Supporting Information

Charge state enhanced propene binding to yttrium-doped gold clusters

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Supporting information contains:

- Method test – Table S1, Table S2
- Optimized structures of neutral clusters and complexes – Figure S1
- Optimized structures of the isomers of cationic clusters and complexes with E_{rel}<0.1 eV – Figure S2
- Proposed growth paths of the lowest energy $Au_{n-1}Y^+$ clusters – Figure S3
- LUMO orbitals of Au_n^+ and $Au_{n-1}Y^+$ (n = 415) – Figures S4 and S5
- Dissociation of propene on the cluster – Figure S6
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- Total electron density transfer – Table S7
- XYZ coordinates and total energies of the optimized clusters and cluster-propene complexes

Table S1: Adsorption energies of propene on Au_4^+, Au_5^+, Au_6^+, Au_3Y^+, Au_4Y^+, Au_5Y^+ (E, eV) calculated using the CCSD(T)/def2-TZVP, TPSSh/def2-TZVP+XDM, CAM-B3LYP/def2-TZVP+XDM, LRC-ωPBE/def2-TZVP+XDM, PBE0/CRENBL, PBE0/CRENBL+XDM and PBE0/CRENBL(SO) methods and the deviation of the adsorption energies from the Au_5^+ adsorption energy (ΔE_1, kJ/mol, to show the accuracy for the size dependence and doping trends) and from the CCSD(T)/def2-TZVP benchmarks (ΔE_2, kJ/mol), respectively. The values are given in eV. Relative to the CCSD(T) benchmark, the LRC-ωPBE method gives the most accurate energies. Using this method, the largest deviation from the) benchmarks is 0.12 eV. This value is used to estimate error bars for the calculated relative adsorption energies. For the neutral case, 0.09 eV was used to estimate error bars, based on the same calculation method.

	CCSD(T)/ def2-TZVP		**TPSSh+XDM/ def2-TZVP**			**CAM-B3LYP+ XDM/ def2-TZVP**			**LRC-ωPBE+ XDM/ def2-TZVP**			**PBE0/ CRENBL**			**PBE0+XDM/ CRENBL**			**PBE0/ CRENBL (SO)[(a)]**		
	E	ΔE_1	E	ΔE_1	ΔE_2	E	ΔE_1	ΔE_2	E	ΔE_1	ΔE_2	E	ΔE_1	ΔE_2	E	ΔE_1	ΔE_2	E	ΔE_1	ΔE_2
Au_4^+	2.01	0.15	1.85	-0.16	0.04	1.69	-0.32	0.22	1.87	-0.14	0.19	1.62	-0.39	-0.08	1.78	-0.23	-0.05	1.60	-0.41	-0.05
Au_5^+	1.86	0.00	1.81	-0.05	0.00	1.48	-0.38	0.00	1.68	-0.18	0.00	1.55	-0.31	0.00	1.73	-0.13	0.00	1.55	-0.31	0.00
Au_6^+	1.83	-0.03	1.68	-0.15	-0.13	1.55	-0.28	0.07	1.68	-0.15	0.00	1.51	-0.32	0.04	1.65	-0.18	0.08	1.50	-0.33	0.05
Au_3Y^+	1.28	-0.58	1.15	-0.13	-0.66	1.15	-0.13	-0.32	1.15	-0.13	-0.53	1.06	-0.22	0.49	1.20	-0.08	0.54	1.10	-0.18	0.45
Au_4Y^+	1.60	-0.26	1.23	-0.37	-0.58	1.27	-0.33	0.21	1.31	-0.29	-0.38	1.04	-0.56	0.51	1.20	-0.40	0.54	0.92	-0.68	0.63
Au_5Y^+	1.29	-0.57	1.22	-0.07	-0.59	1.01	-0.28	-0.47	1.18	-0.11	-0.50	0.98	-0.31	0.57	1.14	-0.15	0.59	1.01	-0.28	0.54

(a) The PBE0(SO) computations were carried out using the NWChem program.[i]

Table S2: Propene adsorption energies on cationic gold and yttrium-doped gold clusters using the LRC-ωPBE/def2-TZVP+XDM method.

n	***LRC-ωPBE/def2-TZVP+XDM***	
	Au_n^+	Au_{n-1Y}^+
4	1.90	1.18
5	1.73	1.33
6	1.72	1.2
7	1.99	1.34
8	1.55	1.42
9	1.35	1.35
10	1.53	1.45
11	1.39	1.27
12	1.35	1.28
13	1.30	1.30
14	1.42	1.23
15	1.49	1.54

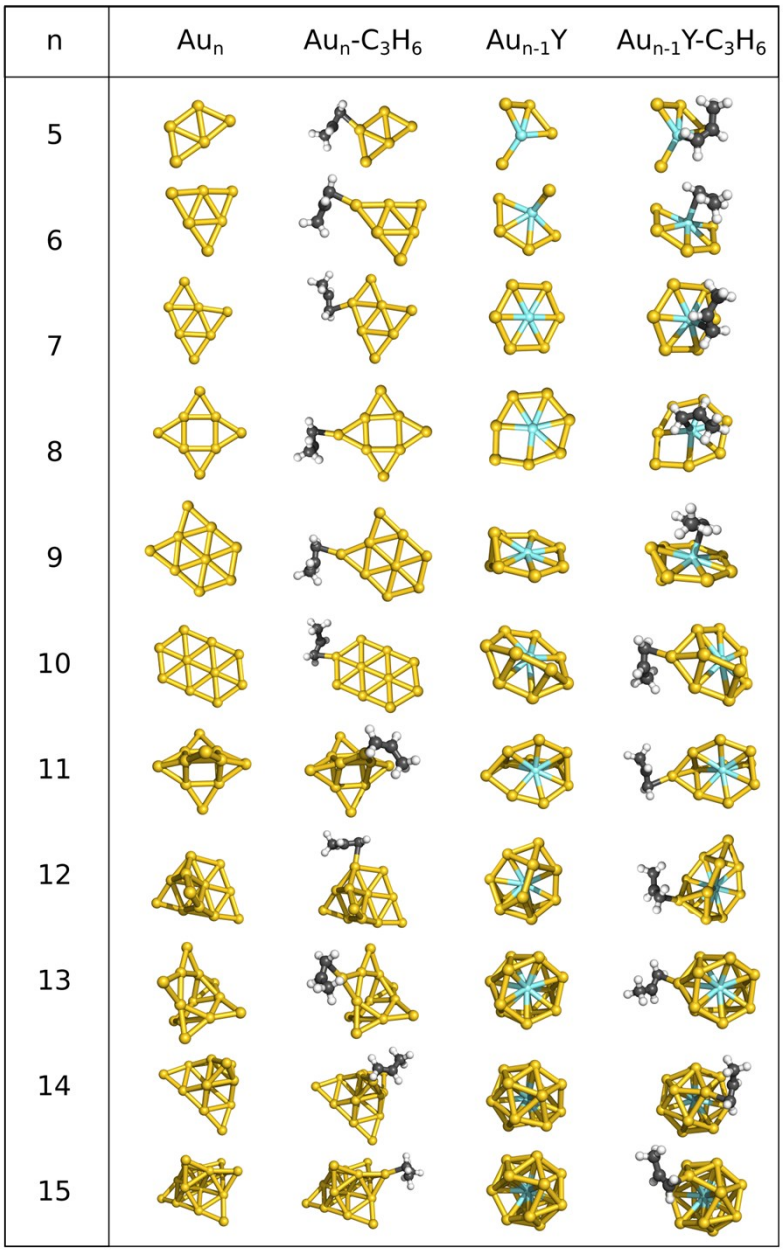

Figure S1: Optimized structures of the lowest energy neutral Au_n and $Au_{n-1}Y$ (n = 5-15) clusters and the corresponding Au_n-C_3H_6 and $Au_{n-1}Y$-C_3H_6 complexes, calculated using the BP86/LANL2DZ method. Au, yellow; Y, blue; C, grey; H, white

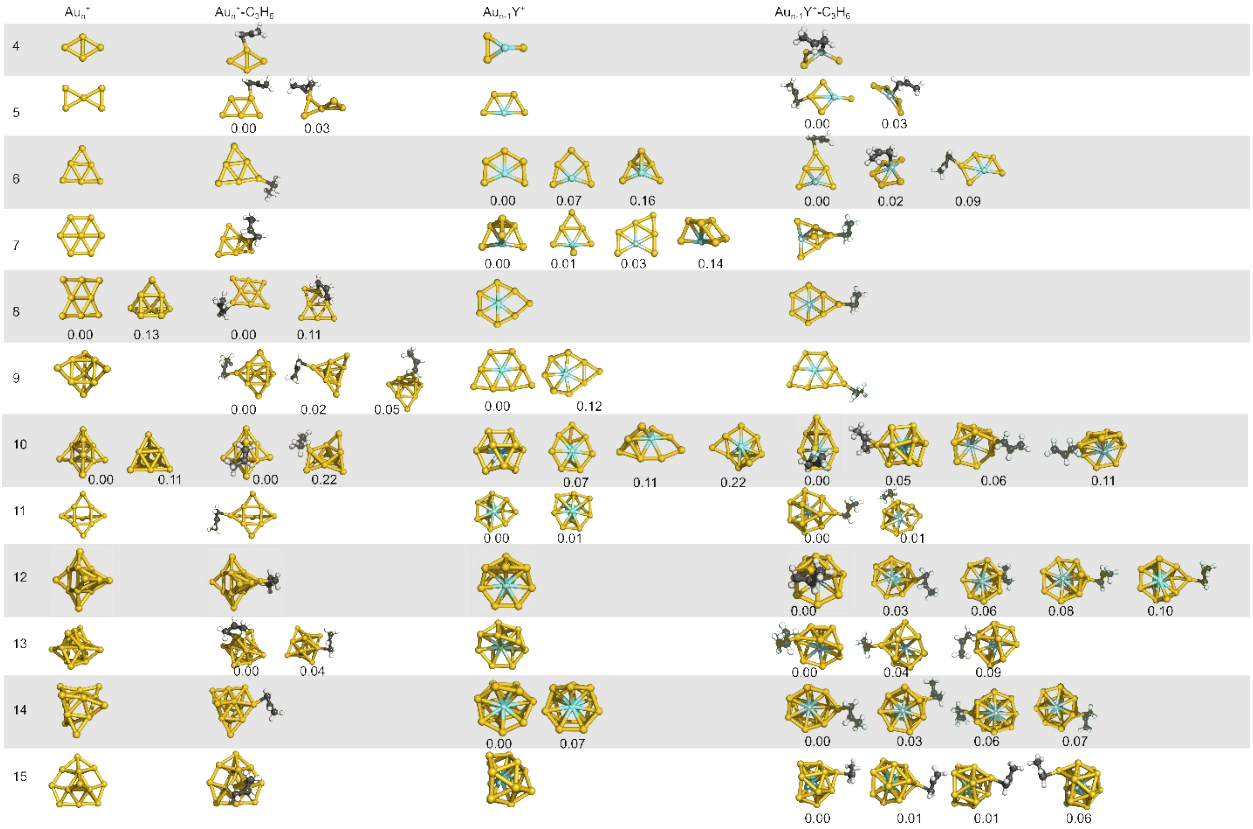

Figure S2: Optimized structures of the lowest energy cationic Au_n^+ and $Au_{n-1}Y^+$ (n = 5-15) clusters and the corresponding Au_n^+-C_3H_6 and $Au_{n-1}Y^+$-C_3H_6 complexes. The relative energies are given in eV. (Method: LRC-ωPBE/def2-TZVP+XDM)

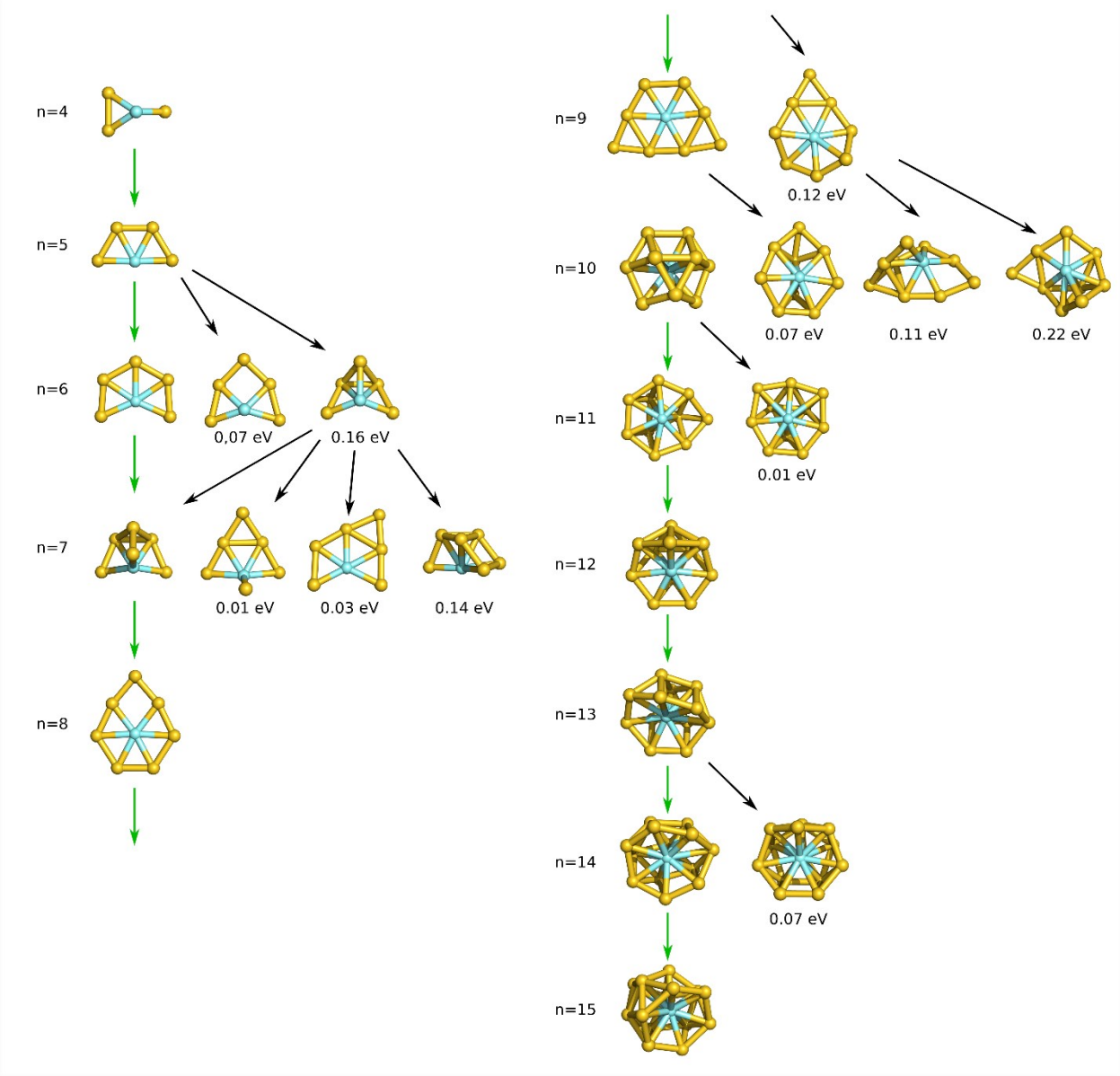

Figure S3: Optimized structures and proposed growth paths of the lowest energy $Au_{n-1}Y^+$ clusters. The most stable Au_9Y^+ cluster was found by using the CALYPSO program. (Method: LRC-ωPBE/def2-TZVP+XDM)

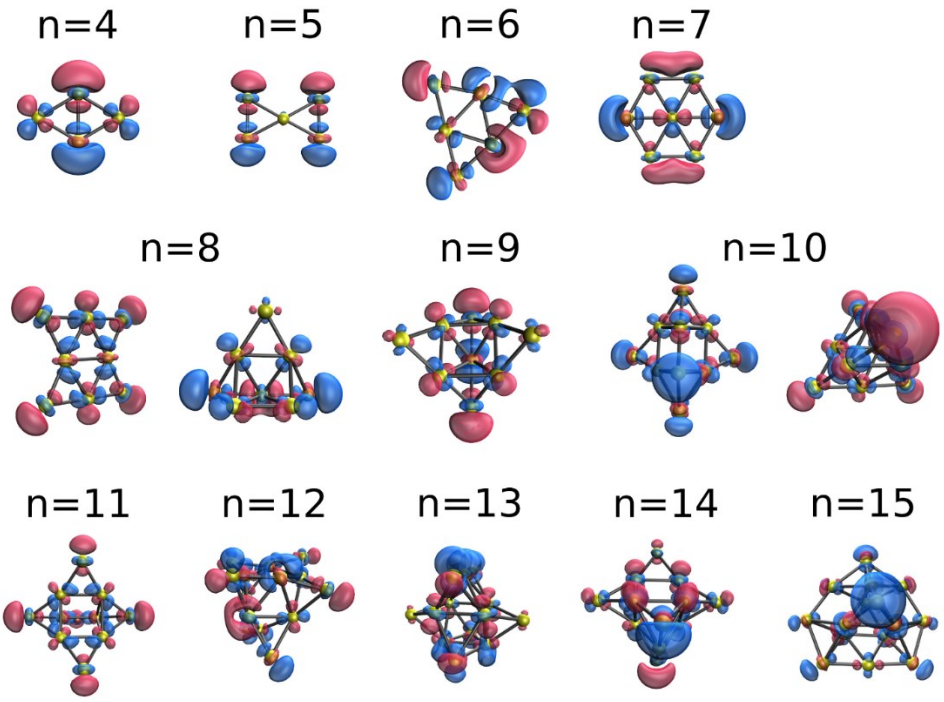

Figure S4:LUMOs of Au_n^+ clusters.

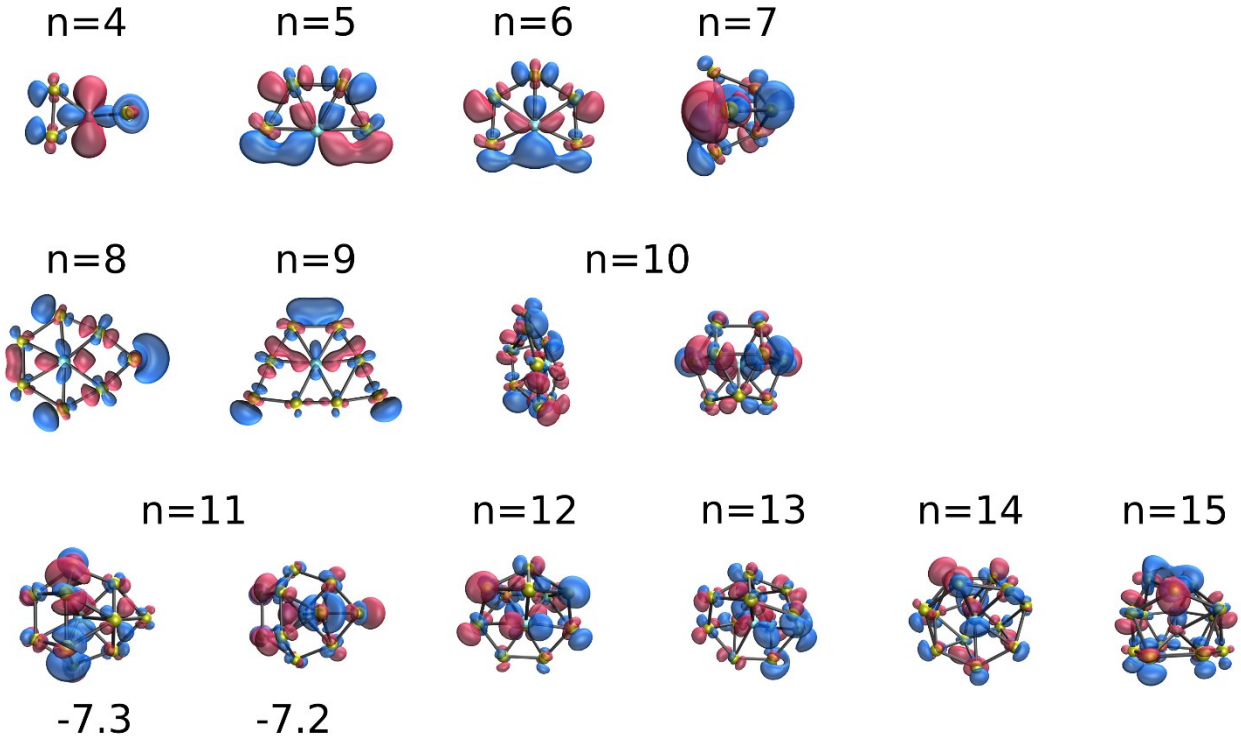

Figure S5: LUMOs of $Au_{n-1}Y^+$. The energies of the orbitals are given in eV. For n=11, LUMO and LUMO+1 are quasi-degenerate.

Dissociation of propene on gold and yttrium-doped gold clusters

To test whether the gold and yttrium-doped gold clusters are able to dissociate propene after the adsorption we remove the different hydrogens from the propene and put on the cluster in the case of Au_6, Au_5Y and Au_6Y clusters. We found that after the geometry optimization the energies of these geometries are larger in every case than that of the undissociated cases.

