Supporting information: 'Systematic cluster growth: a structure search method for transition metal clusters.'

Peter L. Rodríguez-Kessler,*[a] Adán R. Rodríguez-Domínguez,[b] and Alvaro Muñoz-Castro*[a]

[a] *Grupo de Química Inorgánica y Materiales Moleculares, Facultad de Ingeniería, Universidad Autónoma de Chile, El Llano Subercaseaux 2810, Santiago, Chile. E-mail: rodriguezkessler.p@gmail.com, alvaro.munoz@uautonoma.cl*

[b] *Instituto de Física, Universidad Autónoma de San Luis Potosí, San Luis Potosí 78000, México*

I Definitions and complementary data

I.I Effective coordination number and average bond length

To characterize the structures of the clusters, we use the effective coordination number (ECN) and averaged bond length [Angew. Chem. 1970, 9, 25-34] parameters. In our previous work [J. Phys. Chem. C 2015, 119, 22, 12378-12384], we have defined the averaged bond length for the ith atom as

$$d_{av}^{i} = \frac{\sum_{j=1}^{n} |R_i - R_j| \exp\left[1 - \left(\frac{|R_i - R_j|}{d_{av}^{i}}\right)\right]}{\sum_{j=1}^{n} \exp\left[1 - \left(\frac{|R_i - R_j|}{d_{av}^{i}}\right)\right]} \tag{1}$$

where R_i are the positions of the n atoms in the cluster. The initial value of d_{av} is taken as the shortest distance of the i atom at position R_i over all j atomic neighbors at positions R_j (with $j \neq i$). The final value is obtained self-consistently with a convergence criterion of 10^{-4} Å, i.e., the obtained value of d_{av} is used as the initial value for the next iteration. The final value of d_{av} is obtained typically by using 4 iterations, and it is necessary to calculate ECN_i, defined as:

$$\mathrm{ECN}_i = \sum_{j=1}^{n} \exp\left[1 - \left(\frac{|R_i - R_j|}{d_{av}^{i}}\right)\right]. \tag{2}$$

The average ECN and d_{av} for a particular configuration are obtained by

$$\mathrm{ECN} = \frac{1}{n} \sum_{i=1}^{n} \mathrm{ECN}_i \tag{3}$$

and

$$d_{av} = \frac{1}{n} \sum_{i=1}^{n} d_{av}^{i}. \tag{4}$$

The power of 6 and exponential form in d_{av} are used to obtain similar values for the standard coordination number CN for highly symmetric systems such as icosahedral clusters (CN=6.46) and fcc crystalline solids (CN=12) [Phys. Rev. B 2010, 81, 155446].

I.II Descent gradient (DG)

For minimization of the total energy as a function of the atomic coordinates of the LJ clusters, we use the DG algorithm is used. To calculate the force matrix, finite differences are used, i.e., each ion is displaced in the direction of each cartesian coordinate by the following expression

$$\mathbf{r}_{i+1,k} = \mathbf{r}_{i,k} - \gamma \frac{\partial E_k}{\partial \mathbf{r}_{i,k}}, \tag{5}$$

where the sequence

$$E_0\left(\mathbf{r}_i \ldots \mathbf{r}_n\right) \geqslant E_1\left(\mathbf{r}_i \ldots \mathbf{r}_n\right) \geqslant E_2\left(\mathbf{r}_i \ldots \mathbf{r}_n\right) \geqslant \ldots, \tag{6}$$

