

## Electronic Supplementary Information

### Guanine Binding to Gold Nanoparticles through Nonbonding Interactions

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Supporting information includes the following parts:

#### 1. Mulliken Charges

**Figure S1.** Mulliken charges of Au<sub>13</sub>, Au<sub>13</sub>-G1 and Au<sub>13</sub>-G2. Negative values mean electron gain and are observed at the surface shell of NPs.

#### 2. LDOS of Au<sub>13</sub> and Au<sub>147</sub>

**Figure S2.** Comparison of LDOS of Au<sub>13</sub> and Au<sub>13</sub>-G (complex) at the bonding gold atom (Au(B)) and corner atoms in layers with label 1 referring to the surface.

**Figure S3.** Comparison of LDOS of Au<sub>147</sub> and Au<sub>147</sub>-G (complex) at bonding gold atom (Au(B)) and corner atoms in layers with label 1 referring to the surface.

#### 3. FO Analysis of Au<sub>13</sub>-G1 (N(5)-Au; O-Au)

**Table S1.** Gross charges in FO of Au<sub>13</sub>-G1 (N5): spin up.

**Table S2.** Gross charges in FO of Au<sub>13</sub>-G1 (N5): spin down.

**Table S3.** Shape of FO Basis: spin up

**Table S4.** Shape of FO Basis: spin down

**Table S5.** Shape and Coefficients of key MO in Au<sub>13</sub>-G1 Complex

#### 4. FO Analysis of Au<sub>13</sub>-G2 (N(2)-Au; H...Au)

**Table S6.** Gross charges in FO of Au<sub>13</sub>-G2 (N2): spin up.

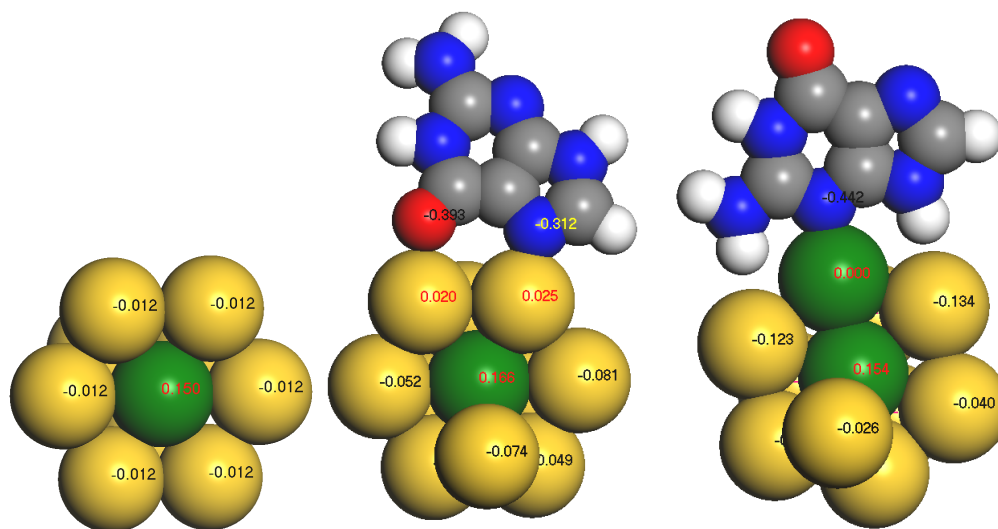
**Table S7.** Gross charges in FO of Au<sub>13</sub>-G2 (N2): spin down.

**Table S8.** Shape of FO basis (spin up and spin down has slight difference)

**Table S9.** Shape and coefficients of key MO in Au<sub>13</sub>-G2 Complex

#### 5. XYZ coordinates of optimized geometries

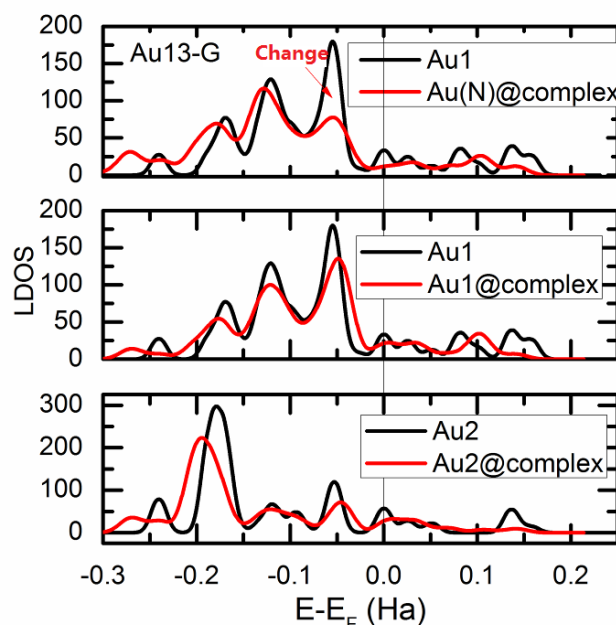
## 1. Mulliken Charges



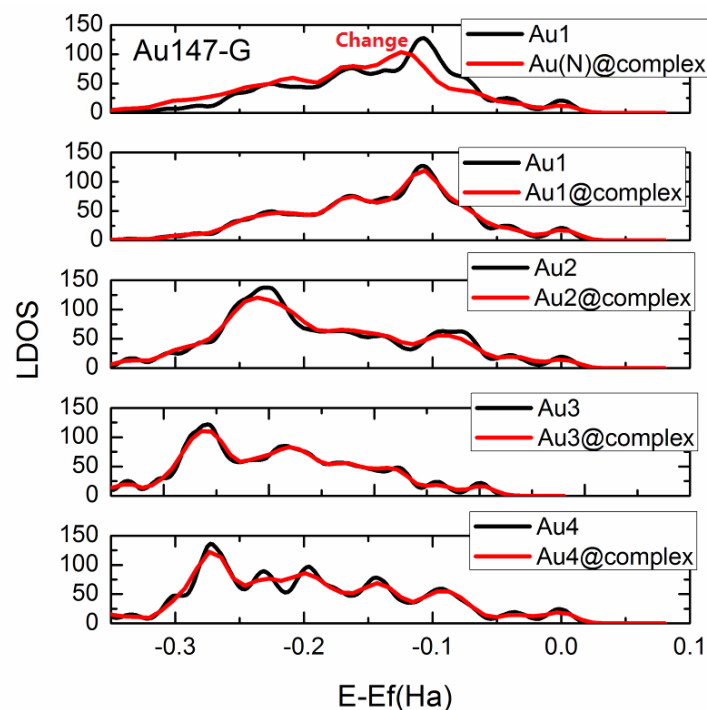
**Figure S1.** Mulliken charges of Au<sub>13</sub>, Au<sub>13</sub>-G1 and Au<sub>13</sub>-G2. Negative values mean electron gain and are observed at the surface shell of NPs. Positive values mean electron loss and are observed in core shells, indicating charge transfer from center to the surface.

## 2. LDOS of Au<sub>13</sub> and Au<sub>147</sub>

As shown in Figures S2 and S3, valence charges at 1<sup>st</sup> atomic shell are polarized upward to  $E_F$ . Au<sub>N</sub> atomic site changes its valence electrons while others remain more or less the same. The results indicate that the polarization occurs mostly at the surface layer of the cluster, and enhances the Au–N bond formation.



**Figure S2** Comparison of LDOS of Au<sub>13</sub> and Au<sub>13</sub>-G1 (complex) at the bonding gold atom (Au(N)) and corner atoms in layers with label 1 referring to the surface.



**Figure S3** Comparison of LDOS of Au<sub>147</sub> and Au<sub>147</sub>-G1 (complex) at the bonding gold atom (Au(N)) and corner atoms in layers with label 1 referring to the surface.

### 3. FO analysis of Au<sub>13</sub>-G1 (N(5)-Au; O-Au)

Au<sub>13</sub> in the doublet spin state has 247 FOs for each spin. 124 FOs are occupied for spin-up while 123 MOs occupied for spin-down. Guanine in the singlet state has 179 FOs with 39 orbitals occupied for each spin. The Au<sub>13</sub>-G complexes in the doublet state have 426 MOs for each spin. 163 MOs are occupied for spin up while 162 MOs occupied for spin down.

Despite the different adsorption sites in Au<sub>13</sub>-G1 and Au<sub>13</sub>-G2, electron donation from the *p<sub>z</sub>* lone pair of N to the Au unoccupied orbital always occurs because of the high electron-donation ability of the N lone pair. In Au<sub>13</sub>-G1, oxygen also donates *p<sub>z</sub>* electrons and forms a Au-O bond with a bond order of 0.247.