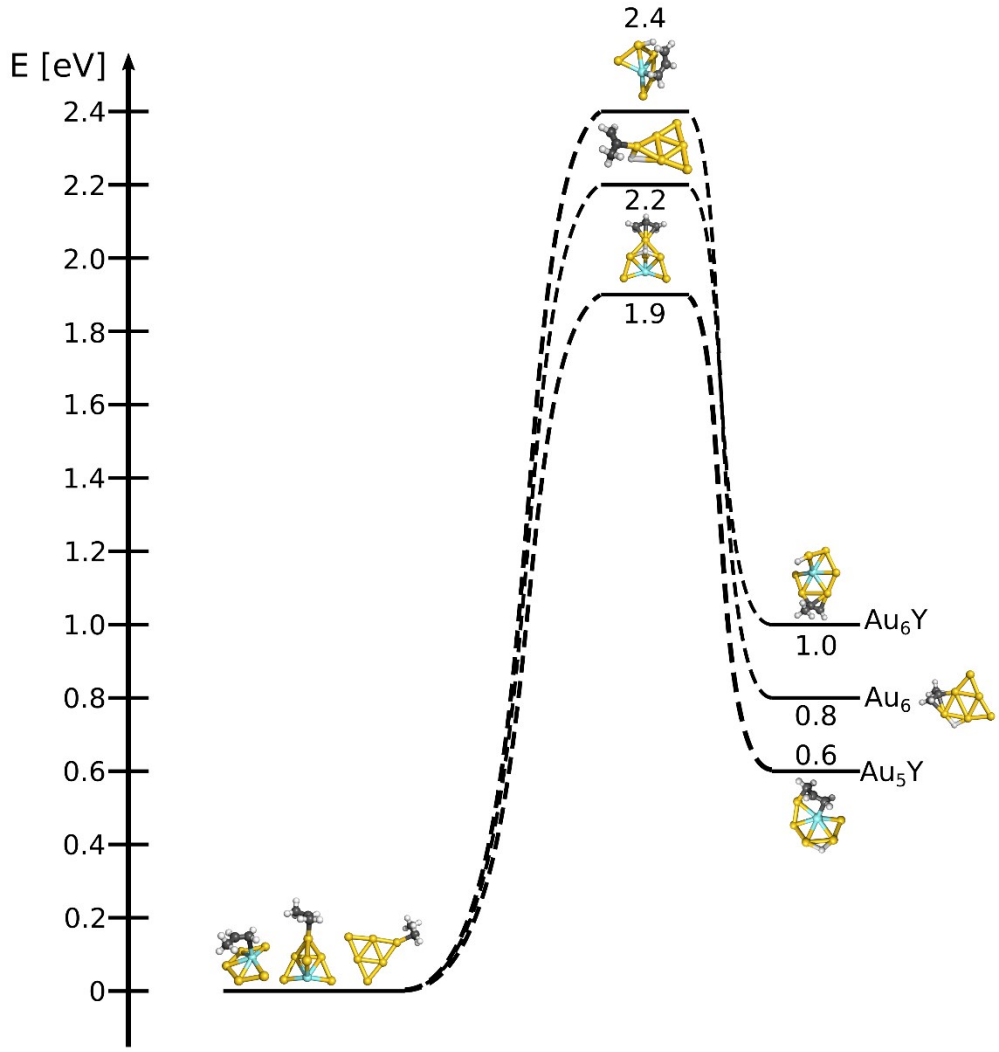

Figure S6: Intact and dissociated propene adduct of Au_5Y^+, Au_6Y^+ and Au_6^+ clusters (Method: LRC-ωPBE/def2-TZVP+XDM)

Table S3: Natural charges of the atoms in the neutral and cationic Au_n clusters. The atoms where the propene is bound are marked with bold.

n	***Au_n^+***	***Au_n***
4		
Au	**0.31**	**-**
Au	0.19	-
Au	0.31	-
Au	0.19	-
5		
Au	0.24	0.11
Au	**0.25**	**0.02**
Au	**0.02**	0.02
Au	0.25	-0.08
Au	0.24	-0.08
6		
Au	**0.09**	0.09
Au	0.25	0.09
Au	0.21	0.09
Au	0.20	-0.09
Au	0.17	-0.09
Au	0.09	**-0.09**
7		
Au	0.15	0.01
Au	0.15	0.09
Au	0.15	0.08
Au	0.15	**0.03**
Au	0.15	-0.05
Au	**0.09**	-0.08
Au	0.15	-0.06
8		
Au	0.12	0.06
Au	0.11	0.06
Au	**0.17**	0.06
Au	0.14	0.06
Au	0.11	**-0.06**
Au	0.10	-0.06
Au	0.11	-0.06
Au	0.14	-0.06
8_2		
Au	0.18	-
Au	0.06	-

Au	0.17	-
Au	0.09	-
Au	**0.18**	-
Au	0.06	-
Au	0.09	-
Au	0.17	-
9		
Au	0.10	0.08
Au	**0.14**	0.05
Au	**0.10**	-0.06
Au	0.14	0.00
Au	0.10	-0.06
Au	0.14	0.05
Au	0.09	0.09
Au	0.09	-0.07
Au	0.09	**-0.07**
10		
Au	0.09	-0.05
Au	0.12	-0.03
Au	0.09	0.12
Au	0.08	-0.05
Au	0.12	0.01
Au	0.15	0.01
Au	0.08	0.12
Au	**0.09**	-0.05
Au	0.07	-0.05
Au	0.04	**-0.03**
10_2		
Au	0.06	
Au	**0.13**	
Au	0.07	
Au	0.12	
Au	0.06	
Au	0.13	
Au	0.12	
Au	0.13	
Au	0.12	
Au	0.06	
11		
Au	0.10	0.09
Au	0.10	0.09

Au	0.10	0.09
Au	0.10	0.09
Au	0.10	0.09
Au	**0.10**	0.09
Au	0.09	-0.11
Au	0.09	-0.11
Au	0.08	-0.11
Au	0.08	-0.11
Au	0.08	**-0.11**
12		
Au	-0.02	0.05
Au	-0.02	0.08
Au	0.1	0.08
Au	0.12	0.08
Au	0.12	0.08
Au	0.10	0.03
Au	0.12	**0.04**
Au	0.12	-0.13
Au	0.01	-0.13
Au	0.10	0.08
Au	**0.10**	-0.11
Au	0.14	-0.16
13		
Au	-0.05	0.04
Au	0.17	0.07
Au	-0.05	0.07
Au	0.17	0.02
Au	**0.14**	**-0.06**
Au	-0.01	0.03
Au	0.14	-0.05
Au	0.14	0.07
Au	-0.01	0.07
Au	0.14	-0.08
Au	0.03	**-0.08**
Au	**0.18**	**-0.05**
Au	0.03	-0.06
14		
Au	0.04	0.12
Au	0.00	0.12
Au	**0.18**	0.04
Au	0.11	0.11

Au	0.18	0.04
Au	0.09	0.04
Au	0.05	0.04
Au	0.09	0.04
Au	0.03	0.04
Au	0.04	**-0.08**
Au	0.05	0.07
Au	0.05	-0.19
Au	0.04	-0.19
Au	0.05	-0.19
15		
Au	0.00	0.13
Au	0.03	0.10
Au	0.10	0.07
Au	0.00	0.10
Au	0.00	0.07
Au	0.10	0.03
Au	0.14	0.03
Au	**0.19**	0.07
Au	0.14	0.07
Au	0.01	**-0.07**
Au	0.03	-0.05
Au	0.00	-0.15
Au	0.11	-0.15
Au	0.14	-0.18
Au	0.01	**-0.08**

Table S4: Natural charges of the atoms in the neutral and cationic yttrium-doped clusters. The atoms where the propene is bound are marked with bold.

n	$Au_{n-1}Y^+$	$Au_{n-1}Y$
4		
Y	**1.46**	**-**
Au	-0.08	-
Au	-0.08	-
Au	-0.31	-
5		
Y	**1.37**	**1.27**
Au	0.02	-0.34
Au	**0.02**	-0.13
Au	-0.21	-0.34
Au	-0.21	-0.46

6		
Y	**1.13**	**1.16**
Au	**0.10**	-0.30
Au	0.10	-0.06
Au	-0.12	-0.06
Au	-0.12	-0.30
Au	-0.09	-0.44
7		
Y	1.03	**0.51**
Au	**0.14**	-0.14
Au	0.14	**0.02**
Au	-0.15	-0.14
Au	-0.15	-0.14
Au	0.14	0.18
Au	0.15	-0.14
8		
Y	0.65	**0.51**
Au	0.06	-0.12
Au	0.02	-0.12
Au	0.05	-0.03
Au	0.02	-0.03
Au	0.06	-0.08
Au	**0.09**	-0.08
Au	0.05	-0.05
9		
Y	0.65	**0.04**
Au	**0.09**	-0.05
Au	0.02	-0.05
Au	0.02	-0.03
Au	0.09	-0.04
Au	0.06	0.03
Au	0.01	0.03
Au	0.01	**0.03**
Au	0.06	**0.03**
10		
Y	0.03	-0.10
Au	**0.07**	-0.05
Au	0.15	0.00
Au	0.05	-0.05
Au	0.12	**0.02**
Au	**0.16**	0.02
Au	0.11	0.04
Au	0.07	0.04

Au	0.07	0.04
Au	**0.16**	0.04
10_2		
Y	-0.23	
Au	**0.19**	
Au	0.09	
Au	0.09	
Au	0.19	
Au	0.05	
Au	0.18	
Au	0.05	
Au	0.22	
Au	0.22	
11		
Y	-0.38	-0.29
Au	0.04	0.02
Au	0.24	0.02
Au	0.06	0.11
Au	0.17	0.00
Au	0.24	0.01
Au	**0.16**	0.14
Au	0.06	0.00
Au	0.16	0.00
Au	0.04	-0.06
Au	**0.21**	**0.03**
12		
Y	-1.06	-1.11
Au	**0.14**	0.10
Au	0.26	**0.15**
Au	0.15	**0.12**
Au	0.20	0.10
Au	0.24	**0.15**
Au	0.20	0.12
Au	0.12	0.06
Au	0.15	0.06
Au	0.12	0.02
Au	**0.24**	0.06
Au	**0.24**	0.17
13		
Y	-1.50	-1.98
Au	0.19	0.13
Au	0.27	0.19
Au	0.16	0.18

Au	0.18	0.13
Au	0.21	**0.19**
Au	0.15	0.18
Au	0.27	0.15
Au	**0.16**	0.15
Au	0.16	0.20
Au	0.29	0.15
Au	**0.27**	0.20
Au	0.19	0.15
14		
Y	-2.08	-2.48
Au	0.21	0.27
Au	0.30	0.15
Au	0.16	0.25
Au	**0.25**	0.15
Au	0.25	**0.29**
Au	0.16	0.24
Au	0.25	0.29
Au	**0.24**	0.13
Au	0.24	0.13
Au	**0.30**	0.16
Au	0.25	0.16
Au	0.21	0.13
Au	**0.27**	0.13
15		
Y	-2.66	-3.67
Au	**0.25**	0.23
Au	0.23	0.23
Au	0.32	0.28
Au	0.33	**0.28**
Au	0.34	0.28
Au	0.28	0.28
Au	0.31	0.28
Au	0.27	0.28
Au	**0.20**	0.26
Au	0.21	0.28
Au	0.27	0.26
Au	0.20	0.28
Au	**0.19**	0.23
Au	**0.24**	0.23

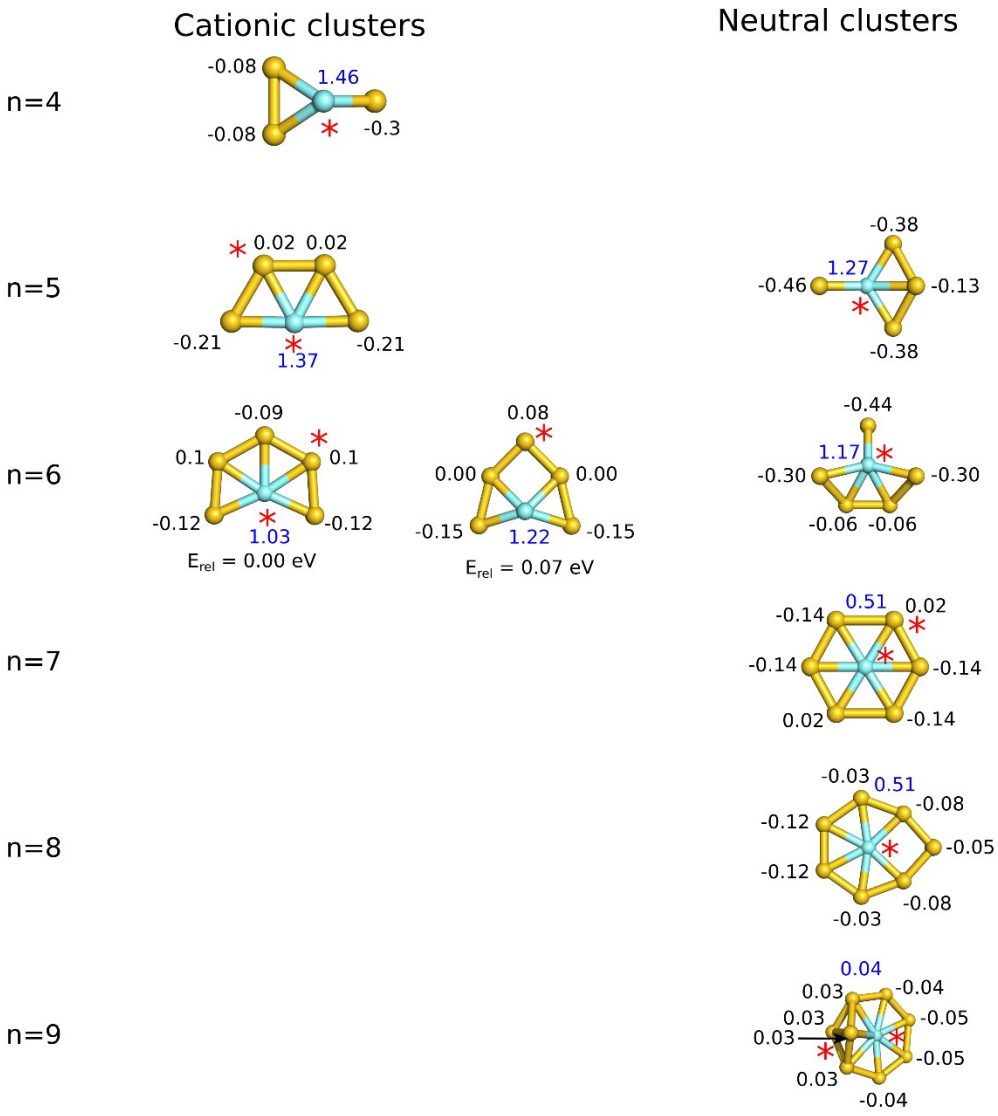

Figure S7: Natural charges of the atoms in the small neutral and cationic yttrium-doped clusters where the propene prefers to bind also to the yttrium atom. The atom where the propene is preferentially bound is marked with red star. The charge of the yttrium atom is colored with blue. For the cationic Au_5Y^+ in the case of the most stable isomer structural reorganization takes place. The original geometry of the most stable cluster is marked with a) and the reorganized cluster is marked with b).

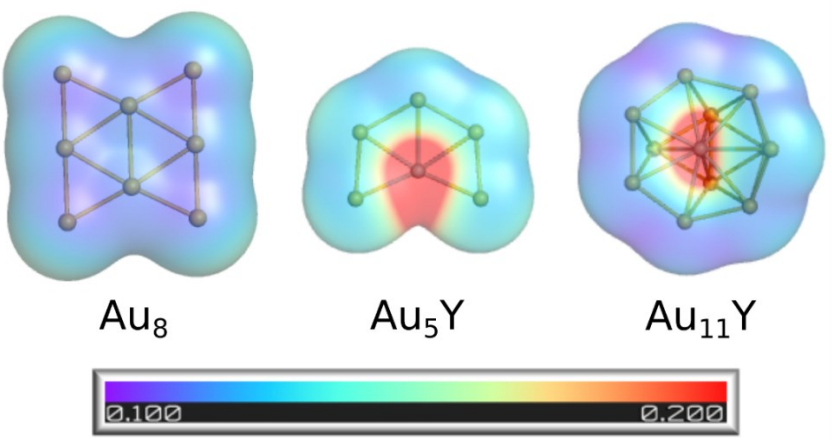

Figure S8: Electrostatic potential of the selected cationic Au_8, Au_5Y and $Au_{11}Y$ clusters.

Table S5: Natural charges of the atoms in the cationic cluster-propene complexes. The atoms where the propene is bound are marked with bold.

n	***Au_n^+-C_3H_6***		***$Au_{n-1}Y^+$-C_3H_6***	
4	isomer		isomer	isomer
Au/Y	0.20	**1.43**		
Au	0.17	-0.10		
Au	**0.36**	-0.08		
Au	0.16	-0.35		
C	-0.51	-0.67		
C	-0.16	-0.02		
C	-0.64	-0.65		
H	0.24	0.23		
H	0.24	0.25		
H	0.23	0.22		
H	0.22	0.27		
H	0.23	0.25		
H	0.25	0.22		
5				
Au/Y	0.16	1.47	**1.24**	
Au	0.19	**0.40**	0.01	
Au	**0.36**	-0.27	0.02	
Au	0.03	-0.29	-0.21	
Au	0.14	-0.36	-0.19	
C	-0.52	-0.51	-0.67	
C	-0.15	-0.19	0.00	

C	-0.64		-0.63	-0.65	
H	0.24		0.23	0.24	
H	0.23		0.24	0.25	
H	0.23		0.23	0.23	
H	0.24		0.23	0.25	
H	0.25		0.22	0.22	
H	0.22		0.24	0.26	
6					
Au/Y	0.23		1.23	**0.97**	1.22
Au	0.09		-0.21	0.09	-0.08
Au	0.09		-0.08	0.10	-0.07
Au	**0.28**		**0.27**	-0.11	-0.21
Au	0.06		-0.07	-0.11	-0.22
Au	0.06		-0.22	-0.06	**0.26**
C	-0.48		-0.51	-0.65	-0.50
C	-0.12		-0.16	-0.02	-0.16
C	-0.64		-0.64	-0.65	-0.64
H	0.24		0.23	0.25	0.23
H	0.24		0.24	0.24	0.24
H	0.23		0.22	0.22	0.23
H	0.22		0.23	0.26	0.24
H	0.25		0.24	0.22	0.23
H	0.24		0.22	0.25	0.22
7					
Au/Y	0.09		1.13		
Au	0.09		0.09		
Au	0.10		0.10		
Au	0.04		-0.33		
Au	0.11		-0.19		
Au	0.05		**0.32**		
Au	**0.40**		-0.18		
C	-0.50		-0.52		
C	-0.16		-0.16		
C	-0.64		-0.64		
H	0.24		0.23		
H	0.24		0.24		
H	0.23		0.23		
H	0.25		0.25		
H	0.23		0.22		
H	0.22		0.23		
8					
Au/Y	0.13	**0.30**	0.73		
Au	0.07	0.00	**0.25**		
Au	**0.41**	0.09	0.01		
Au	-0.01	0.10	-0.07		

Au	0.04	0.13	0.02	
Au	0.07	0.08	-0.07	
Au	0.03	0.07	0.01	
Au	0.17	0.11	0.01	
C	-0.51	-0.48	-0.49	
C	-0.18	-0.15	-0.15	
C	-0.64	-0.64	-0.64	
H	0.23	0.23	0.24	
H	0.24	0.24	0.23	
H	0.23	0.23	0.23	
H	0.22	0.25	0.23	
H	0.25	0.23	0.22	
H	0.23	0.22	0.25	
9				
Au/Y	0.11		0.59	
Au	0.03		-0.01	
Au	0.12		0.01	
Au	**0.20**		**0.26**	
Au	0.06		0.06	
Au	0.12		0.03	
Au	0.10		-0.06	
Au	0.03		-0.02	
Au	0.15		0.02	
C	-0.51		-0.49	
C	-0.14		-0.15	
C	-0.64		-0.64	
H	0.24		0.24	
H	0.23		0.23	
H	0.22		0.23	
H	0.22		0.23	
H	0.23		0.22	
H	0.25		0.25	
10				
Au/Y	0.04	-0.04	0.30	-0.18
Au	0.09	**0.32**	0.03	-0.03
Au	0.04	-0.01	0.08	**0.37**
Au	0.14	0.16	0.12	0.02
Au	0.03	0.06	0.04	0.08
Au	0.09	-0.01	**0.18**	0.15
Au	0.04	0.10	0.00	0.03
Au	**0.30**	0.14	-0.01	0.18
Au	0.13	0.13	0.02	0.18
Au	0.04	0.08	0.12	0.13
C	-0.52	-0.52	-0.48	-0.50
C	-0.17	-0.17	-0.15	-0.18

C	-0.64	-0.64	-0.64	-0.63
H	0.24	0.24	0.23	0.23
H	0.23	0.23	0.23	0.23
H	0.23	0.23	0.22	0.22
H	0.23	0.23	0.23	0.24
H	0.25	0.25	0.25	0.23
H	0.22	0.22	0.22	0.22
11				
Au/Y	0.11		-0.41	
Au	0.10		0.06	
Au	0.10		0.19	
Au	0.09		0.01	
Au	0.09		0.07	
Au	0.08		0.20	
Au	**0.21**		0.13	
Au	0.09		0.12	
Au	0.01		**0.34**	
Au	0.01		0.01	
Au	0.01		0.20	
C	-0.51		-0.49	
C	-0.15		-0.17	
C	-0.64		-0.64	
H	0.24		0.23	
H	0.23		0.23	
H	0.22		0.22	
H	0.25		0.23	
H	0.22		0.24	
H	0.23		0.22	
12				
Au/Y	-0.04		-0.89	
Au	-0.05		0.19	
Au	0.10		0.15	
Au	0.11		0.15	
Au	0.10		0.14	
Au	0.10		0.21	
Au	0.10		0.12	
Au	0.11		0.14	
Au	-0.01		0.12	
Au	**0.24**		0.06	
Au	0.07		**0.37**	
Au	0.07		0.17	
C	-0.51		-0.50	
C	-0.15		-0.17	
C	-0.64		-0.64	
H	0.23		0.23	

H	0.24	0.24
H	0.22	0.23
H	0.23	0.23
H	0.22	0.24
H	0.25	0.22
13		
Au/Y	-0.10	-1.49
Au	0.17	0.19
Au	-0.06	0.26
Au	0.17	0.05
Au	0.12	0.14
Au	-0.05	0.17
Au	0.15	0.14
Au	0.13	0.26
Au	-0.05	**0.37**
Au	0.15	0.15
Au	**0.18**	0.26
Au	0.15	0.26
Au	-0.04	0.16
C	-0.50	-0.49
C	-0.15	-0.17
C	-0.64	-0.64
H	0.24	0.23
H	0.23	0.23
H	0.22	0.22
H	0.24	0.23
H	0.23	0.22
H	0.22	0.24
14		
Au/Y	**0.27**	-2.30
Au	0.11	0.27
Au	0.11	0.21
Au	0.12	**0.43**
Au	0.08	0.21
Au	0.12	0.32
Au	-0.01	0.29
Au	0.12	0.31
Au	0.12	0.20
Au	-0.02	0.15
Au	0.03	0.25
Au	-0.01	0.24
Au	-0.04	0.15
Au	-0.05	0.17
C	-0.50	-0.49
C	-0.18	-0.16

C	-0.63	-0.64
H	0.23	0.23
H	0.24	0.24
H	0.23	0.22
H	0.24	0.23
H	0.23	0.22
H	0.22	0.25
15		
Au/Y	0.00	-2.74
Au	0.00	0.22
Au	0.10	0.23
Au	-0.01	0.32
Au	0.02	0.36
Au	0.11	0.31
Au	0.11	0.23
Au	**0.28**	0.27
Au	0.12	0.27
Au	-0.02	0.21
Au	0.00	0.22
Au	-0.01	0.21
Au	0.10	0.20
Au	0.12	0.20
Au	-0.03	**0.40**
C	-0.50	-0.49
C	-0.16	-0.18
C	-0.64	-0.64
H	0.24	0.23
H	0.23	0.23
H	0.23	0.23
H	0.25	0.22
H	0.23	0.23
H	0.22	0.25

Localized orbital locators (LOL) and bond critical points of the electron density

We used the localized orbital locator (LOL) and the Bader analysis to analyze the chemical bonds between the cluster and propene. LOL is a bonding descriptor, based on the kinetic energy density. It characterizes the atomic shells and the different elements of chemical bonding (e.g. bonds, lone pairs, etc.) correctly, thus it is considered a valuable tool in the analysis of chemical bonding. The Bader analysis defines the chemical bonds by bond critical points (BCP) and the corresponding bond paths, starting from the bond critical point and leading to the nuclei. In this approach, a

covalent bond is characterized by a ~0.1 a.u. electron density at the BCP and a negative Laplacian, while electrostatic interactions and ionic bonds are characterized by a lower, ~0.01 a.u. electron density and a positive Laplacian.

The LOL profiles of the neutral and the cationic clusters indicate the formation of two-electron three-center bonds between the metal atoms in both cases (Figure S9). In the case of the yttrium doped gold clusters, increased localization in the vicinity of the yttrium atom can be observed. The LOL profile of the propene-cluster complex is approximately the union of that of the reactants. Slightly increased localization can be observed near to the propene adsorption site. The absence of the basin between the propene and cluster shows that there is no covalent bond between the two fragments, neither in the neutral, nor in the cationic case.

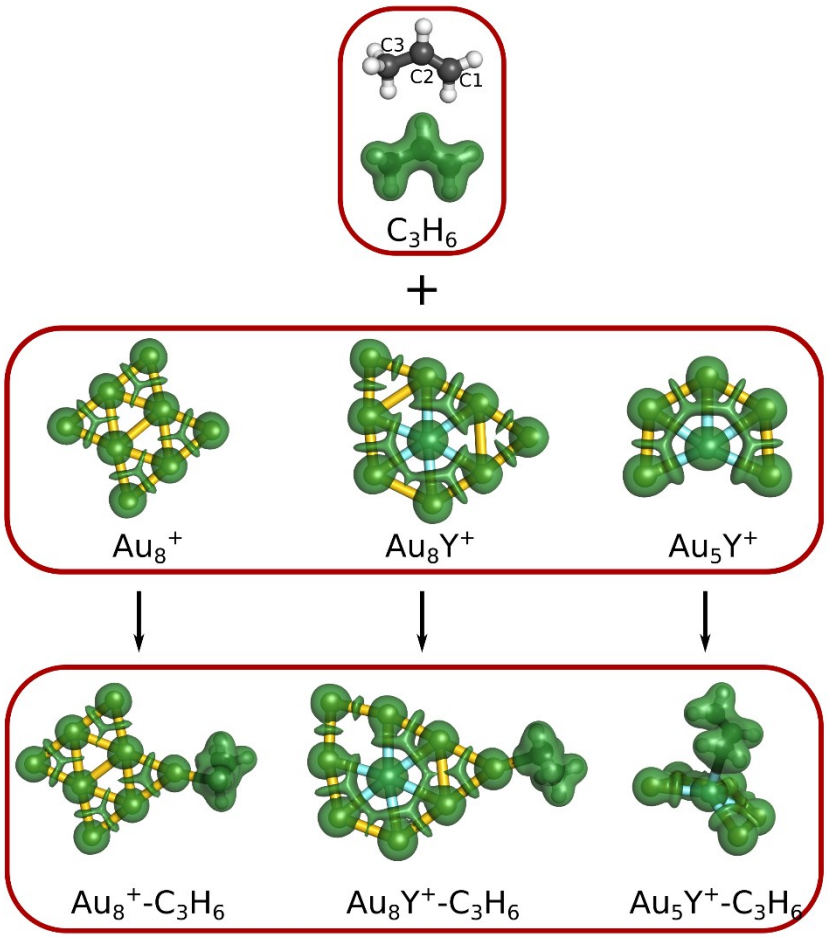

Figure S9: Localized Orbital Locator isosurfaces (green lobes) of propene, selected clusters (Au_8^+, Au_8Y^+, Au_5Y^+) and complexes (Au_8^+-C_3H_6, Au_8Y^+-C_3H_6, Au_5Y^+-C_3H_6). LOL =0.3.

