Electronic Supplementary Material (ESI) for Dalton Transactions.

On the structural landscape in endohedral silicon and germanium clusters, $M@Si_{12}$ and $M@Ge_{12}$.

*José M. Goicoechea and John E. McGrady**

Department of Chemistry, University of Oxford, South Parks Road, Oxford OX1 3QR, U.K.

john.mcgrady@chem.ox.ac.uk

Supporting Information

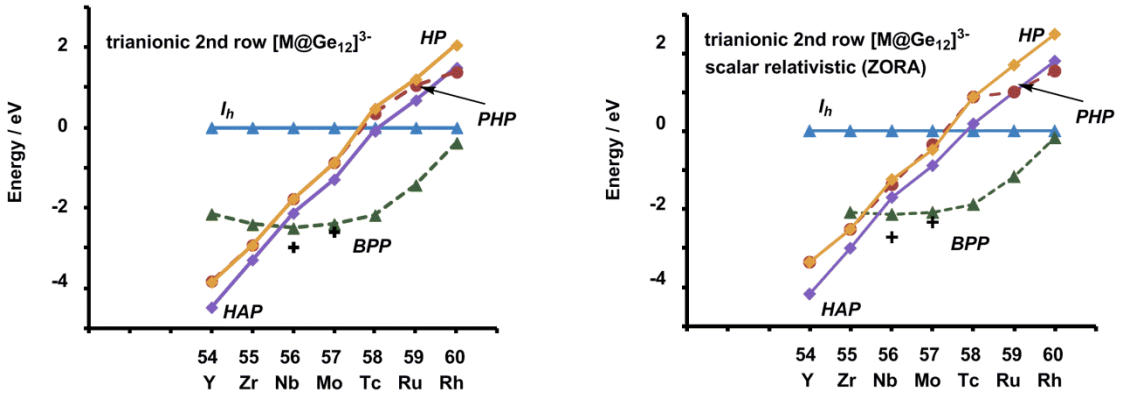

Figure S1 Comparison of non-relativistic and relativistic (scalar, ZORA) energies for $[M@Ge_{12}]^{3-}$.

Table S1(a) Symmetries, MS values and energies of stationary points in Figure 2a

	M_S	Energy /eV
$Ti@Si_{12}$		
I_h	1	-53.48241085
D_{6h}	1	-57.27702003
D_{6d}	1	-56.94695800
D_{3d}	0	-57.40812618
C_s	0	-57.58369086
$V@Si_{12}$		
I_h	3/2	-55.63165666
D_{6h}	1/2	-59.54354768
D_{6d}	1/2	-59.02281205
D_{3d}	1/2	-59.54329499
C_s	1/2	-59.63795649
$Cr@Si_{12}$		
I_h	2	-57.26145147
D_{6h}	0	-61.01693625
D_{6d}	0	-60.17594181
D_{3d}	0	-61.01693625
$Mn@Si_{12}$		
I_h	5/2	-58.23671663
D_{6h}	1/2	-61.58392216
D_{6d}	1/2	-60.67031744

D_{3d}	1/2	-61.58172242
D_{2d}	1/2	-60.50252542
$Fe@Si_{12}$		
I_h	2	-57.98412562
D_{6h}	0	-60.83521038
D_{6d}	0	-59.84549345
D_{3d}	0	-60.87579212
D_{2d}	1	-60.61556907
$Co@Si_{12}$		
I_h	3/2	-57.55774043
D_{6h}	1/2	-59.89231477
D_{6d}	1/2	-59.08864245
D_{3d}	1/2	-59.94679358
D_{2d}	1/2	-60.11484092
C_2	1/2	-60.17781809
$Ni@Si_{12}$		
I_h	1	-54.76578256
D_{6h}	1	-56.60841830
D_{6d}	1	-55.85001251
D_{3d}	1	-56.84920197
D_{2d}	0	-57.00887892
$Cu@Si_{12}$		
I_h	1/2	-52.03802032
D_{6h}	1/2	-53.20707788
D_{6d}	1/2	-52.53983619
D_{2d}	1/2	-53.16202493
C_s	1/2	-53.76424779
$Zn@Si_{12}$		
I_h	0	-49.37542316
D_{6h}	0	-50.05136944
D_{6d}	0	-49.61563855
D_{3d}	0	-50.77517583
D_{2d}	0	-49.34337832

Table S1(b) Symmetries, MS values and energies of stationary points in Figure 2(b)

	M_S	**Energy /eV**
$Ti@Ge_{12}$		
I_h	1	-48.13893638
D_{6h}	1	-48.41745328
D_{6d}	1	-48.79204212
D_{3d}	0	-48.76222690
C_s	0	-48.95253943
$V@Ge_{12}$		
I_h	3/2	-49.64725179
D_{6h}	1/2	-49.97655444
D_{6d}	1/2	-49.79978982
D_{3d}	1/2	-50.23597184
C_{2h}	1/2	-50.31489768
$Cr@Ge_{12}$		
I_h	2	-51.07525889
D_{6h}	0	-50.89063583
D_{6d}	0	-50.92587689
D_{3d}	0	-51.07599264

D_{5d}	2	-51.10913742
$Mn@Ge_{12}$		
I_h	5/2	-51.91531449
D_{6h}	1/2	-51.55631062
D_{6d}	1/2	-51.52449079
D_{3d}	1/2	-51.79362395
D_{2d}	1/2	-50.43174320
$Fe@Ge_{12}$		
I_h	2	-51.11912680
D_{6h}	1	-50.71925177
D_{6d}	1	-50.78245659
D_{3d}	0	-51.17547584
D_{2d}	1	-50.67247866
C_{2h}	1	-51.21831237
$Co@Ge_{12}$		
I_h	3/2	-50.41246223
D_{6h}	1/2	-49.90003258
D_{6d}	1/2	-49.83837433
D_{3d}	1/2	-50.45349209
D_{2d}	1/2	-50.35129821
C_2	1/2	-50.54606567
$Ni@Ge_{12}$		
I_h	1	-47.90054872
D_{6h}	1	-47.03398030
D_{6d}	1	-47.07329344
D_{3d}	1	-47.76143375
D_{2d}	0	-47.99583994
C_2	0	-48.13574252
$Cu@Ge_{12}$		
I_h	1/2	-45.93262864
D_{6h}	1/2	-44.24923328
D_{6d}	1/2	-44.50743374
D_{3d}	1/2	-45.16841288
D_{2d}	1/2	-45.04549589
D_{5d}	1/2	-46.06438376
$Zn@Ge_{12}$		
I_h	0	-44.10613350
D_{6h}	0	-41.57571765
D_{6d}	0	-42.17556810
D_{3d}	0	-42.78048155
D_{2d}	0	-42.13417242

Table S1(c) Symmetries, MS values and energies of stationary points in Figure 2(c)

	M_S	**Energy /eV**
$Zr@Ge_{12}$		
I_h	1	-47.34493893
D_{6h}	1	-48.79235834
D_{6d}	1	-49.56463956
D_{3d}	0	-48.86325932
$Nb@Ge_{12}$		
I_h	3/2	-49.41426902
D_{6h}	1/2	-51.33409707
D_{6d}	1/2	-51.71134368

D_{3d}	1/2	-51.35496303
$Mo@Ge_{12}$		
I_h	2	-50.15988557
D_{6h}	0	-51.96425349
D_{6d}	0	-52.04040007
D_{3d}	0	-52.05688141
$Tc@Ge_{12}$		
I_h	5/2	-51.98896822
D_{6h}	1/2	-53.42169828
D_{6d}	1/2	-53.38290536
D_{3d}	1/2	-53.52404322
D_{2d}	1/2	-52.50804253
$Ru@Ge_{12}$		
I_h	2	-49.79830012
D_{6h}	0	-51.05636836
D_{6d}	0	-50.89807695
D_{3d}	0	-51.24467965
D_{2d}	1	-50.80332020
$Rh@Ge_{12}$		
I_h	3/2	-48.84334783
D_{6h}	1/2	-49.46024174
D_{6d}	1/2	-49.42511296
D_{3d}	1/2	-49.68801998
D_{2d}	1/2	-49.88469445
C_2	1/2	-50.05029677
$Pd@Ge_{12}$		
I_h	1	-44.80362916
D_{6h}	1	-44.84692417
D_{6d}	1	-44.94282086
D_{3d}	1	-45.21397629
D_{2d}	0	-45.65138710
C_2	0	-45.79434111
$Ag@Ge_{12}$		
I_h	1/2	-43.68053624
D_{6h}	1/2	-42.95580076
D_{6d}	1/2	-43.30972340
D_{3d}	1/2	-43.48316148
D_{2d}	1/2	-43.56341872
D_{5d}	1/2	-43.77742101
$Cd@Ge_{12}$		
I_h	0	-42.61588077
D_{6h}	0	-41.08322348
D_{6d}	0	-41.78923319
D_{3d}	0	-41.92021214

Table S1(d) Symmetries, MS values and energies of stationary points in Figure 2(d)

	M_S	**Energy /eV**
$[Y@Ge_{12}]^{3-}$		
I_h	2	-53.84275076
D_{6h}	0	-57.68544841
D_{6d}	0	-58.30489319

D_{3d}	0	-57.66147779
	$[Zr@Ge_{12}]^{3-}$	
I_h	5/2	-57.61095778
D_{6h}	1/2	-60.54278908
D_{6d}	1/2	-60.89265685
D_{3d}	1/2	-60.53178205
D_{2d}	1/2	-59.52238210
	$[Nb@Ge_{12}]^{3-}$	
I_h	2	-60.04616672
D_{6h}	1	-61.80474039
D_{6d}	1	-62.03780751
D_{3d}	1	-61.81645844
D_{2d}	0	-62.54317810
S_4	0	-63.01781248
	$[Mo@Ge_{12}]^{3-}$	
I_h	3/2	-60.92326263
D_{6h}	1/2	-61.79212541
D_{6d}	1/2	-62.09152785
D_{3d}	1/2	-61.65726149
D_{2d}	1/2	-63.31548232
S_4	1/2	-63.50884962
	$[Tc@Ge_{12}]^{3-}$	
I_h	1	-62.87822950
D_{6h}	1	-62.40877066
D_{6d}	1	-62.97342148
D_{3d}	1	-62.57147015
D_{2d}	0	-65.05959488
C_2	0	
	$[Ru@Ge_{12}]^{3-}$	
I_h	1/2	-61.33131095
D_{6h}	1/2	-60.12700694
D_{6d}	1/2	-60.64510422
D_{3d}	1/2	-60.28277460
D_{2d}	1/2	-62.75486768
D_{5d}	1/2	
	$[Rh@Ge_{12}]^{3-}$	
I_h	0	-60.98370180
D_{6h}	0	-58.92507094
D_{6d}	0	-59.49248649
D_{3d}	0	-59.60223198
D_{2d}	0	-61.35565711

Table S2
Cartesian coordinates (Angstrom) and total energies (eV) for all structures reported in the text.

$M@Si_{12}$ Figure 2(a)

I_h $Ti@Si_{12}$ MS=1
Bond Energy -53.48241085 eV

1.Ti	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.616737
5.Si	-2.340379	0.000000	-1.170442

6.Si	-0.723217	-2.225833	-1.170442
7.Si	-0.723217	2.225833	-1.170442
8.Si	1.893407	-1.375640	-1.170442
9.Si	1.893407	1.375640	-1.170442
10.Si	0.000000	0.000000	2.616737
12.Si	2.340379	0.000000	1.170442
13.Si	-1.893407	1.375640	1.170442
14.Si	-1.893407	-1.375640	1.170442
15.Si	0.723217	2.225833	1.170442
16.Si	0.723217	-2.225833	1.170442

D_{6h} $Ti@Si_{12}$ MS=1

Bond Energy -57.27702003 eV

1.Si	2.083724	1.203039	1.228110
2.Si	2.083724	-1.203039	1.228110
3.Si	0.000000	2.406077	1.228110
4.Si	0.000000	-2.406077	1.228110
5.Si	-2.083724	1.203039	1.228110
6.Si	-2.083724	-1.203039	1.228110
7.Si	2.083724	1.203039	-1.228110
8.Si	2.083724	-1.203039	-1.228110
9.Si	0.000000	2.406077	-1.228110
10.Si	0.000000	-2.406077	-1.228110
11.Si	-2.083724	1.203039	-1.228110
12.Si	-2.083724	-1.203039	-1.228110
13.Ti	0.000000	0.000000	0.000000

D_{6d} $TiSi_{12}$ MS=1

Bond Energy -56.94695800 eV

1.Ti	0.000000	0.000000	0.000000
2.Si	-0.646130	-2.411389	-1.087256
3.Si	1.765259	-1.765259	-1.087256
4.Si	-2.411389	-0.646130	-1.087256
5.Si	2.411389	0.646130	-1.087256
6.Si	-1.765259	1.765259	-1.087256
7.Si	0.646130	2.411389	-1.087256
8.Si	0.646130	-2.411389	1.087256
9.Si	2.411389	-0.646130	1.087256
10.Si	-1.765259	-1.765259	1.087256
11.Si	1.765259	1.765259	1.087256
12.Si	-2.411389	0.646130	1.087256
13.Si	-0.646130	2.411389	1.087256

D_{3d} $Ti@Si_{12}$ MS=0

Bond Energy -57.40812618 eV

1.Si	-2.070675	1.195505	1.135411
2.Si	0.000000	2.454233	1.283661
3.Si	-2.125428	-1.227116	1.283661
4.Si	2.070675	1.195505	1.135411
5.Si	0.000000	-2.391010	1.135411
6.Si	2.125428	-1.227116	1.283661
7.Si	-2.125428	1.227116	-1.283661
8.Si	0.000000	2.391010	-1.135411
9.Si	-2.070675	-1.195505	-1.135411
10.Si	2.125428	1.227116	-1.283661
11.Si	0.000000	-2.454233	-1.283661
12.Si	2.070675	-1.195505	-1.135411
13.Ti	0.000000	0.000000	0.000000

C_s Ti@Si_{12} MS=0

Bond Energy -57.58369086 eV

1.Si	0.369290	-1.179761	-2.639821
2.Si	-1.672749	-1.374025	-1.520813
3.Si	2.249160	-0.885779	-1.182852
4.Si	-1.672749	-1.374025	1.520813
5.Si	2.249160	-0.885779	1.182852
6.Si	0.369290	-1.179761	2.639821
7.Si	-0.287413	1.191781	-2.391018
8.Si	-2.346043	0.891927	-1.211624
9.Si	1.754681	1.452028	-1.200374
10.Si	-2.346043	0.891927	1.211624
11.Si	1.754681	1.452028	1.200374
12.Si	-0.287413	1.191781	2.391018
13.Ti	-0.078184	-0.112348	0.000000

I_h V@Si_{12} MS=3/2

Bond Energy -55.63165666 eV

1.V	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.571202
5.Si	-2.299654	0.000000	-1.150075
6.Si	-0.710632	-2.187101	-1.150075
7.Si	-0.710632	2.187101	-1.150075
8.Si	1.860459	-1.351703	-1.150075
9.Si	1.860459	1.351703	-1.150075
10.Si	0.000000	0.000000	2.571202
12.Si	2.299654	0.000000	1.150075
13.Si	-1.860459	1.351703	1.150075
14.Si	-1.860459	-1.351703	1.150075
15.Si	0.710632	2.187101	1.150075
16.Si	0.710632	-2.187101	1.150075

D_{6h} V@Si_{12} MS=1/2

Bond Energy -59.54354768 eV

1.Si	2.056180	1.187136	1.208650
2.Si	2.056180	-1.187136	1.208650
3.Si	0.000000	2.374272	1.208650
4.Si	0.000000	-2.374272	1.208650
5.Si	-2.056180	1.187136	1.208650
6.Si	-2.056180	-1.187136	1.208650
7.Si	2.056180	1.187136	-1.208650
8.Si	2.056180	-1.187136	-1.208650
9.Si	0.000000	2.374272	-1.208650
10.Si	0.000000	-2.374272	-1.208650
11.Si	-2.056180	1.187136	-1.208650
12.Si	-2.056180	-1.187136	-1.208650
13.V	0.000000	0.000000	0.000000

D_{6d} V@Si_{12} MS=1/2

Bond Energy -59.02281205 eV

1.V	0.000000	0.000000	0.000000
2.Si	-0.633660	-2.364852	-1.090583
3.Si	1.731192	-1.731192	-1.090583
4.Si	-2.364852	-0.633660	-1.090583
5.Si	2.364852	0.633660	-1.090583
6.Si	-1.731192	1.731192	-1.090583
7.Si	0.633660	2.364852	-1.090583

