Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information For Modulation of Structural, Energetic and Electronic Properties of DNA and Size-Expanded DNA Bases Upon Binding to Gold Clusters

Sandhya Rai, Supriya Ranjan, Harjinder Singh, and U. Deva Priyakumar*

Center for Computational Natural Science and Bioinformatics, International Institute of Information Technology, Hyderabad, India

E-mail: deva@iiit.ac.in

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*To whom correspondence should be addressed

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Table S1(a): Geometrical features of complexes with Au_3. All the bond distances are in Å and bond angles in degrees.

Complex	Anchor Bond	△R(N-H)*	r(H-Au)	∠N-H ⋯ Au
A-Au_3(N1)	2.121(N1)	0.0117(N6-Ha)	2.784(N6-Ha)	176.27(N6-Ha)
A-Au_3(N3)	2.120(N3)	—	—	—
A-Au_3(N6)	2.200(N6)	0.0101(N6-Ha)	4.784(N6-Ha)	75.54(N6-Ha)
A-Au_3(N7)	2.097(N7)	0.0008(N6-Hb)	2.770(N6-Hb)	164.15(N6-Hb)
xA-Au_3(N1)	2.117(N1)	0.0108(N6-Ha)	2.793(N6-Ha)	179.27(N6-Ha)
xA-Au_3(N3)	2.122(N3)	—	2.973(benz C)	172.41(benz C)
xA-Au_3(N7)	2.098(N7)	0.0008(N6-Hb)	3.503(N6-Hb)	175.18(N6-Hb)
C-Au_3(N3)	2.130(N3)	0.0156(N4-Ha)	2.621(N6-Ha)	179.44(N6-Ha)
C-Au_3(N3*)	2.197(N4)	0.0095(N4-Ha)	4.514(N4-Hb)	80.74(N4-Hb)
xC-Au_3(N3)	2.131(N3)	0.0164(N4-Ha)	2.601(N4-Ha)	177.60(N4-Ha)
xC-Au_3(N4)	2.131(N3)	0.0189(N4-Ha)	2.600(N4-Ha)	177.60(N4-Ha)
G-Au_3(O6)	2.167(O6)	0.0189(N1-H)	2.515(N1-H)	171.13(N1-H)
G-Au_3(N3)	2.133(N3)	0.0103(N2-Hb)	2.735(N2-Hb)	179.06(N2-Hb)
G-Au_3(N7)	2.112(N7)	0.0020(C8-H)	4.000(C8-H)	114.80(C8-H)
xG-Au_3(N7)	2.103(N7)	0.0020(C8-H)	4.269(C8-H)	110.90(C8-H)
xG-Au_3(N3)	2.132(N3)	0.0104(N2-Hb)	2.761(N2-Hb)	179.71(N2-H)
xG-Au_3(O6)	2.174(O6)	0.0188(N1-H)	2.529(N1-H)	172.01(N1-H)
xG-Au_3(N7-bH)	2.103(N7)	0.0020(C8-H)	4.269(C8-H)	110.90(C8-H)
T-Au_3(O2)	2.205(O2)	0.0041(N3-H)	2.868(N3-H)	174.70(N3-H)
T-Au_3(O4)	2.188(O4)	0.0146(N3-H)	2.828(N3-H)	175.63(N3-H)
xT-Au_3(O2)	2.204(O4)	0.0130(N3-H)	2.857(N3-H)	174.60(N3-H)
xT-Au_3(O4)	2.191(O4)	0.0151(N3-H)	2.793(N3-H)	175.88(N3-H)

- $*\triangle$R(N-H) = R (N-H)$_{bonded\,base}$ − R (N-H)$_{unbonded\,base}$
- The bonds have been specified where ever they are not the usual N-H bonds.

Table S1(b): Geometrical features of complexes with Au_4. All the bond distances are in Å and bond angles in degrees.

Complex	Anchor Bond	△R(N-H)*	r(H-Au)	∠N-H ⋯ Au
A-Au_4(N1)	2.129(N1)	0.0110(N6-Ha)	2.734(N6-Ha)	174.63(N6-H)
A-Au_4(N3)	2.122(N3)	—	—	—
A-Au_4(N7)	2.095(N7)	0.0063(N6-Hb)	2.771(N6-Hb)	166.10(N6-Hb)
A-Au_4(N6)	2.111(N1)	0.0113(N6-Ha)	2.780(N6-Ha)	172.20(N6-Ha)
xA-Au_4(N1)	2.019(N1)	0.0101(N6-Ha)	2.734(N6-Ha)	177.19(N6-Ha)
xA-Au_4(N3)	2.117(N3)	—	—	—
xA-Au_4(N7)	2.089(N7)	0.0075(N6-Hb)	3.923(N6-Hb)	170.74(N6-Hb)
C-Au_4(N3)	2.137(N3)	0.0137(N4-Ha)	2.703(N4-Ha)	159.73(N4-Ha)
C-Au_4(N3*)	2.123(N3)	0.0122(N4-Ha)	2.643(N4-Ha)	176.18(N4-Ha)
xC-Au_4(N3)	2.136(N3)	0.0146(N4-Ha)	2.678(N4-Ha)	158.71(N4-Ha)
xC-Au_4(N3*)	2.124(N3)	0.0131(N4-Ha)	2.612(N4-Ha)	179.08(N4-Ha)
G-Au_4(O6)	2.184(O6)	0.0147(N1-H)	2.691(N1-H)	173.85(N1-H)
G-Au_4(N3)	2.134(N3)	0.0037(N2-Hb)	3.995(N2-Hb)	159.29(N2-Hb)
G-Au_4(N7)	2.105(N7)	0.0030(C8-H)	3.123(C8-H)	171.11(C8-H)
xG-Au_4(b-H)	2.095(N7)	0.0050(b C-H)	3.085(b C-H)	168.70(b C-H)
xG-Au_4(N3)	2.129(N3)	0.0041(N2-Hb)	4.019(N2-Hb)	156.47(N2-Hb)
xG-Au_4(N7)	2.095(N7)	0.0112(C8-H)	3.235(C8-H)	169.10(C8-h)
xG-Au_4(N1)	2.182(O6)	0.0191(N1-H)	2.530(N1-H)	172.37(N1-H)
xG-Au_4(N1_Y)	2.181(O6)	0.0183(N1-H)	2.548(N1-H)	160.92(N1-H)
T-Au_4(O2)	2.219(O2)	0.0143(N3-H)	2.691(N3-H)	179.90(N3-H)
T-Au_4(O4)	2.202(O4)	0.0159(N3-H)	2.683(N3-H)	179.48(N3-H)
xT-Au_4(O2)	2.208(O2)	0.0070(N3-H)	3.041(N3-H)	177.60(N3-H)
xT-Au_4(O4)	2.210(O4)	0.0153(N3-H)	2.694(N3-H)	179.84(N3-H)

- *△R(N-H) = R (N-H)$_{bonded\,base}$ − R (N-H)$_{unbonded\,base}$
- The bonds have been specified where ever they are not the usual N-H bonds.

Table S2(a): Geometrical coordinates of A-Au_3(N1) in Å

Atom	x	y	z
N	6.11023	0.16671	-0.00097
C	6.20027	-1.20091	-0.00115
H	7.15906	-1.69784	-0.00206
N	5.044	-1.80779	-0.00088
C	4.13771	-0.77974	-0.0001
C	2.73395	-0.77421	-0.00015
N	2.01329	-1.89013	-0.00047
H	0.99884	-1.85131	-0.00046
H	2.48768	-2.77502	-0.00057
N	2.13215	0.43829	0.00008
C	2.88225	1.5649	-0.00001
H	2.31753	2.48827	-0.00008
N	4.19013	1.65265	0.00006
C	4.77542	0.45097	0.00004
C	7.18748	1.13059	0.00234
H	6.74487	2.12356	-0.03314
H	7.78334	1.03862	0.90999
H	7.82638	0.99341	-0.86936
Au	0.01556	0.57094	-0.00012
Au	-1.76987	-1.56423	0.00033
Au	-2.53997	1.08711	-0.00015

$E_{electronic}$=-913.314836 a.u.

Table S2(b): Geometrical coordinates of A-Au_3(N3) in Å

Atom	x	y	z
N	3.00097	1.51429	0.92611
C	4.25141	2.04401	1.11799
H	4.37258	2.9938	1.61725
N	5.22214	1.30959	0.65281
C	4.57949	0.22364	0.11991
C	5.06492	-0.92102	-0.52775
N	6.36979	-1.12806	-0.73385
H	6.66526	-1.95994	-1.21002
H	7.04085	-0.44715	-0.43073
N	4.18731	-1.83988	-0.95233
C	2.89912	-1.63832	-0.75071
H	2.22383	-2.40469	-1.10916
N	2.31927	-0.58969	-0.14987
C	3.20206	0.33086	0.27806
C	1.75497	2.11197	1.36222
H	1.0701	2.24062	0.52365
H	1.27103	1.48769	2.11252
H	1.98137	3.08413	1.79588
Au	-1.73841	1.40508	-0.54106
Au	0.20774	-0.45497	-0.02218
Au	-2.30266	-1.11169	0.42276

$E_{electronic}$=-913.310607 a.u.

Table S2(c): Geometrical coordinates of A-Au_3(N6) in Å

Atom	x	y	z
N	5.44555	0.68007	0.89833
C	4.73435	0.32587	2.01447
H	5.04359	0.65323	2.99645
N	3.69229	-0.42286	1.77498
C	3.70918	-0.57073	0.41138
C	2.89584	-1.23948	-0.49337
N	1.73299	-1.92594	-0.08327
H	1.51869	-2.67403	-0.73287
H	1.81663	-2.27557	0.86457
N	3.18552	-1.23784	-1.78157
C	4.26158	-0.55342	-2.18773
H	4.4592	-0.57738	-3.25299
N	5.10865	0.14489	-1.44334
C	4.79442	0.10385	-0.15597
C	6.61424	1.52659	0.82208
H	7.13615	1.30481	-0.10621
H	6.33381	2.5802	0.82594
H	7.27383	1.32206	1.66348
Au	-1.38412	1.64516	-0.2298
Au	-2.72853	-0.72023	0.28212
Au	-0.06196	-0.65351	-0.05586

$E_{electronic}$=-913.291944 a.u.