The topological analysis of the electron density (Bader analysis) fully supports this conclusion. The electron density at the BCP is small (~0.07 a.u.) and the Laplacian of the electron density is positive in the BCP of the carbon - gold chemical bond. If propene binds to the yttrium atom, the electron density at the BCP is even smaller (~0.03 a.u.) while the Laplacian is also positive. These values indicate electrostatic interactions between the cluster and propene, similarly to what we observed in the neutral case.

Natural charges and bond indices

The natural charges clearly show that the positive charge resides mainly in the metal atoms of the cluster-propene complex cations, while the propene is approximately neutral with an overall charge of ~0.1 in all cases (Figure S10).

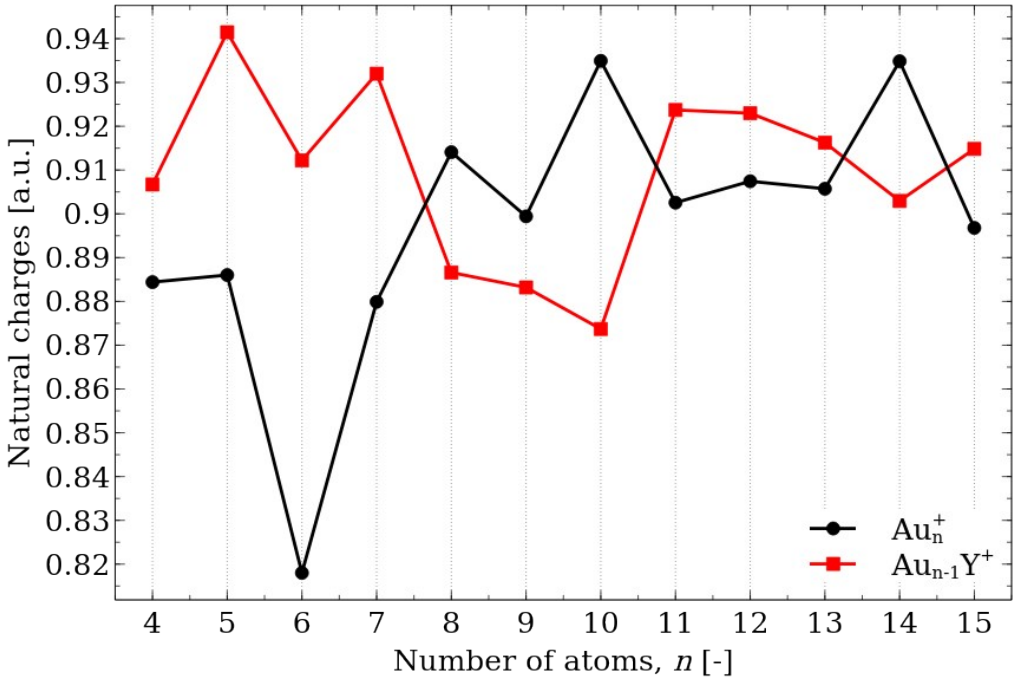

Figure S10: Total natural charge of clusters with respect to the cluster size

The Wiberg bond indices between the carbon atom and the adjacent metal atom (~0.3 for Au-C and ~0.15 for Y-C) are small, clearly showing that there is no covalent bond between the propene and the cluster (Table S5).

Upon propene adsorption the C1-C2 (single C-C bond in propene) bond indices are decreasing, while the C2-C3 (double C-C bond in propene) bond indices are increasing slightly. The C1-C2 decrease is smaller if propene binds to the yttrium atom. The natural charges change also with the adsorption: the charge of C1 becomes more negative, that of C2 becomes slightly less negative, and that of C3 changes only a slightly. For M=Y these values change more significantly. These changes imply donation-back donation mechanism for the adsorption – for the yttrium connected propene complexes in somewhat less extent, similarly to the neutral case.

Table S6: Natural charges of carbon atoms in propene and Wiberg bond indices between the carbon atoms in propene and between the carbon atoms and the adjacent metal atom of the cluster (M=Au or Y). See Figure S9 for labelling of the carbon atoms.

	C_3H_6	Au_8^+-C_3H_6	Au_8Y^+-C_3H_6	Au_5Y^+-C_3H_6
Natural charge				
C1	-0.39	-0.48	-0.49	-0.65
C2	-0.17	-0.15	-0.15	-0.02
C3	-0.61	-0.64	-0.64	-0.65
Wiberg bond index				
C1-C2	1.98	1.64	1.67	1.82
C2-C3	1.06	1.08	1.08	1.09
M-C1	-	0.28	0.26	0.16
M-C2	-	0.22	0.21	0.07

Table S7: Total electron density transfer (dQ) due to the donation/back-donation

	Au_n		$Au_{n-1}Y$	
n	donation [e^-]	back-donation [e^-]	donation [e^-]	back-donation [e^-]
4	0.049	0.019	0.017	0.008
5	0.050	0.024	0.047	0.031
6	0.031	0.013	0.040	0.016
7	0.048	0.019	0.042	0.020
8	0.050	0.023	0.040	0.015
9	0.036	0.013	0.040	0.016
10	0.045	0.020	0.037	0.008
11	0.038	0.015	0.038	0.016
12	0.037	0.010	0.041	0.015
13	0.035	0.010	0.039	0.017
14	0.042	0.011	0.041	0.017
15	0.039	0.011	0.042	0.018

XYZ coordinates of the optimized clusters and cluster-propene complexes on BP86/LANL2DZ level and total energies (in Hartree) on TPSSh/DEF2-TZVP level. The imaginary frequencies are also collected.

Au_4
E = -542.5743802783
Imaginary frequencies: no

Au	0.0000000000	-1.3803040121	-0.0007572594
Au	-2.3393335920	0.0000000000	0.0007572819
Au	0.0000000000	1.3803040121	-0.0007572594
Au	2.3393335920	0.0000000000	0.0007572819

Au_5
E = -678.3407782094
Imaginary frequencies: no

Au	2.3895648628	-0.2122536028	-1.3066017067
Au	2.3758360989	-0.1006243499	1.3145272555
Au	0.0000000000	0.0000000000	-0.0158509752
Au	-2.3758360989	0.1006243499	1.3145272555
Au	-2.3895648628	0.2122536028	-1.3066017067

Au_6
E = -814.0738594346
Imaginary frequencies: 7.69i

Au	3.0712936987	0.5507920995	-0.0011969724
Au	0.5588870226	1.4579207060	-0.0043913798
Au	1.0897603175	-1.2295960643	0.0058922629
Au	-1.0299810566	-2.8557853623	0.0006903003
Au	-1.9547718750	2.3635730766	0.0060239140
Au	-1.7351881074	-0.2869044556	-0.0070181250

Au_7
E = -949.8430618484
Imaginary frequencies: 15.68i

Au	0.0000043728	-2.7633400310	-0.0019236486
Au	-2.3903138740	-1.3808124924	0.0009751180
Au	2.3903173091	-1.3808049435	0.0009762656
Au	-2.3903173091	1.3808049435	0.0009762656
Au	-0.0000043728	2.7633400310	-0.0019236486
Au	2.3903138740	1.3808124924	0.0009751180
Au	0.0000000000	0.0000000000	-0.0000554339

Au_8
E = -1085.57469121
Imaginary frequencies: no

Au	1.1006707262	-1.4565183166	-0.3746391609
Au	1.2572762841	1.2995896245	0.2929809925

Au	-1.1174583150	0.3142991095	-1.1066985955
Au	-1.3537382201	-1.5491602035	1.0898381950
Au	-0.8289563470	2.9427446016	-0.4422446878
Au	3.3712748464	-0.3245249559	0.4631711771
Au	-1.1898894154	-2.3687301544	-1.5937890532
Au	-1.2391795592	1.1423002948	1.6713811328

Au_8_2
E = -1085.5772889538
Imaginary frequencies: no

Au	2.2560829760	-2.7946706324	0.0000000000
Au	1.4514516312	-0.2454413555	0.0000000000
Au	3.0438221840	1.9011571129	0.0000000000
Au	0.3946151437	2.3487843741	0.0000000000
Au	-2.2557145182	2.7943797303	0.0000000000
Au	-1.4517762135	0.2449200541	0.0000000000
Au	-0.3941948172	-2.3484931196	0.0000000000
Au	-3.0442863860	-1.9006361639	0.0000000000

Au_9
E = -1221.3450007571
Imaginary frequencies: no

Au	-1.4435679158	-1.4253483185	-0.3044344582
Au	-3.0310180985	0.0000000000	-1.9094080701
Au	-1.4435679158	1.4253483185	-0.3044344582
Au	-0.0000000000	-2.7434437009	1.6267357212
Au	0.0000000000	2.7434437009	1.6267357212
Au	1.4435679158	1.4253483185	-0.3044344582
Au	1.4435679158	-1.4253483185	-0.3044344582
Au	3.0310180985	-0.0000000000	-1.9094080701
Au	0.0000000000	-0.0000000000	1.7830825309

Au_{10}
E = -1357.0743424524
Imaginary frequencies: no

Au	1.4723020649	-2.7937434748	1.1856879886
Au	-0.8447522962	-1.4461003856	1.1884080831
Au	-3.1911941706	-0.0004392188	1.1419107511
Au	0.9882220622	-1.4004237831	-1.2119723024
Au	-0.1583335436	0.0002066204	-3.3669848424
Au	-1.6916889563	-0.0000761359	-1.1692589273
Au	1.8094643899	0.0000169920	1.0704248418
Au	-0.8449913801	1.4465765277	1.1885435328
Au	0.9882788243	1.4004857976	-1.2120886686
Au	1.4726930056	2.7934970604	1.1853295433

Au_{10}_2
E = -1357.0779997346
Imaginary frequencies: no

Au	-0.1059420176	-3.2429463268	-1.7215855269
Au	-1.6338403814	-1.4676510742	-0.4497245567
Au	-0.1057264103	3.2431287249	-1.7213156338
Au	1.1740989409	-1.4338172805	-0.2300140244
Au	3.5475599423	-0.0001865396	-0.1336925807
Au	-1.6336440922	1.4677699438	-0.4495679711
Au	1.8705060017	-0.0000973144	2.1101162716
Au	-0.8226002083	-0.0000781573	1.8652707430
Au	1.1743258559	1.4337809459	-0.2300299119
Au	-3.4647376310	0.0000970782	0.9605431910

Au_{11}
E = -1492.85438007
Imaginary frequencies: no

Au	-1.4358424706	-0.8266298692	-1.4096452454
Au	1.4357642393	-0.8267661147	-1.4096448933
Au	0.0000791966	1.6593430361	-1.4103971578
Au	1.4357642393	-0.8267661147	1.4096448933
Au	-1.4358424706	-0.8266298692	1.4096452454
Au	0.0000791966	1.6593430361	1.4103971578
Au	-0.0000002774	0.0014043241	3.5904155375
Au	-0.0000002774	0.0014043241	-3.5904155375
Au	-3.3879797627	-1.9663448369	0.0000000000
Au	0.0001865696	3.9183117669	0.0000000000
Au	3.3877918174	-1.9666696823	0.0000000000

Au_{12}
E = -1628.582367701
Imaginary frequencies: no

Au	-3.6379985979	0.0000000000	-0.4119190203
Au	3.6379985979	0.0000000000	-0.4119190203
Au	-1.3966754453	0.0000000000	-2.0284178046
Au	-1.3983923214	-1.4244599880	0.4225767235
Au	-1.3983923214	1.4244599880	0.4225767235
Au	1.3966754453	0.0000000000	-2.0284178046
Au	1.3983923214	1.4244599880	0.4225767235
Au	1.3983923214	-1.4244599880	0.4225767235
Au	0.0000000000	0.0000000000	-4.3145044807
Au	0.0000000000	-2.7117405798	2.4419596052
Au	0.0000000000	2.7117405798	2.4419596052
Au	0.0000000000	0.0000000000	2.6209520260

Au_{13}

E = -1764.3412932263
Imaginary frequencies: no

Au	-2.4443402821	0.0000000000	-2.0902142638
Au	0.0000000000	-1.3898978257	-1.9832211282
Au	2.4443402821	0.0000000000	-2.0902142638
Au	0.0000000000	1.3898978257	-1.9832211282
Au	-1.5764748052	-1.4128110124	0.3448918302
Au	0.0000000000	-3.5999229622	-0.2546448751
Au	1.5764748052	-1.4128110124	0.3448918302
Au	-1.5764748052	1.4128110124	0.3448918302
Au	0.0000000000	3.5999229622	-0.2546448751
Au	1.5764748052	1.4128110124	0.3448918302
Au	-2.7148161391	0.0000000000	2.4542639267
Au	0.0000000000	0.0000000000	2.3680506348
Au	2.7148161391	0.0000000000	2.4542639267

Au_{14}
E = -1900.0795148249
Imaginary frequencies: no

Au	1.5274999491	-1.9594068076	-0.5676136476
Au	-1.3933653360	-0.3521212564	1.2074845085
Au	0.2634624187	1.9267490237	1.5920075150
Au	2.0975824720	0.7719943676	-0.2908772430
Au	1.3008138540	-0.7528289077	2.0030792151
Au	-1.2147317404	-2.1680295764	-0.9520551661
Au	-3.6770601977	-1.4872954525	0.0365060970
Au	-2.3101346917	0.4334484470	-1.3515773401
Au	-0.1502782018	2.1753092874	-1.2129862853
Au	-2.1185534929	2.5003932608	-3.0183514741
Au	-0.4757241324	0.4026228663	3.7500969278
Au	1.9183332954	3.5145850599	0.0790212787
Au	0.4645123353	-3.8727404911	-2.1256000290
Au	3.7676434684	-1.1326798211	0.8508656431

Au_{15}
E = -2035.8493584813
Imaginary frequencies: 12.78i; 2.01i

Au	2.5531996531	-2.0434859199	0.2578637122
Au	3.6848153730	0.4419246214	0.2453348085
Au	1.2935548031	0.9601525846	1.6738958874
Au	2.4627224821	3.0757640058	0.1347620335
Au	-0.3019728230	2.8863786541	0.1761552467
Au	-1.4596039635	0.5795233537	1.6666031366
Au	-1.5529294427	0.5420618914	-1.1962044769
Au	-0.0315840861	-0.0127860363	-3.4209799499
Au	0.2097235208	-1.6941739901	-1.2619361830

Au	0.3637100929	-3.9412367791	0.3139578801
Au	-3.7903185225	-0.2842190011	0.2799128119
Au	-2.0239235084	-2.3575430181	0.3461130874
Au	0.2597767219	-1.5385106630	1.8151087371
Au	1.3555655962	0.8872270834	-1.2227335331
Au	-3.0227358970	2.4989232133	0.1921468015

Au_4-C_3H_6
E = -660.5986783356
Imaginary frequencies: 6.83i

Au	-2.3564336420	1.0602483273	0.7837987913
Au	1.7663462450	0.1054283177	-1.2115459320
Au	-0.3013113758	-0.8119534148	0.4286785731
Au	-0.2023248536	1.7774238690	-0.6101611756
C	-0.9523131055	-2.6216505878	1.6175834936
C	0.2787548506	-3.0443011634	1.0757554990
C	1.5814303092	-3.0578847538	1.8252832582
H	-1.8942971162	-2.9134276930	1.1380310709
H	-1.0101465384	-2.2902520757	2.6620705733
H	0.2590859158	-3.5721240173	0.1101424364
H	1.5543549234	-2.4396863591	2.7367622245
H	2.4285518528	-2.7403278957	1.1920616314
H	1.7993764259	-4.1038672805	2.1268604381

Au_5-C_3H_6
E = -796.3611800924
Imaginary frequencies: 3.52i

Au	2.4642437464	-0.5715435256	2.6310072150
Au	2.2965717266	0.1859450070	0.1069465118
Au	-0.2757123225	0.0025893833	-1.1957600006
Au	-2.3299372958	-0.8933635047	0.3204308599
Au	0.0153836133	-0.7002872986	1.4869104496
C	0.8937008588	0.8513202001	-2.9435947587
C	-0.4204630249	0.6751904883	-3.4385974414
C	-1.4278813268	1.7774646551	-3.5948330267
H	1.6638544100	0.1046334294	-3.1707292410
H	1.2385497534	1.8529658459	-2.6580278755
H	-0.6498239580	-0.2763532442	-3.9424300244
H	-2.4510866362	1.4353669413	-3.3619342527
H	-1.4412571290	2.0853705032	-4.6616052634
H	-1.1896475565	2.6648554769	-2.9871218594

Au_5-C_3H_6_2
E = -796.3606700129
Imaginary frequencies: 21.79i; 10.15i

Au	2.6515095544	-2.3356910003	-0.6207402125

Au	3.2420470962	-0.5523037574	1.2057611261
Au	0.6171173846	-0.9843451895	0.5974078863
Au	-1.2162746270	0.7098187071	-0.7210248693
Au	-1.8489937314	-0.6772204364	1.4673353819
C	-0.7956788300	2.0772396795	-2.4540452249
C	-2.2018734863	2.0757144165	-2.3899260817
C	-3.0340050475	3.1609860545	-1.7652139267
H	-0.2220198002	2.9188880016	-2.0459678877
H	-0.2761752018	1.4268677912	-3.1678207339
H	-2.7425946455	1.3369121262	-3.0007092222
H	-3.9131329507	2.7542471887	-1.2364054737
H	-2.4569387000	3.7980134439	-1.0758742561
H	-3.4301014447	3.8057097822	-2.5766062452

Au_6-C_3H_6
E = -932.0906520675
Imaginary frequencies: 14.18i

Au	2.0961903078	0.0976945570	0.2699359294
Au	-0.4133695825	1.3556735734	0.2155947815
Au	-0.1372576183	-1.3562406278	-0.6109526408
Au	-2.5451513065	-0.1133484148	-0.5842078158
Au	1.8043832533	2.6578237041	0.9900425159
Au	2.3046365771	-2.4652567257	-0.4649749055
C	-4.6329327251	0.0312293462	-1.4812496210
C	-4.9284787853	-0.5074264505	-0.2172576251
C	-5.4091262818	0.2824523606	0.9632167610
H	-4.5458385417	-0.6213364684	-2.3590111843
H	-4.7757017729	1.1020412042	-1.6775119596
H	-4.9530412692	-1.6031615123	-0.1184550913
H	-5.2770756551	1.3684001934	0.8335257683
H	-6.4921565795	0.0801650216	1.0987844277
H	-4.9210998284	-0.0401673557	1.8997737128

Au_7-C_3H_6
E = -1067.8630511446
Imaginary frequencies: 4.94i

Au	1.7849037577	-2.0166291273	-0.3234018417
Au	1.3691802588	0.5734204255	-1.0823412945
Au	-0.8280078966	-1.2728774549	-0.6708131149
Au	0.7803295595	2.9891721169	-2.0110385971
Au	-1.3176390625	1.3624461616	-1.6518544977
Au	-3.2698629800	-0.4332340311	-1.2820818758
Au	0.7336419883	-0.3423114477	1.5648202052
C	0.4901940103	-0.1308419129	3.7768376295
C	0.0989119370	1.1379414152	3.3041433425
C	0.9657405023	2.3666111753	3.3320488940

H	1.4849345819	-0.2758069496	4.2170882411
H	-0.2648077472	-0.8918332317	4.0094092488
H	-0.9671912902	1.2962304346	3.0819718049
H	0.6244768922	3.0136686130	4.1661084948
H	0.8612824250	2.9649710371	2.4109278636
H	2.0302031143	2.1338270641	3.4964575819

Au_8-C_3H_6
E = -1203.5832454148
Imaginary frequencies: no

Au	2.2543992765	0.5990349980	-0.0752119415
Au	-0.4796946924	1.1363020938	0.0546064847
Au	-1.6532374677	-1.2739272023	-1.0991787434
Au	0.6106557529	-1.5824102548	0.7887430362
Au	-3.1858582523	0.9513099737	-0.1458095769
Au	1.2866141895	3.0340743917	-0.5649014213
Au	3.2360112225	-1.8576821957	0.3592536901
Au	-1.8496848697	-0.8096751851	1.6240453826
C	-2.2116632854	-1.9862552308	-3.1474050227
C	-1.0847347640	-2.7738637785	-2.8262226020
C	0.3069340254	-2.5196729537	-3.3399541978
H	-2.1118791431	-1.1248195094	-3.8197079219
H	-3.2238857749	-2.3851287019	-3.0090745200
H	-1.2608680742	-3.7508577172	-2.3513996930
H	0.4359163702	-1.4957010683	-3.7267489007
H	0.5096064881	-3.2284267200	-4.1689305568
H	1.0697458271	-2.7114035930	-2.5658905939

Au_8-C_3H_6_2
E = -1203.5872494836
Imaginary frequencies: no

Au	-1.5323589504	0.5123424531	1.6198883329
Au	0.7259814075	0.4726824650	0.1436485211
Au	2.7115653400	2.2419385639	0.4000234871
Au	3.0710416145	0.3567986987	-1.4641943579
Au	3.3682135117	-1.5455421216	-3.3180909513
Au	1.1249941245	-1.6046872443	-1.8779204423
Au	-1.1440700533	-1.4664632242	-0.2474998062
Au	-0.8432276475	-3.4020652834	-2.1083315008
C	-3.3746769442	1.2165901508	2.7872987826
C	-2.3648020174	1.2926543613	3.7569718153
C	-2.1125022613	0.2637367818	4.8219469909
H	-4.0675909278	0.3659437155	2.7734878245
H	-3.6744991162	2.1062927617	2.2206382234
H	-1.8151675643	2.2420960546	3.8517128331
H	-2.4888659540	0.6582379454	5.7879759269

H	-1.0343959859	0.0749422538	4.9651651550
H	-2.6254917772	-0.6892933707	4.6162023060

Au_9-C_3H_6
E = -1339.3552724777
Imaginary frequencies: no

Au	0.3759054702	-1.6406084396	0.3715047785
Au	-1.5427879270	-3.3352255592	1.1606256058
Au	-2.2983223886	-0.7853130548	1.0043744499
Au	2.4292494341	0.1899526761	-0.0948998247
Au	-2.6744869883	1.9148591092	1.2527173483
Au	-2.3176265125	0.9783278441	-1.2914872156
Au	0.2987329989	-0.0255986603	-1.9143714423
Au	-1.5935957975	0.3419874094	-3.7752934571
Au	-0.1007989412	1.1265142475	0.6434254392
C	4.6839407026	0.3240365439	0.4707916384
C	4.6584754865	1.1765187337	-0.6315947223
C	4.5726836097	2.6756110457	-0.5708614868
H	4.9834403560	-0.7251417418	0.3570096078
H	4.6769825747	0.7262080212	1.4922005100
H	4.8429106253	0.7399365576	-1.6248486020
H	4.3275246483	3.0488631568	0.4366857148
H	3.8404353407	3.0729440992	-1.2959952821
H	5.5555212942	3.0974585460	-0.8633261809

Au_9-C_3H_6_2
E = -1339.3547337395
Imaginary frequencies: 19.65i

Au	-1.0088439502	0.9676875048	1.0379550800
Au	0.6696679962	1.8492603120	2.9285187940
Au	1.4974167080	-0.2926232936	1.5770931954
Au	-2.9899233105	-0.2038266456	-0.5413023157
Au	1.9619784623	-2.6557872628	0.3009719571
Au	1.9348939024	-0.4216874468	-1.2847525393
Au	-0.6574289856	0.7362995940	-1.7381963561
Au	1.5248116420	1.4586646658	-3.1193747490
Au	-0.5478916157	-1.5661536352	-0.1387973586
C	-5.2772222157	-0.0860826287	-0.9576282436
C	-5.2654814263	-1.1228155714	-0.0261643725
C	-5.5293138185	-0.9676895833	1.4451433469
H	-5.5317012400	0.9375489233	-0.6529494407
H	-5.3072542204	-0.3015324164	-2.0326281086
H	-5.1778867777	-2.1532302626	-0.4026197120
H	-4.8132162581	-1.5481921108	2.0535998817
H	-6.5330807462	-1.3809478611	1.6719485829
H	-5.5101420258	0.0854428634	1.7685323434

