Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Electronic Supplementary Information

Trends in Structural, Electronic and Energetic Properties of Bimetallic Vanadium Gold Clusters Au_nV with n = 1–14

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Figure S1. MO shapes of AuV ($C_{\infty v}$)

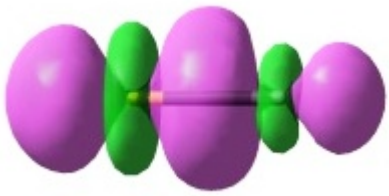
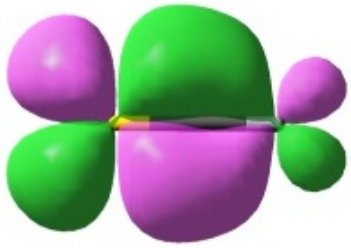
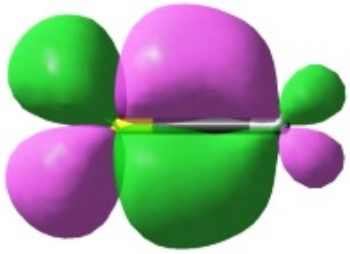
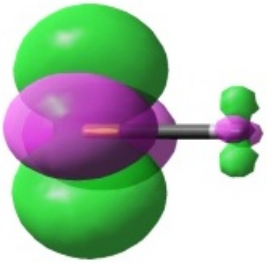
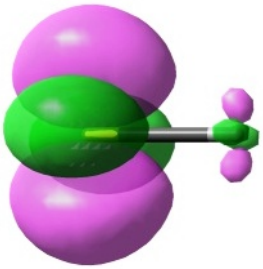
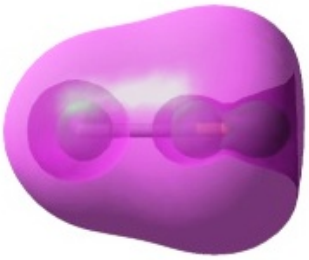
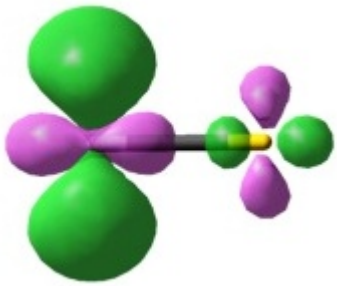
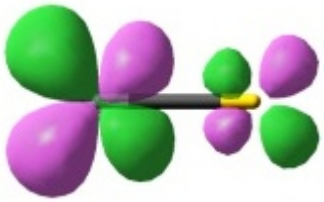
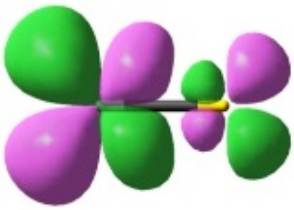
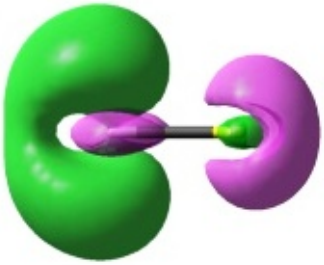
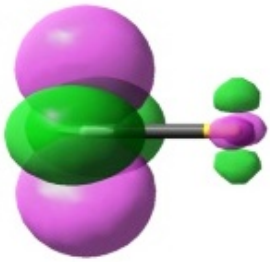
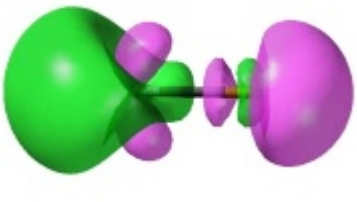
 HOMO-9 (1σ)	 HOMO-8 (1π)	 HOMO-7 (1π)
 HOMO-6 (1δ)	 HOMO-5 (2δ)	 HOMO-4 (2σ)
 SOMO-3 (3δ)	 SOMO-2 (2π)	 SOMO-1 (2π)
 SOMO (3σ)	 LUMO (4δ)	 LUMO+1 (4σ)

Figure S2. MO shapes of Au_3V giving rise from the interactions between valence AOs of V and Au atoms.