8.Si	0.633660	-2.364852	1.090583
9.Si	2.364852	-0.633660	1.090583
10.Si	-1.731192	-1.731192	1.090583
11.Si	1.731192	1.731192	1.090583
12.Si	-2.364852	0.633660	1.090583
13.Si	-0.633660	2.364852	1.090583

D_{3d} V@Si_{12} MS=1/2

Bond Energy -59.54329499 eV

1.Si	-2.053999	1.185877	1.207161
2.Si	0.000000	2.374913	1.208970
3.Si	-2.056735	-1.187457	1.208970
4.Si	2.053999	1.185877	1.207161
5.Si	0.000000	-2.371754	1.207161
6.Si	2.056735	-1.187457	1.208970
7.Si	-2.056735	1.187457	-1.208970
8.Si	0.000000	2.371754	-1.207161
9.Si	-2.053999	-1.185877	-1.207161
10.Si	2.056735	1.187457	-1.208970
11.Si	0.000000	-2.374913	-1.208970
12.Si	2.053999	-1.185877	-1.207161
13.V	0.000000	0.000000	0.000000

C_s V@Si_{12} MS=1/2

Bond Energy -59.63795649 eV

1.Si	2.000934	1.254813	-1.195754
2.Si	2.000934	1.254813	1.195754
3.Si	-0.058388	1.212759	-2.367006
4.Si	-0.058388	1.212759	2.367006
5.Si	-2.117390	1.142814	-1.192959
6.Si	-2.117390	1.142814	1.192959
7.Si	2.050969	-1.139250	-1.194343
8.Si	2.050969	-1.139250	1.194343
9.Si	0.066575	-1.228359	-2.467607
10.Si	0.066575	-1.228359	2.467607
11.Si	-1.934319	-1.242784	-1.225353
12.Si	-1.934319	-1.242784	1.225353
13.V	-0.009205	0.000008	0.000000

I_h Cr@Si_{12} MS=2

Bond Energy -57.26145147 eV

1.Cr	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.548802
5.Si	-2.279619	0.000000	-1.140056
6.Si	-0.704441	-2.168047	-1.140056
7.Si	-0.704441	2.168047	-1.140056
8.Si	1.844251	-1.339926	-1.140056
9.Si	1.844251	1.339926	-1.140056
10.Si	0.000000	0.000000	2.548802
12.Si	2.279619	0.000000	1.140056
13.Si	-1.844251	1.339926	1.140056
14.Si	-1.844251	-1.339926	1.140056
15.Si	0.704441	2.168047	1.140056
16.Si	0.704441	-2.168047	1.140056

D_{6h} Cr@Si_{12} MS=0

Bond Energy -61.01693625 eV

1.Si	2.040957	1.178347	1.193047

2.Si	2.040957	-1.178347	1.193047
3.Si	0.000000	2.356694	1.193047
4.Si	0.000000	-2.356694	1.193047
5.Si	-2.040957	1.178347	1.193047
6.Si	-2.040957	-1.178347	1.193047
7.Si	2.040957	1.178347	-1.193047
8.Si	2.040957	-1.178347	-1.193047
9.Si	0.000000	2.356694	-1.193047
10.Si	0.000000	-2.356694	-1.193047
11.Si	-2.040957	1.178347	-1.193047
12.Si	-2.040957	-1.178347	-1.193047
13.Cr	0.000000	0.000000	0.000000

D_{6d} $Cr@Si_{12}$ MS=0

Bond Energy -60.17594181 eV

1.Cr	0.000000	0.000000	0.000000
2.Si	-0.623050	-2.325254	-1.106220
3.Si	1.702204	-1.702204	-1.106220
4.Si	-2.325254	-0.623050	-1.106220
5.Si	2.325254	0.623050	-1.106220
6.Si	-1.702204	1.702204	-1.106220
7.Si	0.623050	2.325254	-1.106220
8.Si	0.623050	-2.325254	1.106220
9.Si	2.325254	-0.623050	1.106220
10.Si	-1.702204	-1.702204	1.106220
11.Si	1.702204	1.702204	1.106220
12.Si	-2.325254	0.623050	1.106220
13.Si	-0.623050	2.325254	1.106220

D_{3d} $Cr@Si_{12}$ MS=0

Bond Energy -61.01293266 eV

1.Si	-2.039412	1.177455	1.195045
2.Si	0.000000	2.353795	1.192254
3.Si	-2.038446	-1.176897	1.192254
4.Si	2.039412	1.177455	1.195045
5.Si	0.000000	-2.354910	1.195045
6.Si	2.038446	-1.176897	1.192254
7.Si	-2.038446	1.176897	-1.192254
8.Si	0.000000	2.354910	-1.195045
9.Si	-2.039412	-1.177455	-1.195045
10.Si	2.038446	1.176897	-1.192254
11.Si	0.000000	-2.353795	-1.192254
12.Si	2.039412	-1.177455	-1.195045
13.Cr	0.000000	0.000000	0.000000

D_{6h} $[Mn@Si_{12}]^{+}$ MS=0 (closed-shell)

Bond Energy -53.95677959 eV

1.Si	2.037593	1.176405	1.186418
2.Si	2.037593	-1.176405	1.186418
3.Si	0.000000	2.352810	1.186418
4.Si	0.000000	-2.352810	1.186418
5.Si	-2.037593	1.176405	1.186418
6.Si	-2.037593	-1.176405	1.186418
7.Si	2.037593	1.176405	-1.186418
8.Si	2.037593	-1.176405	-1.186418
9.Si	0.000000	2.352810	-1.186418
10.Si	0.000000	-2.352810	-1.186418
11.Si	-2.037593	1.176405	-1.186418

12.Si	-2.037593	-1.176405	-1.186418
13.Mn	0.000000	0.000000	0.000000

C_{6v} $[Mn@Si_{12}]^{+}$ MS=0 (open-shell)

Bond Energy -54.05103822 eV

1.Si	2.058883	1.188697	1.185377
2.Si	2.058883	-1.188697	1.185377
3.Si	0.000000	2.377394	1.185377
4.Si	0.000000	-2.377394	1.185377
5.Si	-2.058883	1.188697	1.185377
6.Si	-2.058883	-1.188697	1.185377
7.Si	2.042875	1.179454	-1.174876
8.Si	2.042875	-1.179454	-1.174876
9.Si	0.000000	2.358909	-1.174876
10.Si	0.000000	-2.358909	-1.174876
11.Si	-2.042875	1.179454	-1.174876
12.Si	-2.042875	-1.179454	-1.174876
13.Mn	0.000000	0.000000	0.067915

I_h $Mn@Si_{12}$ MS=5/2

Bond Energy -58.23671663 eV

1.Mn	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.532057
5.Si	-2.264643	0.000000	-1.132566
6.Si	-0.699813	-2.153804	-1.132566
7.Si	-0.699813	2.153804	-1.132566
8.Si	1.832135	-1.331124	-1.132566
9.Si	1.832135	1.331124	-1.132566
10.Si	0.000000	0.000000	2.532057
12.Si	2.264643	0.000000	1.132566
13.Si	-1.832135	1.331124	1.132566
14.Si	-1.832135	-1.331124	1.132566
15.Si	0.699813	2.153804	1.132566
16.Si	0.699813	-2.153804	1.132566

D_{6h} $Mn@Si_{12}$ MS=1/2

Bond Energy -61.58392216 eV

1.Si	2.033974	1.174315	1.192369
2.Si	2.033974	-1.174315	1.192369
3.Si	0.000000	2.348631	1.192369
4.Si	0.000000	-2.348631	1.192369
5.Si	-2.033974	1.174315	1.192369
6.Si	-2.033974	-1.174315	1.192369
7.Si	2.033974	1.174315	-1.192369
8.Si	2.033974	-1.174315	-1.192369
9.Si	0.000000	2.348631	-1.192369
10.Si	0.000000	-2.348631	-1.192369
11.Si	-2.033974	1.174315	-1.192369
12.Si	-2.033974	-1.174315	-1.192369
13.Mn	0.000000	0.000000	0.000000

D_{6d} $Mn@Si_{12}$ MS=1/2

Bond Energy -60.67031744 eV

1.Mn	0.000000	0.000000	0.000000
2.Si	-0.620307	-2.315019	-1.110279
3.Si	1.694711	-1.694711	-1.110279
4.Si	-2.315019	-0.620307	-1.110279
5.Si	2.315019	0.620307	-1.110279

6.Si	-1.694711	1.694711	-1.110279
7.Si	0.620307	2.315019	-1.110279
8.Si	0.620307	-2.315019	1.110279
9.Si	2.315019	-0.620307	1.110279
10.Si	-1.694711	-1.694711	1.110279
11.Si	1.694711	1.694711	1.110279
12.Si	-2.315019	0.620307	1.110279
13.Si	-0.620307	2.315019	1.110279

D_{3d} $Mn@Si_{12}$ MS=1/2

Bond Energy -61.58172242 eV

1.Si	-2.021464	1.167093	1.183011
2.Si	0.000000	2.363893	1.200466
3.Si	-2.047191	-1.181946	1.200466
4.Si	2.021464	1.167093	1.183011
5.Si	0.000000	-2.334185	1.183011
6.Si	2.047191	-1.181946	1.200466
7.Si	-2.047191	1.181946	-1.200466
8.Si	0.000000	2.334185	-1.183011
9.Si	-2.021464	-1.167093	-1.183011
10.Si	2.047191	1.181946	-1.200466
11.Si	0.000000	-2.363893	-1.200466
12.Si	2.021464	-1.167093	-1.183011
13.Mn	0.000000	0.000000	0.000000

D_{2d} $Mn@Si_{12}$ MS= 1/2

Bond Energy -60.50252542 eV

1.Mn	0.000000	0.000000	0.000000
2.Si	-0.820715	-0.820715	2.421209
3.Si	0.499571	-2.227237	1.063698
4.Si	-2.227237	0.499571	1.063698
5.Si	-2.227237	-0.499571	-1.063698
6.Si	0.499571	2.227237	-1.063698
7.Si	-0.820715	0.820715	-2.421209
8.Si	2.227237	-0.499571	1.063698
9.Si	-0.499571	-2.227237	-1.063698
10.Si	0.820715	0.820715	2.421209
11.Si	0.820715	-0.820715	-2.421209
12.Si	-0.499571	2.227237	1.063698
13.Si	2.227237	0.499571	-1.063698

I_h $Fe@Si_{12}$ MS=2

Bond Energy -57.98412562 eV

1.Fe	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.505093
5.Si	-2.240526	0.000000	-1.120505
6.Si	-0.692361	-2.130867	-1.120505
7.Si	-0.692361	2.130867	-1.120505
8.Si	1.812624	-1.316948	-1.120505
9.Si	1.812624	1.316948	-1.120505
10.Si	0.000000	0.000000	2.505093
12.Si	2.240526	0.000000	1.120505
13.Si	-1.812624	1.316948	1.120505
14.Si	-1.812624	-1.316948	1.120505
15.Si	0.692361	2.130867	1.120505
16.Si	0.692361	-2.130867	1.120505

D_{6h} $Fe@Si_{12}$ MS=0

Bond Energy -60.83521038 eV

1.Si	2.020838	1.166731	1.190515
2.Si	2.020838	-1.166731	1.190515
3.Si	0.000000	2.333463	1.190515
4.Si	0.000000	-2.333463	1.190515
5.Si	-2.020838	1.166731	1.190515
6.Si	-2.020838	-1.166731	1.190515
7.Si	2.020838	1.166731	-1.190515
8.Si	2.020838	-1.166731	-1.190515
9.Si	0.000000	2.333463	-1.190515
10.Si	0.000000	-2.333463	-1.190515
11.Si	-2.020838	1.166731	-1.190515
12.Si	-2.020838	-1.166731	-1.190515
13.Fe	0.000000	0.000000	0.000000

D_{6d} Fe@Si_{12} MS=0

Bond Energy -59.84549345 eV

1.Fe	0.000000	0.000000	0.000000
2.Si	-0.615548	-2.297255	-1.112819
3.Si	1.681708	-1.681708	-1.112819
4.Si	-2.297255	-0.615548	-1.112819
5.Si	2.297255	0.615548	-1.112819
6.Si	-1.681708	1.681708	-1.112819
7.Si	0.615548	2.297255	-1.112819
8.Si	0.615548	-2.297255	1.112819
9.Si	2.297255	-0.615548	1.112819
10.Si	-1.681708	-1.681708	1.112819
11.Si	1.681708	1.681708	1.112819
12.Si	-2.297255	0.615548	1.112819
13.Si	-0.615548	2.297255	1.112819

D_{3d} Fe@Si_{12} MS=0

Bond Energy -60.87579212 eV

1.Si	-2.130670	1.230143	1.229398
2.Si	0.000000	2.213769	1.144224
3.Si	-1.917180	-1.106884	1.144224
4.Si	2.130670	1.230143	1.229398
5.Si	0.000000	-2.460286	1.229398
6.Si	1.917180	-1.106884	1.144224
7.Si	-1.917180	1.106884	-1.144224
8.Si	0.000000	2.460286	-1.229398
9.Si	-2.130670	-1.230143	-1.229398
10.Si	1.917180	1.106884	-1.144224
11.Si	0.000000	-2.213769	-1.144224
12.Si	2.130670	-1.230143	-1.229398
13.Fe	0.000000	0.000000	0.000000

D_{2d} Fe@Si_{12} MS= 1

Bond Energy -60.61556907 eV

1.Fe	0.000000	0.000000	0.000000
2.Si	-0.821764	-0.821764	2.413845
3.Si	0.506932	-2.205270	1.052835
4.Si	-2.205270	0.506932	1.052835
5.Si	-2.205270	-0.506932	-1.052835
6.Si	0.506932	2.205270	-1.052835
7.Si	-0.821764	0.821764	-2.413845
8.Si	2.205270	-0.506932	1.052835
9.Si	-0.506932	-2.205270	-1.052835

10.Si	0.821764	0.821764	2.413845
11.Si	0.821764	-0.821764	-2.413845
12.Si	-0.506932	2.205270	1.052835
13.Si	2.205270	0.506932	-1.052835

I_h $Co@Si_{12}$ MS=3/2

Bond Energy -57.55774043 eV

1.Co	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.497301
5.Si	-2.233558	0.000000	-1.117020
6.Si	-0.690207	-2.124240	-1.117020
7.Si	-0.690207	2.124240	-1.117020
8.Si	1.806986	-1.312852	-1.117020
9.Si	1.806986	1.312852	-1.117020
10.Si	0.000000	0.000000	2.497301
12.Si	2.233558	0.000000	1.117020
13.Si	-1.806986	1.312852	1.117020
14.Si	-1.806986	-1.312852	1.117020
15.Si	0.690207	2.124240	1.117020
16.Si	0.690207	-2.124240	1.117020

D_{6h} $Co@Si_{12}$ MS=1/2

Bond Energy -59.89231477 eV

1.Si	2.035897	1.175426	1.183858
2.Si	2.035897	-1.175426	1.183858
3.Si	0.000000	2.350852	1.183858
4.Si	0.000000	-2.350852	1.183858
5.Si	-2.035897	1.175426	1.183858
6.Si	-2.035897	-1.175426	1.183858
7.Si	2.035897	1.175426	-1.183858
8.Si	2.035897	-1.175426	-1.183858
9.Si	0.000000	2.350852	-1.183858
10.Si	0.000000	-2.350852	-1.183858
11.Si	-2.035897	1.175426	-1.183858
12.Si	-2.035897	-1.175426	-1.183858
13.Co	0.000000	0.000000	0.000000

D_{6d} $Co@Si_{12}$ MS=1/2

Bond Energy -59.08864245 eV

1.Co	0.000000	0.000000	0.000000
2.Si	-0.617372	-2.304063	-1.109478
3.Si	1.686691	-1.686691	-1.109478
4.Si	-2.304063	-0.617372	-1.109478
5.Si	2.304063	0.617372	-1.109478
6.Si	-1.686691	1.686691	-1.109478
7.Si	0.617372	2.304063	-1.109478
8.Si	0.617372	-2.304063	1.109478
9.Si	2.304063	-0.617372	1.109478
10.Si	-1.686691	-1.686691	1.109478
11.Si	1.686691	1.686691	1.109478
12.Si	-2.304063	0.617372	1.109478
13.Si	-0.617372	2.304063	1.109478