Besides the donation from guanine to Au, because of the filled *d* shells of Au, the back-donation from Au to guanine is also considerable. In Au<sub>13</sub>-G1, the back-donation occurs through the  $\pi$  bond between Au *d<sub>yz</sub>* orbital and N, O *p<sub>y</sub>* orbitals, while in Au<sub>13</sub>-G2, back donation is through the Au... H-N hydrogen bond. The results of gross FO population analysis in Tables S6 and S7 show that charge gain of unoccupied FO of guanine occurs mainly in orbitals *g<sub>42</sub>*, *g<sub>44</sub>* and *g<sub>45</sub>*, which are all dominated by the H unoccupied orbital as shown in Table S8. The coefficients of MOs 161 and 162 in Au<sub>13</sub>-G2 in Table S9 also indicate the formation of a bond between the occupied Au 6*s* orbital in FO *a<sub>122</sub>* and *a<sub>123</sub>* with the H unoccupied orbital in *g<sub>42</sub>*, *g<sub>44</sub>* and *g<sub>45</sub>*.

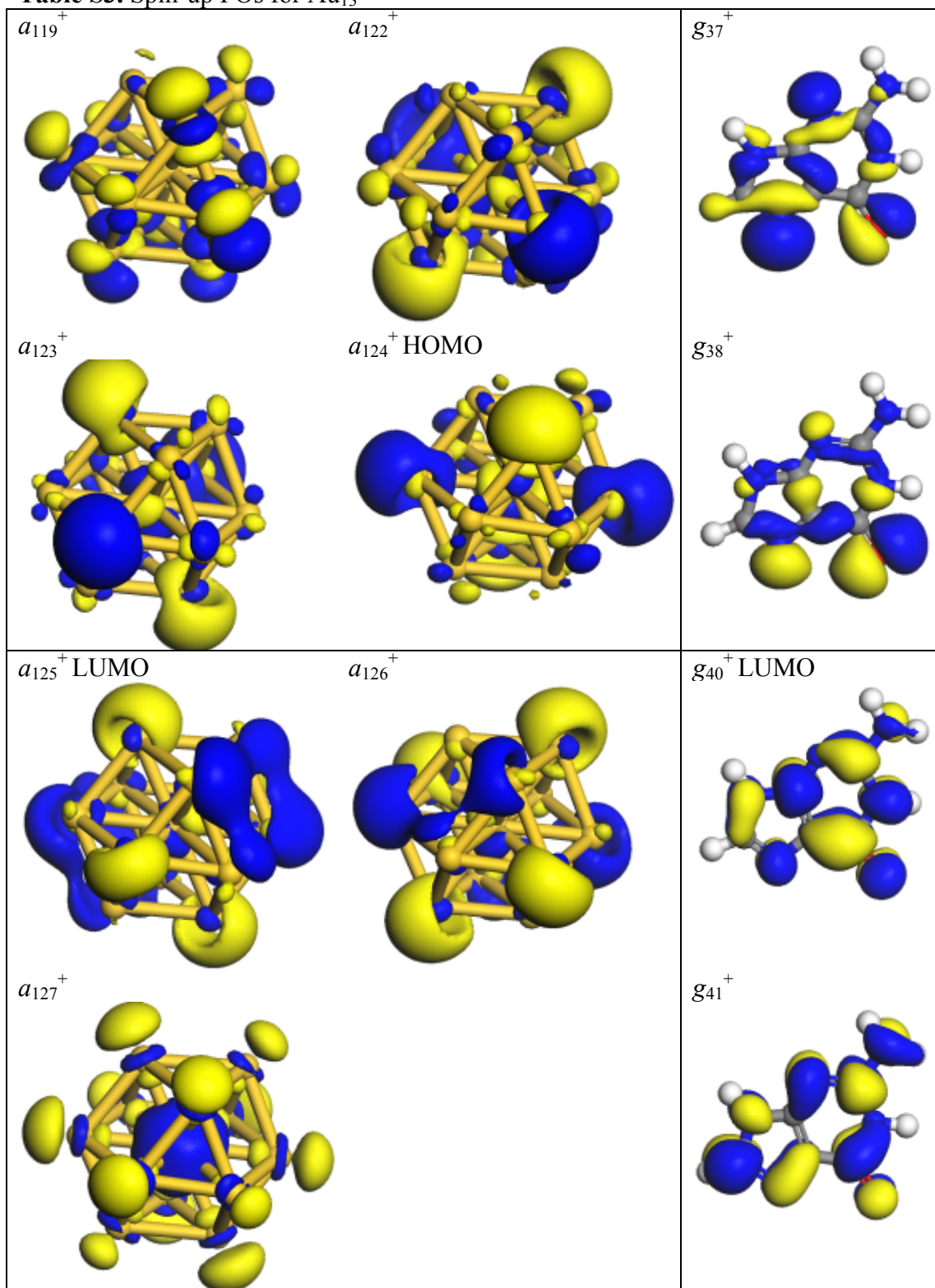
**Table S1.** Gross populations in FO of Au<sub>13</sub>-G1 (N5) for the spin-up electrons. HOMO is 124 for Au<sub>13</sub> and is 39 for guanine.

<b>Au13</b>				<b>Guanine</b>							
1	1.000	41	1.000	81	0.999	121	0.999	1	1.000	<b>41</b>	<b>0.018</b>
2	1.000	42	1.000	82	0.999	<b>122</b>	<b>0.979</b>	2	1.000	42	0.002
3	1.000	43	1.000	83	0.999	<b>123</b>	<b>0.820</b>	3	1.000	<b>43</b>	<b>0.012</b>
4	1.000	44	1.000	84	0.999	<b>124</b>	<b>0.985</b>	4	1.000	44	0.002
5	1.000	45	1.000	85	0.998	<b>125</b>	<b>0.270</b>	5	1.000	45	0.001
6	1.000	46	1.000	86	0.999	<b>126</b>	<b>0.062</b>	6	1.000	46	0.001
7	1.000	47	1.000	87	0.998	<b>127</b>	<b>0.050</b>	7	1.000	47	0.003
8	1.000	48	1.000	88	1.000	128	0.004	8	1.000	48	0.003
9	1.000	49	1.000	89	0.999	129	0.038	9	1.000	49	0.001
10	1.000	50	1.000	90	1.000	130	0.016	10	1.000	50	0.001
11	1.000	51	1.000	91	0.998	131	0.008	11	1.000	51	0.000
12	1.000	52	1.000	92	0.998	132	0.002	12	1.001	52	0.002
13	1.000	53	0.999	93	0.997	133	0.020	13	0.997	53	0.003
14	1.000	54	1.004	94	0.993	134	0.006	14	0.997	54	0.001
15	1.000	55	1.000	95	0.999	135	0.003	15	0.999	55	0.000
16	1.000	56	1.000	96	0.999	136	0.009	16	0.998	56	0.001
17	0.999	57	1.000	97	0.999	137	0.004	17	0.994	57	0.000
18	1.000	58	1.001	98	0.998	138	0.003	18	0.997	58	0.000
19	1.000	59	1.001	99	0.999	139	0.003	19	0.998	59	0.000
20	1.000	60	1.004	100	0.992	140	0.008	20	0.998	60	0.001
21	1.000	61	1.003	101	0.999	141	0.002	21	0.995	61	0.001
22	1.000	62	1.000	102	0.995	142	0.008	22	0.998	62	0.000
23	1.000	63	1.000	103	0.997	143	0.001	23	0.999	63	0.000
24	1.000	64	1.000	104	0.998	144	0.001	24	0.998	64	0.002
25	1.000	65	1.000	105	0.998	145	0.001	25	0.999	65	0.001
26	1.000	66	0.999	106	0.999	146	0.000	26	0.998	66	0.001
27	1.000	67	1.000	107	0.998	147	0.001	27	1.000	67	0.000
28	1.000	68	1.000	108	0.992	148	0.000	28	0.999	68	0.000
29	1.000	69	1.000	109	0.997	149	0.000	29	1.000	69	-0.003
30	1.000	70	1.000	110	0.997	150	0.001	30	0.999	70	-0.001
31	1.000	71	0.998	111	0.998	151	0.002	31	0.966	71	-0.001
32	1.000	72	1.000	112	0.999	152	0.001	32	0.999	72	-0.001
33	1.000	73	0.999	113	0.997	153	0.001	33	0.999	73	0.000
34	1.000	74	1.000	114	0.996	154	0.001	34	0.975	74	0.000
35	1.000	75	0.999	115	0.988	155	0.001	35	0.998	75	-0.002
36	1.000	76	0.999	116	0.997	156	0.001	36	0.994	76	0.000
37	1.000	77	1.000	117	0.999	157	0.000	<b>37</b>	<b>0.895</b>	77	0.000
38	1.000	78	0.999	118	0.998	158	0.001	<b>38</b>	<b>0.930</b>	78	0.000
39	1.000	79	1.000	<b>119</b>	<b>0.988</b>	159	0.001	39	0.994	79	-0.002
40	1.000	80	1.000	120	0.992	160	0.000	<b>40</b>	<b>0.019</b>	80	0.000