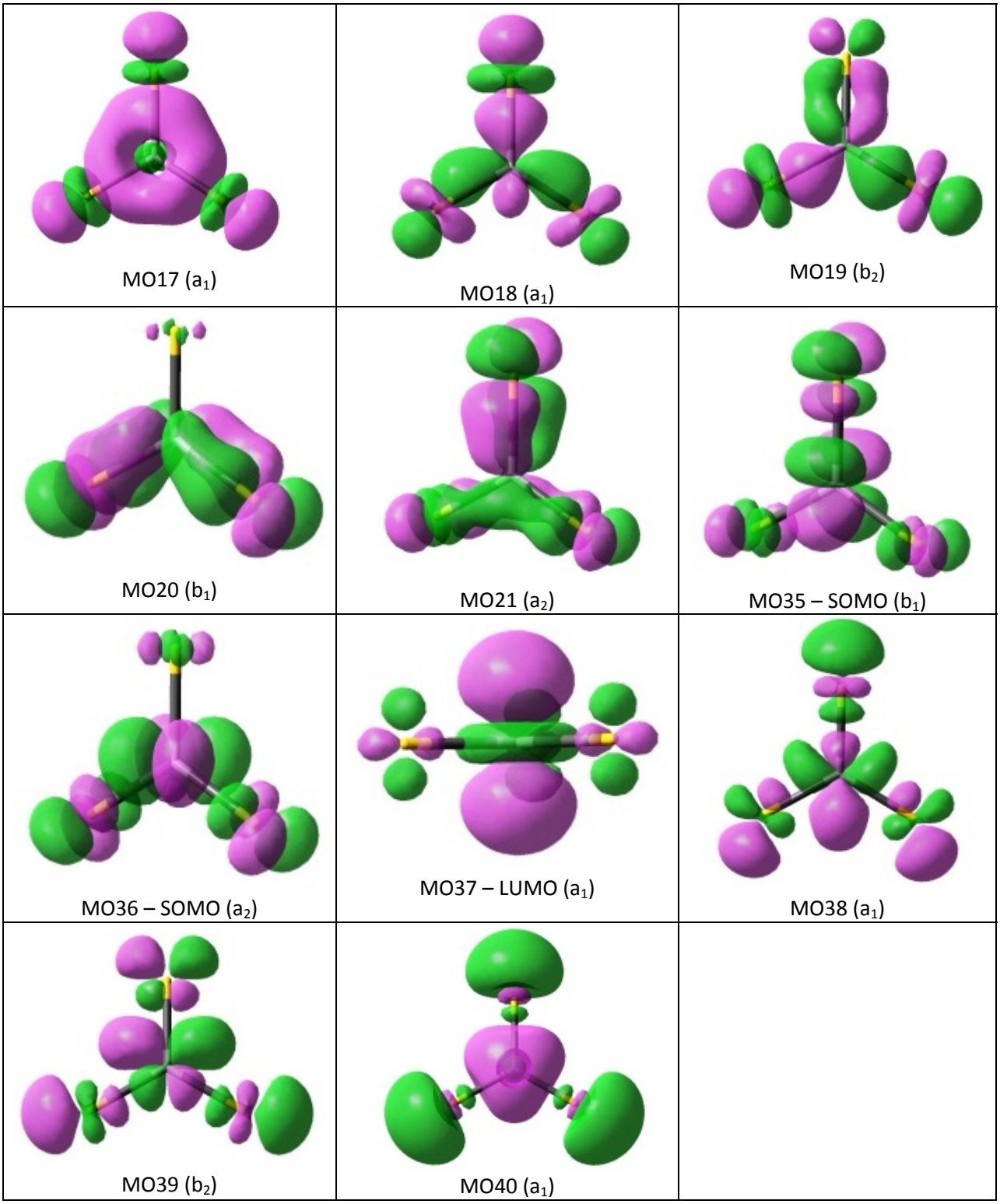
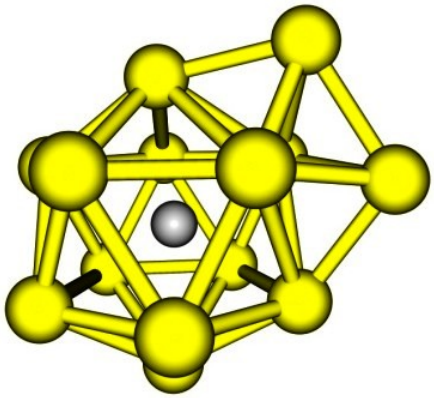
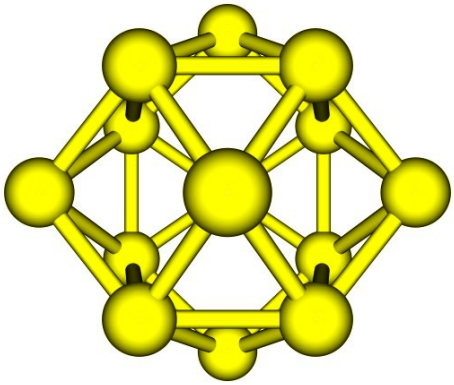
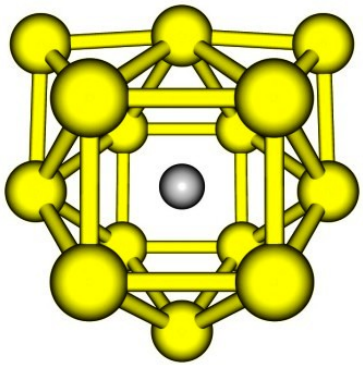
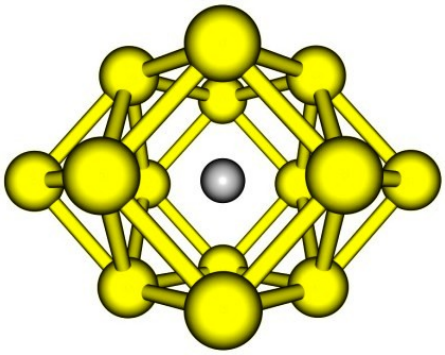
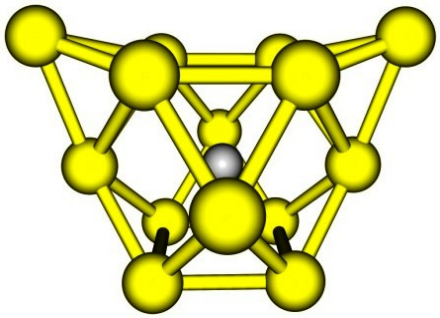
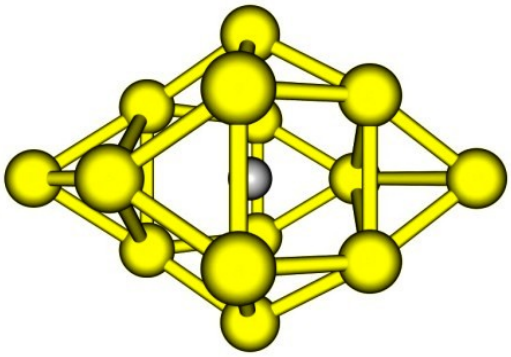
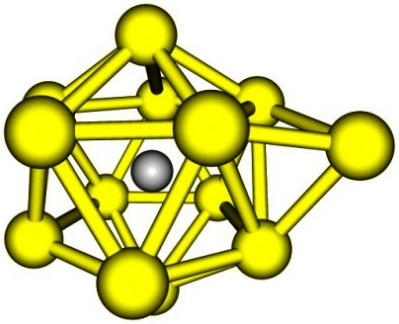
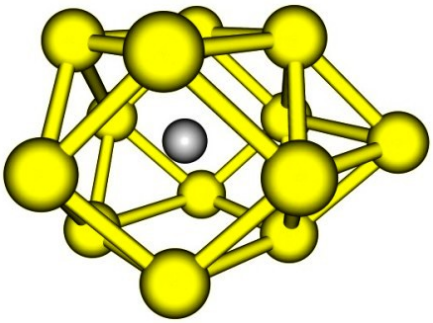
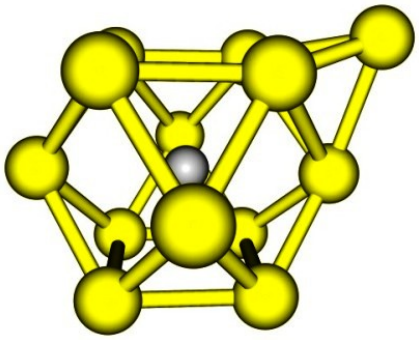
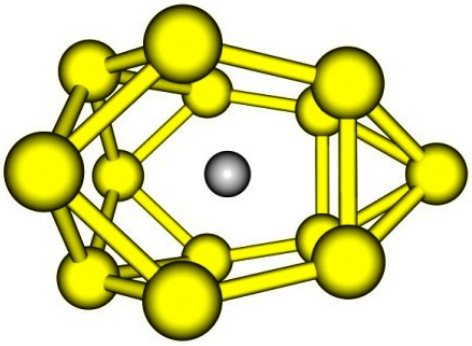
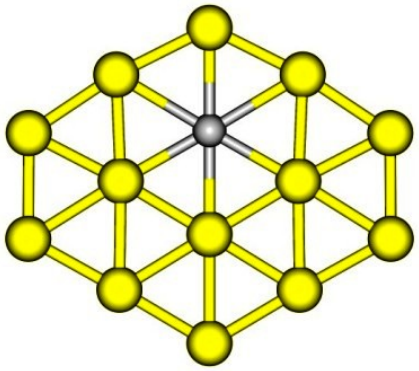
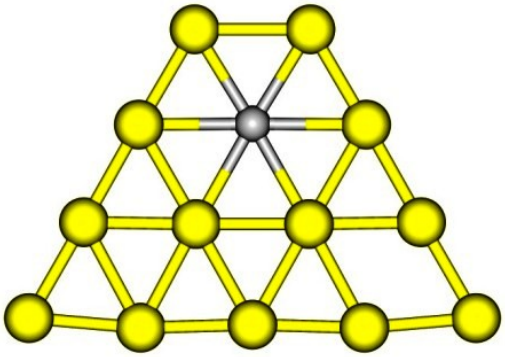
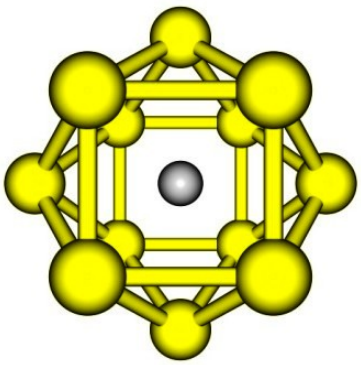
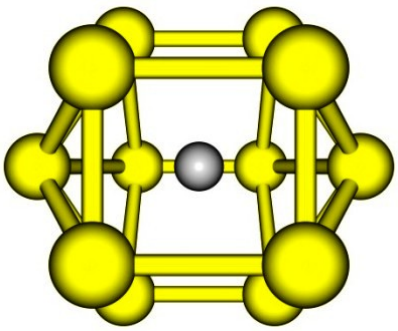
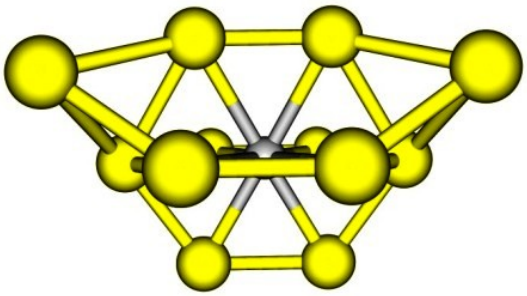
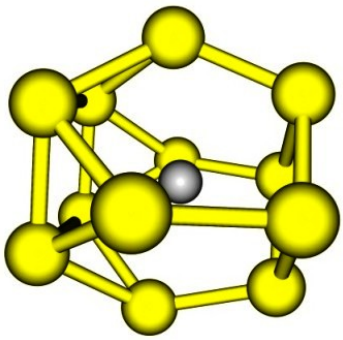
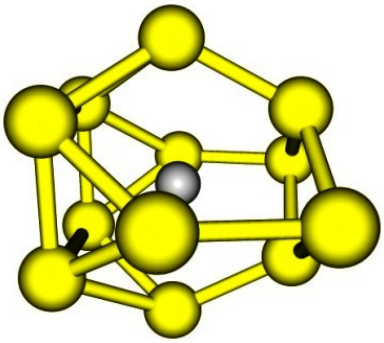
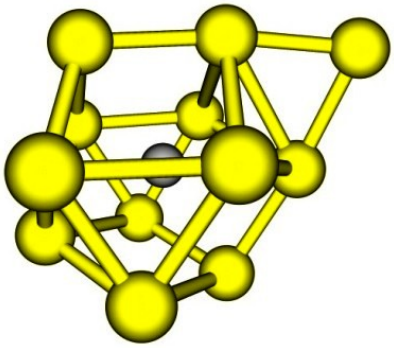
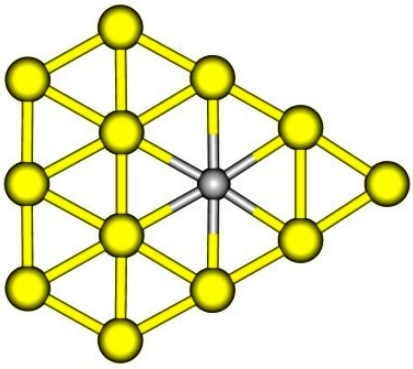
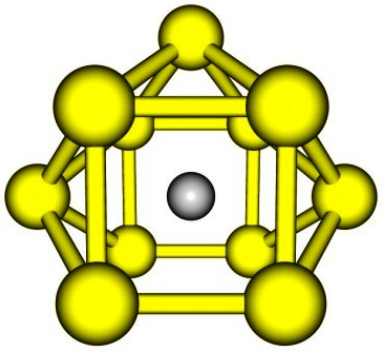
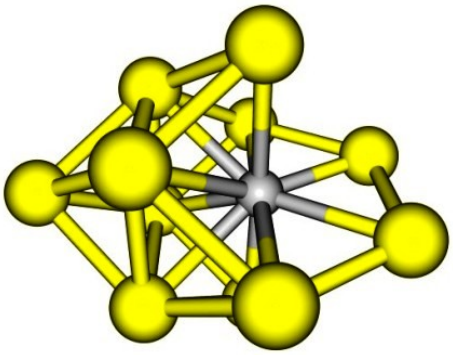
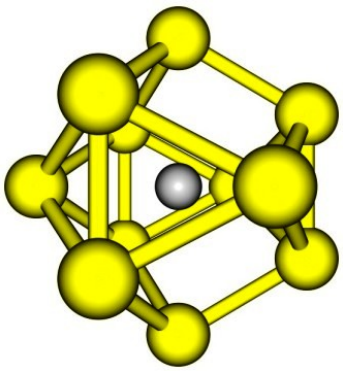
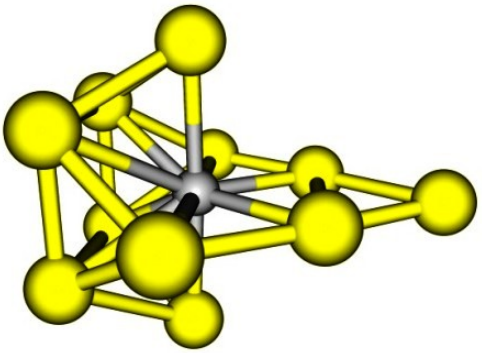
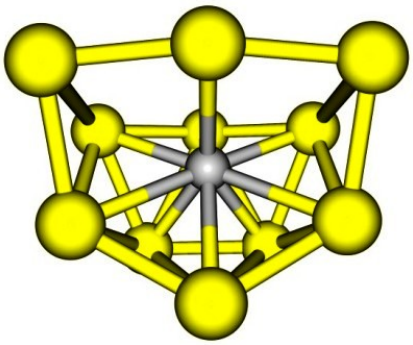
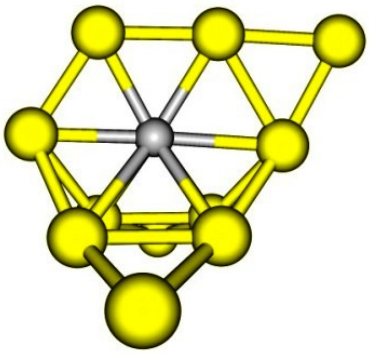
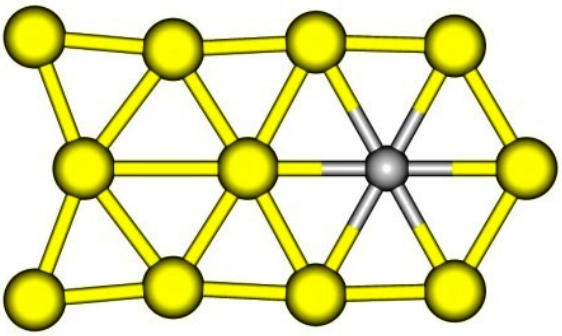
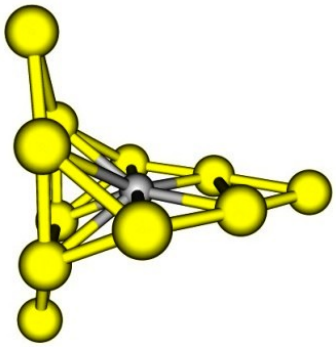
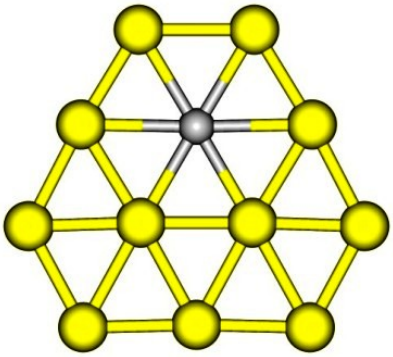
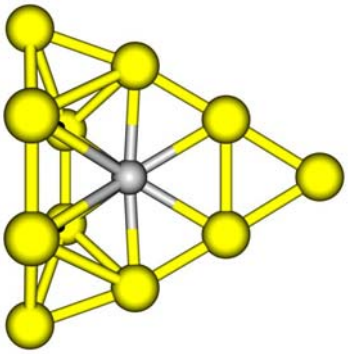