D_{3d} $Co@Si_{12}$ MS=1/2

Bond Energy -59.94679358 eV

1.Si	-1.925621	1.111758	1.117840
2.Si	0.000000	2.485367	1.247872
3.Si	-2.152391	-1.242684	1.247872

4.Si	1.925621	1.111758	1.117840
5.Si	0.000000	-2.223516	1.117840
6.Si	2.152391	-1.242684	1.247872
7.Si	-2.152391	1.242684	-1.247872
8.Si	0.000000	2.223516	-1.117840
9.Si	-1.925621	-1.111758	-1.117840
10.Si	2.152391	1.242684	-1.247872
11.Si	0.000000	-2.485367	-1.247872
12.Si	1.925621	-1.111758	-1.117840
13.Co	0.000000	0.000000	0.000000

D2d $Co@Si_{12}$ MS= 1/2

Bond Energy -60.11484092 eV

1.Co	0.000000	0.000000	0.000000
2.Si	-0.822374	-0.822374	2.396598
3.Si	0.520802	-2.238023	1.062548
4.Si	-2.238023	0.520802	1.062548
5.Si	-2.238023	-0.520802	-1.062548
6.Si	0.520802	2.238023	-1.062548
7.Si	-0.822374	0.822374	-2.396598
8.Si	2.238023	-0.520802	1.062548
9.Si	-0.520802	-2.238023	-1.062548
10.Si	0.822374	0.822374	2.396598
11.Si	0.822374	-0.822374	-2.396598
12.Si	-0.520802	2.238023	1.062548
13.Si	2.238023	0.520802	-1.062548

C_2 $Co@Si_{12}$ MS=1/2

Bond Energy -60.17781809 eV

1.Co	0.000000	0.000000	-0.002259
2.Si	-0.799060	-0.840644	2.400840
3.Si	0.562341	-2.191147	1.032875
4.Si	-2.278268	0.471248	1.094035
5.Si	-2.281484	-0.471099	-1.088552
6.Si	0.561552	2.196123	-1.035568
7.Si	-0.800964	0.839504	-2.401251
8.Si	2.278268	-0.471248	1.094035
9.Si	-0.561552	-2.196123	-1.035568
10.Si	0.799060	0.840644	2.400840
11.Si	0.800964	-0.839504	-2.401251
12.Si	-0.562341	2.191147	1.032875
13.Si	2.281484	0.471099	-1.088552

I_h $Ni@Si_{12}$ MS=1

Bond Energy -54.76578256 eV

1.Ni	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.511987
5.Si	-2.246692	0.000000	-1.123589
6.Si	-0.694266	-2.136731	-1.123589
7.Si	-0.694266	2.136731	-1.123589
8.Si	1.817612	-1.320572	-1.123589
9.Si	1.817612	1.320572	-1.123589
10.Si	0.000000	0.000000	2.511987
12.Si	2.246692	0.000000	1.123589
13.Si	-1.817612	1.320572	1.123589
14.Si	-1.817612	-1.320572	1.123589
15.Si	0.694266	2.136731	1.123589
16.Si	0.694266	-2.136731	1.123589

D_{6h} $Ni@Si_{12}$ MS=1

Bond Energy -56.60841830 eV

1.Si	2.058086	1.188236	1.180522
2.Si	2.058086	-1.188236	1.180522
3.Si	0.000000	2.376473	1.180522
4.Si	0.000000	-2.376473	1.180522
5.Si	-2.058086	1.188236	1.180522
6.Si	-2.058086	-1.188236	1.180522
7.Si	2.058086	1.188236	-1.180522
8.Si	2.058086	-1.188236	-1.180522
9.Si	0.000000	2.376473	-1.180522
10.Si	0.000000	-2.376473	-1.180522
11.Si	-2.058086	1.188236	-1.180522
12.Si	-2.058086	-1.188236	-1.180522
13.Ni	0.000000	0.000000	0.000000

D_{6d} $Ni@Si_{12}$ MS=1

Bond Energy -55.85001251 eV

1.Ni	0.000000	0.000000	0.000000
2.Si	-0.624720	-2.331487	-1.105162
3.Si	1.706767	-1.706767	-1.105162
4.Si	-2.331487	-0.624720	-1.105162
5.Si	2.331487	0.624720	-1.105162
6.Si	-1.706767	1.706767	-1.105162
7.Si	0.624720	2.331487	-1.105162
8.Si	0.624720	-2.331487	1.105162
9.Si	2.331487	-0.624720	1.105162
10.Si	-1.706767	-1.706767	1.105162
11.Si	1.706767	1.706767	1.105162
12.Si	-2.331487	0.624720	1.105162
13.Si	-0.624720	2.331487	1.105162

D_{3d} $Ni@Si_{12}$ MS=1

Bond Energy -56.84920197 eV

1.Si	-1.928779	1.113581	1.069067
2.Si	0.000000	2.524170	1.295584
3.Si	-2.185995	-1.262085	1.295584
4.Si	1.928779	1.113581	1.069067
5.Si	0.000000	-2.227162	1.069067
6.Si	2.185995	-1.262085	1.295584
7.Si	-2.185995	1.262085	-1.295584
8.Si	0.000000	2.227162	-1.069067
9.Si	-1.928779	-1.113581	-1.069067
10.Si	2.185995	1.262085	-1.295584
11.Si	0.000000	-2.524170	-1.295584
12.Si	1.928779	-1.113581	-1.069067
13.Ni	0.000000	0.000000	0.000000

D_{2d} $Ni@Si_{12}$ MS= 0

Bond Energy -57.00887892 eV

1.Ni	0.000000	0.000000	0.000000
2.Si	-0.824517	-0.824517	2.390773
3.Si	0.533528	-2.277504	1.077392
4.Si	-2.277504	0.533528	1.077392
5.Si	-2.277504	-0.533528	-1.077392
6.Si	0.533528	2.277504	-1.077392
7.Si	-0.824517	0.824517	-2.390773

8.Si	2.277504	-0.533528	1.077392
9.Si	-0.533528	-2.277504	-1.077392
10.Si	0.824517	0.824517	2.390773
11.Si	0.824517	-0.824517	-2.390773
12.Si	-0.533528	2.277504	1.077392
13.Si	2.277504	0.533528	-1.077392

I_h $Cu@Si_{12}$ MS=1/2

Bond Energy -52.03802032 eV

1.Cu	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.550925
5.Si	-2.281518	0.000000	-1.141006
6.Si	-0.705028	-2.169853	-1.141006
7.Si	-0.705028	2.169853	-1.141006
8.Si	1.845787	-1.341043	-1.141006
9.Si	1.845787	1.341043	-1.141006
10.Si	0.000000	0.000000	2.550925
12.Si	2.281518	0.000000	1.141006
13.Si	-1.845787	1.341043	1.141006
14.Si	-1.845787	-1.341043	1.141006
15.Si	0.705028	2.169853	1.141006
16.Si	0.705028	-2.169853	1.141006

D_{6h} $Cu@Si_{12}$ MS=1/2

Bond Energy -53.20707788 eV

1.Si	2.091270	1.207395	1.182016
2.Si	2.091270	-1.207395	1.182016
3.Si	0.000000	2.414791	1.182016
4.Si	0.000000	-2.414791	1.182016
5.Si	-2.091270	1.207395	1.182016
6.Si	-2.091270	-1.207395	1.182016
7.Si	2.091270	1.207395	-1.182016
8.Si	2.091270	-1.207395	-1.182016
9.Si	0.000000	2.414791	-1.182016
10.Si	0.000000	-2.414791	-1.182016
11.Si	-2.091270	1.207395	-1.182016
12.Si	-2.091270	-1.207395	-1.182016
13.Cu	0.000000	0.000000	0.000000

D_{6d} $Cu@Si_{12}$ MS=1/2

Bond Energy -52.53983619 eV

1.Cu	0.000000	0.000000	0.000000
2.Si	-0.636919	-2.377014	-1.101433
3.Si	1.740095	-1.740095	-1.101433
4.Si	-2.377014	-0.636919	-1.101433
5.Si	2.377014	0.636919	-1.101433
6.Si	-1.740095	1.740095	-1.101433
7.Si	0.636919	2.377014	-1.101433
8.Si	0.636919	-2.377014	1.101433
9.Si	2.377014	-0.636919	1.101433
10.Si	-1.740095	-1.740095	1.101433
11.Si	1.740095	1.740095	1.101433
12.Si	-2.377014	0.636919	1.101433
13.Si	-0.636919	2.377014	1.101433

D_{2d} $Cu@Si_{12}$ MS= 1/2

Bond Energy -53.16202493 eV

1.Cu	0.000000	0.000000	0.000000
2.Si	-0.831230	-0.831230	2.310969
3.Si	0.568737	-2.369565	1.090134
4.Si	-2.369565	0.568737	1.090134
5.Si	-2.369565	-0.568737	-1.090134
6.Si	0.568737	2.369565	-1.090134
7.Si	-0.831230	0.831230	-2.310969
8.Si	2.369565	-0.568737	1.090134
9.Si	-0.568737	-2.369565	-1.090134
10.Si	0.831230	0.831230	2.310969
11.Si	0.831230	-0.831230	-2.310969
12.Si	-0.568737	2.369565	1.090134
13.Si	2.369565	0.568737	-1.090134

C_s $CuSi_{12}$ MS=1/2

Bond Energy -53.76424779 eV

1.Si	-2.726412	1.125741	-0.019535
2.Si	-1.213165	0.952344	-1.936288
3.Si	-1.261550	0.882703	1.942916
4.Si	1.150801	1.489296	-2.265992
5.Si	1.096348	1.423791	2.120224
6.Si	2.166658	1.201851	-0.044247
7.Si	-2.166658	-1.201851	0.044247
8.Si	-1.096348	-1.423791	-2.120224
9.Si	-1.150801	-1.489296	2.265992
10.Si	1.261550	-0.882703	-1.942916
11.Si	1.213165	-0.952344	1.936288
12.Si	2.726412	-1.125741	0.019535
13.Cu	0.000000	0.000000	0.000000

I_h $Zn@Si_{12}$ MS=0

Bond Energy -49.37542316 eV

1.Zn	0.000000	0.000000	0.000000
3.Si	0.000000	0.000000	-2.593858
5.Si	-2.319917	0.000000	-1.160209
6.Si	-0.716894	-2.206372	-1.160209
7.Si	-0.716894	2.206372	-1.160209
8.Si	1.876852	-1.363613	-1.160209
9.Si	1.876852	1.363613	-1.160209
10.Si	0.000000	0.000000	2.593858
12.Si	2.319917	0.000000	1.160209
13.Si	-1.876852	1.363613	1.160209
14.Si	-1.876852	-1.363613	1.160209
15.Si	0.716894	2.206372	1.160209
16.Si	0.716894	-2.206372	1.160209

D_{6h} $Zn@Si_{12}$ MS=0

Bond Energy -50.05136944 eV

1.Si	2.120323	1.224169	1.183802
2.Si	2.120323	-1.224169	1.183802
3.Si	0.000000	2.448338	1.183802
4.Si	0.000000	-2.448338	1.183802
5.Si	-2.120323	1.224169	1.183802
6.Si	-2.120323	-1.224169	1.183802
7.Si	2.120323	1.224169	-1.183802
8.Si	2.120323	-1.224169	-1.183802
9.Si	0.000000	2.448338	-1.183802
10.Si	0.000000	-2.448338	-1.183802

11.Si	-2.120323	1.224169	-1.183802
12.Si	-2.120323	-1.224169	-1.183802
13.Zn	0.000000	0.000000	0.000000

D_{6d} $Zn@Si_{12}$ MS=0

Bond Energy -49.61563855 eV

1.Zn	0.000000	0.000000	0.000000
2.Si	-0.647941	-2.418148	-1.094696
3.Si	1.770207	-1.770207	-1.094696
4.Si	-2.418148	-0.647941	-1.094696
5.Si	2.418148	0.647941	-1.094696
6.Si	-1.770207	1.770207	-1.094696
7.Si	0.647941	2.418148	-1.094696
8.Si	0.647941	-2.418148	1.094696
9.Si	2.418148	-0.647941	1.094696
10.Si	-1.770207	-1.770207	1.094696
11.Si	1.770207	1.770207	1.094696
12.Si	-2.418148	0.647941	1.094696
13.Si	-0.647941	2.418148	1.094696

D_{3d} $Zn@Si_{12}$ MS=0

Bond Energy -50.77517583 eV

1.Si	-2.001189	1.155387	0.968782
2.Si	0.000000	2.553383	1.420089
3.Si	-2.211295	-1.276692	1.420089
4.Si	2.001189	1.155387	0.968782
5.Si	0.000000	-2.310773	0.968782
6.Si	2.211295	-1.276692	1.420089
7.Si	-2.211295	1.276692	-1.420089
8.Si	0.000000	2.310773	-0.968782
9.Si	-2.001189	-1.155387	-0.968782
10.Si	2.211295	1.276692	-1.420089
11.Si	0.000000	-2.553383	-1.420089
12.Si	2.001189	-1.155387	-0.968782
13.Zn	0.000000	0.000000	0.000000

D_{2d} $Zn@Si_{12}$ MS= 0

Bond Energy -49.34337832 eV

1.Zn	0.000000	0.000000	0.000000
2.Si	-0.845874	-0.845874	2.261248
3.Si	0.585748	-2.450067	1.102958
4.Si	-2.450067	0.585748	1.102958
5.Si	-2.450067	-0.585748	-1.102958
6.Si	0.585748	2.450067	-1.102958
7.Si	-0.845874	0.845874	-2.261248
8.Si	2.450067	-0.585748	1.102958
9.Si	-0.585748	-2.450067	-1.102958
10.Si	0.845874	0.845874	2.261248
11.Si	0.845874	-0.845874	-2.261248
12.Si	-0.585748	2.450067	1.102958
13.Si	2.450067	0.585748	-1.102958

$M@Ge_{12}$ First row transition metals (Figure 3(c))

I_h $Zn@Ge_{12}$ MS=0

Bond Energy -44.10613350 eV

1.Zn	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.813945

5.Ge	-2.516760	0.000000	-1.258652
6.Ge	-0.777722	-2.393581	-1.258652
7.Ge	-0.777722	2.393581	-1.258652
8.Ge	2.036102	-1.479315	-1.258652
9.Ge	2.036102	1.479315	-1.258652
10.Ge	0.000000	0.000000	2.813945
12.Ge	2.516760	0.000000	1.258652
13.Ge	-2.036102	1.479315	1.258652
14.Ge	-2.036102	-1.479315	1.258652
15.Ge	0.777722	2.393581	1.258652
16.Ge	0.777722	-2.393581	1.258652

D_{6h} $Zn@Ge_{12}$ MS=0

Bond Energy -41.57571765 eV

1.Ge	2.321019	1.340041	1.296135
2.Ge	2.321019	-1.340041	1.296135
3.Ge	0.000000	2.680082	1.296135
4.Ge	0.000000	-2.680082	1.296135
5.Ge	-2.321019	1.340041	1.296135
6.Ge	-2.321019	-1.340041	1.296135
7.Ge	2.321019	1.340041	-1.296135
8.Ge	2.321019	-1.340041	-1.296135
9.Ge	0.000000	2.680082	-1.296135
10.Ge	0.000000	-2.680082	-1.296135
11.Ge	-2.321019	1.340041	-1.296135
12.Ge	-2.321019	-1.340041	-1.296135
13.Zn	0.000000	0.000000	0.000000

D_{6d} $Zn@Ge_{12}$ MS=0

Bond Energy -42.17556810 eV

1.Zn	0.000000	0.000000	0.000000
2.Ge	-0.710685	-2.652312	-1.230363
3.Ge	1.941627	-1.941627	-1.230363
4.Ge	-2.652312	-0.710685	-1.230363
5.Ge	2.652312	0.710685	-1.230363
6.Ge	-1.941627	1.941627	-1.230363
7.Ge	0.710685	2.652312	-1.230363
8.Ge	0.710685	-2.652312	1.230363
9.Ge	2.652312	-0.710685	1.230363
10.Ge	-1.941627	-1.941627	1.230363
11.Ge	1.941627	1.941627	1.230363
12.Ge	-2.652312	0.710685	1.230363
13.Ge	-0.710685	2.652312	1.230363