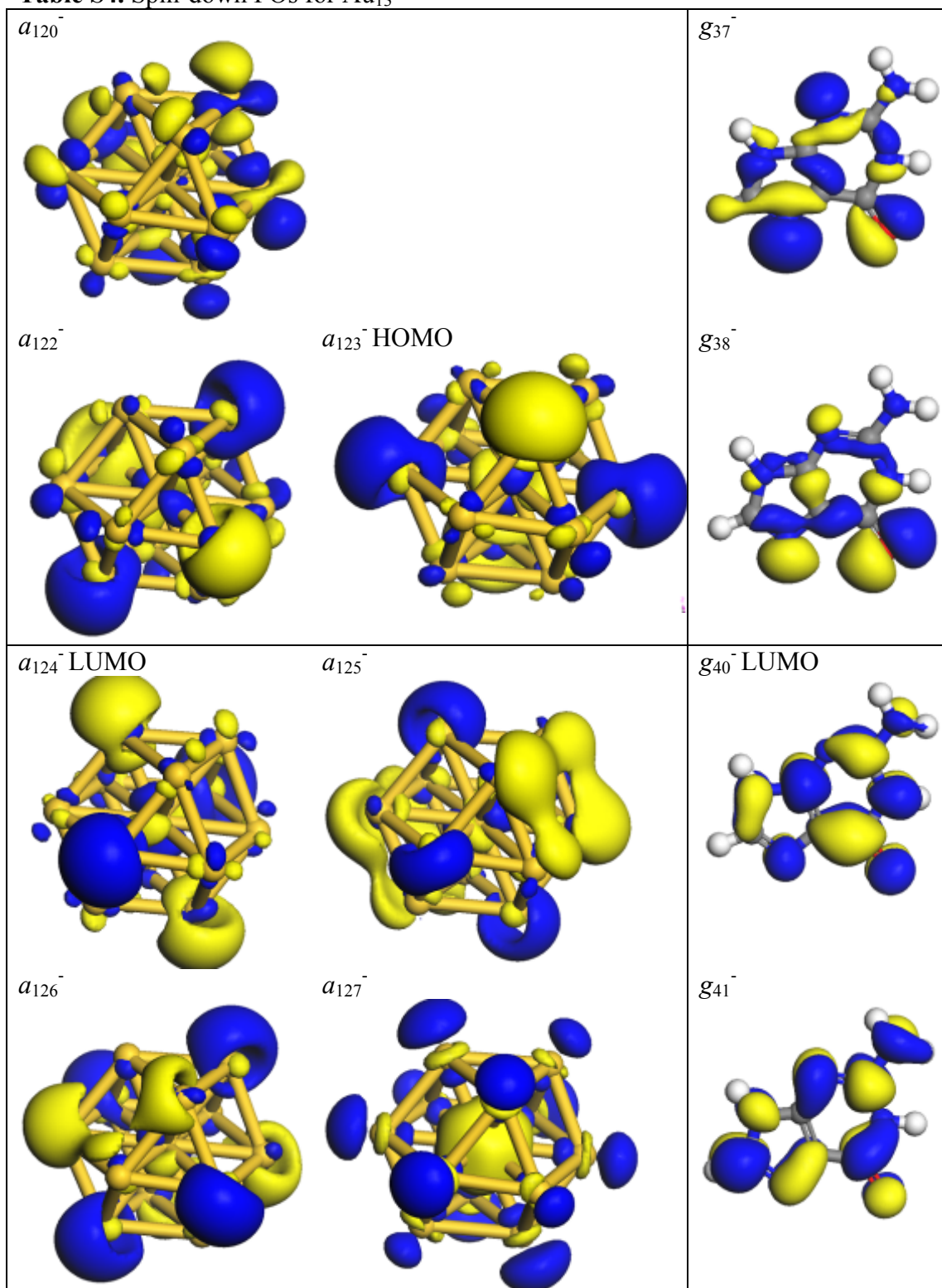
**Table S2.** Gross populations in FO of Au<sub>13</sub>-G1 (N5) for the spin-down electrons.  
 HOMO is 124 for Au<sub>13</sub> and is 39 for guanine.

1	1.000	41	1.000	81	0.999	121	0.999	1	1.000	<b>41</b>	<b>0.012</b>
2	1.000	42	1.000	82	0.999	<b>122</b>	<b>0.976</b>	2	1.000	42	0.002
3	1.000	43	1.000	83	1.000	123	0.993	3	1.000	<b>43</b>	<b>0.011</b>
4	1.000	44	1.000	84	0.998	<b>124</b>	<b>0.131</b>	4	1.000	44	0.001
5	1.000	45	1.000	85	0.998	<b>125</b>	<b>0.040</b>	5	1.000	45	0.001
6	1.000	46	1.000	86	0.999	<b>126</b>	<b>0.044</b>	6	1.000	46	0.001
7	1.000	47	1.000	87	0.999	<b>127</b>	<b>0.036</b>	7	1.000	47	0.003
8	1.000	48	1.000	88	1.000	128	0.004	8	1.000	48	0.003
9	1.000	49	1.000	89	0.999	129	0.009	9	1.000	49	0.001
10	1.000	50	1.000	90	1.000	130	0.037	10	1.000	50	0.001
11	1.000	51	1.000	91	0.998	131	0.006	11	1.000	51	0.000
12	1.000	52	1.000	92	0.997	132	0.002	12	1.001	52	0.002
13	1.000	53	0.999	93	0.997	133	0.015	13	0.997	53	0.003
14	1.000	54	1.003	94	0.992	134	0.009	14	0.997	54	0.001
15	1.000	55	1.000	95	0.999	135	0.003	15	0.999	55	0.000
16	1.000	56	1.001	96	0.999	136	0.007	16	0.998	56	0.001
17	0.999	57	1.000	97	0.999	137	0.004	17	0.994	57	0.000
18	1.000	58	1.001	98	0.999	138	0.003	18	0.997	58	0.000
19	1.000	59	1.001	99	0.998	139	0.002	19	0.998	59	0.000
20	1.000	60	1.004	100	0.992	140	0.009	20	0.998	60	0.001
21	1.000	61	1.003	101	0.999	141	0.001	21	0.995	61	0.001
22	1.000	62	1.000	102	0.995	142	0.008	22	0.998	62	0.000
23	1.000	63	1.000	103	0.997	143	0.001	23	0.999	63	0.000
24	1.000	64	1.000	104	0.998	144	0.001	24	0.998	64	0.002
25	1.000	65	1.000	105	0.997	145	0.001	25	0.999	65	0.001
26	1.000	66	1.000	106	0.999	146	0.000	26	0.998	66	0.001
27	1.000	67	1.000	107	0.998	147	0.001	27	1.000	67	0.001
28	1.000	68	1.000	108	0.995	148	0.000	28	0.999	68	0.000
29	1.000	69	1.000	109	0.994	149	0.001	29	1.000	69	-0.002
30	1.000	70	1.000	110	0.998	150	0.001	30	0.999	70	0.000
31	1.000	71	0.998	111	0.997	151	0.002	31	0.966	71	-0.001
32	1.000	72	1.000	112	0.998	152	0.001	32	0.999	72	-0.001
33	1.000	73	0.999	113	0.997	153	0.001	33	0.999	73	0.000
34	1.000	74	1.000	114	0.996	154	0.001	34	0.973	74	0.000
35	1.000	75	1.000	115	0.997	155	0.001	35	0.997	75	-0.002
36	1.000	76	0.999	116	0.990	156	0.001	36	0.994	76	0.000
37	1.000	77	1.000	117	0.998	157	0.000	<b>37</b>	<b>0.890</b>	77	0.000
38	1.000	78	0.999	118	0.996	158	0.001	<b>38</b>	<b>0.924</b>	78	0.001
39	1.000	79	1.000	119	0.995	159	0.001	39	0.992	79	-0.002
40	1.000	80	1.000	<b>120</b>	<b>0.979</b>	160	0.000	<b>40</b>	<b>0.014</b>	80	0.000