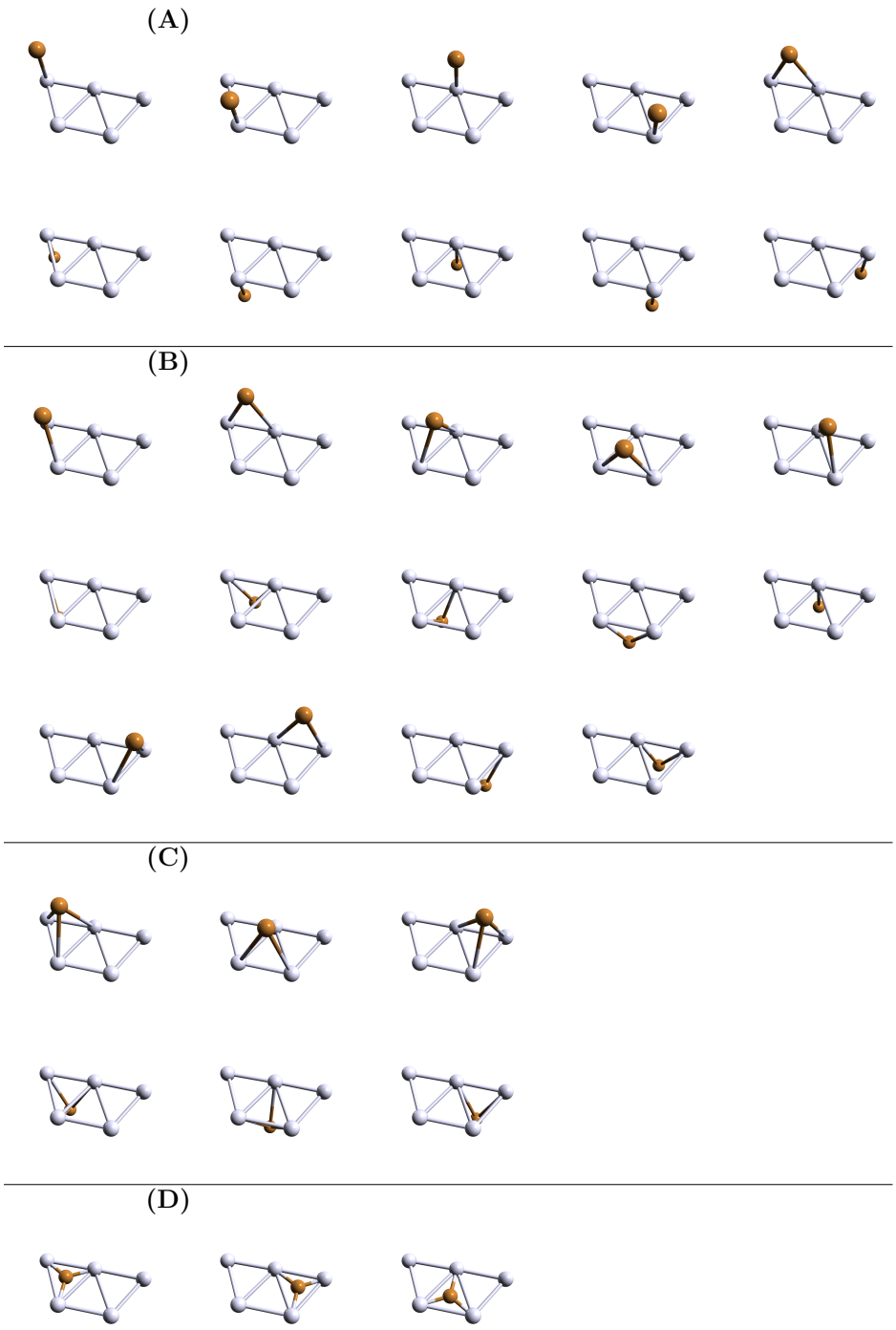
converges to the desired local minimum. The step size γ changes at every iteration as follows:

$$\gamma = \gamma_{min} + \left(\left(\gamma_{max} - \gamma_{min}\right) \Big/ N\right) * k, \tag{7}$$

where N is the number of iterations, γ (in the range of 0.003-0.05), and k the current iteration.

I.III Atomic decoration

Fig. S1 The atomic decoration of a 5 atom cluster in the (A) top, (B) bridge, (C) hollow and (D) iterstitial sites.



II Performance of the SCG method as a function of the number of seeds

Table S1 The total energies of the LJ_n clusters by using 4, 8, 16 and 32 seeds, obtained with the SCG method. The asterisk denotes when the global minimum is not found according to the number of seeds used.