Au_9-C_3H_6_3
E = -1339.3537893227
Imaginary frequencies: 5.54i

Au	-0.7337439190	-1.2552235141	0.9031868038
Au	-3.1400559784	-0.1201435695	0.3204882495
Au	-0.8907702586	1.3950160827	0.3014259529
Au	1.6950840973	-2.3942810161	1.6109989592
Au	1.4547141473	2.9108537431	0.3624954193
Au	1.2600437471	1.0881546005	-1.6514294827
Au	1.4172605675	-1.6802541631	-1.0096775407
Au	1.4451365765	-0.7974148311	-3.5283829010
Au	1.7473841449	0.2973330915	1.1014172094
C	-5.2535056870	-0.5215304502	-0.5565722822
C	-5.5157641760	-0.5168227830	0.8133368808
C	-6.0818473757	0.6451860738	1.5830745864
H	-5.4676346845	0.3615931027	-1.1719105365
H	-5.0785630156	-1.4627911934	-1.0908773153
H	-5.4523235678	-1.4734052536	1.3538272415
H	-7.1336833919	0.4168696207	1.8478045910
H	-6.0711667754	1.5816749795	1.0023227540
H	-5.5499754535	0.8049226531	2.5376625954

Au_{10}-C_3H_6
E = -1475.0768603224
Imaginary frequencies: no

Au	1.0569687541	0.7756889500	3.0387495520
Au	1.9654531827	1.4030434677	0.3825890973
Au	0.6853094258	-0.4415773230	-3.8112356820
Au	-0.7920229911	1.3609321908	1.0794412516
Au	-2.9208322392	1.3367201508	-0.6134491921
Au	-0.1571855078	0.8451470167	-1.5713616216
Au	0.6954993929	-1.0620513555	1.0235755891
Au	0.3054618263	-1.9683656415	-1.6685206407
Au	-2.0067985426	-1.1309466769	-0.1205214891
Au	-0.6095532247	-3.4196673273	0.4631161369
C	3.5904062368	2.5246822595	-0.7297800924
C	4.2866815938	2.0952258703	0.4133371652
C	5.1976773225	0.8978119262	0.4576191553
H	3.1771032341	3.5399276130	-0.7754707336
H	3.7154532372	2.0024769604	-1.6861737597
H	4.3128303375	2.7644076174	1.2856945986
H	5.0676096800	0.3135781398	1.3853914238
H	6.2485811316	1.2529057751	0.4560331521
H	5.0618484941	0.2332265240	-0.4109672207

Au_{10}_2-C_3H_6
E = -1475.0876247066
Imaginary frequencies: 9.52i

Au	-0.4725488300	-3.0333933995	2.3437983639
Au	-1.1297839044	-0.8699538705	0.9091454453
Au	0.8622982968	-0.8017114068	-3.7710175719
Au	1.5557093609	-1.6631266946	1.3138013583
Au	3.7445681057	-0.2002385890	0.6882221589
Au	-0.5788573714	0.0668369455	-1.6866576904
Au	1.1707666944	1.0721519685	0.5985871886
Au	-1.4760782381	1.9178285574	0.3273393346
Au	2.1475341562	-0.6505657713	-1.4538341303
Au	-3.1651395426	-0.0259496020	-0.7544875122
C	-1.2627657833	4.0288995193	1.1491648623
C	-2.5890671332	4.0251300585	0.6807123706
C	-3.0344262256	4.6147698156	-0.6294289522
H	-1.0500506769	3.8550480124	2.2103900955
H	-0.4686650084	4.5047652698	0.5604725174
H	-3.3839913772	3.7389884790	1.3851757967
H	-3.7838052834	3.9799781497	-1.1332573845
H	-3.5315076183	5.5860849360	-0.4298912230
H	-2.1937746889	4.7993893274	-1.3180511912

Au_{11}-C_3H_6
E = -1610.8596794
Imaginary frequencies: no

Au	1.6158650072	-1.4937475596	-0.8961989333
Au	1.8381073870	1.3652251445	-0.6459440714
Au	1.4373530777	-0.2612212511	1.6956816939
Au	-0.9767512655	1.5824296092	-0.9206465275
Au	-1.1828003129	-1.1931369854	-1.1739400254
Au	-1.3623248187	0.0109063023	1.3569438979
Au	-3.4242184731	0.3274272185	-0.4957328104
Au	3.7869105252	-0.3182961285	0.2896824815
Au	0.1502280796	-3.1900707385	-2.3440355294
Au	-0.2440172823	-0.3034211593	3.7647671285
Au	0.6861420058	3.5076649297	-1.7381375648
C	-5.5987533716	0.9403079834	-0.9844711319
C	-5.8067614574	-0.3320127974	-0.4509178185
C	-6.2247514507	-0.6177328009	0.9647869221
H	-5.5312005287	1.0865313910	-2.0694133912
H	-5.7701342018	1.8376445115	-0.3762600751
H	-5.7975097749	-1.1888801438	-1.1413690804
H	-7.2811297316	-0.9542149601	0.9632104353
H	-6.1483258748	0.2690569416	1.6145108807
H	-5.6384142104	-1.4431940518	1.4060937850

Au_{12}-C_3H_6
E = -1746.5849473961
Imaginary frequencies: no

Au	0.3548275735	3.4308483974	1.3947595198
Au	0.4225247718	-3.6703228094	0.0528711315
Au	1.6116993984	1.0750749191	2.0503333977
Au	0.6693871085	1.5453963504	-0.6163998168
Au	-1.1709679461	1.1082531845	1.5593356702
Au	1.6091858669	-1.6736238457	1.5328892773
Au	-1.1740397266	-1.6093047609	1.0323330093
Au	0.6809438232	-1.1737850382	-1.1262383623
Au	3.4885942375	-0.5423534599	3.0605238557
Au	0.2093127043	0.6276838876	-3.2238633553
Au	-3.5036600870	-0.1532799482	0.7582429310
Au	-1.7835876227	0.2644779839	-1.3068879422
C	0.0463784963	1.0620343757	-5.4925610114
C	1.4107134708	0.7864582891	-5.3910176348
C	2.4974323789	1.8204286673	-5.2913970403
H	-0.3139966289	2.0976254933	-5.5405171659
H	-0.6592537746	0.2807320350	-5.8002627286
H	1.7372892269	-0.2556176313	-5.5271746586
H	3.2433384382	1.5572090261	-4.5205486610
H	2.1032688145	2.8286656683	-5.0852154554
H	3.0457284893	1.8546934218	-6.2543589913

Au_{13}-C_3H_6
E = -1882.3408445957
Imaginary frequencies: no

Au	-1.1485328152	-0.3808597121	-2.6581516597
Au	-1.5337493890	-2.2273836915	-0.5888193842
Au	0.5135622457	-4.0229399364	0.1122769698
Au	0.9661566319	-2.0084396640	-1.7874890668
Au	-1.3899821273	0.4886020467	0.1901297816
Au	-3.0199926115	-1.2584139917	1.5731307456
Au	-0.3453326867	-1.8854186399	1.9461387426
Au	1.0966475644	0.7068815231	-1.0080531818
Au	3.4136300578	-0.6804700737	-1.5737845856
Au	2.1931383398	-1.6538903551	0.7222206367
Au	0.0009153787	2.9332972186	0.3305358631
Au	0.9157422675	0.7829963892	1.8083021592
Au	1.8999374963	-1.1648902467	3.4375125258
C	-0.1710747875	5.1654552244	-0.3528690210
C	-0.5665350044	5.2629702203	0.9790496069
C	-1.9923260755	5.3025874877	1.4567796665
H	0.8653029919	5.3715610406	-0.6459943670

H	-0.9156946078	5.1348936649	-1.1582231545
H	0.2075839237	5.4611450777	1.7356926742
H	-2.2220529143	6.3278985334	1.8094350609
H	-2.1532461852	4.6326332197	2.3201345137
H	-2.7099456886	5.0453185404	0.6610343580

Au_{13}-C_3H_6_2
E = -1882.3377232783
Imaginary frequencies: no

Au	-0.3608708990	-1.7426906331	-2.5906479504
Au	-1.2613166183	-1.5746975339	-0.0349994274
Au	0.3163329637	-3.5234169732	1.5256833336
Au	1.5798679544	-1.8972845440	-0.2288588324
Au	-1.8524791413	0.6595935736	-1.8132631967
Au	-2.6828694464	-0.2585482110	1.8603624591
Au	0.1534974250	-0.9362464454	2.3506940068
Au	0.9149469409	0.5396384014	-1.5094410982
Au	3.5860771669	-0.2152195118	-1.1062122201
Au	2.2544581763	0.6583456569	1.0884540167
Au	-0.2940209789	3.0007784293	-1.3015728165
Au	-0.6804031477	1.3716538489	0.8612335899
Au	0.9445243066	1.5149525924	3.2686024962
C	-3.9826604493	0.3085336065	-2.6056450002
C	-3.9863296781	1.6617604761	-2.2320402599
C	-4.5825233407	2.1960669032	-0.9548317712
H	-4.4274921296	-0.4512543914	-1.9519383295
H	-3.8036401166	0.0179589648	-3.6472015132
H	-3.7279571142	2.4048607544	-3.0007307773
H	-5.5799826165	2.6264662964	-1.1765723675
H	-3.9713050653	3.0083658911	-0.5260919935
H	-4.7106523532	1.4091999558	-0.1920834512

Au_{14}-C_3H_6
E = -2018.0847339652
Imaginary frequencies: no

Au	2.3848007591	2.4615901510	0.2218278973
Au	-1.9516872213	-0.9885546837	1.3044835570
Au	-1.8484752349	-0.8571353938	-1.4777220503
Au	0.4293797965	1.0362597980	-1.3110067390
Au	-2.2746175286	1.6204415698	0.0169887442
Au	0.3409117561	0.8930447814	1.4615014532
Au	-0.3809398246	-0.7485003661	3.5678614961
Au	0.6138282676	-2.0474462971	1.3145584682
Au	0.7144688856	-1.9143019871	-1.4757065265
Au	2.7735448858	-3.0521596640	-0.0599116462
Au	-4.2132871766	-0.2817730802	-0.1407689394

Au	-0.1640509327	-0.3732708528	-3.6189073522
Au	2.6254397244	-0.2561629333	0.0747380945
Au	-0.3658198382	3.4535283799	0.1914192654
C	3.1573346000	4.6494171649	0.3978731174
C	4.3141959869	3.8629670510	0.2928240397
C	5.1164604298	3.6832328688	-0.9689166342
H	2.7719732153	5.1907244066	-0.4745780900
H	2.7857145428	4.9638886712	1.3796912240
H	4.7860523404	3.5150008057	1.2237770954
H	6.0282460470	4.3105700387	-0.9018805285
H	5.4602705121	2.6413408875	-1.0909350088
H	4.5584440694	3.9867380180	-1.8697856655

Au_{15}-C_3H_6
E = -2153.856271005
Imaginary frequencies: 14.96i; 12.31i

Au	0.7075524072	0.4209341100	-1.4733057208
Au	-1.2517596030	-1.7221302867	-1.4261843114
Au	-1.9199295644	2.5999985807	0.8320860709
Au	-2.1136126791	1.1012151246	-1.5172285395
Au	-0.2671864243	-2.7315136103	0.9892147300
Au	-3.8647032799	0.6305063283	0.5752175412
Au	-2.9820292906	-2.2168239738	0.6788248593
Au	0.9672288001	2.0534137450	0.8045276633
Au	1.8195237146	-0.6690452858	0.8637243409
Au	-0.8793313989	-0.1387770899	-3.6592111872
Au	-1.1046500578	-0.0666731448	0.9999787685
Au	-0.0631334297	4.2349332194	1.9309671678
Au	2.1841630614	-2.9921284234	2.1064172578
Au	-5.5477626935	-1.4396469387	0.9086814300
Au	3.2496666671	1.2234480169	-0.5918762196
C	5.4234949114	1.3719265187	-1.2899864319
C	5.0187130981	2.7106235200	-1.3407815076
C	5.3022618004	3.7388109719	-0.2808562043
H	5.4111230234	0.7515309268	-2.1941994509
H	6.0164664276	0.9986245346	-0.4452971970
H	4.5976499708	3.0871035847	-2.2848981727
H	4.4220513690	4.3748628937	-0.0823465207
H	6.1021682762	4.4132478530	-0.6472789169
H	5.6448203039	3.2879469925	0.6642973955

Au_3Y
E = -445.281022319
Imaginary frequencies: no

Y	0.5542823043	0.9348077511	0.0000000000
Au	-1.5192264553	-0.2308946657	-1.3903137889

Au	-1.5192264553	-0.2308946657	1.3903137889
Au	2.7393634478	-0.4440412103	0.0000000000

Au_4Y
E = -581.0487429007
Imaginary frequencies: no

Y	0.0012802707	-1.1266405950	0.0564069460
Au	-1.3247791224	1.3484526282	-0.0026388099
Au	1.3224278679	1.3498623788	0.0032654151
Au	-2.7567953211	-1.0721617794	-0.0127848433
Au	2.7585296545	-1.0700156793	-0.0156184686

Au_5Y
E = -716.7900775479
Imaginary frequencies: no

Y	-0.6373357992	0.2908661779	-0.3552022448
Au	1.9312315829	1.5236078289	-0.1189476177
Au	-0.6765671472	-2.3865286560	0.6408851663
Au	-2.9704744844	-1.2919012419	-0.3607424823
Au	-0.1201012656	2.8965810924	-1.2915185634
Au	1.6792848370	-1.0296569064	0.7954545520

Au_5Y_2
E = -716.7829136443
Imaginary frequencies: no

Y	0.2475540305	0.1870421423	1.3526635523
Au	1.0677376230	0.3154002962	-1.4338746935
Au	1.7321314008	2.3098291435	0.3290036222
Au	-2.5383705260	0.2078847763	1.3947959697
Au	1.0656993701	-2.1688515160	0.0504533471
Au	-1.3511461306	-0.8394709953	-0.8447720369

Au_5Y_3
E = -716.7870133368
Imaginary frequencies: no

Y	0.6434609236	0.9211594511	-0.7074684630
Au	-0.6654357760	3.0665849111	0.4685684117
Au	-1.9000938756	0.6138227937	0.3393070955
Au	3.1746663433	-0.1767339753	-0.3937468725
Au	0.9591225251	-1.7978139367	-0.2982835687
Au	-1.6986341633	-2.0044865857	-0.1467253091

Au_6Y
E = -852.5531487049
Imaginary frequencies: no

Y	0.3276573742	-0.0013777457	1.1880223800

Au	0.6330235302	1.3800798381	-1.4124627037
Au	-1.7227779260	-0.0105025996	-0.9441529020
Au	1.6931051356	-2.4397325453	0.8712119227
Au	1.6418944083	2.4667193269	0.8764593324
Au	0.6354233185	-1.3931515212	-1.4160223826
Au	-2.4426129081	-0.0007214168	1.6862629894

Au_6Y_2
E = -852.5527778571
Imaginary frequencies: no

Y	-0.6970096919	0.9531576641	0.0360721003
Au	2.1550329026	0.3285251905	0.2347116310
Au	-2.4722849496	-1.2195048423	-0.0699255495
Au	-3.3698737264	1.5158189265	-0.0893132523
Au	1.3961631184	2.8698402391	0.2385552167
Au	0.0721590953	-1.8452177729	0.0543776907
Au	2.7365323372	-2.2459868090	0.2013457273

Au_6Y_3
E = -852.5497493906
Imaginary frequencies: no

Y	0.0113395126	-1.3063309119	0.0936071213
Au	-2.6943809920	-2.0288910681	-0.0167066096
Au	-2.1583263928	0.6881597972	-0.0885659047
Au	2.3749561493	-0.5419742514	-1.3274743501
Au	2.2263766488	-0.4249118414	1.6699490375
Au	0.0519127497	1.2118240182	1.4954751713
Au	0.2010086907	1.0937731946	-1.4838285132

Au_6Y_4
E = -852.5486169239
Imaginary frequencies: no

Y	-0.1472471019	-0.6695064221	-1.2728888763
Au	-0.9491766715	-3.1441901587	-1.2925576000
Au	-1.0399506840	1.2000896193	0.8214734770
Au	2.7354456832	-0.6407605942	-1.4179804460
Au	1.7087204186	0.2820012055	0.8162832715
Au	0.4618340289	1.1125196770	3.0182812641
Au	-2.4344566693	1.0920981506	-1.4008448467

Au_7Y
E = -988.2992975214
Imaginary frequencies: no

Y	0.4179799244	-0.2582517716	-0.0076451993
Au	-2.3709253275	-0.7546291566	-0.2561209333
Au	1.8409193337	2.1739244826	0.6691225012

Au	3.2772180482	-0.2659772329	0.3268546429
Au	-0.7456652858	-2.8490325155	-0.5684990079
Au	-0.8213004198	2.2512658287	0.4901086467
Au	-3.3963882329	1.6652457827	0.1510993972
Au	2.0813790310	-2.5939892902	-0.2761471521

Au_8Y
E = -1124.0629679158
Imaginary frequencies: 7.56i

Y	-0.1738106943	-0.4520732352	0.1224969822
Au	2.3738015142	-1.7850164831	0.4570388248
Au	-0.4332660898	2.3783335336	0.0449825355
Au	-2.8836048458	0.4389820120	-0.3933045203
Au	0.2397199117	-3.3052155795	0.0778552300
Au	1.9743633743	1.3753484944	0.4277528626
Au	4.2802469249	0.0097272201	0.8122556411
Au	-2.4362040772	-2.1687259438	-0.3691765254
Au	-3.0191180682	3.0794037519	-0.3491576235

Au_8Y_2
E = -1124.057551584
Imaginary frequencies: 8.50i

Y	0.4639896780	0.0804908471	0.0652212170
Au	-1.7380892985	-1.9162510985	-0.1713884684
Au	-0.5320160460	2.7931300558	-0.0250233122
Au	3.2425883877	0.7945354949	0.1341729236
Au	0.6987421247	-2.8297569660	0.1609330240
Au	-2.3481443984	0.9457815246	-0.3989558702
Au	-4.1905185996	-0.9756927345	-0.6509292863
Au	2.7335967976	-1.4425506165	-1.1978089191
Au	1.7310828710	2.4345551779	1.5815492164

Au_9Y
E = -1259.7987370179
Imaginary frequencies: no

Y	0.2243130744	-0.5291672149	-0.4990128275
Au	2.7820239677	-1.5031286669	0.5860408414
Au	-0.9728955866	1.4110158744	1.3925082919
Au	-2.6247882577	0.0328524801	-0.6219903749
Au	0.6215422946	-3.1240375439	0.8448631892
Au	0.5412400517	-0.5300872250	2.3476218244
Au	2.7324028981	0.8934805043	-0.9453115199
Au	-1.8870430480	-2.5379588328	-0.3764042565
Au	-2.2364902490	2.7380256023	-0.7665250410
Au	0.4578307537	2.3231315762	-1.0189291632

Au_9Y_2
E = -1259.7983957749
Imaginary frequencies: no

Y	0.2377691374	-0.1385571039	0.7828038868
Au	2.7824449548	1.1507589773	0.6778046629
Au	-0.7536591894	-0.9151117797	-1.8313537569
Au	-3.3452346693	0.2160043482	-1.8506270993
Au	0.5943982934	2.7676816640	0.8535822297
Au	1.8037527681	-1.2709432264	-1.2822092844
Au	4.1329400279	-1.0653252192	0.0851688533
Au	-1.6256781043	1.8092431118	-0.3592005427
Au	-2.6465015577	-0.8119230182	0.5278089932
Au	-1.3850454905	-1.5957276122	2.7044369105

Au_9Y_3
E = -1259.7960531339
Imaginary frequencies: no

Y	-0.6067652677	-0.1629053067	0.7392155250
Au	2.1396064878	0.5328777486	-0.2831490442
Au	-0.9051125465	-3.0658016109	0.4807057360
Au	-2.7423754560	1.1957456524	-0.8518070828
Au	0.4129885392	2.5639193434	0.2740717370
Au	1.5556589316	-2.1187719093	0.9277333800
Au	3.9281670759	-0.8702945918	1.1243944003
Au	-2.0255580664	2.4108070087	1.5246961170
Au	-2.1123618007	-1.4057873943	-1.4043543601
Au	-0.1188858420	0.8025514208	-1.9370238224

$Au_{10}Y$
E = -1395.5781359152
Imaginary frequencies: 6.25i

Y	-0.0784158867	0.4064953002	0.9207820118
Au	2.5224853487	-0.9904508698	0.9510249671
Au	-1.5229178498	0.0996604431	-1.6565239850
Au	-2.1878417481	2.3673765838	-0.0264459093
Au	2.6754582433	1.6534245175	0.4991637016
Au	1.1095320580	0.9075861377	-1.7564196721
Au	1.1287487252	-3.3559079882	1.0429475735
Au	0.4282414834	3.1879684766	-0.1344416387
Au	-3.0597488880	-0.1750914792	0.7325057697
Au	-1.3807321551	-2.2334734357	1.1367340469
Au	0.5016791952	-1.7261480358	-1.1066252353

$Au_{10}Y\_2$
E = -1395.5776027734

Imaginary frequencies: 14.96i

Y	-0.1289769415	-0.2349178442	0.9483767847
Au	2.8672257819	-1.9303987531	0.2611960402
Au	-1.4718729594	-0.1673657351	-1.6805927771
Au	-1.4911143306	2.3963407487	1.1006389400
Au	2.6336109679	0.7289208800	0.7340533697
Au	1.2301953051	-0.7575239720	-1.6449469395
Au	0.3360647433	-3.0157102746	0.0146432557
Au	1.2074146261	2.9742302468	1.2527256182
Au	-3.1324789706	0.3031224959	0.6177541059
Au	-2.2623203061	-2.2758978422	0.1014534735
Au	0.3505287439	1.8386091018	-1.1288797092

$Au_{11}Y$

E = -1531.3192627014

Imaginary frequencies: no

Y	-0.0868813772	-0.1813726645	0.8392844116
Au	1.9865697806	1.6842681721	1.9936696027
Au	-1.5809039993	-1.3320600240	-1.4626531972
Au	-3.0201548245	-1.1283505375	1.0090690112
Au	-0.2652583706	2.9177961276	0.7969346000
Au	-0.8820521473	1.3803105904	-1.6059607229
Au	2.9682238964	-0.3914698122	0.3391484070
Au	-2.6251386960	1.5331501567	0.6677864669
Au	-1.0965510757	-3.1033474364	0.7375897438
Au	1.5028247216	-2.6911564165	0.0805902143
Au	1.1025799430	-0.6434671519	-1.8904732428
Au	1.8076849274	1.9059479000	-0.8511623072

$Au_{12}Y$

E = -1667.0851452714

Imaginary frequencies: no

Y	-0.0689837175	-0.2250646866	0.4670346233
Au	2.1899728175	1.1285532827	2.1750575002
Au	-2.1496606346	-0.3997261205	-1.7497425665
Au	-2.9699554262	-0.8019908571	1.0251316410
Au	0.2988542680	2.8803106913	1.0678467166
Au	0.3922898844	0.5312371635	-2.4641872839
Au	2.3936854244	-1.5121051873	1.6653722629
Au	-1.4207322508	2.1362071269	-1.0397081807
Au	-1.7549437024	-2.8329941539	-0.4191412746
Au	0.8972331986	-3.1564534016	0.0236361597
Au	2.3194441206	-1.0722543977	-1.2194502498
Au	2.1987885788	1.5897002157	-0.5930350262
Au	-2.1940406221	1.7026403887	1.6390070735

$Au_{13}Y$
E = -1802.839659287
Imaginary frequencies: no

Y	0.0387511245	0.0010188891	0.5453532720
Au	2.9159059493	0.1535891947	1.4619507914
Au	-2.4208988761	0.9226576553	-1.0512944191
Au	-2.2111536311	1.6167649220	1.7948952866
Au	2.4020198534	2.4297751793	-0.0385368645
Au	-0.1333836418	0.0335658806	-2.5040165593
Au	1.7569159318	-2.3054830790	1.5262632389
Au	-0.1736184735	2.5172440274	-1.1845295159
Au	-2.8645045914	-0.9699224967	1.1309077818
Au	-0.8647519141	-2.9433941876	0.9985979041
Au	0.8714076774	-2.3351412760	-1.2719899668
Au	2.4351429080	-0.0646329267	-1.3588829691
Au	0.2250289151	2.8141559817	1.6397256169
Au	-1.9503272475	-1.8802137894	-1.3816032180

$Au_{13}Y\_2$
E = -1802.8353747458
Imaginary frequencies: no

Y	-0.0826523218	0.0396210567	0.5683087821
Au	2.2227370453	1.4488374775	2.0150913549
Au	-2.0533357828	-0.0713877025	-1.6725334421
Au	-2.2855277997	-2.0151751889	0.5821107658
Au	0.5097956530	3.1148773279	0.6159016777
Au	0.7778427344	-0.2328571058	-2.6095070463
Au	2.1383580725	-1.2688774254	2.2239337668
Au	-0.3863017054	2.2190704074	-1.8873502947
Au	-0.5347184556	-2.4685984221	-1.5282451837
Au	0.3150854244	-3.0192091061	1.0916352167
Au	2.1635687907	-1.5757008225	-0.5981108061
Au	2.2560230414	1.3102004329	-0.8189629468
Au	-2.1512466066	2.2038153181	0.2625337484
Au	-2.7405741367	0.2355026032	2.0583665380