Table S2(d): Geometrical coordinates of A-Au_3(N7) in Å

Atom	x	y	z
N	-4.26938	1.64291	0.04172
C	-2.93352	1.84479	0.038
H	-2.49259	2.82792	0.06111
N	-2.25498	0.71886	0.00348
C	-3.20162	-0.28629	-0.01688
C	-3.15156	-1.69587	-0.05584
N	-2.0226	-2.4066	-0.08694
H	-2.0986	-3.40769	-0.10069
H	-1.10579	-1.97861	-0.0636
N	-4.31917	-2.35286	-0.06475
C	-5.45853	-1.66735	-0.03827
H	-6.3626	-2.26701	-0.04756
N	-5.63322	-0.35059	-0.00193
C	-4.46674	0.28352	0.00697
C	-5.31041	2.64487	0.07634
H	-5.94454	2.55198	-0.80384
H	-5.9236	2.51329	0.96639
H	-4.85153	3.63072	0.09244
Au	2.40438	1.10095	-0.02763
Au	1.62662	-1.53676	0.03788
Au	-0.16507	0.54499	-0.00274

$E_{electronic}$=-913.314759 a.u.

Table S2(e): Geometrical coordinates of xA-Au_3(N1) in Å

Atom	x	y	z
N	-7.66528	-0.04232	0.00025
C	-7.89782	1.30774	0.0005
N	-6.82698	2.0424	0.0005
C	-3.58422	0.22702	-0.00014
C	-4.11327	-1.09586	-0.00029
C	-2.15067	0.33651	-0.00024
N	-1.53926	1.5196	-0.00011
N	-1.39968	-0.76793	-0.00043
C	-2.0262	-1.97912	-0.0006
N	-3.29721	-2.19527	-0.00054
C	-6.30216	-0.19283	0.00008
C	-5.78912	1.13186	0.00023
C	-4.42944	1.34355	0.00011
C	-5.49654	-1.30742	-0.00017
H	-8.90923	1.68996	0.00067
H	-0.52389	1.56202	-0.00015
H	-2.05977	2.37431	0.00001
H	-1.35902	-2.83299	-0.00081
H	-4.05926	2.36052	0.00024
H	-5.86827	-2.32299	-0.00029
C	-8.64648	-1.09702	0.00022
H	-8.54159	-1.72148	-0.88823
H	-8.54156	-1.72156	0.88862
H	-9.64078	-0.65512	0.00026
Au	2.26802	1.64304	-0.00014
Au	0.71426	-0.6641	-0.00014
Au	3.31162	-0.91153	0.00033

$E_{electronic}$=-1066.765274 a.u.

Table S2(f): Geometrical coordinates of xA-Au_3(N3) in Å

Atom	x	y	z
N	-3.66563	2.8237	0.00048
C	-5.00874	3.08449	-0.00624
N	-5.76916	2.02939	-0.01013
C	-4.0084	-1.24781	-0.00139
C	-2.67804	-0.73604	-0.00027
C	-4.12826	-2.67676	0.00499
N	-5.32599	-3.28392	0.00458
N	-3.06796	-3.46968	-0.00274
C	-1.86897	-2.89483	-0.01056
N	-1.60742	-1.60522	-0.00518
C	-3.54661	1.45948	0.00117
C	-4.88123	0.97323	-0.00515
C	-5.11113	-0.3829	-0.00742
C	-2.44347	0.64038	0.00249
H	-5.3693	4.10375	-0.00803
H	-5.33617	-4.2852	0.07808
H	-6.17979	-2.77815	0.13138
H	-1.01487	-3.56116	-0.01847
H	-6.13083	-0.74502	-0.02161
H	-1.42272	1.01086	0.00343
C	-2.58234	3.77788	0.00584
H	-1.96666	3.65515	0.89744
H	-1.9513	3.64709	-0.87379
H	-2.99815	4.78329	-0.00246
Au	1.48203	1.6473	0.00265
Au	3.00356	-0.64351	0.00036
Au	0.40006	-0.91864	-0.00296

$E_{electronic}$= -1066.765880 a.u.

Table S2(g): Geometrical coordinates of xA-Au_3(N7) in Å

Atom	x	y	z
N	-3.14198	3.07097	0.00225
C	-1.79047	3.02052	0.00118
N	-1.32518	1.79709	-0.00055
C	-3.78968	-0.97706	-0.00188
C	-4.96773	-0.17075	-0.00009
C	-4.01298	-2.40021	-0.00299
N	-2.98521	-3.26521	-0.00595
N	-5.23195	-2.90338	-0.00236
C	-6.25476	-2.02893	-0.00096
N	-6.21309	-0.72454	0.00024
C	-3.59821	1.76612	0.00101
C	-2.43644	0.9662	-0.00078
C	-2.51672	-0.40423	-0.00237
C	-4.86371	1.23014	0.00135
H	-1.18078	3.91037	0.00185
H	-3.20159	-4.24505	-0.00155
H	-2.0245	-2.9766	0.00107
H	-7.2421	-2.48171	-0.00064
H	-1.59913	-0.98469	-0.00394
H	-5.76962	1.82059	0.00264
C	-3.96099	4.25826	0.00356
H	-4.59251	4.28397	-0.88501
H	-4.59269	4.28181	0.89206
H	-3.31772	5.13537	0.00471
Au	0.63449	1.04787	-0.00078
Au	1.23416	-1.69109	0.00295
Au	3.13075	0.31247	-0.00159

$E_{electronic}$=-1066.763726 a.u.

Table S2(h): Geometrical coordinates of C-Au_3(N3) in Å

Atom	x	y	z
N	4.78457	0.42238	0.00034
C	5.14255	-0.87537	0.00036
H	6.20583	-1.07681	0.00059
C	4.22589	-1.86783	0.00016
H	4.52464	-2.90417	0.0003
C	2.85287	-1.49094	-0.00001
N	1.89976	-2.41842	-0.00006
H	0.91613	-2.14615	-0.00012
H	2.13775	-3.39199	-0.00021
N	2.5002	-0.20382	-0.00011
C	3.43378	0.80693	-0.00009
O	3.14666	1.98185	-0.00039
C	5.76253	1.49567	0.00035
H	5.63073	2.11975	-0.88197
H	5.62761	2.12228	0.88036
H	6.75967	1.06082	0.00271
Au	-1.61706	-1.47134	0.00003
Au	-2.0004	1.2714	0.00015
Au	0.45578	0.39424	-0.00023

$E_{electronic}$=-841.008805 a.u.

Table S2(i): Geometrical coordinates of C-Au_3(N3*) in Å

Atom	x	y	z
N	5.04245	0.6643	-0.61449
C	4.14145	1.48095	-0.04692
H	4.28	2.5412	-0.21486
C	3.10567	0.99322	0.68521
H	2.34482	1.63693	1.09885
C	3.06151	-0.4127	0.79033
N	1.99341	-1.01866	1.51046
H	2.19435	-2.00719	1.61834
H	1.85542	-0.58973	2.41841
N	3.91475	-1.23256	0.26335
C	4.96096	-0.74534	-0.48008
O	5.80436	-1.43197	-1.0086
C	6.14954	1.17144	-1.40407
H	7.09347	0.85963	-0.95962
H	6.1024	0.75951	-2.41082
H	6.0923	2.25707	-1.44032
Au	0.04346	-0.72729	0.54212
Au	-1.30475	1.62847	0.07929
Au	-2.30285	-0.87357	-0.5888

$E_{electronic}$=-840.984035 a.u.

Table S2(j): Geometrical coordinates of xC-Au_3(N3) in Å

Atom	x	y	z
C	4.48466	-0.76684	-0.00007
C	2.32424	-1.89407	0.00048
O	1.7066	-2.93361	0.00093
N	1.70818	-0.65394	0.00034
C	2.40119	0.47775	0.00031
N	1.73092	1.62261	0.00041
C	3.85428	0.47918	0.00013
N	3.70437	-1.89006	0.00001
C	4.63343	1.64272	0.00011
C	6.60982	0.31495	-0.00036
C	5.88857	-0.86038	-0.00033
C	6.00998	1.58291	-0.00016
C	6.85476	2.82161	-0.00039
H	0.709	1.61195	0.00041
H	2.20449	2.50442	0.00004
H	4.12421	-2.80416	0.00022
H	4.16379	2.61875	0.00036
H	7.69318	0.2518	-0.00053
H	6.24006	3.72133	0.00205
H	7.49946	2.85951	-0.88118
H	7.50326	2.85728	0.87767
C	6.55913	-2.19909	-0.00051
H	6.28964	-2.78674	0.88211
H	6.28915	-2.78674	-0.88296
H	7.6419	-2.08754	-0.0008
Au	-3.02563	-0.83349	-0.00029
Au	-0.42243	-0.67841	0.00014
Au	-1.89037	1.69375	0.00008

$E_{electronic}$=-1033.735066 a.u.

Table S2(k): Geometrical coordinates of xC-Au_3(N3*) in Å

Atom	x	y	z
C	4.48459	-0.76683	-0.00009
C	2.3242	-1.8941	-0.00053
O	1.70656	-2.93365	-0.00107
N	1.70812	-0.65396	-0.00007
C	2.40111	0.47773	0.00027
N	1.73079	1.62257	0.00074
C	3.85419	0.47917	0.00019
N	3.70432	-1.89007	-0.00029
C	4.63333	1.64273	0.00048
C	6.60973	0.31498	0.00024
C	5.88851	-0.86035	-0.00002
C	6.00988	1.58294	0.00044
C	6.85464	2.82164	0.00022
H	0.70888	1.61188	0.00057
H	2.20431	2.50441	0.00054
H	4.12417	-2.80416	-0.00072
H	4.16366	2.61875	0.00079
H	7.69309	0.25186	0.00036
H	6.23994	3.72135	0.00569
H	7.49714	2.86105	-0.88213
H	7.50534	2.85583	0.8767
C	6.55907	-2.19905	-0.00013
H	6.28918	-2.78686	0.88225
H	6.28951	-2.78656	-0.88282
H	7.64184	-2.0875	0.00008
Au	-1.89015	1.69383	-0.00035
Au	-3.02569	-0.83336	0.00035
Au	-0.42249	-0.67862	-0.00002

$E_{electronic}$=-1033.735066 a.u.

Table S2(l): Geometrical coordinates of G-Au_3(O6) in Å

Atom	x	y	z
N	-6.05561	-0.28762	0.04713
C	-5.95901	-1.66108	0.08792
H	-6.84466	-2.27727	0.13457
N	-4.73719	-2.10154	0.06385
C	-3.97345	-0.96299	0.00251
C	-2.57515	-0.76748	-0.03749
O	-1.69023	-1.64773	-0.01953
N	-2.2368	0.57226	-0.09966
H	-1.23012	0.77526	-0.11762
C	-3.1137	1.61866	-0.10864
N	-2.56789	2.8498	-0.21257
H	-1.58181	2.97181	-0.03705
H	-3.17966	3.62465	-0.03291
N	-4.41293	1.46643	-0.05696
C	-4.77898	0.17524	-0.00838
Au	2.9404	-0.54086	-0.01048
Au	1.14461	1.58695	0.05
Au	0.40938	-1.11019	-0.01585
C	-7.25464	0.51528	0.05807
H	-7.27029	1.16567	0.93209
H	-7.30761	1.13114	-0.83905
H	-8.11763	-0.14633	0.08926

$E_{electronic}$=-988.491555 a.u.