D_{3d} $Zn@Ge_{12}$ MS=0

Bond Energy -42.78048155 eV

1.Ge	-2.407027	1.389698	1.629070
2.Ge	0.000000	2.518690	1.006092
3.Ge	-2.181249	-1.259345	1.006092
4.Ge	2.407027	1.389698	1.629070
5.Ge	0.000000	-2.779396	1.629070
6.Ge	2.181249	-1.259345	1.006092
7.Ge	-2.181249	1.259345	-1.006092
8.Ge	0.000000	2.779396	-1.629070
9.Ge	-2.407027	-1.389698	-1.629070
10.Ge	2.181249	1.259345	-1.006092
11.Ge	0.000000	-2.518690	-1.006092
12.Ge	2.407027	-1.389698	-1.629070

13.Zn	0.000000	0.000000	0.000000

D_{2d} $Zn@Ge_{12}$ MS= 0

Bond Energy -42.13417242 eV

1.Zn	0.000000	0.000000	0.000000
2.Ge	-0.930553	-0.930553	2.445920
3.Ge	0.641733	-2.667585	1.170432
4.Ge	-2.667585	0.641733	1.170432
5.Ge	-2.667585	-0.641733	-1.170432
6.Ge	0.641733	2.667585	-1.170432
7.Ge	-0.930553	0.930553	-2.445920
8.Ge	2.667585	-0.641733	1.170432
9.Ge	-0.641733	-2.667585	-1.170432
10.Ge	0.930553	0.930553	2.445920
11.Ge	0.930553	-0.930553	-2.445920
12.Ge	-0.641733	2.667585	1.170432
13.Ge	2.667585	0.641733	-1.170432

I_h $Cu@Ge_{12}$ MS=1/2

Bond Energy -45.93262864 eV

1.Cu	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.780546
5.Ge	-2.486888	0.000000	-1.243713
6.Ge	-0.768491	-2.365171	-1.243713
7.Ge	-0.768491	2.365171	-1.243713
8.Ge	2.011935	-1.461756	-1.243713
9.Ge	2.011935	1.461756	-1.243713
10.Ge	0.000000	0.000000	2.780546
12.Ge	2.486888	0.000000	1.243713
13.Ge	-2.011935	1.461756	1.243713
14.Ge	-2.011935	-1.461756	1.243713
15.Ge	0.768491	2.365171	1.243713
16.Ge	0.768491	-2.365171	1.243713

D_{6h} $Cu@Ge_{12}$ MS=1/2

Bond Energy -44.24923328 eV

1.Ge	2.288829	1.321456	1.292359
2.Ge	2.288829	-1.321456	1.292359
3.Ge	0.000000	2.642912	1.292359
4.Ge	0.000000	-2.642912	1.292359
5.Ge	-2.288829	1.321456	1.292359
6.Ge	-2.288829	-1.321456	1.292359
7.Ge	2.288829	1.321456	-1.292359
8.Ge	2.288829	-1.321456	-1.292359
9.Ge	0.000000	2.642912	-1.292359
10.Ge	0.000000	-2.642912	-1.292359
11.Ge	-2.288829	1.321456	-1.292359
12.Ge	-2.288829	-1.321456	-1.292359
13.Cu	0.000000	0.000000	0.000000

D_{6d} $Cu@Ge_{12}$ MS=1/2

Bond Energy -44.50743374 eV

1.Cu	0.000000	0.000000	0.000000
2.Ge	-0.699133	-2.609201	-1.228444
3.Ge	1.910068	-1.910068	-1.228444
4.Ge	-2.609201	-0.699133	-1.228444
5.Ge	2.609201	0.699133	-1.228444
6.Ge	-1.910068	1.910068	-1.228444

7.Ge	0.699133	2.609201	-1.228444
8.Ge	0.699133	-2.609201	1.228444
9.Ge	2.609201	-0.699133	1.228444
10.Ge	-1.910068	-1.910068	1.228444
11.Ge	1.910068	1.910068	1.228444
12.Ge	-2.609201	0.699133	1.228444
13.Ge	-0.699133	2.609201	1.228444

D_{3d} $Cu@Ge_{12}$ MS=1/2

Bond Energy -45.16841288 eV

1.Ge	-2.481513	1.432702	1.471879
2.Ge	0.000000	2.376568	1.134158
3.Ge	-2.058168	-1.188284	1.134158
4.Ge	2.481513	1.432702	1.471879
5.Ge	0.000000	-2.865405	1.471879
6.Ge	2.058168	-1.188284	1.134158
7.Ge	-2.058168	1.188284	-1.134158
8.Ge	0.000000	2.865405	-1.471879
9.Ge	-2.481513	-1.432702	-1.471879
10.Ge	2.058168	1.188284	-1.134158
11.Ge	0.000000	-2.376568	-1.134158
12.Ge	2.481513	-1.432702	-1.471879
13.Cu	0.000000	0.000000	0.000000

D_{2d} $Cu@Ge_{12}$ MS= 1/2

Bond Energy -45.04549589 eV

1.Cu	0.000000	0.000000	0.000000
2.Ge	-0.907704	-0.907704	2.520248
3.Ge	0.619120	-2.582644	1.171105
4.Ge	-2.582644	0.619120	1.171105
5.Ge	-2.582644	-0.619120	-1.171105
6.Ge	0.619120	2.582644	-1.171105
7.Ge	-0.907704	0.907704	-2.520248
8.Ge	2.582644	-0.619120	1.171105
9.Ge	-0.619120	-2.582644	-1.171105
10.Ge	0.907704	0.907704	2.520248
11.Ge	0.907704	-0.907704	-2.520248
12.Ge	-0.619120	2.582644	1.171105
13.Ge	2.582644	0.619120	-1.171105

D_{5d} $Cu@Ge_{12}$

Bond Energy -46.06438376 eV

1.Ge	1.481628	2.039286	1.242567
2.Ge	2.397325	-0.778938	1.242567
3.Ge	-1.481628	2.039286	1.242567
4.Ge	-2.397325	-0.778938	1.242567
5.Ge	0.000000	-2.520697	1.242567
6.Ge	1.481628	-2.039286	-1.242567
7.Ge	-1.481628	-2.039286	-1.242567
8.Ge	2.397325	0.778938	-1.242567
9.Ge	0.000000	2.520697	-1.242567
10.Ge	-2.397325	0.778938	-1.242567
11.Cu	0.000000	0.000000	0.000000
12.Ge	0.000000	0.000000	2.637052
13.Ge	0.000000	0.000000	-2.637052

I_h $Ni@Ge_{12}$ MS=1

Bond Energy -47.90054872 eV

1.Ni	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.754986
5.Ge	-2.464028	0.000000	-1.232280
6.Ge	-0.761426	-2.343429	-1.232280
7.Ge	-0.761426	2.343429	-1.232280
8.Ge	1.993440	-1.448319	-1.232280
9.Ge	1.993440	1.448319	-1.232280
10.Ge	0.000000	0.000000	2.754986
12.Ge	2.464028	0.000000	1.232280
13.Ge	-1.993440	1.448319	1.232280
14.Ge	-1.993440	-1.448319	1.232280
15.Ge	0.761426	2.343429	1.232280
16.Ge	0.761426	-2.343429	1.232280

D_{6h} Ni@Ge_{12} MS=1

Bond Energy -47.03398030 eV

1.Ge	2.246521	1.297029	1.293081
2.Ge	2.246521	-1.297029	1.293081
3.Ge	0.000000	2.594058	1.293081
4.Ge	0.000000	-2.594058	1.293081
5.Ge	-2.246521	1.297029	1.293081
6.Ge	-2.246521	-1.297029	1.293081
7.Ge	2.246521	1.297029	-1.293081
8.Ge	2.246521	-1.297029	-1.293081
9.Ge	0.000000	2.594058	-1.293081
10.Ge	0.000000	-2.594058	-1.293081
11.Ge	-2.246521	1.297029	-1.293081
12.Ge	-2.246521	-1.297029	-1.293081
13.Ni	0.000000	0.000000	0.000000

D_{6d} Ni@Ge_{12} MS=1

Bond Energy -47.07329344 eV

1.Ni	0.000000	0.000000	0.000000
2.Ge	-0.686551	-2.562244	-1.232278
3.Ge	1.875692	-1.875692	-1.232278
4.Ge	-2.562244	-0.686551	-1.232278
5.Ge	2.562244	0.686551	-1.232278
6.Ge	-1.875692	1.875692	-1.232278
7.Ge	0.686551	2.562244	-1.232278
8.Ge	0.686551	-2.562244	1.232278
9.Ge	2.562244	-0.686551	1.232278
10.Ge	-1.875692	-1.875692	1.232278
11.Ge	1.875692	1.875692	1.232278
12.Ge	-2.562244	0.686551	1.232278
13.Ge	-0.686551	2.562244	1.232278

D_{3d} Ni@Ge_{12} MS=1

Bond Energy -47.76143375 eV

1.Ge	-2.502678	1.444922	1.328804
2.Ge	0.000000	2.262576	1.254906
3.Ge	-1.959448	-1.131288	1.254906
4.Ge	2.502678	1.444922	1.328804
5.Ge	0.000000	-2.889844	1.328804
6.Ge	1.959448	-1.131288	1.254906
7.Ge	-1.959448	1.131288	-1.254906
8.Ge	0.000000	2.889844	-1.328804
9.Ge	-2.502678	-1.444922	-1.328804
10.Ge	1.959448	1.131288	-1.254906

11.Ge	0.000000	-2.262576	-1.254906
12.Ge	2.502678	-1.444922	-1.328804
13.Ni	0.000000	0.000000	0.000000

D_{2d} $Ni@Ge_{12}$ MS= 0

Bond Energy -47.99583994 eV

1.Ni	0.000000	0.000000	0.000000
2.Ge	-0.898146	-0.898146	2.643871
3.Ge	0.570952	-2.470332	1.166688
4.Ge	-2.470332	0.570952	1.166688
5.Ge	-2.470332	-0.570952	-1.166688
6.Ge	0.570952	2.470332	-1.166688
7.Ge	-0.898146	0.898146	-2.643871
8.Ge	2.470332	-0.570952	1.166688
9.Ge	-0.570952	-2.470332	-1.166688
10.Ge	0.898146	0.898146	2.643871
11.Ge	0.898146	-0.898146	-2.643871
12.Ge	-0.570952	2.470332	1.166688
13.Ge	2.470332	0.570952	-1.166688

C_2 $Ni@Ge_{12}$ MS=0

Bond Energy -48.13574252 eV

1.Ni	0.000000	0.000000	-0.000009
2.Ge	-0.662534	-1.128783	2.493860
3.Ge	0.581879	-2.642365	0.829903
4.Ge	-2.355714	0.687327	1.477516
5.Ge	-2.642277	-0.581872	-0.829883
6.Ge	0.687294	2.355763	-1.477515
7.Ge	-1.128765	0.662556	-2.493878
8.Ge	2.355714	-0.687327	1.477516
9.Ge	-0.687294	-2.355763	-1.477515
10.Ge	0.662534	1.128783	2.493860
11.Ge	1.128765	-0.662556	-2.493878
12.Ge	-0.581879	2.642365	0.829903
13.Ge	2.642277	0.581872	-0.829883

I_h $Co@Ge_{12}$ MS=3/2

Bond Energy -50.41246223 eV

1.Co	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.758616
5.Ge	-2.467275	0.000000	-1.233904
6.Ge	-0.762430	-2.346518	-1.233904
7.Ge	-0.762430	2.346518	-1.233904
8.Ge	1.996067	-1.450228	-1.233904
9.Ge	1.996067	1.450228	-1.233904
10.Ge	0.000000	0.000000	2.758616
12.Ge	2.467275	0.000000	1.233904
13.Ge	-1.996067	1.450228	1.233904
14.Ge	-1.996067	-1.450228	1.233904
15.Ge	0.762430	2.346518	1.233904
16.Ge	0.762430	-2.346518	1.233904

D_{6h} $Co@Ge_{12}$ MS=1/2

Bond Energy -49.90003258 eV

1.Ge	2.220533	1.282025	1.295797
2.Ge	2.220533	-1.282025	1.295797
3.Ge	0.000000	2.564051	1.295797
4.Ge	0.000000	-2.564051	1.295797

5.Ge	-2.220533	1.282025	1.295797
6.Ge	-2.220533	-1.282025	1.295797
7.Ge	2.220533	1.282025	-1.295797
8.Ge	2.220533	-1.282025	-1.295797
9.Ge	0.000000	2.564051	-1.295797
10.Ge	0.000000	-2.564051	-1.295797
11.Ge	-2.220533	1.282025	-1.295797
12.Ge	-2.220533	-1.282025	-1.295797
13.Co	0.000000	0.000000	0.000000

D_{6d} $Co@Ge_{12}$ MS=1/2

Bond Energy -49.83837433 eV

1.Co	0.000000	0.000000	0.000000
2.Ge	-0.678599	-2.532565	-1.236388
3.Ge	1.853966	-1.853966	-1.236388
4.Ge	-2.532565	-0.678599	-1.236388
5.Ge	2.532565	0.678599	-1.236388
6.Ge	-1.853966	1.853966	-1.236388
7.Ge	0.678599	2.532565	-1.236388
8.Ge	0.678599	-2.532565	1.236388
9.Ge	2.532565	-0.678599	1.236388
10.Ge	-1.853966	-1.853966	1.236388
11.Ge	1.853966	1.853966	1.236388
12.Ge	-2.532565	0.678599	1.236388
13.Ge	-0.678599	2.532565	1.236388

D_{3d} $Co@Ge_{12}$ MS=1/2

Bond Energy -50.45349209 eV

1.Ge	-2.484842	1.434624	1.298545
2.Ge	0.000000	2.245568	1.286161
3.Ge	-1.944719	-1.122784	1.286161
4.Ge	2.484842	1.434624	1.298545
5.Ge	0.000000	-2.869248	1.298545
6.Ge	1.944719	-1.122784	1.286161
7.Ge	-1.944719	1.122784	-1.286161
8.Ge	0.000000	2.869248	-1.298545
9.Ge	-2.484842	-1.434624	-1.298545
10.Ge	1.944719	1.122784	-1.286161
11.Ge	0.000000	-2.245568	-1.286161
12.Ge	2.484842	-1.434624	-1.298545
13.Co	0.000000	0.000000	0.000000

D_{2d} $Co@Ge_{12}$ MS= 1/2

Bond Energy -50.35129821 eV

1.Co	0.000000	0.000000	0.000000
2.Ge	-0.901232	-0.901232	2.711349
3.Ge	0.530184	-2.422719	1.170137
4.Ge	-2.422719	0.530184	1.170137
5.Ge	-2.422719	-0.530184	-1.170137
6.Ge	0.530184	2.422719	-1.170137
7.Ge	-0.901232	0.901232	-2.711349
8.Ge	2.422719	-0.530184	1.170137
9.Ge	-0.530184	-2.422719	-1.170137
10.Ge	0.901232	0.901232	2.711349
11.Ge	0.901232	-0.901232	-2.711349
12.Ge	-0.530184	2.422719	1.170137
13.Ge	2.422719	0.530184	-1.170137

C_2 Co@Ge_{12} MS=1/2

Bond Energy -50.54606567 eV

1.Co	0.051055	0.059938	0.020270
2.Ge	-0.729956	-1.050777	2.569624
3.Ge	0.260347	-2.574863	0.713358
4.Ge	-2.164373	0.860436	1.468079
5.Ge	-2.489406	-0.718377	-0.719012
6.Ge	0.379198	2.313951	-1.431806
7.Ge	-1.079759	0.398848	-2.598268
8.Ge	2.210928	-0.729237	1.308525
9.Ge	-0.611522	-2.467581	-1.748757
10.Ge	0.742968	1.103936	2.650236
11.Ge	1.268420	-0.731629	-2.405859
12.Ge	-0.409458	2.764372	0.997639
13.Ge	2.581745	0.783164	-0.819920

I_h Fe@Ge_{12} MS=2

Bond Energy -51.11912680 eV

1.Fe	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.777059
5.Ge	-2.483770	0.000000	-1.242153
6.Ge	-0.767527	-2.362205	-1.242153
7.Ge	-0.767527	2.362205	-1.242153
8.Ge	2.009412	-1.459923	-1.242153
9.Ge	2.009412	1.459923	-1.242153
10.Ge	0.000000	0.000000	2.777059
12.Ge	2.483770	0.000000	1.242153
13.Ge	-2.009412	1.459923	1.242153
14.Ge	-2.009412	-1.459923	1.242153
15.Ge	0.767527	2.362205	1.242153
16.Ge	0.767527	-2.362205	1.242153