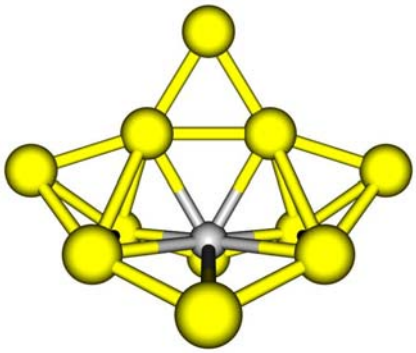
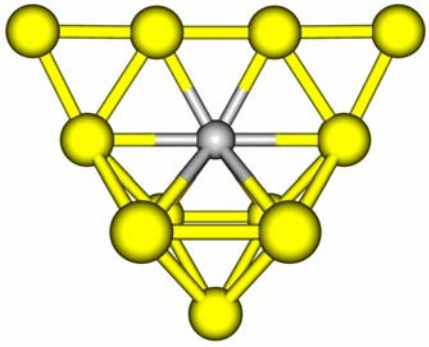
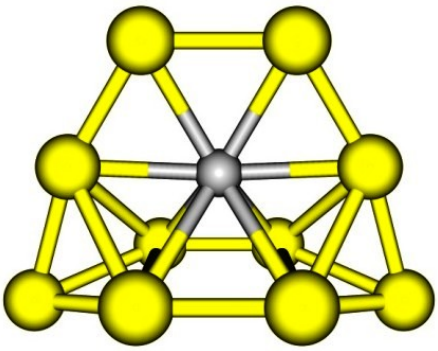
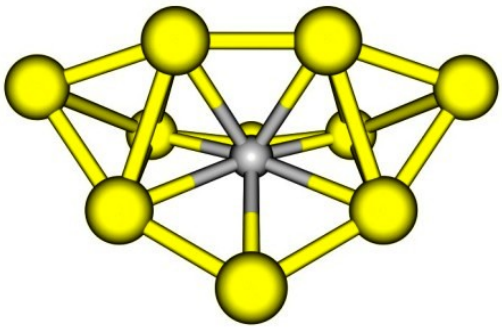
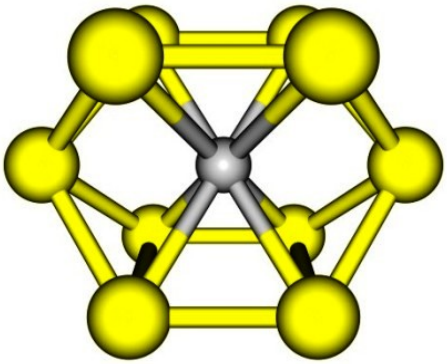
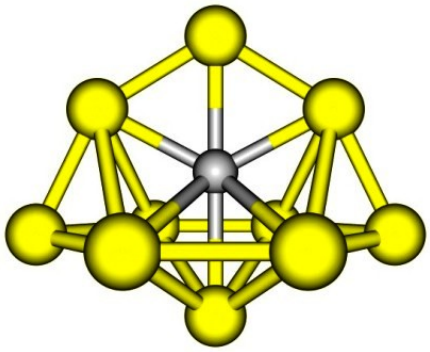
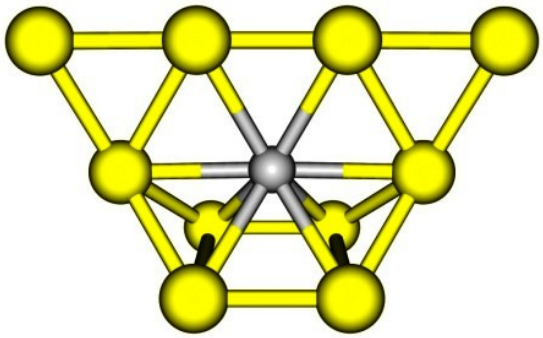
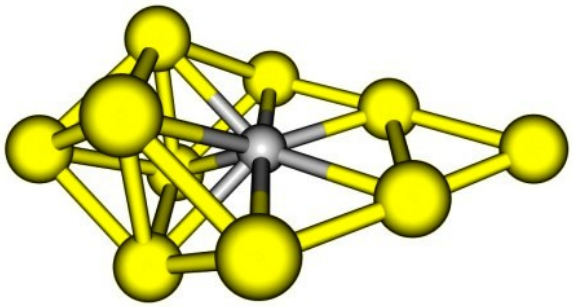
Figure S3. Selected Geometries and Relative Energies of Gold doped Vanadium Clusters Au_nV (BP86/LanL2DZ)