$Au_{14}Y$
E = -1938.6082485850
Imaginary frequencies: 8.11i

Au	0.574219	0.041331	2.630682
Y	0.146944	-0.027446	-0.476025
Au	-0.504725	-2.346699	1.498588
Au	2.201616	-1.717274	1.097380
Au	2.621784	1.177067	1.136371
Au	-2.684744	-1.309422	-0.020608
Au	-2.443877	1.596931	0.366562

Au	0.086726	2.461016	1.270899
Au	3.178616	-0.310614	-1.193434
Au	1.974496	2.252098	-1.411075
Au	-0.740219	2.640929	-1.649169
Au	-2.402916	0.403546	-2.226535
Au	-1.152507	-2.174129	-2.186741
Au	1.482685	-2.533901	-1.550549
Au	-2.263696	-0.167332	2.472628

Au_3Y-C_3H_6
E = -563.2784397983
Imaginary frequencies: no

Y	0.4113196605	0.8397840658	-1.0215625178
Au	-1.9454181965	0.8459993326	0.4649511761
Au	-1.5764700807	-1.0588351754	-1.4960807205
Au	2.6003162358	0.1180741663	0.2042980306
C	0.8063141397	3.2978064888	-1.8876590832
C	-0.3728075315	3.8868366576	-1.5036480716
C	-1.5761251168	4.0784554715	-2.3712108856
H	0.9759362487	3.0348807168	-2.9465521928
H	1.7047915276	3.3727117735	-1.2519478879
H	-0.4476254427	4.2849335093	-0.4790987589
H	-1.7573668731	5.1659782970	-2.4931465264
H	-2.4912067716	3.6793374847	-1.8932449858
H	-1.4621866510	3.6379434679	-3.3749060019

Au_4Y-C_3H_6
E = -699.0480296263
Imaginary frequencies: no

Y	1.0240996616	-1.4147147721	1.1206791162
Au	-0.7204504677	0.6917051978	-1.0636707861
Au	0.3539086529	1.2296927685	1.3811203123
Au	0.0528396431	-1.9566337947	-1.3565828465
Au	3.4175626027	-2.1938971526	1.7758339945
C	-1.8080617146	1.2938675907	-2.9214824749
C	-1.8925718368	2.4440707700	-2.0990602148
C	-3.1247743769	2.8469868395	-1.3326046193
H	-2.6720537350	0.6263741554	-3.0277832591
H	-1.0437138835	1.2312935261	-3.7051779023
H	-1.1145012660	3.2127771416	-2.2156387785
H	-2.8774313639	3.3299727059	-0.3724842139
H	-3.8047513262	1.9990467666	-1.1484184625
H	-3.6774602971	3.6006808547	-1.9306835813

Au_4Y-C_3H_6_2
E = -699.0471736197

Imaginary frequencies: 18.36i; 10.85i

Y	0.1048623003	-0.2939471924	0.8564819601
Au	1.2867252505	0.2887961134	-1.6522835179
Au	-1.1892304542	1.1103649638	-1.2510703837
Au	2.5017069945	-1.5105974920	0.1275218670
Au	-2.6636557501	0.0640381725	0.8829838727
C	0.7349697176	1.5030152634	2.6486374711
C	1.5197171397	2.3238638801	1.8755156589
C	3.0087017733	2.2660506374	1.7789611070
H	1.2014183893	0.8145638697	3.3737364852
H	-0.3328125957	1.7382731229	2.7961577723
H	1.0222605285	3.1032441059	1.2770206656
H	3.3322064760	2.1234514120	0.7292225634
H	3.4522165111	1.4762265959	2.4056972317
H	3.4319378946	3.2427234143	2.0891442019

Au_5Y-C_3H_6

E = -834.7891816867

Imaginary frequencies: no

Y	0.8230661417	-2.1779539276	0.4470177652
Au	2.6221299635	-1.5517079989	-1.5036309125
Au	1.0975926179	0.4905080160	-0.3134909539
Au	-0.7343866186	1.9328143085	1.1250098463
Au	-1.4862543966	-0.6273550551	0.7161818660
Au	-1.6189650698	-3.3703367766	0.1822662403
C	-1.5379167383	3.7677384802	2.2307225201
C	-0.5432444610	4.3428697099	1.4294668325
C	-0.7938238172	5.0469807825	0.1237945053
H	-2.5935526777	3.8297374085	1.9376033055
H	-1.3316536265	3.5140926419	3.2771719785
H	0.4688894076	4.4356300198	1.8516623873
H	-0.0308282584	4.7945895508	-0.6330520837
H	-0.7181658338	6.1408556560	0.2901388759
H	-1.7945671051	4.8341371206	-0.2858471657

Au_5Y-C_3H_6_2

E = -834.7886222835

Imaginary frequencies: 8.98i

Y	0.1664609533	1.6021506360	2.4566983657
Au	1.3982198695	0.8313879896	0.0684119206
Au	-1.4697490130	0.2115495783	0.6749703320
Au	-2.5409632047	2.0279477265	2.4942957997
Au	2.2556693193	3.0860163117	1.5125839443
Au	0.0638208178	-1.3149965639	-0.9460107825
C	-0.1763957601	-3.3810678696	-1.9467891307
C	0.5893481219	-2.6885102206	-2.8906660020

C	0.0419321842	-2.0306862628	-4.1281913304
H	-1.2586375001	-3.4985877675	-2.0838225641
H	0.3032753041	-4.0435591182	-1.2170958779
H	1.6851054955	-2.7581680834	-2.8167630182
H	0.3231834187	-2.6409577424	-5.0099264924
H	0.4819875929	-1.0306414561	-4.2890394403
H	-1.0566749517	-1.9433400321	-4.1074726447

Au_5Y-C_3H_6_3
E = -834.7861309501
Imaginary frequencies: no

Y	-0.0240284794	0.0560655430	0.6866119072
Au	2.1277710968	-0.7844504891	-0.9848727264
Au	-2.4375785800	-0.7212088336	-0.6477494289
Au	-2.4325014258	1.5503162201	0.8468642161
Au	2.5618870347	1.2467168735	0.7637685244
Au	-0.2138982074	-2.0688901842	-1.4068933477
C	-0.0137576194	-1.1286180331	3.0334285718
C	0.1864200386	-2.4210729255	2.6184311351
C	1.5133211496	-3.0993186803	2.4929322303
H	-1.0287790489	-0.7688084761	3.2667762404
H	0.8294601945	-0.5327016161	3.4220665842
H	-0.6970513821	-3.0310362728	2.3729428973
H	1.5688912773	-3.9158062775	3.2422188975
H	2.3639957273	-2.4194165757	2.6621670902
H	1.6235197356	-3.5913299460	1.5086238932

Au_6Y-C_3H_6
E = -970.5538712545
Imaginary frequencies: 13.38i

Y	-0.6736049745	1.2604106715	1.9301380150
Au	1.4218443265	0.8124206146	0.0111603965
Au	-1.1657774578	0.4635117444	-0.8018700893
Au	-0.4577111480	-1.3733105992	2.4453288427
Au	1.7662631608	2.6970910005	1.9286041193
Au	0.4368636242	-1.7344935273	-0.3612725190
Au	-2.9725545414	2.0299996529	0.4710679570
C	0.6677431605	-4.0052215248	-0.4956855670
C	1.1802051992	-3.5594775016	-1.7253640519
C	2.6459585758	-3.4224176540	-2.0401603276
H	1.3460508562	-4.2939709053	0.3165038793
H	-0.3695840470	-4.3524508708	-0.4184163077
H	0.4885139879	-3.4855893647	-2.5774454210
H	2.9510367881	-4.2729050059	-2.6828186789
H	3.2731573162	-3.4380710412	-1.1339332637
H	2.8598714878	-2.5047126455	-2.6149487742

$Au_7Y\text{-}C_3H_6$
E = -1106.303856521
Imaginary frequencies: no

Y	-1.3965404107	-0.2097040541	0.2682568801
Au	3.2457739078	0.9012314534	0.2717635234
Au	1.3531325433	-1.0526050598	0.2356381267
Au	-0.5895835158	-2.9449427963	0.2690635385
Au	0.7015026398	1.6864216805	-0.2681740167
Au	-1.8667864621	2.4178886251	-0.7337168149
Au	-3.3088301101	-2.2056390086	-0.4175129925
Au	-3.9220890767	0.3728353028	-0.9073404008
C	5.4725753643	1.3966669816	-0.0393461879
C	5.3745362804	1.4455296393	1.3534649757
C	5.7685258262	0.3305306116	2.2830789636
H	5.4055863121	2.3136473469	-0.6370116270
H	5.8823166160	0.5115247524	-0.5419623920
H	5.1330849154	2.4127490332	1.8199658865
H	5.0295305155	0.1869716622	3.0909596897
H	5.9187013044	-0.6252645707	1.7547396122
H	6.7216164977	0.6015452697	2.7805085007

$Au_8Y\text{-}C_3H_6$
E = -1242.0673841134
Imaginary frequencies: 2.20i

Y	0.9943981743	0.5728881532	-0.0515722736
Au	1.5630287053	-2.1190508936	0.6337199306
Au	-0.9593356663	-1.3273573022	0.8142959175
Au	-3.5734696400	-0.4579006736	1.0014612590
Au	4.2376118470	-2.2966743987	0.2672973303
Au	3.8219725461	0.2399309004	-0.3644701762
Au	-0.0172087044	3.1827330415	-0.7208457369
Au	-1.8051851120	1.3621183532	0.1412874565
Au	2.8061398027	2.6350919314	-0.8732327023
C	-5.4503312957	-1.1525299436	2.1315937054
C	-5.6486088438	-1.7305681472	0.8739223408
C	-6.5232787063	-1.1619656998	-0.2093459764
H	-5.0091707719	-1.7323822298	2.9510770574
H	-5.9646782988	-0.2228254165	2.4078717163
H	-5.2632662139	-2.7477067017	0.7075055512
H	-6.0396389680	-1.2245184120	-1.2000124355
H	-6.8135403572	-0.1169344750	-0.0134670331
H	-7.4479977648	-1.7696553289	-0.2753876670

$Au_9Y\text{-}C_3H_6$
E = -1377.7989311046

Imaginary frequencies: no

Y	0.3917336847	-0.3954936617	0.3283126608
Au	2.1102361829	-2.5551670010	-0.6868508798
Au	-1.6896781194	1.5217956891	-0.2311264578
Au	-1.2714940141	0.6443414195	2.6065563161
Au	3.1656205197	-0.9022060984	1.1606620269
Au	0.4666621711	1.9354417925	-1.6395250180
Au	-0.6657325693	-2.9734138632	-0.4105785248
Au	1.3357161925	0.2785913495	2.9654257569
Au	-3.7790318015	0.8839556472	1.5543633225
Au	-2.4585264860	-1.2925572845	0.5857310064
C	2.5768704642	2.6493639828	-2.3906199632
C	1.9910882589	2.2156120696	-3.5764266270
C	1.2909344291	3.1042262728	-4.5673160604
H	3.2566366329	1.9980073429	-1.8300000153
H	2.5803354187	3.7129018958	-2.1201342346
H	2.1594892505	1.1739603567	-3.8865313083
H	0.3408372633	2.6618408816	-4.9174947290
H	1.9309108422	3.2117787264	-5.4661683845
H	1.0953483349	4.1124206624	-4.1663777988

$Au_9Y\text{-}C_3H_6\_2$

E = -1377.7981761747

Imaginary frequencies: 2.60i

Y	-0.1076413408	0.6927824335	1.9946407409
Au	2.4266414446	-0.4294880134	2.9643373250
Au	0.1390652897	-0.7650160837	-1.6878402116
Au	-0.1370795200	1.7677495104	-0.7365686293
Au	2.5255659032	2.1488616161	2.0536606367
Au	2.0834238191	0.1322937216	0.1287317947
Au	0.1170778305	-1.3238066843	4.1026365622
Au	0.3062476923	3.6076070933	1.2594644606
Au	-2.1281188347	-0.1691137533	0.0528354126
Au	-2.1762816862	-1.2575343512	2.5033800004
C	0.8384475969	-2.5383480132	-2.9770269244
C	-0.5496346267	-2.5431448477	-3.1752523500
C	-1.2516598414	-1.9406937906	-4.3633100933
H	1.5095473470	-2.0924129096	-3.7214085796
H	1.2964421777	-3.2083662527	-2.2400728393
H	-1.1604571509	-3.1763377216	-2.5144255336
H	-2.1745302151	-1.4112086207	-4.0686285731
H	-1.5633082260	-2.7585186569	-5.0438684356
H	-0.6064294614	-1.2525225400	-4.9332564722

$Au_9Y\text{-}C_3H_6\_3$

E = -1377.7968437111

Imaginary frequencies: 20.04i; 16.65i; 7.85i

Y	0.3530148721	-0.3560859103	0.3975884316
Au	3.2985043515	-0.4098193640	0.0411115022
Au	-1.0784665003	1.4228427555	-1.4567891919
Au	-3.0212181336	1.3312365315	0.4484856039
Au	2.1327640784	2.0030811592	0.8605469746
Au	1.6601109981	1.0786819059	-1.8288808705
Au	2.0645991911	-2.7291437623	0.6298747198
Au	-0.5118728989	2.3035056857	1.3392531627
Au	-2.2240480113	-1.1084467011	-0.7849165349
Au	-0.6421236153	-3.0791751643	0.0884154830
C	-4.5307973270	2.0817545128	2.0127549503
C	-5.2530988417	1.0762892779	1.3551910451
C	-6.2677884238	1.3263057570	0.2725537492
H	-4.6941556412	3.1373815592	1.7630410152
H	-4.0152884104	1.8742745681	2.9575241808
H	-5.2119273401	0.0571494560	1.7670204392
H	-6.2006641118	2.3455934645	-0.1423770159
H	-6.1848631934	0.5955747853	-0.5511569721
H	-7.2819866890	1.1965111616	0.7021012799

$Au_{10}Y\text{-}C_3H_6$

E = -1513.5771640883

Imaginary frequencies: no

Y	0.4058676855	0.7026335038	0.8777426990
Au	3.0797012972	1.8105128911	0.2439527107
Au	-1.0710676585	-0.6807541732	-1.2755808430
Au	-2.5708005615	0.5459455576	0.8098036346
Au	1.0728974966	3.5778892552	0.5296187932
Au	-0.4891616635	2.1055429584	-1.5504955805
Au	3.0151897080	-0.9491109126	0.2197587154
Au	-1.6312213671	3.0859498688	0.8485045122
Au	-2.1721073696	-2.2328025952	0.7240618997
Au	0.6244490623	-2.2108526848	0.4708650788
Au	1.5260068136	0.2964250131	-1.8293371486
C	-2.8901076104	-4.1069847201	1.8968402302
C	-4.0583082839	-3.3435176597	1.8039529521
C	-5.1418387808	-3.5631472315	0.7809349310
H	-2.7154947339	-4.9439034947	1.2093660033
H	-2.2666375546	-4.0698108285	2.7970973996
H	-4.2874745523	-2.6436489719	2.6210008150
H	-5.5149653950	-2.6114750516	0.3634956442
H	-6.0069176296	-4.0519213375	1.2726666818
H	-4.8097319974	-4.2137006215	-0.0447062330

$Au_{10}Y\text{-}C_3H_6\_2$

E = -1513.5747342932
Imaginary frequencies: no

Y	-0.5378778938	-0.1485986898	1.4601270062
Au	2.1043565494	0.8889699880	2.2524846947
Au	0.1306365145	-1.4788063554	-1.0014379482
Au	-3.0007415764	0.6794118776	0.0479290598
Au	0.3104051996	2.6738051361	1.3644965597
Au	2.2664273154	0.2546727414	-0.6461249923
Au	1.9018049666	-1.7741594558	1.6709638964
Au	-1.9504889970	3.2180283855	-0.0659725603
Au	-2.5519865532	-1.9507534106	0.2949645348
Au	-0.2801286939	-3.3404688932	1.0501707183
Au	-0.3567186446	1.1963882420	-1.1463134940
C	4.4841447363	0.8189701198	-0.9267316158
C	4.0264363953	0.6757662104	-2.2448563610
C	4.2436507457	-0.5423643026	-3.1027062405
H	5.0568988976	0.0168785837	-0.4454820318
H	4.5381560109	1.8103254791	-0.4624159642
H	3.6438234298	1.5703221858	-2.7583061928
H	4.5682264895	-1.4178095254	-2.5168601136
H	5.0310978535	-0.3145788260	-3.8492941290
H	3.3370249004	-0.8059636608	-3.6749689205

$Au_{11}Y\text{-}C_3H_6$
E = -1649.3160582259
Imaginary frequencies: 7.65i

Y	0.0142590044	0.1698645790	1.3150233709
Au	3.1487293021	-0.5862734124	1.2889798494
Au	-2.3254658477	0.9461049290	-0.2886486967
Au	-2.0738353899	2.2371659642	2.2574267397
Au	2.4662572937	1.9222747419	0.4871479341
Au	0.1538491530	1.8243161698	-1.1787903434
Au	1.2509107810	-2.5703230653	0.9972927232
Au	0.2004058253	3.2839386612	1.2538504498
Au	-2.9417957130	-0.3696297451	2.1581587085
Au	-1.1650700850	-2.3911123785	2.1422447849
Au	-0.9135854141	-0.4204633139	-2.3356370557
Au	1.6396953852	-0.5965663304	-1.0661059744
C	-1.1157800543	-2.1589512884	-3.8297171095
C	-2.4516816316	-1.8984221025	-3.4940145855
C	-3.4080406391	-1.0978258262	-4.3365289343
H	-0.6910713986	-1.7776799267	-4.7669447447
H	-0.5624936404	-2.9630298266	-3.3312968314
H	-2.8895697423	-2.4584841922	-2.6543988533
H	-4.0732874225	-0.4667851574	-3.7219726765
H	-4.0656907987	-1.8007158287	-4.8877377475

H -2.8913565486 -0.4650161603 -5.0765151821

$Au_{11}Y\text{-}C_3H_6\_2$
E = -1649.3143012406
Imaginary frequencies: 17.06i

Y	0.3887035239	0.5417319834	0.6024513067
Au	3.0678671901	0.0482915902	1.8833747802
Au	-1.7346943561	0.0918032171	-1.4041120061
Au	-2.0461860969	2.2416281571	0.4865700094
Au	2.7695146719	2.3413698874	0.2528747848
Au	0.7027732559	1.2943737548	-2.2406691068
Au	1.6193798263	-2.1493032951	0.9780603949
Au	0.3129351072	3.4088564889	-0.3298820473
Au	-3.1655856153	-0.3268099076	0.8842028207
Au	-1.0825285506	-2.1559891082	0.4165408998
Au	0.6646040745	-1.4859879569	-1.7315883527
Au	2.9438250735	-0.1941979995	-0.9564297411
C	-4.5804147976	-1.3237105495	2.4202930213
C	-4.9783692322	0.0192122715	2.4529707897
C	-6.1624539449	0.5813089618	1.7106251057
H	-3.8864207664	-1.7198445822	3.1702467509
H	-5.1452491935	-2.0583877427	1.8331113724
H	-4.5129121925	0.6785194485	3.2001452972
H	-6.5355070285	-0.1071279378	0.9348971021
H	-5.9302860223	1.5567237831	1.2478950342
H	-6.9834773016	0.7626035311	2.4328897645

$Au_{11}Y\text{-}C_3H_6\_3$
E = -1649.3136373615
Imaginary frequencies: 18.50i

Y	-0.2578055735	-0.5116766828	1.1549886141
Au	2.0671731262	-2.0072166540	2.3866775421
Au	-1.3266016879	1.2225821388	-0.9693083999
Au	-2.5074954765	1.9671848615	1.4569623014
Au	2.3130415334	0.7997184261	1.9631585562
Au	1.4902079466	1.5346108861	-1.0168541127
Au	0.8303016985	-3.1933357416	0.1490539867
Au	0.1757794284	2.3977977702	1.5914864604
Au	-3.1942357810	-0.5110520221	0.4614726503
Au	-1.7781479579	-2.6394066883	-0.4063051504
Au	0.2105718782	-0.9411013090	-1.7158229820
Au	2.6047059440	-0.9905460626	-0.2063307496
C	3.1093305402	3.1670189262	-1.4142433053
C	2.4071920726	3.1609056445	-2.6234257504
C	1.3638363092	4.1717671077	-3.0146337636
H	4.0275410590	2.5797829286	-1.2984248001

H	2.9290322328	3.9533977479	-0.6715043382
H	2.7462840373	2.4764588585	-3.4152758409
H	0.5024213593	3.7002542074	-3.5195196336
H	1.8089105511	4.8753231974	-3.7474546288
H	1.0039632860	4.7586782840	-2.1532417151

$Au_{11}Y\text{-}C_3H_6\_4$
E = -1649.3134334636
Imaginary frequencies: 13.88i

Y	-0.6051377943	0.1621928665	0.9807631533
Au	2.1128025596	0.3435727815	2.2693241770
Au	-2.2913384976	0.1794278483	-1.4310098157
Au	-3.4327481506	1.2345124437	1.0696394766
Au	1.2076349690	2.6415551481	0.9620975049
Au	-0.0149525051	1.8271434891	-1.4713701991
Au	1.6912544045	-1.8567749980	0.6024319402
Au	-1.4944368295	3.0838143773	0.6546962175
Au	-3.1607592793	-1.4833450208	0.7973787410
Au	-0.8684910922	-2.7880880651	0.1950110206
Au	0.2967877499	-0.9189467206	-1.6781305181
Au	2.5355635886	0.6355539542	-0.6531866772
C	4.3409594262	0.5383827282	-2.1162426568
C	4.8058706947	1.4480503811	-1.1595552059
C	5.7533859389	1.1043704849	-0.0424098188
H	4.6670335180	-0.5084257186	-2.0955189971
H	3.8815291426	0.8918576392	-3.0463725351
H	4.6061544721	2.5171252218	-1.3242031533
H	5.4670841771	1.5924944169	0.9056771288
H	6.7625031041	1.4861737075	-0.2982945526
H	5.8305453112	0.0170404596	0.1210829040

$Au_{11}Y\text{-}C_3H_6\_5$
E = -1649.3122838016
Imaginary frequencies: no

Y	-0.6193010160	-0.2809302437	0.9724151172
Au	1.0349595842	-2.3940472575	2.3433371451
Au	-1.8699127807	1.3655319845	-1.1973492083
Au	-1.6730952752	2.4709282587	1.4928809935
Au	3.2907276581	1.2391755054	-0.3880305750
Au	0.8203056249	0.6904077869	-1.5327564480
Au	-0.1989112920	-3.0647561972	-0.1006190082
Au	0.9448391265	2.2436791821	0.8834448672
Au	-3.5230176128	0.3802846534	1.0417143921
Au	-2.8142274288	-2.1545515545	0.3089049507
Au	-1.1759517245	-1.2195560950	-1.9034932867
Au	2.0613091326	-1.2125380829	0.0711640545

C	5.5825351962	1.6023082801	-0.4573131506
C	5.1125767850	2.8453409733	-0.0257790638
C	5.1070047501	3.3124718698	1.4048777371
H	6.0010131235	0.8834134448	0.2581814856
H	5.7942524510	1.4215426125	-1.5180330849
H	4.8773547879	3.6012098367	-0.7900822497
H	4.1664593537	3.8294628970	1.6650572072
H	5.9194014951	4.0546101023	1.5410616655
H	5.2746779705	2.4882587547	2.1174119294

$Au_{12}Y\text{-}C_3H_6$
E = -1785.0846655903
Imaginary frequencies: no

Y	0.5178624961	0.3641909575	0.3716730726
Au	2.8332672023	-0.5940817652	1.9998507148
Au	-1.7568721474	0.3569907734	-1.5634536617
Au	-1.7690103341	2.2490564284	0.6590542434
Au	3.0475474090	1.9395211468	0.7880394168
Au	0.9162275113	-0.0764927607	-2.5926384027
Au	0.7569207053	-2.3168314771	1.8059229324
Au	0.0825029201	2.4142031652	-1.8878459993
Au	-3.3314426543	-0.0950071490	0.6258498938
Au	-1.3472550247	-1.9886055965	-0.0543285037
Au	1.2726530940	-2.3463889175	-1.0229526342
Au	3.1728256479	-0.3958081864	-0.8432477644
Au	0.7302529304	3.3913011914	0.6982225124
C	-4.8919623937	-1.2080370858	1.9247923298
C	-5.0992528395	0.1277046177	2.2871909328
C	-6.1887163989	1.0069764297	1.7353520030
H	-4.2601806529	-1.8608239486	2.5381148040
H	-5.5534333807	-1.6981067623	1.1988010126
H	-4.5434860114	0.5198540853	3.1515845195
H	-5.8165484257	2.0207318018	1.5067880602
H	-6.6562765955	0.5821990198	0.8321088106
H	-6.9772514812	1.1275880023	2.5052950818