seeds	4		8		16		3 2		-	
size (N)	E(ε)	Eval.	E(ε)	Eval.	E(ε)	Eval	E(ε)	Eval	E(ε)[a,b]	Eval[a]
13	-44.3267	1202	-44.3267	2371	-44.326	4808	-44.326	10160	-44.326	754
14	-47.8451	1484	-47.8451	2805	-47.845	5623	-47.845	10529	-47.845	112
15	-52.3226	1526	-52.3226	2991	-52.322	5915	-52.322	12554	-52.322	132
16	-56.8157	1746	-56.8157	3355	-56.815	6580	-56.815	13559	-56.815	177
17	-61.3179	1831	-61.3179	3617	-61.317	7054	-61.317	14088	-61.317	153
18	-66.5309	1931	-66.5309	3842	-66.530	7366	-66.530	14619	-66.530	6,620
19	-72.6597	2010	-72.6597	4064	-72.659	7815	-72.659	15693	-72.659	9,901
20	-77.1770	2146	-77.1770	4270	-77.177	8335	-77.177	16879	-77.177	866
21	-81.6845	2251	-81.6845	4443	-81.684	8822	-81.684	17472	-81.684	175
22	-86.8097	2380	-86.8097	4702	-86.809	9433	-86.809	19294	-86.809	1542
23	-92.8444	2472	-92.8444	4910	-92.844	9703	-92.844	19558	-92.844	2041
24	-97.3488	2551	-97.3488	5137	-97.348	10247	-97.348	20503	-97.348	163
25	-102.372	2706	-102.372	5404	-102.372	10621	-102.372	21594	-102.372	283
26	-108.315	2817	-108.315	5655	-108.315	11233	-108.315	22678	-108.315	2213
27	-112.873	2932	-112.873	5860	-112.873	11755	-112.873	23653	-112.873	3599
28	-117.822	3081	-117.822	6092	-117.822	12213	-117.822	24415	-117.822	411
29	-123.587	3172	-123.587	6390	-123.587	12903	-123.587	25811	-123.587	3949
30	-128.286	3300	-128.286	6568	-128.286	13085	-128.286	26252	-128.286	11198
31	-133.293*	3413	-133.293*	6845	-133.586	13532	-133.586	26879	-133.586	115531
32	-138.823*	3575	-138.823*	7056	-139.635	13953	-139.635	28109	-139.635	1431
33	-143.622*	3740	-144.714*	7080	-144.842	14239	-144.842	28815	-144.842	1174
34	-149.672*	3678	-149.996*	7192	-150.044	14412	-150.044	28530	-150.044	10632
35	-154.592*	3610	-155.756	7173	-155.756	14316	-155.756	28575	-155.756	9988
36	-159.600*	3345	-161.825	7487	-161.825	14809	-161.825	28690	-161.825	249
37	-165.424*	3441	-167.033	7575	-167.033	14790	-167.033	29577	-167.033	12306
38	-171.500*	3541	-173.134*	7828	-173.134*	15587	-173.134*	30730	-173.928	2226
39	-176.757*	3627	-180.033	8213	-180.033	16196	-180.033	31996	-180.033	14832
40	-182.713*	3758	-185.249	8342	-185.249	16562	-185.249	32968	-185.249	7505

[a] Baron et al.
[b] Leary et al.

III Cartesian coordinates

III.I The lowest energy structures of the clusters calculated by using the VASP code and the PBE approach.

Ti_6 geometry:

Ti 0.85088 0.29233 -1.66194
Ti -0.84832 -0.28940 1.65441
Ti 0.74483 -1.49392 0.15582
Ti 1.45315 0.85383 0.85346
Ti -0.75281 1.48622 -0.15172
Ti -1.44773 -0.84905 -0.85004

Ti_7 geometry:

Ti 1.72126 0.06441 -1.26345
Ti -1.87238 0.93916 0.41893
Ti -0.65116 -0.88496 -0.93051
Ti 0.65104 0.88455 0.93058
Ti -0.91199 -1.04109 1.62779

Ti 1.31014 -1.58255 0.58709
Ti -0.24690 1.62047 -1.37042

Ti_8 geometry:
Ti 1.40944 1.77731 -0.73902
Ti -1.54190 -0.73297 -0.43863
Ti 0.88452 -0.67933 -1.36683
Ti 1.37402 -0.03890 1.10342
Ti -0.71674 1.45095 0.70216
Ti -0.74804 1.26372 -1.88019
Ti 0.26135 -2.30810 0.54449
Ti -0.92265 -0.73267 2.07459

Ti_9 geometry:
Ti 1.112368 0.490570 -1.359070
Ti -2.550852 -0.719280 0.257260
Ti -0.696362 -1.477240 -1.409830
Ti -1.751972 1.205110 1.602360
Ti -1.205972 1.083670 -0.833920
Ti 0.040588 -0.676700 0.943860
Ti 1.787888 -1.832600 -0.728320
Ti 0.675418 1.835790 0.910720
Ti 2.588898 0.090680 0.616940

Ti_{10} geometry:
Ti 0.196859 2.406431 0.626521
Ti -0.257081 -1.147229 -1.642329
Ti 0.167289 -0.251059 1.045261
Ti 1.106569 1.021811 -1.343669
Ti -1.461121 1.039061 -0.883609
Ti -2.123831 -1.297929 0.128911
Ti 0.023369 -2.733689 0.259661
Ti -2.137671 1.156871 1.413421
Ti 2.402119 1.064261 0.784401
Ti 2.083499 -1.258529 -0.388569