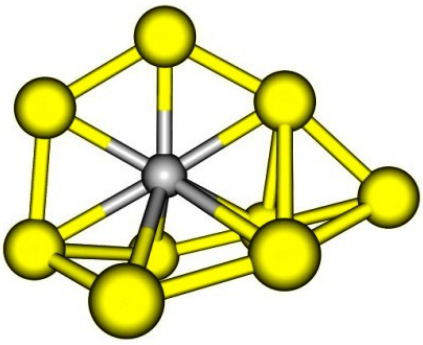
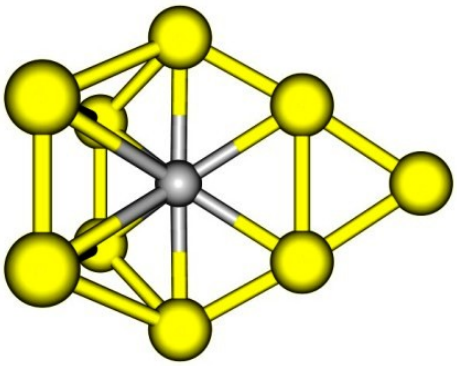
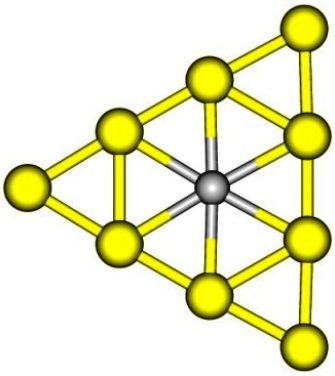
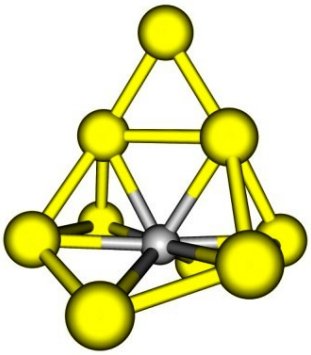
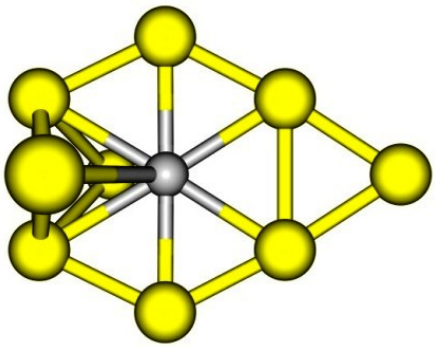
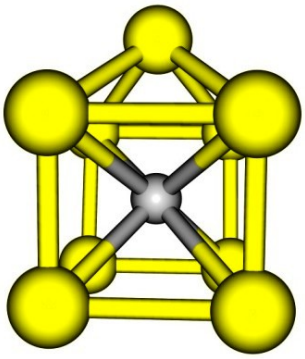
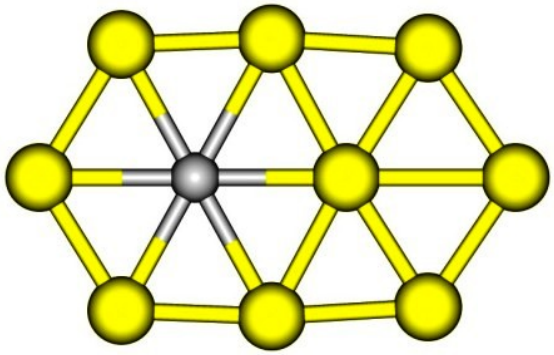
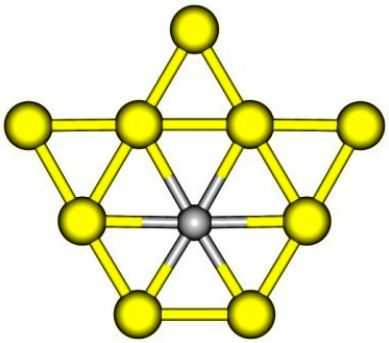
n	Structure, symmetry, elctronic state and relative energy (eV)	
14	 C_s – ^{2}A′ (0.00); ^{4}A″ (0.49)	 D_{2d} – $^2B_2$ (0.09)
	 C_{2v} – $^2B_2$ (0.18); $^4B_2$ (0.53)	 D_{4h} – $^2A_{1g}$ (0.34); $^4A_{2g}$ (0.63)
	 C_{2v} – $^4B_2$ (0.59); $^2A_1$ (0.63)	 C_{2h} – ^4B_u (0.79); ^2B_u (0.80)
13		