$Au_{12}Y\text{-}C_3H_6\_2$
E = -1785.0824904491
Imaginary frequencies: no

Y	0.6749600785	-0.2355863891	-0.8318534189
Au	0.9703686678	-3.0812410205	-1.9032099047
Au	-0.9135731516	1.8866288847	0.5626561188
Au	-1.0143070616	3.0959132162	-1.9860296386
Au	-1.6211062140	-2.0743209984	-1.3559258484
Au	-0.0554410205	-0.2151501211	2.0475740552
Au	3.2463383313	-1.7222742917	-1.3373364649

Au	-2.6276008853	-0.3058076271	0.7816204649
Au	1.4852110796	2.5941168329	-0.9758639928
Au	3.3884334255	0.8661987275	-0.2147988955
Au	2.4435000783	-1.3381863885	1.3889585474
Au	0.1781875328	-2.7617998398	0.7941921301
Au	-2.0026325090	0.5538451199	-1.9344934680
C	-4.5968014267	-1.3475105769	1.3270609495
C	-4.3689084144	-0.4731576506	2.4041243984
C	-5.0402659803	0.8652707270	2.5723470836
H	-4.3120669806	-2.4032049466	1.3989268574
H	-5.3068507181	-1.0807767156	0.5354825892
H	-3.8268916682	-0.8631390429	3.2784626904
H	-5.8304605345	0.7731852420	3.3447723187
H	-5.5136804158	1.2169468823	1.6409442794
H	-4.3373406148	1.6363816516	2.9328960174

$Au_{13}Y$-C_3H_6
E = -1920.8367526031
Imaginary frequencies: 4.48i

Au	0.2718913948	-0.1900214893	2.4756023021
Y	0.4125797525	0.1241703318	-0.4967567725
Au	-1.5244829263	-1.7183191704	0.8993631263
Au	-3.3489708841	0.4535812753	0.2095195640
Au	-1.1439960829	1.9756990087	1.3065248107
Au	1.1312937559	-2.4738754716	1.0122017824
Au	2.9784504857	-0.3547585716	1.3931975401
Au	1.6133872482	2.1301402772	1.5215655981
Au	-1.7115309269	1.9269308575	-1.5301071086
Au	0.8534098374	2.9720887654	-1.2079892493
Au	3.1035424536	1.3537566189	-0.8848692085
Au	2.8037774603	-1.5200326322	-1.2007371961
Au	0.2801965463	-2.5336535064	-1.8135877755
Au	-2.0165682073	-0.9417194927	-1.8466079215
C	-5.0357634361	0.8969697050	1.7215348762
C	-5.5229223327	-0.2437779395	1.0695590618
C	-6.5257615473	-0.2282596420	-0.0514859710
H	-5.3986516454	1.8949365760	1.4461817343
H	-4.5171540523	0.8095049488	2.6827878822
H	-5.2874074313	-1.2259367296	1.5047481320
H	-6.2638417692	-0.9467958936	-0.8478432227
H	-6.6471671202	0.7737949432	-0.4941517880
H	-7.5100558082	-0.5494374701	0.3462372368

$Au_{13}Y$-C_3H_6_2
E = -1920.8339221636
Imaginary frequencies: no

Y	0.4991012265	-0.3367501409	-0.6324727102
Au	1.1273245324	-3.3702125020	-0.8064935761
Au	-1.4891949612	1.8605585605	-0.1070854507
Au	-1.4476425724	2.0744893828	-2.9440435382
Au	-1.5182348896	-2.5577771958	-0.5194853026
Au	-0.6038282957	0.3655805261	2.0890647418
Au	3.1916401405	-1.6197136227	-0.5097599295
Au	-2.9905354476	-0.4282429900	0.8067191441
Au	1.0501037539	2.3162893219	-1.9109380502
Au	3.1628941882	1.1391983653	-0.6164903539
Au	2.2242337620	-0.1931085966	1.8598156534
Au	0.3118658454	-2.2239642744	1.7024678661
Au	-2.2047830295	-0.3578533236	-1.9601833365
Au	1.0948702939	2.3443182253	0.9553044372
C	-5.0412580214	-1.2694119956	1.4750437975
C	-4.7732014691	-0.2821291966	2.4344981604
C	-5.3641545449	1.1032446752	2.4244113787
H	-5.7209267145	-1.0625138016	0.6393063331
H	-4.8117128822	-2.3217002371	1.6762373123
H	-4.2533866688	-0.5874966432	3.3544411778
H	-4.6196354377	1.8692249647	2.7026424253
H	-6.1688712137	1.1542300161	3.1853826888
H	-5.8018645324	1.3641222357	1.4467642535

$Au_{13}Y$-C_3H_6_3
E = -1920.8338644617
Imaginary frequencies: 20.46i

Y	-0.3390153978	0.0384126533	-0.7776775524
Au	-2.3361396316	-2.1511703097	-1.4532176486
Au	0.7879317947	2.4556267716	0.7193165812
Au	-0.0770158410	2.8230027293	-2.0463360994
Au	-3.5041407599	-0.1400981141	0.0408488049
Au	0.1653728476	0.2016924198	2.2453260534
Au	0.2706747689	-2.7698837980	-1.8022020702
Au	-1.8668443018	1.8164543255	1.2219571985
Au	2.3019258346	1.5403219160	-1.5329911764
Au	2.4814820763	-1.1857597413	-1.4531106825
Au	1.1309086380	-2.0553958165	0.9154482654
Au	-1.5987814638	-1.7790236108	1.3272407957
Au	-2.5765802255	1.8977190948	-1.5884508703
Au	2.8291545816	0.3191074744	1.0289420641
C	4.8358410432	1.0094196416	2.0033901442
C	4.4918046097	-0.0786402371	2.8107462669
C	3.8644839346	0.0329529878	4.1740217407
H	4.6551354067	2.0357479780	2.3450032917
H	5.5208810954	0.8848396268	1.1569341742

H	4.8532165054	-1.0748928987	2.5164118690
H	3.4272617603	1.0287776538	4.3543483649
H	4.6460891327	-0.1408330484	4.9413178510
H	3.0922630335	-0.7386066191	4.3370408475

$Au_{13}Y$-C_3H_6_4
E = -1920.8336726618
Imaginary frequencies: 22.15i

Y	-0.6477058468	0.0312975793	0.8855119011
Au	1.8670986034	-0.3164444584	2.4879659716
Au	-2.0357508083	0.4973550905	-1.7628541207
Au	-3.3210721292	1.4025817559	0.7020530348
Au	1.4108428289	2.1754365336	1.4895342312
Au	0.7683359104	-0.1459823388	-1.7869700846
Au	0.9481506172	-2.8669701587	2.8607192779
Au	-0.1027005870	2.3501285628	-0.9572564923
Au	-3.3021301288	-1.3120337513	0.2223670357
Au	-1.3628919574	-2.8414103462	1.4355664890
Au	1.3509740298	-2.0862891859	0.1409868641
Au	2.9777405990	0.2977541031	-0.0736512313
Au	-1.2596292354	2.9182084740	1.6440042799
Au	-1.0924499183	-2.2245946488	-1.3373361379
C	4.9994745147	1.3442142116	-0.5063723036
C	4.8411526646	0.4927989169	-1.6078920835
C	5.5263242095	-0.8384687045	-1.7676947519
H	4.7041018745	2.3972442374	-0.5680369777
H	5.6514244347	1.0614832922	0.3290941849
H	4.3434108530	0.8966345057	-2.5019710015
H	4.8439318252	-1.6040748294	-2.1760125320
H	5.9579926826	-1.2054950766	-0.8219422508
H	6.3507684105	-0.7305783394	-2.5011906781

$Au_{14}Y$-C_3H_6
E = -2056.6151237891
Imaginary frequencies: 11.21i

Au	0.1013394426	-2.0887116441	-1.4971967591
Y	-0.4160179728	0.4520574051	0.2094598981
Au	0.2792048470	-2.2230101497	1.4384515065
Au	-2.1819506691	-2.2234417855	0.1145332437
Au	-2.0896453768	-0.5587022590	-2.2632805953
Au	2.0763076571	-0.1237587168	1.8242629800
Au	2.4727431545	0.9343295566	-0.7628522027
Au	0.5119506230	0.4425503367	-2.6832904709
Au	-3.4738900053	0.2993597005	0.0587952511
Au	-2.1061618812	2.1747734273	-1.5998098075
Au	0.4909347426	2.9789655717	-1.2084698937

Au	1.3623101500	2.6234018262	1.4185798664
Au	-0.0850863037	1.0310160112	3.1957996384
Au	-2.1482820114	-0.5843701486	2.4311392718
Au	2.7053188071	-1.8855488894	-0.1799141308
C	3.4345218049	-3.8496987852	-1.1814733804
C	4.2791263692	-2.8697435218	-1.7206169273
C	5.6755525451	-2.5905290828	-1.2301958306
H	2.5592387512	-4.2045892173	-1.7373621124
H	3.7662653543	-4.4716766829	-0.3408535734
H	3.9879123011	-2.3999217804	-2.6712165387
H	5.8684593444	-3.0377269087	-0.2411728274
H	5.8895132539	-1.5086607451	-1.1872459301
H	6.3979905895	-3.0258449262	-1.9498903923

$Au_{14}Y\text{-}C_3H_6\_2$
E = -2056.6148499307
Imaginary frequencies: no

Au	-0.7653288097	2.0214934420	1.9337506554
Y	0.2435703583	-0.5434156370	-0.7386564649
Au	-0.5648904450	-1.8533953237	1.8619288928
Au	1.3818370262	0.1202783286	2.0810507587
Au	1.2675095660	2.1548181815	0.0935038173
Au	-2.0588265830	-2.5822831591	-0.4093943092
Au	-2.7143859388	-0.1747187219	-2.0124212341
Au	-1.3220610760	2.0236542558	-0.9344952763
Au	3.2157902845	0.0698617364	-0.2135194058
Au	2.0519070694	1.2074719116	-2.4533732749
Au	-0.4011296481	0.5875441153	-3.4570155209
Au	-1.0305542554	-2.1869904205	-3.0171759084
Au	0.5112787905	-3.5281665014	-1.0323495454
Au	2.1566213382	-2.3221165158	0.7967987231
Au	-2.4619780214	-0.0843619579	0.7514541323
C	-1.7614772556	2.2681459337	4.0042012863
C	-2.6135378331	2.9954652362	3.1622083190
C	-2.5738716156	4.4897272188	2.9808064783
H	-1.0015147765	2.7793014612	4.6083450071
H	-2.0017196493	1.2377249459	4.2881364060
H	-3.4864648652	2.4762568800	2.7400586412
H	-3.4212448052	4.9388822620	3.5370980379
H	-2.7055993406	4.7785774782	1.9233611629
H	-1.6407673619	4.9362951021	3.3615816086

$Au_{14}Y\text{-}C_3H_6\_3$
E = -2056.6146695937
Imaginary frequencies: no

Au	0.8619873507	-2.6787578337	-1.8249367798
Y	-0.2146641539	-0.6218475261	0.1293673834
Au	0.9892880828	0.2198297535	-2.5055506091
Au	2.7783182116	-0.8891997831	-0.6910952976
Au	1.5636637011	-3.0144031485	0.8829392806
Au	0.2192162347	2.3515568775	-0.8244283008
Au	-3.2771700170	-0.5119365890	-0.1885148930
Au	-1.7511815141	-1.9306994773	-2.1137643190
Au	2.1004904488	-0.4298979914	2.0373548759
Au	-0.1044603985	-1.9949932980	2.8598057718
Au	-2.1244070979	-0.2200324547	2.4196130718
Au	-2.1281239319	1.9404773121	0.6026896102
Au	0.2805788948	1.6805210831	2.0195157434
Au	2.7854699423	1.7168179524	0.4666096930
Au	-1.7294604084	0.8724140757	-2.1262538637
C	4.0714869717	3.1949938512	-0.7650969444
C	3.7032926196	3.9652599093	0.3451617513
C	4.5720854122	4.1907162797	1.5539664737
H	5.0572995319	2.7161355459	-0.8107439982
H	3.5218748061	3.2736383122	-1.7095805655
H	2.8018866450	4.5904852924	0.2682621037
H	5.4191003381	3.4871435345	1.5990617846
H	3.9954732783	4.1252186228	2.4932152798
H	4.9818133287	5.2201533008	1.5095647849

$Au_{14}Y$-C_3H_6_4
E = -2056.6124983503
Imaginary frequencies: 20.99i; 16.88i

Au	0.5048467908	-0.4091961421	-3.2758597078
Y	-0.0103808582	0.1606916705	-0.2800464902
Au	1.1755429179	-2.5577851796	-0.0119819807
Au	-0.7112916607	-2.5110481976	-2.0513303556
Au	-1.1150255824	1.8541659803	-2.4621867375
Au	2.4002582827	-0.5657301700	1.5423512505
Au	2.5960716652	1.9743298245	0.2344596558
Au	1.7367984400	1.9255644802	-2.3777718105
Au	-2.5949131630	-0.4260918486	-1.6182928583
Au	-2.6821439007	2.0778713226	-0.2631693106
Au	-0.0160329383	3.1288839222	-0.0839131281
Au	0.6825542233	1.6588169144	2.2876117243
Au	-0.2263774598	-0.9792933978	2.5208017591
Au	-1.7702197704	-2.1127943633	0.5699449395
Au	2.7221363259	-0.5266234352	-1.2435143018
C	-3.7817885021	2.9101051133	1.5710610708
C	-4.6656977007	1.9407904408	1.0696202194
C	-5.8573447353	2.2384016207	0.1972142735

H	-3.9316431946	3.9739365657	1.3481501543
H	-3.1118168944	2.6760671555	2.4054222476
H	-4.6045025894	0.9253421393	1.4861098857
H	-5.8004300141	3.2340315260	-0.2729733713
H	-6.7719973608	2.2096236895	0.8232557939
H	-5.9906403804	1.4737410802	-0.5872410608

XYZ coordinates of the optimized cluster-propene complexes with one hydrogen dissociated from the propene to the cluster for Au_6, Au_5Y and Au_6Y on BP86/LANL2DZ level and total energies (in Hartree) on TPSSh/DEF2-TZVP level. The imaginary frequencies are also collected.

Au_6-C_3H_6_1
E = -932.0380041454
Imaginary frequencies: no

Au	1.7735547903	0.6954551700	0.0593961193
Au	-0.9946588131	0.9240531312	-0.0848282185
Au	0.1887806277	-1.7104021797	-0.0556975119
Au	-2.6996729030	-1.2177911083	-0.1793935185
Au	0.5396010905	3.0893985708	-0.0320925895
Au	2.8579636239	-1.7333478597	0.1315166035
C	-4.6311357212	-0.6118243638	-0.2263060206
C	-5.3456025429	-0.3096655886	0.9018129303
C	-6.5915479165	0.5287316733	0.9054806543
H	-5.0503436710	-0.5230346248	-1.2403321713
H	-4.9969511765	-0.6616759628	1.8846729510
H	-6.8939297020	0.8536620134	-0.1013819326
H	-7.4158295050	-0.0584460922	1.3629137006
H	-6.4624770057	1.4185105893	1.5514189401
H	-1.3506567455	-2.4143584644	-0.2163867325

Au_6-C_3H_6_2
E = -932.0680784138
Imaginary frequencies: no

Au	1.1395146896	-1.1279786930	-0.0299369560
Au	0.8715487320	1.7444409178	0.0249112202
Au	-1.5964314598	-0.5772264529	0.0412424290
Au	-1.8328941409	2.2668141115	-0.1583283284
Au	3.2235279001	0.5322297433	0.0818804437
Au	-0.6847981706	-3.0885456710	-0.0930479596
C	-3.8396724091	1.2499433500	-0.7768536024
C	-3.3746606747	0.4817022658	0.2933095367
C	-4.0121036689	0.3855504036	1.6454804151
H	-3.5518725983	1.0401639298	-1.8151108909
H	-4.7236593163	1.8921745228	-0.6402742978
H	-4.7671735627	1.1832263461	1.7876250262

H	-4.5360066832	-0.5879964252	1.7205845673
H	-3.2827302761	0.4252799488	2.4711711013
H	-0.2968735214	3.1149930557	0.0334393262

Au_5Y-C_3H_6_1
E = -834.7481763940
Imaginary frequencies: 10.47i

Y	-0.0100753465	-0.5615205866	-0.1075080385
Au	-2.5033481294	0.7385368406	0.4695820530
Au	2.2693862276	1.2392977300	-0.4357936416
Au	2.7488142901	-1.4301817182	-0.0119926529
Au	-2.3471961601	-1.8094804361	-0.8409297949
Au	-0.3715704178	2.3020980850	0.2113975774
C	1.2823330513	-2.5761144702	1.0096876921
C	0.8981982763	-2.2725253231	2.2890153577
C	0.0534792610	-3.1555139939	3.1698627014
H	1.0190332368	-3.5452791080	0.5544712847
H	1.2534071729	-1.3364017396	2.7579224069
H	0.6519622632	-3.4699543412	4.0481277362
H	-0.2968755966	-4.0595713825	2.6471301225
H	-0.8194576194	-2.6066282494	3.5705360418
H	1.2900265026	2.7606908132	-0.1855883408

Au_5Y-C_3H_6_2
E = -834.7390237583
Imaginary frequencies: 17.68i

Y	0.1664094621	-0.8732671924	0.4913525973
Au	-2.6354514313	0.6058049798	0.3703773396
Au	2.1349401886	1.2465765764	-0.2777329622
Au	3.0272644852	-1.2119322294	-0.2307598411
Au	-2.1970705334	-1.6802433245	-0.9985709002
Au	-0.4593083909	2.0823204116	0.0463212440
C	0.2672418821	-3.0631411815	1.9276879736
C	0.0935425080	-1.8441909394	2.5187118766
C	-0.0220559013	-1.6250021488	4.0024620259
H	0.3408002376	-3.2141176982	0.8159445821
H	0.3549413121	-4.0310781749	2.4416107743
H	0.7855775497	-0.9577431335	4.3580738740
H	0.0204191112	-2.5628550849	4.5870334344
H	-0.9712052211	-1.1122671908	4.2471572847
H	1.1875559229	2.7699006978	-0.1668980354

Au_5Y-C_3H_6_3
E = -834.7747595710
Imaginary frequencies: 9.12i

Y	0.0120726769	-0.6659371952	0.2925744522

Au	-2.5839662406	0.6205876541	0.4126748318
Au	1.9545209020	1.1821960034	-0.9268240218
Au	2.7804061680	-1.2048436585	0.1118857959
Au	-2.3439487677	-1.7689304727	-0.8293505656
Au	-0.1794420882	2.2088861019	0.4704423867
C	2.4897700455	-2.8371613645	1.5229287066
C	1.4740683144	-2.2616496637	2.4029320763
C	0.0918616750	-2.3571908991	2.2386309060
H	3.4911043616	-2.9468757323	1.9658588688
H	2.1866987213	-3.7025596150	0.9133744702
H	1.8482920743	-1.6424890190	3.2323237175
H	-0.3342747318	-3.1240975977	1.5651265397
H	-0.5812026624	-1.9966449091	3.0265222952
H	-1.9936802684	2.1264744305	1.0319946100

Au_6Y-C_3H_6_1
E = -970.4854220650
Imaginary frequencies: no

Y	-1.0838297179	-0.4339842207	-1.0261558913
Au	0.3083200159	-1.2806378394	1.3548204305
Au	-0.8197394703	1.1620347203	1.3647709763
Au	1.2513702726	0.5522469963	-2.0517011617
Au	-0.7071363656	-3.1523465820	-0.3829514428
Au	1.9392247477	0.9434968983	0.5963218553
Au	-2.8351329615	1.6966143249	-0.4104322064
C	3.6688141465	1.9000733434	-0.0234538455
C	4.8634064294	1.2884484606	-0.1358106521
C	5.2430149751	-0.1127103564	0.2533700001
H	3.4705381773	2.9562890270	-0.2403841522
H	5.6704170459	1.8977520222	-0.5796145575
H	5.5918186246	-0.6853739470	-0.6265859787
H	4.3971743343	-0.6532857594	0.7127240843
H	6.0815917247	-0.0992550737	0.9745583257
H	2.5908129258	1.2631166948	2.0193013856

Au_6Y-C_3H_6_2
E = -970.5288599421
Imaginary frequencies: 17.42i

Y	0.0898643033	0.4771893386	-0.1732320867
Au	2.0604876452	1.1177072474	1.6762554625
Au	-1.1058859468	-2.3403761728	-0.0347590840
Au	-1.6196986121	2.6253407149	-0.8036631602
Au	2.9497749198	0.4769205925	-0.8209562692
Au	-2.7918452253	0.4184696457	0.1935865106
Au	1.4319837222	-1.9871373431	-0.5050703712
C	-3.4209914336	-2.5036060640	-0.0277176362

C	-3.2383202850	-1.4616496072	0.8933777721
C	-3.3712918388	-1.6579116287	2.3809200859
H	-3.7337232552	-3.4959290002	0.3327790446
H	-3.5720719952	-2.3100939835	-1.0970686334
H	-2.5638322014	-1.1659969930	2.9496592865
H	-3.4061110431	-2.7281772035	2.6556280720
H	-4.3178378968	-1.1887821886	2.7156754571
H	1.2119861613	1.4545488798	2.9938428332

Au_6Y-C_3H_6_3
E = -970.5536714556
Imaginary frequencies: 9.74i

Y	1.3383374955	0.1203139409	-0.9484732442
Au	-0.2709448113	1.3527252387	1.1010268382
Au	0.0757686574	-1.3584064752	1.1816851251
Au	-0.9173644608	-0.2365029819	-2.3732979261
Au	1.7502426493	2.7723320841	-0.0397886807
Au	-2.2985756399	-0.3154028071	0.2105683148
Au	2.4329905833	-2.2483343347	0.1540325072
C	-4.4594907877	-0.6385627864	-0.4301338494
C	-4.5618667103	-0.5048904286	0.9657562816
C	-4.9995124608	0.7477362897	1.6761873662
H	-4.7131973181	0.2011909578	-1.0889375837
H	-4.4286876531	-1.6324948844	-0.8921275284
H	-4.5127172388	-1.4200124152	1.5742484684
H	-6.0524059889	0.6197941665	2.0000565435
H	-4.4115737050	0.9281845532	2.5925761398
H	-4.9486019299	1.6389482893	1.0299136013

XYZ coordinates of the optimized clusters and cluster-propene complexes and total energies (in Hartree) on LRC-ωPBE/def2-TZVP+XDM level.

