900	-4.488868	-31.656722
H	-0.195777	-6.474874	-29.611509
H	-12.963125	0.809767	-15.448047
H	-13.085704	-1.545440	-16.295132
H	-12.140023	-6.285313	-21.559133
H	-11.142529	-4.120795	-20.574368
H	-11.849729	-8.120992	-19.088549
H	-13.522298	-2.262413	-21.244067
H	-2.603047	-8.342073	-30.212993
H	-1.488583	-2.568255	-29.264572
H	-1.476753	-4.335548	-29.166624
H	-2.645537	-6.574773	-30.293237
H	-5.299658	-4.219171	-25.680458
H	-6.453115	-6.461417	-26.792856
H	-5.803868	-4.323193	-28.157020
H	-10.250902	-8.125940	-23.255949
H	-4.030069	-6.403014	-26.067502

H	-9.198323	-4.109954	-22.241257
H	-9.659517	-4.197480	-24.722060
H	-8.356076	-6.403195	-25.027668
H	-4.548475	-6.523633	-28.545059
H	-3.383192	-4.268678	-27.417514
H	-7.250632	-4.174938	-23.952215
H	-10.251487	-6.357121	-23.273275
H	-8.337925	-8.172545	-24.979928
H	-6.436057	-8.229449	-26.720703
H	-7.834972	-6.332807	-22.548081
H	-7.716321	-4.271145	-26.432530
H	-5.314592	-2.449682	-25.749582
H	-9.175780	-2.341162	-22.300344
H	-3.900282	-4.390898	-29.891628
H	-7.822117	-8.102575	-22.501709
H	-9.657539	-2.429167	-24.792511
H	-2.123886	-6.450471	-27.819123
H	-5.932256	-6.351510	-24.319810
H	-7.244673	-2.405511	-24.014231
H	-4.521766	-8.291352	-28.463678
H	-4.009696	-8.170765	-25.987595
H	-5.821325	-2.555371	-28.231277
H	-3.397858	-2.500921	-27.499218
H	-11.607929	-4.088824	-23.056434
H	-9.772004	-8.111796	-20.775913
H	-5.911089	-8.119596	-24.242659
H	-7.732986	-2.504134	-26.504928
H	-3.915192	-2.623942	-29.978997
H	-2.093336	-8.217634	-27.737766
H	-11.585019	-2.318551	-23.047003
H	-9.735204	-6.341770	-20.787164
Au	-21.204709	-2.976326	-11.687121
Au	-19.202072	-3.111686	-13.622238
Au	-21.501006	-3.423637	-15.985910
Au	-21.292476	-5.241299	-13.627379
Au	-23.264490	-4.962527	-11.741510
Au	-23.509817	-3.286317	-14.044211
Au	-21.410515	-1.323794	-14.026786
Au	-19.332748	-5.234864	-15.544429

2) Glycerol Site

a) Au_{4a}-DMPG

116

C	-1.761805	-3.576678	-31.286271
C	-2.133899	-3.486532	-29.788440
C	-3.657515	-3.510811	-29.523211
C	-4.024296	-3.436135	-28.022533

C	-5.547468	-3.468097	-27.757704
C	-5.922239	-3.402374	-26.258375
C	-7.448380	-3.433888	-26.006102
C	-7.830369	-3.371517	-24.508969
C	-9.356596	-3.387804	-24.263833
C	-9.737658	-3.321423	-22.767730
C	-11.264628	-3.308371	-22.525248
C	-11.632873	-3.263968	-21.026742
C	-13.162933	-3.253915	-20.788749
C	-13.518123	-3.320521	-19.305863
O	-12.843516	-2.823953	-18.401038
O	-14.685552	-4.020834	-19.114091
C	-15.075045	-4.335970	-17.731850
C	-14.958995	-5.867681	-17.565363
O	-13.597832	-6.276473	-17.910020
C	-13.431482	-6.967214	-19.100604
O	-14.358276	-7.373133	-19.796321
C	-16.519291	-3.863126	-17.498547
O	-16.637389	-2.410610	-17.574589
P	-16.534454	-1.514290	-16.195105
O	-16.771401	-0.046948	-16.538397
O	-14.891483	-1.710652	-15.744826
C	-13.927423	-0.710956	-16.179755
C	-13.309496	-0.049427	-14.928352
O	-12.392628	1.042539	-15.362059
C	-14.321052	0.631386	-13.979332
O	-15.266647	-0.274055	-13.357193
O	-17.301082	-2.099457	-15.009677
C	-11.945133	-7.146362	-19.405864
C	-11.644593	-7.212152	-20.924459
C	-10.128412	-7.262458	-21.225834
C	-9.801973	-7.305107	-22.738963
C	-8.282273	-7.285984	-23.034849
C	-7.938651	-7.337462	-24.543289
C	-6.418292	-7.306589	-24.829927
C	-6.067099	-7.370275	-26.335099
C	-4.545455	-7.340098	-26.613358
C	-4.188657	-7.409024	-28.117168
C	-2.667419	-7.374184	-28.394387
C	-2.311548	-7.438497	-29.898100
C	-0.791299	-7.385894	-30.169341
Na	-17.547361	0.319299	-14.334206
H	-13.773640	1.142908	-13.171288
H	-0.666913	-3.553993	-31.425179
H	-0.575778	-7.434417	-31.250081
H	-14.386627	-3.819252	-17.050227
H	-15.675158	-6.403508	-18.205743
H	-15.111121	-6.135855	-16.509094
H	-13.654625	-4.090624	-21.310229
H	-11.391557	-6.326587	-18.920620
H	-17.181862	-4.257490	-18.284446
H	-14.424786	0.060359	-16.792462

