Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Thiolated Au_{18} cluster: Preferred Ag sites for doping, structures, optical and chiroptical properties

Bertha Molina and Alfredo Tlahuice-Flores

CICFIM-Facultad de Ciencias Físico-Matemáticas, Universidad Autónoma de Nuevo León, San Nicolás de los Garza, NL 66450, México.

Email: tlahuicef@gmail.com

Part I. **Figure S1**. Comparison of calculated optical absorption spectra of thiolated Au_{18} cluster.

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Part VIII. Cartesian coordinates of relaxed isomers.

PART I

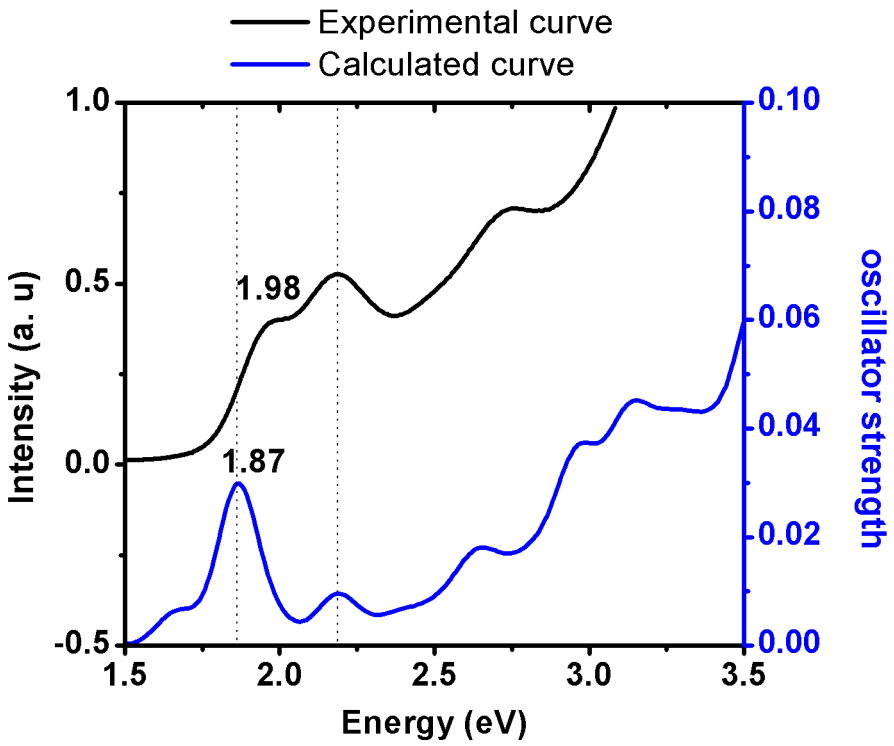


Figure S1. Calculated optical absorption spectrum for $[Au_{18}(SH)_{14}]$ cluster in good agreement with the experimental data of reference: A. Das, C. Liu, H. Y. Byun, K. Nobusada, S. Zhao, N. Rosi and R. Jin. *Angew. Chem.*, 2015, 127, 3183–3187.

PART II

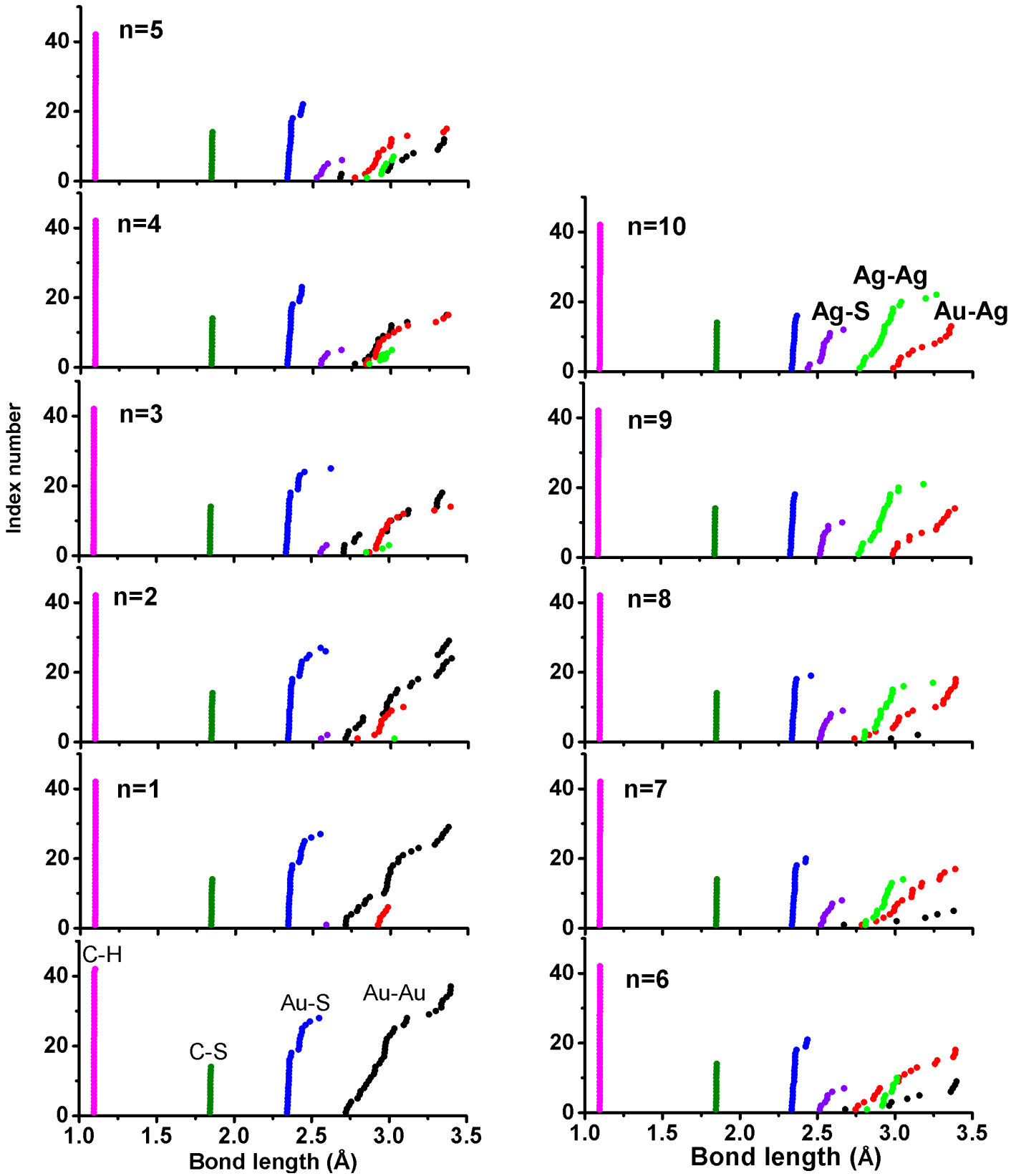
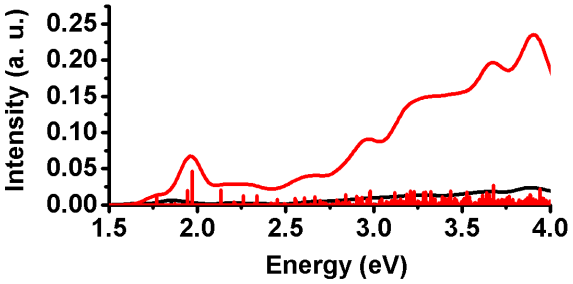


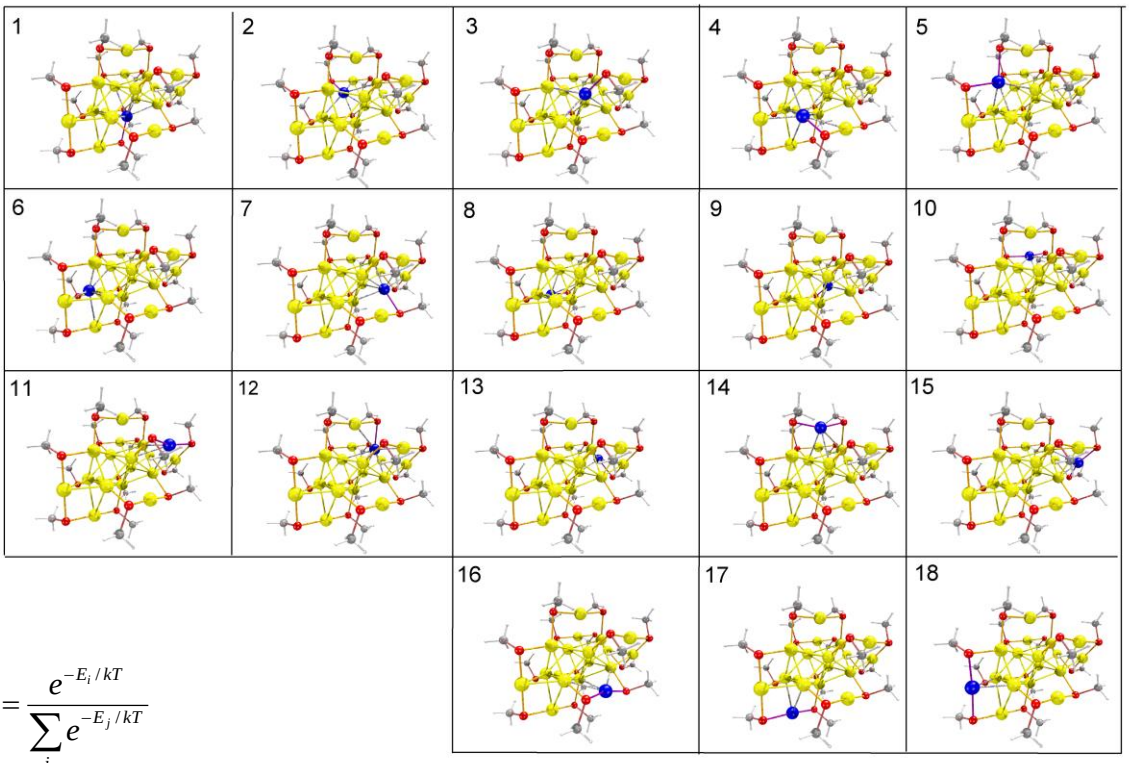
Figure S2. Calculated bond lengths of studied structures. Type of bonds are indicated by labels.

PART III

Table S1. Table reporting Boltzmann weights of an extended set of isomers for various compositions (n). Absorption spectra belong to the more stable isomers and show contribution to the first HOMO-LUMO transition mainly.

n=1



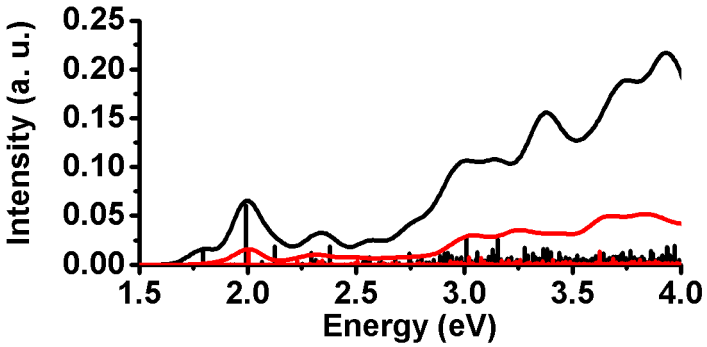


$$BW(i) = \frac{e^{-E_i/kT}}{\sum_j e^{-E_j/kT}}$$

1.20373 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight	Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	**0.8307506**	13	0.1927910	0.0004560
2	0.0593000	**0.0825256**	14	0.2115240	0.0002199
3	0.0897000	0.0252617	15	0.2241160	0.0001347
4	0.0943290	0.0210949	16	0.2350330	0.0000880
5	0.0987320	0.0177711	17	0.2506960	0.0000478
6	0.1032470	0.0149058	18	0.2582250	0.0000357
7	0.1487690	0.0025321			
8	0.1576790	0.0017898			
9	0.1782780	0.0008025			
10	0.1854680	0.0006065			
11	0.1897360	0.0005136			
12	0.1923660	0.0004636			

n=2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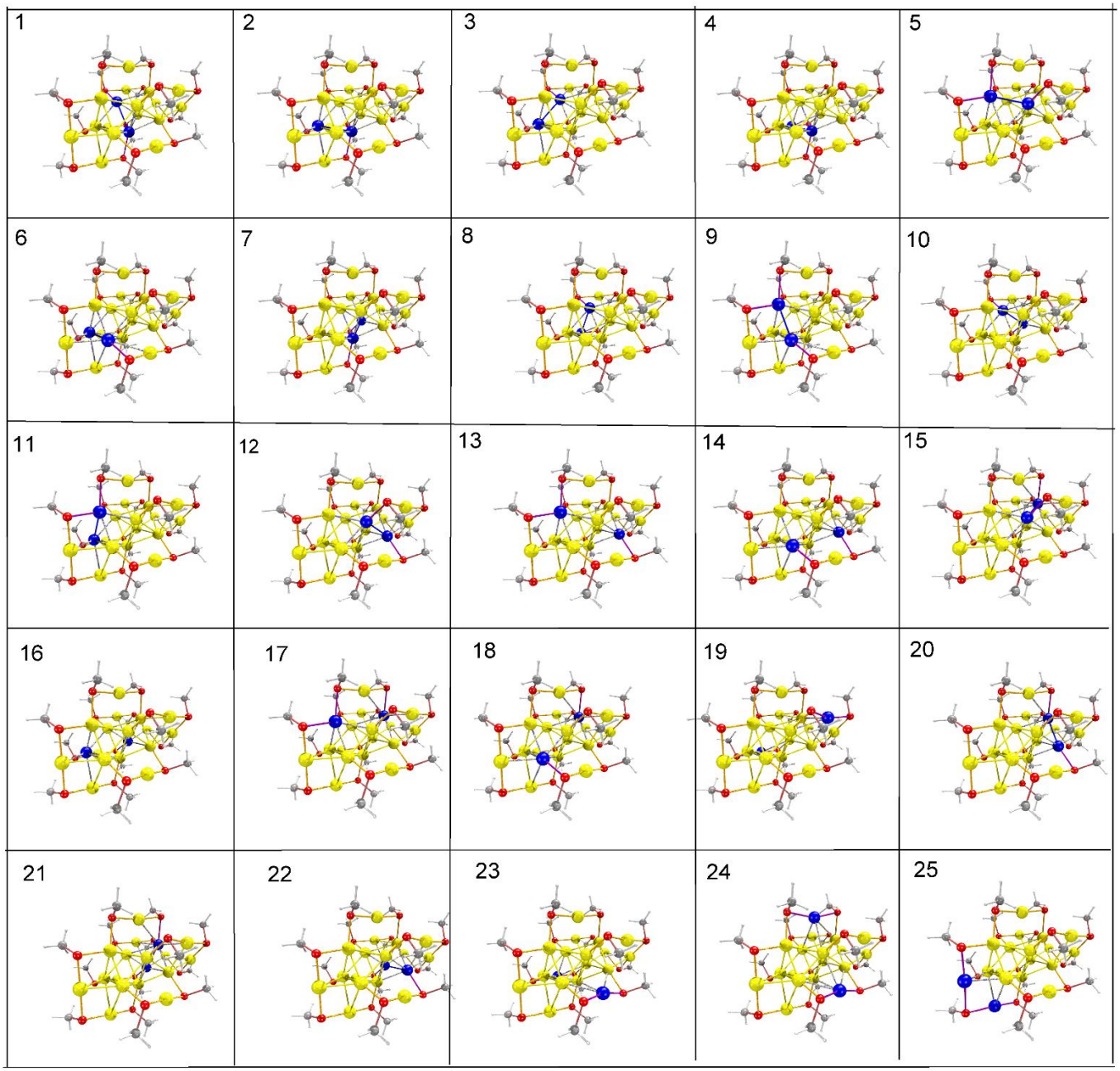
Energy (eV)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n=2