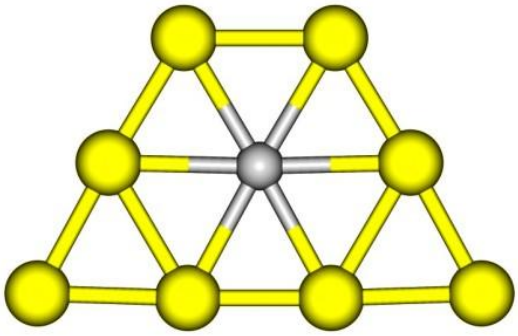
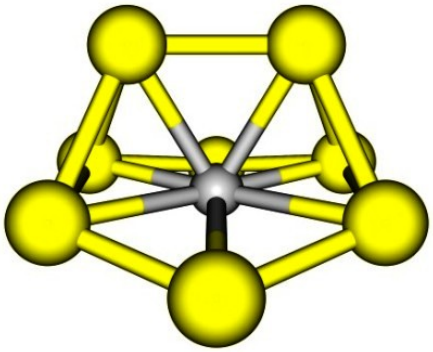
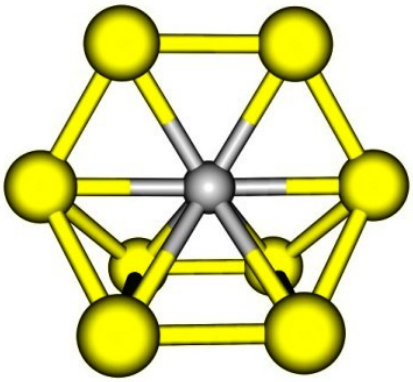
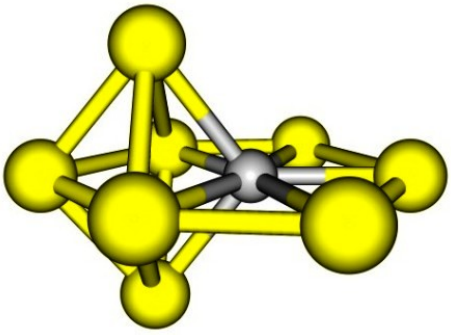
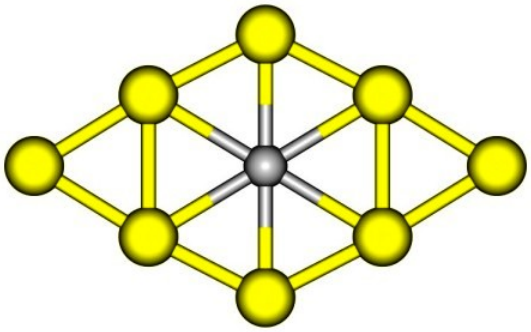
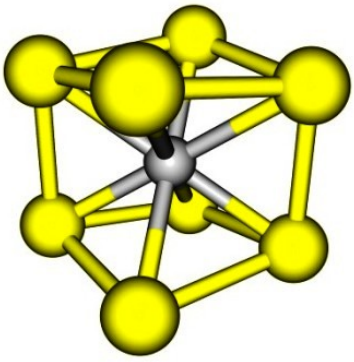
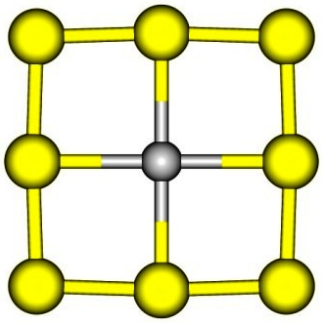
	C_s – ^{1}A’ (0.00); ^{3}A” (0.28)	C_{4v} – $^3B_1$ (0.013); $^1A_1$ (0.29)
	 C_s – ^{3}A’ (0.19); ^{1}A’ (0.46)	 C_{4v} – $^3B_1$ (0.42)
	 C_{2v} – $^3A_2$ (1.88)	 C_{2v} – $^3A_1$ (1.97)
12	 D_{4h} – $^2A_{1g}$ (0.00); $^4A_{2g}$ (0.27)	 C_{2v} – $^2B_1$ (0.52); $^4B_1$ (1.09)
	 C_{2v} – $^4A_2$ (0.67); $^2A_1$ (0.80)	 C_{4v} – $^2B_1$ (0.81)

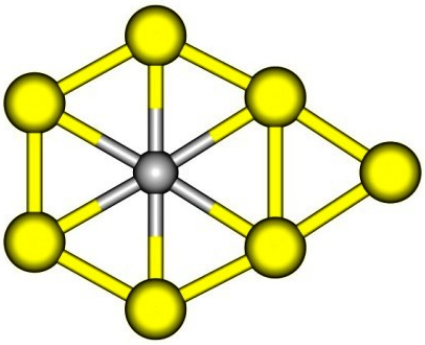
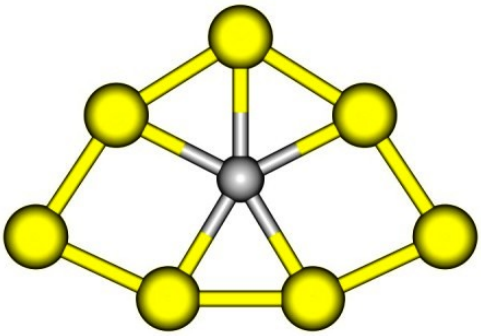
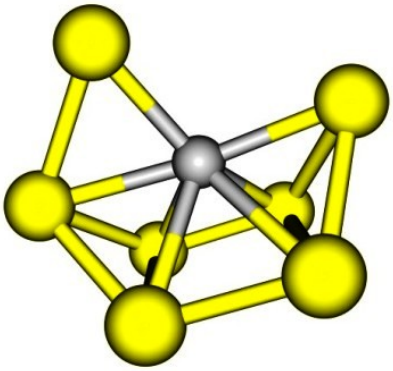
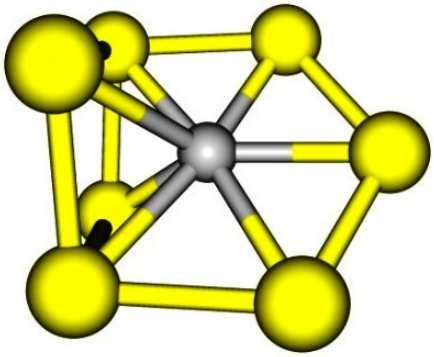
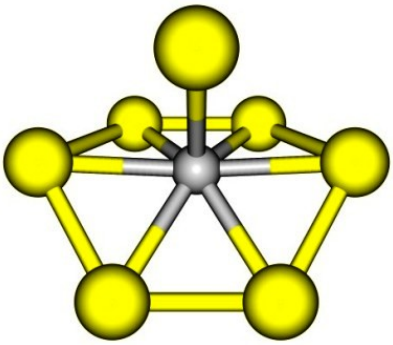
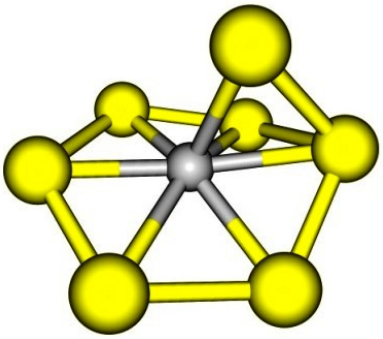
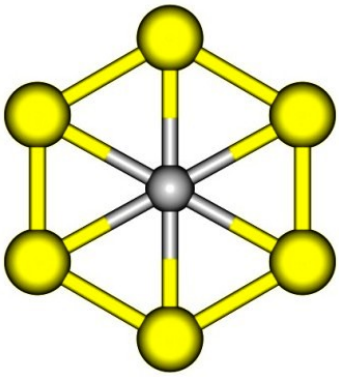
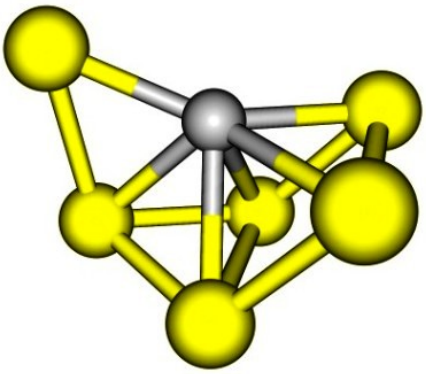
	 C_{2v} – $^4B_2$ (0.92)	 C_{2v} – $^4B_2$ (1.03); $^2A_2$ (1.07)
	 C_{2v} – $^4A_1$ (1.63); $^2A_2$ (1.83)	
11	 C_{2v} – $^3B_2$ (0.00); $^1A_1$ (0.46) [**11-I**]	 C_{2v} – $^3B_2$ (0.41)

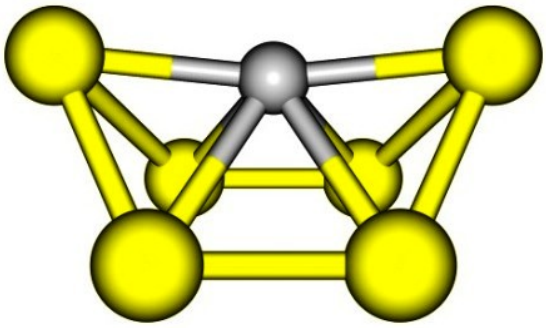
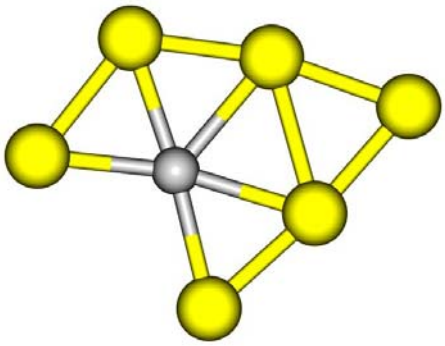
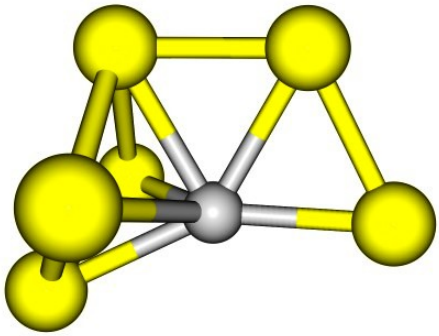
11	 C_{2v} – $^3B_1$ (0.48)	 C_{2v} – $^3B_2$ (0.50); $^1A_1$ (1.00)
	 C_{2v} – $^3B_1$ (0.51); $^1A_1$ (0.87)	 C_s – $^3A''$ (0.73); $^1A'$ (1.75)
	 C_{2v} – $^3B_2$ (0.84)	 C_{2v} – $^3B_2$ (1.07)
	 C_{2v} – $^3B_2$ (1.14)	 C_{2v} – $^3A_2$ (0.46) [**11-II**]