H	-12.698080	-0.774954	-14.363742
H	-12.150335	-8.091843	-21.356519
H	-16.868282	-4.224117	-16.515970
H	-11.181645	-2.377732	-20.549667
H	-2.189962	-2.733884	-31.857629
H	-0.270125	-8.229503	-29.683120
H	-2.138437	-4.512322	-31.736285
H	-0.350197	-6.450066	-29.783660
H	-13.153462	-1.224974	-16.774560
H	-12.088027	-6.329351	-21.418920
H	-11.195194	-4.141806	-20.518473
H	-11.617735	-8.082059	-18.914608
H	-13.604543	-2.323078	-21.190679
H	-2.732507	-8.365120	-30.332283
H	-1.707448	-2.559546	-29.361436
H	-1.659727	-4.324810	-29.245066
H	-2.805531	-6.599183	-30.421738
H	-5.449118	-4.248523	-25.725479
H	-6.550131	-6.523451	-26.857664
H	-5.974007	-4.389791	-28.196959
H	-10.252970	-8.210780	-23.187384
H	-4.115139	-6.416863	-26.180372
H	-9.293444	-4.185891	-22.238419
H	-9.789939	-4.303721	-24.710209
H	-8.422195	-6.485345	-25.057597
H	-4.672194	-6.565111	-28.644953
H	-3.544323	-4.277680	-27.488796
H	-7.365121	-4.223748	-23.978147
H	-10.279924	-6.441037	-23.238479
H	-8.374551	-8.253585	-24.985403
H	-6.500424	-8.289729	-26.772670
H	-7.837891	-6.373471	-22.592165
H	-7.871375	-4.355147	-26.450599
H	-5.497848	-2.481479	-25.814692
H	-9.288564	-2.416972	-22.314397
H	-4.088108	-4.433017	-29.958324
H	-7.801045	-8.141407	-22.522871
H	-9.820023	-2.534176	-24.794877
H	-2.239227	-6.450516	-27.959544
H	-5.985458	-6.385719	-24.395077
H	-7.399512	-2.455955	-24.060312
H	-4.617745	-8.331988	-28.552616
H	-4.061447	-8.183562	-26.084351
H	-6.027618	-2.624519	-28.289364
H	-3.597799	-2.512124	-27.587630
H	-11.714245	-4.208975	-22.985329
H	-9.683080	-8.146253	-20.729963
H	-5.930336	-8.150989	-24.306793
H	-7.923826	-2.588528	-26.540081
H	-4.135009	-2.667522	-30.058341
H	-2.178784	-8.216629	-27.867533
H	-11.713565	-2.439752	-23.044023

H	-9.636776	-6.377268	-20.777875
H	-11.854251	0.708399	-16.111765
H	-14.870501	1.401068	-14.561967
H	-15.277908	-1.112387	-13.879918
Au	-14.271991	5.501585	-16.599686
Au	-13.399347	3.097540	-15.946771
Au	-16.004317	3.979745	-15.089010
Au	-18.044819	3.234519	-13.596944

b) Au_3-DMPE

112

C	-1.569560	-3.566297	-31.201871
C	-1.933110	-3.482214	-29.701992
C	-3.458014	-3.479699	-29.445340
C	-3.838600	-3.411502	-27.948278
C	-5.365364	-3.414502	-27.702525
C	-5.753218	-3.357900	-26.206299
C	-7.282286	-3.363032	-25.972312
C	-7.687007	-3.306695	-24.480709
C	-9.217907	-3.294264	-24.259847
C	-9.625910	-3.236700	-22.769145
C	-11.157462	-3.212578	-22.552939
C	-11.561925	-3.222137	-21.061402
C	-13.097968	-3.213751	-20.871304
C	-13.519883	-3.354888	-19.409653
O	-12.876409	-2.949079	-18.442252
O	-14.731037	-4.007220	-19.322985
C	-15.234464	-4.380289	-17.991242
C	-15.254661	-5.923260	-17.923542
O	-13.894620	-6.406800	-18.154239
C	-13.634895	-6.978411	-19.388078
O	-14.502791	-7.274614	-20.205133
C	-16.642000	-3.790082	-17.812147
O	-16.596608	-2.362244	-17.495535
P	-16.539754	-1.937470	-15.903155
O	-16.938781	-0.384281	-16.034772
O	-14.941957	-1.953622	-15.482692
C	-13.999074	-0.982593	-16.053290
C	-13.708821	0.115068	-15.016766
N	-14.959143	0.861364	-14.633251
O	-17.306436	-2.844277	-14.994031
C	-12.131469	-7.170222	-19.577468
C	-11.726017	-7.184776	-21.069029
C	-10.196061	-7.221346	-21.277611
C	-9.803386	-7.236645	-22.773329
C	-8.276595	-7.234017	-23.016046
C	-7.897326	-7.270177	-24.515293
C	-6.372221	-7.262212	-24.769276
C	-5.994734	-7.320820	-26.268353
C	-4.467996	-7.314491	-26.518174

C	-4.085493	-7.377860	-28.016002
C	-2.558926	-7.364363	-28.267647
C	-2.175645	-7.425108	-29.765408
C	-0.649813	-7.397839	-30.013437
H	-16.292862	0.196639	-15.483603
H	-14.835248	1.883606	-14.782347
H	-15.157445	0.740698	-13.633888
H	-0.476204	-3.568146	-31.350222
H	-0.420561	-7.441608	-31.092182
H	-14.547039	-3.981531	-17.232758
H	-15.933670	-6.362815	-18.668770
H	-15.536231	-6.246127	-16.910301
H	-13.574566	-4.019326	-21.451864
H	-11.608137	-6.371774	-19.026129
H	-17.205558	-3.866268	-18.753929
H	-14.395460	-0.558721	-16.991038
H	-13.257368	-0.342804	-14.123001
H	-12.198367	-8.047775	-21.567075
H	-17.180962	-4.329353	-17.015727
H	-11.120744	-2.355846	-20.540031
H	-1.984814	-2.708875	-31.760901
H	-0.150699	-8.254674	-29.526998
H	-1.971892	-4.488930	-31.656720
H	-0.195932	-6.474804	-29.611506
H	-12.962812	0.810475	-15.448220
H	-13.085360	-1.544944	-16.294875
H	-12.139886	-6.285463	-21.559310
H	-11.142582	-4.120874	-20.574467
H	-11.849735	-8.121261	-19.088680
H	-13.522433	-2.262572	-21.244003
H	-2.603144	-8.342048	-30.212982
H	-1.488588	-2.568322	-29.264680
H	-1.476865	-4.335465	-29.166641
H	-2.645610	-6.574728	-30.293295
H	-5.299791	-4.219151	-25.680366
H	-6.453135	-6.461324	-26.792930
H	-5.804007	-4.323362	-28.157046
H	-10.250740	-8.126102	-23.256083
H	-4.030036	-6.403057	-26.067690
H	-9.198384	-4.110122	-22.241338
H	-9.659594	-4.197683	-24.722182
H	-8.356160	-6.403153	-25.027725
H	-4.548441	-6.523526	-28.545155
H	-3.383206	-4.268817	-27.417529
H	-7.250549	-4.175032	-23.952067
H	-10.251466	-6.357059	-23.273382
H	-8.338148	-8.172688	-24.979995
H	-6.435974	-8.229569	-26.720712
H	-7.834968	-6.332875	-22.548252
H	-7.716402	-4.271283	-26.432431
H	-5.314799	-2.449824	-25.749534
H	-9.175804	-2.341141	-22.300236

H	-3.900443	-4.391054	-29.891659
H	-7.822127	-8.102606	-22.501881
H	-9.657482	-2.429149	-24.792541
H	-2.123883	-6.450423	-27.819168
H	-5.932230	-6.351435	-24.319678
H	-7.244536	-2.405457	-24.014328
H	-4.521696	-8.291449	-28.463817
H	-4.009504	-8.170886	-25.987584
H	-5.821409	-2.555353	-28.231232
H	-3.397826	-2.500788	-27.499247
H	-11.607997	-4.089102	-23.056697
H	-9.771983	-8.112044	-20.775931
H	-5.911028	-8.119661	-24.242741
H	-7.733175	-2.503900	-26.504968
H	-3.915207	-2.623868	-29.978976
H	-2.093250	-8.217808	-27.737731
H	-11.584914	-2.318697	-23.047015
H	-9.735289	-6.341809	-20.787317
Au	-14.816699	6.087466	-14.617257
Au	-16.196678	3.885075	-13.632871
Au	-13.547635	3.760363	-15.403010