Ti_{11} geometry:
Ti -0.436280 0.671051 -2.460610
Ti -0.913530 -0.115849 -0.013000
Ti 1.175980 -1.226969 -1.613950
Ti -0.694580 2.477251 -0.287460
Ti -1.618430 1.510751 2.009140
Ti -0.320090 -0.768939 2.449070
Ti 0.787400 1.475911 1.640030
Ti -1.138010 -1.857689 -2.042640
Ti 1.492050 1.215701 -0.831230
Ti -0.060790 -2.573529 0.275790
Ti 1.726280 -0.807689 0.874860

Ti_{12} geometry:
Ti 1.860070 0.156700 -1.561531

Ti 0.083900 0.678570 2.324989
Ti -0.535600 0.156740 -0.285761
Ti 1.939290 -0.619130 0.979619
Ti 1.457740 1.903880 0.426349
Ti 0.803240 -2.176950 -0.774341
Ti -0.378450 -1.832460 1.541259
Ti -2.263320 -0.004660 1.594719
Ti -1.781240 -2.048900 -0.660671
Ti -0.234220 -0.847220 -2.683491
Ti 0.074160 2.146370 -1.732591
Ti -1.025570 2.487060 0.831449

Ti_{13} geometry:
Ti 11.14016 9.09168 7.50967
Ti 9.20229 9.63348 11.50332
Ti 9.10099 9.00796 8.98427
Ti 11.16482 8.19169 10.26330
Ti 10.62964 10.98239 9.57448
Ti 9.94031 6.65803 8.30848
Ti 8.85902 7.06766 10.71865
Ti 6.86864 8.96151 10.48658
Ti 7.36928 7.06909 8.37903
Ti 8.69390 8.35638 6.48251
Ti 9.10888 10.95111 7.26662
Ti 8.07516 11.33279 9.71729
Ti 6.84690 9.69623 7.80580

Ti_{14} geometry:
Ti 10.79125 10.63769 8.86129
Ti 6.50606 9.78706 9.38263
Ti 8.98784 8.98674 8.97737
Ti 8.34312 11.31553 10.32984
Ti 8.33551 8.56327 11.29720
Ti 7.07128 7.22412 9.08491
Ti 11.17562 7.87230 8.00919
Ti 7.06274 8.94877 7.00443
Ti 9.67006 9.43486 6.50228
Ti 9.55653 6.49430 9.62267
Ti 8.93464 6.91859 7.15565
Ti 11.15664 8.28282 10.54815
Ti 10.28142 10.36590 11.45376
Ti 8.12731 11.16804 7.77062

Ni_6 geometry:
Ni 0.706140 0.245420 -1.462800
Ni -0.706550 -0.243660 1.462710
Ni 0.760980 -1.444090 0.177790
Ni 1.261250 0.707100 0.778660
Ni -0.761510 1.443970 -0.177970
Ni -1.260310 -0.708740 -0.778390

Ni_7 geometry:

Ni	0.067421	-0.399930	-1.388210
Ni	-1.026499	1.020010	0.058460
Ni	0.628741	0.671250	1.669010
Ni	1.738881	-0.759510	0.202390
Ni	-0.505739	-1.148630	0.738890
Ni	-2.139959	-0.790830	-0.838900
Ni	1.237151	1.407640	-0.441640

Ni_8 geometry:

Ni	1.288051	1.617869	-0.669420
Ni	-1.233169	-0.633631	-0.303430
Ni	0.837541	-0.641391	-1.297170
Ni	1.077591	-0.082571	0.919270
Ni	-0.678169	1.376639	0.664080
Ni	-0.686059	1.148229	-1.712790
Ni	0.307481	-2.202451	0.413380
Ni	-0.913269	-0.582691	1.986080

Ni_9 geometry:

Ni	0.080580	2.412210	-0.059490
Ni	-1.456640	0.742830	0.632960
Ni	0.333240	-1.410060	-1.006710
Ni	1.934530	-1.237270	0.750050
Ni	0.735610	0.688980	1.433610
Ni	1.502100	0.610800	-0.664780
Ni	-0.424360	-1.333220	1.072220
Ni	-2.014490	-1.138850	-0.691700
Ni	-0.690570	0.664580	-1.466160