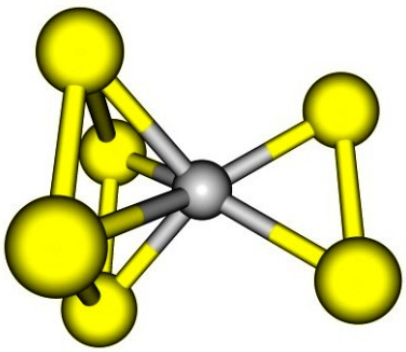
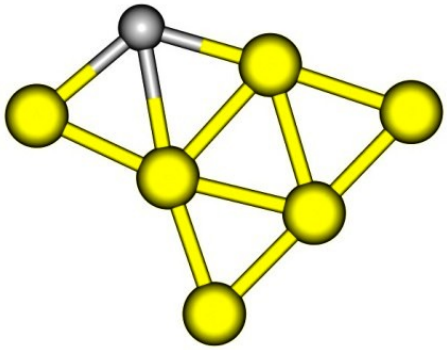
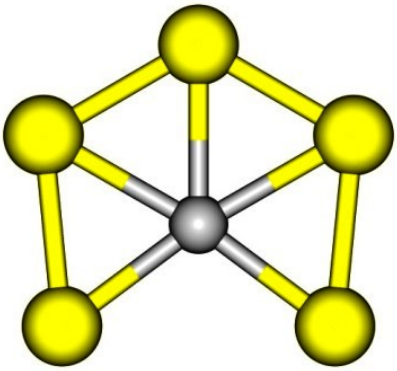
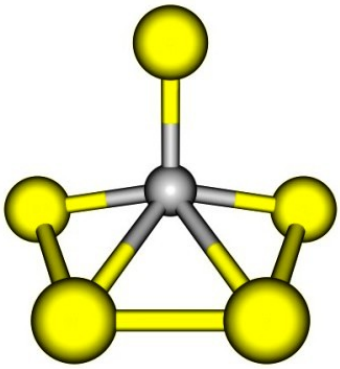
	 C_{2v} – $^3B_1$ (1.13) [**11-III**]	 C_{2v} – $^3A_2$ (0.98)
10	 C_{2v} – $^4A_2$ (0.00); $^2A_2$ (0.23)	 C_{2v} – $^2B_1$ (0.025); $^4A_2$ (0.072)
	 D_{2h} – $^4B_{2g}$ (0.05); $^2B_{2g}$ (0.09)	 C_{2v} – $^4B_2$ (0.39); $^2A_1$ (0.44)
	 C_{2v} – $^2A_2$ (0.43)	 C_{2v} – $^2A_2$ (0.76)

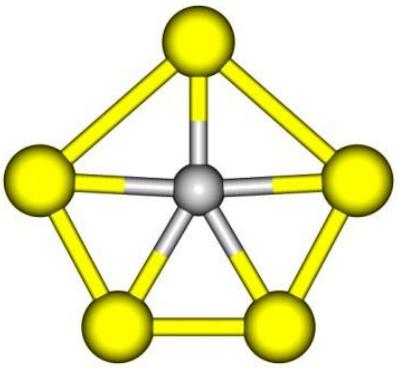
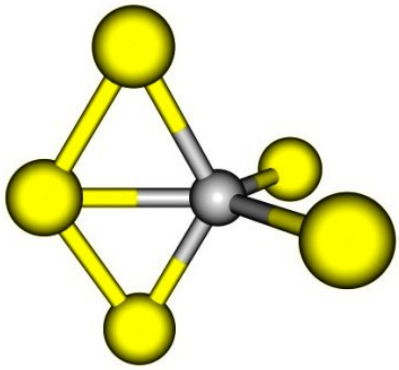
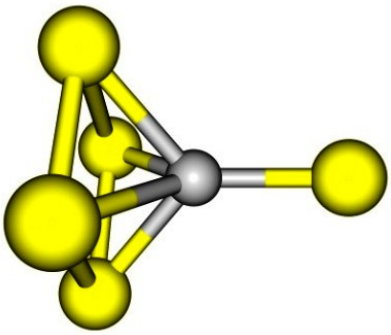
9	 $C_s - {}^3A''$ (0.00)	 $C_{2v} - {}^3A_2$ (0.18)
	 $C_{2v} - {}^3B_2$ (0.19)	 $C_{2v} - {}^3A_2$ (0.25); ${}^1A_1$ (1.06)
	 $C_{2v} - {}^3A_2$ (0.44); ${}^1A_1$ (1.03)	 $C_{2v} - {}^3B_1$ (0.49)
	 $C_{2v} - {}^3B_1$ (0.58)	 $C_{2v} - {}^3B_1$ (1.04)

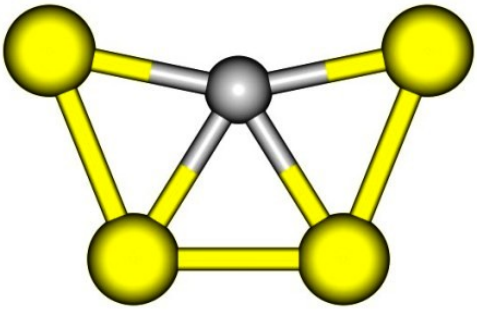
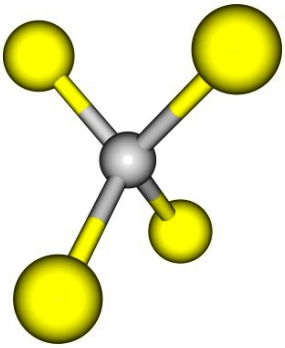
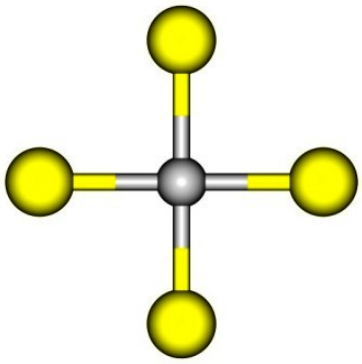
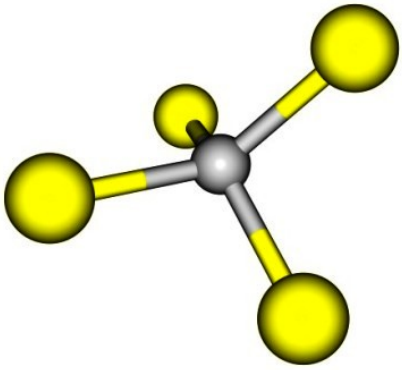
8	 C_{2v} – $^4B_2$ (0.00); $^2B_1$ (0.53)	 C_{2v} – $^4A_2$ (0.15); $^2A_2$ (0.38)
	 C_{2v} – $^4A_2$ (0.20); $^2A_1$ (0.27)	 C_{2v} – $^4B_1$ (0.53); $^2A_1$ (0.76)
	 D_{2h} – $^2B_{3u}$ (0.62)	 C_i – ^4A_g (0.73); ^2A_g (0.81)
	 D_{4h} – $^4B_{2g}$ (0.86)	

7	 C_{2v} – $^3A_2$ (0.00) [**7-I**]	 C_{2v} – $^3B_2$ (0.05) [**7-II**]
	 C_s – $^3A''$ (0.30)	 C_{2v} – $^3A_2$ (0.47); $^1A_1$ (0.87)
	 C_{2v} – $^3B_2$ (0.57)	 C_s – $^3A'$ (0.58)
6	 D_{2h} – $^4B_{3g}$ (0.00); $^4B_{2g}$ (0.10); $^2B_{3g}$ (0.24)	 C_s – $^4A''$ (0.15) **[6-III]**

	 C_{2v} – $^4B_1$ (0.16)	 C_s – $^4A'$ (0.14) [**6-II**]
	 C_s – $^4A''$ (0.38)	