D_{6h} Fe@Ge_{12} MS=1

Bond Energy -50.71925177 eV

1.Ge	2.238431	1.292359	1.298315
2.Ge	2.238431	-1.292359	1.298315
3.Ge	0.000000	2.584718	1.298315
4.Ge	0.000000	-2.584718	1.298315
5.Ge	-2.238431	1.292359	1.298315
6.Ge	-2.238431	-1.292359	1.298315
7.Ge	2.238431	1.292359	-1.298315
8.Ge	2.238431	-1.292359	-1.298315
9.Ge	0.000000	2.584718	-1.298315
10.Ge	0.000000	-2.584718	-1.298315
11.Ge	-2.238431	1.292359	-1.298315
12.Ge	-2.238431	-1.292359	-1.298315
13.Fe	0.000000	0.000000	0.000000

D_{6d} Fe@Ge_{12} MS=1

Bond Energy -50.78245659 eV

1.Fe	0.000000	0.000000	0.000000
2.Ge	-0.684624	-2.555052	-1.236787
3.Ge	1.870428	-1.870428	-1.236787
4.Ge	-2.555052	-0.684624	-1.236787
5.Ge	2.555052	0.684624	-1.236787
6.Ge	-1.870428	1.870428	-1.236787
7.Ge	0.684624	2.555052	-1.236787
8.Ge	0.684624	-2.555052	1.236787

9.Ge	2.555052	-0.684624	1.236787
10.Ge	-1.870428	-1.870428	1.236787
11.Ge	1.870428	1.870428	1.236787
12.Ge	-2.555052	0.684624	1.236787
13.Ge	-0.684624	2.555052	1.236787

D_{3d} $Fe@Ge_{12}$ MS=1

Bond Energy -51.17547584 eV

1.Ge	-2.465342	1.423366	1.349236
2.Ge	0.000000	2.320475	1.239207
3.Ge	-2.009591	-1.160238	1.239207
4.Ge	2.465342	1.423366	1.349236
5.Ge	0.000000	-2.846732	1.349236
6.Ge	2.009591	-1.160238	1.239207
7.Ge	-2.009591	1.160238	-1.239207
8.Ge	0.000000	2.846732	-1.349236
9.Ge	-2.465342	-1.423366	-1.349236
10.Ge	2.009591	1.160238	-1.239207
11.Ge	0.000000	-2.320475	-1.239207
12.Ge	2.465342	-1.423366	-1.349236
13.Fe	0.000000	0.000000	0.000000

D_{2d} $Fe@Ge_{12}$ MS= 1

Bond Energy -50.67247866 eV

1.Fe	0.000000	0.000000	0.000000
2.Ge	-0.915896	-0.915896	2.735991
3.Ge	0.535069	-2.441148	1.200613
4.Ge	-2.441148	0.535069	1.200613
5.Ge	-2.441148	-0.535069	-1.200613
6.Ge	0.535069	2.441148	-1.200613
7.Ge	-0.915896	0.915896	-2.735991
8.Ge	2.441148	-0.535069	1.200613
9.Ge	-0.535069	-2.441148	-1.200613
10.Ge	0.915896	0.915896	2.735991
11.Ge	0.915896	-0.915896	-2.735991
12.Ge	-0.535069	2.441148	1.200613
13.Ge	2.441148	0.535069	-1.200613

C_{2h} $Fe@Ge_{12}$ MS= 1

Bond Energy -51.21831237 eV

1.Ge	-1.499757	1.203521	2.443390
2.Ge	-2.455659	0.961621	0.000000
3.Ge	1.056887	1.375124	1.969986
4.Ge	-1.499757	1.203521	-2.443390
5.Ge	2.795123	1.651665	0.000000
6.Ge	1.056887	1.375124	-1.969986
7.Ge	-1.056887	-1.375124	1.969986
8.Ge	-2.795123	-1.651665	0.000000
9.Ge	1.499757	-1.203521	2.443390
10.Ge	-1.056887	-1.375124	-1.969986
11.Ge	2.455659	-0.961621	0.000000
12.Ge	1.499757	-1.203521	-2.443390
13.Fe	0.000000	0.000000	0.000000

D_{3d} $Fe@Ge_{12}$ MS= 2 (trigonally distorted icosahedron)

Bond Energy -51.24288795 eV

1.Fe	0.000000	0.000000	0.000000
2.Ge	0.000000	1.661379	-2.282572

3.Ge	-1.438796	-0.830689	-2.282572
4.Ge	1.438796	-0.830689	-2.282572
5.Ge	0.000000	-2.697184	-0.493205
6.Ge	-2.335830	1.348592	-0.493205
7.Ge	2.335830	1.348592	-0.493205
8.Ge	0.000000	2.697184	0.493205
9.Ge	-2.335830	-1.348592	0.493205
10.Ge	2.335830	-1.348592	0.493205
11.Ge	0.000000	-1.661379	2.282572
12.Ge	-1.438796	0.830689	2.282572
13.Ge	1.438796	0.830689	2.282572

I_h $Mn@Ge_{12}$ MS=5/2

Bond Energy -51.91531449 eV

1.Mn	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.802432
5.Ge	-2.506463	0.000000	-1.253502
6.Ge	-0.774540	-2.383788	-1.253502
7.Ge	-0.774540	2.383788	-1.253502
8.Ge	2.027771	-1.473262	-1.253502
9.Ge	2.027771	1.473262	-1.253502
10.Ge	0.000000	0.000000	2.802432
12.Ge	2.506463	0.000000	1.253502
13.Ge	-2.027771	1.473262	1.253502
14.Ge	-2.027771	-1.473262	1.253502
15.Ge	0.774540	2.383788	1.253502
16.Ge	0.774540	-2.383788	1.253502

D_{6h} $Mn@Ge_{12}$ MS=1/2

Bond Energy -51.55631062 eV

1.Ge	2.223539	1.283761	1.307156
2.Ge	2.223539	-1.283761	1.307156
3.Ge	0.000000	2.567522	1.307156
4.Ge	0.000000	-2.567522	1.307156
5.Ge	-2.223539	1.283761	1.307156
6.Ge	-2.223539	-1.283761	1.307156
7.Ge	2.223539	1.283761	-1.307156
8.Ge	2.223539	-1.283761	-1.307156
9.Ge	0.000000	2.567522	-1.307156
10.Ge	0.000000	-2.567522	-1.307156
11.Ge	-2.223539	1.283761	-1.307156
12.Ge	-2.223539	-1.283761	-1.307156
13.Mn	0.000000	0.000000	0.000000

D_{6d} $Mn@Ge_{12}$ MS=1/2

Bond Energy -51.52449079 eV

1.Mn	0.000000	0.000000	0.000000
2.Ge	-0.679353	-2.535379	-1.247139
3.Ge	1.856027	-1.856027	-1.247139
4.Ge	-2.535379	-0.679353	-1.247139
5.Ge	2.535379	0.679353	-1.247139
6.Ge	-1.856027	1.856027	-1.247139
7.Ge	0.679353	2.535379	-1.247139
8.Ge	0.679353	-2.535379	1.247139
9.Ge	2.535379	-0.679353	1.247139
10.Ge	-1.856027	-1.856027	1.247139
11.Ge	1.856027	1.856027	1.247139
12.Ge	-2.535379	0.679353	1.247139

13.Ge	-0.679353	2.535379	1.247139

D_{3d} $Mn@Ge_{12}$ MS=1/2

Bond Energy -51.79362395 eV

1.Ge	-2.442553	1.410208	1.312906
2.Ge	0.000000	2.318918	1.291107
3.Ge	-2.008242	-1.159459	1.291107
4.Ge	2.442553	1.410208	1.312906
5.Ge	0.000000	-2.820417	1.312906
6.Ge	2.008242	-1.159459	1.291107
7.Ge	-2.008242	1.159459	-1.291107
8.Ge	0.000000	2.820417	-1.312906
9.Ge	-2.442553	-1.410208	-1.312906
10.Ge	2.008242	1.159459	-1.291107
11.Ge	0.000000	-2.318918	-1.291107
12.Ge	2.442553	-1.410208	-1.312906
13.Mn	0.000000	0.000000	0.000000

D_{2d} $Mn@Ge_{12}$ MS= 1/2

Bond Energy -50.43174320 eV

1.Mn	0.000000	0.000000	0.000000
2.Ge	-0.896059	-0.896059	2.685459
3.Ge	0.546291	-2.488530	1.177072
4.Ge	-2.488530	0.546291	1.177072
5.Ge	-2.488530	-0.546291	-1.177072
6.Ge	0.546291	2.488530	-1.177072
7.Ge	-0.896059	0.896059	-2.685459
8.Ge	2.488530	-0.546291	1.177072
9.Ge	-0.546291	-2.488530	-1.177072
10.Ge	0.896059	0.896059	2.685459
11.Ge	0.896059	-0.896059	-2.685459
12.Ge	-0.546291	2.488530	1.177072
13.Ge	2.488530	0.546291	-1.177072

I_h $Cr@Ge_{12}$ MS=2

Bond Energy -51.07525889 eV

1.Cr	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.807827
5.Ge	-2.511288	0.000000	-1.255915
6.Ge	-0.776031	-2.388377	-1.255915
7.Ge	-0.776031	2.388377	-1.255915
8.Ge	2.031675	-1.476098	-1.255915
9.Ge	2.031675	1.476098	-1.255915
10.Ge	0.000000	0.000000	2.807827
12.Ge	2.511288	0.000000	1.255915
13.Ge	-2.031675	1.476098	1.255915
14.Ge	-2.031675	-1.476098	1.255915
15.Ge	0.776031	2.388377	1.255915
16.Ge	0.776031	-2.388377	1.255915

D_{6h} $Cr@Ge_{12}$ MS=0

Bond Energy -50.89063583 eV

1.Ge	2.222106	1.282933	1.304567
2.Ge	2.222106	-1.282933	1.304567
3.Ge	0.000000	2.565867	1.304567
4.Ge	0.000000	-2.565867	1.304567
5.Ge	-2.222106	1.282933	1.304567
6.Ge	-2.222106	-1.282933	1.304567

7.Ge	2.222106	1.282933	-1.304567
8.Ge	2.222106	-1.282933	-1.304567
9.Ge	0.000000	2.565867	-1.304567
10.Ge	0.000000	-2.565867	-1.304567
11.Ge	-2.222106	1.282933	-1.304567
12.Ge	-2.222106	-1.282933	-1.304567
13.Cr	0.000000	0.000000	0.000000

D_{6d} $Cr@Ge_{12}$ MS=0

Bond Energy -50.92587689 eV

1.Cr	0.000000	0.000000	0.000000
2.Ge	-0.680281	-2.538845	-1.238630
3.Ge	1.858563	-1.858563	-1.238630
4.Ge	-2.538845	-0.680281	-1.238630
5.Ge	2.538845	0.680281	-1.238630
6.Ge	-1.858563	1.858563	-1.238630
7.Ge	0.680281	2.538845	-1.238630
8.Ge	0.680281	-2.538845	1.238630
9.Ge	2.538845	-0.680281	1.238630
10.Ge	-1.858563	-1.858563	1.238630
11.Ge	1.858563	1.858563	1.238630
12.Ge	-2.538845	0.680281	1.238630
13.Ge	-0.680281	2.538845	1.238630

D_{3d} $Cr@Ge_{12}$ MS=0

Bond Energy -51.07599264 eV

1.Ge	-2.428292	1.401975	1.344845
2.Ge	0.000000	2.344478	1.256852
3.Ge	-2.030378	-1.172239	1.256852
4.Ge	2.428292	1.401975	1.344845
5.Ge	0.000000	-2.803951	1.344845
6.Ge	2.030378	-1.172239	1.256852
7.Ge	-2.030378	1.172239	-1.256852
8.Ge	0.000000	2.803951	-1.344845
9.Ge	-2.428292	-1.401975	-1.344845
10.Ge	2.030378	1.172239	-1.256852
11.Ge	0.000000	-2.344478	-1.256852
12.Ge	2.428292	-1.401975	-1.344845
13.Cr	0.000000	0.000000	0.000000

D_{5d} $Cr@Ge_{12}$ MS=2

Bond Energy -51.10913742 eV

1.Ge	1.469755	2.022945	1.287247
2.Ge	2.378114	-0.772696	1.287247
3.Ge	-1.469755	2.022945	1.287247
4.Ge	-2.378114	-0.772696	1.287247
5.Ge	0.000000	-2.500497	1.287247
6.Ge	1.469755	-2.022945	-1.287247
7.Ge	-1.469755	-2.022945	-1.287247
8.Ge	2.378114	0.772696	-1.287247
9.Ge	0.000000	2.500497	-1.287247
10.Ge	-2.378114	0.772696	-1.287247
11.Cr	0.000000	0.000000	0.000000
12.Ge	0.000000	0.000000	2.791458
13.Ge	0.000000	0.000000	-2.791458

I_h $V@Ge_{12}$ MS=3/2

Bond Energy -49.64725179 eV

1.V	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.816734
5.Ge	-2.519254	0.000000	-1.259899
6.Ge	-0.778492	-2.395953	-1.259899
7.Ge	-0.778492	2.395953	-1.259899
8.Ge	2.038120	-1.480781	-1.259899
9.Ge	2.038120	1.480781	-1.259899
10.Ge	0.000000	0.000000	2.816734
12.Ge	2.519254	0.000000	1.259899
13.Ge	-2.038120	1.480781	1.259899
14.Ge	-2.038120	-1.480781	1.259899
15.Ge	0.778492	2.395953	1.259899
16.Ge	0.778492	-2.395953	1.259899

D_{6h} V@Ge_{12} MS=1/2

Bond Energy -49.97655444 eV

1.Ge	2.236384	1.291177	1.321353
2.Ge	2.236384	-1.291177	1.321353
3.Ge	0.000000	2.582354	1.321353
4.Ge	0.000000	-2.582354	1.321353
5.Ge	-2.236384	1.291177	1.321353
6.Ge	-2.236384	-1.291177	1.321353
7.Ge	2.236384	1.291177	-1.321353
8.Ge	2.236384	-1.291177	-1.321353
9.Ge	0.000000	2.582354	-1.321353
10.Ge	0.000000	-2.582354	-1.321353
11.Ge	-2.236384	1.291177	-1.321353
12.Ge	-2.236384	-1.291177	-1.321353
13.V	0.000000	0.000000	0.000000

D_{6d} V@Ge_{12} MS=1/2

Bond Energy -49.79978982 eV

1.V	0.000000	0.000000	0.000000
2.Ge	-0.693002	-2.586320	-1.236379
3.Ge	1.893317	-1.893317	-1.236379
4.Ge	-2.586320	-0.693002	-1.236379
5.Ge	2.586320	0.693002	-1.236379
6.Ge	-1.893317	1.893317	-1.236379
7.Ge	0.693002	2.586320	-1.236379
8.Ge	0.693002	-2.586320	1.236379
9.Ge	2.586320	-0.693002	1.236379
10.Ge	-1.893317	-1.893317	1.236379
11.Ge	1.893317	1.893317	1.236379
12.Ge	-2.586320	0.693002	1.236379
13.Ge	-0.693002	2.586320	1.236379

D_{3d} V@Ge_{12} MS=1/2

Bond Energy -50.23597184 eV

1.Ge	-2.459817	1.420176	1.362644
2.Ge	0.000000	2.339954	1.273819
3.Ge	-2.026460	-1.169977	1.273819
4.Ge	2.459817	1.420176	1.362644
5.Ge	0.000000	-2.840352	1.362644
6.Ge	2.026460	-1.169977	1.273819
7.Ge	-2.026460	1.169977	-1.273819
8.Ge	0.000000	2.840352	-1.362644
9.Ge	-2.459817	-1.420176	-1.362644
10.Ge	2.026460	1.169977	-1.273819

11.Ge	0.000000	-2.339954	-1.273819
12.Ge	2.459817	-1.420176	-1.362644
13.V	0.000000	0.000000	0.000000

C_{2h} VGe_{12} MS=1/2

Bond Energy -50.31489768 eV

1.Ge	1.334825	1.439713	-2.429937
2.Ge	1.266565	-1.187658	-1.991648
3.Ge	1.321439	2.372437	0.000000
4.Ge	1.387632	-2.862438	0.000000
5.Ge	1.334825	1.439713	2.429937
6.Ge	1.266565	-1.187658	1.991648
7.Ge	-1.266565	1.187658	-1.991648
8.Ge	-1.334825	-1.439713	-2.429937
9.Ge	-1.387632	2.862438	0.000000
10.Ge	-1.321439	-2.372437	0.000000
11.Ge	-1.266565	1.187658	1.991648
12.Ge	-1.334825	-1.439713	2.429937
13.V	0.000000	0.000000	0.000000