Table S2(m): Geometrical coordinates of G-Au_3(N3) in Å

Atom	x	y	z
N	3.2994	-1.89437	0.10889
C	4.61747	-2.27944	0.20187
H	4.88057	-3.3234	0.28168
N	5.45342	-1.28638	0.18196
C	4.65932	-0.1791	0.07049
C	5.02463	1.20246	-0.00652
O	6.10247	1.74313	0.00842
N	3.85137	2.00436	-0.12557
H	4.05138	2.98782	-0.22493
C	2.56459	1.5892	-0.16306
N	1.61137	2.52221	-0.32422
H	1.82411	3.48425	-0.13277
H	0.64134	2.23529	-0.21646
N	2.24735	0.30377	-0.08091
C	3.32051	-0.53645	0.02351
C	2.16748	-2.79413	0.10268
H	1.51058	-2.6043	0.95157
H	1.59299	-2.6937	-0.81795
H	2.54838	-3.81154	0.17174
Au	-1.96523	1.47805	0.11572
Au	0.1882	-0.25351	-0.0561
Au	-2.21326	-1.27241	-0.05677

$E_{electronic}$=-988.493232 a.u.

Table S2(n): Geometrical coordinates of G-Au_3(N7) in Å

Atom	x	y	z
N	3.63404	2.01048	-0.00577
C	2.29181	1.79815	-0.00945
H	1.56906	2.59795	-0.01413
N	1.99667	0.52049	-0.00586
C	3.1993	-0.14082	0.00071
C	3.51226	-1.53874	-0.00166
O	2.78995	-2.50517	-0.01094
N	4.92387	-1.70397	0.00101
H	5.2151	-2.66807	-0.05669
C	5.85675	-0.71227	0.00699
N	7.16381	-1.09158	-0.04592
H	7.42073	-1.98036	0.34656
H	7.81283	-0.344	0.13154
N	5.55759	0.55905	0.01475
C	4.22892	0.78062	0.00019
C	4.3136	3.28637	-0.00994
H	4.94209	3.3789	0.87437
H	4.93596	3.37711	-0.89879
H	3.56883	4.07859	-0.00806
Au	-2.33054	-1.3562	0.00014
Au	-2.25026	1.4089	0.00441
Au	0.00951	-0.19573	-0.00349

$E_{electronic}$=-988.305674 a.u.

Table S2(o): Geometrical coordinates of xG-Au_3(N3) in Å

Atom	x	y	z
N	4.59804	-2.61964	0.08723
C	5.96786	-2.57422	0.15154
N	6.46636	-1.37556	0.15831
C	2.82786	0.6223	-0.03841
C	4.00968	1.40581	0.00476
N	1.56664	1.21681	-0.09462
C	1.47841	2.52359	-0.13522
N	0.2904	3.14411	-0.25284
N	2.58402	3.31353	-0.09945
C	3.90177	2.85568	-0.02856
O	4.80903	3.65681	-0.00806
C	4.17848	-1.31809	0.04945
C	5.36399	-0.5468	0.09457
C	5.27515	0.83009	0.07085
C	2.9127	-0.76462	-0.01657
H	6.54565	-3.48699	0.19167
H	0.21357	4.11094	0.00699
H	-0.54643	2.57521	-0.14734
H	2.48955	4.31414	-0.17598
H	6.14829	1.46788	0.10145
H	2.00654	-1.35924	-0.05017
C	3.76392	-3.79446	0.06391
H	3.08252	-3.8006	0.91582
H	3.18069	-3.83626	-0.85714
H	4.3969	-4.67788	0.11685
Au	-2.18927	-1.66042	-0.072
Au	-2.81053	1.023	0.14781
Au	-0.22306	0.05828	-0.07487

$E_{electronic}$=-1141.961833 a.u.

Table S2(p): Geometrical coordinates of xG-Au_3(N7) in Å

Atom	x	y	z
N	2.57348	2.97615	-0.00558
C	1.29739	2.52471	-0.00745
N	1.22129	1.21788	-0.00517
C	5.29922	0.46045	0.00616
C	4.42108	-0.65927	0.00405
N	6.66941	0.32579	0.02361
C	7.15326	-0.86904	0.00688
N	8.50653	-1.06045	-0.05068
N	6.38808	-2.00319	-0.00615
C	4.99686	-2.00253	-0.00745
O	4.38544	-3.04809	-0.02593
C	3.39369	1.86937	-0.00169
C	2.52801	0.75765	-0.00191
C	3.03886	-0.52349	-0.00014
C	4.76947	1.75222	0.00252
H	0.44562	3.18682	-0.01047
H	8.88032	-1.88117	0.39507
H	9.02844	-0.21845	0.12722
H	6.81477	-2.91324	-0.08531
H	2.40576	-1.40172	-0.00312
H	5.43985	2.60055	0.00368
C	2.9975	4.35483	-0.00833
H	3.59093	4.57133	0.88049
H	3.59214	4.56748	-0.89728
H	2.11932	4.99649	-0.01027
Au	-3.2053	0.97433	0.00277
Au	-0.58056	0.13382	-0.0025
Au	-2.4709	-1.68165	0.00175

$E_{electronic}$=-1141.958052 a.u.

Table S2(q): Geometrical coordinates of xG-Au_3(O6) in Å

Atom	x	y	z
N	-7.53426	-0.40284	0.06522
C	-7.59631	-1.77464	0.08874
N	-6.44238	-2.36555	0.06925
C	-4.15954	1.11757	-0.04545
C	-3.47633	-0.13557	-0.04265
N	-3.4956	2.31921	-0.07799
C	-2.20663	2.28986	-0.12454
N	-1.47638	3.42847	-0.22022
N	-1.47547	1.12577	-0.1254
C	-2.03855	-0.10831	-0.07482
O	-1.33031	-1.13857	-0.05799
C	-6.20343	-0.08196	0.02654
C	-5.5272	-1.32981	0.02947
C	-4.15107	-1.35749	-0.00447
C	-5.55547	1.13659	-0.00884
H	-8.55186	-2.27944	0.12086
H	-0.496	3.40232	0.01379
H	-1.97495	4.27784	-0.02453
H	-0.44972	1.16724	-0.13971
H	-3.59543	-2.28517	-0.0025
H	-6.0696	2.088	-0.01091
C	-8.64045	0.51818	0.07728
H	-8.59384	1.16746	0.95313
H	-8.6397	1.13575	-0.82243
H	-9.57039	-0.04599	0.11146
Au	0.83922	-0.99898	-0.03387
Au	2.04542	1.51872	0.07228
Au	3.43033	-0.89824	-0.00347

$E_{electronic}$=-1141.951365 a.u.

Table S2(r): Geometrical coordinates of xG-Au_3(N7-bH) in Å

Atom	x	y	z
N	-2.57345	2.97604	0.00546
C	-1.29738	2.52456	0.00776
N	-1.22134	1.21773	0.00574
C	-5.29929	0.46044	-0.00635
C	-4.42119	-0.65931	-0.00388
N	-6.66947	0.32583	-0.02399
C	-7.15339	-0.86898	-0.00721
N	-8.50665	-1.06029	0.05008
N	-6.38824	-2.00316	0.00611
C	-4.99702	-2.00254	0.00771
O	-4.38564	-3.04812	0.02641
C	-3.3937	1.86929	0.00163
C	-2.52808	0.75754	0.00223
C	-3.03897	-0.52359	0.00053
C	-4.7695	1.75219	-0.00281
H	-0.44558	3.18664	0.01087
H	-8.88046	-1.88133	-0.39502
H	-9.02858	-0.21839	-0.12813
H	-6.81495	-2.91322	0.08508
H	-2.40588	-1.40185	0.00375
H	-5.43983	2.60056	-0.0042
C	-2.99742	4.35473	0.0082
H	-3.59209	4.57077	-0.87991
H	-3.5908	4.56789	0.89787
H	-2.11922	4.99637	0.00849
Au	0.58061	0.13379	0.00278
Au	2.47109	-1.68158	-0.0019
Au	3.20516	0.97435	-0.00291

$E_{electronic}$=-1141.958053 a.u.

Table S2(s): Geometrical coordinates of T-Au_3(O2) in Å

Atom	x	y	z
N	-4.13668	-1.47947	-0.00008
C	-5.23985	-0.6563	0.00002
H	-6.18835	-1.17728	0.00001
C	-5.17106	0.68518	0.00011
C	-6.36302	1.57809	0.00024
H	-6.3528	2.23081	0.87488
H	-6.35289	2.23093	-0.87432
H	-7.28831	1.00278	0.00025
C	-3.85219	1.30556	0.00002
O	-3.64011	2.49497	0.0002
N	-2.78698	0.39218	-0.00001
H	-1.84404	0.78594	-0.00002
C	-2.87885	-0.95731	0.00003
O	-1.90259	-1.72467	0.
Au	0.18325	-1.01038	-0.00008
Au	0.89359	1.64176	-0.00009
Au	2.72507	-0.47829	0.00013
C	-4.26463	-2.92848	-0.00006
H	-3.78789	-3.35048	-0.88322
H	-3.78975	-3.35036	0.88418
H	-5.32224	-3.17898	-0.00116

$E_{electronic}$=-900.126277 a.u.

Table S2(t): Geometrical coordinates of T-Au_3(O4) in Å

Atom	x	y	z
N	5.04405	-0.71804	-0.00053
C	5.22328	0.63205	-0.00017
H	6.25638	0.95634	-0.00019
C	4.21272	1.52799	0.00023
C	4.41106	3.00591	0.00066
H	3.94553	3.46141	-0.87497
H	3.94601	3.46086	0.87683
H	5.47164	3.25595	0.00044
C	2.87274	1.00157	0.00025
O	1.88057	1.75102	0.00066
N	2.75022	-0.35797	-0.00015
H	1.80531	-0.75093	0.00004
C	3.77949	-1.28211	-0.0006
O	3.59815	-2.47456	-0.001
Au	-0.18357	1.02606	0.00022
Au	-2.7213	0.47141	-0.00061
Au	-0.88142	-1.63494	0.00056
C	6.1626	-1.64575	-0.00112
H	6.12115	-2.28323	0.88069
H	6.12149	-2.28179	-0.884
H	7.08805	-1.07539	-0.00048

$E_{electronic}$=-900.129548 a.u.