1.319507 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight	Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	**0.7578586**	14	0.1723990	0.0009204
2	0.0352000	**0.1924356**	15	0.1871080	0.0005191
3	0.1111000	0.0100153	16	0.1904390	0.0004559
4	0.1164440	0.0081337	17	0.2084480	0.0002261
5	0.1218970	0.0065776	18	0.2145720	0.0001781
6	0.1297720	0.0048404	19	0.2634220	0.0000266
7	0.1312190	0.0045752	20	0.2857200	0.0000112
8	0.1399500	0.0032565	21	0.2977420	0.0000070
9	0.1444000	0.0027384	22	0.3027800	0.0000057
10	0.1487150	0.0023148	23	0.3219260	0.0000027
11	0.1536700	0.0019086	24	0.3831690	0.0000003
12	0.1552340	0.0017958	25	0.4527130	0.0000000
13	0.1656650	0.0011964			

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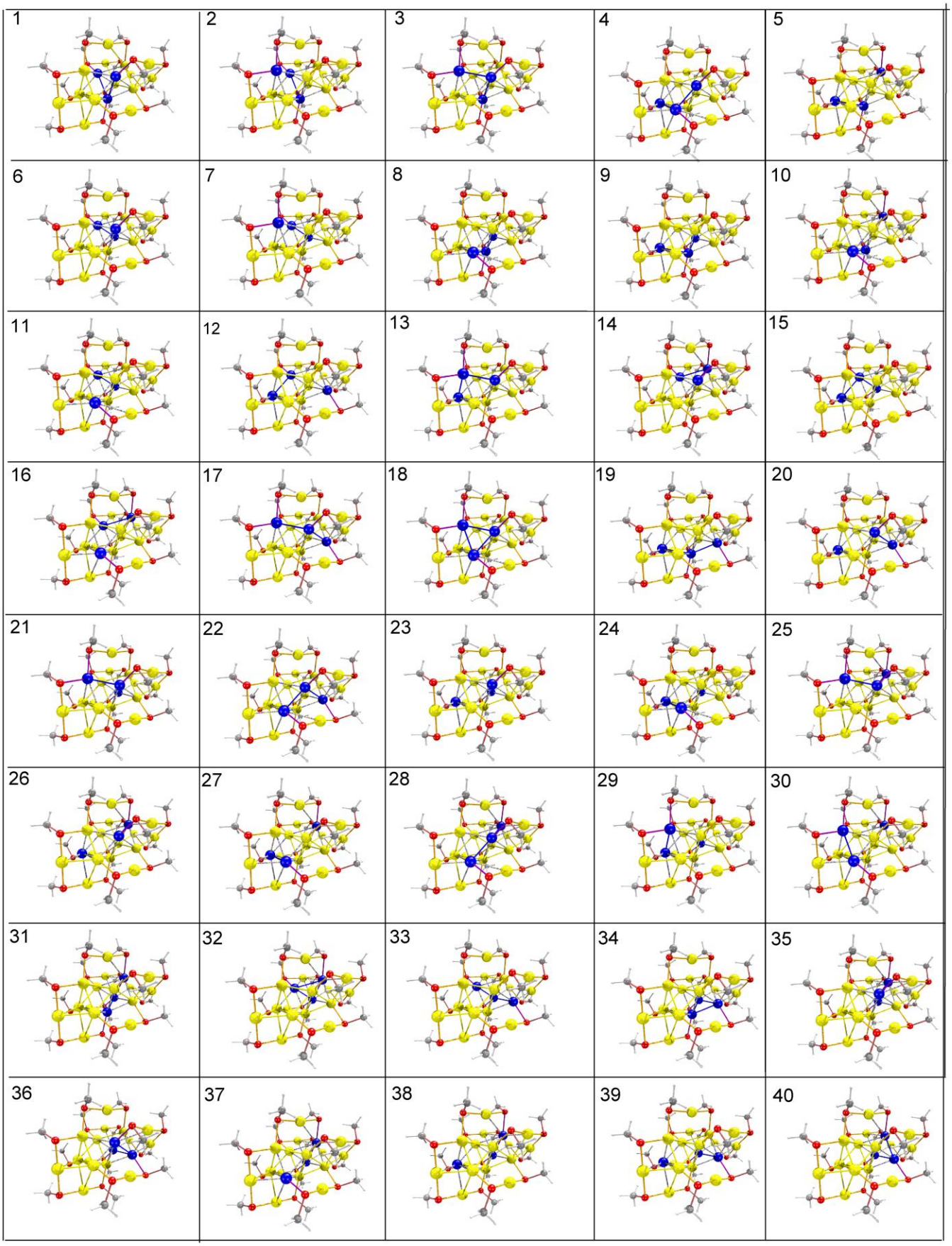
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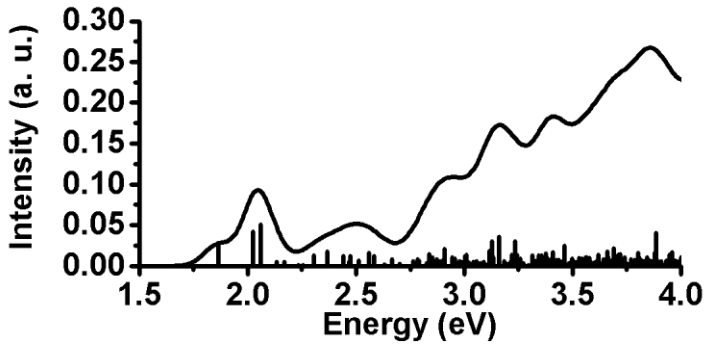
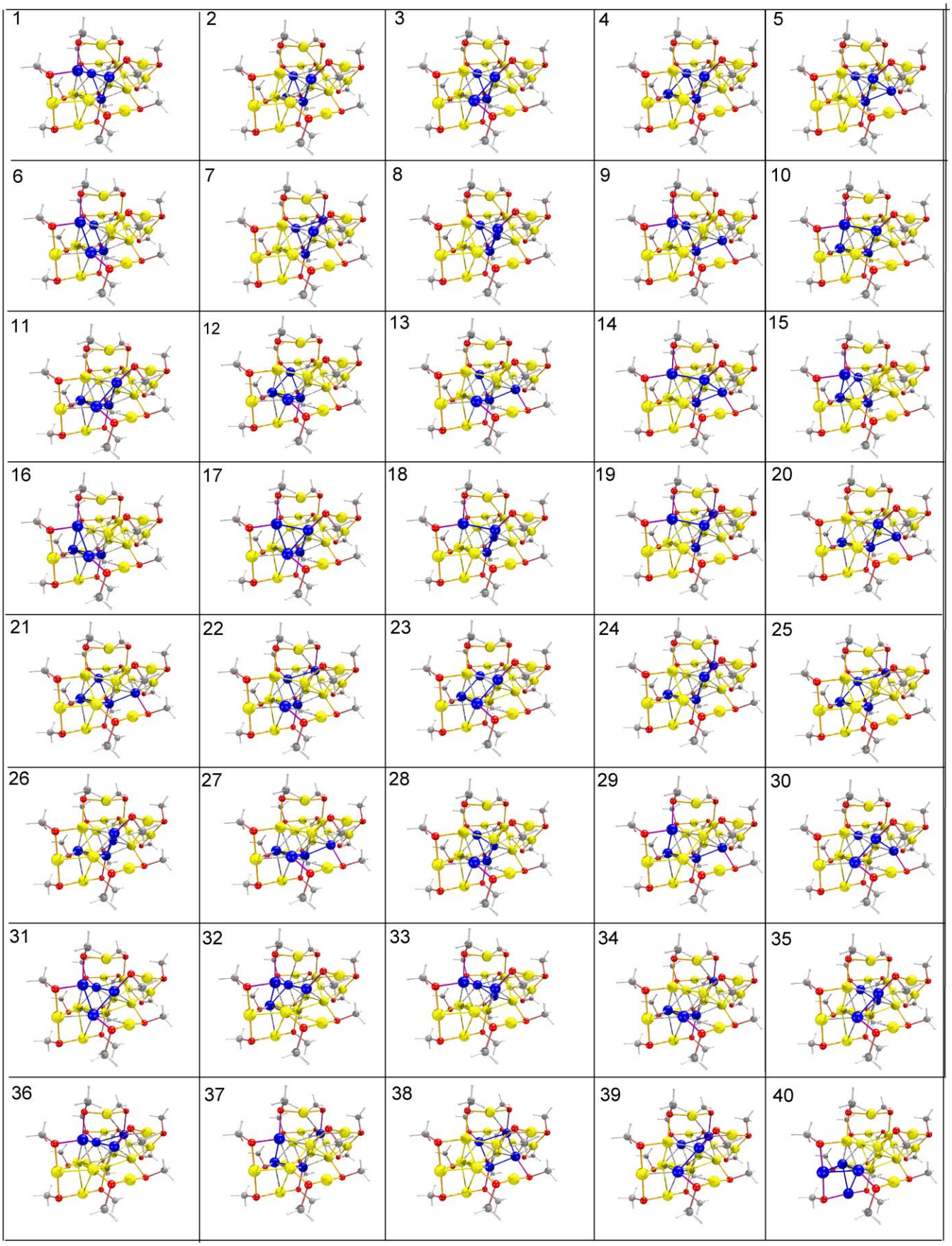


1.01672 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight	Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	**0.9835512**	21	0.2153070	0.0002247
2	0.1441000	0.0035956	22	0.2168450	0.0002116
3	0.1727000	0.0011806	23	0.2251490	0.0001531
4	0.1751890	0.0010715	24	0.2278100	0.0001381
5	0.1768250	0.0010054	25	0.2346270	0.0001059
6	0.1773130	0.0009865	26	0.2373330	0.0000953
7	0.1814390	0.0008400	27	0.2407360	0.0000835
8	0.1816250	0.0008340	28	0.2419830	0.0000795
9	0.1817290	0.0008306	29	0.2551890	0.0000475
10	0.1858200	0.0007083	30	0.2592150	0.0000406
11	0.1903430	0.0005939	31	0.2725870	0.0000241
12	0.1906250	0.0005874	32	0.2922840	0.0000112
13	0.1922080	0.0005523	33	0.2945350	0.0000103
14	0.1985260	0.0004318	34	0.3098510	0.0000057
15	0.2006400	0.0003977	35	0.3164480	0.0000044
16	0.2026560	0.0003677	36	0.3220320	0.0000035
17	0.2047510	0.0003389	37	0.3278630	0.0000028
18	0.2055160	0.0003289	38	0.3286900	0.0000027
19	0.2074150	0.0003055	39	0.3408720	0.0000017
20	0.2129750	0.0002460	40	0.4304140	0.0000001

n=4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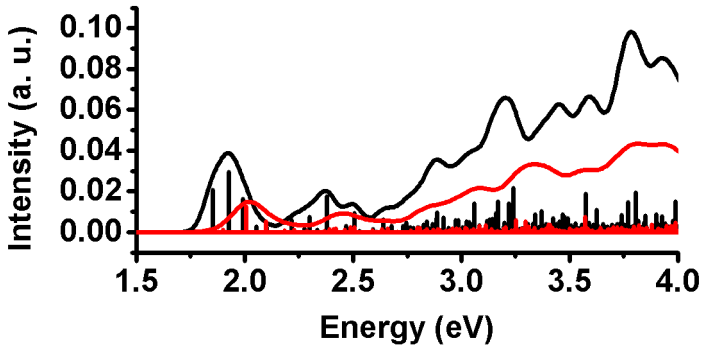

2.055586 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight	Isomer	Erelative (eV)	Boltzmann weight
1	**0.0000000**	**0.4864792**	21	0.1289063	0.0032137
2	**0.0292000**	**0.1560391**	22	0.1308594	0.0029783
3	0.0461000	0.0808017	23	0.1347656	0.0025580
4	0.0546875	0.0578347	24	0.1386719	0.0021971
5	0.0683594	0.0339602	25	0.1406250	0.0020362
6	0.0761719	0.0250521	26	0.1425781	0.0018870
7	0.0800781	0.0215170	27	0.1445313	0.0017488
8	0.0820313	0.0199412	28	0.1503906	0.0013921
9	0.0917969	0.0136331	29	0.1523438	0.0012901
10	0.0937500	0.0126347	30	0.1542969	0.0011956
11	0.0937500	0.0126347	31	0.1562500	0.0011081
12	0.1054688	0.0080053	32	0.1582031	0.0010269
13	0.1074219	0.0074190	33	0.1640625	0.0008174
14	0.1074219	0.0074190	34	0.1699219	0.0006506
15	0.1074219	0.0074190	35	0.1699219	0.0006506
16	0.1132813	0.0059054	36	0.1777344	0.0004800
17	0.1171875	0.0050721	37	0.1933594	0.0002612
18	0.1191406	0.0047006	38	0.1933594	0.0002612
19	0.1230469	0.0040373	39	0.5253906	0.0000000
20	0.1250000	0.0037416	40	0.5859375	0.0000000

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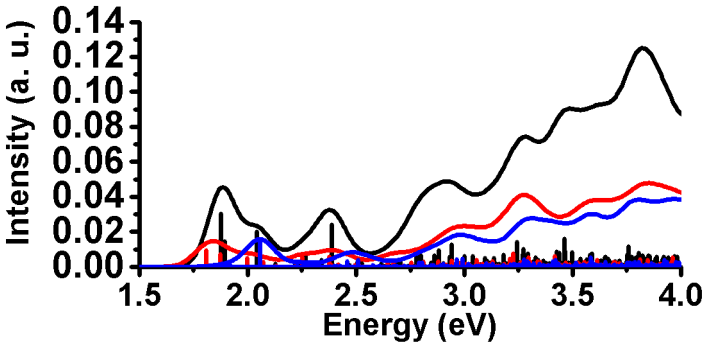
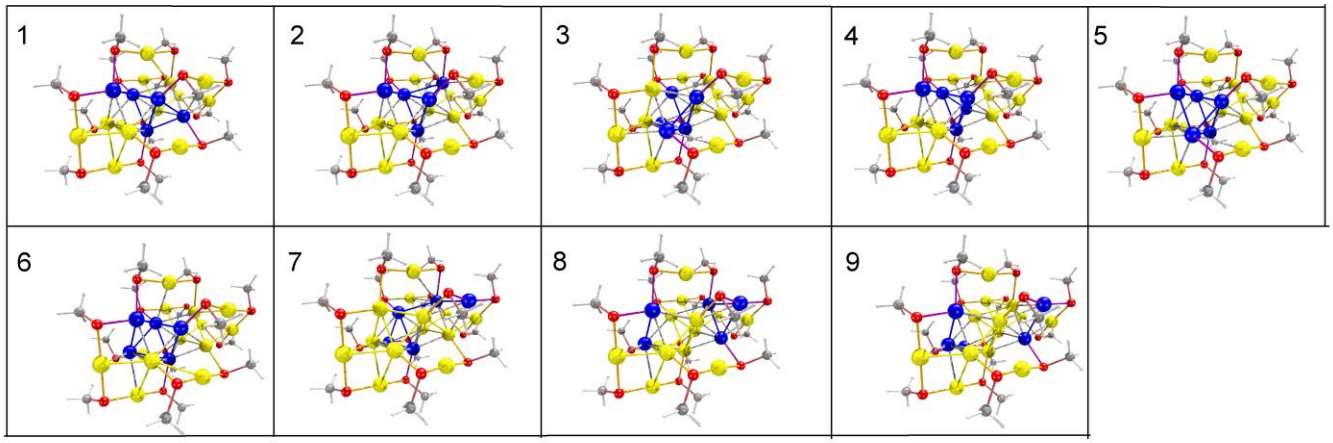
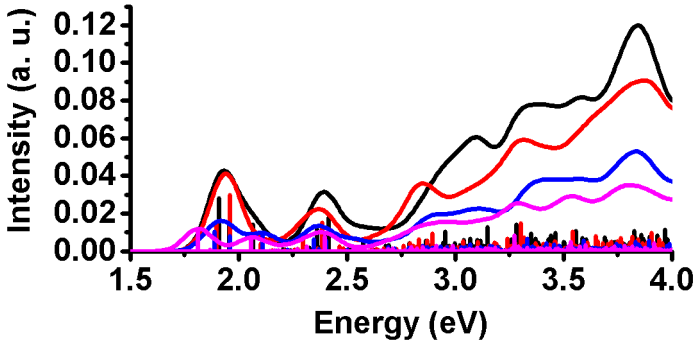