3) Carboxylate site

a) Au_{5b}-DMPG

117

C	-1.596522	-3.508246	-31.143248
C	-1.963661	-3.429568	-29.644427
C	-3.488524	-3.433314	-29.388282
C	-3.868556	-3.369303	-27.890801
C	-5.395408	-3.379160	-27.644596
C	-5.781914	-3.322747	-26.148445
C	-7.309878	-3.328446	-25.912093
C	-7.706170	-3.272593	-24.418983
C	-9.235586	-3.261160	-24.191442
C	-9.636662	-3.206443	-22.699014
C	-11.167142	-3.177023	-22.475861
C	-11.561324	-3.166456	-20.982448
C	-13.094131	-3.152013	-20.771683
C	-13.484023	-3.304691	-19.303859
O	-12.799915	-2.940750	-18.347801
O	-14.709755	-3.929470	-19.192997
C	-15.183240	-4.265768	-17.843511
C	-15.086055	-5.798893	-17.673238
O	-13.717413	-6.231158	-18.028444
C	-13.526332	-6.847314	-19.214499
O	-14.483574	-7.130255	-19.967738

C	-16.644466	-3.802156	-17.700271
O	-16.754317	-2.353706	-17.684257
P	-16.693052	-1.560373	-16.229006
O	-17.004033	-0.083753	-16.485655
O	-15.095306	-1.747603	-15.754022
C	-14.110990	-0.749646	-16.144902
C	-13.681198	0.102631	-14.925830
O	-12.561163	0.951439	-15.291175
C	-14.745717	1.092749	-14.385819
O	-15.761532	0.467962	-13.527761
O	-17.517160	-2.259066	-15.141354
C	-12.053401	-7.107484	-19.497659
C	-11.691738	-7.114801	-21.004290
C	-10.163155	-7.170271	-21.241875
C	-9.790370	-7.196895	-22.742805
C	-8.264223	-7.202234	-22.997983
C	-7.893116	-7.245775	-24.500219
C	-6.368108	-7.237515	-24.760477
C	-5.988462	-7.288887	-26.259499
C	-4.460171	-7.278028	-26.507594
C	-4.086524	-7.335560	-28.008256
C	-2.564241	-7.321270	-28.273735
C	-2.191422	-7.375316	-29.773217
C	-0.665007	-7.345689	-30.013681
Na	-17.905067	-0.088818	-14.332108
H	-14.219431	1.878587	-13.816596
H	-0.502874	-3.502714	-31.289643
H	-0.423391	-7.386639	-31.089948
H	-14.543831	-3.755904	-17.111703
H	-15.813180	-6.335972	-18.296423
H	-15.206119	-6.069741	-16.615112
H	-13.586586	-3.949791	-21.350891
H	-11.478089	-6.339131	-18.957830
H	-17.232940	-4.138497	-18.568235
H	-14.498684	-0.093715	-16.941413
H	-13.390597	-0.587228	-14.102190
H	-12.181769	-7.973164	-21.498419
H	-17.076279	-4.233750	-16.779732
H	-11.113742	-2.295738	-20.474763
H	-2.016389	-2.652528	-31.700982
H	-0.170606	-8.202757	-29.522418
H	-1.991847	-4.432134	-31.600757
H	-0.218309	-6.422539	-29.603499
H	-13.241806	-1.309152	-16.531476
H	-12.101414	-6.205963	-21.479694
H	-11.137602	-4.058894	-20.486720
H	-11.794186	-8.077625	-19.033352
H	-13.525056	-2.198464	-21.128852
H	-2.619206	-8.290178	-30.224514
H	-1.523356	-2.515502	-29.204204
H	-1.504985	-4.281450	-29.109715
H	-2.662072	-6.523014	-30.297229

H	-5.327274	-4.183336	-25.622405
H	-6.445725	-6.427839	-26.783618
H	-5.830317	-4.290171	-28.098802
H	-10.242597	-8.089510	-23.214631
H	-4.023211	-6.366014	-26.056332
H	-9.207892	-4.082676	-22.175833
H	-9.679668	-4.162850	-24.655732
H	-8.354039	-6.380989	-25.013180
H	-4.553802	-6.478555	-28.528999
H	-3.408666	-4.225540	-27.361961
H	-7.265165	-4.139733	-23.891726
H	-10.239295	-6.318283	-23.243398
H	-8.338024	-8.149068	-24.959437
H	-6.423387	-8.198370	-26.717042
H	-7.814588	-6.301111	-22.538177
H	-7.745308	-4.237168	-26.370254
H	-5.343649	-2.414357	-25.692354
H	-9.182059	-2.313066	-22.230334
H	-3.928594	-4.344891	-29.836459
H	-7.809606	-8.071697	-22.485349
H	-9.676200	-2.394255	-24.719965
H	-2.124324	-6.409744	-27.826597
H	-5.927820	-6.329112	-24.307384
H	-7.261258	-2.370797	-23.956740
H	-4.526188	-8.246838	-28.457173
H	-3.996648	-8.135095	-25.981436
H	-5.855341	-2.522040	-28.173357
H	-3.431663	-2.456931	-27.441157
H	-11.622223	-4.057834	-22.968941
H	-9.739748	-8.062464	-20.742897
H	-5.905847	-8.097171	-24.238994
H	-7.762586	-2.468722	-26.442562
H	-3.948654	-2.577445	-29.919015
H	-2.092261	-8.176399	-27.753260
H	-11.594043	-2.288417	-22.978520
H	-9.687662	-6.291319	-20.765531
H	-11.904041	0.397766	-15.760350
H	-15.304180	1.546357	-15.216832
H	-15.300567	-0.119639	-12.895389
Au	-15.073288	-8.886264	-21.271749
Au	-17.492104	-10.182577	-20.648959
Au	-18.974721	-9.500714	-18.536904
Au	-21.142357	-9.118575	-17.026633
Au	-15.821667	-10.911028	-22.798876