Ni_{10} geometry:

Ni	-0.208749	2.777821	0.091720
Ni	-1.429019	0.891481	-0.279780
Ni	-0.338439	-0.969169	-1.364150
Ni	1.429341	-0.891899	0.278090
Ni	0.338551	0.969521	1.363870
Ni	0.871311	1.086211	-0.987840
Ni	-0.869939	-1.086799	0.988430
Ni	-2.487129	-1.097199	-0.615120
Ni	0.845761	-0.949869	2.479890
Ni	1.848311	-0.730099	-1.955110

Ni_{11} geometry:

Ni	1.826210	1.170711	0.449821
Ni	-1.900820	0.773281	0.837201
Ni	-0.173650	0.958641	-0.680039
Ni	-0.110490	2.259281	1.258741
Ni	0.175610	0.007621	1.713651
Ni	-1.069980	-1.343029	0.128281
Ni	1.331260	-1.085139	-0.121239
Ni	-2.187860	0.007641	-1.381679

Ni	1.809660	0.437031	-1.798409
Ni	0.409410	-2.259309	1.603361
Ni	-0.109350	-0.926729	-2.009689

Ni_{12} geometry:

Ni	-0.207098	1.342521	0.482832
Ni	0.704572	-0.212829	-1.198828
Ni	2.133702	0.957581	0.280572
Ni	-0.502298	-1.104369	0.727572
Ni	1.844022	-1.376359	0.524942
Ni	-1.160658	1.157251	-1.690618
Ni	-1.448218	-1.176929	-1.445208
Ni	-2.324438	0.299551	0.177282
Ni	0.954272	2.103071	-1.381468
Ni	0.959902	0.100401	2.142912
Ni	-1.347838	0.424041	2.293902
Ni	0.394082	-2.513929	-0.913888

Ni_{13} geometry:

Ni	-0.485920	1.328840	0.304911
Ni	0.423080	-0.194800	-1.368469
Ni	1.920350	0.977010	0.153261
Ni	-0.783570	-1.078830	0.557261
Ni	1.630400	-1.360730	0.397071
Ni	-1.457670	1.170700	-1.858219
Ni	-1.742370	-1.141180	-1.615359
Ni	-2.615980	0.322230	-0.008979
Ni	0.732430	2.097360	-1.508169
Ni	0.747640	0.118970	2.022771
Ni	-1.558120	0.421120	2.145721
Ni	0.168410	-2.473190	-1.031119
Ni	3.021320	-0.187500	1.809321

Ni_{14} geometry:

Ni	-0.203271	1.321331	0.475749
Ni	0.710249	-0.214529	-1.210521
Ni	2.160329	0.971721	0.286579
Ni	-0.503821	-1.107219	0.730279
Ni	1.868319	-1.384989	0.533409
Ni	-1.178741	1.176551	-1.708791
Ni	-1.470601	-1.180559	-1.461791
Ni	-2.357381	0.310651	0.180789
Ni	0.959779	2.093241	-1.391501
Ni	0.975809	0.107001	2.173279
Ni	-1.345371	0.406821	2.293089
Ni	0.390899	-2.501369	-0.910531
Ni	3.246959	-0.198569	1.947639
Ni	-3.253161	0.199911	-1.937681

Cu_6 geometry:

Cu 1.159738 0.512508 -0.567762
Cu -0.592712 0.648568 1.076298
Cu -0.572592 -1.156052 -0.514182
Cu 1.154748 -1.262222 -2.086892
Cu 1.108448 2.250618 0.993338
Cu -2.257632 -0.993422 1.099198

Cu_7 geometry:
Cu 0.152901000 2.09899300 0.000457000
Cu -1.357307000 -1.60823100 0.000249000
Cu -0.000185000 0.00050800 -1.281519000
Cu 0.000215000 -0.00074100 1.281339000
Cu 2.043240000 0.50305600 0.000126000
Cu 1.110143000 -1.78748100 -0.000579000
Cu -1.949008000 0.79389500 -0.000073000

Cu_8 geometry:
Cu 1.169873 0.307390 -1.119610
Cu 1.873453 -0.930020 0.787850
Cu -0.490427 2.031740 -0.792000
Cu -1.054917 -0.102100 -1.968220
Cu -1.591897 0.220220 0.365300
Cu -0.143367 -1.602940 -0.360850
Cu -0.328477 -0.999690 1.972250
Cu 0.565762 1.075400 1.115280