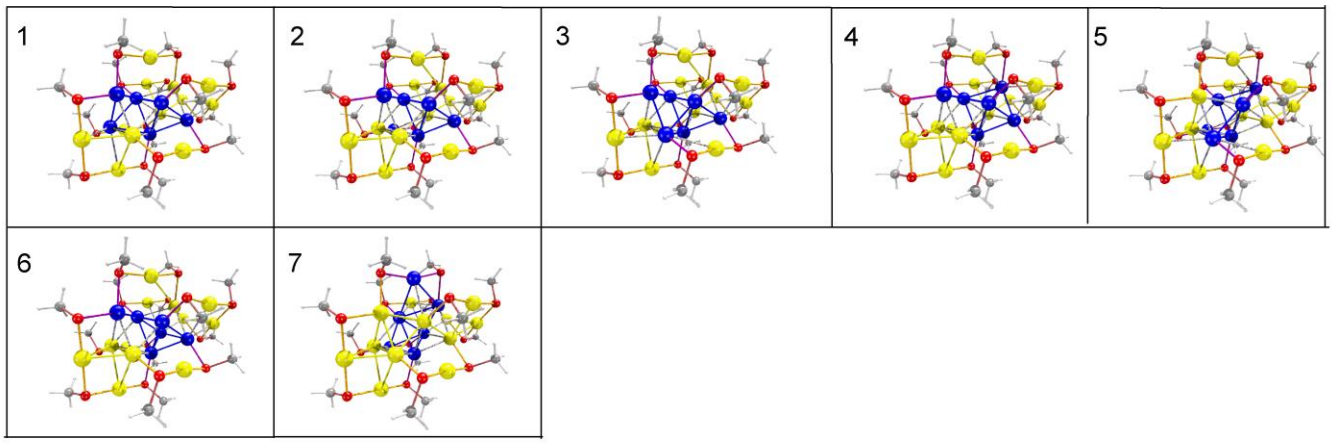


2.352318 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	0.4251126
2	0.0225000	0.1770043
3	0.0293740	0.1354349
4	0.0370340	0.1005043
5	0.0384880	0.0949718
6	0.0478000	0.0660861
7	0.1591160	0.0008660
8	0.3061420	0.0000028
9	0.2598500	0.0000171

n=6

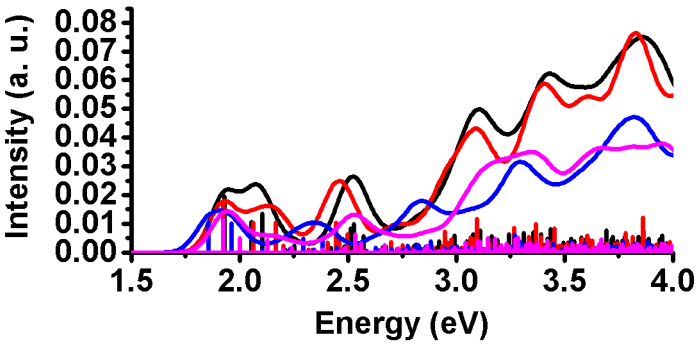




2.62108 Sum of denominador terms

Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	0.3815229
2	0.0051000	0.3128019
3	0.0206000	0.1710540
4	0.0283000	0.1267391
5	0.1051520	0.0063561
6	0.1418570	0.0015221
7	0.2943800	0.0000040

n=7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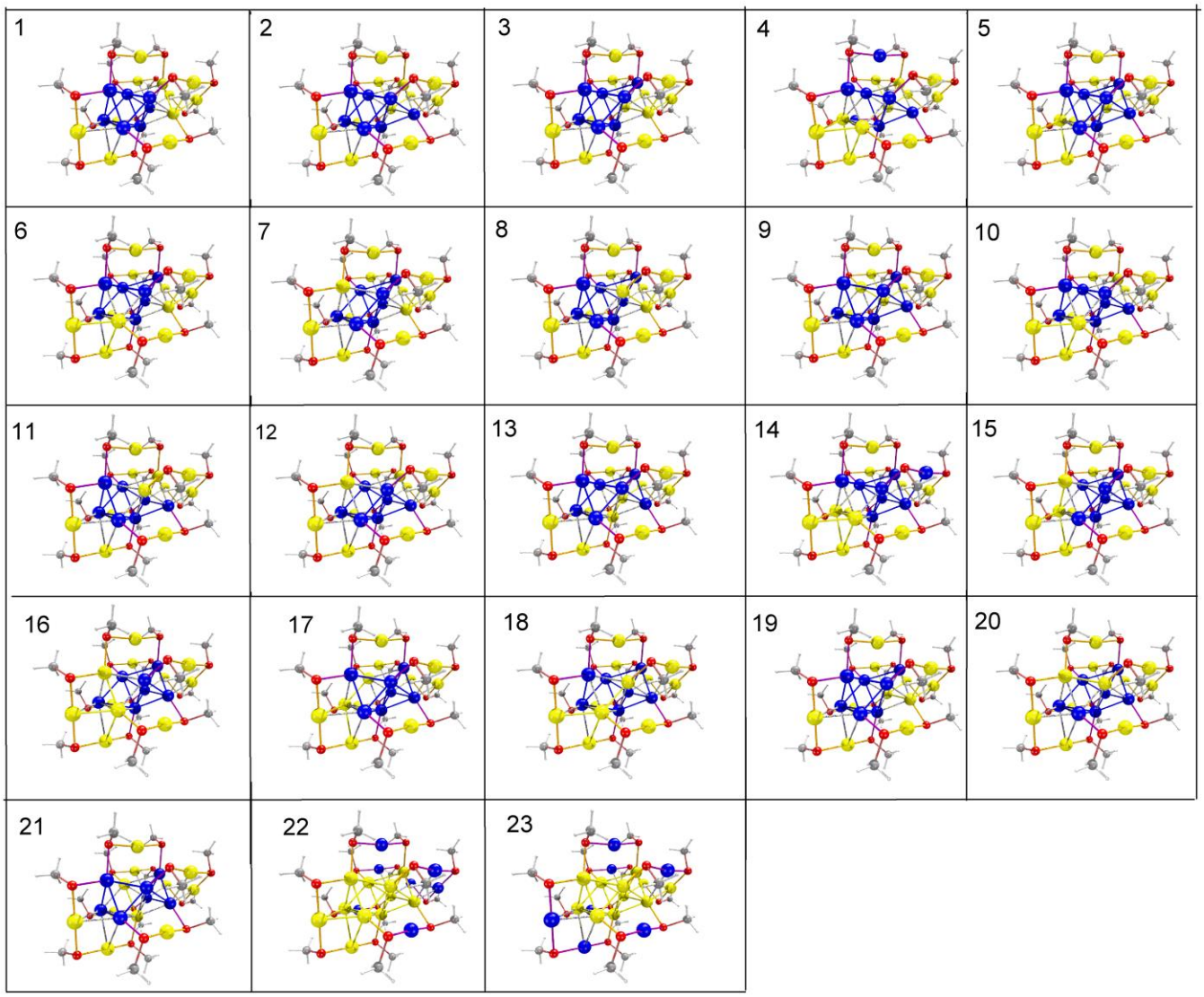
Energy (eV)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n=7

3.8016 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight	Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	0.2630473	14	0.1018920	0.0049755
2	0.0021000	0.2423922	15	0.1165280	0.0028139
3	0.0143300	0.1505514	16	0.1634230	0.0004531
4	0.0152000	0.1455363	17	0.1703910	0.0003454
5	0.0413060	0.0526583	18	0.1740700	0.0002993
6	0.0565460	0.0290889	19	0.1761050	0.0002765
7	0.0587640	0.0266819	20	0.1778200	0.0002587
8	0.0598570	0.0255701	21	0.1782010	0.0002549
9	0.0710910	0.0165098	22	0.1859230	0.0001887
10	0.0730740	0.0152829	23	0.4684090	0.0000000
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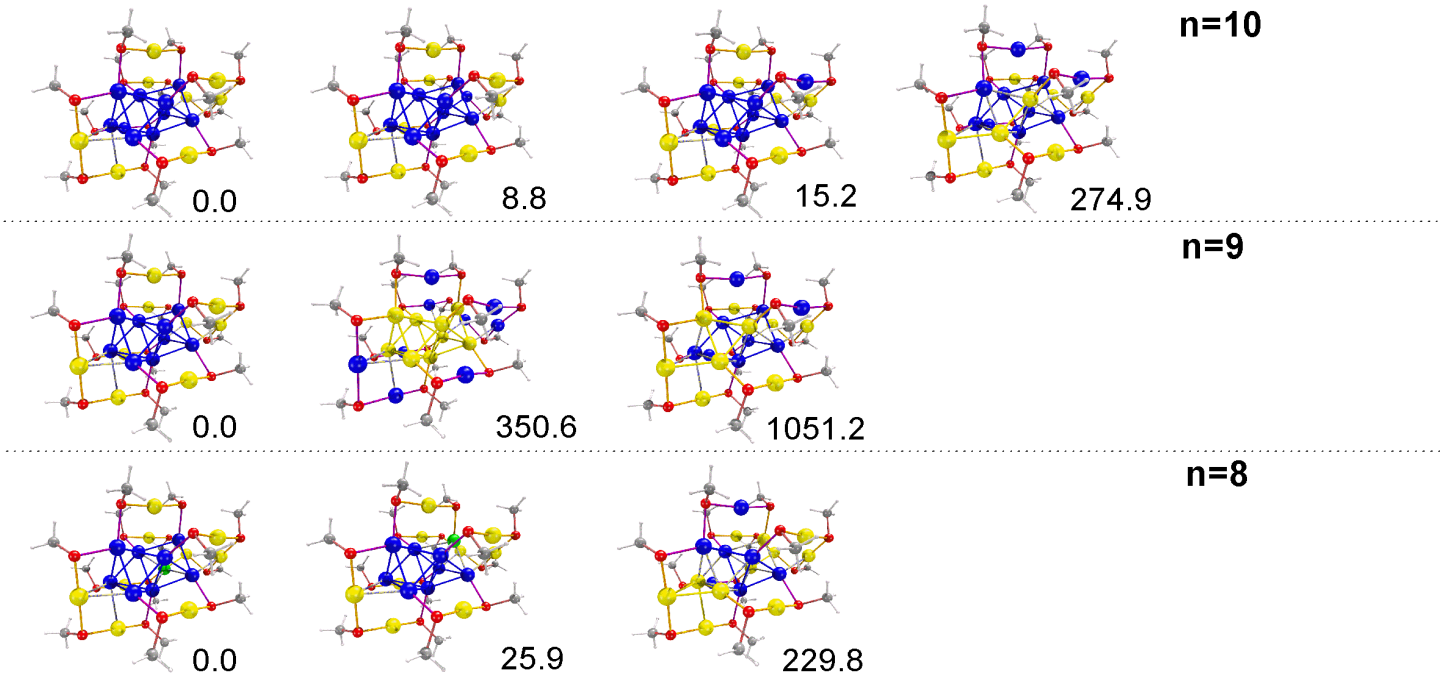

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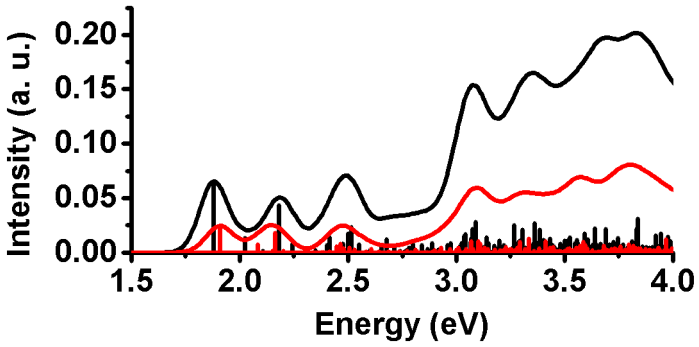

1.3648662 Sum of denominador term.

Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	0.7326726
2	0.0259000	0.2672323
3	0.2298000	0.0000952

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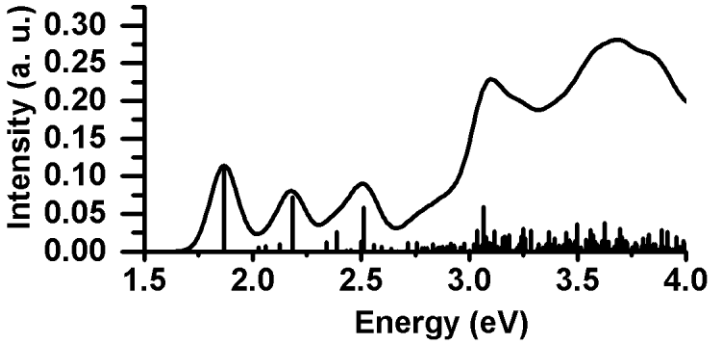
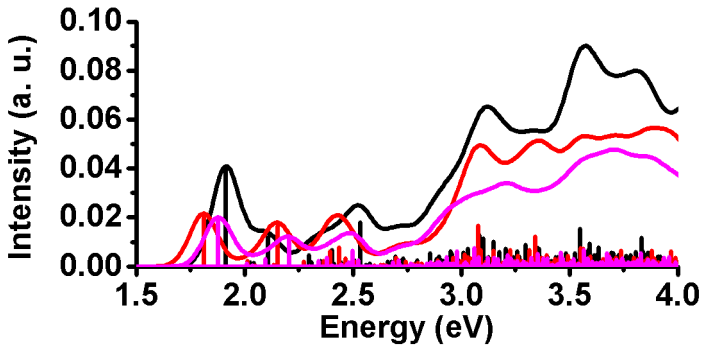


1.00 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	0.9999988
2	0.3506000	0.0000012
3	1.0512000	0.0000000

n=10



3.35657 Sum of denominador terms.

Isomer	Erelative (eV)	Boltzmann weight
1	0.0000000	0.2979236
2	0.0088000	0.2114848
3	0.0152000	0.1648323
4	0.0274900	0.1021395
5	0.0292710	0.0952957
6	0.0334060	0.0811227
7	0.0607680	0.0279509
8	0.0850940	0.0108391
9	0.1068190	0.0046514
10	0.1122970	0.0037578
11	0.3087980	0.0000018
12	0.3512800	0.0000003

PART IV

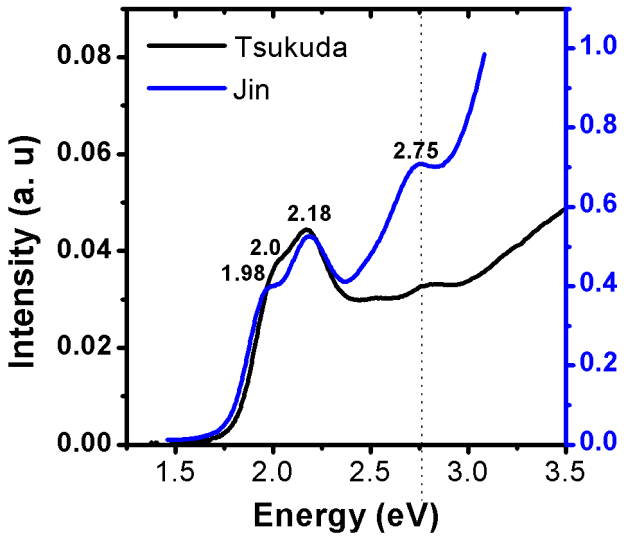


Figure S3. Comparison between experimental absorption spectra reported for the thiolated Au_{18} cluster. Tsukuda data correspond with the curve included in reference 32, While Jin curve corresponds with the X-Ray solved structure (Ref. 21b). Noteworthy is that Jin reported thiolated Au_{18} cluster as non-chiral rather a chiral one by Tsukuda, but both curves look similar.