I_h $Ti@Ge_{12}$ MS=1

Bond Energy -48.13893638 eV

1.Ti	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.842652
5.Ge	-2.542435	0.000000	-1.271492
6.Ge	-0.785656	-2.418000	-1.271492
7.Ge	-0.785656	2.418000	-1.271492
8.Ge	2.056873	-1.494406	-1.271492
9.Ge	2.056873	1.494406	-1.271492
10.Ge	0.000000	0.000000	2.842652
12.Ge	2.542435	0.000000	1.271492
13.Ge	-2.056873	1.494406	1.271492
14.Ge	-2.056873	-1.494406	1.271492
15.Ge	0.785656	2.418000	1.271492
16.Ge	0.785656	-2.418000	1.271492

D_{6h} $Ti@Ge_{12}$ MS=1

Bond Energy -48.41745328 eV

1.Ge	2.287428	1.320647	1.308371
2.Ge	2.287428	-1.320647	1.308371
3.Ge	0.000000	2.641295	1.308371
4.Ge	0.000000	-2.641295	1.308371
5.Ge	-2.287428	1.320647	1.308371
6.Ge	-2.287428	-1.320647	1.308371
7.Ge	2.287428	1.320647	-1.308371
8.Ge	2.287428	-1.320647	-1.308371
9.Ge	0.000000	2.641295	-1.308371
10.Ge	0.000000	-2.641295	-1.308371
11.Ge	-2.287428	1.320647	-1.308371
12.Ge	-2.287428	-1.320647	-1.308371
13.Ti	0.000000	0.000000	0.000000

D_{6d} $Ti@Ge_{12}$ MS=1

Bond Energy -48.79204212 eV

1.Ti	0.000000	0.000000	0.000000
2.Ge	-0.701445	-2.617828	-1.235130
3.Ge	1.916383	-1.916383	-1.235130
4.Ge	-2.617828	-0.701445	-1.235130

5.Ge	2.617828	0.701445	-1.235130
6.Ge	-1.916383	1.916383	-1.235130
7.Ge	0.701445	2.617828	-1.235130
8.Ge	0.701445	-2.617828	1.235130
9.Ge	2.617828	-0.701445	1.235130
10.Ge	-1.916383	-1.916383	1.235130
11.Ge	1.916383	1.916383	1.235130
12.Ge	-2.617828	0.701445	1.235130
13.Ge	-0.701445	2.617828	1.235130

D_{3d} $Ti@Ge_{12}$ MS=1

Bond Energy -48.76222690 eV

1.Ge	-2.406078	1.389150	1.491124
2.Ge	0.000000	2.509023	1.150269
3.Ge	-2.172878	-1.254512	1.150269
4.Ge	2.406078	1.389150	1.491124
5.Ge	0.000000	-2.778300	1.491124
6.Ge	2.172878	-1.254512	1.150269
7.Ge	-2.172878	1.254512	-1.150269
8.Ge	0.000000	2.778300	-1.491124
9.Ge	-2.406078	-1.389150	-1.491124
10.Ge	2.172878	1.254512	-1.150269
11.Ge	0.000000	-2.509023	-1.150269
12.Ge	2.406078	-1.389150	-1.491124
13.Ti	0.000000	0.000000	0.000000

C_1 $TiGe_{12}$ MS=0

Bond Energy -48.95253943 eV

1.Ge	-1.860108	2.465187	-1.097048
2.Ge	-2.545736	-0.041627	-1.280214
3.Ge	0.775821	2.294383	-1.057947
4.Ge	-1.349769	-2.315180	-1.532623
5.Ge	2.947574	0.857109	-1.335453
6.Ge	1.820571	-1.500445	-1.346800
7.Ge	-1.671168	1.468052	1.349988
8.Ge	-2.795621	-0.911053	1.382841
9.Ge	0.981662	2.367846	1.554036
10.Ge	-0.675759	-2.403604	1.002376
11.Ge	2.407881	0.171955	1.282926
12.Ge	1.964953	-2.404495	1.133336
13.Ti	-0.000038	-0.074737	-0.086399

$M@Ge_{12}$ Second row transition metals (Figure 2(c))

I_h $Zr@Ge_{12}$ MS=1

Bond Energy -47.34493893 eV

1.Zr	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.920667
5.Ge	-2.612211	0.000000	-1.306388
6.Ge	-0.807218	-2.484360	-1.306388
7.Ge	-0.807218	2.484360	-1.306388
8.Ge	2.113323	-1.535419	-1.306388
9.Ge	2.113323	1.535419	-1.306388
10.Ge.1	0.000000	0.000000	2.920667
12.Ge	2.612211	0.000000	1.306388
13.Ge	-2.113323	1.535419	1.306388
14.Ge	-2.113323	-1.535419	1.306388
15.Ge	0.807218	2.484360	1.306388

16.Ge	0.807218	-2.484360	1.306388

D_{6h} $Zr@Ge_{12}$ MS=1

Bond Energy -48.79235834 eV

1.Ge	2.317288	1.337887	1.337528
2.Ge	2.317288	-1.337887	1.337528
3.Ge	0.000000	2.675774	1.337528
4.Ge	0.000000	-2.675774	1.337528
5.Ge	-2.317288	1.337887	1.337528
6.Ge	-2.317288	-1.337887	1.337528
7.Ge	2.317288	1.337887	-1.337528
8.Ge	2.317288	-1.337887	-1.337528
9.Ge	0.000000	2.675774	-1.337528
10.Ge	0.000000	-2.675774	-1.337528
11.Ge	-2.317288	1.337887	-1.337528
12.Ge	-2.317288	-1.337887	-1.337528
13.Zr	0.000000	0.000000	0.000000

D_{6d} $Zr@Ge_{12}$ MS=0

Bond Energy -49.56463956 eV

1.Zr	0.000000	0.000000	0.000000
2.Ge	-0.718644	-2.682016	-1.214841
3.Ge	1.963372	-1.963372	-1.214841
4.Ge	-2.682016	-0.718644	-1.214841
5.Ge	2.682016	0.718644	-1.214841
6.Ge	-1.963372	1.963372	-1.214841
7.Ge	0.718644	2.682016	-1.214841
8.Ge	0.718644	-2.682016	1.214841
9.Ge	2.682016	-0.718644	1.214841
10.Ge	-1.963372	-1.963372	1.214841
11.Ge	1.963372	1.963372	1.214841
12.Ge	-2.682016	0.718644	1.214841
13.Ge	-0.718644	2.682016	1.214841

D_{3d} $Zr@Ge_{12}$ MS=1

Bond Energy -48.86325932 eV

1.Ge	-2.491552	1.438498	1.383670
2.Ge	0.000000	2.467992	1.341278
3.Ge	-2.137343	-1.233996	1.341278
4.Ge	2.491552	1.438498	1.383670
5.Ge	0.000000	-2.876996	1.383670
6.Ge	2.137343	-1.233996	1.341278
7.Ge	-2.137343	1.233996	-1.341278
8.Ge	0.000000	2.876996	-1.383670
9.Ge	-2.491552	-1.438498	-1.383670
10.Ge	2.137343	1.233996	-1.341278
11.Ge	0.000000	-2.467992	-1.341278
12.Ge	2.491552	-1.438498	-1.383670
13.Zr	0.000000	0.000000	0.000000

I_h $Nb@Ge_{12}$ MS=3/2

Bond Energy -49.41426902 eV

1.Nb	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.874391
5.Ge	-2.570823	0.000000	-1.285689
6.Ge	-0.794428	-2.444998	-1.285689
7.Ge	-0.794428	2.444998	-1.285689
8.Ge	2.079839	-1.511092	-1.285689

9.Ge	2.079839	1.511092	-1.285689
10.Ge.1	0.000000	0.000000	2.874391
12.Ge	2.570823	0.000000	1.285689
13.Ge	-2.079839	1.511092	1.285689
14.Ge	-2.079839	-1.511092	1.285689
15.Ge	0.794428	2.444998	1.285689
16.Ge	0.794428	-2.444998	1.285689

D_{6h} $Nb@Ge_{12}$ MS=3/2

Bond Energy -51.33409707 eV

1.Ge	2.284335	1.318861	1.312056
2.Ge	2.284335	-1.318861	1.312056
3.Ge	0.000000	2.637723	1.312056
4.Ge	0.000000	-2.637723	1.312056
5.Ge	-2.284335	1.318861	1.312056
6.Ge	-2.284335	-1.318861	1.312056
7.Ge	2.284335	1.318861	-1.312056
8.Ge	2.284335	-1.318861	-1.312056
9.Ge	0.000000	2.637723	-1.312056
10.Ge	0.000000	-2.637723	-1.312056
11.Ge	-2.284335	1.318861	-1.312056
12.Ge	-2.284335	-1.318861	-1.312056
13.Nb	0.000000	0.000000	0.000000

D_{6d} $Nb@Ge_{12}$ MS=1/2

Bond Energy -51.71134368 eV

1.Nb	0.000000	0.000000	0.000000
2.Ge	-0.700253	-2.613380	-1.233561
3.Ge	1.913127	-1.913127	-1.233561
4.Ge	-2.613380	-0.700253	-1.233561
5.Ge	2.613380	0.700253	-1.233561
6.Ge	-1.913127	1.913127	-1.233561
7.Ge	0.700253	2.613380	-1.233561
8.Ge	0.700253	-2.613380	1.233561
9.Ge	2.613380	-0.700253	1.233561
10.Ge	-1.913127	-1.913127	1.233561
11.Ge	1.913127	1.913127	1.233561
12.Ge	-2.613380	0.700253	1.233561
13.Ge	-0.700253	2.613380	1.233561

D_{3d} $Nb@Ge_{12}$ MS=1/2

Bond Energy -51.35496303 eV

1.Ge	-2.466560	1.424069	1.375340
2.Ge	0.000000	2.418827	1.305357
3.Ge	-2.094766	-1.209414	1.305357
4.Ge	2.466560	1.424069	1.375340
5.Ge	0.000000	-2.848138	1.375340
6.Ge	2.094766	-1.209414	1.305357
7.Ge	-2.094766	1.209414	-1.305357
8.Ge	0.000000	2.848138	-1.375340
9.Ge	-2.466560	-1.424069	-1.375340
10.Ge	2.094766	1.209414	-1.305357
11.Ge	0.000000	-2.418827	-1.305357
12.Ge	2.466560	-1.424069	-1.375340
13.Nb	0.000000	0.000000	0.000000

I_h $Mo@Ge_{12}$ MS=2

Bond Energy -50.15988557 eV

1.Mo	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.842219
5.Ge	-2.542048	0.000000	-1.271298
6.Ge	-0.785536	-2.417631	-1.271298
7.Ge	-0.785536	2.417631	-1.271298
8.Ge	2.056560	-1.494178	-1.271298
9.Ge	2.056560	1.494178	-1.271298
10.Ge.1	0.000000	0.000000	2.842219
12.Ge	2.542048	0.000000	1.271298
13.Ge	-2.056560	1.494178	1.271298
14.Ge	-2.056560	-1.494178	1.271298
15.Ge	0.785536	2.417631	1.271298
16.Ge	0.785536	-2.417631	1.271298

D_{6h} $Mo@Ge_{12}$ MS=0

Bond Energy -51.96425349 eV

1.Ge	2.252832	1.300673	1.320000
2.Ge	2.252832	-1.300673	1.320000
3.Ge	0.000000	2.601347	1.320000
4.Ge	0.000000	-2.601347	1.320000
5.Ge	-2.252832	1.300673	1.320000
6.Ge	-2.252832	-1.300673	1.320000
7.Ge	2.252832	1.300673	-1.320000
8.Ge	2.252832	-1.300673	-1.320000
9.Ge	0.000000	2.601347	-1.320000
10.Ge	0.000000	-2.601347	-1.320000
11.Ge	-2.252832	1.300673	-1.320000
12.Ge	-2.252832	-1.300673	-1.320000
13.Mo	0.000000	0.000000	0.000000

D_{6d} $Mo@Ge_{12}$ MS=0

Bond Energy -52.04040007 eV

1.Mo	0.000000	0.000000	0.000000
2.Ge	-0.688183	-2.568336	-1.248624
3.Ge	1.880152	-1.880152	-1.248624
4.Ge	-2.568336	-0.688183	-1.248624
5.Ge	2.568336	0.688183	-1.248624
6.Ge	-1.880152	1.880152	-1.248624
7.Ge	0.688183	2.568336	-1.248624
8.Ge	0.688183	-2.568336	1.248624
9.Ge	2.568336	-0.688183	1.248624
10.Ge	-1.880152	-1.880152	1.248624
11.Ge	1.880152	1.880152	1.248624
12.Ge	-2.568336	0.688183	1.248624
13.Ge	-0.688183	2.568336	1.248624

D_{3d} $Mo@Ge_{12}$ MS=0

Bond Energy -52.05688141 eV

1.Ge	-2.416613	1.395232	1.362457
2.Ge	0.000000	2.429922	1.268934
3.Ge	-2.104374	-1.214961	1.268934
4.Ge	2.416613	1.395232	1.362457
5.Ge	0.000000	-2.790465	1.362457
6.Ge	2.104374	-1.214961	1.268934
7.Ge	-2.104374	1.214961	-1.268934
8.Ge	0.000000	2.790465	-1.362457
9.Ge	-2.416613	-1.395232	-1.362457

10.Ge	2.104374	1.214961	-1.268934
11.Ge	0.000000	-2.429922	-1.268934
12.Ge	2.416613	-1.395232	-1.362457
13.Mo	0.000000	0.000000	0.000000

I_h $Tc@Ge_{12}$ MS=5/2

Bond Energy -51.98896822 eV

1.Tc	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.818955
5.Ge	-2.521241	0.000000	-1.260893
6.Ge	-0.779106	-2.397843	-1.260893
7.Ge	-0.779106	2.397843	-1.260893
8.Ge	2.039727	-1.481949	-1.260893
9.Ge	2.039727	1.481949	-1.260893
10.Ge.1	0.000000	0.000000	2.818955
12.Ge	2.521241	0.000000	1.260893
13.Ge	-2.039727	1.481949	1.260893
14.Ge	-2.039727	-1.481949	1.260893
15.Ge	0.779106	2.397843	1.260893
16.Ge	0.779106	-2.397843	1.260893

D_{6h} $Tc@Ge_{12}$ MS=1/2

Bond Energy -53.42169828 eV

1.Ge	2.239930	1.293224	1.314219
2.Ge	2.239930	-1.293224	1.314219
3.Ge	0.000000	2.586448	1.314219
4.Ge	0.000000	-2.586448	1.314219
5.Ge	-2.239930	1.293224	1.314219
6.Ge	-2.239930	-1.293224	1.314219
7.Ge	2.239930	1.293224	-1.314219
8.Ge	2.239930	-1.293224	-1.314219
9.Ge	0.000000	2.586448	-1.314219
10.Ge	0.000000	-2.586448	-1.314219
11.Ge	-2.239930	1.293224	-1.314219
12.Ge	-2.239930	-1.293224	-1.314219
13.Tc	0.000000	0.000000	0.000000

D_{6d} $Tc@Ge_{12}$ MS=1/2

Bond Energy -53.38290536 eV

1.Tc	0.000000	0.000000	0.000000
2.Ge	-0.684104	-2.553109	-1.246707
3.Ge	1.869006	-1.869006	-1.246707
4.Ge	-2.553109	-0.684104	-1.246707
5.Ge	2.553109	0.684104	-1.246707
6.Ge	-1.869006	1.869006	-1.246707
7.Ge	0.684104	2.553109	-1.246707
8.Ge	0.684104	-2.553109	1.246707
9.Ge	2.553109	-0.684104	1.246707
10.Ge	-1.869006	-1.869006	1.246707
11.Ge	1.869006	1.869006	1.246707
12.Ge	-2.553109	0.684104	1.246707
13.Ge	-0.684104	2.553109	1.246707

D_{3d} $Tc@Ge_{12}$ MS=1/2

Bond Energy -53.52404322 eV

1.Ge	-2.419076	1.396654	1.317315
2.Ge	0.000000	2.393161	1.305777
3.Ge	-2.072538	-1.196581	1.305777