**Table S3.** Spin-up FOs for Au<sub>13</sub>

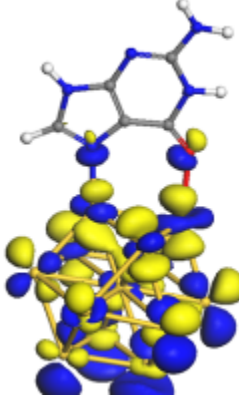
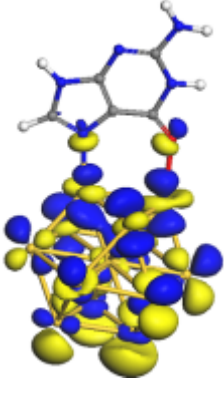
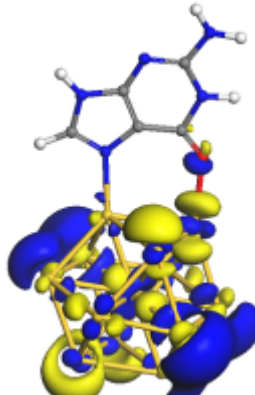
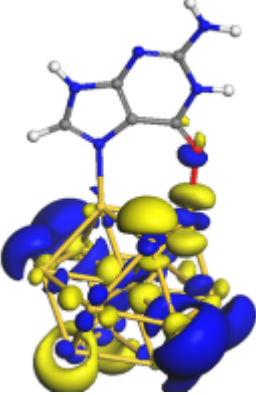
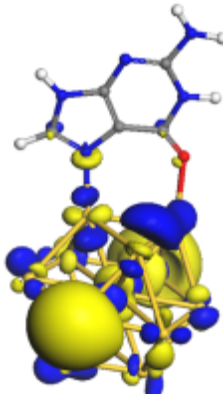
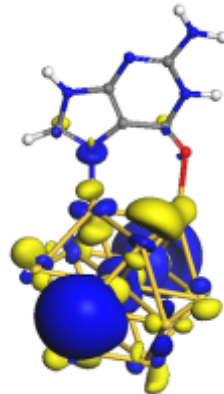


**Table S4.** Spin-down FOs for Au<sub>13</sub>





**Table S5.** Shape and coefficients of key MO in the Au<sub>13</sub>-G1 Complex (bold numbers indicate occupied FOs)

$\psi_{159}^+$ : -0.20117 Ha $0.66 a_{119} - 0.49 a_{120} - 0.22 a_{123}$ $- 0.079 a_{125} - 0.062 a_{126} - 0.075 a_{127}$ $- 0.21 g_{38} - 0.02 g_{40} + 0.023 g_{41}$ 	$\psi_{159}^-$ : -0.20029 Ha $-0.78 a_{120} + 0.25 a_{119} + 0.21 a_{124}$ $-0.075 a_{125} - 0.06 a_{126} - 0.08 a_{127}$ $+ 0.21 g_{38} + 0.02 g_{40} - 0.023 g_{41}$ 
$\psi_{162}^+$ : -0.16224 Ha $+0.73 a_{122} - 0.17 a_{123} + 0.62 a_{124}$ $- 0.13 a_{126} - 0.095 g_{37} - 0.071 g_{38}$ $- 0.031 g_{40} + 0.049 g_{41}$ 	$\psi_{162}^-$ : -0.16118 Ha $-0.75 a_{122} + 0.62 a_{123} - 0.06 a_{124}$ $+ 0.13 a_{126} - 0.091 g_{37} - 0.077 g_{38}$ $- 0.035 g_{40} + 0.053 g_{41}$ 
$\psi_{163}^+$ (HOMO): -0.15274 Ha $-0.83 a_{123} - 0.16 a_{124} + 0.46 a_{125}$ $+ 0.13 a_{126} + 0.12 a_{127} - 0.089 g_{37}$ $+ 0.11 g_{38} + 0.07 g_{40} + 0.07 g_{41}$ 	$\psi_{161}^-$ (LUMO): -0.14682 Ha 

#### 4. Au<sub>13</sub>-G2 (N(2)-Au; H...Au)

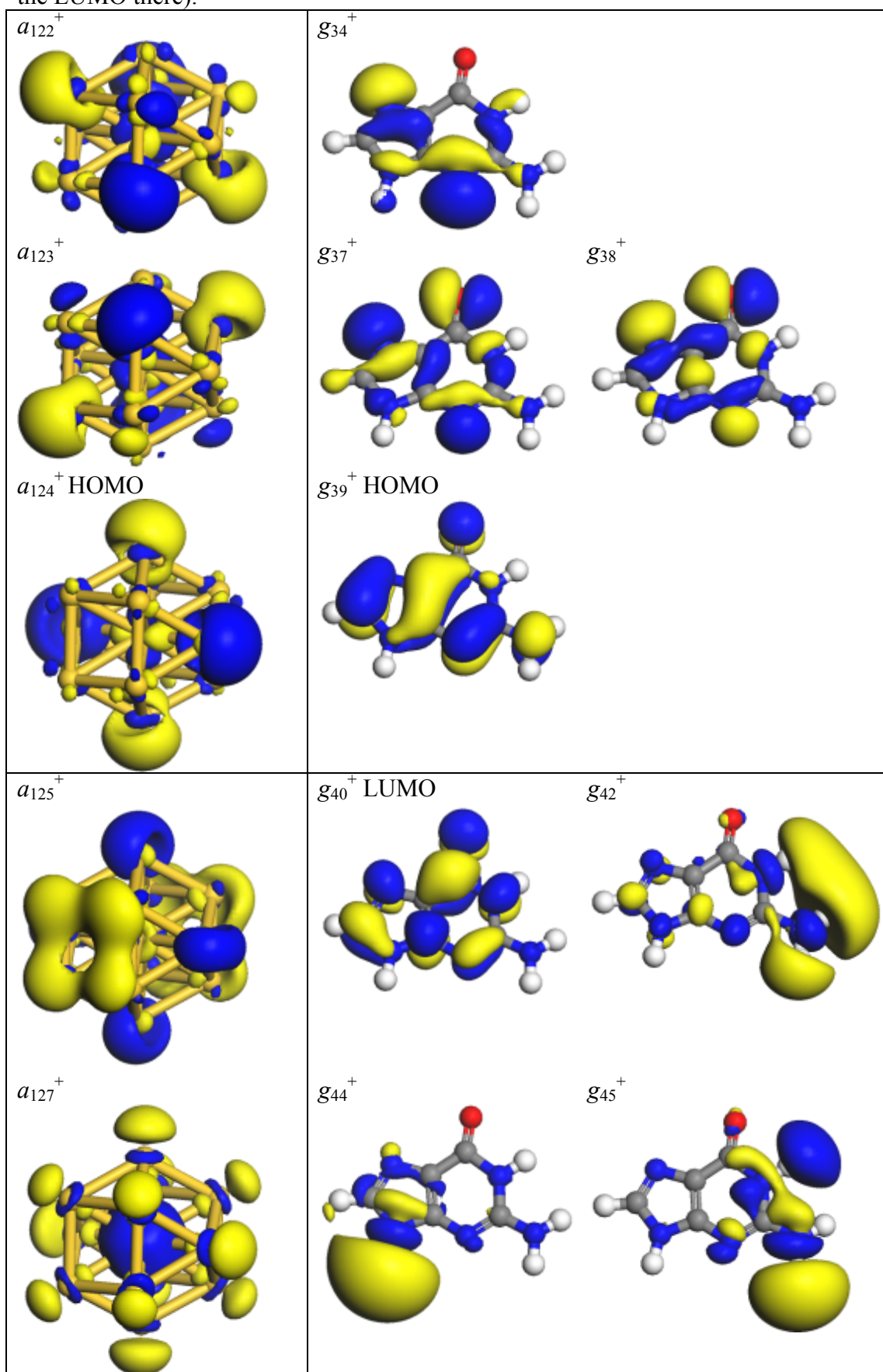
**Table S6.** Gross population changes of spin-up FOs.