Cu_9 geometry:
Cu 0.706991 -2.682730 1.247830
Cu 1.094691 0.626300 -1.260890
Cu 1.783851 -0.609750 0.671870
Cu -0.596189 2.359250 -1.043950
Cu -1.130059 0.218300 -2.118510
Cu -1.673109 0.580580 0.211640
Cu -0.241079 -1.284540 -0.491340
Cu -0.422049 -0.643510 1.846270
Cu 0.476951 1.436100 0.937080

Cu_{10} geometry:
Cu -0.705672 -0.905659 -1.013069
Cu 0.399008 1.294921 -0.714299
Cu -1.990732 1.160431 -0.808299
Cu 1.527278 -0.569189 -1.817429
Cu -0.990242 2.719941 0.789291
Cu 1.005258 1.555951 1.589431
Cu -0.964312 0.255641 1.162261
Cu 0.989568 -2.721929 -0.785729
Cu 1.269298 -0.644789 0.564981
Cu -0.539452 -2.145319 1.032861

Cu_{11} geometry:
Cu -2.007881 0.104090 0.179501

Cu	0.025279	0.268790	-1.353229
Cu	-2.112161	1.364980	-1.894809
Cu	-0.712161	2.131380	-0.013909
Cu	0.102079	0.208840	1.359901
Cu	-0.475211	-1.787040	-0.024449
Cu	1.675569	1.496010	0.065131
Cu	-1.913261	-1.053170	-1.918809
Cu	1.124149	-1.915570	1.877221
Cu	2.498069	0.083920	1.914481
Cu	1.795529	-0.902230	-0.191029

Cu_{12} geometry:

Cu	1.077319	2.317029	1.436202
Cu	-2.096141	-0.091621	0.162532
Cu	-0.229331	-0.196011	-1.500868
Cu	-2.330181	0.914089	-1.977528
Cu	-0.791761	1.916419	-0.311398
Cu	0.110749	0.149579	1.161982
Cu	-0.586991	-2.005991	0.173562
Cu	1.565509	1.214929	-0.618448
Cu	-2.195831	-1.600701	-1.670848
Cu	1.291979	-1.773101	1.944892
Cu	2.495579	0.319309	1.523052
Cu	1.689099	-1.163931	-0.323128

Cu_{13} geometry:

Cu	-0.005472	-2.359540	-1.720669
Cu	-2.092852	0.191750	0.370201
Cu	-0.272562	0.033700	-1.352499
Cu	-2.343412	1.167790	-1.794979
Cu	-0.706982	2.170530	-0.158939
Cu	0.142238	0.362800	1.323961
Cu	-0.674382	-1.777050	0.482911
Cu	1.596858	1.331260	-0.480739
Cu	-2.232372	-1.343980	-1.498629
Cu	1.316298	-1.660260	2.012661
Cu	2.529868	0.429420	1.566711
Cu	1.608678	-1.088200	-0.273019
Cu	1.134088	2.541780	1.523031

Cu_{14} geometry:

Cu	1.423531	-1.425330	-0.162920
Cu	0.240541	0.070550	3.345560
Cu	-0.746089	-1.210130	-1.141330
Cu	-2.309819	0.065510	0.306480
Cu	1.946131	-0.013310	1.684800
Cu	1.496361	1.340390	-0.224590
Cu	-0.414659	-1.158160	1.340460
Cu	-0.682519	1.188500	-1.194950
Cu	-0.351929	1.240440	1.285940
Cu	-2.068189	0.121050	2.687170

Cu	1.436921	-0.085660	-2.133600
Cu	3.374621	-0.098300	-0.445950
Cu	-2.700679	0.024150	-2.054250
Cu	-0.644219	-0.059700	-3.292820

Ag_6 geometry:

Ag	2.184252	-2.132910	-0.539880
Ag	-1.127458	1.112760	0.274000
Ag	-2.345768	0.352400	-1.994200
Ag	0.156452	1.774580	2.537660
Ag	-0.076098	-0.912710	-1.320390
Ag	1.208622	-0.194120	1.042810

Ag_7 geometry:

Ag	1.253589	-1.930391	-0.561741
Ag	-1.764171	1.411969	-0.711711
Ag	-0.831791	-0.843321	-2.051441
Ag	-0.258041	1.717949	1.611709
Ag	-0.974571	-0.844621	0.739749
Ag	1.599389	-0.356611	1.711609
Ag	0.975599	0.845029	-0.738171

Ag_8 geometry:

Ag	1.575090	0.406530	0.632030
Ag	-1.071040	1.365770	0.189780
Ag	0.136310	-0.404080	-1.693270
Ag	1.031310	2.193050	-1.406380
Ag	-0.641660	-1.368180	0.873210
Ag	-2.529200	-0.649020	-1.012980
Ag	-0.220410	0.647200	2.720720
Ag	1.719600	-2.191270	-0.303110

Ag_9 geometry:

Ag	2.862311	-0.862410	-0.496130
Ag	-1.229669	-0.380960	1.897910
Ag	0.530371	-0.357980	-1.976340
Ag	-3.315589	0.913790	0.589630
Ag	1.362471	0.394950	1.517200
Ag	1.921501	1.786160	-0.844090
Ag	0.445631	-1.989530	0.325110
Ag	-1.884269	-0.976910	-0.862470
Ag	-0.692759	1.472890	-0.150820

Ag_{10} geometry:

Ag	1.613051	0.331421	0.620701
Ag	-0.912619	1.502841	0.070851
Ag	0.184291	-0.635689	-1.630889
Ag	1.225941	1.930111	-1.638569
Ag	-0.881459	-1.197189	0.939161
Ag	-2.532259	-0.380849	-1.158289
Ag	-0.172579	0.837721	2.678461

Ag	1.308391	-1.551249	2.794601
Ag	-1.310459	1.553151	-2.792929
Ag	1.477701	-2.390269	0.116901

Ag_{11} geometry:

Ag	-0.815230	0.960898	-1.015989
Ag	-2.682540	1.807968	0.855821
Ag	0.817600	-1.284622	0.546761
Ag	2.659260	0.172838	2.027461
Ag	-0.015410	1.200848	1.744771
Ag	1.253700	-0.632742	-2.147979
Ag	3.470060	-0.927272	-0.391889
Ag	-1.840710	-0.822612	1.141821
Ag	1.834060	1.376928	-0.338199
Ag	-1.223430	-1.790222	-1.373289
Ag	-3.457360	-0.062012	-1.049289

Ag_{12} geometry:

Ag	0.833940	-0.966719	-1.257250
Ag	0.859780	2.986381	1.341540
Ag	-0.005400	0.154001	-3.671960
Ag	-1.806540	0.219981	-1.590620
Ag	1.045930	-1.539599	1.472180
Ag	2.202180	0.744001	0.477980
Ag	-1.227750	-2.274279	-2.609330
Ag	0.426510	1.866031	-1.443480
Ag	-0.724410	0.769731	0.914420
Ag	-1.466770	-1.881459	0.194020
Ag	-1.135020	-0.934459	3.043100
Ag	0.997550	0.856391	3.129400

Ag_{13} geometry:

Ag	0.861021	-0.508479	-1.274041
Ag	0.610981	3.259311	1.510969
Ag	-0.070329	0.670561	-3.582751
Ag	-1.884309	0.503061	-1.487181
Ag	1.099701	-1.400169	1.362489
Ag	2.104901	1.081541	0.652079
Ag	-1.096159	-1.882129	-2.698631
Ag	0.316051	2.285621	-1.203351
Ag	-0.799969	0.938091	1.044839
Ag	-1.521739	-1.634249	0.236479
Ag	-1.044679	-1.013979	3.038229
Ag	0.964561	0.938521	3.196859
Ag	0.459971	-3.237699	-0.795991

Ag_{14} geometry:

Ag	1.492449	-1.335199	-0.615271
Ag	0.766189	0.892721	3.689789
Ag	-0.512601	-0.797779	-2.667731
Ag	-3.344811	0.240051	0.732439

Ag 0.651899 -1.297339 1.999429
Ag 2.361739 0.792241 1.338449
Ag -1.233721 -1.327919 0.012569
Ag 1.063079 1.336421 -1.216511
Ag -0.408201 1.324331 1.160549
Ag -1.764471 -0.234889 2.941679
Ag 2.144139 -0.337309 -3.200681
Ag 3.720849 0.338241 -1.007361
Ag -3.254751 -0.889459 -1.902931
Ag -1.681791 1.295891 -1.264411

Pt_6 geometry:
Pt 0.000000 -1.578847 -0.177908
Pt 0.000000 0.621563 1.406382
Pt 0.000000 -1.113597 -2.591928
Pt 0.000000 2.814703 0.316752
Pt 0.000000 0.918473 -1.232568
Pt 0.000000 -1.662297 2.279272