Table S2(u): Geometrical coordinates of xT-Au_3(O2) in Å

Atom	x	y	z
Au	-1.55366	1.62937	0.00023
Au	-3.39648	-0.48136	-0.00037
Au	-0.85724	-1.02683	0.00023
C	2.20443	-0.97891	0.00016
O	1.22768	-1.74329	0.00054
N	2.11271	0.37387	-0.00003
C	3.18182	1.2786	-0.00024
O	2.97466	2.46642	-0.00039
C	4.50781	0.64942	-0.00022
C	4.61501	-0.73811	-0.00012
N	3.45396	-1.49768	-0.00011
C	5.65438	1.44031	-0.00025
C	6.98513	-0.53621	-0.00007
C	5.87166	-1.35781	-0.00005
C	6.90893	0.86232	-0.00018
C	8.15825	1.6915	-0.00023
H	1.17148	0.77104	0.00015
H	3.49969	-2.5026	0.00007
H	5.52571	2.51547	-0.00032
H	7.964	-1.0048	-0.00001
H	7.92418	2.75519	-0.00003
H	8.77075	1.48202	-0.87993
H	8.77103	1.48174	0.87921
C	5.99262	-2.85151	0.00004
H	5.52578	-3.29735	0.88352
H	5.52594	-3.29743	-0.88347
H	7.03865	-3.15271	0.00015

$E_{electronic}$=-1053.604838 a.u.

Table S2(v): Geometrical coordinates of xT-Au_3(O4) in Å

Atom	x	y	z
Au	1.78313	1.56575	-0.00048
Au	0.55269	-0.89555	-0.00012
Au	3.14825	-0.87886	0.00049
C	-2.81034	2.2373	0.00044
O	-2.35921	3.35447	0.00069
N	-2.00381	1.10319	0.00004
C	-2.42259	-0.18981	-0.00014
O	-1.62445	-1.13861	-0.00048
C	-3.8603	-0.40709	-0.00008
C	-4.70692	0.70186	0.00027
N	-4.15382	1.96476	0.00052
C	-4.38639	-1.70012	-0.00034
C	-6.57877	-0.77129	0.00013
C	-6.09935	0.52533	0.00039
C	-5.75034	-1.90276	-0.00025
C	-6.3441	-3.27954	-0.00072
H	-0.99567	1.28055	0.00001
H	-4.74429	2.77922	0.00078
H	-3.69366	-2.53174	-0.00058
H	-7.65455	-0.91541	0.00025
H	-5.56718	-4.04294	0.00107
H	-6.96998	-3.43939	-0.88144
H	-6.97334	-3.4386	0.87771
C	-7.01914	1.70781	0.0008
H	-6.87092	2.33616	0.88409
H	-6.87107	2.33666	-0.88215
H	-8.0592	1.38674	0.00079

$E_{electronic}$=-1053.606158 a.u.

Table S3(a): Geometrical coordinates of A-Au_4(N1) in Å

Atom	x	y	z
N	-6.34848	-0.42968	0.04883
C	-6.61906	0.89981	-0.14226
H	-7.63672	1.25748	-0.19458
N	-5.55478	1.64859	-0.24834
C	-4.52032	0.7585	-0.11926
C	-3.12843	0.93695	-0.14319
N	-2.56263	2.12593	-0.32175
H	-1.55216	2.21297	-0.28664
H	-3.1484	2.93681	-0.40662
N	-2.36965	-0.17082	0.0182
C	-2.96297	-1.37675	0.1901
H	-2.27611	-2.20444	0.30941
N	-4.24798	-1.63487	0.22547
C	-4.9878	-0.53305	0.06581
C	-7.2914	-1.51268	0.2031
H	-7.14516	-2.255	-0.58042
H	-7.16029	-1.99339	1.17169
H	-8.30018	-1.11156	0.13433
Au	1.29381	-2.4255	-0.04393
Au	1.1526	2.41089	0.06154
Au	2.37787	0.02016	-0.00885
Au	-0.24372	-0.06446	0.00986

$E_{electronic}$= -1049.08997a.u.

Table S3(b): Geometrical coordinates of A-Au_4(N3) in Å

Atom	x	y	z
Au	0.87359	-2.64221	0.00942
Au	1.57099	-0.0565	-0.003
Au	-1.0941	-0.90612	0.00003
Au	2.6832	2.2688	-0.01121
N	-2.5992	2.35565	0.03946
C	-3.47146	3.4132	0.04796
H	-3.10081	4.42712	0.06972
N	-4.72945	3.07145	0.0276
C	-4.69194	1.7031	0.00406
C	-5.71404	0.74507	-0.02421
N	-7.00848	1.07786	-0.03287
H	-7.70163	0.35316	-0.05478
H	-7.2791	2.04362	-0.0207
N	-5.37825	-0.55265	-0.0429
C	-4.10253	-0.88428	-0.03415
H	-3.87597	-1.94278	-0.04997
N	-3.04154	-0.06363	-0.00784
C	-3.37992	1.23966	0.01093
C	-1.15208	2.44919	0.05623
H	-0.73833	1.96141	0.93709
H	-0.71908	1.98672	-0.82896
H	-0.87549	3.50105	0.07385

$E_{electronic}$= –1049.090718 a.u.

Table S3(c): Geometrical coordinates of A-Au_4(N6) in Å

Atom	x	y	z
N	-6.38067	0.6404	-0.00064
C	-6.12022	1.98553	-0.00068
H	-6.92361	2.70721	-0.00107
N	-4.84818	2.27937	-0.00055
C	-4.23357	1.055	-0.00022
C	-2.87401	0.69784	-0.00002
N	-1.90625	1.60399	0.00025
H	-0.92154	1.3587	0.
H	-2.15848	2.57655	0.00019
N	-2.60244	-0.63023	0.00004
C	-3.61487	-1.53049	-0.00021
H	-3.30268	-2.56696	-0.00035
N	-4.90153	-1.28554	-0.00023
C	-5.16208	0.02683	-0.00019
C	-7.66886	-0.01258	0.00133
H	-7.76771	-0.65427	-0.87312
H	-7.78467	-0.61956	0.89837
H	-8.44675	0.74742	-0.02107
Au	-0.60397	-1.31101	0.00009
Au	1.71111	2.90259	0.00023
Au	1.78752	-2.36337	0.0001
Au	1.66004	0.32701	-0.00036

$E_{electronic}$= -1049.095637a.u.

Table S3(d): Geometrical coordinates of A-Au_4(N7) in Å

Atom	x	y	z
N	-5.16214	-0.13161	0.00061
C	-4.06854	-0.92337	0.00077
H	-4.12443	-1.99949	0.00119
N	-2.94897	-0.23194	0.00032
C	-3.32706	1.09693	-0.00017
C	-2.63655	2.32991	-0.00078
N	-1.31113	2.45337	-0.001
H	-0.91767	3.37777	-0.00139
H	-0.6718	1.67207	-0.00066
N	-3.37838	3.44727	-0.00115
C	-4.70386	3.35714	-0.00093
H	-5.23502	4.30317	-0.00127
N	-5.46065	2.26461	-0.00034
C	-4.71309	1.16826	0.00002
C	-6.55001	-0.54149	0.00117
H	-7.15386	0.36303	-0.00117
H	-6.77603	-1.12746	-0.88869
H	-6.77668	-1.1232	0.89366
Au	-1.03144	-1.07474	0.00009
Au	1.54719	0.01184	0.00003
Au	1.07276	-2.62981	-0.00029
Au	2.4049	2.43952	0.00028

$E_{electronic}$=-1049.094211 a.u.

Table S3(e): Geometrical coordinates of xA-Au_4(N1) in Å

Atom	x	y	z
N	7.94205	0.18831	0.00022
C	7.99714	1.55746	-0.00028
N	6.83974	2.14622	-0.00062
C	3.85982	-0.07454	-0.0002
C	4.55687	-1.31673	0.00023
C	2.42185	-0.14931	-0.00026
N	1.66924	0.94547	-0.00058
N	1.82384	-1.34612	0.
C	2.60398	-2.46505	0.00035
N	3.89124	-2.51413	0.00049
C	6.6104	-0.13796	0.00011
C	5.9295	1.10824	-0.00038
C	4.55353	1.14166	-0.00053
C	5.95549	-1.34753	0.00039
H	8.95017	2.0681	-0.00031
H	0.65508	0.89304	-0.00051
H	2.07849	1.85929	-0.0006
H	2.05523	-3.39963	0.00051
H	4.05563	2.10228	-0.00092
H	6.45513	-2.30667	0.0007
C	9.05228	-0.72954	0.00039
H	9.02853	-1.36339	0.88806
H	9.03068	-1.3614	-0.88877
H	9.98046	-0.16173	0.00221
Au	-0.27677	-1.53562	-0.00003
Au	-1.49564	3.13132	0.00012
Au	-2.85469	-1.95799	-0.0001
Au	-2.06526	0.61813	0.00006

$E_{electronic}$=-1202.546558 a.u.

Table S3(f): Geometrical coordinates of xA-Au_4(N3) in Å

Atom	x	y	z
N	6.12681	-1.2867	0.00576
C	7.39233	-0.76196	0.00406
N	7.44205	0.53601	0.00097
C	4.16856	2.30253	-0.00219
C	3.33897	1.14476	-0.00044
C	3.48119	3.56251	-0.0034
N	4.14489	4.72751	-0.00599
N	2.15966	3.64008	-0.00601
C	1.47293	2.50248	-0.00629
N	1.96967	1.28134	-0.0027
C	5.27305	-0.21525	0.00349
C	6.11817	0.92654	0.00061
C	5.5645	2.18528	-0.00254
C	3.90073	-0.13456	0.00271
H	8.25557	-1.41292	0.00534
H	3.60341	5.57275	0.01177
H	5.14287	4.78111	0.02732
H	0.392	2.58561	-0.00876
H	6.21856	3.04737	-0.00716
H	3.24585	-0.9983	0.00388
C	5.75732	-2.68024	0.00867
H	5.17198	-2.92115	0.89702
H	5.17366	-2.92542	-0.87963
H	6.66153	-3.28533	0.011
Au	0.62914	-0.35692	-0.00133
Au	-3.75209	1.72532	0.0024
Au	-0.73744	-2.58783	-0.002
Au	-2.15952	-0.29606	0.00052

$E_{electronic}$=-1202.541733 a.u.