1	1.000	41	1.000	81	1.000	121	0.999	1	1.000	41	0.005
2	1.000	42	1.000	82	0.999	<b>122</b>	<b>0.980</b>	2	1.000	<b>42</b>	<b>0.013</b>
3	1.000	43	1.000	83	0.999	<b>123</b>	<b>0.970</b>	3	1.000	43	0.008
4	1.000	44	1.000	84	0.998	<b>124</b>	<b>0.800</b>	4	1.000	<b>44</b>	<b>0.046</b>
5	1.000	45	1.000	85	0.999	<b>125</b>	<b>0.322</b>	5	1.000	<b>45</b>	<b>0.032</b>
6	1.000	46	1.000	86	1.000	126	0.010	6	1.000	46	0.003
7	1.000	47	1.000	87	0.999	<b>127</b>	<b>0.055</b>	7	1.000	47	0.002
8	1.000	48	1.000	88	0.999	128	0.001	8	1.000	48	0.003
9	1.000	49	1.000	89	0.999	129	0.037	9	1.000	49	0.000
10	1.000	50	1.000	90	0.999	130	0.007	10	1.000	50	-0.001
11	1.000	51	1.000	91	1.000	131	0.004	11	1.000	51	0.001
12	1.000	52	1.000	92	0.998	132	0.002	12	1.000	52	0.001
13	1.000	53	0.997	93	0.999	133	0.028	13	0.998	53	0.003
14	1.000	54	1.004	94	0.989	134	0.002	14	0.997	54	0.003
15	1.000	55	1.001	95	1.000	135	0.001	15	0.998	55	0.001
16	1.000	56	1.000	96	1.000	136	0.007	16	0.992	56	-0.001
17	0.999	57	1.000	97	1.000	137	0.004	17	0.997	57	-0.001
18	1.000	58	1.000	98	1.000	138	0.001	18	0.998	58	0.000
19	1.000	59	1.000	99	0.998	139	0.004	19	0.997	59	0.000
20	1.000	60	1.011	100	0.997	140	0.001	20	0.996	60	0.000
21	1.000	61	1.000	101	1.000	141	0.001	21	0.992	61	0.000
22	1.000	62	1.000	102	0.996	142	0.009	22	0.995	62	0.000
23	1.000	63	1.000	103	0.999	143	0.001	23	0.997	63	-0.001
24	1.000	64	1.000	104	0.995	144	0.000	24	0.999	64	-0.002
25	1.000	65	0.999	105	0.997	145	0.002	25	0.995	65	0.000
26	1.000	66	0.999	106	1.000	146	0.000	26	0.994	66	-0.001
27	1.000	67	1.000	107	0.999	147	0.001	27	1.001	67	-0.001
28	1.000	68	1.000	108	0.999	148	0.000	28	0.999	68	0.000
29	1.000	69	1.000	109	1.000	149	0.001	29	1.000	69	0.000
30	1.000	70	1.000	110	0.998	150	0.000	30	1.000	70	-0.001
31	1.000	71	0.998	111	0.998	151	0.001	31	0.999	71	0.000
32	1.000	72	0.999	112	0.998	152	0.002	32	0.999	72	0.000
33	1.000	73	0.999	113	0.999	153	0.001	33	0.998	73	0.000
34	1.000	74	1.000	114	0.995	154	0.000	<b>34</b>	<b>0.869</b>	74	0.000
35	1.000	75	1.000	115	0.979	155	0.002	35	0.999	75	0.000
36	1.000	76	0.995	116	0.999	156	0.000	36	0.999	76	-0.001
37	1.000	77	1.000	117	0.995	157	0.000	<b>37</b>	<b>0.951</b>	77	-0.001
38	1.000	78	1.000	118	0.998	158	0.001	<b>38</b>	<b>0.975</b>	78	-0.002
39	1.000	79	1.000	119	0.984	159	0.000	39	0.992	79	0.000
40	1.000	80	0.999	120	0.997	160	0.000	40	0.003	80	0.000

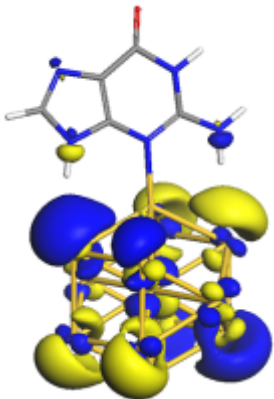
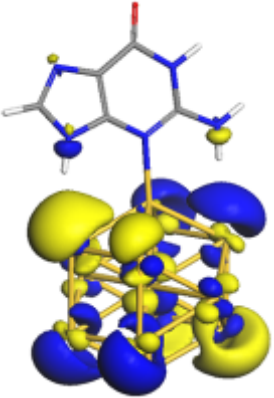
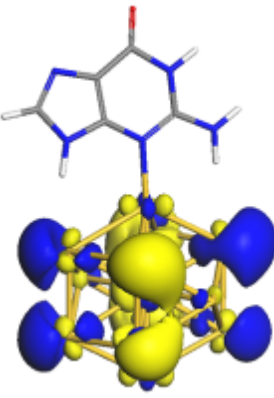
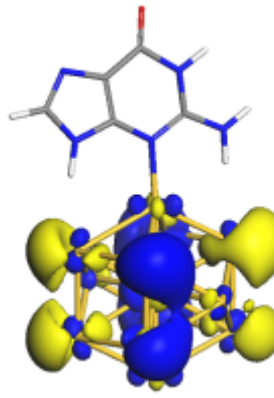
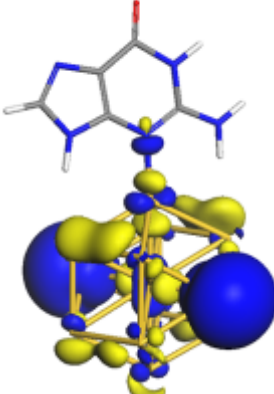
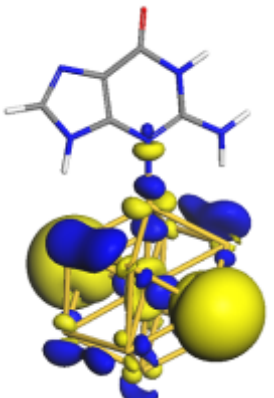
**Table S7.** Gross population changes of spin-down FOs.

1	1.000	41	1.000	81	1.000	121	0.999	1	1.000	41	0.005
2	1.000	42	1.000	82	0.999	<b>122</b>	<b>0.976</b>	2	1.000	<b>42</b>	<b>0.013</b>
3	1.000	43	1.000	83	0.999	<b>123</b>	<b>0.975</b>	3	1.000	43	0.008
4	1.000	44	1.000	84	0.998	<b>124</b>	<b>0.137</b>	4	1.000	<b>44</b>	<b>0.045</b>
5	1.000	45	1.000	85	0.999	<b>125</b>	<b>0.038</b>	5	1.000	<b>45</b>	<b>0.030</b>
6	1.000	46	1.000	86	1.000	126	0.010	6	1.000	46	0.003
7	1.000	47	1.000	87	0.999	127	0.044	7	1.000	47	0.001
8	1.000	48	1.000	88	0.999	128	0.001	8	1.000	48	0.003
9	1.000	49	1.000	89	0.999	129	0.015	9	1.000	49	0.000
10	1.000	50	1.000	90	0.999	130	0.013	10	1.000	50	-0.001
11	1.000	51	1.000	91	1.000	131	0.004	11	1.000	51	0.001
12	1.000	52	1.000	92	0.998	132	0.002	12	1.000	52	0.001
13	1.000	53	0.997	93	0.999	133	0.025	13	0.998	53	0.003
14	1.000	54	1.003	94	0.987	134	0.002	14	0.997	54	0.003
15	1.000	55	1.001	95	1.000	135	0.001	15	0.998	55	0.001
16	1.000	56	1.000	96	1.000	136	0.006	16	0.992	56	-0.001
17	0.999	57	1.000	97	1.000	137	0.004	17	0.997	57	-0.001
18	1.000	58	1.000	98	0.999	138	0.001	18	0.998	58	0.000
19	1.000	59	1.000	99	0.998	139	0.005	19	0.997	59	0.000
20	1.000	60	1.011	100	0.997	140	0.001	20	0.996	60	0.000
21	1.000	61	1.000	101	1.000	141	0.001	21	0.992	61	0.000
22	1.000	62	0.999	102	0.995	142	0.007	22	0.995	62	0.000
23	1.000	63	1.000	103	0.999	143	0.001	23	0.997	63	-0.001
24	1.000	64	1.000	104	0.994	144	0.001	24	0.999	64	-0.002
25	1.000	65	0.999	105	0.997	145	0.002	25	0.995	65	0.000
26	1.000	66	0.999	106	1.000	146	0.000	26	0.994	66	-0.001
27	1.000	67	1.000	107	0.999	147	0.001	27	1.001	67	-0.001
28	1.000	68	1.000	108	0.999	148	0.000	28	0.999	68	0.000
29	1.000	69	1.000	109	1.000	149	0.001	29	1.000	69	0.000
30	1.000	70	1.000	110	0.998	150	0.000	30	1.000	70	-0.001
31	1.000	71	0.998	111	0.998	151	0.001	31	0.999	71	0.000
32	1.000	72	0.999	112	0.999	152	0.002	32	0.999	72	0.000
33	1.000	73	0.999	113	0.997	153	0.001	33	0.998	73	0.000
34	1.000	74	1.000	114	0.995	154	0.000	<b>34</b>	<b>0.861</b>	74	0.000
35	1.000	75	1.000	115	0.998	155	0.001	35	0.999	75	0.000
36	1.000	76	0.995	116	0.995	156	0.000	36	0.999	76	-0.001
37	1.000	77	1.000	117	0.980	157	0.000	<b>37</b>	<b>0.947</b>	77	-0.001
38	1.000	78	1.000	118	0.997	158	0.001	<b>38</b>	<b>0.972</b>	78	-0.001
39	1.000	79	1.000	119	0.984	159	0.000	39	0.993	79	0.000
40	1.000	80	0.999	120	0.997	160	0.000	40	0.002	80	0.000