Pt_7 geometry:
Pt 0.406934 1.375131 0.193007
Pt 2.403794 0.911431 1.561937
Pt -0.430596 1.167361 -2.233183
Pt -2.101746 1.411141 -0.357113
Pt 1.054754 -1.073979 1.078787
Pt -0.923286 -0.849489 -0.720843
Pt -0.409856 -2.941599 0.477407

Pt_6 geometry:
Pt 0.809780 -1.256130 -1.183198
Pt -1.746610 1.267850 -1.199348
Pt 0.860120 0.000000 1.021743
Pt -1.611960 0.000000 1.046302
Pt 2.979980 0.000000 -0.508397
Pt -1.746610 -1.267850 -1.199348
Pt 0.809780 1.256130 -1.183198
Pt -0.354480 0.000000 3.205443

Pt_6 geometry:
Pt 2.518480 0.000000 1.753858
Pt 0.000000 -1.306540 -2.321272
Pt -1.369720 1.258740 -0.184822
Pt -1.369720 -1.258740 -0.184822
Pt -2.518480 0.000000 1.753858
Pt 0.000000 1.306540 -2.321272
Pt 0.000000 0.000000 1.874118
Pt 1.369720 -1.258740 -0.184822
Pt 1.369720 1.258740 -0.184822

Pt_6 geometry:
Pt 0.000000 2.538300 -1.794850

Pt	2.538300	0.000000	1.794850
Pt	-2.538300	0.000000	1.794850
Pt	-1.380720	-1.380720	0.000000
Pt	1.380720	-1.380720	0.000000
Pt	0.000000	0.000000	1.952630
Pt	-1.380720	1.380720	0.000000
Pt	0.000000	0.000000	-1.952630
Pt	1.380720	1.380720	0.000000
Pt	0.000000	-2.538300	-1.794850

Pt_6 geometry:

Pt	2.502715	-0.986654	-1.402414
Pt	-1.955475	-1.004374	-2.266444
Pt	0.667525	2.760226	1.377786
Pt	0.395395	0.410336	2.362096
Pt	-1.475935	-1.457134	0.158706
Pt	-1.004045	1.040336	0.369906
Pt	1.107405	-1.543534	0.609276
Pt	1.959615	1.047486	0.031836
Pt	0.296725	0.209776	-1.788264
Pt	-0.553045	-1.957144	2.490886
Pt	-1.940885	1.480676	-1.943374

Pt_6 geometry:

Pt	-2.773283	-0.861403	0.542467
Pt	1.938517	-0.229633	0.854548
Pt	0.212267	0.251827	-3.248053
Pt	-0.709553	-2.401153	0.826477
Pt	-1.239393	1.397467	-0.040183
Pt	0.327198	-1.274023	-1.175083
Pt	-1.887473	-0.250493	-1.814433
Pt	-0.410583	-0.123983	1.830967
Pt	1.015268	1.499847	-1.210763
Pt	-0.273243	2.407067	2.090348
Pt	1.823057	-2.703773	0.363407
Pt	1.977218	2.288257	0.980297

Pt_6 geometry:

Pt	0.322251	1.603981	0.679062
Pt	0.421831	-0.589279	2.718662
Pt	-1.183599	-0.738679	-1.864658
Pt	-0.320899	-3.088079	-1.438958
Pt	-0.258269	-2.449179	1.062552
Pt	0.809521	1.157881	-1.760918
Pt	1.329441	-1.316649	-0.546518
Pt	2.339261	0.191411	1.197052
Pt	-1.496829	-0.315999	0.591052
Pt	3.166331	0.362921	-1.245558
Pt	-1.623449	1.742361	-2.267018
Pt	-1.398069	1.339481	2.659282
Pt	-2.107519	2.099831	0.215972

Pt_6 geometry:

Pt	-0.798051	-1.374619	1.663814
Pt	2.039889	2.515591	-1.649466
Pt	2.039919	-2.515649	-1.649516
Pt	1.104059	-0.000009	2.665994
Pt	-0.445061	0.000061	-1.074476
Pt	1.740639	-1.374369	0.612344
Pt	-0.351911	-2.518279	-0.849776
Pt	-0.798101	1.374661	1.663754
Pt	1.975089	0.000051	-1.812276
Pt	-0.351901	2.518191	-0.849726
Pt	-2.608691	-2.515959	0.275744
Pt	-2.608611	2.515871	0.275754
Pt	1.740639	1.374401	0.612274
Pt	-2.677901	0.000061	0.115564