Au_4
E = -542.876207478283

Au	0.0000000000	-1.3319672315	0.0000500623
Au	-2.3103296544	0.0000000000	-0.0000500623
Au	0.0000000000	1.3319672315	0.0000500623
Au	2.3103296544	0.0000000000	-0.0000500623

Au_5
E = -678.721463100737

Au	2.3473859286	0.0541456636	1.2801965724
Au	2.3286944660	-0.0546678997	-1.2870463118
Au	0.0000000000	0.0000000000	0.0136994789
Au	-2.3286944660	0.0546678997	-1.2870463118
Au	-2.3473859286	-0.0541456636	1.2801965724

Au_6
E = -814.521701019185

Au	3.0090369630	0.5717176954	0.0002161333
Au	0.5379974476	1.4358532960	0.0011092181
Au	1.0250958034	-1.1369178220	-0.0014543346
Au	-0.9633014463	-2.8423698188	-0.0003812031
Au	-1.9372493812	2.2903678862	-0.0014366718
Au	-1.6715793866	-0.3186512368	0.0019468580

Au_7
E = -950.370953199763

Au	2.6917207532	-0.0001917551	0.0018159984
Au	1.3456004375	2.3290192669	-0.0009160986
Au	1.3452706249	-2.3292095017	-0.0009170368
Au	-1.3452706249	2.3292095017	-0.0009170368
Au	-2.6917207532	0.0001917551	0.0018159984
Au	-1.3456004375	-2.3290192669	-0.0009160986
Au	0.0000000000	0.0000000000	0.0000342741

Au_8
E = -1086.18306961367

Au	1.4787232259	1.0393341837	-0.1818874140
Au	-1.2730516833	1.2555595423	-0.1619137797
Au	-0.0914706580	-1.1994123342	-0.9656308943
Au	1.2370224742	-1.2183602814	1.5055989693
Au	-2.7438783542	-0.8697048289	-0.9333740105
Au	0.2776142764	3.3374788348	0.1394184925
Au	2.5785458083	-1.3151673667	-0.8898017861
Au	-1.4635050893	-1.0297277495	1.4875904229

Au_8_2
E = -1086.1781595999

Au	2.3866804899	-2.5586680240	0.0000000000
Au	0.0443025060	-1.4059327586	0.0000000000
Au	-2.2191122881	-2.7053609757	0.0000000000
Au	-2.3268472442	-0.0738887542	0.0000000000
Au	-2.3867488903	2.5586699887	0.0000000000
Au	-0.0443284038	1.4059902153	0.0000000000
Au	2.3269295693	0.0738719354	0.0000000000
Au	2.2191242610	2.7053183731	0.0000000000

Au_9
E = -1222.03093754233

Au	3.0332718976	0.4957181757	0.7722388805
Au	0.5746240362	1.5198428574	0.8267479315
Au	-1.9458673520	2.3797375474	0.7680954925
Au	1.0285528425	-1.2578311156	0.8263314846
Au	-1.0878370903	-2.8759999472	0.7642421113
Au	-1.6032951249	-0.2621007773	0.8253296979
Au	1.5492793321	0.2527292472	-1.5927600174
Au	-0.9931929190	1.2152830337	-1.5947804079
Au	-0.5555356222	-1.4673790212	-1.5954451729

Au_{10}
E = -1357.83861841529

Au	1.0325638322	-2.8453035146	1.3406215362
Au	-1.1212901581	-1.4641374886	0.7855088452
Au	-3.2944859999	0.0062477628	0.1869574337
Au	1.2464090960	-1.3141337291	-0.9498429418
Au	0.7830942535	0.2098444511	-3.2082372939
Au	-1.2526318271	0.1103651949	-1.5623946349
Au	1.3890148297	-0.1075402350	1.4987530072
Au	-1.1064459910	1.3600536693	0.9734487777
Au	1.2599745984	1.4140124602	-0.7687897824
Au	1.0637973663	2.6305914290	1.7039750530

Au_{10}_2
E = -1357.84295424075

Au	-0.1126455899	-3.2439011826	-1.6145197744
Au	-1.5845773802	-1.4359301060	-0.4554235704
Au	-0.1124586787	3.2439424276	-1.6144880787
Au	1.1563753245	-1.4018476331	-0.2625925467
Au	3.4761344136	-0.0001338126	-0.0977828528
Au	-1.5844322775	1.4360020742	-0.4553956519
Au	1.8208291370	-0.0000248425	2.0548480465

Au	-0.8215633104	-0.0000231906	1.8036565919
Au	1.1565227410	1.4018040254	-0.2626458400
Au	-3.3941843792	0.0001122402	0.9043436765

Au_{11}
E = -1493.70513722813

Au	-1.4063552794	-0.8113274057	-1.3723926563
Au	1.4063034868	-0.8114175691	-1.3723926634
Au	0.0000522204	1.6265869499	-1.3728827135
Au	1.4063034868	-0.8114175691	1.3723926634
Au	-1.4063552794	-0.8113274057	1.3723926563
Au	0.0000522204	1.6265869499	1.3728827135
Au	-0.0000001249	0.0024415917	3.5058271100
Au	-0.0000001249	0.0024415917	-3.5058271100
Au	-3.3211254747	-1.9268761955	0.0000000000
Au	0.0001237726	3.8413990570	0.0000000000
Au	3.3210010891	-1.9270899951	0.0000000000

Au_{12}
E = -1629.50396897513

Au	-3.5527771546	0.0000000000	-0.4161795928
Au	3.5527771546	0.0000000000	-0.4161795928
Au	-1.3528779790	0.0000000000	-1.9812786808
Au	-1.3713355292	-1.3879813927	0.4251714314
Au	-1.3713355292	1.3879813927	0.4251714314
Au	1.3528779790	0.0000000000	-1.9812786808
Au	1.3713355292	1.3879813927	0.4251714314
Au	1.3713355292	-1.3879813927	0.4251714314
Au	0.0000000000	0.0000000000	-4.2256940357
Au	0.0000000000	-2.6634966857	2.3864548339
Au	0.0000000000	2.6634966857	2.3864548339
Au	0.0000000000	0.0000000000	2.5470151895

Au_{13}
E = -1765.34510914659

Au	0.0000000000	2.3980328318	2.0543429160
Au	1.3486181164	0.0000000000	1.9274349750
Au	0.0000000000	-2.3980328318	2.0543429160
Au	-1.3486181164	0.0000000000	1.9274349750
Au	1.3818140118	1.5290364429	-0.3469897570
Au	3.5310080953	0.0000000000	0.2743414264
Au	1.3818140118	-1.5290364429	-0.3469897570
Au	-1.3818140118	1.5290364429	-0.3469897570
Au	-3.5310080953	0.0000000000	0.2743414264
Au	-1.3818140118	-1.5290364429	-0.3469897570
Au	0.0000000000	2.6641815513	-2.3990645075

Au	0.0000000000	0.0000000000	-2.3261505919
Au	0.0000000000	-2.6641815513	-2.3990645075

Au_{14}
E = -1901.16031962883

Au	-0.2596528712	2.1810937533	-1.0262815925
Au	0.5915231175	0.0199130863	1.6001590594
Au	-1.6532051012	-1.5352052323	1.0942124493
Au	-1.7439443343	-0.1004723885	-1.2975124879
Au	-1.8295702110	1.2935679156	1.1177140617
Au	2.1845839776	1.5408404619	-0.0697422475
Au	3.3220362689	0.1904894782	1.9351483162
Au	2.3600514880	-1.2447092680	-0.1043176694
Au	0.0152678079	-2.1822505050	-1.0637982889
Au	2.3136734660	-3.2913589473	-1.7096976103
Au	-1.5272815298	-0.1258813963	3.3657189752
Au	-2.6670025914	-2.6484361310	-1.1235160291
Au	1.8739012434	3.5955394499	-1.6364933387
Au	-2.9803807304	2.3068697231	-1.0815935975

Au_{15}
E = -2037.00166314082

Au	2.4747049492	-1.8709086442	0.0999636165
Au	3.6812251771	0.4954076721	0.3693993781
Au	1.2640905700	0.9236462294	1.7204927594
Au	2.3888830097	3.0091445471	0.2101229513
Au	-0.2911264678	2.7404089524	0.1330575050
Au	-1.4321138890	0.5911326587	1.6922373261
Au	-1.5303426458	0.4595579857	-1.0892777720
Au	-0.0079421700	0.1649515866	-3.2933907327
Au	0.1477449301	-1.7148020825	-1.3787196588
Au	0.4104572457	-3.8530007334	0.2003046400
Au	-3.7166494012	-0.2836636581	0.3436969333
Au	-2.0164872642	-2.3330954043	0.1995519742
Au	0.2020274244	-1.5086674658	1.6256163987
Au	1.3927567228	0.7379952059	-1.0606490295
Au	-2.9672281908	2.4418931503	0.2275937105

Au_4-C_3H_6
E = -660.791671589258

Au	2.3184603369	-0.2296047049	-0.1246222151
Au	-2.2065452550	0.6510273863	0.2377019738
Au	-0.2290428548	-1.2301889441	0.0807216270
Au	0.2663755827	1.4037544213	-0.1498021013
C	0.0941220253	-3.3833946138	0.2028820972
C	-1.2779902266	-3.2040457477	0.1991738031

C	-2.1492921721	-3.4285615695	-0.9962320187
H	0.6274164643	-3.5289781158	1.1407845681
H	0.6072138754	-3.6894258770	-0.7082745029
H	-1.7841813884	-3.1531237928	1.1655593373
H	-1.5841543888	-3.3947359029	-1.9315819977
H	-2.9715213666	-2.7086878637	-1.0448407387
H	-2.6035100496	-4.4239542963	-0.9073568175

Au_5-C_3H_6
E = -796.630577707172

Au	2.8651560836	-0.3876384505	0.0994894043
Au	1.1905120274	1.5791902778	-0.0106264193
Au	-1.6219873063	0.9257641534	-0.1022026260
Au	-2.2026021527	-1.6596343769	-0.0671591636
Au	0.2835126735	-0.9879870454	0.0124621020
C	-1.7007578668	3.1008284971	-0.1424771509
C	-3.0087065142	2.6356234777	-0.1940989437
C	-3.9441640596	2.6241072413	0.9712124330
H	-1.2095701104	3.4243838989	-1.0595045537
H	-1.3094894879	3.4942149105	0.7959602543
H	-3.4671843976	2.5259542028	-1.1792253416
H	-4.5844503858	1.7368424527	0.9642975052
H	-4.6076270220	3.4949080586	0.8883793476
H	-3.4169950019	2.6838450049	1.9270495976

Au_6-C_3H_6
E = -932.430161077037

Au	1.6731470593	0.1252470394	0.0874070349
Au	-0.7616932188	1.3023854608	0.0859753340
Au	-0.5095132290	-1.4439083758	-0.1749617325
Au	-2.9047129798	-0.2725635871	-0.1226347186
Au	1.4498034411	2.7223826945	0.3124929204
Au	1.9223281919	-2.4686252257	-0.1391454630
C	-4.9891549645	-0.4187956964	-0.7797348701
C	-5.0403062790	-0.4532873252	0.5983086643
C	-5.3951184678	0.7119655133	1.4635608982
H	-5.0083336814	-1.3417400020	-1.3578179185
H	-5.2080685639	0.5028424232	-1.3186762003
H	-5.0376812521	-1.4317933625	1.0838472476
H	-5.3377647438	1.6612092489	0.9242251741
H	-6.4266423945	0.5769565318	1.8133907039
H	-4.7635942238	0.7597570036	2.3560340958

Au_7-C_3H_6
E = -1068.28880327553

Au	2.3308074318	-0.7570058802	-1.3652036763

Au	0.7409882323	1.2852046843	-0.6146437939
Au	0.0358225143	-1.4062813755	-0.1205940362
Au	-1.0691368612	3.1112635995	-0.2279858201
Au	-1.7747108361	0.6379324988	0.3256228583
Au	-2.3604780022	-1.8880034977	0.7682222668
Au	2.1938744760	-0.2461684548	1.2499863657
C	3.3282391310	-0.0600229477	3.1002325764
C	2.0023331771	0.1277348936	3.4402903251
C	1.3673336183	1.4610114586	3.6818233873
H	3.9929504047	0.7953012467	2.9814083151
H	3.7985621004	-1.0334164414	3.2301414843
H	1.4382236786	-0.7427598652	3.7824262195
H	1.2733537163	1.6081402116	4.7652128895
H	0.3579322883	1.5060357483	3.2621514380
H	1.9641489499	2.2810247715	3.2735197739

Au_8-C_3H_6
E = -1204.08463024198

Au	2.1054779499	0.6817116531	-0.2402088314
Au	-0.5740670830	1.0698659959	0.0736006817
Au	-1.5807746206	-1.2513385504	-1.1837465867
Au	0.7368245684	-1.5813325342	0.5168399545
Au	-3.2370059693	0.6560925250	-0.0028055727
Au	1.0234891133	3.0496296101	-0.5040660109
Au	3.3062553665	-1.6433593185	0.0280451444
Au	-1.6935142604	-1.0312261770	1.5097373199
C	-2.1205669068	-1.8084503513	-3.2088032612
C	-0.9173143836	-2.4397776791	-2.9346994764
C	0.4107155294	-1.9634078538	-3.4377175222
H	-2.1385109014	-0.8974735648	-3.8058747106
H	-3.0614596793	-2.3469573773	-3.1096294891
H	-0.9555378794	-3.4688437733	-2.5718802681
H	0.3863187894	-0.9075125012	-3.7214154538
H	0.6769463310	-2.5525018302	-4.3244428784
H	1.2008529163	-2.1148432186	-2.6966888032

Au_8-C_3H_6_2
E = -1204.08052270780

Au	3.4565072446	0.3251035275	0.1213396746
Au	0.9151843494	0.9883124068	0.4132881936
Au	0.1128157802	3.2725090747	1.4034395262
Au	-1.7595226175	1.6032135014	0.6316154907
Au	-3.5987789417	-0.0995250851	-0.1484066795
Au	-1.1078935381	-0.8238383561	-0.4098547000
Au	1.5232276582	-1.3975509037	-0.6084074022
Au	-0.3201192582	-3.1393778776	-1.3687864679

C	5.5674501931	0.3162793679	0.7244334535
C	5.5717263434	0.5897573352	-0.6254759689
C	5.8720365403	-0.4120518257	-1.6942027833
H	5.7834852097	-0.6879793581	1.0875015141
H	5.6244401376	1.1238110531	1.4530767211
H	5.5760218010	1.6376094537	-0.9336486493
H	6.8921953825	-0.2365953737	-2.0583458935
H	5.2043612155	-0.2961251199	-2.5535541837
H	5.8119698132	-1.4389042180	-1.3236033045

Au_9-C_3H_6
E = -1339.93714896661

Au	0.7136102540	-1.6303029414	-0.7608857490
Au	-1.4908796131	-2.8354074312	-1.5355507251
Au	-1.7850632053	-0.9897969057	0.2839980077
Au	3.0302840345	-0.7453015245	0.3993786936
Au	-1.8556803073	0.5944474689	2.4523614866
Au	-1.0825266430	1.7736976406	0.1691258080
Au	1.3696078575	1.0241501367	-0.9027324653
Au	0.0200053831	3.0950220066	-1.7945639321
Au	0.6108210276	-0.0732772079	1.5290166698
C	4.9471096536	-1.7034562090	1.0494511356
C	5.2424124092	-0.3704829880	0.9383401931
C	5.3015359299	0.5880869807	2.0840252150
H	5.1592585719	-2.3891158339	0.2304379040
H	4.7323026666	-2.1460053915	2.0218650560
H	5.6424233561	-0.0133268277	-0.0133124267
H	4.8501361246	0.1734893281	2.9894724091
H	4.8156664643	1.5383655714	1.8398977864
H	6.3536157570	0.8158891193	2.2965381335

Au_{10}-C_3H_6
E = -1475.73259927424

Au	3.3406577288	-0.5894002822	-0.7477627850
Au	1.9367481057	1.7544811427	-0.2163437490
Au	-2.5979847206	2.5846210219	0.1022867766
Au	1.5331415721	-0.5289988757	1.2827469556
Au	-0.4796320695	-1.0413872893	2.9648403131
Au	-0.5709295326	1.1789768936	1.0880793072
Au	0.7305798490	-0.4952324064	-1.3839680944
Au	-1.9053860157	0.4452137309	-1.2076588513
Au	-1.0338605179	-1.6891996646	0.4775727379
Au	-1.3676070438	-1.9876530003	-2.1942531487
C	2.0105727030	3.9292648040	-0.2374227618
C	3.0886855452	3.5137224041	-0.9983319969
C	3.1056469619	3.5119543338	-2.4960363577

H	2.1470272426	4.2117377983	0.8049219417
H	1.0959900605	4.2711351157	-0.7201768940
H	4.0572428411	3.4244831057	-0.5034166909
H	3.6407763887	2.6451928160	-2.8943793761
H	3.6383441294	4.4064791207	-2.8428879798
H	2.0959406072	3.5334231112	-2.9155828018

Au_{10}_2-C_3H_6
E = -1475.72420023605

Au	0.7249846755	-3.2770954206	-1.4180312068
Au	-0.8836626264	-1.4654172845	-0.4017919509
Au	0.2276354088	3.2315268857	-1.6642940699
Au	1.8451534370	-1.3197783902	-0.1203085905
Au	3.1623180506	0.2990070005	1.5419602381
Au	-1.0985995997	1.2744515224	-0.5210734495
Au	0.4072450277	0.0920628153	1.8045582925
Au	-2.3147962830	-0.1185750943	1.5855197326
Au	1.6168001335	1.5657058143	-0.2258996682
Au	-3.2723837086	-0.2922437763	-0.9452242520
C	-2.7411243586	-0.0832396690	3.7232717665
C	-3.9756854120	-0.0786779082	3.0959100929
C	-4.8256367584	1.1423169196	2.9293983572
H	-2.3229321731	-1.0114402590	4.1079708499
H	-2.3300387733	0.8413572918	4.1261720077
H	-4.4713524184	-1.0387719000	2.9411263877
H	-5.3540210350	1.1416425373	1.9717398113
H	-5.5896569075	1.1467926441	3.7175327948
H	-4.2424199774	2.0631839304	3.0172252572

Au_{11}-C_3H_6
E = -1611.60128828568

Au	1.4507569611	-0.0871385939	1.6376985617
Au	1.5778771625	-1.1432327052	-0.9749325396
Au	1.2984117286	1.6328316843	-0.5885436150
Au	-1.1729839951	-1.3757860891	-0.9765434771
Au	-1.2927824206	-0.3565657343	1.5547091963
Au	-1.4399523150	1.3263053984	-0.6124600215
Au	-3.5242518363	-0.3436839629	-0.0325137699
Au	3.5642472055	0.3439934704	0.0452835529
Au	0.0456602872	-0.5235281556	3.7915465212
Au	-0.2891401046	3.5219121266	-1.4353621856
Au	0.3552838979	-3.0010061772	-2.3358161349
C	-5.6393072296	-0.8786253662	-0.4604918989
C	-5.7070440349	0.0889186918	0.5092937023
C	-5.9985682765	1.5332996037	0.2542064635
H	-5.6825763725	-1.9338003019	-0.1951628710

H	-5.8000778932	-0.6255814419	-1.5082148524
H	-5.7469247092	-0.2346023777	1.5516822617
H	-7.0281822895	1.7439714236	0.5697269362
H	-5.9034668044	1.7905418272	-0.8042405930
H	-5.3465393188	2.1853016257	0.8442930034

Au_{12}-C_3H_6
E = -1747.39864506264

Au	-0.4150304932	-3.5053319775	-0.1205496634
Au	-0.4322245942	3.5644190628	0.0402550281
Au	-1.9563166789	-1.3183963195	-0.4563591084
Au	0.7559516777	-1.3113765696	-1.1814896469
Au	-0.0187586450	-1.3568813143	1.5186010615
Au	-1.9688598269	1.3951453425	-0.3973910142
Au	-0.0315496602	1.3451334561	1.5798898887
Au	0.7451886440	1.4219906765	-1.1186788778
Au	-4.0524608019	0.0461097812	-1.2382731923
Au	2.9062130767	0.0870510690	-2.1487392294
Au	1.7216169162	-0.0347329645	3.1385862926
Au	2.4344276121	0.0265025140	0.5720185811
C	4.7773138148	0.0997287582	-3.3535748668
C	3.7692847669	0.0201303631	-4.2801309213
C	3.3223353722	-1.2404233157	-4.9482079621
H	5.3235622851	-0.7934231374	-3.0506754051
H	5.2222619797	1.0606658916	-3.0994033114
H	3.3899603221	0.9525037023	-4.7039539042
H	2.2303641410	-1.3020845033	-5.0003491621
H	3.7108189295	-2.1309193859	-4.4465263998
H	3.6891273303	-1.2391088243	-5.9824091052

Au_{13}-C_3H_6
E = -1883.23813788974

Au	-0.2899625575	0.8241613619	-3.0698376964
Au	1.2332591438	-1.0887440346	-1.8058937745
Au	3.2109748000	-0.3671800552	-0.0231628589
Au	1.4998383273	1.5055739781	-1.0992592480
Au	-1.4186862277	-0.9964715513	-1.0871961940
Au	-0.1189526641	-3.3765925353	-1.1593117405
Au	0.8364578694	-1.7783902384	0.8203319109
Au	-1.1482610473	1.6051336518	-0.3700678429
Au	0.6064850193	3.3932387509	0.6678137272
Au	1.1040866769	0.8730817607	1.5461697812
Au	-3.5862727482	0.3666146129	-0.0602975542
Au	-1.5214668054	-0.3185627344	1.5939464594
Au	0.3650886523	-0.9937139093	3.3824441516
C	-5.6387591973	0.7169418994	-0.8749166419

C	-5.8050678952	0.5434817118	0.4743921767
C	-6.2498529372	-0.7296349000	1.1212195787
H	-5.5671668202	1.7157137047	-1.3019337817
H	-5.8232475913	-0.1046240974	-1.5664681219
H	-5.8091206273	1.4344001437	1.1064423081
H	-7.2985983678	-0.6225792372	1.4256276433
H	-5.6762430152	-0.9412109899	2.0293921917
H	-6.1751798565	-1.5825851451	0.4411146497

Au_{14}-C_3H_6
E = -2019.05700433738

Au	2.3858356312	2.4488796457	0.2115318831
Au	-1.8474985698	-0.9093782722	1.2681495860
Au	-1.7467079860	-0.7833997852	-1.4531351320
Au	0.4833152540	1.0682612964	-1.2927065044
Au	-2.1494951348	1.6155130240	0.0065131742
Au	0.3905963165	0.9280829927	1.4267597048
Au	-0.3187954020	-0.6821147588	3.4813723990
Au	0.6622876217	-1.9446354901	1.2776738093
Au	0.7649261448	-1.8090811086	-1.4451721887
Au	2.7640946558	-2.9573125366	-0.0629025620
Au	-4.0638198932	-0.2382630235	-0.1460030335
Au	-0.1006011732	-0.3133535941	-3.5448733178
Au	2.6175204814	-0.2214951834	0.0689620460
Au	-0.2949048369	3.4316752491	0.1703585161
C	3.1031732915	4.5369528774	0.3524733717
C	4.2149296934	3.7165391820	0.3127468934
C	5.0618126480	3.5030500228	-0.9033122689
H	2.7821508406	5.0652648618	-0.5444271550
H	2.7300198226	4.9102386567	1.3042083274
H	4.6582316191	3.4149200337	1.2638092886
H	5.9543696285	4.1368271564	-0.8247857683
H	5.4063662350	2.4671783751	-0.9743408807
H	4.5332280494	3.7695784638	-1.8227286264

Au_{15}-C_3H_6
E = -2154.90156606888

Au	-1.9284680910	-2.3617233382	-0.2412920317
Au	-3.7359204237	-0.4032420874	-0.2728969940
Au	-1.4670768146	0.4309676068	-1.6756557998
Au	-3.0330141291	2.3176827744	-0.2591852333
Au	-0.3791148518	2.7295972648	-0.1534431675
Au	1.1835941952	0.9919183508	-1.7859175029
Au	1.2951385477	0.7331403319	1.0166074571
Au	-0.0288873094	0.2711985592	3.3872869755
Au	0.1318991369	-1.6802523183	1.4553312638

Au	0.4715771822	-3.8540223423	-0.1002909991
Au	3.5906072274	0.5214738307	-0.3798985025
Au	2.5346206171	-1.8893229460	0.0950445046
Au	0.3657123321	-1.5173492984	-1.5583546608
Au	-1.5264851212	0.4328948440	1.1117414693
Au	2.3107929443	3.0237428658	-0.2160297151
C	0.0586107131	0.2136529094	5.5993674962
C	0.2829595899	1.5232229842	5.2482738738
C	1.6322500559	2.1657256658	5.1722945142
H	-0.9368143627	-0.1204710765	5.8875531006
H	0.8904152024	-0.4450235313	5.8475972624
H	-0.5754434587	2.1979221704	5.2191476253
H	1.7611500944	2.8230050989	6.0412142339
H	1.7252264905	2.7936756782	4.2800012789
H	2.4380569637	1.4265773916	5.1763850570

Au_3Y
E = -445.515149007483

Y	0.5462894587	-1.0330002416	0.0000000000
Au	-1.5269615948	0.1280323367	1.3417287169
Au	-1.5269615948	0.1280323367	-1.3417287169
Au	2.7797439585	0.2329271810	0.0000000000

Au_4Y
E = -581.355107907814

Y	0.0005403741	-1.1374626624	0.0572855741
Au	-1.2891362486	1.2897585257	-0.0002766846
Au	1.2883081767	1.2908949357	-0.0001249425
Au	-2.7607217544	-1.0078249595	-0.0140708525
Au	2.7615599800	-1.0058115808	-0.0142695648

Au_5Y
E = -717.173496900705

Y	0.0007530712	-0.6932704341	0.0144401714
Au	-2.3340313127	0.8622322037	0.0144558110
Au	2.3319532952	0.8672008613	-0.0244251837
Au	2.6122683407	-1.7663832498	0.0181399909
Au	-2.6083480138	-1.7720319268	-0.0200093994
Au	-0.0023684473	2.1538778251	0.0045900194