b) Au_{5c} - DMPE

114

C	-1.565663	-3.572011	-31.201584
C	-1.939490	-3.481320	-29.705039

C	-3.465379	-3.478252	-29.454806
C	-3.848814	-3.405972	-27.958412
C	-5.376667	-3.409387	-27.715642
C	-5.767254	-3.346336	-26.219881
C	-7.296913	-3.349320	-25.985715
C	-7.697763	-3.289673	-24.492490
C	-9.228119	-3.277786	-24.264516
C	-9.631089	-3.224177	-22.771807
C	-11.162352	-3.187544	-22.553683
C	-11.562883	-3.178161	-21.061098
C	-13.096293	-3.141390	-20.860186
C	-13.506579	-3.280360	-19.394329
O	-12.826190	-2.944842	-18.425280
O	-14.757492	-3.854029	-19.307777
C	-15.253475	-4.268554	-17.988378
C	-15.291749	-5.814213	-17.972605
O	-13.948588	-6.327100	-18.243915
C	-13.684024	-6.788039	-19.516857
O	-14.540147	-6.917983	-20.392317
C	-16.662385	-3.689422	-17.785841
O	-16.630426	-2.265621	-17.459559
P	-16.570809	-1.855707	-15.863147
O	-16.974101	-0.304043	-15.978831
O	-14.971565	-1.872500	-15.449680
C	-14.026958	-0.917911	-16.045666
C	-13.713174	0.198399	-15.034585
N	-14.944216	0.990135	-14.674125
O	-17.333738	-2.777630	-14.967228
C	-12.194851	-7.088897	-19.673546
C	-11.750336	-7.128134	-21.152627
C	-10.218082	-7.204646	-21.331414
C	-9.800139	-7.229162	-22.820449
C	-8.268608	-7.224424	-23.030286
C	-7.862170	-7.260563	-24.521825
C	-6.334281	-7.248092	-24.766519
C	-5.966993	-7.305678	-26.269768
C	-4.443770	-7.300728	-26.536993
C	-4.072666	-7.366909	-28.037531
C	-2.546625	-7.359036	-28.291009
C	-2.161347	-7.421743	-29.788267
C	-0.633979	-7.400481	-30.032151
H	-16.313958	0.275757	-15.446345
H	-14.826301	1.976383	-14.928835
H	-15.095761	0.963847	-13.659997
H	-0.471083	-3.571034	-31.341341
H	-0.401135	-7.447120	-31.110222
H	-14.560235	-3.901578	-17.218650
H	-16.001331	-6.211784	-18.713396
H	-15.548747	-6.166798	-16.962565
H	-13.592000	-3.943270	-21.430596
H	-11.638920	-6.326766	-19.102452
H	-17.237368	-3.767330	-18.721326

H	-14.429764	-0.508439	-16.987472
H	-13.283459	-0.254133	-14.126169
H	-12.231426	-7.985149	-21.653832
H	-17.180010	-4.242627	-16.984260
H	-11.101366	-2.317611	-20.547755
H	-1.979926	-2.719605	-31.768758
H	-0.138803	-8.258711	-29.543647
H	-1.960901	-4.498354	-31.654423
H	-0.177813	-6.477815	-29.631446
H	-12.941239	0.856237	-15.471833
H	-13.118149	-1.489675	-16.283455
H	-12.127258	-6.221918	-21.658487
H	-11.159791	-4.081803	-20.569557
H	-11.991848	-8.055730	-19.176116
H	-13.513144	-2.188555	-21.237024
H	-2.590346	-8.337785	-30.237007
H	-1.497749	-2.565500	-29.269082
H	-1.486779	-4.332177	-29.163120
H	-2.626131	-6.569875	-30.319094
H	-5.314911	-4.205916	-25.689925
H	-6.433759	-6.446327	-26.787667
H	-5.813875	-4.321002	-28.166593
H	-10.238071	-8.121414	-23.306897
H	-4.002640	-6.388389	-26.091954
H	-9.209859	-4.104104	-22.249417
H	-9.671831	-4.179810	-24.728409
H	-8.314417	-6.393609	-25.040361
H	-4.535426	-6.511502	-28.565538
H	-3.394625	-4.262134	-27.424335
H	-7.257203	-4.156250	-23.963787
H	-10.241159	-6.354571	-23.335624
H	-8.293516	-8.164306	-24.994462
H	-6.415976	-8.214437	-26.714719
H	-7.842254	-6.320230	-22.553999
H	-7.730993	-4.259165	-26.443171
H	-5.328495	-2.436911	-25.766119
H	-9.172706	-2.334362	-22.299295
H	-3.908164	-4.390799	-29.898623
H	-7.825903	-8.092741	-22.505526
H	-9.669451	-2.410455	-24.792454
H	-2.108410	-6.446451	-27.842677
H	-5.894830	-6.336342	-24.317670
H	-7.253548	-2.386668	-24.031450
H	-4.513574	-8.279724	-28.482548
H	-3.982168	-8.156639	-26.008322
H	-5.832748	-2.552926	-28.248910
H	-3.409600	-2.493441	-27.510936
H	-11.620192	-4.065502	-23.048794
H	-9.821525	-8.104202	-20.823159
H	-5.867959	-8.104787	-24.242342
H	-7.747521	-2.490782	-26.520107
H	-3.922051	-2.623581	-29.990753

H	-2.084417	-8.214606	-27.761280
H	-11.581904	-2.295514	-23.057148
H	-9.744042	-6.334929	-20.836846
Au	-16.170157	-8.952334	-21.949632
Au	-14.433364	-13.193275	-20.700487
Au	-15.174854	-11.405994	-22.702549
Au	-15.613844	-10.673335	-19.932999
Au	-14.868484	-12.473842	-18.051014

Optimized co-ordinates for silver quantum dots

Phosphate site

a) Ag_{5b}-DMPG

117

C	-1.421095	-3.366663	-31.219801
C	-1.798952	-3.313923	-29.721864
C	-3.324151	-3.347430	-29.464269
C	-3.697079	-3.301631	-27.963347
C	-5.221411	-3.336092	-27.700502
C	-5.593860	-3.307217	-26.197911
C	-7.120252	-3.345754	-25.945385
C	-7.516015	-3.335193	-24.448336
C	-9.048764	-3.360949	-24.231878
C	-9.485780	-3.349324	-22.746235
C	-11.025417	-3.352143	-22.575802
C	-11.496114	-3.378953	-21.102331
C	-13.044270	-3.373924	-20.991274
C	-13.544266	-3.541037	-19.557272
O	-13.041465	-3.005842	-18.566701
O	-14.646293	-4.365995	-19.521667
C	-15.171733	-4.785933	-18.212345
C	-14.892275	-6.299067	-18.048808
O	-13.484511	-6.573082	-18.322001
C	-13.205805	-7.277828	-19.481409
O	-14.063236	-7.777362	-20.205757
C	-16.692217	-4.550131	-18.183452
O	-17.074727	-3.189312	-17.828023
P	-17.241072	-2.790273	-16.229343
O	-18.166150	-1.581699	-16.168625
O	-15.700225	-2.358818	-15.762343
C	-15.062721	-1.227018	-16.450049
C	-14.198112	-0.457044	-15.429007
O	-13.239665	0.389536	-16.107986
C	-14.989251	0.520656	-14.528231
O	-16.155035	-0.079015	-13.885193
O	-17.537239	-4.062653	-15.412646
C	-11.700476	-7.340187	-19.720093
C	-11.347146	-7.333514	-21.226335