PART V

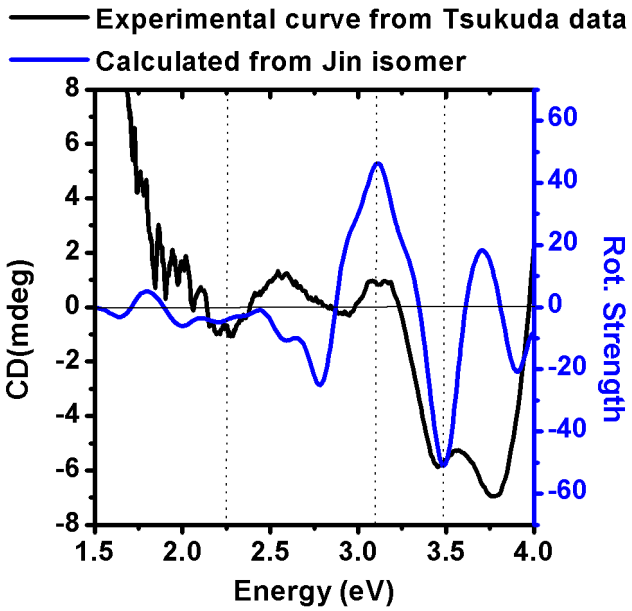


Figure S4. Comparison between calculated CD profile of thiolated Au_{18} cluster, from relaxed experimental Au_9 core structure (published by Jin et al.) and Tsukuda data. Interestingly, both curves show coincidence in the position and sign of peaks located at 3.13 and 3.49 eV. Noteworthy is that one isomer reported by Tlahuice et al. (Ref. 22a) depicts a good agreement with experimental curve by Tsukuda.

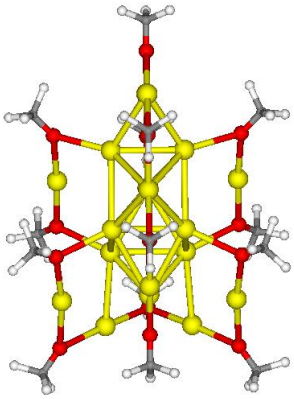
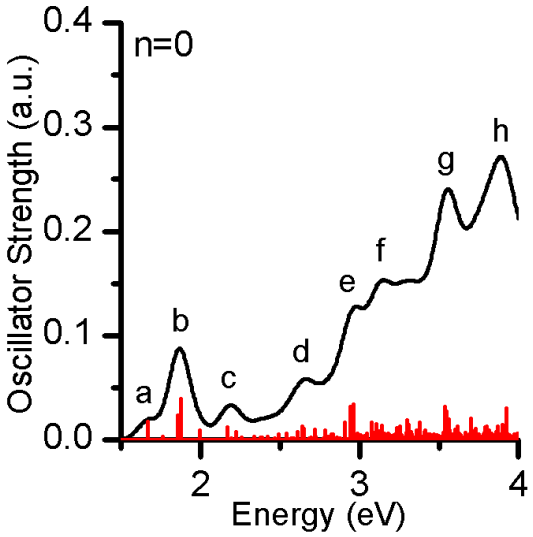


Figure S5. C_s isomer of thiolated Au_{18} cluster. A vertical plane in the middle region is present.

Tabla S2. Excitation energy (E_{peak}), oscillator strength (f $X10^{-2}$), electronic transitions and their contribution weights for peaks of studied isomers.

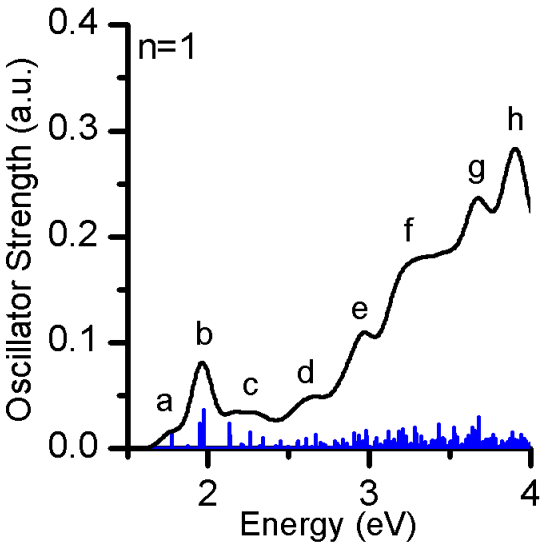
$Au_{18}C_{14}H_{56}$

Peak	E_{peak} (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.667	1.77	HOMO →LUMO	85.6
b	1.855	4.68	HOMO-2 → LUMO	46.6
	1.878	3.96	HOMO-3 → LUMO	61.8
c	2.225	7.42	HOMO→ LUMO+1	66.8
d	2.639		HOMO-2 → LUMO+3	24.8
		1.33	HOMO-11 → LUMO	21.7
			HOMO-12 → LUMO	21.0
	2.650	1.12	HOMO-2 → LUMO+3	37.3
			HOMO-13 → LUMO	27.5
	2.718	1.07	HOMO-14 → LUMO	29.4
			HOMO-2 → LUMO+4	24.6
e	2.903	1.91	HOMO-21 → LUMO	20.0
			HOMO-7 → LUMO+1	16.7
			HOMO-4 → LUMO+3	14.0
	2.942	3.32	HOMO-7 → LUMO+1	31.9
			HOMO-4 → LUMO+4	13.8
			HOMO-4 → LUMO+3	7.0
	2.962	3.37	HOMO-6 → LUMO+1	30.3
			HOMO-6 → LUMO+2	13.0
			HOMO-4 → LUMO+3	10.6
f	3.073	1.69	HOMO-7 → LUMO+2	45.7
			HOMO-2 → LUMO+6	11.9
	3.105	1.67	HOMO-3 → LUMO	21.8
			HOMO-1 → LUMO+6	20.5
			HOMO-7 → LUMO+3	12.9
	3.141	1.79	HOMO-27 → LUMO	40.1
			HOMO → LUMO+10	17.7
	3.297	2.10	HOMO-13 → LUMO+1	19.9
			HOMO → LUMO+11	17.8
			HOMO-11 → LUMO+1	15.5
	3.310	1.83	HOMO-13 → LUMO+1	28.5
			HOMO-12 → LUMO+1	19.8
			HOMO-4 → LUMO+6	16.5
	3.377	2.12	HOMO-2 → LUMO+10	23.4
			HOMO-33 → LUMO	14.2
			HOMO-5 → LUMO+5	14.2
g	3.539	4.07	HOMO-6 → LUMO+6	13.0
			HOMO-9 → LUMO+4	12.6
			HOMO-14 → LUMO+3	8.9
	3.545	2.81	HOMO-15 → LUMO+2	24.8
			HOMO-39 → LUMO	12.3
			HOMO-10 → LUMO+4	8.5
	3.562	2.03	HOMO-4 → LUMO+9	55.6
h	3.868	1.69	HOMO-53 → LUMO	57.5
	3.900	1.60	HOMO-31 → LUMO+1	17.1
			HOMO-13 → LUMO+5	12.1
			HOMO-29 → LUMO+1	9.6
	3.915	1.55	HOMO-8 → LUMO+7	28.7
			HOMO → LUMO+18	24.9
	3.922	3.86	HOMO-8 → LUMO+7	20.9
			HOMO → LUMO+18	15.0



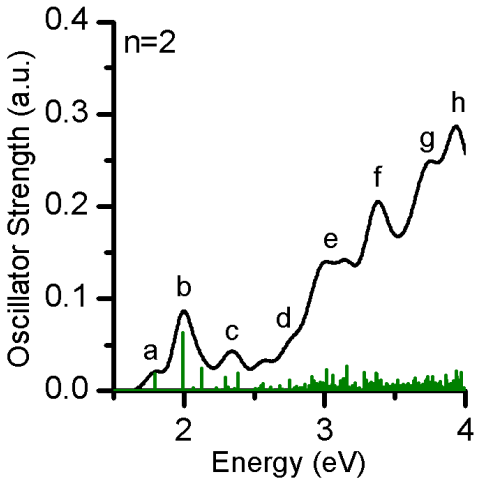
$Au_{17}AgC_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.771	1.47	HOMO → LUMO	87.7
b	1.945	2.42	HOMO-3 → LUMO	61.2
	1.971	5.66	HOMO-1 → LUMO	44.5
			HOMO-3 → LUMO	38.1
c	2.134	2.48	HOMO-4 → LUMO	89.3
	2.26	1.54	HOMO-6 → LUMO	88.3
	2.339	1.56	HOMO → LUMO+2	62.0
d	2.606	1.21	HOMO-9 → LUMO	71.0
	2.666	1.34	HOMO-3→ LUMO+2	54.2
e	2.841	1.71	HOMO-5 → LUMO+2	35.5
			HOMO-5 → LUMO+1	23.0
	2.978	2.18	HOMO-6→ LUMO+2	52.3
	2.982	2.33	HOMO-4 → LUMO+3	31.4
			HOMO-8 → LUMO+1	12.8
			HOMO-3→ LUMO+3	6.7
f	3.120	2.03	HOMO-5 → LUMO+4	46.8
			HOMO-2 → LUMO+4	6.4
	3.187	1.83	HOMO → LUMO+10	37.1
			HOMO-2 → LUMO+6	28.4
	3.207	2.34	HOMO → LUMO+10	33.5
			HOMO-8 → LUMO+2	17.9
	3.228	2.25	HOMO-6 → LUMO+4	16.4
			HOMO-10 → LUMO+1	16.1
			HOMO-7 → LUMO+4	10.5
	3.284	2.06	HOMO-8 → LUMO+3	22.9
			HOMO-13 → LUMO+1	14.4
			HOMO-11 → LUMO+1	10.6
	3.295	2.16	HOMO-8 → LUMO+3	27.0
			HOMO-2 → LUMO+7	21.6
	3.323	2.22	HOMO-30 → LUMO	33.6
			HOMO-14 → LUMO+1	28.7
	3.526	2.16	HOMO-3 → LUMO+10	27.9
			HOMO-35 → LUMO	12.5
			HOMO-12 → LUMO+3	11.3
g	3.617	1.64	HOMO-7 → LUMO+6	26.7
			HOMO-15 → LUMO+3	12.2
			HOMO-22 → LUMO+1	11.0
	3.640	2.09	HOMO-39 → LUMO	27.3
			HOMO-18 → LUMO+2	20.4
	3.656	1.74	HOMO-19 → LUMO+2	23.6
			HOMO-23 → LUMO+1	14.3
			HOMO-39 → LUMO	10.6
	3.677	3.30	HOMO-3 → LUMO+11	33.3
			HOMO-4 → LUMO+10	20.7
h	3.885	1.69	HOMO-30 → LUMO+1	32.4
			HOMO-10 → LUMO+5	6.3
	3.888	1.66	HOMO-7 → LUMO+10	22.3
			HOMO-9 → LUMO+6	15.8
			HOMO-22 → LUMO+3	13.2
	3.941	2.65	HOMO-1 → LUMO+14	19.9
			HOMO-31 → LUMO+1	12.7
			HOMO-5 → LUMO+11	11.4



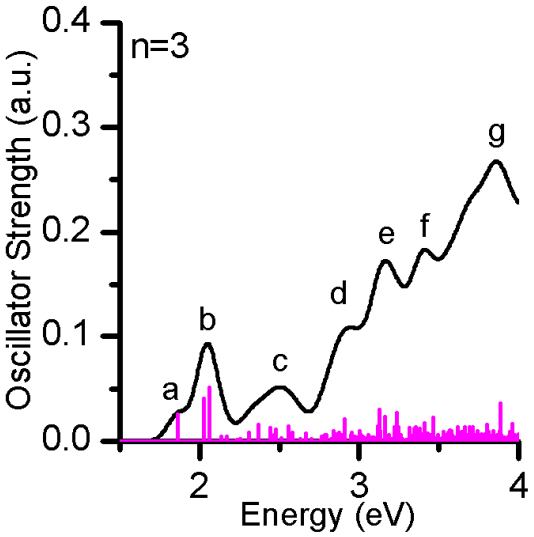
$Au_{16}Ag_2C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.795	2.03	HOMO → LUMO	86.0
b	1.991	8.05	HOMO-1 → LUMO	78.2
	2.126	2.48	HOMO-4 → LUMO	86.2
c	2.294	1.59	HOMO-6 → LUMO	79.5
	2.379	2.47	HOMO → LUMO+3	65.7
d	2.746	1.57	HOMO-3 → LUMO+2	67.4
e	2.908	1.56	HOMO-5 → LUMO+2	28.0
			HOMO → LUMO+6	10.0
	2.926	1.65	HOMO-3 → LUMO+4	32.7
			HOMO-5 → LUMO+1	13.1
	3.011	3.61	HOMO-19 → LUMO	48.9
	3.059	1.74	HOMO → LUMO+8	28.1
			HOMO → LUMO+7	19.4
	3.133	2.04	HOMO-5 → LUMO+4	46.6
			HOMO → LUMO+9	31.8
	3.156	3.44	HOMO → LUMO+9	52.0
f	3.279	2.28	HOMO-1 → LUMO+7	25.5
			HOMO-3 → LUMO+5	10.7
	3.365	2.13	HOMO-3 → LUMO+6	17.2
			HOMO-29 → LUMO	17.0
			HOMO-14 → LUMO+1	12.2
	3.374	1.86	HOMO-14 → LUMO+1	39.0
			HOMO-9 → LUMO+3	15.7
	3.382	2.15	HOMO-13 → LUMO+1	32.9
			HOMO-11 → LUMO+2	15.2
	3.400	1.74	HOMO-10 → LUMO+3	21.0
			HOMO-10 → LUMO+2	20.3
	3.438	1.59	HOMO-12 → LUMO+2	32.7
			HOMO-4 → LUMO+6	16.2
g	3.642	1.56	HOMO-11 → LUMO+4	30.5
			HOMO-5 → LUMO+7	12.1
	3.727	1.49	HOMO-6 → LUMO+8	29.6
			HOMO-23 → LUMO+1	13.3
	3.732	1.66	HOMO-20 → LUMO+2	25.6
			HOMO → LUMO+14	17.6
	3.768	1.91	HOMO-5 → LUMO+10	42.2
			HOMO-42 → LUMO	22.6
h	3.860	1.90	HOMO-27 → LUMO+1	27.3
			HOMO-18 → LUMO+4	13.5
	3.935	2.36	HOMO-26 → LUMO+2	20.9
	3.938	2.34	HOMO-8 → LUMO+7	15.2
			HOMO-25 → LUMO+3	13.6
	3.971	2.55	HOMO-9 → LUMO+6	16.7
			HOMO-1 → LUMO+14	14.4



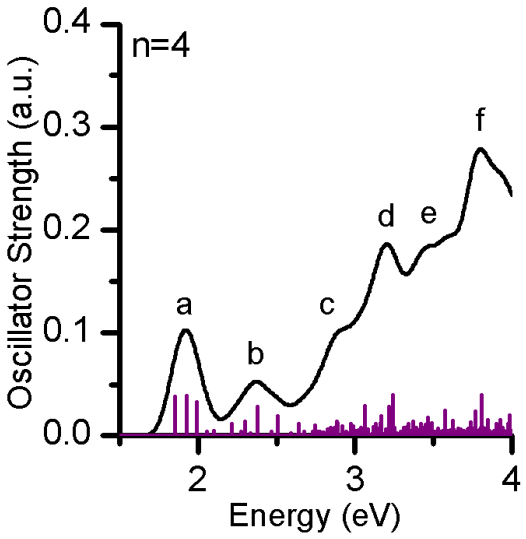
$Au_{15}Ag_3C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.863	2.57	HOMO → LUMO	79.4
b	2.025	4.22	HOMO-1 → LUMO	45.3
			HOMO-2 → LUMO	42.5
	2.060	5.08	HOMO-2 → LUMO	53.8
c	2.304	1.30	HOMO-5 → LUMO	88.7
	2.366	1.75	HOMO-6 → LUMO	90.1
	2.559	1.65	HOMO-1→ LUMO+1	59.8
d	2.838	1.46	HOMO-11 → LUMO	22.2
			HOMO-10 → LUMO	20.4
	2.909	2.07	HOMO-14 → LUMO	17.5
			HOMO-6 →LUMO+1	14.5
			HOMO-3 → LUMO+3	12.2
e	3.116	1.88	HOMO-6 → LUMO+3	38.6
			HOMO-1 → LUMO+5	28.9
	3.122	1.90	HOMO-8 → LUMO+2	35.8
			HOMO-5 → LUMO+4	20.3
	3.129	3.02	HOMO → LUMO+9	17.0
			HOMO-5 → LUMO+4	16.9
			HOMO-1 → LUMO+5	15.3
	3.162	3.62	HOMO → LUMO+9	62.3
	3.235	3.02	HOMO-23 → LUMO	32.2
			HOMO → LUMO+10	21.6
f	3.378	1.54	HOMO → LUMO+11	26.7
			HOMO-27 → LUMO	24.4
	3.408	1.68	HOMO-2 → LUMO+7	37.1
			HOMO-3 → LUMO+6	27.5
	3.462	2.52	HOMO-5 → LUMO+5	76.0
g	3.660	1.75	HOMO-33 → LUMO	21.4
			HOMO-3 → LUMO+10	12.0
	3.690	2.18	HOMO-4 → LUMO+10	24.5
			HOMO-2 → LUMO+11	13.4
	3.804	1.63	HOMO-6 → LUMO+9	23.9
			HOMO-18 → LUMO+3	17.4
	3.878	1.60	HOMO-25 → LUMO+2	30.9
			HOMO-7 → LUMO+9	23.1
	3.886	4.05	HOMO-27 → LUMO+1	15.8
			HOMO-7 → LUMO+9	11.4
	3.960	1.68	HOMO-47 → LUMO	15.4
			HOMO-10 → LUMO+5	13.7
			HOMO-23 → LUMO+3	12.3