Table S3(g): Geometrical coordinates of xA-Au_4(N7) in Å

Atom	x	y	z
N	-3.38294	3.57857	0.29734
C	-2.03347	3.57006	0.27811
N	-1.53351	2.36885	0.12575
C	-3.93077	-0.45506	-0.19268
C	-5.12682	0.31922	-0.08821
C	-4.12876	-1.87295	-0.37401
N	-3.09547	-2.71613	-0.50786
N	-5.34287	-2.39075	-0.43838
C	-6.38009	-1.54493	-0.32594
N	-6.36222	-0.25036	-0.15598
C	-3.8007	2.26975	0.14301
C	-2.61887	1.50603	0.03609
C	-2.66841	0.14159	-0.12995
C	-5.05305	1.71036	0.08605
H	-1.44927	4.47099	0.3791
H	-3.31964	-3.69309	-0.57301
H	-2.13093	-2.46608	-0.34049
H	-7.35942	-2.01162	-0.38356
H	-1.74734	-0.42686	-0.20531
H	-5.9713	2.27595	0.16366
C	-4.23758	4.7309	0.44582
H	-4.87545	4.84473	-0.43122
H	-4.86391	4.62536	1.33208
H	-3.62158	5.62099	0.55269
Au	0.32947	-3.19392	0.21035
Au	0.46365	1.76752	0.01423
Au	1.41582	-0.86424	0.00976
Au	3.02181	1.28277	-0.17117

$E_{electronic}$=-1202.546934 a.u.

Table S3(h): Geometrical coordinates of C-Au_4(N3) in Å

Atom	x	y	z
N	4.88645	-0.45051	-0.33153
C	5.38319	0.57995	0.37685
H	6.4619	0.64475	0.43386
C	4.5775	1.48283	0.97858
H	4.98444	2.30661	1.54341
C	3.1736	1.29889	0.84144
N	2.32195	2.14401	1.42446
H	1.33434	2.08652	1.18124
H	2.66633	2.98567	1.84716
N	2.68088	0.27208	0.14842
C	3.50152	-0.63497	-0.48613
O	3.09469	-1.55773	-1.15158
C	5.74246	-1.41988	-0.99177
H	5.51214	-2.4219	-0.63415
H	5.57173	-1.398	-2.06695
H	6.78021	-1.17649	-0.77446
Au	-0.9513	2.3886	-0.23002
Au	0.57679	-0.0621	-0.01264
Au	-2.05478	-0.04719	-0.02148
Au	-0.88164	-2.43329	0.19678

$E_{electronic}$=-976.781775 a.u.

Table S3(i): Geometrical coordinates of C-Au_4(N3*) in Å

Atom	x	y	z
N	4.8793	1.90846	-0.00014
C	4.42687	3.17785	-0.00003
H	5.18236	3.95258	-0.00009
C	3.10766	3.46516	0.00007
H	2.75812	4.48549	0.00006
C	2.19471	2.37062	0.00011
N	0.88646	2.59137	0.00008
H	0.20817	1.83236	0.00007
H	0.52749	3.5277	0.00052
N	2.64945	1.11419	0.00006
C	3.99344	0.8224	-0.00003
O	4.4272	-0.30817	-0.00002
C	6.29619	1.59043	-0.00019
H	6.54652	1.00343	0.88194
H	6.54573	1.00089	-0.88082
H	6.86329	2.51867	-0.00176
Au	-2.81338	1.91964	-0.00013
Au	-1.4175	-0.25099	0.0002
Au	-0.20824	-2.66073	-0.00012
Au	1.36229	-0.5739	0.00006

$E_{electronic}$=-976.791933 a.u.

Table S3(j): Geometrical coordinates of xC-Au_4(N3) in Å

Atom	x	y	z
C	-4.7749	-0.87575	0.32618
C	-2.51488	-1.59932	0.89069
O	-1.80459	-2.40823	1.43823
N	-2.02236	-0.48661	0.22426
C	-2.82602	0.40525	-0.33832
N	-2.27098	1.45596	-0.93724
C	-4.26896	0.24833	-0.3293
N	-3.88875	-1.7417	0.90378
C	-5.15574	1.14726	-0.93519
C	-6.99237	-0.18874	-0.21907
C	-6.16159	-1.1059	0.3896
C	-6.51827	0.94771	-0.89118
C	-7.47712	1.90199	-1.53785
H	-1.27366	1.618	-0.79673
H	-2.83654	2.21727	-1.25936
H	-4.21653	-2.55635	1.39454
H	-4.78218	2.0176	-1.46098
H	-8.0633	-0.35875	-0.1761
H	-6.9528	2.73384	-2.0074
H	-8.17501	2.31655	-0.80715
H	-8.07131	1.40443	-2.30748
C	-6.69766	-2.31179	1.09703
H	-6.33314	-3.23979	0.64665
H	-6.41021	-2.32257	2.1526
H	-7.78514	-2.33209	1.05405
Au	2.08217	-2.18146	-0.40523
Au	0.10309	-0.29505	0.14197
Au	2.62458	0.4143	-0.12414
Au	0.97416	2.46424	0.38754

$E_{electronic}$=-1169.50788 a.u.

Table S3(k): Geometrical coordinates of xC-Au_4(N3*) in Å

Atom	x	y	z
C	4.89624	-0.66136	-0.00017
C	2.98028	-2.16405	-0.00037
O	2.55737	-3.2984	-0.00073
N	2.14871	-1.05878	0.00012
C	2.61925	0.18426	0.00037
N	1.75673	1.18805	0.0008
C	4.04908	0.44839	0.00024
N	4.3347	-1.90988	-0.00041
C	4.60251	1.73465	0.00049
C	6.78815	0.78983	-0.0001
C	6.29329	-0.49751	-0.00036
C	5.96698	1.92681	0.00036
C	6.57072	3.29917	0.00091
H	0.75143	1.02365	0.00067
H	2.06011	2.14248	0.0009
H	4.91531	-2.73132	-0.0008
H	3.96228	2.60822	0.00076
H	7.86482	0.92541	-0.00028
H	5.80173	4.07109	-0.00141
H	7.20167	3.45304	-0.87715
H	7.1974	3.45415	0.88185
C	7.1965	-1.69189	-0.00086
H	7.03812	-2.31862	0.88172
H	7.0378	-2.31813	-0.88373
H	8.24089	-1.38525	-0.00097
Au	-1.49342	3.122	-0.00031
Au	-1.8195	0.56073	0.00009
Au	-2.48049	-2.05467	0.00008
Au	0.07203	-1.50505	0.00011

$E_{electronic}$=-1169.518388 a.u.

Table S3(l): Geometrical coordinates of G-Au_4(O6) in Å

Atom	x	y	z
N	6.47572	-1.21622	-0.00557
C	6.0392	-2.5127	-0.10542
H	6.74285	-3.32979	-0.15537
N	4.74033	-2.62925	-0.13166
C	4.29018	-1.33303	-0.04353
C	2.99097	-0.79083	-0.02492
O	1.91636	-1.43303	-0.09105
N	2.98889	0.58325	0.07793
H	2.06098	1.01338	0.09576
C	4.10229	1.37503	0.15102
N	3.89688	2.69914	0.29651
H	3.00605	3.09704	0.05189
H	4.70049	3.28754	0.16056
N	5.32266	0.89393	0.12858
C	5.35928	-0.44314	0.03585
C	7.84581	-0.75466	0.0441
H	8.05157	-0.09571	-0.7978
H	8.02876	-0.21857	0.97384
H	8.50415	-1.61781	-0.00719
Au	-0.28185	2.32799	-0.05774
Au	-2.40514	0.64387	0.0265
Au	-0.05496	-0.49372	-0.04238
Au	-2.37405	-2.0507	0.04201

$E_{electronic}$=-1124.262363 a.u.

Table S3(m): Geometrical coordinates of G-Au_4(N3) in Å

Atom	x	y	z
N	-2.58724	2.08256	1.15669
C	-3.43817	3.10853	1.49339
H	-3.09701	3.92168	2.11598
N	-4.63185	2.98417	0.99561
C	-4.58061	1.81676	0.28827
C	-5.59924	1.17573	-0.48547
O	-6.74379	1.48085	-0.70825
N	-5.07953	-0.02143	-1.06656
H	-5.73623	-0.48587	-1.67515
C	-3.83566	-0.52739	-0.93249
N	-3.54183	-1.65711	-1.61362
H	-4.2891	-2.2776	-1.86974
H	-2.65564	-2.08756	-1.38824
N	-2.91231	0.0695	-0.19813
C	-3.31996	1.2446	0.37655
C	-1.20142	1.98315	1.56643
H	-1.02948	1.07139	2.13874
H	-0.52702	2.00019	0.70989
H	-0.97773	2.83913	2.19994
Au	0.92069	-2.60591	0.31401
Au	1.66534	-0.05063	-0.06774
Au	-0.99358	-0.83944	0.01883
Au	2.65289	2.30812	-0.33249

$E_{electronic}$=-1124.268679 a.u.

Table S3(n): Geometrical coordinates of G-Au_4(N7) in Å

Atom	x	y	z
N	3.16059	2.17746	-0.00463
C	2.00546	1.46494	-0.00596
H	1.0221	1.91862	-0.00887
N	2.23389	0.17074	-0.00256
C	3.59781	0.02625	0.0017
C	4.4253	-1.14033	-0.00161
O	4.12728	-2.3116	-0.01002
N	5.78956	-0.7495	-0.00141
H	6.43179	-1.52496	-0.06229
C	6.26597	0.52712	0.00387
N	7.61873	0.68158	-0.05168
H	8.19772	-0.03446	0.35114
H	7.92675	1.62328	0.12211
N	5.4989	1.58341	0.01256
C	4.18745	1.27564	-0.00028
C	3.28461	3.61864	-0.00831
H	3.82227	3.94987	0.87865
H	3.82521	3.94518	-0.8952
H	2.28736	4.05184	-0.01107
Au	-1.62138	-2.51493	0.00081
Au	-1.81195	0.19345	0.00163
Au	0.61454	-1.17461	-0.00137
Au	-1.98175	2.77311	0.00023

$E_{electronic}$=-1124.276384 a.u.

Table S3(o): Geometrical coordinates of xG-Au_4(O6) in Å

Atom	x	y	z
N	-7.94444	-0.97375	0.01698
C	-7.81586	-2.3181	-0.23248
N	-6.59223	-2.7255	-0.36654
C	-4.81592	0.99554	0.2194
C	-3.96618	-0.12408	-0.02588
N	-4.32399	2.26119	0.43104
C	-3.04631	2.42289	0.37884
N	-2.4875	3.65552	0.50962
N	-2.16113	1.39869	0.14711
C	-2.54636	0.1119	-0.05288
O	-1.70295	-0.78773	-0.24657
C	-6.67209	-0.46815	0.04572
C	-5.83013	-1.58433	-0.19786
C	-4.4643	-1.41163	-0.23324
C	-6.1993	0.81204	0.25582
H	-8.69143	-2.94838	-0.30342
H	-1.52221	3.72292	0.78653
H	-3.10647	4.36218	0.86583
H	-1.1527	1.58301	0.08645
H	-3.78559	-2.23378	-0.41442
H	-6.8395	1.66335	0.4426
C	-9.16654	-0.23822	0.21092
H	-9.18733	0.22399	1.19925
H	-9.27459	0.53956	-0.54685
H	-10.00836	-0.92299	0.12926
Au	2.41927	-2.35507	0.12907
Au	2.96338	0.26584	0.1075
Au	0.44557	-0.42412	-0.13553
Au	1.24639	2.33375	-0.19787

$E_{electronic}$=-1277.723642 a.u.