C	-9.823873	-7.347002	-21.478018
C	-9.461407	-7.328004	-22.980764
C	-7.938504	-7.302207	-23.238761
C	-7.568477	-7.300601	-24.738871
C	-6.044460	-7.262522	-24.991322
C	-5.667499	-7.286957	-26.489033
C	-4.143155	-7.252396	-26.738702
C	-3.769379	-7.292549	-28.237268
C	-2.247126	-7.246425	-28.498019
C	-1.881036	-7.282056	-29.999648
C	-0.360149	-7.199836	-30.259463
Na	-18.416653	-0.026020	-14.619548
H	-14.313293	0.940040	-13.762568
H	-0.325806	-3.342800	-31.354264
H	-0.135568	-7.232199	-31.339484
H	-14.660651	-4.213519	-17.427292
H	-15.515067	-6.903000	-18.725183
H	-15.076290	-6.583747	-17.001660
H	-13.485669	-4.165972	-21.615106
H	-11.222467	-6.501791	-19.188537
H	-17.106191	-4.723186	-19.188400
H	-15.820231	-0.564688	-16.900862
H	-13.682372	-1.205302	-14.791493
H	-11.822992	-8.200983	-21.713135
H	-17.152190	-5.253536	-17.470926
H	-11.086609	-2.515753	-20.551513
H	-1.848755	-2.510757	-31.771580
H	0.170848	-8.039412	-29.776275
H	-1.795696	-4.290783	-31.693942
H	0.060512	-6.261052	-29.857608
H	-14.416742	-1.637675	-17.242318
H	-11.790133	-6.436370	-21.695634
H	-11.098330	-4.281639	-20.604955
H	-11.330800	-8.269449	-19.248087
H	-13.441649	-2.411413	-21.364028
H	-2.283646	-8.209536	-30.449181
H	-1.375435	-2.397637	-29.269037
H	-1.326071	-4.165415	-29.198323
H	-2.386674	-6.443679	-30.514031
H	-5.118235	-4.167185	-25.689781
H	-6.140372	-6.426286	-26.998059
H	-5.647751	-4.246995	-28.162236
H	-9.903028	-8.214344	-23.474618
H	-3.718371	-6.339372	-26.279617
H	-9.059968	-4.232122	-22.232808
H	-9.465507	-4.261208	-24.723032
H	-8.041208	-6.429961	-25.232057
H	-4.252422	-6.441180	-28.753159
H	-3.220732	-4.155525	-27.445873
H	-7.057212	-4.206283	-23.943252
H	-9.927836	-6.444382	-23.456170
H	-7.997406	-8.199829	-25.221200

H	-6.092163	-8.194599	-26.958769
H	-7.501794	-6.408030	-22.753716
H	-7.542814	-4.250006	-26.424346
H	-5.167294	-2.397431	-25.733428
H	-9.060266	-2.460671	-22.242401
H	-3.749358	-4.262945	-29.918854
H	-7.471393	-8.178183	-22.749128
H	-9.500630	-2.492264	-24.748541
H	-1.827410	-6.328976	-28.042249
H	-5.621470	-6.353189	-24.522860
H	-7.091696	-2.435827	-23.962457
H	-4.190374	-8.209206	-28.693302
H	-3.668444	-8.106920	-26.219766
H	-5.699793	-2.479295	-28.213012
H	-3.269183	-2.387476	-27.508701
H	-11.442034	-4.231691	-23.103726
H	-9.380566	-8.244252	-21.004607
H	-5.567644	-8.122200	-24.482675
H	-7.592091	-2.481002	-26.450263
H	-3.801754	-2.495324	-29.985244
H	-1.759657	-8.096841	-27.982810
H	-11.449818	-2.461298	-23.077748
H	-9.360096	-6.473158	-20.980171
H	-12.647370	-0.188224	-16.631583
H	-15.370618	1.350935	-15.145273
H	-15.907637	-0.983774	-13.601688
Ag	-18.948109	-4.232364	-13.673475
Ag	-20.261433	-2.273659	-12.018549
Ag	-20.502768	0.507853	-12.373841
Ag	-20.425659	-5.086313	-11.514900
Ag	-19.927943	2.774147	-13.876581

b) Ag_{4b}-DMPE

113

C	-1.432474	-3.825266	-31.445502
C	-1.796657	-3.741261	-29.945764
C	-3.321666	-3.738964	-29.688966
C	-3.701658	-3.670469	-28.191543
C	-5.228749	-3.673793	-27.946098
C	-5.617155	-3.617019	-26.450007
C	-7.146336	-3.621566	-26.216290
C	-7.550073	-3.565658	-24.724100
C	-9.081347	-3.553344	-24.503188
C	-9.489096	-3.495641	-23.012138
C	-11.020819	-3.472211	-22.796692
C	-11.425131	-3.481035	-21.305043
C	-12.961084	-3.473037	-21.114353

C	-13.382464	-3.613143	-19.652837
O	-12.742431	-3.208224	-18.682585
O	-14.596028	-4.262946	-19.566298
C	-15.096427	-4.639234	-18.236353
C	-15.117085	-6.182937	-18.167159
O	-13.758130	-6.664805	-18.397079
C	-13.498200	-7.237965	-19.631959
O	-14.367805	-7.532796	-20.447295
C	-16.504640	-4.054115	-18.056476
O	-16.467702	-2.623228	-17.735020
P	-16.392727	-2.185810	-16.157923
O	-16.806540	-0.643756	-16.266874
O	-14.808096	-2.214480	-15.721221
C	-13.861867	-1.241265	-16.294557
C	-13.572893	-0.141186	-15.260456
N	-14.825118	0.610043	-14.880528
O	-17.162281	-3.102062	-15.245828
C	-11.995033	-7.429617	-19.821246
C	-11.589253	-7.443971	-21.313027
C	-10.059210	-7.480681	-21.521345
C	-9.666583	-7.495263	-23.017418
C	-8.139719	-7.492685	-23.260262
C	-7.760413	-7.529289	-24.759486
C	-6.234805	-7.520901	-25.012802
C	-5.857584	-7.579522	-26.512026
C	-4.330888	-7.573878	-26.761926
C	-3.948911	-7.636848	-28.259842
C	-2.422242	-7.623506	-28.510917
C	-2.039494	-7.683993	-30.008867
C	-0.513651	-7.657047	-30.256442
H	-16.154200	-0.056237	-15.723419
H	-14.699885	1.617435	-15.025846
H	-15.018632	0.485706	-13.880378
H	-0.338837	-3.827289	-31.593699
H	-0.283846	-7.700729	-31.335098
H	-14.408712	-4.242170	-17.476821
H	-15.796610	-6.620797	-18.913427
H	-15.398819	-6.504140	-17.152751
H	-13.439645	-4.278020	-21.694613
H	-11.472240	-6.631122	-19.269430
H	-17.070492	-4.124607	-18.996809
H	-14.260294	-0.820067	-17.232594
H	-13.121301	-0.599751	-14.365779
H	-12.061988	-8.306794	-21.811203
H	-17.043966	-4.591651	-17.260477
H	-10.984663	-2.614635	-20.783237
H	-1.848146	-2.967979	-32.004480
H	-0.014722	-8.514269	-29.770323
H	-1.834756	-4.747897	-31.900012
H	-0.060402	-6.733519	-29.854849
H	-12.827772	0.549267	-15.691779
H	-12.950268	-1.804822	-16.535936