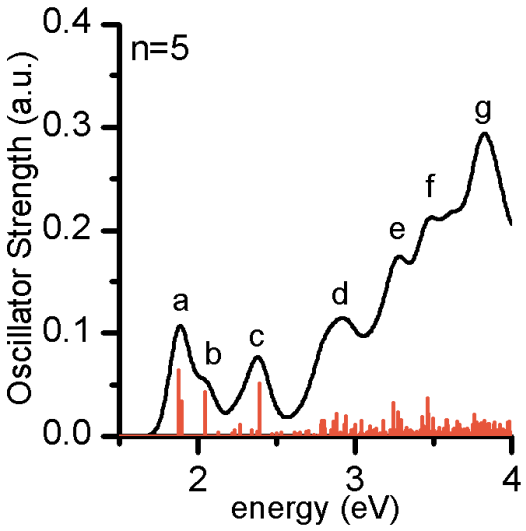
$Au_{14}Ag_4C_{14}H_{56}$

Peak	Energy (eV)	F	Transition from occupied → unoccupied orbital	Weight (%)
a	1.852	4.26	HOMO → LUMO	65.7
	1.926	6.07	HOMO-1 → LUMO	54.7
	1.993	3.35	HOMO-2→ LUMO	77.6
b	2.298	1.53	HOMO → LUMO+1	62.2
	2.380	3.62	HOMO-7 → LUMO	87.7
	2.507	1.92	HOMO-1→ LUMO+1	84.5
c	2.640	1.27	HOMO → LUMO+4	82.8
	2.885	1.41	HOMO-2 → LUMO+3	50.0
	2.889	1.98	HOMO-2 → LUMO+4	26.8
			HOMO-5→ LUMO+1	23.8
	2.919	1.46	HOMO-16 → LUMO	33.5
			HOMO-2 → LUMO+4	30.5
	3.062	2.89	HOMO → LUMO+6	31.3
			HOMO-7 → LUMO+2	22.9
d	3.160	1.96	HOMO-23 → LUMO	46.8
			HOMO → LUMO+8	15.9
	3.171	3.07	HOMO-23 → LUMO	28.2
			HOMO → LUMO+8	9.8
	3.220	2.90	HOMO-6→ LUMO+4	26.5
			HOMO → LUMO+9	18.4
	3.240	4.45	HOMO → LUMO+9	68.4
e	3.341	1.79	HOMO-2 → LUMO+6	26.6
			HOMO-3 → LUMO+5	19.9
			HOMO-10 → LUMO+2	18.6
	3.371	2.14	HOMO-4 → LUMO+5	37.1
			HOMO-29 → LUMO	14.9
	3.467	1.83	HOMO-5→ LUMO+5	31.3
			HOMO-13 → LUMO+2	17.5
	3.575	3.86	HOMO-2→ LUMO+10	45.6
	3.624	2.27	HOMO-10 → LUMO+3	32.6
			HOMO-18 → LUMO+2	14.2
f	3.740	1.73	HOMO-41 → LUMO	23.9
			HOMO-2 → LUMO+11	16.9
	3.770	3.03	HOMO-6→ LUMO+7	10.5
	3.806	3.98	HOMO-5→ LUMO+10	25.4
			HOMO-3 → LUMO+11	14.0
	3.899	1.84	HOMO-26 → LUMO+1	16.6
			HOMO-16 → LUMO+3	13.7
	3.989	3.12	HOMO-2→ LUMO+13	40.3



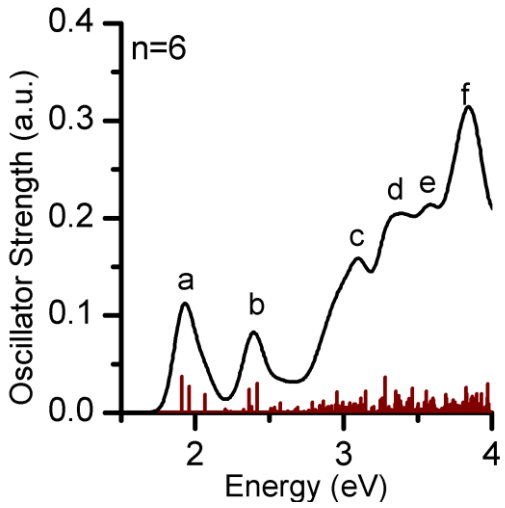
$Au_{13}Ag_5C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.877	7.13	HOMO → LUMO	73.6
	1.894	3.43	HOMO-1→ LUMO	77.0
b	2.043	4.76	HOMO-2 → LUMO	83.2
c	2.389	5.72	HOMO-7 → LUMO	47.2
			HOMO-1 → LUMO+1	23.6
d	2.780	1.69	HOMO-10 → LUMO	58.1
	2.788	1.64	HOMO-3 → LUMO+2	15.7
			HOMO-4 → LUMO+2	14.9
			HOMO-1 → LUMO+3	13.8
	2.800	1.54	HOMO-4 → LUMO+2	24.3
			HOMO-10 → LUMO	13.7
			HOMO-5 → LUMO+2	13.2
	2.862	1.57	HOMO-1 → LUMO+4	14.5
			HOMO-6 → LUMO+1	14.5
			HOMO-5 → LUMO+2	12.7
	2.884	2.23	HOMO-5→ LUMO+2	28.2
			HOMO-7 → LUMO+1	14.4
	2.943	3.02	HOMO-2→ LUMO+3	35.6
			HOMO-7 → LUMO+3	23.5
e	3.183	1.62	HOMO → LUMO+9	45.8
	3.243	3.31	HOMO-5→ LUMO+4	29.1
			HOMO → LUMO+10	21.6
	3.271	1.75	HOMO-1→ LUMO+8	59.7
	3.274	2.40	HOMO-10 → LUMO+1	24.0
			HOMO-2 → LUMO+1	17.6
	3.295	1.76	HOMO-1 → LUMO+1	52.9
f	3.427	2.07	HOMO-14 → LUMO+1	30.8
			HOMO-2 → LUMO+7	17.0
	3.439	1.89	HOMO-12 → LUMO+2	23.4
			HOMO-2 → LUMO+8	10.9
	3.463	3.79	HOMO-8 → LUMO+4	14.9
			HOMO-2 → LUMO+8	14.3
			HOMO-2 → LUMO+9	13.5
	3.465	2.16	HOMO-8→ LUMO+4	36.6
			HOMO-2 → LUMO+8	13.3
	3.498	1.93	HOMO-5 → LUMO+5	35.4
			HOMO.30 → LUMO	23.6
	3.588	1.78	HOMO-5 → LUMO+6	31.4
			HOMO-16 → LUMO+2	10.7
g	3.753	1.62	HOMO-8 → LUMO+5	30.7
			HOMO-23 → LUMO+1	12.1
	3.759	2.71	HOMO-11 → LUMO+4	18.7
			HOMO-8 → LUMO+5	12.6
	3.807	1.92	HOMO-8 → LUMO+6	27.5
			HOMO-15 → LUMO+3	11.6
	3.824	1.51	HOMO-3 → LUMO+11	24.6
			HOMO-25 → LUMO+1	18.8
	3.849	1.50	HOMO-4 → LUMO+11	23.7
			HOMO-14 → LUMO+3	13.1
			HOMO-15 → LUMO+3	12.4
	3.971	1.47	HOMO-19 → LUMO+3	37.4
			HOMO-2 → LUMO+13	25.9



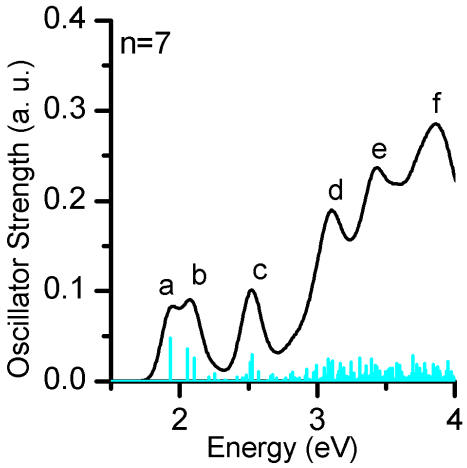
$Au_{12}Ag_6C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.909	7.39	HOMO → LUMO	56.48
			HOMO-1 → LUMO	31.4
	1.957	4.18	HOMO-1→ LUMO	65.4
			HOMO→ LUMO	27.3
	2.064	3.74	HOMO-2 → LUMO	88.5
b	2.362	3.06	HOMO-6 → LUMO	42.0
			HOMO → LUMO+2	27.8
	2.416	4.67	HOMO-7 → LUMO	77.2
c	2.955	2.74	HOMO-6 → LUMO+2	16.0
			HOMO → LUMO+5	10.1
	3.149	3.42	HOMO-4 → LUMO+4	36.7
			HOMO → LUMO+8	14.7
d	3.282	3.76	HOMO-1 → LUMO+8	37.0
			HOMO-21 → LUMO	13.9
	3.351	2.49	HOMO-3 → LUMO+5	19.6
			HOMO-2 → LUMO+6	17.4
	3.443	2.25	HOMO-2 → LUMO+8	46.8
			HOMO-27 → LUMO	13.7
	3.462	2.57	HOMO-12 → LUMO+2	19.0
			HOMO-8 → LUMO+4	10.6
e	3.558	2.79	HOMO-14 → LUMO+2	31.3
			HOMO-2 → LUMO+10	16.0
	3.588	1.87	HOMO-3 → LUMO+8	41.7
			HOMO-5 → LUMO+6	22.1
	3.689	1.96	HOMO-5 → LUMO+8	24.2
			HOMO-2 → LUMO+11	16.4
f	3.827	2.86	HOMO-3 → LUMO+11	26.7
			HOMO-37 → LUMO	15.3
	3.830	2.00	HOMO-37 → LUMO	30.1
			HOMO-38 → LUMO	12.4
	3.858	2.26	HOMO-2 → LUMO+12	29.2
			HOMO-4 → LUMO+11	21.8
	3.898	2.01	HOMO-7 → LUMO+10	51.4
	3.932	2.21	HOMO-5 → LUMO+11	54.1
	3.969	2.99	HOMO-46 → LUMO	23.5
			HOMO-2 → LUMO+13	20.2



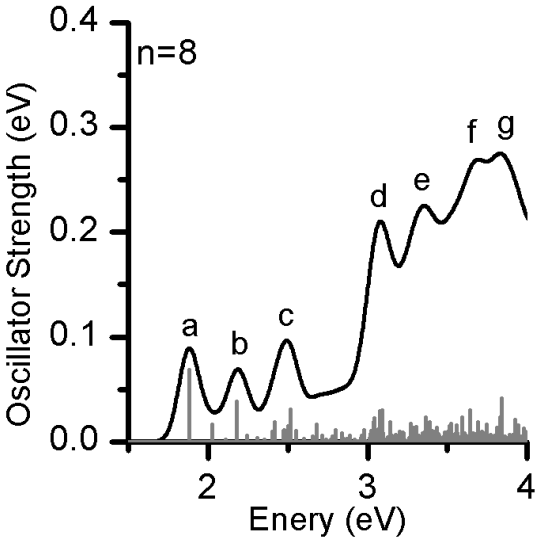
$Au_{11}Ag_7C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.928	7.45	HOMO → LUMO	69.4
			HOMO- 1 → LUMO	24.6
b	2.055	4.05	HOMO-1 → LUMO	62.8
	2.105	5.15	HOMO-2 → LUMO	75.1
c	2.511	3.21	HOMO → LUMO+3	46.2
			HOMO-7 → LUMO	24.6
	2.526	3.76	HOMO-5 → LUMO	34.7
			HOMO-2 → LUMO+2	28.5
	2.570	2.16	HOMO-2 → LUMO+2	42.8
			HOMO-2 → LUMO+1	31.2
d	2.993	2.26	HOMO-7 → LUMO+1	24.2
			HOMO-3 → LUMO+3	12.9
	3.078	2.45	HOMO-14 → LUMO	21.0
			HOMO-8 → LUMO+2	17.4
	3.088	2.15	HOMO-8 → LUMO+2	14.6
			HOMO-1 → LUMO+5	12.7
	3.104	2.32	HOMO-5 → LUMO+3	38.3
			HOMO-15 → LUMO	16.3
	3.110	2.94	HOMO-15 → LUMO	56.3
	3.165	2.15	HOMO-17 → LUMO	56.1
	3.244	2.42	HOMO-19 → LUMO	26.9
			HOMO-3 → LUMO+4	11.8
e	3.311	2.62	HOMO-8 → LUMO+3	23.5
			HOMO-5 → LUMO+4	17.9
	3.355	2.65	HOMO-10 → LUMO+1	33.9
			HOMO-6 → LUMO+4	27.8
	3.392	2.43	HOMO-10 → LUMO+2	19.8
			HOMO-12 → LUMO+1	11.6
	3.435	3.12	HOMO-3 → LUMO+6	21.5
			HOMO-12 → LUMO+1	16.9
	3.579	1.97	HOMO-1 → LUMO+11	49.9
			HOMO-3 → LUMO+8	27.3
f	3.693	2.92	HOMO-1 → LUMO+12	22.6
			HOMO-2 → LUMO+11	22.0
	3.722	2.12	HOMO-21 → LUMO+1	24.2
			HOMO-13 → LUMO+3	13.1
	3.779	2.16	HOMO-5 → LUMO+9	16.5
			HOMO-4 → LUMO+10	14.4
	3.841	2.09	HOMO-34 → LUMO	29.6
			HOMO-10 → LUMO+4	16.6
			HOMO-16 → LUMO+3	15.2
	3.950	2.24	HOMO-1 → LUMO+14	13.0
			HOMO-14 → LUMO+4	12.3