Table S3(p): Geometrical coordinates of xG-Au_4(N3) in Å

Atom	x	y	z
N	2.74126	3.39296	0.91556
C	3.86747	4.17292	0.93192
N	4.96275	3.5486	0.61504
C	3.18872	-0.1528	-0.00939
C	4.59194	-0.05448	-0.19884
N	2.51982	-1.36651	-0.21022
C	3.20758	-2.42247	-0.55236
N	2.61444	-3.63386	-0.68516
N	4.54822	-2.37538	-0.7478
C	5.34415	-1.23418	-0.59102
O	6.53691	-1.31714	-0.77671
C	3.15527	2.14281	0.55147
C	4.55455	2.25506	0.36632
C	5.27756	1.14265	-0.01331
C	2.4547	0.9634	0.36872
H	3.8052	5.21971	1.19417
H	3.0323	-4.30013	-1.31144
H	1.60352	-3.61656	-0.67445
H	5.05823	-3.22141	-0.94834
H	6.34749	1.17243	-0.16935
H	1.3793	0.90044	0.49472
C	1.39457	3.79588	1.24526
H	0.70633	3.55917	0.43111
H	1.04953	3.28759	2.14666
H	1.38212	4.86994	1.41904
Au	-2.04826	-2.3314	0.40343
Au	-1.71744	0.28996	-0.07095
Au	0.41144	-1.51148	0.04509
Au	-1.96959	2.81941	-0.48103

$E_{electronic}$=-1277.739475 a.u.

Table S3(q): Geometrical coordinates of xG-Au_4(N7) in Å

Atom	x	y	z
N	3.16059	2.17746	-0.00463
C	2.00546	1.46494	-0.00596
H	1.0221	1.91862	-0.00887
N	2.23389	0.17074	-0.00256
C	3.59781	0.02625	0.0017
C	4.4253	-1.14033	-0.00161
O	4.12728	-2.3116	-0.01002
N	5.78956	-0.7495	-0.00141
H	6.43179	-1.52496	-0.06229
C	6.26597	0.52712	0.00387
N	7.61873	0.68158	-0.05168
H	8.19772	-0.03446	0.35114
H	7.92675	1.62328	0.12211
N	5.4989	1.58341	0.01256
C	4.18745	1.27564	-0.00028
C	3.28461	3.61864	-0.00831
H	3.82227	3.94987	0.87865
H	3.82521	3.94518	-0.8952
H	2.28736	4.05184	-0.01107
Au	-1.62138	-2.51493	0.00081
Au	-1.81195	0.19345	0.00163
Au	0.61454	-1.17461	-0.00137
Au	-1.98175	2.77311	0.00023

$E_{electronic}$=-1277.738861 a.u.

Table S3(r): Geometrical coordinates of xG-Au_4(benz C) in Å

Atom	x	y	z
N	2.66106	3.93157	0.01002
C	1.33131	3.68493	0.00502
N	1.05245	2.40614	-0.00193
C	4.96693	1.02976	0.0048
C	3.92851	0.05503	-0.00603
N	6.30219	0.69525	0.0223
C	6.60458	-0.55799	-0.00185
N	7.91527	-0.94554	-0.05898
N	5.68028	-1.56436	-0.02314
C	4.30204	-1.35985	-0.02704
O	3.55101	-2.30834	-0.05475
C	3.29837	2.71004	0.00612
C	2.2734	1.74393	-0.00201
C	2.58107	0.39683	-0.00929
C	4.64001	2.38623	0.01013
H	0.5976	4.47512	0.00666
H	8.16283	-1.81692	0.37842
H	8.55461	-0.19117	0.12837
H	5.96635	-2.52754	-0.1069
H	1.81931	-0.37786	-0.01757
H	5.43134	3.12279	0.01789
C	3.29596	5.22619	0.01779
H	3.91376	5.34098	0.90899
H	3.9193	5.3489	-0.86848
H	2.52963	5.99813	0.01885
Au	-3.4097	0.94049	-0.00467
Au	-1.65536	-1.10682	0.00527
Au	-0.85888	1.5485	-0.00396
Au	0.12755	-2.95758	0.00776

$E_{electronic}$=-1277.738861 a.u.

Table S3(s): Geometrical coordinates of xG-Au_4(N1-Y) in Å

Atom	x	y	z
N	7.94324	-0.94168	-0.09032
C	7.83038	-2.25303	-0.4822
N	6.61075	-2.66465	-0.63803
C	4.78913	0.93879	0.38335
C	3.95226	-0.1625	0.03325
N	4.28242	2.16866	0.7287
C	3.00065	2.30349	0.74906
N	2.42029	3.4701	1.13748
N	2.12699	1.29051	0.43661
C	2.52905	0.05025	0.0567
O	1.69616	-0.82928	-0.24543
C	6.66405	-0.46431	0.01611
C	5.83473	-1.56196	-0.33246
C	4.46602	-1.41021	-0.32472
C	6.17579	0.77731	0.37192
H	8.71383	-2.85681	-0.63675
H	1.47417	3.6573	0.84666
H	3.04251	4.25845	1.16839
H	1.11616	1.46495	0.41144
H	3.7968	-2.21943	-0.58301
H	6.80643	1.61454	0.63807
C	9.1574	-0.2106	0.16164
H	9.2399	0.64598	-0.50941
H	9.18908	0.14278	1.19361
H	10.00789	-0.86813	-0.0073
Au	-1.16171	2.31766	-0.34606
Au	-0.45372	-0.4746	-0.14523
Au	-2.94177	0.33007	0.07767
Au	-2.49392	-2.30616	0.219

$E_{electronic}$=-1277.723622 a.u.

Table S3(t): Geometrical coordinates of T-Au_4(O2) in Å

Atom	x	y	z
N	4.11493	2.21952	-0.00003
C	5.39685	1.71889	0.00165
H	6.17267	2.47337	0.00275
C	5.68895	0.40712	0.00171
C	7.07637	-0.13448	0.00324
H	7.24064	-0.76587	0.8782
H	7.24249	-0.76608	-0.87121
H	7.81385	0.66757	0.00394
C	4.5829	-0.54165	0.00029
O	4.69334	-1.74596	-0.00019
N	3.31646	0.05612	-0.00182
H	2.50419	-0.56579	-0.00266
C	3.04228	1.37993	-0.00111
O	1.8946	1.85132	-0.00137
C	3.85178	3.65027	0.00131
H	3.27658	3.92959	-0.87985
H	3.28421	3.92987	0.88739
H	4.80433	4.17364	-0.0029
Au	-2.50345	1.6875	0.00017
Au	-2.03594	-0.95981	0.00151
Au	0.06091	0.60203	-0.00142
Au	0.36586	-2.19971	-0.00068

$E_{electronic}$=-1035.901716 a.u.

Table S3(u): Geometrical coordinates of T-Au_4(O4) in Å

Atom	x	y	z
N	5.58641	0.36898	-0.00016
C	5.38891	1.71741	0.00015
H	6.29433	2.31122	0.00014
C	4.17252	2.30433	0.00043
C	3.96123	3.78041	0.00069
H	3.38985	4.09199	-0.87531
H	3.38914	4.09154	0.87637
H	4.91402	4.30911	0.0012
C	3.02736	1.43103	0.00039
O	1.8662	1.87297	0.00058
N	3.28439	0.09121	0.00013
H	2.47472	-0.53667	0.00012
C	4.52386	-0.5179	-0.00012
O	4.67279	-1.71595	-0.00032
C	6.91626	-0.21671	-0.00035
H	7.0517	-0.83979	0.88235
H	7.05102	-0.8406	-0.88257
H	7.65005	0.58539	-0.001
Au	0.36964	-2.19971	-0.00011
Au	-2.02954	-0.95884	0.00038
Au	0.06393	0.60847	-0.00015
Au	-2.51243	1.68121	-0.00025

$E_{electronic}$=-1035.90462 a.u.

Table S3(v): Geometrical coordinates of xT-Au_4(O2) in Å

Atom	x	y	z
C	2.625516	0.93941	0.000751
O	1.541324	1.539173	0.00146
N	2.744374	-0.410883	-0.000194
C	3.935689	-1.142275	-0.001099
O	3.910158	-2.348798	-0.002042
C	5.150242	-0.318613	-0.000753
C	5.044045	1.069485	0.000284
N	3.781106	1.643894	0.000912
C	6.404374	-0.924794	-0.001473
C	7.417619	1.231834	-0.000121
C	6.191655	1.873637	0.000612
C	7.555824	-0.162014	-0.001149
C	8.916977	-0.790983	-0.001692
H	1.869247	-0.939245	-0.000341
H	3.672878	2.644073	0.001618
H	6.442026	-2.006988	-0.002303
H	8.313446	1.844551	0.000091
H	8.847676	-1.877933	-0.005091
H	9.489804	-0.493354	0.879363
H	9.491686	-0.48788	-0.879626
C	6.08284	3.368207	0.001654
H	5.553064	3.737778	-0.881517
H	5.553092	3.736554	0.885352
H	7.070454	3.825866	0.001962
Au	-0.48907	-2.279998	0.000744
Au	-0.432991	0.536738	0.000614
Au	-2.713566	-0.74241	-0.000504
Au	-2.839591	1.941355	-0.000625

$E_{electronic}$=-1189.5722337 a.u.

Table S3(w): Geometrical coordinates of xT-Au_4(O4) in Å

Atom	x	y	z
C	-3.63499	-2.16536	0.00445
O	-3.36852	-3.34151	0.0064
N	-2.65853	-1.17722	0.00241
C	-2.85801	0.16676	-0.00009
O	-1.91162	0.96576	-0.00184
C	-4.24141	0.61529	-0.00053
C	-5.25649	-0.34243	0.00165
N	-4.91625	-1.67942	0.00409
C	-4.55069	1.97634	-0.00308
C	-6.86461	1.41437	-0.00124
C	-6.60167	0.05702	0.00127
C	-5.8641	2.39675	-0.00341
C	-6.22755	3.85146	-0.00546
H	-1.68852	-1.50485	0.00244
H	-5.63153	-2.3867	0.00551
H	-3.73226	2.68474	-0.00481
H	-7.90281	1.731	-0.00164
H	-5.33757	4.47933	-0.01511
H	-6.81363	4.11324	0.87829
H	-6.82869	4.10711	-0.88078
C	-7.70208	-0.95945	0.00346
H	-7.65963	-1.60598	-0.87823
H	-7.6596	-1.60217	0.88793
H	-8.67552	-0.47231	0.00242
Au	2.28261	2.2458	0.00177
Au	0.21695	0.37192	-0.00064
Au	2.714	-0.4048	0.00017
Au	0.86244	-2.37249	-0.00206

$E_{electronic}$=-1189.381592 a.u.