H	-12.002279	-6.544831	-21.804322
H	-11.006123	-4.380034	-20.818556
H	-11.713521	-8.381156	-19.332922
H	-13.386767	-2.522434	-21.486900
H	-2.467404	-8.600857	-30.456344
H	-1.351843	-2.827417	-29.508741
H	-1.340719	-4.594317	-29.410009
H	-2.509473	-6.833555	-30.537025
H	-5.164109	-4.478007	-25.923186
H	-6.316240	-6.719965	-27.036695
H	-5.667843	-4.582746	-28.400440
H	-10.112894	-8.385279	-23.500261
H	-3.892912	-6.662117	-26.312379
H	-9.061891	-4.369861	-22.485181
H	-9.523172	-4.456936	-24.965951
H	-8.219441	-6.662309	-25.271449
H	-4.411456	-6.781995	-28.789086
H	-3.246536	-4.528357	-27.661109
H	-7.113382	-4.433925	-24.194963
H	-10.114652	-6.615463	-23.517616
H	-8.202467	-8.431766	-25.223639
H	-6.298653	-8.488707	-26.963939
H	-7.697858	-6.591643	-22.792783
H	-7.580297	-4.530523	-26.675361
H	-5.179237	-2.709113	-25.992625
H	-9.039118	-2.599837	-22.542902
H	-3.764604	-4.650418	-30.135037
H	-7.685569	-8.361535	-22.746360
H	-9.520287	-2.687925	-25.036096
H	-1.987250	-6.709248	-28.062955
H	-5.795344	-6.610111	-24.562378
H	-7.107045	-2.664243	-24.258770
H	-4.384546	-8.550546	-28.708167
H	-3.871775	-8.430196	-26.231253
H	-5.685040	-2.814419	-28.474320
H	-3.260887	-2.759134	-27.743047
H	-11.471180	-4.348647	-23.301188
H	-9.635445	-8.371735	-21.019762
H	-5.773689	-8.378903	-24.486732
H	-7.597430	-2.761790	-26.748423
H	-3.778491	-2.882690	-30.222161
H	-1.956501	-8.477239	-27.981359
H	-11.447536	-2.578314	-23.290763
H	-9.598902	-6.600641	-21.031540
Ag	-19.060250	-3.255591	-13.609763
Ag	-21.056996	-4.490970	-11.951009
Ag	-22.996061	-3.006757	-10.373247
Ag	-20.963964	-1.797956	-12.027504

Cartesian coordinates for lowest energy conformers of Au with DMPC, DMPE and DMPG

1) Au4a-Pendate-DMPC-Choline

C	1.896966	-2.435856	-2.842709
N	1.134400	-3.454611	-1.991879
C	1.431092	-4.912273	-2.447590
C	1.271483	-5.264549	-3.932705
O	-0.111612	-5.285475	-4.329888
P	-0.622513	-4.188862	-5.547799
O	0.108559	-4.836624	-6.907016
C	-0.522988	-5.990836	-7.522409
C	0.067828	-7.317443	-7.017395
C	-0.811484	-8.507607	-7.457208
O	-0.141567	-9.755987	-7.087479
C	0.348548	-10.532543	-8.120907
O	0.113567	-10.328257	-9.309691
C	1.598418	-3.341647	-0.547576
C	-0.364398	-3.141640	-2.042394
O	-2.127401	-4.344407	-5.588658
O	0.089990	-2.865617	-5.275092
O	1.398651	-7.502892	-7.624637
C	2.461095	-7.801017	-6.810289
O	2.418439	-7.831617	-5.577896
C	3.708256	-8.091939	-7.644336
C	4.629677	-9.152646	-6.994559
C	5.801562	-9.554871	-7.917230
C	6.738770	-10.613167	-7.289178
C	7.876752	-11.057467	-8.237601
C	8.838926	-12.093280	-7.610837
C	9.965177	-12.539157	-8.572239
C	10.944707	-13.562456	-7.951394
C	12.064870	-14.003354	-8.922715
C	13.052331	-15.025314	-8.311954
C	14.167437	-15.461740	-9.290819
C	15.155869	-16.488282	-8.689549

C	16.264224	-16.919999	-9.676768
H	16.950689	-17.650382	-9.214785
C	1.216096	-11.665031	-7.573931
C	2.374226	-12.035894	-8.531470
C	3.325984	-13.093504	-7.930200
C	4.476173	-13.479809	-8.889430
C	5.462916	-14.505717	-8.286177
C	6.590744	-14.921138	-9.259204
C	7.578871	-15.942979	-8.650745
C	8.697981	-16.378880	-9.625253
C	9.683004	-17.400653	-9.010259
C	10.803401	-17.844347	-9.980007
C	11.785254	-18.865242	-9.359099
C	12.911071	-19.308844	-10.322403
C	13.888531	-20.327227	-9.692537
H	14.676371	-20.621866	-10.407045
H	0.175812	-7.303818	-5.925307
H	-0.996495	-8.502261	-8.540918
H	-1.764027	-8.482487	-6.907427
H	3.391816	-8.403687	-8.652123
H	1.595125	-11.371492	-6.581994
H	-0.354871	-5.897047	-8.607371
H	1.875736	-4.603151	-4.574405
H	0.764609	-5.548880	-1.844990
H	1.956136	-12.397950	-9.485376
H	-1.607014	-5.974856	-7.317849
H	5.012578	-8.768919	-6.033701
H	16.864619	-16.052837	-10.005053
H	13.358951	-21.243506	-9.376332
H	15.832096	-17.388690	-10.578586
H	14.384738	-19.902898	-8.801798
H	2.475736	-5.102582	-2.152932