**Table S8.** Spin-up FOs (spin-down FOs are similar; the only difference is that  $a_{124}^-$  is the LUMO there).



**Table S9.** MO of Au<sub>13</sub>-G2 Complex

<p><math>\psi_{161}^+</math>: -0.20522 Ha  <b>-0.59</b> <math>a_{122}</math> <b>+0.76</b> <math>a_{123}</math>                  +0.044 <math>g_{42}</math> -0.078 <math>g_{44}</math> +0.048 <math>g_{45}</math></p> 	<p><math>\psi_{161}^-</math>: -0.20420 Ha  <b>+0.68</b> <math>a_{122}</math> <b>-0.69</b> <math>a_{123}</math>                  -0.044 <math>g_{42}</math> +0.078 <math>g_{44}</math> -0.048 <math>g_{45}</math></p> 
<p><math>\psi_{162}^+</math>: -0.20162 Ha  <b>-0.78</b> <math>a_{122}</math> <b>-0.61</b> <math>a_{123}</math>                  -0.015 <math>g_{44}</math> -0.017 <math>g_{45}</math></p> 	<p><math>\psi_{162}^-</math>: -0.20055 Ha  <b>+0.71</b> <math>a_{122}</math> <b>+0.70</b> <math>a_{123}</math>                  +0.016 <math>g_{44}</math> +0.017 <math>g_{45}</math></p> 
<p><math>\psi_{163}^+</math> (HOMO): -0.18670 Ha                  0.83 <math>a_{124}</math> +0.52 <math>a_{125}</math> -0.11 <math>a_{127}</math>  <b>+0.12</b> <math>g_{34}</math> <b>+0.081</b> <math>g_{37}</math> <b>-0.061</b> <math>g_{38}</math></p> 	<p><math>\psi_{163}^-</math> (LUMO): -0.18049 Ha</p> 

## 5. XYZ coordinates of optimized geometries

=====Au13-G1 29 atoms=====

	x	y	z
Au	0.000000	0.000000	0.000000
Au	2.816750	-0.064064	-0.556080
Au	0.740504	-0.354383	-2.523204
Au	3.442945	-0.490983	-3.144352
Au	2.209357	1.941327	-2.373402
Au	-2.004901	-0.242897	-1.926548
Au	-0.728089	-2.652187	-2.737096
Au	1.293648	-2.439207	-0.779629
Au	-1.219371	-0.629523	-4.543557
Au	0.289067	1.682068	-4.414792
Au	-0.524427	2.085102	-1.790241
Au	1.504473	-0.719696	-5.126196
Au	1.970518	-2.819826	-3.448752
N	0.000000	0.000000	2.090529
O	3.160881	0.000000	1.737880
N	-0.778248	-0.481342	4.092344
C	-1.085880	-0.103666	2.822086
H	-2.097853	0.063868	2.458667
C	1.057751	-0.300998	2.910070
C	2.463990	-0.304639	2.705757
N	3.128595	-0.723742	3.873360
H	4.148007	-0.714605	3.767572
C	2.552996	-1.042394	5.067372
N	3.366698	-1.390481	6.083146
H	4.325573	-1.685186	5.920176
H	2.904340	-1.716140	6.930363
N	1.257200	-0.990538	5.262206
C	0.575128	-0.617086	4.177714
H	-1.432525	-0.641656	4.858657

=====Au13-G2 29 atoms=====

	x	y	z
Au	0.000000	0.000000	0.000000
Au	2.570681	0.035270	-1.169323
Au	0.134830	-0.143763	-2.627005
Au	-0.636141	-2.522232	-3.938744
Au	1.708632	-2.347707	-2.376218
Au	-0.837359	-2.403472	-1.213025
Au	0.950339	2.262907	-1.405223
Au	-1.429196	2.056096	-2.892468
Au	-2.429556	-0.148167	-1.422393
Au	1.095891	2.037494	-4.127642
Au	2.683383	-0.224391	-3.928926
Au	0.291327	-0.316904	-5.330995
Au	-2.241763	-0.269010	-4.194727
N	0.000000	0.000000	2.078679
H	2.630334	0.000000	1.252593
N	2.411013	-0.058692	2.271497
C	3.263027	-0.133498	3.346703
H	4.345036	-0.152942	3.218869
N	2.628429	-0.173314	4.486115
C	1.305933	-0.121347	4.157199
C	0.138803	-0.133711	4.978596
O	0.001325	-0.181395	6.182197
N	-1.036925	-0.071347	4.155754
H	-1.895322	-0.049411	4.713565
C	-1.110878	-0.013674	2.806796
N	-2.304564	0.049381	2.205153
H	-3.158699	-0.145857	2.720969
H	-2.320606	-0.037533	1.169789
C	1.159698	-0.049932	2.779468

=====Au55-G1 71 atoms=====

	x	y	z
Au	-1.33948	0.10129	1.6634
Au	-1.72893	2.05951	3.660949
Au	0.598228	0.458045	3.675795

Au	0.235196	2.419324	1.684966
Au	-4.93811	-2.59558	-0.3531
Au	-2.57856	-4.23842	-0.3166
Au	-2.91155	-2.23536	-2.36978
Au	-0.6337	-3.80023	-2.20358
Au	-0.96207	-1.86219	-0.32542
Au	1.357515	-3.53727	-0.30936
Au	0.971177	-1.54342	-2.34198
Au	2.985271	-1.13938	-0.26164
Au	-5.14745	-0.60178	-2.26147
Au	-5.67255	1.340565	-0.36007
Au	-3.28378	-0.25825	-0.32914
Au	-3.64876	1.718157	-2.36613
Au	-1.32811	0.112345	-2.44239
Au	-1.7028	2.069048	-0.31197
Au	0.650392	0.465828	-0.33659
Au	0.245399	2.4432	-2.33396
Au	2.505278	0.81498	-2.21301
Au	2.243551	2.803618	-0.28574
Au	-4.04115	3.72691	-0.32716
Au	-2.0561	3.969563	-2.21828
Au	-0.11994	4.457224	-0.31033
Au	-4.49477	-4.43974	1.651352
Au	-4.97843	-2.59343	3.637056
Au	-2.60807	-4.23024	3.655932
Au	-2.94456	-2.21854	1.658745
Au	-0.60756	-3.97274	1.683554
Au	-1.00764	-1.86352	3.657232
Au	1.321179	-3.51727	3.685602
Au	0.965587	-1.50992	1.684957
Au	3.186457	-3.06484	1.705279
Au	2.966367	-1.13785	3.683535
Au	-5.40791	-0.64834	1.633255
Au	-5.70468	1.33099	3.634846
Au	-3.32717	-0.26172	3.645804
Au	-3.67221	1.704667	1.658497
Au	2.697709	0.848199	1.69614
Au	2.24803	2.794488	3.683936
Au	-5.91122	3.235358	1.648074
Au	-4.06461	3.706728	3.652942
Au	-2.10262	4.174424	1.678898
Au	-0.13502	4.42807	3.683494
Au	1.764584	4.650002	1.697399
Au	-2.9922	-2.22588	5.688306
Au	-0.68653	-3.74594	5.578879
Au	0.942614	-1.51092	5.719391
Au	-5.22651	-0.61113	5.541205
Au	-3.70787	1.696356	5.684909
Au	-1.37968	0.099329	5.790522
Au	0.218227	2.424905	5.70835
Au	2.453104	0.800547	5.597389
Au	-2.0879	3.936965	5.573811
N	5.413739	1.237179	-5.33406
C	4.782119	1.589126	-4.18065
H	5.024137	2.476899	-3.59929
N	3.851845	0.718162	-3.8729
C	3.86875	-0.23722	-4.85342
C	3.085715	-1.40557	-5.05942
O	2.162329	-1.90038	-4.41865
N	3.492971	-2.06108	-6.2383
H	2.927123	-2.89122	-6.44139
C	4.484794	-1.6663	-7.08883
N	4.708275	-2.41431	-8.18434
H	4.322009	-3.34722	-8.29463
H	5.506093	-2.1376	-8.7716
N	5.199606	-0.58441	-6.88933
C	4.852704	0.079139	-5.78533
H	6.16251	1.738446	-5.79122