Table S4(a): Dipole moments (μ), polarizability (α), hyperpolarizability (β) and electrophilicity index (ω) values of Au_3 complexes. All the calculations were performed at PBE0/SDD∪6-311++G(2d,2p).

Complex	μ (Debye)	α (esu)	β (a.u.)	ω (eV)
A-Au_3(N1)	8.62	241.84	438.25	3.77
A-Au_3(N3)	7.25	244.60	526.55	3.80
A-Au_3(N6)	8.85	246.00	545.50	4.91
A-Au_3(N7)	6.34	238.41	709.68	4.03
xA-Au_3(N1)	10.17	304.33	601.49	4.90
xA-Au_3(N3)	7.25	295.80	806.01	5.27
xA-Au_3(N7)	7.01	292.63	1089.57	4.63
C-Au_3(N3)	10.27	216.94	279.57	3.98
C-Au_3(N3*)	5.79	221.48	700.79	5.35
xC-Au_3(N3)	11.62	284.65	677.46	5.28
xC-Au_3(N3*)	11.62	284.68	677.46	5.28
G-Au_3(O6)	7.19	244.75	522.71	4.82
G-Au_3(N3)	1.54	240.25	1130.44	4.78
G-Au_3(N7)	14.14	248.19	290.56	2.85
xG-Au_3(N7)	13.33	307.05	517.19	4.27
xG-Au_3(N3)	1.80	297.06	1293.85	4.23
xG-Au_3(O6)	7.37	307.50	700.33	4.89
xG-Au_3(N7-bH)	13.33	307.52	517.04	4.26
T-Au_3(O2)	9.12	222.28	489.10	4.89
T-Au_3(O4)	9.32	224.62	389.41	4.59
xT-Au_3(O2)	10.05	275.81	782.00	4.80
xT-Au_3(O4)	10.07	276.86	705.81	5.16

Table S4(b): Dipole moments (μ), polarizability (α), hyperpolarizability (β) and electrophilicity index (ω) values of Au_4 complexes. All the calculations were performed at PBE0/SDD∪6-311++G(2d,2p).

Complex	μ (Debye)	α (esu)	β (a.u.)	ω (eV)
A-Au_4(N1)	8.11	283.18	467.49	4.62
A-Au_4(N3)	7.52	277.30	561.54	4.99
A-Au_4(N7)	8.34	275.19	717.49	5.37
xA-Au_4(N1)	9.91	338.98	611.56	4.77
xA-Au_4(N3)	12.00	341.14	918.94	6.35
xA-Au_4(N7)	8.94	325.99	1137.07	5.08
C-Au_4(N3)	10.17	261.49	279.02	4.46
C-Au_4(N3*)	9.54	253.35	309.72	4.51
xC-Au_4(N3)	11.54	331.66	716.04	4.78
xC-Au_4(N3*)	10.54	318.61	728.96	4.68
G-Au_4(O6)	8.60	295.13	511.22	5.69
G-Au_4(N3)	5.61	281.73	281.73	5.67
G-Au_4(N7)	12.34	281.31	297.13	4
xG-Au_4(N3)	4.52	332.20	1373.90	4.48
xG-Au_4(N7)	11.62	342.91	564.30	4.31
xG-Au_4(O6)	8.07	354.10	727.64	5.78
T-Au_4(O2)	8.39	264.34	551.09	5.38
T-Au_4(O4)	9.00	267.15	412.86	8.72
xT-Au_4(O2)	9.51	320.03	731.22	5.29
xT-Au_4(O4)	9.63	318.24	760.90	5.20

Table S5(a): Data for calculating Pearson correlation coefficient for Au_3 complexes.

Bond length	E_{int}
2.121	32.27546
2.200	17.91073
2.097	32.22714
2.130	33.60764
2.197	18.06447
2.167	27.77942
2.112	29.45360
2.098	32.30119
2.117	33.27256
2.103	30.46701
2.174	17.06047
2.131	33.80782
2.202	18.22386
2.205	17.06047
2.188	20.30527
2.191	19.25672
2.205	18.42842

Table S5(b): Data for calculating Pearson correlation coefficient for Au_4 complexes.

Bond length	E_{int}
2.117	24.84084
2.108	24.54780
2.095	27.63510
2.109	29.82947
2.247	13.71213
2.089	30.06603
2.292	13.16871
2.204	10.85512
2.290	13.63369
2.136	25.05984
2.313	4.25948
2.105	26.56459
2.105	26.56333
2.184	18.37508
2.182	17.17656
2.095	26.72585
2.219	11.14252
2.202	12.96478
2.442	0.03138
2.210	12.14338

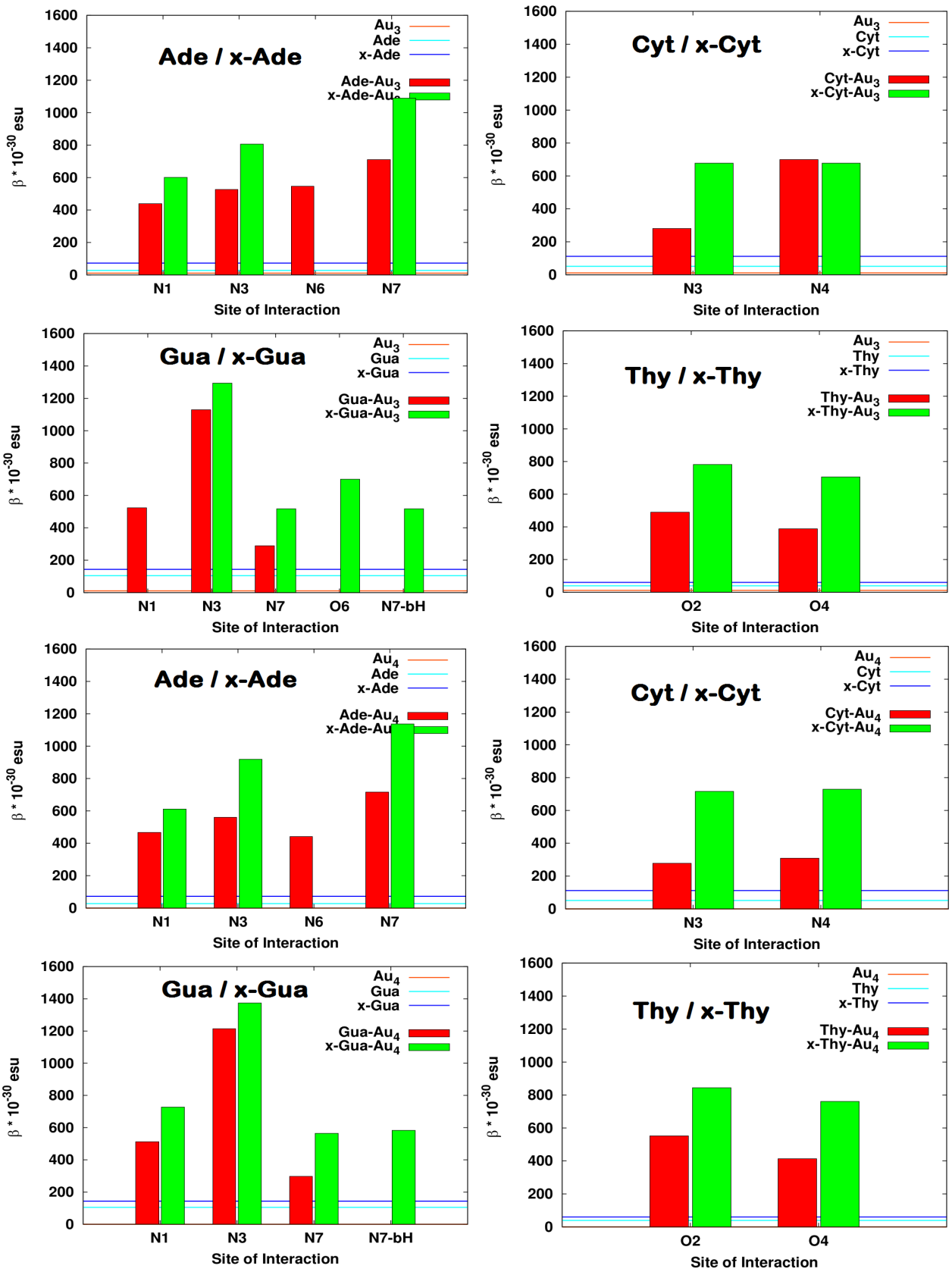

Figure S3: Comparison of Hyperpolarizability values before and after complexation for complexes with Au_3 and Au_4.