Au_6Y
E = -853.014796933774

Y	0.0156755856	0.0154977239	1.1733764321
Au	1.1101804136	-1.0974766514	-1.2582674842
Au	0.3458245972	1.4948576883	-1.2876550944
Au	-2.6932549805	-0.7820723016	1.1184031813

Au	2.0706572997	-1.9232941907	1.0655748343
Au	-1.5161430171	-0.4623724444	-1.2322320739
Au	0.6723041016	2.7592949555	1.0150343147

Au_7Y
E = -988.837958146004

Y	0.5829510092	0.0011386801	0.6408944751
Au	-1.7272342817	1.4514185762	-0.1024536625
Au	0.5271871085	-2.7418608416	-0.0714546540
Au	2.9686800641	-1.3070893637	-0.1302012728
Au	0.5266950690	2.7386944688	-0.0832852764
Au	-1.7274063227	-1.4552763222	-0.0914663559
Au	-3.8997386985	-0.0020858455	-0.0292419984
Au	2.9778756434	1.3155122910	-0.0966730922

Au_8Y
E = -1124.67894772093

Y	-0.0069893829	-0.4993787413	-0.5270363057
Au	-2.7777354479	-0.5931486639	0.1043386953
Au	1.3003342926	1.8912721380	0.0571564759
Au	2.7692391275	-0.6285121271	0.0781288290
Au	-1.5085647750	-2.8411517026	0.1196797210
Au	-1.2855811505	1.9124065765	0.0459422879
Au	-3.9368535147	1.7204774082	0.0019116819
Au	1.4902042779	-2.8707939655	0.0348473243
Au	3.9500381811	1.6764947463	0.0508346963

Au_9Y
E = -1260.48673823265

Y	0.3864161418	-0.0046358185	0.8166979632
Au	2.8743708752	-1.3376062581	0.1248829105
Au	-1.3178868728	0.0116753905	-1.5709595185
Au	-1.7555802342	1.8638537298	0.5635347720
Au	2.8843871894	1.3139721506	0.1358399906
Au	1.2335042594	0.0008897716	-1.8772371364
Au	0.6198020864	-2.8736442613	0.8116129910
Au	0.6425521643	2.8625148495	0.8330896952
Au	-3.6087631927	0.0143013110	-0.0112815943
Au	-1.7701126931	-1.8540637771	0.5487123234

Au_9Y_2
E = -1260.49021333860

Au	-1.9716472185	-2.2012027028	-0.7227172268
Au	-2.8781379262	0.3222504791	-0.6601109009
Au	-1.2963055211	2.5236439382	-0.4640700687
Au	1.5032649906	2.3898314653	-0.5046958674

Au	2.8827066271	0.0616698795	-0.7665352365
Au	1.7353976531	-2.3641420512	-0.7666415070
Au	-0.0776870410	-1.8057392386	1.2934477268
Au	-1.2812155294	0.6276773804	1.5774472267
Au	1.3978481938	0.4747234477	1.5233614791
Y	-0.0190789013	-0.0661585789	-1.0275295972

$Au_{10}Y$
E = -1396.34428893178

Y	-0.1085274750	0.0029979900	-0.9753408038
Au	1.8004538363	-2.1380389064	-0.4421580433
Au	-0.8338625897	1.3354977428	1.4903529079
Au	-2.7733310040	1.3137111934	-0.5795952192
Au	-0.6648722524	-3.0414835281	-0.7072669602
Au	-0.7988698622	-1.3612828031	1.4838949170
Au	3.3993770349	0.0173575318	-0.5051160118
Au	-2.7532497864	-1.3396776832	-0.5764225726
Au	-0.6966775757	3.0307145880	-0.6932098347
Au	1.7835001546	2.1629063192	-0.4494777577
Au	1.5331840913	0.0182295191	1.4598748489

$Au_{11}Y$
E = -1532.16232228304

Y	-0.1324582996	0.0012914553	0.8283918772
Au	2.6975732491	-0.0090313525	1.8257841113
Au	-2.0561178089	0.0033800030	-1.3675864944
Au	-2.8694835728	1.3675989481	0.9257682894
Au	1.8326460563	2.2745662905	0.4563141317
Au	0.2700419235	1.3779632914	-1.7483706848
Au	1.8140166653	-2.2877714297	0.4600274077
Au	-0.7677047677	2.8967021898	0.3860284351
Au	-2.8827634353	-1.3437205612	0.9305179075
Au	-0.7918276879	-2.8872780425	0.3884133277
Au	0.2625515834	-1.3824579149	-1.7483309581
Au	2.5469929597	-0.0102222791	-0.9168962600

$Au_{12}Y$
E = -1668.00820269477

Y	-0.0258506216	-0.1693815418	0.4904945044
Au	2.4938742572	1.4099848903	1.6579661069
Au	-2.2368260280	-0.8085982585	-1.4993352371
Au	-2.8788078346	-0.1916163363	1.2321860697
Au	0.5127871895	2.7656193024	0.2907931585
Au	0.0526610793	0.3915030540	-2.4378962976
Au	2.6408962173	-1.2093306140	1.1981910641
Au	-1.7803942977	1.7607925828	-0.9702809300

Au	-1.8302745715	-2.5986233353	0.5574652221
Au	0.7900220220	-3.0823696532	0.5541419608
Au	1.7735373600	-1.5510634990	-1.5190682221
Au	2.2773289976	1.0134162536	-1.0086173446
Au	-1.7983500400	2.1978487216	1.6985314249

$Au_{13}Y$

E = -1803.83865000443

Y	0.0905338779	0.0005355636	0.5268434228
Au	2.2388547582	-1.9840055400	1.3668740556
Au	-1.1198182087	2.2612973952	-1.1012035152
Au	-0.2960769742	2.7992141888	1.5777285275
Au	3.2242155703	0.0036650688	-0.1834751656
Au	-0.1908671771	-0.0021250825	-2.4156280579
Au	-0.2896128327	-2.7977669319	1.5821172376
Au	1.5273283009	1.8480484570	-1.3323848944
Au	-2.5407570869	1.3720414928	1.2301651376
Au	-2.5373690777	-1.3760408223	1.2322390541
Au	-1.1144456865	-2.2656392662	-1.0977132301
Au	1.5317345791	-1.8465179926	-1.3295349011
Au	2.2344664908	1.9915617628	1.3637851187
Au	-2.7259564387	-0.0040830964	-1.1460455420

$Au_{14}Y$

E = -1939.69622908470

Au	1.4140540798	0.0731007790	2.5364061780
Y	-0.0037090994	0.0059053469	-0.3805204973
Au	0.1423026146	-2.2704153799	1.5158914394
Au	2.5835367666	-1.3504713262	0.5837584611
Au	2.3870238815	1.5837729803	0.5335024206
Au	-2.3821010484	-1.5972056042	0.5391378408
Au	-2.5584197713	1.3479460907	0.6568260103
Au	-0.1099188308	2.2351671515	1.5915619084
Au	2.7474737705	0.0789493796	-1.7403170437
Au	1.2351972152	2.3806346842	-1.8033169497
Au	-1.4058200398	2.3636672515	-1.6000608727
Au	-2.7817379710	-0.0389214973	-1.6888334835
Au	-1.2742170760	-2.3391987427	-1.8359776407
Au	1.3694267304	-2.3281232478	-1.6570437528
Au	-1.3666549887	-0.1377996478	2.5531207530

$Au_3Y\text{-}C_3H_6$

E = -563.401969138099

Y	0.5122550675	0.6330121186	-0.4299826166
Au	-1.5382311943	0.5380379916	1.4168198900
Au	-1.8490081855	-0.7162096396	-0.9254914035

Au	2.8307282367	-0.4728316514	-0.0687076022
C	0.9806929130	3.0129296593	-1.5357552496
C	-0.1603665028	3.4871258845	-1.0066320926
C	-1.4925180623	3.4619158363	-1.6646058635
H	1.0060697963	2.6285429135	-2.5613029495
H	1.9424929834	3.1503357845	-1.0354892709
H	-0.1186184256	3.9529066001	-0.0176738735
H	-1.8473399867	4.4929984929	-1.7861247455
H	-2.2337494820	2.9612051913	-1.0285950826
H	-1.4689004012	2.9849647131	-2.6486749887

Au_4Y-C_3H_6
E = -699.249267729939

Y	-1.0200962166	0.0389210806	-0.6302674012
Au	2.1314537191	-0.1941523457	0.1704597114
Au	0.7862024501	2.0651468914	-0.3027823857
Au	0.4427554041	-2.2333663257	-0.2821762172
Au	-3.3373794362	0.2872900101	0.5044029540
C	4.0284024498	-1.0374112127	0.7774979474
C	4.1966924196	0.3439085029	0.7353818128
C	4.9297732169	1.0583570006	-0.3607568123
H	4.4083782691	-1.6577729881	-0.0333241936
H	3.8419216858	-1.5398368072	1.7247375812
H	4.0833693297	0.8929670400	1.6719172661
H	4.5065462709	2.0474301378	-0.5569985997
H	4.9386816685	0.4835776078	-1.2911535273
H	5.9698173323	1.2093557718	-0.0454380927

Au_4Y-C_3H_6_2
E = -699.248258403245

Y	0.0605802693	-1.0869487390	-0.0886846325
Au	-1.6696634834	1.0716462918	0.1334191865
Au	0.7846273240	1.5671314910	-0.4721866729
Au	-2.5361302220	-1.3823943614	0.9024913578
Au	2.7345898784	-0.3234637050	-0.3033416913
C	-0.1474506925	-2.3882450258	-2.3535040871
C	-0.4098753989	-1.2467532661	-3.0156343467
C	-1.7623637182	-0.7462228471	-3.3633946395
H	-0.9550259390	-3.0693567101	-2.0687588998
H	0.8843531289	-2.7427349014	-2.2551863309
H	0.4365672954	-0.6403734739	-3.3508594143
H	-1.8845422943	0.2957103961	-3.0453202287
H	-2.5602047106	-1.3604945549	-2.9382616285
H	-1.8614569583	-0.7449913577	-4.4568140411

Au_5Y-C_3H_6

E = -835.063234245562

Y	1.5883736583	0.1414017149	0.8352314228
Au	1.7045405738	2.7013517923	-0.0905280014
Au	-0.6488030625	1.3662357046	-0.1489251759
Au	-2.7406554463	-0.2903665550	0.1264993835
Au	-0.3865897695	-1.4823044244	-0.1453246340
Au	2.1750298619	-2.3417446878	-0.1404249100
C	-4.8215413052	-0.9186882819	0.5078405701
C	-4.9000781668	0.4074880172	0.1510147548
C	-5.2968023991	0.8970668904	-1.2056903164
H	-5.0448326809	-1.6990332157	-0.2192191891
H	-4.8106665916	-1.2112800613	1.5563506296
H	-4.8924620711	1.1519424067	0.9500696471
H	-4.6907094922	1.7519018665	-1.5212714248
H	-6.3372470086	1.2433701982	-1.1622893825
H	-5.2290175812	0.1098719719	-1.9614002221

Au_5Y-C_3H_6_2

E = -835.06233900462

Y	-0.0383109777	-0.6268998807	0.4793384373
Au	-2.1549110376	1.0230724974	-0.3405254028
Au	2.3463542032	0.7386259943	-0.1040456489
Au	2.4425488904	-1.8998235242	-0.1083976142
Au	-2.6579656144	-1.5624809206	-0.1466465042
Au	0.1642705180	2.2521642308	0.0419437174
C	0.0388689034	-0.9816750807	3.0865756120
C	-0.3340304568	0.2890244219	3.3187965915
C	-1.7268011286	0.7459710355	3.5551239685
H	1.0965978083	-1.2555270858	3.0358084608
H	-0.6960375144	-1.7927754984	3.1114331337
H	0.4449731832	1.0543220642	3.3694471772
H	-1.8021449071	1.1194641942	4.5845690068
H	-2.4595983957	-0.0538058453	3.4182449422
H	-1.9755594891	1.5914327762	2.9033946674

Au_6Y-C_3H_6

E = -970.908460946390

Y	1.1704532867	0.0627547578	-0.9302544524
Au	-0.3493827365	1.3557451699	1.0430164349
Au	-0.0390065495	-1.2915228875	1.2083725684
Au	-1.0791931443	-0.2863188718	-2.3262337514
Au	1.6100154822	2.7428263142	-0.0371475655
Au	-2.3632998940	-0.2767802835	0.2738612908
Au	2.2114470420	-2.3028083915	0.2889440566
C	-4.4139380088	-0.5694636784	-0.4353884014
C	-4.4980383203	-0.4043761564	0.9343890565

C	-4.9267222312	0.8635957600	1.6050682253
H	-4.6530259970	0.2580680499	-1.1024709102
H	-4.4180746033	-1.5672605611	-0.8706727087
H	-4.5078209784	-1.3018705939	1.5555617860
H	-5.9790600288	0.7640522524	1.9000505506
H	-4.8395682464	1.7281169654	0.9409650685
H	-4.3542125640	1.0507933680	2.5182586177

Au_7Y-C_3H_6

E = -1106.73390290117

Y	-0.7614315572	0.0398879940	-0.7101262741
Au	3.8467957012	-0.1467200832	0.1260340010
Au	1.6160940180	1.3094801230	0.1055925817
Au	-0.5682790058	2.7693770274	0.0172870543
Au	1.5222355940	-1.4405699622	0.0200034504
Au	-0.7624134854	-2.7347173292	-0.1527257541
Au	-3.0604933875	1.4093349749	0.1536853681
Au	-3.1510360508	-1.2103231558	0.0822539722
C	5.9565344007	-0.2445092875	0.8044276079
C	6.0190779948	-0.0878780755	-0.5576069614
C	6.2887383047	1.2093363897	-1.2525057856
H	6.0238268159	-1.2337161600	1.2544317367
H	6.0967277316	0.6077559268	1.4687678151
H	6.0857248793	-0.9874919058	-1.1733020793
H	5.6442089827	1.3398804806	-2.1274741589
H	6.1678276529	2.0662303153	-0.5841258435
H	7.3232350061	1.2017869864	-1.6179151671

Au_8Y-C_3H_6

E = -1242.57213385282

Y	-0.3029036254	-0.5279212501	-0.0238231890
Au	-0.9703565964	2.1666971110	0.0655722717
Au	1.5569304847	1.5171441449	0.0665194360
Au	4.1773739629	0.8295710334	0.0936367444
Au	-3.6219460731	2.4294626062	0.0462886054
Au	-3.0794711708	-0.0982351512	-0.0100474054
Au	0.7300146044	-3.1471002645	-0.1325194515
Au	2.4550215685	-1.1486428076	-0.0370556174
Au	-2.2719552545	-2.5602088699	-0.0738807022
C	6.0524573759	1.7959599017	0.7828522886
C	6.0564600581	1.9294404249	-0.5828836591
C	6.8316371876	1.0585762803	-1.5203936733
H	5.6950415935	2.6019804362	1.4212285034
H	6.6310196524	1.0077116752	1.2641869591
H	5.6411904836	2.8453464785	-1.0085893393
H	6.2425432676	0.7930830902	-2.4038753433

H	7.1848191449	0.1447269292	-1.0347550791
H	7.7053907812	1.6183718476	-1.8766111780

Au_9Y-C_3H_6
E = -1378.38460273518

Y	-0.7014925511	-0.1513304324	0.0120312916
Au	-3.1893197257	0.6263656305	-1.2584888221
Au	1.7234312586	-1.6405272139	-0.0357284353
Au	1.6227297789	0.8533011258	1.4907266801
Au	-3.1762524724	0.5265168548	1.3724741601
Au	-0.3465105215	-3.1498525686	-0.0214033885
Au	-0.7505608760	1.2693505505	-2.4570914750
Au	-0.7160516282	1.1552322803	2.5413123348
Au	3.7520655278	0.2192170490	-0.0108956811
Au	1.6020521295	0.9200645952	-1.4495359649
C	-2.1460489443	-4.3335226029	0.6031342154
C	-1.9784125109	-4.6104373660	-0.7271233733
C	-1.2894015318	-5.8248141319	-1.2631556053
H	-2.8600299879	-3.5793730749	0.9292838516
H	-1.7719420544	-5.0164640046	1.3656805885
H	-2.5375608883	-4.0142773473	-1.4509467799
H	-0.6198908562	-5.5753370056	-2.0931315648
H	-2.0463312036	-6.5108524216	-1.6632560838
H	-0.7245095199	-6.3527450498	-0.4897268586

Au_9Y-C_3H_6_2
E = -1378.38304275921

Au	-1.5437174099	-2.4046803524	-0.3026786156
Au	-3.1914656339	-0.1832578295	-0.3670682410
Au	-1.6761497916	2.0908976188	0.0976228391
Au	0.9591992152	2.7194663773	-0.4889679423
Au	2.7230641784	0.7367953415	-0.9099653475
Au	2.2551848039	-1.8828597548	-1.2450323970
Au	0.8782077289	-1.8304364236	1.1317899269
Au	-1.2890657248	-0.2229422849	1.5647514089
Au	1.2357854381	0.8282181828	1.5498864114
Y	-0.0269509628	-0.0378493158	-0.9889624525
C	-4.9771435441	-0.7407459867	-1.5290905978
C	-5.1016262330	0.6072999225	-1.2525858070
C	-5.9780040536	1.1633568276	-0.1711879716
H	-5.5133776616	-1.4771274633	-0.9317691700
H	-4.6048107758	-1.0781493407	-2.4939901637
H	-4.7689817538	1.3168334517	-2.0118373138
H	-6.9204299166	1.5004863927	-0.6209780852
H	-5.5225333732	2.0314131287	0.3139859817
H	-6.2155686291	0.4134995411	0.5888374149

$Au_{10}Y\text{-}C_3H_6$
E = -1514.23578077636

Y	0.0930685256	0.0534323621	0.9205970814
Au	2.8299471436	-1.0457270325	0.8906470333
Au	-1.4425416096	-0.2252938489	-1.5133927539
Au	-1.9453750584	1.9942122264	0.0606282641
Au	2.6082051712	1.5697459410	0.7391337752
Au	0.8354474082	1.3207509022	-1.5721177945
Au	0.9388752269	-2.9595516671	0.8257631363
Au	0.4300557625	3.1304441414	0.4816255165
Au	-3.4773379343	-0.2780996632	0.2836436253
Au	-1.5927816659	-2.2848506389	0.3269302706
Au	1.0727682600	-1.3408156048	-1.4115147005
C	-5.3217244141	-1.0184569987	1.2689211230
C	-5.4886635188	0.3414741569	1.1364712090
C	-6.3104705111	0.9907949636	0.0658999635
H	-5.7849270562	-1.7039022500	0.5600412946
H	-4.9746360382	-1.4467250615	2.2070408712
H	-5.2141098409	0.9737117349	1.9828022933
H	-5.8424232503	1.9081026739	-0.3036688415
H	-7.2819355941	1.2740557212	0.4903190585
H	-6.4910140534	0.3170488048	-0.7763635366

$Au_{11}Y\text{-}C_3H_6$
E = -1650.05580482520

Y	0.0150572736	-0.1957326401	0.4606350449
Au	3.1016860177	0.0530042225	1.2643824433
Au	-2.0896039587	0.5727765131	-1.4155108648
Au	-2.9032886497	0.9712943048	1.1375261965
Au	1.7473023468	2.2645046964	0.5412102713
Au	0.3458628549	1.7061823836	-1.8315446769
Au	2.0866367137	-2.3135473933	0.3786735287
Au	-0.9119710356	2.6642406116	0.5013285721
Au	-2.5915144568	-1.5998289564	0.2968014615
Au	-0.4266294633	-3.0730171958	0.5643105490
Au	-0.0201835792	-0.7991184636	-2.7174178309
Au	2.3284548047	-0.0912828301	-1.3282407420
C	0.3430149722	-2.7728035588	-3.6295554309
C	-1.0257560250	-2.6058519480	-3.6258325783
C	-1.8331086676	-2.2085002704	-4.8221822911
H	0.9184724918	-2.5928848816	-4.5371189288
H	0.8330095094	-3.3371429267	-2.8388464448
H	-1.5824173280	-3.0108231357	-2.7783321693
H	-2.6446560251	-1.5259825277	-4.5528632283
H	-2.2967024208	-3.1080793934	-5.2466493730
H	-1.2174839296	-1.7449988612	-5.5982067377

$Au_{12}Y\text{-}C_3H_6$
E = -1785.90065080658

Y	0.0795881801	0.0872109237	-0.4590646981
Au	-2.2032387368	-1.0855678304	-1.8691352421
Au	2.1197203159	0.2394907919	1.5984433542
Au	2.4088572521	1.9036702372	-0.6652939516
Au	-2.2802922191	1.6137349032	-1.4476145654
Au	-0.5255553990	-0.0246379133	2.4369100709
Au	-0.1961278463	-2.7928109826	-1.4876098086
Au	0.4073810902	2.3308407543	1.5440922241
Au	3.4365675352	-0.6546824013	-0.5707663214
Au	1.5362803596	-2.2829988794	0.6434319311
Au	-1.2271879703	-2.2253188278	0.9968778926
Au	-2.7193740245	-0.0369931024	0.7149046695
Au	-0.0239135471	3.0121169392	-1.1280591014
C	4.6347011590	-2.0147060743	-1.8447243098
C	4.9820945811	-0.7357547621	-2.2207216450
C	6.2269684850	-0.0330311713	-1.7752043953
H	3.9016713936	-2.5808412248	-2.4155213760
H	5.2682741801	-2.5816691214	-1.1635317676
H	4.4609544974	-0.2953637045	-3.0726208009
H	6.0420970265	1.0265482657	-1.5745795593
H	6.6628953277	-0.4952631980	-0.8850505605
H	6.9674476400	-0.0834227501	-2.5834565870

$Au_{13}Y\text{-}C_3H_6$
E = -1921.72867424674

Au	-0.0676592502	-0.2279755067	2.3350043719
Y	0.1183617533	0.0401991952	-0.5142495598
Au	-1.6981793165	-1.8787985875	0.8067356495
Au	-3.4608537463	0.3041148577	0.2656011359
Au	-1.3343091674	1.9657215541	1.1946436749
Au	0.9177758911	-2.4642086891	1.0107026900
Au	2.6887241226	-0.3798208570	1.2387912329
Au	1.3405187729	2.0006452909	1.4562643954
Au	-2.0009558496	1.7696487111	-1.5386788339
Au	0.4782994315	2.8693700079	-1.1603518010
Au	2.7025202068	1.2923205585	-0.9871731302
Au	2.4331091383	-1.5500465168	-1.2721687531
Au	-0.0416002225	-2.6254887734	-1.7085256423
Au	-2.2685260262	-1.0329802677	-1.8172852795
C	-5.0790991590	0.9384400862	1.6329997956
C	-5.2450860678	-0.4189621978	1.4583681539
C	-6.2512943704	-1.0368214474	0.5383540093
H	-5.6880695338	1.6457825823	1.0713283274

H	-4.5650307810	1.3219173043	2.5118649810
H	-4.7979293244	-1.0823358988	2.2009647853
H	-5.8503392709	-1.9228590584	0.0371700413
H	-6.6065934257	-0.3283780538	-0.2150614078
H	-7.1135418738	-1.3665091306	1.1318623636

$Au_{14}Y\text{-}C_3H_6$

E = -2057.58965173836

Au	-0.2379468688	-1.1738654397	2.3066426944
Y	0.2608477020	0.1812394633	-0.3516083832
Au	-0.7861412949	-2.5928022589	-0.0972609713
Au	1.7780777771	-2.2712805466	0.8169017048
Au	2.0693949978	0.2369438231	2.1133766850
Au	-2.3305994759	-0.7235481538	-1.3625514312
Au	-2.3816993520	1.4306510893	0.3720062176
Au	-0.3373722487	1.5823978392	2.1952448591
Au	3.2300558093	-0.2308561693	-0.3617516288
Au	2.2495912103	2.2906262695	0.3118042763
Au	-0.2523293155	3.1222806252	-0.2310714497
Au	-1.4335048629	1.7434597027	-2.3019410622
Au	-0.3146558121	-0.5879918438	-3.2094101164
Au	1.6150608940	-1.9207570411	-1.9105236328
Au	-2.8802635891	-1.1870121488	1.2333792248
C	-3.6070205834	-2.2497119553	3.0340807746
C	-4.1558605723	-0.9859354345	3.0860634268
C	-5.5577233135	-0.6565240328	2.6781297665
H	-2.7249418141	-2.4951527024	3.6228169240
H	-4.1874659264	-3.0909417849	2.6570118492
H	-3.6347168786	-0.2294968289	3.6751227438
H	-5.9896655220	-1.4277562234	2.0343594959
H	-5.6124852779	0.3095328073	2.1673627724
H	-6.1762937111	-0.5784776736	3.5813140707

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