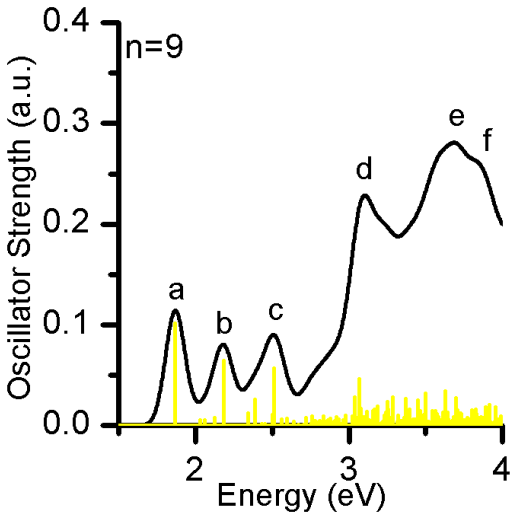
$Au_{10}Ag_8C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.879	8.78	HOMO → LUMO	81.9
b	2.180	5.94	HOMO-2→ LUMO	84.5
c	2.415	1.92	HOMO-5 → LUMO	45.7
			HOMO → LUMO+3	35.4
	2.499	2.38	HOMO-7 → LUMO	29.4
			HOMO-6 → LUMO	25.7
	2.515	3.17	HOMO-7 → LUMO	63.0
	2.678	1.69	HOMO-8 → LUMO	56.2
d	3.038	2.11	HOMO-1 → LUMO+5	46.9
	3.042	2.34	HOMO-5 → LUMO+3	31.1
			HOMO-8 → LUMO+1	12.2
	3.076	2.99	HOMO-12 → LUMO	37.1
			HOMO-3 → LUMO+4	27.5
	3.089	3.82	HOMO-3 → LUMO+4	41.1
	3.141	1.95	HOMO-13 → LUMO	29.9
			HOMO-2 → LUMO+5	15.1
e	3.268	3.41	HOMO-6 → LUMO+4	45.9
			HOMO-2 → LUMO+6	37.1
	3.306	2.90	HOMO-20 → LUMO	39.3
	3.362	3.68	HOMO-10 → LUMO+1	20.6
			HOMO-2 → LUMO+8	16.6
	3.387	2.88	HOMO-11 → LUMO+1	59.3
f	3.523	1.91	HOMO-21 → LUMO	54.8
	3.592	2.36	HOMO-6 → LUMO+6	51.5
	3.639	3.07	HOMO-19 → LUMO+1	30.5
			HOMO-2 → LUMO+11	19.1
	3.689	2.93	HOMO-17 → LUMO+2	19.4
			HOMO-1 → LUMO+12	13.8
g	3.776	2.01	HOMO-30 → LUMO	74.0
	3.831	2.98	HOMO-11 → LUMO+4	26.6
			HOMO-21 → LUMO+1	11.1
	3.838	4.24	HOMO-6 → LUMO+10	33.0
			HOMO-31 → LUMO	21.9
	3.922	2.17	HOMO-2 → LUMO+13	18.3
			HOMO-25 → LUMO+1	15.3
	3.943	2.43	HOMO-23 → LUMO+2	67.5



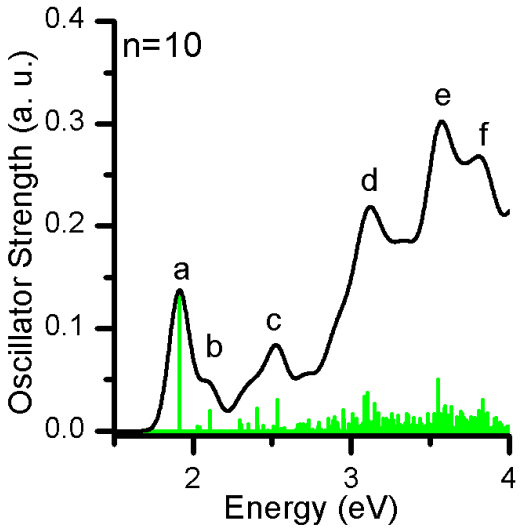
$Au_9Ag_9C_{15}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.868	11.38	HOMO → LUMO	83.8
b	2.184	7.18	HOMO → LUMO+1	85.1
c	2.389	2.65	HOMO → LUMO+3	60.5
	2.510	5.82	HOMO-6 → LUMO	57.1
			HOMO-4 → LUMO	30.9
d	3.038	2.79	HOMO-10 → LUMO	41.6
	3.065	5.98	HOMO-8 → LUMO+2	16.7
			HOMO-6 → LUMO+3	13.4
	3.117	2.71	HOMO-6 → LUMO+3	23.4
			HOMO-4 → LUMO+3	19.4
	3.164	2.02	HOMO-2 → LUMO+5	44.5
			HOMO-7 → LUMO+3	24.7
	3.185	2.15	HOMO-14 → LUMO	51.1
	3.240	2.01	HOMO-9 → LUMO+1	26.7
			HOMO-7 → LUMO+3	21.7
	3.250	3.08	HOMO-6 → LUMO+4	35.0
			HOMO-9 → LUMO+1	22.1
	3.285	2.79	HOMO-17 → LUMO	77.3
e	3.367	2.32	HOMO-19 → LUMO	37.8
			HOMO-2 → LUMO+8	16.6
	3.368	2.63	HOMO-9 → LUMO+2	43.2
	3.448	2.56	HOMO-21 → LUMO	42.9
	3.497	3.60	HOMO-1 → LUMO+11	43.9
	3.560	2.89	HOMO-4 → LUMO+6	19.5
			HOMO-15 → LUMO+1	14.3
	3.572	2.23	HOMO → LUMO+14	14.3
			HOMO-12 → LUMO+2	13.7
			HOMO-16 → LUMO+1	13.3
	3.625	3.83	HOMO-2 → LUMO+11	67.2
	3.695	3.07	HOMO-19 → LUMO+1	41.1
f	3.831	2.26	HOMO → LUMO+18	19.2
			HOMO-22 → LUMO+1	13.7
	3.889	2.84	HOMO-2 → LUMO+13	42.0
	3.914	2.66	HOMO-7 → LUMO+10	22.6
			HOMO-25 → LUMO+5	21.3



$Au_8Ag_{10}C_{14}H_{56}$

Peak	Energy (eV)	f	Transition from occupied → unoccupied orbital	Weight (%)
a	1.912	13.52	HOMO → LUMO	83.3
b	2.105	4.01	HOMO-1 → LUMO+2	69.2
c	2.403	2.23	HOMO→ LUMO+3	67.3
	2.532	6.07	HOMO-6→ LUMO	75.9
d	2.950	2.06	HOMO → LUMO+9	27.5
			HOMO-5 → LUMO+2	13.6
	3.032	2.40	HOMO-9 → LUMO+1	38.6
			HOMO-3 → LUMO+3	14.9
	3.085	4.30	HOMO-9 → LUMO+1	31.0
			HOMO-9 → LUMO+2	16.2
	3.103	3.86	HOMO-9 → LUMO+2	28.2
			HOMO-6 → LUMO+3	23.4
	3.148	3.44	HOMO-13 → LUMO	28.9
			HOMO-10 → LUMO+1	13.2
	3.204	2.44	HOMO-10 → LUMO+2	20.7
			HOMO-15 → LUMO	15.8
			HOMO-4 → LUMO+4	12.6
	3.259	2.11	HOMO-10 → LUMO+2	25.9
			HOMO-10 → LUMO+1	15.5
e	3.296	3.00	HOMO-17 → LUMO	31.0
			HOMO-2 → LUMO+6	20.8
	3.350	2.58	HOMO-3→ LUMO+5	43.5
			HOMO-7 → LUMO+4	11.2
	3.360	2.41	HOMO-3 → LUMO+6	42.3
			HOMO-11 → LUMO+1	14.7
	3.549	5.14	HOMO-9 → LUMO+4	9.4
			HOMO-2 → LUMO+9	8.7
	3.588	2.28	HOMO-17 → LUMO+1	19.1
			HOMO-24 → LUMO	19.1
			HOMO-16 → LUMO+2	17.4
	3.593	3.13	HOMO-3 → LUMO+9	32.7
			HOMO-7 → LUMO+5	16.2
	3.634	2.65	HOMO-4 → LUMO+7	41.8
f	3.807	1.99	HOMO-9 → LUMO+6	21.4
			HOMO-11 → LUMO+4	20.5
	3.831	3.95	HOMO-5 → LUMO+10	30.0
			HOMO-3 → LUMO+11	28.9
	3.838	2.13	HOMO → LUMO+18	54.5
	3.861	1.92	HOMO-23 → LUMO+2	35.3
			HOMO-12 → LUMO+5	28.9



Part VIII. Cartesian coordinates of relaxed isomers.

N=1

88

Au	-1.27992	-1.32696	0.58046
Au	1.13051	-2.50796	-0.87613
Au	0.96496	0.19023	0.46344
Ag	-1.23501	0.84158	-1.42346
Au	-1.5407	-4.55379	-0.59807
Au	-1.07559	-1.93806	-2.35025
Au	1.24172	-0.31586	-2.48105
Au	1.26381	-2.43212	2.42409
Au	-4.16993	-0.72505	-1.5172
Au	3.98935	-0.52326	-1.10128
Au	-2.8886	1.14025	0.96564
Au	-0.60754	2.66742	0.85177
Au	1.38	3.08972	-1.80045
Au	-2.97496	3.78619	-0.71438
Au	-0.77353	0.55918	2.68067
Au	0.13189	-4.28359	-3.74682
Au	2.89458	-2.28016	-4.01016
Au	-2.69849	3.46791	2.81588
S	-2.22652	2.84357	-2.72618
S	-2.32669	-3.40974	1.2917
S	-3.25143	-1.77368	-3.40503
S	2.04246	-3.97626	0.82129
S	3.30027	0.9009	0.62482
S	-5.07325	0.28455	0.4075
S	2.04613	1.70304	-3.56996
S	0.75301	4.47629	-0.00146
S	0.56703	-0.97031	4.11549
S	-0.80863	-5.92639	-2.36408
S	4.88215	-1.82735	-2.84518
S	-3.72893	4.89506	1.23577
S	-1.87832	2.00813	4.46201
S	1.02946	-2.8049	-5.34343
C	-4.15652	-3.31819	1.08434
C	-3.95775	-3.48049	-3.42499
C	0.63806	-6.81495	-1.6323
C	-6.09288	1.71441	-0.16118

C	3.87951	-3.78781	0.79286
C	3.94928	0.15491	2.18351
C	-0.76331	-1.87317	5.02286
C	0.85019	2.03802	-4.93665
C	-3.74732	2.29603	-3.61661
C	1.69493	-3.91389	-6.66803
C	5.72392	-0.56026	-3.89783
C	2.25435	4.56144	1.07143
C	-2.70901	6.43511	1.27036
C	-0.38948	2.82466	5.18757
H	-4.56529	-4.32774	1.21277
H	-4.42417	-2.9157	0.09949
H	-4.54521	-2.65198	1.86455
H	-3.80903	-3.98135	-2.4614
H	-3.43306	-4.03675	-4.21205
H	-5.02591	-3.41057	-3.66285
H	1.1558	-7.33786	-2.44503
H	0.24393	-7.54033	-0.91035
H	1.31323	-6.11449	-1.12897
H	-6.95935	1.32259	-0.70724
H	-5.50652	2.38893	-0.79672
H	-6.42696	2.25306	0.73414
H	4.26246	-4.42768	-0.01208
H	4.27785	-4.12301	1.75798
H	4.16636	-2.74712	0.59452
H	5.04467	0.20045	2.16145
H	3.60576	-0.88053	2.29988
H	3.56546	0.75599	3.01765
H	-0.29205	-2.61995	5.67306
H	-1.44831	-2.36248	4.32202
H	-1.30828	-1.13614	5.62648
H	0.94802	1.22415	-5.66539
H	1.12576	2.99378	-5.39883
H	-0.17477	2.08843	-4.55333
H	-4.32557	1.58225	-3.01548
H	-3.42135	1.7998	-4.53977
H	-4.35591	3.17387	-3.86261
H	0.83888	-4.34188	-7.20388
H	2.3147	-4.71191	-6.24885
H	2.28922	-3.295	-7.35144
H	6.05253	-1.05599	-4.81904
H	6.5927	-0.18967	-3.3408
H	5.04319	0.26531	-4.13043
H	2.97698	5.22718	0.58364
H	2.69382	3.56713	1.20837

H	1.95079	4.98648	2.03622
H	-3.07629	7.09058	0.4716
H	-1.65001	6.20542	1.10982
H	-2.85708	6.91362	2.24581
H	0.21273	3.30734	4.41132
H	0.20394	2.04411	5.68099
H	-0.72224	3.56663	5.92351

N=2

88

Au	-1.27191	-1.25419	0.54514
Ag	1.05151	0.28078	0.45775
Ag	-1.23977	0.86566	-1.42716
Au	-2.94399	1.14593	0.93395
Au	-0.68469	2.6742	0.85316
Au	-0.86186	0.55577	2.67021
Au	1.10453	-2.50134	-0.86762
Au	-1.49729	-4.53248	-0.58622
Au	-1.08877	-1.92192	-2.34851
Au	1.22438	-0.3145	-2.48198
Au	1.27183	-2.39591	2.42312
Au	-4.20557	-0.7383	-1.51981
Au	4.00137	-0.53504	-1.06359
Au	1.4291	3.05652	-1.69754
Au	-3.01807	3.79451	-0.74698
Au	0.07996	-4.27825	-3.77919
Au	2.82291	-2.29629	-4.02587
Au	-2.77775	3.49012	2.80038
S	-2.21897	2.86827	-2.74701
S	-2.22224	-3.38429	1.32251
S	-3.26887	-1.78654	-3.39714
S	2.04131	-3.95074	0.82914
S	3.50976	0.91713	0.70305
S	-5.13218	0.27831	0.38924
S	2.10542	1.70779	-3.49392
S	0.77159	4.43968	0.09248
S	0.55525	-0.90594	4.07935
S	-0.82568	-5.91655	-2.36863
S	4.79879	-1.87209	-2.83457
S	-3.824	4.87817	1.19548
S	-1.91109	2.08303	4.46617

S	0.95886	-2.78882	-5.37594
C	-4.05811	-3.29808	1.1729
C	-3.95528	-3.50153	-3.40725
C	0.64169	-6.80273	-1.67571
C	-6.15323	1.69871	-0.20211
C	3.87908	-3.77478	0.78811
C	4.12913	0.07302	2.22461
C	-0.72562	-1.83066	5.03573
C	0.94881	2.12019	-4.87366
C	-3.71601	2.2869	-3.65659
C	1.61628	-3.88848	-6.71232
C	5.68205	-0.63652	-3.88982
C	2.22248	4.47818	1.23528
C	-2.85037	6.44762	1.24697
C	-0.39586	2.91845	5.11131
H	-4.46336	-4.30678	1.31759
H	-4.35736	-2.89948	0.19576
H	-4.42244	-2.62901	1.96233
H	-3.80286	-3.99396	-2.43995
H	-3.4231	-4.0571	-4.18979
H	-5.02379	-3.44482	-3.6469
H	1.13619	-7.32888	-2.5007
H	0.26868	-7.52509	-0.93966
H	1.33099	-6.10041	-1.19478
H	-7.01629	1.29866	-0.74753
H	-5.56565	2.36702	-0.84286
H	-6.49284	2.24722	0.68514
H	4.25237	-4.41986	-0.01715
H	4.27966	-4.1103	1.75217
H	4.17113	-2.73623	0.58542
H	5.2182	-0.0333	2.16043
H	3.65334	-0.90704	2.35779
H	3.86958	0.7136	3.07732
H	-0.21676	-2.54814	5.69064
H	-1.41005	-2.35602	4.3608
H	-1.27916	-1.09706	5.63579
H	1.04409	1.32995	-5.62831
H	1.25871	3.08392	-5.2958
H	-0.08341	2.18309	-4.51253
H	-4.29264	1.57068	-3.05712
H	-3.36706	1.78658	-4.56906
H	-4.33471	3.15198	-3.92189
H	0.75716	-4.30938	-7.24883
H	2.23534	-4.69176	-6.30221
H	2.20984	-3.26536	-7.3925

H	5.99306	-1.14309	-4.81123
H	6.56329	-0.29501	-3.33368
H	5.0297	0.2121	-4.1215
H	2.97735	5.13935	0.7923
H	2.63982	3.47492	1.3746
H	1.88112	4.89302	2.19178
H	-3.21703	7.08996	0.4374
H	-1.78147	6.24937	1.11397
H	-3.03526	6.92446	2.21694
H	0.18865	3.35778	4.29659
H	0.20491	2.15483	5.62209
H	-0.6979	3.69681	5.82239