=====Au55-G2 71 atoms=====

	x	y	z
Au	0.095787	0.044853	-0.08032
Au	-0.29295	2.00835	1.891746
Au	2.050051	0.422002	1.935129
Au	1.726597	2.376914	-0.04013
Au	-3.55819	-2.64121	-2.10604
Au	-1.17274	-4.27629	-2.05176
Au	-1.46846	-2.27362	-4.06909
Au	0.87135	-3.80016	-3.89663
Au	0.487817	-1.92442	-2.06087
Au	2.878527	-3.50935	-1.96861
Au	2.517079	-1.5444	-4.02601
Au	4.537586	-1.15959	-1.98085
Au	-3.71805	-0.66013	-4.00866
Au	-4.25446	1.283339	-2.11946
Au	-1.86702	-0.31011	-2.06543
Au	-2.17681	1.632574	-4.11304
Au	0.161194	0.028342	-4.13317
Au	-0.22074	1.992931	-2.05518
Au	2.126871	0.412469	-1.99778
Au	1.785143	2.346512	-4.04501
Au	4.037159	0.758707	-3.88723
Au	3.793225	2.751323	-1.98767
Au	-2.57803	3.641171	-2.09607
Au	-0.53828	3.870325	-3.96112
Au	1.389233	4.362641	-2.03708
Au	-3.10539	-4.4822	-0.10684
Au	-3.61323	-2.62344	1.861484
Au	-1.20972	-4.25417	1.886937
Au	-1.54801	-2.25344	-0.09651
Au	0.830397	-3.96381	-0.0603
Au	0.420762	-1.89453	1.90166
Au	2.78298	-3.5283	1.951242
Au	2.446936	-1.52307	-0.02751
Au	4.706515	-3.0433	0.027494
Au	4.45735	-1.14804	1.997303
Au	-4.01213	-0.68247	-0.12957
Au	-4.30692	1.285498	1.850359
Au	-1.92137	-0.30169	1.87359
Au	-2.24601	1.647063	-0.10822
Au	4.204622	0.817673	0.002919
Au	3.73013	2.757777	1.976712
Au	-4.47756	3.185029	-0.13906
Au	-2.64471	3.647503	1.866541
Au	-0.64261	4.073285	-0.0844
Au	1.32362	4.389674	1.933288
Au	3.262801	4.604466	-0.01686
Au	-1.58557	-2.25606	3.909791
Au	0.732565	-3.77286	3.805455
Au	2.372133	-1.53592	3.973147
Au	-3.82839	-0.64089	3.768094
Au	-2.29955	1.652703	3.907411
Au	0.03566	0.059853	3.997688
Au	1.656146	2.386881	3.957133
Au	3.894478	0.773115	3.881877
Au	-0.65975	3.885788	3.790576
N	-0.41378	-6.86003	-4.26918
C	-0.7673	-8.17383	-4.46534
H	-1.67463	-8.59338	-4.03144
N	0.09302	-8.8167	-5.20554
C	1.053764	-7.89826	-5.51197
C	2.257324	-8.02504	-6.26912
O	2.739003	-8.96645	-6.86253
N	2.956668	-6.77147	-6.28308
H	3.814188	-6.81462	-6.8412
C	2.593775	-5.60798	-5.69514
N	3.374878	-4.52735	-5.83168
H	4.333159	-4.61663	-6.15942
H	3.127422	-3.69342	-5.26859
N	1.462447	-5.52589	-5.0082

C	0.746837	-6.67326	-4.93755
H	-0.86857	-6.14003	-3.6755

=====Au147-G1 163 atoms=====

	x	y	z
Au	0.187854	-0.86118	0.829162
Au	0.12682	1.287665	2.648831
Au	2.159542	-0.65975	2.839003
Au	2.146861	1.166686	0.686723
Au	4.337778	-0.77794	0.884961
Au	4.146347	1.350421	2.683426
Au	6.405791	-0.5763	2.877849
Au	6.400205	1.228204	0.742974
Au	0.121746	3.267471	0.484233
Au	0.054328	5.512345	2.283114
Au	2.070358	3.335525	2.492567
Au	2.063265	5.385896	0.334264
Au	0.137209	-0.51758	4.960452
Au	0.064914	1.629525	6.877323
Au	2.078697	-0.30798	7.06923
Au	2.077174	1.477828	4.688123
Au	0.073187	3.406098	4.438676
Au	-0.00107	5.45622	6.175382
Au	2.047331	3.599657	6.503744
Au	2.039082	5.492146	4.273924
Au	4.092389	-0.45498	4.821402
Au	4.012479	1.715943	6.692799
Au	5.953531	-0.26505	6.743365
Au	6.102352	1.585253	4.664898
Au	4.078548	3.153919	0.551916
Au	4.022626	5.347193	2.399854
Au	6.104304	3.338203	2.572102
Au	5.959421	5.082239	0.391914
Au	4.216523	3.695632	4.669622
Au	-5.55558	-6.80802	1.252309
Au	-5.70319	-5.06916	-0.92357
Au	-5.71202	-3.2995	-3.00131
Au	-5.76955	-4.7309	3.090325
Au	-6.00558	-2.95525	0.920076
Au	-5.82196	-2.65693	4.848997
Au	-5.57968	-1.44424	-5.07367
Au	-6.01048	-1.142	-1.22718
Au	-5.78788	0.69936	-3.34117
Au	-6.06794	-0.81676	2.718776
Au	-6.0726	0.988995	0.586551
Au	-5.73224	-0.94229	6.59249
Au	-5.89451	1.356219	4.514375
Au	-5.84161	2.793512	-1.582
Au	-5.9022	3.109303	2.423712
Au	-5.77213	4.859286	0.254996
Au	-3.63239	-7.07202	-0.74558
Au	-1.64173	-7.21136	-2.6092
Au	-3.67165	-6.74276	3.283135
Au	-1.67511	-7.11258	1.323244
Au	-1.76666	-6.54706	5.231352
Au	-3.6248	-3.43719	-5.03217
Au	-1.65854	-5.31871	-4.84482
Au	-3.81873	-5.41785	-3.01316
Au	-3.75538	-3.07086	-1.02687
Au	-1.686	-5.06205	-0.82825
Au	-1.69126	-3.19823	-3.02894
Au	-3.69401	-4.87461	1.105669
Au	-3.80535	-2.74409	2.941766
Au	-1.75581	-4.73291	3.101028
Au	-1.7622	-2.88461	0.974048
Au	-3.94335	-4.72668	5.258683
Au	-3.79651	-2.4446	6.922744
Au	-1.83419	-4.32225	7.107085
Au	-1.80445	-2.55643	4.961917
Au	-3.69645	0.573798	-5.36427