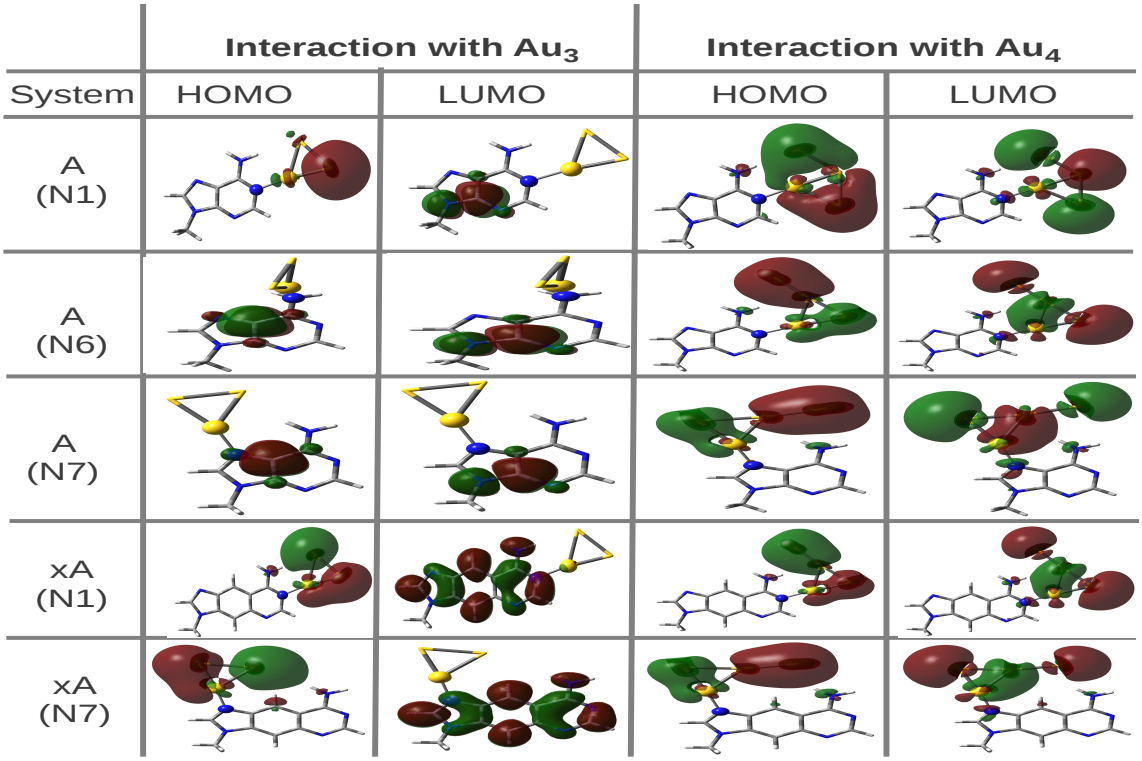

Figure S5(a): The natural orbital plots corresponding to the HOMO and LUMO orbitals of Adenine and x-Adenine complexes calculated at PBE0/SDD∪6-311++G(2d,2p) level of theory.

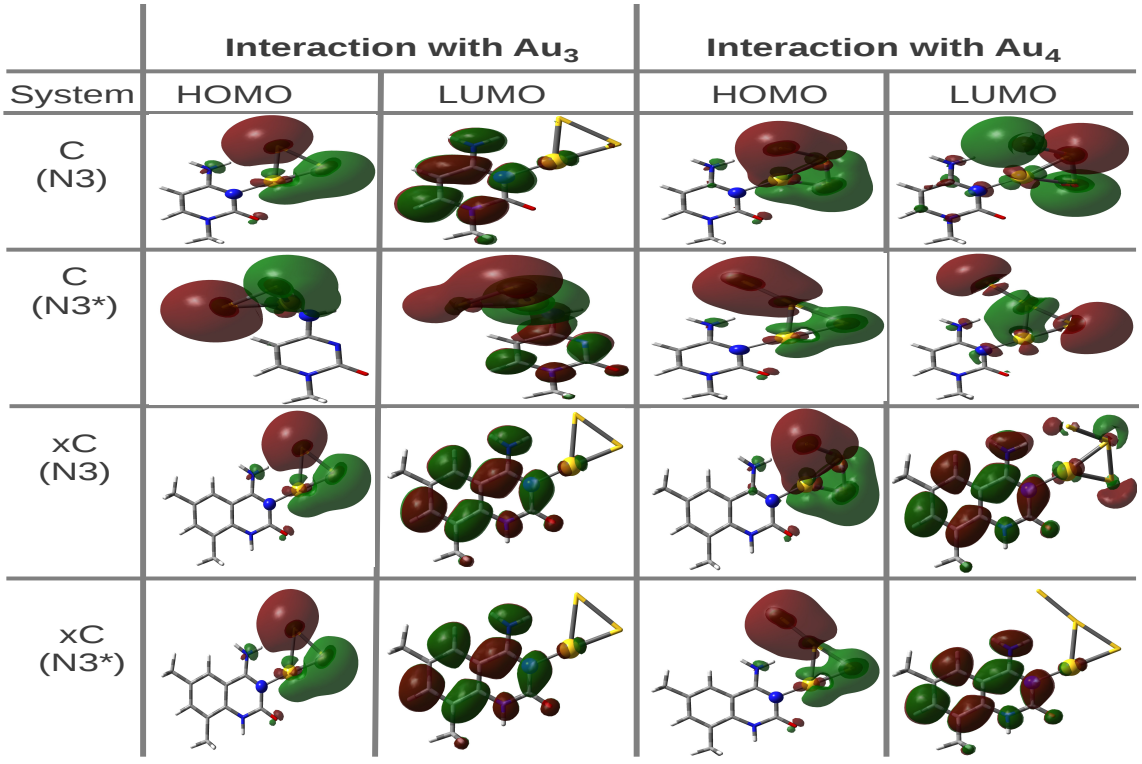

Figure S5(b): The natural orbital plots corresponding to the HOMO and LUMO orbitals of Cytosine and x-Cytosine complexes calculated at PBE0/SDD∪6-311++G(2d,2p) level of theory.

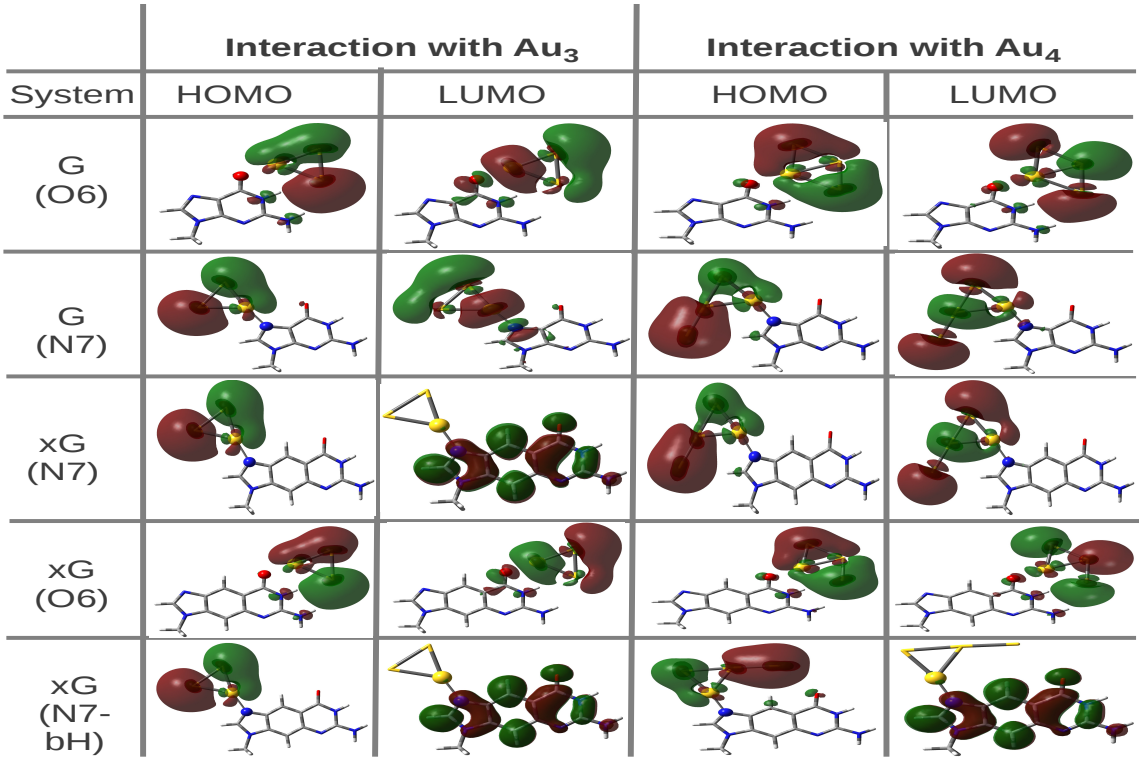

Figure S5(c): The natural orbital plots corresponding to the HOMO and LUMO orbitals of Guanine and x-Guanine complexes calculated at PBE0/SDD∪6-311++G(2d,2p) level of theory.

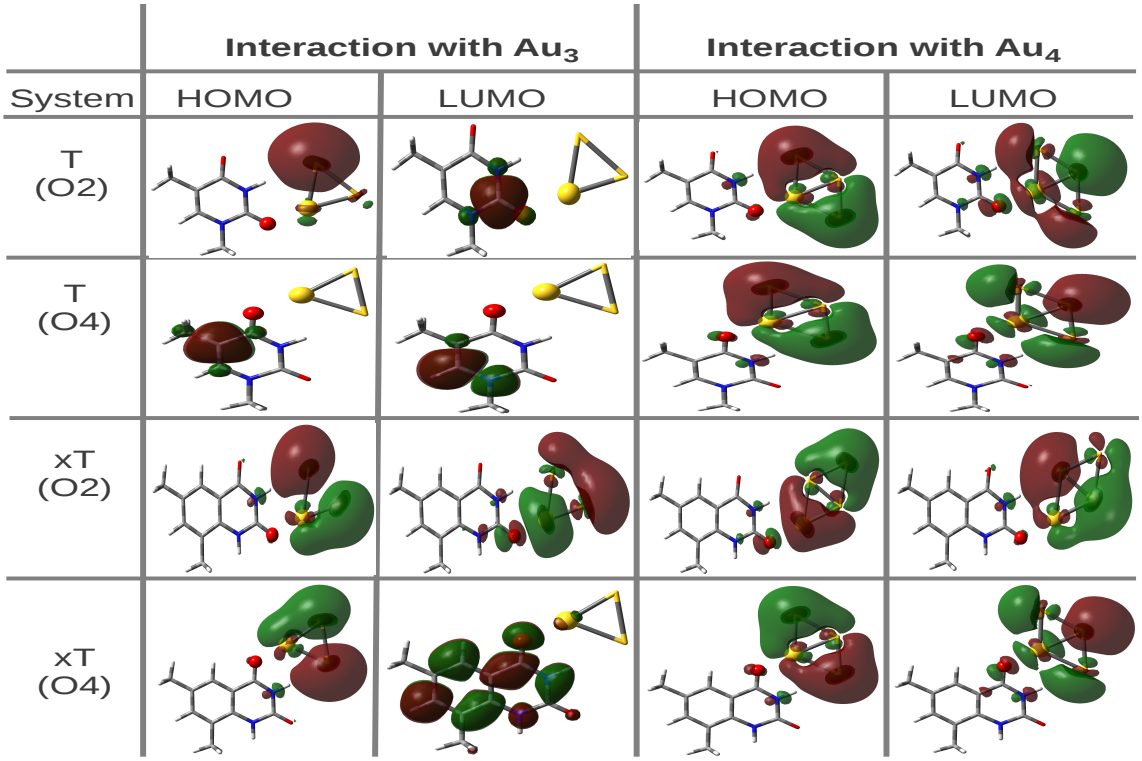

Figure S5(d): The natural orbital plots corresponding to the HOMO and LUMO orbitals of Thymine and x-Thymine complexes calculated at PBE0/SDD∪6-311++G(2d,2p) level of theory.