N=3

88

Au	-0.63394	2.71789	0.81244
Ag	1.01876	0.25372	0.43598
Ag	-1.19702	0.92452	-1.47187
Au	1.24637	-0.27996	-2.5145
Au	-2.89077	1.2217	0.90158
Au	-1.07867	-1.85232	-2.42475
Ag	-1.38497	-1.28197	0.48784
Au	-0.80367	0.6149	2.62889
Au	1.09155	-2.47713	-0.92926
Au	1.2215	-2.39871	2.37702
Au	-4.17248	-0.7507	-1.45424
Au	4.01389	-0.52322	-1.08173
Au	-1.51951	-4.52402	-0.52141
Au	1.46453	3.09444	-1.72451
Au	-2.99686	3.84667	-0.7817
Au	0.10582	-4.24643	-3.76303
Au	2.86116	-2.26675	-4.0565
Au	-2.76379	3.54651	2.7781
S	-2.24855	2.89915	-2.79082
S	-2.30368	-3.48153	1.42006
S	-3.29791	-1.77553	-3.37461
S	1.98762	-3.94254	0.77261
S	3.49592	0.88996	0.70452
S	-5.06693	0.27558	0.46419
S	2.13231	1.74142	-3.52011
S	0.82859	4.48908	0.06499

S	0.51287	-0.90826	4.0345
S	-0.83174	-5.85508	-2.3408
S	4.83456	-1.81928	-2.87219
S	-3.75258	4.96274	1.16127
S	-1.97986	2.09809	4.44816
S	0.99418	-2.79101	-5.38805
C	-4.14256	-3.47655	1.24632
C	-3.93915	-3.50738	-3.35628
C	0.61185	-6.7875	-1.66156
C	-6.13354	1.66097	-0.13354
C	3.82677	-3.77454	0.74602
C	4.11492	0.03003	2.21705
C	-0.81517	-1.79726	4.96054
C	0.97563	2.15841	-4.89898
C	-3.76456	2.28507	-3.64566
C	1.64902	-3.91842	-6.70226
C	5.69012	-0.5522	-3.91285
C	2.28197	4.5027	1.20594
C	-2.72051	6.49498	1.19931
C	-0.49265	2.91592	5.176
H	-4.51045	-4.50714	1.31129
H	-4.45233	-3.01976	0.29873
H	-4.54546	-2.88461	2.07786
H	-3.73183	-3.9935	-2.39568
H	-3.42818	-4.05013	-4.16147
H	-5.01821	-3.47669	-3.54874
H	1.09662	-7.31117	-2.49388
H	0.21948	-7.51345	-0.93915
H	1.31565	-6.11024	-1.16559
H	-7.00483	1.23098	-0.6418
H	-5.57936	2.32345	-0.80851
H	-6.45666	2.22493	0.75019
H	4.20273	-4.42027	-0.05751
H	4.2187	-4.11388	1.71228
H	4.12512	-2.73687	0.54713
H	5.2043	-0.07426	2.15538
H	3.6401	-0.95197	2.33883
H	3.85188	0.66106	3.07583
H	-0.33875	-2.52055	5.6333
H	-1.49161	-2.31215	4.26968
H	-1.3675	-1.04599	5.53947
H	1.07201	1.37162	-5.65706
H	1.28578	3.12399	-5.31662
H	-0.05704	2.21925	-4.53888
H	-4.31198	1.5688	-3.01979

H	-3.43712	1.7785	-4.56262
H	-4.40416	3.13753	-3.90207
H	0.78883	-4.34955	-7.22876
H	2.26797	-4.71354	-6.27643
H	2.24213	-3.30992	-7.39587
H	6.00867	-1.04004	-4.84173
H	6.56583	-0.20122	-3.35394
H	5.02039	0.28645	-4.13106
H	3.04618	5.15454	0.76526
H	2.68399	3.49283	1.34192
H	1.94701	4.91845	2.16428
H	-3.06589	7.14564	0.38705
H	-1.65998	6.25636	1.06457
H	-2.88501	6.98404	2.16689
H	0.14256	3.34777	4.39586
H	0.07026	2.14529	5.71845
H	-0.82017	3.6982	5.8712

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Au	-0.63599	2.70437	0.77221
Ag	0.98523	0.26698	0.39825
Ag	-1.1872	0.96844	-1.51523
Au	1.24073	-0.22629	-2.57118
Au	-2.88831	1.24628	0.8317
Au	-1.09915	-1.77977	-2.51757
Ag	-1.45073	-1.23753	0.39583
Ag	-0.84275	0.60316	2.69569
Au	1.05172	-2.4393	-1.01085
Au	1.23298	-2.38345	2.33447
Au	-4.19618	-0.76318	-1.44623
Au	4.01127	-0.48142	-1.07942
Au	-1.5435	-4.49611	-0.46244
Au	1.54336	3.12121	-1.65945
Au	-2.97687	3.83199	-0.87215
Au	0.08876	-4.25158	-3.71035
Au	2.86578	-2.25284	-4.04352
Au	-2.7684	3.54989	2.72432
S	-2.23524	2.90038	-2.8905
S	-2.27648	-3.40492	1.47109
S	-3.3455	-1.74921	-3.3992

S	1.94485	-3.90547	0.68283
S	3.46293	0.8803	0.73765
S	-5.06984	0.23937	0.49719
S	2.19842	1.80343	-3.48769
S	0.89608	4.48282	0.15265
S	0.59977	-0.97697	4.08658
S	-0.88921	-5.83547	-2.2848
S	4.84199	-1.73883	-2.89117
S	-3.73287	4.94244	1.06884
S	-2.0399	2.19708	4.49213
S	1.0068	-2.84107	-5.35883
C	-4.12092	-3.44754	1.36796
C	-3.93969	-3.49761	-3.37614
C	0.53129	-6.80313	-1.60677
C	-6.17716	1.60104	-0.08256
C	3.7857	-3.76943	0.63283
C	4.09397	-0.00537	2.22942
C	-0.69483	-1.92893	5.00127
C	1.08767	2.30994	-4.87428
C	-3.74973	2.24816	-3.71973
C	1.67469	-4.0053	-6.63376
C	5.63597	-0.4425	-3.94398
C	2.31375	4.45148	1.33549
C	-2.70225	6.47571	1.10792
C	-0.55054	3.05249	5.17607
H	-4.45999	-4.48196	1.49703
H	-4.4769	-3.04641	0.41214
H	-4.50659	-2.82467	2.18489
H	-3.69906	-3.98178	-2.42236
H	-3.43358	-4.0235	-4.19531
H	-5.02331	-3.49366	-3.54387
H	1.00686	-7.33339	-2.44023
H	0.12082	-7.52383	-0.88917
H	1.24771	-6.14328	-1.1049
H	-7.06146	1.15203	-0.55021
H	-5.65961	2.25841	-0.78996
H	-6.47437	2.17601	0.80317
H	4.14091	-4.40546	-0.18769
H	4.18367	-4.13374	1.5875
H	4.09925	-2.73278	0.45116
H	5.18474	-0.09111	2.16455
H	3.63337	-0.99686	2.32744
H	3.82117	0.60006	3.10338
H	-0.20474	-2.70604	5.59952
H	-1.4073	-2.38695	4.30627

H	-1.21548	-1.22189	5.65951
H	1.19205	1.56038	-5.66813
H	1.42674	3.28871	-5.23484
H	0.04618	2.37202	-4.54075
H	-4.28539	1.54292	-3.07197
H	-3.42229	1.72192	-4.62546
H	-4.40023	3.08695	-3.99332
H	0.81967	-4.4551	-7.15299
H	2.29356	-4.78505	-6.18022
H	2.27033	-3.41549	-7.3412
H	5.94728	-0.91622	-4.88253
H	6.51371	-0.06957	-3.40274
H	4.93703	0.37777	-4.14084
H	3.09774	5.10664	0.93656
H	2.70188	3.43414	1.45583
H	1.95336	4.84522	2.29396
H	-3.03562	7.11933	0.28513
H	-1.63943	6.23693	0.99237
H	-2.8821	6.97272	2.06872
H	0.13679	3.35581	4.37909
H	-0.04426	2.33822	5.83809
H	-0.86621	3.93043	5.75195

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Au	-0.60451	2.73884	0.78481
Ag	1.02201	0.34664	0.38253
Ag	-1.15669	0.94982	-1.49673
Au	1.28323	-0.15082	-2.56975
Au	-2.81837	1.2249	0.86296
Ag	-1.07349	-1.84945	-2.488
Ag	-1.33125	-1.25417	0.44973
Ag	-0.75981	0.64417	2.72493
Au	1.21168	-2.31	-0.99095
Au	1.18318	-2.42391	2.34844
Au	-4.14882	-0.79026	-1.45244
Au	3.99457	-0.53021	-1.01715
Au	-1.52145	-4.53441	-0.55092
Au	1.50182	3.18283	-1.7387
Au	-2.97647	3.80273	-0.85543
Au	0.11403	-4.28769	-3.78002

Au	2.84389	-2.25442	-3.99447
Au	-2.72951	3.55721	2.74195
S	-2.25326	2.85581	-2.87323
S	-2.2462	-3.45089	1.38684
S	-3.40706	-1.7703	-3.44491
S	1.8875	-3.93132	0.6787
S	3.50453	0.88576	0.77764
S	-4.97682	0.18587	0.52782
S	2.14065	1.8871	-3.59073
S	0.89027	4.52496	0.10089
S	0.59212	-1.01413	4.11223
S	-0.85028	-5.88038	-2.36296
S	4.82057	-1.81688	-2.81212
S	-3.73256	4.91697	1.08247
S	-1.95918	2.24159	4.52044
S	0.99294	-2.77822	-5.35232
C	-4.08969	-3.46315	1.27357
C	-4.03509	-3.50724	-3.39025
C	0.58281	-6.81802	-1.66682
C	-6.11387	1.54041	-0.00864
C	3.73435	-3.89193	0.74117
C	4.052	-0.02198	2.28856
C	-0.75299	-1.91399	5.00595
C	0.97402	2.34556	-4.94655
C	-3.77794	2.20689	-3.68533
C	1.66373	-3.85862	-6.69775
C	5.67612	-0.544	-3.84568
C	2.34861	4.50874	1.23406
C	-2.73138	6.46997	1.10161
C	-0.48202	3.13667	5.17962
H	-4.44303	-4.49565	1.37702
H	-4.43371	-3.03439	0.32507
H	-4.47103	-2.85374	2.10244
H	-3.72784	-4.01105	-2.46594
H	-3.60459	-4.03224	-4.2523
H	-5.12807	-3.49364	-3.47155
H	1.07549	-7.34412	-2.49287
H	0.17896	-7.54223	-0.94906
H	1.28128	-6.14149	-1.16201
H	-6.9996	1.08536	-0.46774
H	-5.61878	2.21585	-0.71536
H	-6.40386	2.09761	0.89072
H	4.10539	-4.50944	-0.08645
H	4.05695	-4.31813	1.69858
H	4.11033	-2.86776	0.6274

H	5.13892	-0.15926	2.25421
H	3.54291	-0.9906	2.3764
H	3.78412	0.59919	3.15289
H	-0.30329	-2.71235	5.60789
H	-1.47402	-2.34099	4.30031
H	-1.25339	-1.18813	5.65929
H	1.0768	1.59039	-5.73537
H	1.27092	3.32984	-5.32845
H	-0.05814	2.37985	-4.58139
H	-4.3064	1.50051	-3.03281
H	-3.46239	1.68111	-4.59551
H	-4.42995	3.04744	-3.94961
H	0.81007	-4.28694	-7.23682
H	2.29479	-4.65573	-6.29418
H	2.2474	-3.22075	-7.37258
H	5.99988	-1.02913	-4.77421
H	6.54849	-0.19226	-3.28205
H	5.00554	0.29354	-4.06561
H	3.11845	5.15804	0.79966
H	2.74055	3.49326	1.35734
H	2.02136	4.91619	2.19871
H	-3.08379	7.10072	0.27681
H	-1.66517	6.25089	0.97917
H	-2.91302	6.97069	2.06015
H	0.19692	3.43491	4.37354
H	0.03845	2.44547	5.85506
H	-0.81004	4.02117	5.73827

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Ag	-0.50375	2.75051	0.79977
Ag	0.97149	0.19277	0.40136
Ag	-1.14642	0.945	-1.49141
Au	1.25012	-0.192	-2.58793
Au	-2.78966	1.22862	0.83455
Ag	-1.12403	-1.84191	-2.57097
Ag	-1.42572	-1.29272	0.37716
Ag	-0.80892	0.53463	2.68935
Au	1.13059	-2.40146	-1.07579
Au	1.22706	-2.44612	2.29625
Au	-4.18617	-0.75458	-1.49221
Au	3.98646	-0.40779	-1.02404
Au	-1.57879	-4.56086	-0.511

Au	1.47469	3.22028	-1.76657
Au	-2.91978	3.81739	-0.83007
Au	0.15575	-4.34149	-3.68937
Au	2.91449	-2.25119	-3.95328
Au	-2.73657	3.47616	2.76622
S	-2.20653	2.88254	-2.85561
S	-2.33133	-3.44726	1.39788
S	-3.47202	-1.78386	-3.47135
S	1.9011	-3.95561	0.61776
S	3.38851	0.95801	0.77588
S	-5.00249	0.27832	0.46268
S	2.10026	1.85914	-3.57701
S	0.94837	4.66018	0.01692
S	0.65629	-1.04837	4.07889
S	-0.88078	-5.91752	-2.30244
S	4.87497	-1.66285	-2.80919
S	-3.64989	4.91452	1.12564
S	-2.04951	2.06044	4.49902
S	1.08601	-2.89134	-5.28775
C	-4.17353	-3.45007	1.25824
C	-4.0821	-3.5248	-3.36021
C	0.50824	-6.89129	-1.5685
C	-6.10242	1.64864	-0.10795
C	3.74624	-3.85721	0.5984
C	4.0245	0.08867	2.2761
C	-0.63929	-1.98712	5.00664
C	0.95948	2.30136	-4.95911
C	-3.73913	2.25843	-3.67371
C	1.78672	-4.02232	-6.5747
C	5.62341	-0.35281	-3.87869
C	2.47715	4.70006	1.055
C	-2.60308	6.43646	1.1897
C	-0.59029	2.89336	5.27023
H	-4.53623	-4.47797	1.37418
H	-4.50146	-3.03487	0.2983
H	-4.56143	-2.82401	2.07152
H	-3.75154	-4.00209	-2.42969
H	-3.66327	-4.06766	-4.21692
H	-5.17654	-3.52346	-3.42037
H	1.00953	-7.42893	-2.38193
H	0.06683	-7.60599	-0.8634
H	1.21	-6.23308	-1.04397
H	-6.99036	1.20753	-0.57642
H	-5.58207	2.30571	-0.81358
H	-6.39512	2.22201	0.7803

H	4.10089	-4.46674	-0.2422
H	4.12426	-4.26713	1.54258
H	4.08313	-2.82146	0.4647
H	5.11967	0.06268	2.23976
H	3.617	-0.92727	2.34944
H	3.69549	0.66719	3.14878
H	-0.15392	-2.77943	5.58851
H	-1.37316	-2.42495	4.32108
H	-1.13665	-1.27856	5.68108
H	1.07237	1.53563	-5.73617
H	1.26561	3.27976	-5.34882
H	-0.07813	2.34439	-4.61055
H	-4.26705	1.5395	-3.03407
H	-3.42931	1.75177	-4.59673
H	-4.38932	3.10652	-3.91763
H	0.9453	-4.48213	-7.10705
H	2.41879	-4.79487	-6.12731
H	2.37487	-3.40876	-7.26798
H	5.95996	-0.82967	-4.80689
H	6.48164	0.06398	-3.33816
H	4.89378	0.43538	-4.09472
H	3.2304	5.30792	0.54008
H	2.8666	3.69014	1.22468
H	2.21331	5.17305	2.0094
H	-2.94042	7.09965	0.38424
H	-1.54358	6.19196	1.05648
H	-2.7704	6.91386	2.16256
H	0.12025	3.24388	4.51402
H	-0.09829	2.15064	5.91138
H	-0.93389	3.738	5.87892