4.Ge	2.419076	1.396654	1.317315
5.Ge	0.000000	-2.793309	1.317315
6.Ge	2.072538	-1.196581	1.305777
7.Ge	-2.072538	1.196581	-1.305777
8.Ge	0.000000	2.793309	-1.317315
9.Ge	-2.419076	-1.396654	-1.317315
10.Ge	2.072538	1.196581	-1.305777
11.Ge	0.000000	-2.393161	-1.305777
12.Ge	2.419076	-1.396654	-1.317315
13.Tc	0.000000	0.000000	0.000000

D_{2d} $Tc@Ge_{12}$ MS=1/2

Bond Energy -52.50804253 eV

1.Tc	0.000000	0.000000	0.000000
2.Ge	-0.905677	-0.905677	2.809747
3.Ge	0.485120	-2.463440	1.214197
4.Ge	-2.463440	0.485120	1.214197
5.Ge	-2.463440	-0.485120	-1.214197
6.Ge	0.485120	2.463440	-1.214197
7.Ge	-0.905677	0.905677	-2.809747
8.Ge	2.463440	-0.485120	1.214197
9.Ge	-0.485120	-2.463440	-1.214197
10.Ge	0.905677	0.905677	2.809747
11.Ge	0.905677	-0.905677	-2.809747
12.Ge	-0.485120	2.463440	1.214197
13.Ge	2.463440	0.485120	-1.214197

I_h $Ru@Ge_{12}$ MS=2

Bond Energy -49.79830012 eV

1.Ru	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.798036
5.Ge	-2.502532	0.000000	-1.251536
6.Ge	-0.773325	-2.380049	-1.251536
7.Ge	-0.773325	2.380049	-1.251536
8.Ge	2.024591	-1.470951	-1.251536
9.Ge	2.024591	1.470951	-1.251536
10.Ge.1	0.000000	0.000000	2.798036
12.Ge	2.502532	0.000000	1.251536
13.Ge	-2.024591	1.470951	1.251536
14.Ge	-2.024591	-1.470951	1.251536
15.Ge	0.773325	2.380049	1.251536
16.Ge	0.773325	-2.380049	1.251536

D_{6h} $Ru@Ge_{12}$ MS=0

Bond Energy -51.05636836 eV

1.Ge	2.223833	1.283930	1.311678
2.Ge	2.223833	-1.283930	1.311678
3.Ge	0.000000	2.567861	1.311678
4.Ge	0.000000	-2.567861	1.311678
5.Ge	-2.223833	1.283930	1.311678
6.Ge	-2.223833	-1.283930	1.311678
7.Ge	2.223833	1.283930	-1.311678
8.Ge	2.223833	-1.283930	-1.311678
9.Ge	0.000000	2.567861	-1.311678
10.Ge	0.000000	-2.567861	-1.311678
11.Ge	-2.223833	1.283930	-1.311678
12.Ge	-2.223833	-1.283930	-1.311678
13.Ru	0.000000	0.000000	0.000000

D_{6d} $Ru@Ge_{12}$ MS=0

Bond Energy -50.89807695 eV

1.Ru	0.000000	0.000000	0.000000
2.Ge	-0.679605	-2.536320	-1.250584
3.Ge	1.856715	-1.856715	-1.250584
4.Ge	-2.536320	-0.679605	-1.250584
5.Ge	2.536320	0.679605	-1.250584
6.Ge	-1.856715	1.856715	-1.250584
7.Ge	0.679605	2.536320	-1.250584
8.Ge	0.679605	-2.536320	1.250584
9.Ge	2.536320	-0.679605	1.250584
10.Ge	-1.856715	-1.856715	1.250584
11.Ge	1.856715	1.856715	1.250584
12.Ge	-2.536320	0.679605	1.250584
13.Ge	-0.679605	2.536320	1.250584

D_{3d} $Ru@Ge_{12}$ MS=0

Bond Energy -51.24467965 eV

1.Ge	-2.437220	1.407129	1.283520
2.Ge	0.000000	2.331792	1.335198
3.Ge	-2.019391	-1.165896	1.335198
4.Ge	2.437220	1.407129	1.283520
5.Ge	0.000000	-2.814259	1.283520
6.Ge	2.019391	-1.165896	1.335198
7.Ge	-2.019391	1.165896	-1.335198
8.Ge	0.000000	2.814259	-1.283520
9.Ge	-2.437220	-1.407129	-1.283520
10.Ge	2.019391	1.165896	-1.335198
11.Ge	0.000000	-2.331792	-1.335198
12.Ge	2.437220	-1.407129	-1.283520
13.Ru	0.000000	0.000000	0.000000

D_{2d} $Ru@Ge_{12}$ MS=1

Bond Energy -50.80332020 eV

1.Ru	0.000000	0.000000	0.000000
2.Ge	-0.905890	-0.905890	2.812957
3.Ge	0.489963	-2.435779	1.206898
4.Ge	-2.435779	0.489963	1.206898
5.Ge	-2.435779	-0.489963	-1.206898
6.Ge	0.489963	2.435779	-1.206898
7.Ge	-0.905890	0.905890	-2.812957
8.Ge	2.435779	-0.489963	1.206898
9.Ge	-0.489963	-2.435779	-1.206898
10.Ge	0.905890	0.905890	2.812957
11.Ge	0.905890	-0.905890	-2.812957
12.Ge	-0.489963	2.435779	1.206898
13.Ge	2.435779	0.489963	-1.206898

I_h $Rh@Ge_{12}$ MS=3/2

Bond Energy -48.84334783 eV

1.Rh	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.793981
5.Ge	-2.498904	0.000000	-1.249722
6.Ge	-0.772204	-2.376599	-1.249722
7.Ge	-0.772204	2.376599	-1.249722
8.Ge	2.021656	-1.468819	-1.249722
9.Ge	2.021656	1.468819	-1.249722

10.Ge.1	0.000000	0.000000	2.793981
12.Ge	2.498904	0.000000	1.249722
13.Ge	-2.021656	1.468819	1.249722
14.Ge	-2.021656	-1.468819	1.249722
15.Ge	0.772204	2.376599	1.249722
16.Ge	0.772204	-2.376599	1.249722

D_{6h} $Rh@Ge_{12}$ MS=1/2

Bond Energy -49.46024174 eV

1.Ge	2.250092	1.299091	1.303911
2.Ge	2.250092	-1.299091	1.303911
3.Ge	0.000000	2.598182	1.303911
4.Ge	0.000000	-2.598182	1.303911
5.Ge	-2.250092	1.299091	1.303911
6.Ge	-2.250092	-1.299091	1.303911
7.Ge	2.250092	1.299091	-1.303911
8.Ge	2.250092	-1.299091	-1.303911
9.Ge	0.000000	2.598182	-1.303911
10.Ge	0.000000	-2.598182	-1.303911
11.Ge	-2.250092	1.299091	-1.303911
12.Ge	-2.250092	-1.299091	-1.303911
13.Rh	0.000000	0.000000	0.000000

D_{6d} $Rh@Ge_{12}$ MS=1/2

Bond Energy -49.42511296 eV

1.Rh	0.000000	0.000000	0.000000
2.Ge	-0.684671	-2.555228	-1.242543
3.Ge	1.870557	-1.870557	-1.242543
4.Ge	-2.555228	-0.684671	-1.242543
5.Ge	2.555228	0.684671	-1.242543
6.Ge	-1.870557	1.870557	-1.242543
7.Ge	0.684671	2.555228	-1.242543
8.Ge	0.684671	-2.555228	1.242543
9.Ge	2.555228	-0.684671	1.242543
10.Ge	-1.870557	-1.870557	1.242543
11.Ge	1.870557	1.870557	1.242543
12.Ge	-2.555228	0.684671	1.242543
13.Ge	-0.684671	2.555228	1.242543

D_{3d} $Rh@Ge_{12}$ MS=1/2

Bond Energy -49.68801998 eV

1.Ge	-2.469809	1.425945	1.252119
2.Ge	0.000000	2.327742	1.351080
3.Ge	-2.015883	-1.163871	1.351080
4.Ge	2.469809	1.425945	1.252119
5.Ge	0.000000	-2.851890	1.252119
6.Ge	2.015883	-1.163871	1.351080
7.Ge	-2.015883	1.163871	-1.351080
8.Ge	0.000000	2.851890	-1.252119
9.Ge	-2.469809	-1.425945	-1.252119
10.Ge	2.015883	1.163871	-1.351080
11.Ge	0.000000	-2.327742	-1.351080
12.Ge	2.469809	-1.425945	-1.252119
13.Rh	0.000000	0.000000	0.000000

D_{2d} $Rh@Ge_{12}$ MS=1/2

Bond Energy -49.88469445 eV

1.Rh	0.000000	0.000000	0.000000

2.Ge	-0.901497	-0.901497	2.721551
3.Ge	0.535839	-2.473703	1.193018
4.Ge	-2.473703	0.535839	1.193018
5.Ge	-2.473703	-0.535839	-1.193018
6.Ge	0.535839	2.473703	-1.193018
7.Ge	-0.901497	0.901497	-2.721551
8.Ge	2.473703	-0.535839	1.193018
9.Ge	-0.535839	-2.473703	-1.193018
10.Ge	0.901497	0.901497	2.721551
11.Ge	0.901497	-0.901497	-2.721551
12.Ge	-0.535839	2.473703	1.193018
13.Ge	2.473703	0.535839	-1.193018

C_2 Rh@Ge_{12} MS=1/2

Bond Energy -50.05029677 eV

1.Rh	0.000000	0.000000	-0.006149
2.Ge	-0.563065	-1.174294	2.625398
3.Ge	0.687332	-2.595629	0.866606
4.Ge	-2.369866	0.471428	1.513920
5.Ge	-2.677692	-0.380494	-0.972590
6.Ge	0.760562	2.269830	-1.384375
7.Ge	-1.049008	0.763987	-2.644679
8.Ge	2.369866	-0.471428	1.513920
9.Ge	-0.760562	-2.269830	-1.384375
10.Ge	0.563065	1.174294	2.625398
11.Ge	1.049008	-0.763987	-2.644679
12.Ge	-0.687332	2.595629	0.866606
13.Ge	2.677692	0.380494	-0.972590

I_h Pd@Ge_{12} MS=1

Bond Energy -44.80362916 eV

1.Pd	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.812121
5.Ge	-2.515129	0.000000	-1.257836
6.Ge	-0.777218	-2.392030	-1.257836
7.Ge	-0.777218	2.392030	-1.257836
8.Ge	2.034782	-1.478356	-1.257836
9.Ge	2.034782	1.478356	-1.257836
10.Ge.1	0.000000	0.000000	2.812121
12.Ge	2.515129	0.000000	1.257836
13.Ge	-2.034782	1.478356	1.257836
14.Ge	-2.034782	-1.478356	1.257836
15.Ge	0.777218	2.392030	1.257836
16.Ge	0.777218	-2.392030	1.257836

D_{6h} Pd@Ge_{12} MS=1

Bond Energy -44.84692417 eV

1.Ge	2.286542	1.320136	1.300188
2.Ge	2.286542	-1.320136	1.300188
3.Ge	0.000000	2.640271	1.300188
4.Ge	0.000000	-2.640271	1.300188
5.Ge	-2.286542	1.320136	1.300188
6.Ge	-2.286542	-1.320136	1.300188
7.Ge	2.286542	1.320136	-1.300188
8.Ge	2.286542	-1.320136	-1.300188
9.Ge	0.000000	2.640271	-1.300188
10.Ge	0.000000	-2.640271	-1.300188
11.Ge	-2.286542	1.320136	-1.300188

12.Ge	-2.286542	-1.320136	-1.300188
13.Pd	0.000000	0.000000	0.000000

D_{6d} Pd@Ge_{12} MS=1

Bond Energy -44.94282086 eV

1.Pd	0.000000	0.000000	0.000000
2.Ge	-0.697162	-2.601843	-1.233560
3.Ge	1.904681	-1.904681	-1.233560
4.Ge	-2.601843	-0.697162	-1.233560
5.Ge	2.601843	0.697162	-1.233560
6.Ge	-1.904681	1.904681	-1.233560
7.Ge	0.697162	2.601843	-1.233560
8.Ge	0.697162	-2.601843	1.233560
9.Ge	2.601843	-0.697162	1.233560
10.Ge	-1.904681	-1.904681	1.233560
11.Ge	1.904681	1.904681	1.233560
12.Ge	-2.601843	0.697162	1.233560
13.Ge	-0.697162	2.601843	1.233560

D_{3d} Pd@Ge_{12} MS=1

Bond Energy -45.21397629 eV

1.Ge	-2.496671	1.441454	1.339318
2.Ge	0.000000	2.392781	1.266308
3.Ge	-2.072209	-1.196391	1.266308
4.Ge	2.496671	1.441454	1.339318
5.Ge	0.000000	-2.882908	1.339318
6.Ge	2.072209	-1.196391	1.266308
7.Ge	-2.072209	1.196391	-1.266308
8.Ge	0.000000	2.882908	-1.339318
9.Ge	-2.496671	-1.441454	-1.339318
10.Ge	2.072209	1.196391	-1.266308
11.Ge	0.000000	-2.392781	-1.266308
12.Ge	2.496671	-1.441454	-1.339318
13.Pd	0.000000	0.000000	0.000000

D_{2d} Pd@Ge_{12} MS=0

Bond Energy -45.65138710 eV

1.Pd	0.000000	0.000000	0.000000
2.Ge	-0.900854	-0.900854	2.665287
3.Ge	0.581364	-2.522445	1.189917
4.Ge	-2.522445	0.581364	1.189917
5.Ge	-2.522445	-0.581364	-1.189917
6.Ge	0.581364	2.522445	-1.189917
7.Ge	-0.900854	0.900854	-2.665287
8.Ge	2.522445	-0.581364	1.189917
9.Ge	-0.581364	-2.522445	-1.189917
10.Ge	0.900854	0.900854	2.665287
11.Ge	0.900854	-0.900854	-2.665287
12.Ge	-0.581364	2.522445	1.189917
13.Ge	2.522445	0.581364	-1.189917

C_2 Pd@Ge_{12} MS=0

Bond Energy -45.79434111 eV

1.Pd	0.000000	0.000000	-0.000001
2.Ge	-0.667499	-1.131012	2.559805
3.Ge	0.582464	-2.685639	0.898996
4.Ge	-2.393239	0.685000	1.468446
5.Ge	-2.685575	-0.582421	-0.898987

6.Ge	0.684999	2.393270	-1.468434
7.Ge	-1.130982	0.667546	-2.559824
8.Ge	2.393239	-0.685000	1.468446
9.Ge	-0.684999	-2.393270	-1.468434
10.Ge	0.667499	1.131012	2.559805
11.Ge	1.130982	-0.667546	-2.559824
12.Ge	-0.582464	2.685639	0.898996
13.Ge	2.685575	0.582421	-0.898987

I_h $Ag@Ge_{12}$ MS=1/2

Bond Energy -43.68053624 eV

1.Ag	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.849251
5.Ge	-2.548337	0.000000	-1.274444
6.Ge	-0.787480	-2.423613	-1.274444
7.Ge	-0.787480	2.423613	-1.274444
8.Ge	2.061648	-1.497875	-1.274444
9.Ge	2.061648	1.497875	-1.274444
10.Ge.1	0.000000	0.000000	2.849251
12.Ge	2.548337	0.000000	1.274444
13.Ge	-2.061648	1.497875	1.274444
14.Ge	-2.061648	-1.497875	1.274444
15.Ge	0.787480	2.423613	1.274444
16.Ge	0.787480	-2.423613	1.274444

D_{6h} $Ag@Ge_{12}$ MS=1/2

Bond Energy -42.95580076 eV

1.Ge	2.332904	1.346903	1.301487
2.Ge	2.332904	-1.346903	1.301487
3.Ge	0.000000	2.693805	1.301487
4.Ge	0.000000	-2.693805	1.301487
5.Ge	-2.332904	1.346903	1.301487
6.Ge	-2.332904	-1.346903	1.301487
7.Ge	2.332904	1.346903	-1.301487
8.Ge	2.332904	-1.346903	-1.301487
9.Ge	0.000000	2.693805	-1.301487
10.Ge	0.000000	-2.693805	-1.301487
11.Ge	-2.332904	1.346903	-1.301487
12.Ge	-2.332904	-1.346903	-1.301487
13.Ag	0.000000	0.000000	0.000000