	 C_{2v} – $^4B_2$ (0.84)	 C_s – $^4A'$ (1.25)
5	 C_{2v} – $^3B_1$ (0.00)	 C_s – $^3A''$ (0.13)

	 C_{2v} – $^3A_2$ (0.19)	 C_{2v} – $^3A_2$ (0.28)
	 C_{4v} – $^3B_1$ (0.36)	

4	 C_{2v} – $^4A_2$ (0.00); $^2A_1$ (0.60)	 C_{2v} – $^2A_2$ (0.46)
		

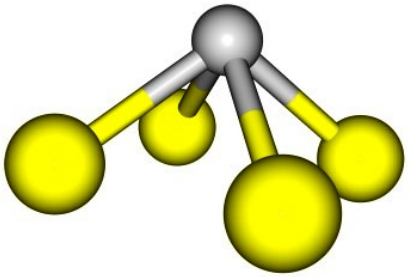
	C_{2v} – $^4B_{1g}$ (0.99)	D_{2d} – $^4A_2$ (1.01)
	 C_{4v} – $^4A_2$ (0.51); $^2A_2$ (0.91)	

Table S1. The natural charges distributed on V of $V@Au_n^{0/+/-}$ clusters (n = 1 – 14) computed at BP86/cc-pVTZ-PP level of theory.

n	neutral	anion	cation
1	0.42	-0.34	1.11
2	0.64	0.06	0.86
3	0.23	-0.02	0.16
4	0.26	0.09	0.43
5	-0.16	-0.39	-0.08
6	-0.41	-0.60	-0.43
7	-0.31	-0.42	-0.16
8	-0.09	-0.18	-0.06
9	-1.62	-1.73	-1.65
10	-1.98	-1.90	-1.92
11	-3.59	-2.75	-3.56
12	-4.37	-4.09	-4.18
13	-4.04	-4.23	-4.25
14	-4.53	-4.31	-4.92

Table S2. Electronegativity of gold clusters as a function of cluster size estimated from the Mulliken formula, EN = 0.187(IE + EA), where IE and EA are experimental ionization energy and electron affinity of gold clusters.

n	Expt IE[2] (eV)	Expt ADE[3] (eV)	Mulliken Electronegativity (eV)
2	9.50	1.92	2.14
3	7.50	3.88	2.13
4	8.60	2.70	2.11
5	8.0	3.06	2.07
6	8.80	2.06	2.03
7	7.8	3.40	2.09
8	8.65	2.73	2.13
9	7.15	3.81	2.05
10	8.2	3.89	2.26
11	7.28	3.76	2.06
12	8.15	3.03	2.09
13	7.70	3.91	2.17
14	8.00	2.94	2.05
15	7.65		

[2] J. Wang, G. Wang and J. Zhao, Phys. Rev. B, **66**, 035418 (2002)
[3] H. Häkkinen, B. Yoon, U. Landman, X. Li, H. J. Zhai and L. S. Wang, *J. Phys. Chem. A*, 2003, **107**, 6168.

Table S3. Coordinates of selected species

Isomer	Coordinates			
14-I	79	0.000000000	3.156362000	0.798275000
	79	-1.394150000	-2.003891000	-1.362846000
	79	-1.394150000	2.003891000	-1.362846000
	79	2.003891000	-1.394150000	1.362846000
	79	3.156362000	0.000000000	-0.798275000
	79	-2.003891000	-1.394150000	1.362846000
	79	-3.156362000	0.000000000	-0.798275000
	79	2.003891000	1.394150000	1.362846000
	79	-2.003891000	1.394150000	1.362846000
	79	1.394150000	-2.003891000	-1.362846000
	79	0.000000000	0.000000000	2.701292000
	79	0.000000000	0.000000000	-2.701292000
	79	1.394150000	2.003891000	-1.362846000
	79	0.000000000	-3.156362000	0.798275000
	23	0.000000000	0.000000000	0.000000000
14-II	79	0.000000000	2.443629000	-0.827814000
	79	-2.332772000	1.458593000	0.545355000
	79	0.000000000	2.265514000	1.954938000
	79	2.332772000	1.458593000	0.545355000
	79	1.818731000	0.000000000	-1.745854000
	79	-1.818731000	0.000000000	-1.745854000
	79	0.000000000	-2.443629000	-0.827814000
	79	2.332772000	-1.458593000	0.545355000
	79	-2.332772000	-1.458593000	0.545355000
	79	1.462807000	0.000000000	2.818965000
	79	-1.462807000	0.000000000	2.818965000
	79	0.000000000	-2.265514000	1.954938000
	23	0.000000000	0.000000000	0.369961000
	79	0.000000000	-1.406406000	-3.344801000
	79	0.000000000	1.406406000	-3.344801000
14-III	79	0.000000000	0.000000000	-2.567023000
	79	2.044112000	1.397721000	-0.987262000
	79	0.000000000	2.844993000	0.450698000
	79	-2.044112000	1.397721000	-0.987262000
	79	-2.044112000	-1.397721000	-0.987262000
	79	-1.998366000	1.417748000	1.810096000
	79	1.998366000	1.417748000	1.810096000
	79	2.044112000	-1.397721000	-0.987262000
	79	1.998366000	-1.417748000	1.810096000
	79	0.000000000	0.000000000	3.178982000
	79	-1.998366000	-1.417748000	1.810096000
	79	0.000000000	-2.844993000	0.450698000
	23	0.000000000	0.000000000	0.372573000
	79	0.000000000	2.738002000	-2.456581000
	79	0.000000000	-2.738002000	-2.456581000

Isomer	Coordinates			
13-I	79	-1.678412000	2.420928000	0.000000000
	79	0.808431000	2.445677000	1.430284000
	79	-2.677677000	-0.274096000	0.000000000
	79	2.670746000	0.860730000	0.000000000
	79	-0.904435000	-1.797692000	-1.614476000
	79	1.855152000	-1.781963000	0.000000000
	79	0.015492000	-3.798178000	0.000000000
	79	-1.344229000	0.836438000	-2.319552000
	79	0.808431000	2.445677000	-1.430284000
	79	1.348670000	-0.225778000	-2.322456000
	79	1.348670000	-0.225778000	2.322456000
	79	-1.344229000	0.836438000	2.319552000
	79	-0.904435000	-1.797692000	1.614476000
	23	-0.006363000	0.228503000	0.000000000
13-II	79	-0.916560000	1.827275000	1.575074000
	79	-2.292104000	-0.670303000	1.457718000
	79	-2.292104000	-0.670303000	-1.457718000
	79	-0.916560000	1.827275000	-1.575074000
	79	1.487683000	2.208747000	0.000000000
	79	0.045146000	-0.342160000	-2.930301000
	79	-1.396459000	-2.868667000	0.000000000
	79	0.045146000	-0.342160000	2.930301000
	79	0.992047000	-2.518748000	1.476984000
	79	0.992047000	-2.518748000	-1.476984000
	79	2.387675000	0.046093000	-1.444011000
	79	2.387675000	0.046093000	1.444011000
	23	0.051832000	-0.378785000	0.000000000
	79	-0.538721000	4.085885000	0.000000000
12-I	79	0.000000000	2.040275000	1.914781000
	79	2.040275000	0.000000000	1.914781000
	79	0.000000000	-2.040275000	1.914781000
	79	-2.040275000	0.000000000	1.914781000
	79	-2.027815000	2.027815000	0.000000000
	79	-2.027815000	-2.027815000	0.000000000
	79	2.027815000	-2.027815000	0.000000000
	79	2.027815000	2.027815000	0.000000000
	79	2.040275000	0.000000000	-1.914781000
	79	0.000000000	-2.040275000	-1.914781000
	79	-2.040275000	0.000000000	-1.914781000
	79	0.000000000	2.040275000	-1.914781000
	23	0.000000000	0.000000000	0.000000000