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Ag	-1.51777	-1.29673	0.39705
Ag	0.94459	0.05926	0.43052
Ag	-1.21254	0.87575	-1.43921
Ag	-2.97081	1.2136	0.86456
Ag	-0.53668	2.61344	0.82196
Ag	-0.87999	0.44484	2.69143
Au	0.93082	-2.58179	-1.02599
Au	-1.63948	-4.51274	-0.41362
Au	-1.17362	-1.85122	-2.49661
Ag	1.24624	-0.29617	-2.58437
Au	1.32661	-2.4574	2.32507

Au	-4.27885	-0.70168	-1.47264
Au	4.03352	-0.32973	-1.07896
Au	1.46212	3.15282	-1.73006
Au	-2.87536	3.82943	-0.81935
Au	0.14451	-4.32918	-3.58229
Au	3.00785	-2.27938	-3.98087
Au	-2.69959	3.50076	2.77335
S	-2.15567	2.8495	-2.81925
S	-2.41552	-3.41091	1.49966
S	-3.40091	-1.66853	-3.42978
S	2.04966	-3.93715	0.64357
S	3.33052	0.9552	0.73791
S	-5.28098	0.26559	0.42002
S	2.15902	1.84869	-3.54754
S	0.87108	4.57662	0.04851
S	0.65327	-1.09971	4.10387
S	-0.95339	-5.87896	-2.20427
S	4.94141	-1.552	-2.87421
S	-3.58643	4.95097	1.12957
S	-2.05393	2.02879	4.47246
S	1.16125	-2.99677	-5.23732
C	-4.25614	-3.4132	1.33546
C	-4.05878	-3.39553	-3.46044
C	0.39781	-6.89584	-1.45941
C	-6.30682	1.65801	-0.2349
C	3.87065	-3.68487	0.48936
C	4.04834	0.12176	2.22262
C	-0.59776	-2.12297	5.00351
C	1.0476	2.32448	-4.94425
C	-3.69308	2.29266	-3.67725
C	1.85552	-4.20972	-6.45049
C	5.60844	-0.22976	-3.9821
C	2.38562	4.66303	1.10403
C	-2.49654	6.44317	1.18184
C	-0.55238	2.78482	5.24304
H	-4.62128	-4.44118	1.44224
H	-4.57194	-2.99388	0.37345
H	-4.65483	-2.79079	2.14633
H	-3.84741	-3.91397	-2.51841
H	-3.56325	-3.91775	-4.28821
H	-5.1396	-3.3504	-3.63921
H	0.8791	-7.45833	-2.26826
H	-0.06945	-7.58769	-0.74815
H	1.12535	-6.26065	-0.94163
H	-7.12513	1.24739	-0.8376

H	-5.70477	2.35107	-0.83331
H	-6.71799	2.18877	0.63296
H	4.21718	-4.29082	-0.3572
H	4.34705	-4.02932	1.41504
H	4.10726	-2.62866	0.30193
H	5.14192	0.17449	2.17189
H	3.7146	-0.92079	2.29441
H	3.69101	0.67013	3.10363
H	-0.07936	-2.91592	5.55515
H	-1.31928	-2.56386	4.30632
H	-1.11723	-1.45918	5.70649
H	1.1956	1.59092	-5.74646
H	1.33729	3.32222	-5.29461
H	-7.62E-4	2.33295	-4.62639
H	-4.28022	1.6167	-3.04326
H	-3.38055	1.75278	-4.58023
H	-4.28617	3.17109	-3.95676
H	1.01014	-4.68182	-6.96566
H	2.46596	-4.96913	-5.95327
H	2.46332	-3.6485	-7.1707
H	5.93828	-0.70679	-4.91253
H	6.4648	0.22524	-3.47013
H	4.84292	0.52695	-4.18522
H	3.12597	5.29354	0.5975
H	2.80386	3.66483	1.27529
H	2.09838	5.12646	2.05642
H	-2.82208	7.11337	0.37734
H	-1.44581	6.16637	1.03941
H	-2.64332	6.9275	2.15456
H	0.15847	3.13137	4.48542
H	-0.07875	2.00473	5.85261
H	-0.85672	3.6223	5.8817

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Ag	-1.46767	-1.23322	0.3607
Ag	0.94725	0.19868	0.37918
Ag	-1.15873	0.9754	-1.46676
Ag	-2.92709	1.28788	0.82214
Ag	-0.53903	2.75209	0.79639
Ag	-0.83474	0.55937	2.65018
Ag	1.16471	-2.48565	-1.06774
Au	-1.52199	-4.51217	-0.50725
Ag	-1.11475	-1.79135	-2.55065

Au	1.22668	-0.19534	-2.56853
Au	1.25701	-2.50772	2.27004
Au	-4.25946	-0.75604	-1.41923
Au	3.95776	-0.45689	-1.0251
Au	1.4857	3.22134	-1.71699
Au	-2.9277	3.87337	-0.85958
Au	0.14703	-4.28222	-3.71941
Au	2.87866	-2.22686	-3.98302
Au	-2.6963	3.59119	2.73714
S	-2.23576	2.87193	-2.85788
S	-2.29727	-3.40548	1.39875
S	-3.49839	-1.77218	-3.39004
S	2.00994	-4.0777	0.69059
S	3.37246	0.91732	0.77225
S	-5.2066	0.25056	0.48496
S	2.16012	1.87214	-3.51686
S	0.93187	4.67999	0.04454
S	0.62806	-1.07508	4.00985
S	-0.84493	-5.86535	-2.30964
S	4.84367	-1.71796	-2.80904
S	-3.60774	5.01939	1.08723
S	-2.02017	2.13626	4.43946
S	1.03407	-2.80895	-5.32322
C	-4.13882	-3.47217	1.25935
C	-4.10076	-3.51628	-3.29581
C	0.55726	-6.84924	-1.61568
C	-6.29858	1.59134	-0.17156
C	3.85081	-3.90973	0.70671
C	4.0005	0.04507	2.27365
C	-0.64663	-2.02745	4.95099
C	1.0442	2.3263	-4.9158
C	-3.77203	2.22582	-3.65164
C	1.70992	-3.91598	-6.64427
C	5.6467	-0.41484	-3.84713
C	2.43375	4.68728	1.12273
C	-2.52105	6.51525	1.10521
C	-0.53488	2.92568	5.20776
H	-4.46549	-4.51285	1.36749
H	-4.48186	-3.05914	0.3037
H	-4.54705	-2.86678	2.07832
H	-3.75962	-4.00371	-2.3744
H	-3.68813	-4.0473	-4.16296
H	-5.19569	-3.51974	-3.34558
H	1.03813	-7.3793	-2.44619
H	0.12748	-7.57005	-0.90964

H	1.27197	-6.19976	-1.0983
H	-7.12715	1.13773	-0.72764
H	-5.74189	2.28079	-0.81613
H	-6.69113	2.13901	0.69442
H	4.24776	-4.58073	-0.06567
H	4.22874	-4.21411	1.6896
H	4.1567	-2.87972	0.48252
H	5.09543	0.0116	2.23721
H	3.5849	-0.96773	2.34663
H	3.67473	0.62674	3.14538
H	-0.14884	-2.82183	5.5194
H	-1.38854	-2.46441	4.27321
H	-1.13703	-1.32775	5.6398
H	1.17914	1.57284	-5.70131
H	1.34772	3.3127	-5.28675
H	-0.00131	2.35399	-4.59035
H	-4.30115	1.5311	-2.98726
H	-3.46399	1.68709	-4.55681
H	-4.41832	3.06837	-3.92334
H	0.85844	-4.3614	-7.17293
H	2.34596	-4.69957	-6.22241
H	2.28956	-3.29013	-7.33379
H	5.98229	-0.88782	-4.7777
H	6.50932	-0.0333	-3.2878
H	4.94502	0.39875	-4.06086
H	3.21158	5.28373	0.6315
H	2.80135	3.66972	1.29572
H	2.15455	5.15903	2.0734
H	-2.8523	7.16985	0.2903
H	-1.46976	6.24013	0.9647
H	-2.66486	7.0168	2.06965
H	0.18131	3.26129	4.45012
H	-0.06108	2.16511	5.8414
H	-0.85346	3.77476	5.82368

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Ag	-1.44827	-1.27268	0.38218
Ag	0.95206	0.15761	0.37945
Ag	-1.19218	0.90557	-1.44114
Ag	-2.94023	1.24155	0.85775
Ag	-0.54532	2.69839	0.80295
Ag	-0.83792	0.52608	2.67089
Ag	1.1121	-2.49209	-1.08741

Au	-1.5563	-4.52562	-0.44173
Ag	-1.16352	-1.82305	-2.52811
Ag	1.24068	-0.16378	-2.6206
Au	1.29085	-2.5053	2.25538
Au	-4.28584	-0.75905	-1.43242
Au	3.98774	-0.43753	-1.0367
Au	1.52872	3.22151	-1.72466
Au	-2.90786	3.82317	-0.86439
Au	0.13956	-4.32109	-3.63421
Au	2.90998	-2.27265	-3.96045
Au	-2.70282	3.56058	2.74106
S	-2.18162	2.82334	-2.85334
S	-2.32291	-3.40624	1.45979
S	-3.54318	-1.76672	-3.41591
S	2.06029	-4.05638	0.66592
S	3.36525	0.92251	0.75466
S	-5.22511	0.23233	0.48308
S	2.24666	1.9724	-3.57485
S	0.91832	4.62677	0.06223
S	0.64942	-1.09936	4.01339
S	-0.87763	-5.89405	-2.2312
S	4.87327	-1.69088	-2.82301
S	-3.61592	4.96883	1.0736
S	-2.01518	2.12399	4.45585
S	1.03952	-2.86938	-5.25017
C	-4.16457	-3.4334	1.31019
C	-4.16271	-3.50598	-3.3265
C	0.5082	-6.88733	-1.51796
C	-6.29915	1.59438	-0.15886
C	3.89774	-3.86319	0.66776
C	4.00783	0.061	2.25683
C	-0.61102	-2.07948	4.94537
C	1.14314	2.50546	-4.95789
C	-3.70906	2.205	-3.6861
C	1.68946	-3.98372	-6.57829
C	5.62378	-0.38059	-3.89203
C	2.40514	4.66294	1.15958
C	-2.54186	6.47365	1.09269
C	-0.52511	2.92387	5.20364
H	-4.51511	-4.4655	1.42572
H	-4.49262	-3.02152	0.3488
H	-4.56365	-2.81129	2.12114
H	-3.82358	-4.00138	-2.40905
H	-3.75978	-4.03728	-4.19803
H	-5.25785	-3.49927	-3.37134

H	0.9876	-7.43178	-2.34002
H	0.06476	-7.59559	-0.80764
H	1.22789	-6.24134	-1.00292
H	-7.13194	1.15778	-0.72219
H	-5.73231	2.28454	-0.79382
H	-6.6868	2.13635	0.71289
H	4.29788	-4.5301	-0.10654
H	4.2882	-4.16024	1.64799
H	4.18724	-2.82922	0.43923
H	5.10328	0.04845	2.22237
H	3.61077	-0.95935	2.32919
H	3.66953	0.63681	3.12775
H	-0.1028	-2.87825	5.49819
H	-1.35249	-2.51198	4.26398
H	-1.10386	-1.39549	5.64807
H	1.3014	1.8099	-5.79151
H	1.42868	3.51924	-5.26237
H	0.0918	2.49306	-4.64984
H	-4.27363	1.52936	-3.03164
H	-3.38862	1.65151	-4.57793
H	-4.32682	3.0607	-3.98216
H	0.8266	-4.42192	-7.09428
H	2.32319	-4.77248	-6.16276
H	2.26526	-3.364	-7.27641
H	5.95047	-0.85599	-4.82448
H	6.48946	0.02409	-3.35413
H	4.89966	0.41544	-4.09703
H	3.17489	5.28029	0.68152
H	2.79423	3.65315	1.33047
H	2.10376	5.12204	2.10969
H	-2.87224	7.12209	0.2725
H	-1.48747	6.20606	0.96081
H	-2.69654	6.97818	2.05391
H	0.18819	3.24517	4.43699
H	-0.04975	2.17345	5.84819
H	-0.83888	3.784	5.8066

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Ag	-1.44406	-1.28652	0.39065
Ag	0.94334	0.16206	0.37632
Ag	-1.21324	0.88732	-1.43407
Ag	-2.95096	1.2311	0.86012
Ag	-0.56147	2.70574	0.80293

Ag	-0.84663	0.52697	2.67085
Ag	1.12302	-2.47802	-1.09748
Au	-1.57445	-4.5343	-0.41614
Ag	-1.15821	-1.82516	-2.53073
Ag	1.23768	-0.14349	-2.63264
Au	1.30997	-2.47545	2.2469
Au	-4.27762	-0.74235	-1.467
Au	3.98352	-0.4413	-1.06939
Ag	1.51466	3.17935	-1.67457
Au	-2.90927	3.82616	-0.85921
Au	0.11425	-4.34589	-3.61275
Au	2.88316	-2.30178	-3.95605
Au	-2.74247	3.54243	2.74228
S	-2.12914	2.84495	-2.83696
S	-2.33968	-3.40198	1.47809
S	-3.52719	-1.76017	-3.44238
S	2.06627	-4.03729	0.66235
S	3.3559	0.95488	0.69169
S	-5.23695	0.24302	0.44139
S	2.28751	1.93512	-3.62303
S	0.88444	4.66502	0.16877
S	0.67883	-1.06739	4.00663
S	-0.89543	-5.91226	-2.19737
S	4.86078	-1.71572	-2.84389
S	-3.64794	4.95702	1.07547
S	-2.04616	2.10572	4.45384
S	1.00709	-2.90008	-5.23719
C	-4.18069	-3.40725	1.31771
C	-4.15476	-3.49634	-3.34472
C	0.4952	-6.89628	-1.48043
C	-6.29064	1.61815	-0.20601
C	3.90485	-3.85543	0.65946
C	4.01898	0.15035	2.21651
C	-0.56054	-2.0585	4.95571
C	1.15614	2.46485	-4.98622
C	-3.6267	2.24463	-3.73514
C	1.64958	-4.02067	-6.56385
C	5.59192	-0.41248	-3.9351
C	2.33952	4.63199	1.30912
C	-2.57202	6.46031	1.11615
C	-0.56225	2.91884	5.20028
H	-4.5443	-4.43435	1.43711
H	-4.49816	-2.99765	0.35192
H	-4.57692	-2.77574	2.12273
H	-3.8206	-3.98779	-2.42335

H	-3.75081	-4.034	-4.21187
H	-5.24967	-3.48556	-3.39332
H	0.97327	-7.44602	-2.29975
H	0.05596	-7.60006	-0.7631
H	1.21506	-6.24436	-0.97321
H	-7.11735	1.19232	-0.78628
H	-5.70837	2.30929	-0.82591
H	-6.68815	2.15583	0.66394
H	4.29892	-4.52619	-0.11464
H	4.29594	-4.1529	1.6393
H	4.19993	-2.82369	0.42813
H	5.11429	0.16062	2.17848
H	3.64432	-0.87571	2.31646
H	3.67008	0.74299	3.07169
H	-0.03768	-2.85089	5.50399
H	-1.30603	-2.49972	4.28437
H	-1.05189	-1.37793	5.66277
H	1.25123	1.74544	-5.80866
H	1.46978	3.45779	-5.33059
H	0.11533	2.50694	-4.64574
H	-4.21797	1.56449	-3.10997
H	-3.27496	1.70149	-4.62141
H	-4.22837	3.10772	-4.04248
H	0.784	-4.45946	-7.07476
H	2.28393	-4.80875	-6.14796
H	2.22346	-3.40429	-7.26653
H	5.91353	-0.89748	-4.86442
H	6.45959	0.00514	-3.4104
H	4.85799	0.37445	-4.14296
H	3.11151	5.29558	0.90076
H	2.74465	3.61852	1.40842
H	2.01884	5.00788	2.28862
H	-2.88744	7.11117	0.29194
H	-1.51554	6.19004	1.00299
H	-2.74358	6.96258	2.07576
H	0.14382	3.25275	4.43226
H	-0.07526	2.17104	5.83917
H	-0.88397	3.77223	5.80861