H	1.679220	-6.285264	-4.040060
H	2.948313	-11.123561	-8.774143
H	4.032145	-10.049577	-6.751649
H	0.558635	-12.540434	-7.418216
H	4.253500	-7.137053	-7.764892
H	12.458833	-19.746686	-11.232252
H	15.618739	-16.058196	-7.781291
H	14.593287	-17.380968	-8.358564
H	13.475212	-18.417382	-10.654340
H	10.378460	-14.453162	-7.619536
H	9.259723	-15.485577	-9.958076
H	11.606149	-14.440615	-9.830243
H	4.047604	-13.889194	-9.823894
H	10.140937	-16.962747	-8.102505
H	6.142826	-11.498689	-6.997051
H	7.433836	-11.483416	-9.158429
H	7.147748	-14.019847	-9.578574
H	11.368290	-16.953880	-10.315497
H	12.491359	-15.918827	-7.978330
H	8.260259	-12.980239	-7.290090
H	5.031208	-12.566696	-9.177158
H	6.141126	-15.348765	-10.175843
H	8.240411	-16.814191	-10.534359
H	5.911680	-14.082220	-7.366830
H	9.511847	-12.976216	-9.482588
H	11.399873	-13.126732	-7.041151
H	7.174310	-10.209440	-6.355085
H	13.705428	-15.893895	-10.199465
H	4.903796	-15.407607	-7.970656
H	8.454669	-10.168288	-8.555451
H	12.238976	-18.427242	-8.448992
H	8.036723	-15.508712	-7.741144

H	9.287587	-11.666300	-6.693193
H	10.347413	-18.282712	-10.888614
H	9.119454	-18.291894	-8.672880
H	12.626645	-13.110908	-9.260041
H	13.513055	-14.591142	-7.403630
H	5.395448	-9.951297	-8.867688
H	2.751010	-14.001200	-7.663357
H	7.017759	-16.837295	-8.317445
H	10.531799	-11.648663	-8.906579
H	14.729743	-14.568510	-9.626084
H	11.221106	-19.757132	-9.023687
H	6.390188	-8.655725	-8.183096
H	3.753814	-12.707628	-6.984407
H	-0.676091	-3.069808	-3.089761
H	2.683117	-3.509218	-0.504453
H	-0.910889	-3.944746	-1.529051
H	1.377380	-2.331861	-0.175918
H	1.071153	-4.093754	0.057948
H	2.962258	-2.705704	-2.840198
H	1.775722	-1.447544	-2.375598
H	-0.528418	-2.180767	-1.533120
H	1.465280	-2.437549	-3.857804
Au	3.927590	-0.193650	1.431476
Au	2.686442	1.415049	-0.308767
Au	4.804163	-0.184953	-1.219598
Au	6.601583	-1.292452	-2.740364

2) Au5b-Pendate-DMPE-Carboxylate

C	-1.565499	-3.531799	-31.170326
C	-1.940388	-3.442516	-29.672954
C	-3.467090	-3.441086	-29.422058
C	-3.851150	-3.371999	-27.925093
C	-5.378589	-3.378581	-27.680408

C	-5.769130	-3.318399	-26.185192
C	-7.297717	-3.323075	-25.949964
C	-7.695514	-3.266251	-24.456666
C	-9.225201	-3.258407	-24.228801
C	-9.628601	-3.211744	-22.736574
C	-11.159554	-3.179460	-22.515328
C	-11.553131	-3.170219	-21.021382
C	-13.084994	-3.140973	-20.810600
C	-13.484753	-3.281068	-19.343271
O	-12.796413	-2.949936	-18.379105
O	-14.735914	-3.856253	-19.242948
C	-15.212938	-4.246972	-17.909066
C	-15.200593	-5.788361	-17.841714
O	-13.829460	-6.257862	-18.139709
C	-13.583504	-6.771063	-19.363167
O	-14.491820	-6.919071	-20.212439
C	-16.637016	-3.699268	-17.709832
O	-16.624992	-2.276237	-17.385077
P	-16.552228	-1.873374	-15.783203
O	-16.965674	-0.325385	-15.887955
O	-14.944271	-1.883331	-15.395250
C	-14.015031	-0.916053	-15.992572
C	-13.706197	0.200923	-14.980956
N	-14.938757	0.989358	-14.618550
O	-17.292860	-2.807308	-14.881665
C	-12.111753	-7.088751	-19.579633
C	-11.700700	-7.105123	-21.070088
C	-10.170521	-7.182385	-21.274231
C	-9.778793	-7.204566	-22.770526
C	-8.250496	-7.200596	-23.002840
C	-7.859356	-7.237242	-24.497602
C	-6.333567	-7.224741	-24.744272

C	-5.964332	-7.278903	-26.244991
C	-4.441037	-7.270479	-26.510107
C	-4.069636	-7.332582	-28.011134
C	-2.543752	-7.323012	-28.266322
C	-2.161117	-7.382559	-29.763824
C	-0.634713	-7.361108	-30.008812
H	-16.302886	0.259108	-15.360172
H	-14.840229	1.969094	-14.905580
H	-15.072798	0.991910	-13.601468
H	-0.470423	-3.528557	-31.309447
H	-0.403405	-7.406315	-31.087116
H	-14.530413	-3.834069	-17.153868
H	-15.908499	-6.247516	-18.543890
H	-15.402142	-6.121508	-16.814871
H	-13.583374	-3.940612	-21.382195
H	-11.527121	-6.343805	-19.016500
H	-17.212696	-3.790609	-18.642738
H	-14.428511	-0.509015	-16.930498
H	-13.278590	-0.251958	-14.072334
H	-12.185987	-7.956578	-21.581251
H	-17.146972	-4.260421	-16.909621
H	-11.094876	-2.306668	-20.511637
H	-1.981246	-2.679461	-31.736958
H	-0.140958	-8.220511	-29.520901
H	-1.958639	-4.459079	-31.623443
H	-0.179497	-6.438821	-29.605838
H	-12.934699	0.860545	-15.415819
H	-13.100902	-1.477249	-16.236001
H	-12.083425	-6.191847	-21.557751
H	-11.138606	-4.068495	-20.529279
H	-11.909468	-8.066308	-19.105986
H	-13.508731	-2.187971	-21.177448

H	-2.592860	-8.296915	-30.212365
H	-1.499134	-2.526276	-29.237112
H	-1.485795	-4.293017	-29.131679
H	-2.628024	-6.529607	-30.290139
H	-5.316028	-4.177957	-25.656365
H	-6.429579	-6.418909	-26.762413
H	-5.813588	-4.289950	-28.133120
H	-10.222141	-8.099148	-23.248107
H	-3.998683	-6.358484	-26.065397
H	-9.205353	-4.092426	-22.216696
H	-9.667786	-4.158864	-24.696033
H	-8.317543	-6.373160	-25.014341
H	-4.531672	-6.476445	-28.538190
H	-3.393378	-4.228145	-27.394379
H	-7.253181	-4.132095	-23.928662
H	-10.226701	-6.327131	-23.274837
H	-8.294463	-8.140503	-24.965214
H	-6.408603	-8.187707	-26.694008
H	-7.813528	-6.298636	-22.532872
H	-7.733092	-4.231962	-26.407323
H	-5.332104	-2.409509	-25.729376
H	-9.172585	-2.322867	-22.260686
H	-3.907366	-4.353018	-29.869270
H	-7.800909	-8.069287	-22.485373
H	-9.667985	-2.390211	-24.753252
H	-2.105797	-6.411486	-27.816042
H	-5.897316	-6.314444	-24.290606
H	-7.253409	-2.363165	-23.994129
H	-4.509004	-8.244262	-28.459428
H	-3.975125	-8.126734	-25.985744
H	-5.835874	-2.522518	-28.212423
H	-3.411603	-2.459743	-27.477643