Isomer	Coordinates			
11-I	79	1.985506000	1.417363000	1.184597000
	79	0.000000000	2.856022000	-0.314063000
	79	-1.985506000	1.417363000	1.184597000
	79	-1.985506000	-1.417363000	1.184597000
	79	1.985506000	-1.417363000	1.184597000
	79	0.000000000	-2.856022000	-0.314063000
	79	2.059605000	-1.375723000	-1.663732000
	79	2.059605000	1.375723000	-1.663732000
	79	-2.059605000	1.375723000	-1.663732000
	79	-2.059605000	-1.375723000	-1.663732000
	79	0.000000000	0.000000000	2.661209000
	23	0.000000000	0.000000000	-0.301784000
10-I	79	0.000000000	2.648426000	1.385906000
	79	-2.315408000	-1.370405000	0.744792000
	79	0.000000000	-2.648426000	1.385906000
	79	2.315408000	-1.370405000	0.744792000
	79	2.315408000	1.370405000	0.744792000
	79	-2.315408000	1.370405000	0.744792000
	79	0.000000000	2.050724000	-1.309071000
	79	-1.821531000	0.000000000	-1.636364000
	79	0.000000000	-2.050724000	-1.309071000
	79	1.821531000	0.000000000	-1.636364000
	23	0.000000000	0.000000000	0.483159000
10-II	79	-1.493866000	2.257000000	0.620014000
	79	-1.493866000	-2.257000000	0.620014000
	79	-2.591208000	0.000000000	1.407601000
	79	1.493866000	-2.257000000	0.620014000
	79	1.493866000	2.257000000	0.620014000
	79	2.591208000	0.000000000	1.407601000
	79	0.000000000	3.908851000	-0.917354000
	79	0.000000000	-1.303411000	-1.802428000
	79	0.000000000	1.303411000	-1.802428000
	79	0.000000000	-3.908851000	-0.917354000
	23	0.000000000	0.000000000	0.495657000
10-III	79	1.323275000	1.866796000	1.421063000
	79	1.323275000	1.866796000	-1.421063000
	79	2.798985000	0.000000000	0.000000000
	79	-1.323275000	1.866796000	-1.421063000
	79	-2.798985000	0.000000000	0.000000000
	79	-1.323275000	1.866796000	1.421063000
	23	0.000000000	0.000000000	0.000000000
	79	1.323275000	-1.866796000	1.421063000
	79	-1.323275000	-1.866796000	1.421063000
	79	-1.323275000	-1.866796000	-1.421063000
	79	1.323275000	-1.866796000	-1.421063000

Isomer	Coordinates			
9-I	79	1.396785000	-1.488001000	1.554856000
	79	1.396785000	-1.488001000	-1.554856000
	79	-0.007086000	-3.360193000	0.000000000
	79	-2.509435000	-2.242654000	0.000000000
	79	-3.035495000	0.430634000	0.000000000
	79	1.396785000	1.183006000	-1.440678000
	79	-1.140315000	2.293434000	0.000000000
	79	1.396785000	1.183006000	1.440678000
	23	-0.510454000	-0.406486000	0.000000000
	79	1.253803000	3.607115000	0.000000000
9-II	79	0.467300000	2.902351000	1.385077000
	79	1.086057000	0.546086000	2.685181000
	79	0.524202000	-1.867399000	-1.639568000
	79	-0.664577000	-3.760109000	0.000000000
	79	0.524202000	-1.867399000	1.639568000
	79	1.086057000	0.546086000	-2.685181000
	79	0.467300000	2.902351000	-1.385077000
	79	-1.831657000	1.583548000	0.000000000
	79	-1.822653000	-1.106648000	0.000000000
	23	0.599590000	0.420965000	0.000000000
9-III	79	0.000000000	1.389500000	2.276401000
	79	0.000000000	2.693062000	0.066129000
	79	0.000000000	-2.693062000	0.066129000
	79	0.000000000	1.284388000	-2.335970000
	79	0.000000000	-1.284388000	-2.335970000
	79	0.000000000	-1.389500000	2.276401000
	23	0.000000000	0.000000000	-0.002721000
	79	0.000000000	3.946425000	-2.282470000
	79	0.000000000	-3.946425000	-2.282470000
	79	0.000000000	0.000000000	4.552611000
8-I	79	0.000000000	1.371708000	2.822238000
	79	0.000000000	2.746084000	0.611490000
	79	0.000000000	-2.746084000	0.611490000
	79	0.000000000	1.289783000	-1.798448000
	79	0.000000000	-1.289783000	-1.798448000
	79	0.000000000	-1.371708000	2.822238000
	79	0.000000000	3.972502000	-1.715713000
	79	0.000000000	-3.972502000	-1.715713000
	23	0.000000000	0.000000000	0.552543000

Isomer	Coordinates			
8-II	79	2.373051000	1.419189000	0.481368000
	79	-2.373051000	1.419189000	0.481368000
	79	0.000000000	2.657541000	0.805623000
	79	-2.373051000	-1.419189000	0.481368000
	79	2.373051000	-1.419189000	0.481368000
	79	0.000000000	-2.657541000	0.805623000
	79	-1.347603000	0.000000000	-1.842689000
	79	1.347603000	0.000000000	-1.842689000
	23	0.000000000	0.000000000	0.510610000
8-III	79	-1.462452000	1.344112000	-1.527361000
	79	1.462452000	1.344112000	-1.527361000
	79	0.000000000	2.698039000	0.361075000
	79	0.000000000	1.372863000	2.642660000
	79	0.000000000	-1.372863000	2.642660000
	79	1.462452000	-1.344112000	-1.527361000
	79	0.000000000	-2.698039000	0.361075000
	79	-1.462452000	-1.344112000	-1.527361000
	23	0.000000000	0.000000000	0.350257000
7-I	79	0.000000000	0.000000000	3.916003000
	79	0.000000000	1.441509000	1.698403000
	79	0.000000000	-1.441509000	1.698403000
	79	0.000000000	2.611979000	-0.610453000
	79	0.000000000	-2.611979000	-0.610453000
	79	0.000000000	1.336927000	-2.955320000
	79	0.000000000	-1.336927000	-2.955320000
	23	0.000000000	0.000000000	-0.622596000
7-II	79	0.000000000	3.716726000	-0.833590000
	79	0.000000000	1.316816000	-1.981461000
	79	0.000000000	-1.316816000	-1.981461000
	79	0.000000000	-3.716726000	-0.833590000
	79	0.000000000	-2.261021000	1.383825000
	79	0.000000000	0.000000000	2.799839000
	79	0.000000000	2.261021000	1.383825000
	23	0.000000000	0.000000000	0.215062000

Isomer	Coordinates			
6-I	79	0.000000000	2.320921000	1.304657000
	79	0.000000000	0.000000000	2.695984000
	79	0.000000000	0.000000000	-2.695984000
	79	0.000000000	-2.320921000	1.304657000
	79	0.000000000	-2.320921000	-1.304657000
	79	0.000000000	2.320921000	-1.304657000
	23	0.000000000	0.000000000	0.000000000
5-I	79	0.000000000	2.273980000	0.873471000
	79	0.000000000	0.000000000	2.183683000
	79	0.000000000	2.063366000	-1.900764000
	79	0.000000000	-2.273980000	0.873471000
	79	0.000000000	-2.063366000	-1.900764000
	23	0.000000000	0.000000000	-0.443424000
5-II	23	0.000000000	0.000000000	-0.450340000
	79	0.000000000	0.000000000	2.204619000
	79	0.000000000	2.242713000	0.813285000
	79	1.939298000	0.000000000	-1.850038000
	79	-1.939298000	0.000000000	-1.850038000
	79	0.000000000	-2.242713000	0.813285000
5-III	79	0.638074000	-0.883482000	2.374631000
	79	0.572490000	1.665387000	1.316274000
	79	0.572490000	1.665387000	-1.316274000
	79	0.638074000	-0.883482000	-2.374631000
	79	-2.358076000	-1.401509000	0.000000000
	23	-0.121780000	-0.541840000	0.000000000
4-I	79	0.000000000	2.516071000	1.176551000
	79	0.000000000	1.313906000	-1.316172000
	79	0.000000000	-1.313906000	-1.316172000
	79	0.000000000	-2.516071000	1.176551000
	23	0.000000000	0.000000000	0.959137000
4-II	79	1.419559000	1.419559000	1.419559000
	79	-1.419559000	-1.419559000	1.419559000
	79	-1.419559000	1.419559000	-1.419559000
	79	1.419559000	-1.419559000	-1.419559000
	23	0.000000000	0.000000000	0.000000000
3-I	79	0.000000000	0.000000000	2.397640000
	79	0.000000000	2.077844000	-1.198723000
	23	0.000000000	0.000000000	-0.000667000
	79	0.000000000	-2.077844000	-1.198723000
2-I	79	0.000000000	2.387230000	-0.064238000
	79	0.000000000	-2.387230000	-0.064238000
	23	0.000000000	0.000000000	0.441287000