Au	-1.69708	-1.41515	-5.41511	Au	4.081449	-2.29579	7.025274
Au	-3.70593	-1.26546	-3.15543	Au	6.169628	-2.42505	5.001254
Au	-3.81375	0.893548	-1.35804	Au	4.187192	0.72368	-5.26766
Au	-1.77331	-1.05973	-1.18056	Au	6.132665	-1.22792	-4.94179
Au	-1.77597	0.735523	-3.36692	Au	4.209959	-1.10706	-3.05616
Au	-3.95392	-0.94274	0.775423	Au	4.193917	1.050005	-1.26397
Au	-3.88212	1.200606	2.59052	Au	6.462453	-0.90695	-1.06452
Au	-1.83078	-0.72964	2.791452	Au	6.216687	0.937917	-3.19819
Au	-1.83472	1.083744	0.641273	Au	4.329841	3.014577	-3.59317
Au	-3.80979	-0.61324	4.721364	Au	4.054754	5.030011	-1.62242
Au	-3.8885	1.583575	6.575759	Au	6.156955	3.014785	-1.43033
Au	-1.87374	-0.38258	7.017991	N	0.220618	7.371151	-8.65902
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Au	-1.79743	2.530525	-5.52648	H	1.599954	7.046276	-7.01671
Au	-3.97281	2.858053	-3.7028	N	-0.10813	5.781579	-7.1738
Au	-3.80754	4.882196	-1.70905	C	-1.12143	5.738814	-8.08813
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Au	-3.82202	3.000335	0.447752	N	-3.16079	5.433288	-9.1437
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Au	-1.88636	3.261754	2.446838	C	-2.90437	6.467132	-10.0007
Au	-1.8871	5.311072	0.287721	N	-3.84383	6.788353	-10.9043
Au	-4.09232	3.537015	4.565174	H	-4.7566	6.346648	-10.9429
Au	-1.96386	3.510994	6.464687	H	-3.62162	7.540431	-11.554
Au	-1.97723	5.410144	4.224516	N	-1.79041	7.162287	-9.96519
Au	0.379495	-7.1706	-4.51502	C	-0.95515	6.769772	-9.00423
Au	0.330436	-7.24103	-0.621	H	0.620462	8.189107	-9.12014
Au	2.363875	-7.13118	-2.56964				
Au	0.28135	-6.91067	3.325119				
Au	2.278652	-7.03855	1.382136				
Au	0.216566	-6.20129	7.135961	=====Au147-G2 163 atoms=====			
Au	2.25684	-6.47346	5.277478	x	y	z	
Au	0.318569	-3.34935	-5.22589	Au	0.101522	0.03444	0.014227
Au	2.348134	-5.23677	-4.80907	Au	0.140273	2.024529	2.029296
Au	0.312579	-5.13379	-2.78535	Au	2.018181	-0.10568	2.089628
Au	0.260872	-3.01139	-0.99152	Au	2.208083	1.905999	0.098778
Au	2.279313	-4.98887	-0.79078	Au	4.185552	-0.22983	0.164089
Au	2.273292	-3.13201	-2.98332	Au	4.161667	1.752394	2.155347
Au	0.259933	-4.9943	1.168874	Au	6.183726	-0.38279	2.223849
Au	0.199548	-2.68662	2.979632	Au	6.392501	1.609451	0.260034
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Au	0.206808	-4.48563	5.106013	Au	2.254642	3.914241	2.089629
Au	0.13411	-2.31389	7.20633	Au	2.448045	6.078662	0.109162
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Au	2.145196	-2.47987	5.013444	Au	-0.00213	1.984287	6.207338
Au	0.251789	0.601292	-5.5635	Au	1.837252	-0.12332	6.275149
Au	2.263965	-1.33979	-5.36808	Au	2.051824	1.877456	4.118635
Au	0.249758	-1.2033	-3.30911	Au	0.19763	3.988829	4.005307
Au	0.190498	0.963979	-1.31635	Au	0.252992	5.899286	5.908137
Au	2.212788	-0.98845	-1.12796	Au	2.11976	3.840274	6.11447
Au	2.217216	0.819748	-3.32122	Au	2.329504	5.896963	4.062272
Au	0.204683	4.599788	-5.43253	Au	3.900913	-0.24502	4.130861
Au	2.220521	2.60609	-5.45144	Au	3.94378	1.763309	6.175654
Au	0.19841	2.739844	-3.49062	Au	5.723989	-0.38268	6.111155
Au	0.114504	5.177242	-1.64392	Au	6.048704	1.631049	4.214553
Au	2.121598	2.998042	-1.4711	Au	4.309686	3.75565	0.18367
Au	2.132647	4.834056	-3.54119	Au	4.343112	5.774721	2.192211
Au	4.274996	-6.92955	-0.62915	Au	6.25934	3.591878	2.270806
Au	4.212566	-6.59264	3.397638	Au	6.329997	5.533171	0.264713
Au	6.156727	-6.58356	1.399413	Au	4.288348	3.856368	4.286984
Au	4.277332	-3.30302	-4.92565	Au	-6.1575	-5.43478	-0.24663
Au	4.476531	-5.26466	-2.91129	Au	-6.0625	-3.50323	-2.26169
Au	4.274928	-2.92378	-0.93086	Au	-5.85122	-1.56045	-4.2078
Au	6.294004	-4.83786	-0.77016	Au	-6.22903	-3.5209	1.769307
Au	6.292646	-3.07784	-2.85454	Au	-6.20094	-1.53071	-0.24186
Au	4.228541	-4.72101	1.21579	Au	-6.16997	-1.59777	3.742388
Au	4.215216	-2.58735	3.027271	Au	-5.52796	0.423809	-6.12117
Au	6.232797	-4.51262	3.251557	Au	-5.99907	0.441601	-2.21556
Au	6.469032	-2.71339	1.073055	Au	-5.62481	2.431457	-4.18363
Au	4.355432	-4.57209	5.368668	Au	-6.14768	0.428023	1.763896
				Au	-5.958	2.400316	-0.2114



Au	-5.98294	0.371768	5.689093	Au	0.456248	2.060294	-6.16078
Au	-5.90725	2.403218	3.77736	Au	2.301167	-0.04624	-6.0889
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Au	-5.73276	4.345809	1.835151	Au	0.291395	2.064715	-1.99335
Au	-5.44429	6.243933	-0.16586	Au	2.167164	-0.0745	-1.92186
Au	-4.16519	-5.69275	-2.18103	Au	2.366819	1.927071	-3.9129
Au	-2.13438	-5.82087	-4.05066	Au	0.622616	6.043083	-5.84242
Au	-4.32303	-5.71338	1.833788	Au	2.548799	3.930455	-5.90581
Au	-2.28835	-6.01021	-0.10109	Au	0.504341	4.074521	-3.97765
Au	-2.45008	-5.84416	3.856723	Au	0.529898	6.218758	-1.93296
Au	-3.72335	-1.69562	-6.17101	Au	2.396825	3.940872	-1.87712
Au	-1.90181	-3.77363	-6.09799	Au	2.594332	5.928781	-3.85842
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Au	-3.95526	-1.67541	-2.14884	Au	3.581195	-6.24455	2.126184
Au	-2.06542	-3.84758	-2.07012	Au	5.589769	-6.22673	0.206604
Au	-1.84649	-1.81274	-4.11055	Au	4.145117	-2.19408	-5.84348
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Au	-4.11731	-1.69472	1.842591	Au	4.051728	-2.21639	-1.81717
Au	-2.21761	-3.86676	1.892915	Au	5.912854	-4.30948	-1.79046
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Au	-4.40066	-3.80264	3.932212	Au	3.795696	-4.2093	0.151667
Au	-4.1968	-1.74984	5.880205	Au	3.907624	-2.22463	2.135481
Au	-2.37808	-3.82436	5.932249	Au	5.759358	-4.3295	2.225231
Au	-2.17954	-1.84605	3.953087	Au	6.130122	-2.34979	0.234088
Au	-3.50511	2.311587	-6.14898	Au	3.760679	-4.3525	4.23191
Au	-1.62032	0.191091	-6.26678	Au	3.678487	-2.26132	6.156793
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Au	-3.722	2.286301	-2.12269	Au	4.374467	1.835686	-5.82893
Au	-1.81475	0.182384	-2.07703	Au	6.170213	-0.30475	-5.63347
Au	-1.612	2.175329	-4.09045	Au	4.212849	-0.2051	-3.78733
Au	-4.00231	0.298158	-0.14722	Au	4.305125	1.787339	-1.80568
Au	-3.86693	2.266919	1.852516	Au	6.33475	-0.36185	-1.73093
Au	-1.97188	0.149025	1.957396	Au	6.35278	1.673074	-3.69785
Au	-1.77669	2.1383	-0.05028	Au	4.590199	3.8955	-3.90958
Au	-4.0226	0.279865	3.839053	Au	4.479806	5.795454	-1.82194
Au	-3.93396	2.253122	5.902017	Au	6.415826	3.617249	-1.74265
Au	-2.0968	0.12679	6.137615	N	-2.64905	6.985166	-6.89054
Au	-1.90836	2.127647	3.984272	C	-3.80377	7.339154	-7.54149
Au	-1.45455	4.124628	-6.02995	H	-4.78378	7.081293	-7.13858
Au	-3.62908	4.427422	-4.23682	N	-3.57159	7.988071	-8.64807
Au	-3.454	6.289772	-2.08915	C	-2.21325	8.064586	-8.73152
Au	-1.55763	4.185514	-2.02041	C	-1.39449	8.679096	-9.72293
Au	-1.44386	6.172497	-3.92844	O	-1.6745	9.278387	-10.7391
Au	-3.62707	4.249887	-0.12539	N	-0.01382	8.521356	-9.37116
Au	-3.56323	6.260279	1.903796	H	0.609205	8.991972	-10.0335
Au	-1.71647	4.161396	1.945826	C	0.499542	7.877386	-8.30017
Au	-1.50842	6.339027	-0.02721	N	1.831311	7.84069	-8.13353
Au	-3.8815	4.364342	3.991411	H	2.459874	8.026468	-8.91077
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Au	-1.67633	6.139185	3.916318	N	-0.28346	7.302544	-7.3975
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Au	1.560046	-6.13121	3.996695				
Au	0.223485	-1.91346	-6.1892				
Au	2.080062	-4.02531	-5.94535				
Au	0.001314	-3.92719	-3.97935				
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Au	1.898675	-4.10884	-1.91821				
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