H	-11.617200	-4.058499	-23.009056
H	-9.766900	-8.082600	-20.773288
H	-5.870942	-8.082759	-24.220249
H	-7.751101	-2.464264	-26.480973
H	-3.922669	-2.585833	-29.957796
H	-2.080589	-8.178668	-27.738266
H	-11.584406	-2.289205	-23.016806
H	-9.692928	-6.312671	-20.783487
Au	-14.979171	-8.781242	-21.421764
Au	-17.137645	-10.256777	-20.365752
Au	-18.452542	-9.388455	-18.208352
Au	-20.233740	-9.315279	-16.222942
Au	-15.613030	-11.050940	-22.613584

3) Au7a-Planar-DMPG-Phosphate

C	-1.591652	-3.548492	-31.188949
C	-1.954585	-3.477411	-29.688205
C	-3.479036	-3.478092	-29.427522
C	-3.853220	-3.415530	-27.928433
C	-5.378756	-3.422235	-27.674800
C	-5.758622	-3.363809	-26.176818
C	-7.285571	-3.368079	-25.933033
C	-7.678090	-3.313567	-24.438312
C	-9.207705	-3.301397	-24.211191
C	-9.614766	-3.260583	-22.719996
C	-11.146829	-3.226745	-22.507936
C	-11.554060	-3.242462	-21.017814
C	-13.089827	-3.221041	-20.824872
C	-13.502531	-3.388020	-19.365105
O	-12.841457	-3.014351	-18.396119
O	-14.723555	-4.022714	-19.279301
C	-15.210402	-4.395994	-17.945719

C	-15.124967	-5.933835	-17.825218
O	-13.754426	-6.352526	-18.103138
C	-13.534184	-7.019324	-19.298827
O	-14.430579	-7.406190	-20.043728
C	-16.664976	-3.922808	-17.808089
O	-16.778901	-2.469354	-17.733753
P	-16.659089	-1.698927	-16.284036
O	-17.034990	-0.234521	-16.477701
O	-15.073832	-1.877914	-15.832986
C	-14.071023	-0.893359	-16.227194
C	-13.638048	-0.034046	-15.017519
O	-12.486769	0.765240	-15.390830
C	-14.680075	1.004361	-14.523213
O	-15.694743	0.450167	-13.618890
O	-17.415804	-2.451139	-15.166705
C	-12.036612	-7.193074	-19.544242
C	-11.678701	-7.196001	-21.050576
C	-10.154546	-7.242865	-21.298672
C	-9.787390	-7.245870	-22.801257
C	-8.262992	-7.246610	-23.060199
C	-7.892466	-7.280378	-24.561271
C	-6.367309	-7.273948	-24.817831
C	-5.991314	-7.328990	-26.317175
C	-4.465185	-7.322062	-26.568763
C	-4.084565	-7.381613	-28.066691
C	-2.558282	-7.371752	-28.315330
C	-2.172714	-7.425369	-29.812169
C	-0.645720	-7.406157	-30.051559
Na	-17.856628	-0.175017	-14.293552
H	-14.133565	1.814432	-14.010217
H	-0.498087	-3.544981	-31.337473
H	-0.408606	-7.446465	-31.128741

H	-14.573246	-3.916405	-17.191881
H	-15.809729	-6.438188	-18.522603
H	-15.343872	-6.234823	-16.788926
H	-13.579334	-4.008679	-21.419351
H	-11.498031	-6.397528	-19.004739
H	-17.244938	-4.216765	-18.696890
H	-14.438954	-0.246458	-17.039739
H	-13.385156	-0.712639	-14.175466
H	-12.172668	-8.051699	-21.540108
H	-17.120927	-4.380610	-16.911190
H	-11.106141	-2.383727	-20.489847
H	-2.010540	-2.688227	-31.740838
H	-0.155634	-8.268309	-29.565004
H	-1.990343	-4.468965	-31.650874
H	-0.190761	-6.486986	-29.641677
H	-13.215050	-1.477298	-16.602747
H	-12.098195	-6.288889	-21.521376
H	-11.142655	-4.147717	-20.536511
H	-11.735005	-8.150269	-19.079324
H	-13.506201	-2.258024	-21.175344
H	-2.605184	-8.336647	-30.266504
H	-1.510247	-2.566602	-29.244300
H	-1.496766	-4.334312	-29.160017
H	-2.635839	-6.568650	-30.336033
H	-5.303262	-4.224217	-25.651136
H	-6.450742	-6.468721	-26.839652
H	-5.818111	-4.332704	-28.125375
H	-10.242594	-8.130290	-23.285875
H	-4.026783	-6.411119	-26.118005
H	-9.195987	-4.145365	-22.203899
H	-9.652507	-4.198559	-24.683053
H	-8.351187	-6.411307	-25.069844

H	-4.544374	-6.523660	-28.592871
H	-3.393459	-4.273707	-27.402583
H	-7.238179	-4.182236	-23.912697
H	-10.238500	-6.360096	-23.287500
H	-8.337131	-8.181061	-25.026184
H	-6.432111	-8.237521	-26.770357
H	-7.814380	-6.348187	-22.594155
H	-7.724434	-4.275813	-26.389676
H	-5.318769	-2.455156	-25.722787
H	-9.158962	-2.375116	-22.237378
H	-3.922540	-4.388037	-29.875766
H	-7.806582	-8.117952	-22.552528
H	-9.646857	-2.429360	-24.732717
H	-2.121065	-6.461653	-27.861065
H	-5.925990	-6.365386	-24.364955
H	-7.232820	-2.412506	-23.974484
H	-4.522435	-8.292412	-28.518569
H	-4.004722	-8.179135	-26.040665
H	-5.840291	-2.564939	-28.201634
H	-3.412276	-2.504786	-27.479229
H	-11.602319	-4.096401	-23.019484
H	-9.727759	-8.142265	-20.814812
H	-5.906296	-8.133928	-24.294963
H	-7.741117	-2.507609	-26.459836
H	-3.938796	-2.620152	-29.955441
H	-2.096428	-8.229971	-27.789760
H	-11.565523	-2.326435	-22.997026
H	-9.676898	-6.372021	-20.809435
H	-11.845229	0.178103	-15.840189
H	-15.245825	1.418168	-15.369576
H	-15.240184	0.119780	-12.818481
Au	-19.806387	-6.021507	-12.458499

Au	-17.849701	-5.749363	-14.311350
Au	-19.132788	-3.343772	-13.801707
Au	-20.651934	-1.121283	-13.181488
Au	-21.136122	-3.512728	-11.893046
Au	-23.168631	-3.552241	-10.030179
Au	-21.806132	-5.921887	-10.600287