D_{6d} $Ag@Ge_{12}$ MS=1/2

Bond Energy -43.30972340 eV

1.Ag	0.000000	0.000000	0.000000
2.Ge	-0.713354	-2.662275	-1.235062
3.Ge	1.948920	-1.948920	-1.235062
4.Ge	-2.662275	-0.713354	-1.235062
5.Ge	2.662275	0.713354	-1.235062
6.Ge	-1.948920	1.948920	-1.235062
7.Ge	0.713354	2.662275	-1.235062
8.Ge	0.713354	-2.662275	1.235062
9.Ge	2.662275	-0.713354	1.235062
10.Ge	-1.948920	-1.948920	1.235062
11.Ge	1.948920	1.948920	1.235062
12.Ge	-2.662275	0.713354	1.235062
13.Ge	-0.713354	2.662275	1.235062

D_{3d} $Ag@Ge_{12}$ MS=1/2

Bond Energy -43.48316148 eV

1.Ge	-2.463252	1.422159	1.516435
2.Ge	0.000000	2.536323	1.102754
3.Ge	-2.196520	-1.268162	1.102754
4.Ge	2.463252	1.422159	1.516435
5.Ge	0.000000	-2.844318	1.516435
6.Ge	2.196520	-1.268162	1.102754
7.Ge	-2.196520	1.268162	-1.102754
8.Ge	0.000000	2.844318	-1.516435
9.Ge	-2.463252	-1.422159	-1.516435
10.Ge	2.196520	1.268162	-1.102754
11.Ge	0.000000	-2.536323	-1.102754
12.Ge	2.463252	-1.422159	-1.516435
13.Ag	0.000000	0.000000	0.000000

D_{2d} $Ag@Ge_{12}$ MS=1/2

Bond Energy -43.56341872 eV

1.Ag	0.000000	0.000000	0.000000
2.Ge	-0.917641	-0.917641	2.604341
3.Ge	0.611094	-2.611500	1.201060
4.Ge	-2.611500	0.611094	1.201060
5.Ge	-2.611500	-0.611094	-1.201060
6.Ge	0.611094	2.611500	-1.201060
7.Ge	-0.917641	0.917641	-2.604341
8.Ge	2.611500	-0.611094	1.201060
9.Ge	-0.611094	-2.611500	-1.201060
10.Ge	0.917641	0.917641	2.604341
11.Ge	0.917641	-0.917641	-2.604341
12.Ge	-0.611094	2.611500	1.201060
13.Ge	2.611500	0.611094	-1.201060

D_{5d} $Ag@Ge_{12}$ MS=1/2

Bond Energy -43.77742101 eV

1.Ge	1.513957	2.083783	1.273749
2.Ge	2.449634	-0.795934	1.273749
3.Ge	-1.513957	2.083783	1.273749
4.Ge	-2.449634	-0.795934	1.273749
5.Ge	0.000000	-2.575697	1.273749
6.Ge	1.513957	-2.083783	-1.273749
7.Ge	-1.513957	-2.083783	-1.273749
8.Ge	2.449634	0.795934	-1.273749
9.Ge	0.000000	2.575697	-1.273749
10.Ge	-2.449634	0.795934	-1.273749
11.Ag	0.000000	0.000000	0.000000
12.Ge	0.000000	0.000000	2.732082
13.Ge	0.000000	0.000000	-2.732082

I_h $Cd@Ge_{12}$ MS=0

Bond Energy -42.61588077 eV

1.Cd	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.884035
5.Ge	-2.579448	0.000000	-1.290003
6.Ge	-0.797093	-2.453201	-1.290003
7.Ge	-0.797093	2.453201	-1.290003
8.Ge	2.086817	-1.516162	-1.290003
9.Ge	2.086817	1.516162	-1.290003
10.Ge.1	0.000000	0.000000	2.884035

12.Ge	2.579448	0.000000	1.290003
13.Ge	-2.086817	1.516162	1.290003
14.Ge	-2.086817	-1.516162	1.290003
15.Ge	0.797093	2.453201	1.290003
16.Ge	0.797093	-2.453201	1.290003

D_{6d} $Cd@Ge_{12}$ MS=0

Bond Energy -41.78923319 eV

1.Cd	0.000000	0.000000	0.000000
2.Ge	-0.725784	-2.708663	-1.236206
3.Ge	1.982879	-1.982879	-1.236206
4.Ge	-2.708663	-0.725784	-1.236206
5.Ge	2.708663	0.725784	-1.236206
6.Ge	-1.982879	1.982879	-1.236206
7.Ge	0.725784	2.708663	-1.236206
8.Ge	0.725784	-2.708663	1.236206
9.Ge	2.708663	-0.725784	1.236206
10.Ge	-1.982879	-1.982879	1.236206
11.Ge	1.982879	1.982879	1.236206
12.Ge	-2.708663	0.725784	1.236206
13.Ge	-0.725784	2.708663	1.236206

D_{6h} $Cd@Ge_{12}$ MS=0

Bond Energy -41.08322348 eV

1.Ge	2.372779	1.369924	1.305741
2.Ge	2.372779	-1.369924	1.305741
3.Ge	0.000000	2.739849	1.305741
4.Ge	0.000000	-2.739849	1.305741
5.Ge	-2.372779	1.369924	1.305741
6.Ge	-2.372779	-1.369924	1.305741
7.Ge	2.372779	1.369924	-1.305741
8.Ge	2.372779	-1.369924	-1.305741
9.Ge	0.000000	2.739849	-1.305741
10.Ge	0.000000	-2.739849	-1.305741
11.Ge	-2.372779	1.369924	-1.305741
12.Ge	-2.372779	-1.369924	-1.305741
13.Cd	0.000000	0.000000	0.000000

D_{3d} $Cd@Ge_{12}$ MS=0

Bond Energy -41.92021214 eV

1.Ge	-2.412613	1.392923	1.652394
2.Ge	0.000000	2.636374	1.007630
3.Ge	-2.283167	-1.318187	1.007630
4.Ge	2.412613	1.392923	1.652394
5.Ge	0.000000	-2.785845	1.652394
6.Ge	2.283167	-1.318187	1.007630
7.Ge	-2.283167	1.318187	-1.007630
8.Ge	0.000000	2.785845	-1.652394
9.Ge	-2.412613	-1.392923	-1.652394
10.Ge	2.283167	1.318187	-1.007630
11.Ge	0.000000	-2.636374	-1.007630
12.Ge	2.412613	-1.392923	-1.652394
13.Cd	0.000000	0.000000	0.000000

$[M@Ge_{12}]^{3-}$ (Figure 2(d))

I_h $[Rh@Ge_{12}]^{3-}$ MS=0

Bond Energy -60.98370180 eV

1.Rh	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.788084
5.Ge	-2.493630	0.000000	-1.247084
6.Ge	-0.770574	-2.371583	-1.247084
7.Ge	-0.770574	2.371583	-1.247084
8.Ge	2.017389	-1.465719	-1.247084
9.Ge	2.017389	1.465719	-1.247084
10.Ge.1	0.000000	0.000000	2.788084
12.Ge	2.493630	0.000000	1.247084
13.Ge	-2.017389	1.465719	1.247084
14.Ge	-2.017389	-1.465719	1.247084
15.Ge	0.770574	2.371583	1.247084
16.Ge	0.770574	-2.371583	1.247084

D_{6h} $[Rh@Ge_{12}]^{3-}$ MS=0

Bond Energy -58.92507094 eV

1.Ge	2.299006	1.327332	1.281646
2.Ge	2.299006	-1.327332	1.281646
3.Ge	0.000000	2.654663	1.281646
4.Ge	0.000000	-2.654663	1.281646
5.Ge	-2.299006	1.327332	1.281646
6.Ge	-2.299006	-1.327332	1.281646
7.Ge	2.299006	1.327332	-1.281646
8.Ge	2.299006	-1.327332	-1.281646
9.Ge	0.000000	2.654663	-1.281646
10.Ge	0.000000	-2.654663	-1.281646
11.Ge	-2.299006	1.327332	-1.281646
12.Ge	-2.299006	-1.327332	-1.281646
13.Rh	0.000000	0.000000	0.000000

D_{6d} $[Rh@Ge_{12}]^{3-}$ MS=0

Bond Energy -59.49248649 eV

1.Rh	0.000000	0.000000	0.000000
2.Ge	-0.703050	-2.623817	-1.208263
3.Ge	1.920768	-1.920768	-1.208263
4.Ge	-2.623817	-0.703050	-1.208263
5.Ge	2.623817	0.703050	-1.208263
6.Ge	-1.920768	1.920768	-1.208263
7.Ge	0.703050	2.623817	-1.208263
8.Ge	0.703050	-2.623817	1.208263
9.Ge	2.623817	-0.703050	1.208263
10.Ge	-1.920768	-1.920768	1.208263
11.Ge	1.920768	1.920768	1.208263
12.Ge	-2.623817	0.703050	1.208263
13.Ge	-0.703050	2.623817	1.208263

D_{3d} $[Rh@Ge_{12}]^{3-}$ MS=0

Bond Energy -59.60223198 eV

1.Ge	-2.352389	1.358153	1.626704
2.Ge	0.000000	2.532334	0.979071
3.Ge	-2.193066	-1.266167	0.979071
4.Ge	2.352389	1.358153	1.626704
5.Ge	0.000000	-2.716305	1.626704
6.Ge	2.193066	-1.266167	0.979071
7.Ge	-2.193066	1.266167	-0.979071
8.Ge	0.000000	2.716305	-1.626704
9.Ge	-2.352389	-1.358153	-1.626704
10.Ge	2.193066	1.266167	-0.979071

11.Ge	0.000000	-2.532334	-0.979071
12.Ge	2.352389	-1.358153	-1.626704
13.Rh	0.000000	0.000000	0.000000

D_{2d} $[Rh@Ge_{12}]^{3-}$ MS=0

Bond Energy -61.35565711 eV

1.Rh	0.000000	0.000000	0.000000
2.Ge	-0.924134	-0.924134	2.509722
3.Ge	0.601693	-2.586468	1.155072
4.Ge	-2.586468	0.601693	1.155072
5.Ge	-2.586468	-0.601693	-1.155072
6.Ge	0.601693	2.586468	-1.155072
7.Ge	-0.924134	0.924134	-2.509722
8.Ge	2.586468	-0.601693	1.155072
9.Ge	-0.601693	-2.586468	-1.155072
10.Ge	0.924134	0.924134	2.509722
11.Ge	0.924134	-0.924134	-2.509722
12.Ge	-0.601693	2.586468	1.155072
13.Ge	2.586468	0.601693	-1.155072

I_h $[Ru@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -61.33131095 eV

1.Ru	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.784274
5.Ge	-2.490223	0.000000	-1.245380
6.Ge	-0.769521	-2.368343	-1.245380
7.Ge	-0.769521	2.368343	-1.245380
8.Ge	2.014633	-1.463716	-1.245380
9.Ge	2.014633	1.463716	-1.245380
10.Ge.1	0.000000	0.000000	2.784274
12.Ge	2.490223	0.000000	1.245380
13.Ge	-2.014633	1.463716	1.245380
14.Ge	-2.014633	-1.463716	1.245380
15.Ge	0.769521	2.368343	1.245380
16.Ge	0.769521	-2.368343	1.245380

D_{6h} $[Ru@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -60.12700694 eV

1.Ge	2.279630	1.316145	1.286700
2.Ge	2.279630	-1.316145	1.286700
3.Ge	0.000000	2.632290	1.286700
4.Ge	0.000000	-2.632290	1.286700
5.Ge	-2.279630	1.316145	1.286700
6.Ge	-2.279630	-1.316145	1.286700
7.Ge	2.279630	1.316145	-1.286700
8.Ge	2.279630	-1.316145	-1.286700
9.Ge	0.000000	2.632290	-1.286700
10.Ge	0.000000	-2.632290	-1.286700
11.Ge	-2.279630	1.316145	-1.286700
12.Ge	-2.279630	-1.316145	-1.286700
13.Ru	0.000000	0.000000	0.000000

D_{6d} $[Ru@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -60.64510422 eV

1.Ru	0.000000	0.000000	0.000000
2.Ge	-0.695739	-2.596533	-1.218065
3.Ge	1.900794	-1.900794	-1.218065
4.Ge	-2.596533	-0.695739	-1.218065

5.Ge	2.596533	0.695739	-1.218065
6.Ge	-1.900794	1.900794	-1.218065
7.Ge	0.695739	2.596533	-1.218065
8.Ge	0.695739	-2.596533	1.218065
9.Ge	2.596533	-0.695739	1.218065
10.Ge	-1.900794	-1.900794	1.218065
11.Ge	1.900794	1.900794	1.218065
12.Ge	-2.596533	0.695739	1.218065
13.Ge	-0.695739	2.596533	1.218065

D_{3d} $[Ru@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -60.28277460 eV

1.Ge	-2.480825	1.432305	1.316481
2.Ge	0.000000	2.404404	1.250369
3.Ge	-2.082275	-1.202202	1.250369
4.Ge	2.480825	1.432305	1.316481
5.Ge	0.000000	-2.864610	1.316481
6.Ge	2.082275	-1.202202	1.250369
7.Ge	-2.082275	1.202202	-1.250369
8.Ge	0.000000	2.864610	-1.316481
9.Ge	-2.480825	-1.432305	-1.316481
10.Ge	2.082275	1.202202	-1.250369
11.Ge	0.000000	-2.404404	-1.250369
12.Ge	2.480825	-1.432305	-1.316481
13.Ru	0.000000	0.000000	0.000000

D_{2d} $[Ru@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -62.75486768 eV

1.Ru	0.000000	0.000000	0.000000
2.Ge	-0.912701	-0.912701	2.612833
3.Ge	0.579170	-2.513781	1.162469
4.Ge	-2.513781	0.579170	1.162469
5.Ge	-2.513781	-0.579170	-1.162469
6.Ge	0.579170	2.513781	-1.162469
7.Ge	-0.912701	0.912701	-2.612833
8.Ge	2.513781	-0.579170	1.162469
9.Ge	-0.579170	-2.513781	-1.162469
10.Ge	0.912701	0.912701	2.612833
11.Ge	0.912701	-0.912701	-2.612833
12.Ge	-0.579170	2.513781	1.162469
13.Ge	2.513781	0.579170	-1.162469

I_h $[Tc@Ge_{12}]^{3-}$ MS=1

Bond Energy -62.87822950 eV

1.Tc	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.796774
5.Ge	-2.501403	0.000000	-1.250972
6.Ge	-0.772976	-2.378976	-1.250972
7.Ge	-0.772976	2.378976	-1.250972
8.Ge	2.023677	-1.470288	-1.250972
9.Ge	2.023677	1.470288	-1.250972
10.Ge.1	0.000000	0.000000	2.796774
12.Ge	2.501403	0.000000	1.250972
13.Ge	-2.023677	1.470288	1.250972
14.Ge	-2.023677	-1.470288	1.250972
15.Ge	0.772976	2.378976	1.250972
16.Ge	0.772976	-2.378976	1.250972

D_{6h} $[Tc@Ge_{12}]^{3-}$ MS=0

Bond Energy -62.40877066 eV

1.Ge	2.285543	1.319559	1.312459
2.Ge	2.285543	-1.319559	1.312459
3.Ge	0.000000	2.639117	1.312459
4.Ge	0.000000	-2.639117	1.312459
5.Ge	-2.285543	1.319559	1.312459
6.Ge	-2.285543	-1.319559	1.312459
7.Ge	2.285543	1.319559	-1.312459
8.Ge	2.285543	-1.319559	-1.312459
9.Ge	0.000000	2.639117	-1.312459
10.Ge	0.000000	-2.639117	-1.312459
11.Ge	-2.285543	1.319559	-1.312459
12.Ge	-2.285543	-1.319559	-1.312459
13.Tc	0.000000	0.000000	0.000000

D_{6d} $[Tc@Ge_{12}]^{3-}$ MS=1

Bond Energy -62.97342148 eV

1.Tc	0.000000	0.000000	0.000000
2.Ge	-0.697421	-2.602811	-1.217729
3.Ge	1.905390	-1.905390	-1.217729
4.Ge	-2.602811	-0.697421	-1.217729
5.Ge	2.602811	0.697421	-1.217729
6.Ge	-1.905390	1.905390	-1.217729
7.Ge	0.697421	2.602811	-1.217729
8.Ge	0.697421	-2.602811	1.217729
9.Ge	2.602811	-0.697421	1.217729
10.Ge	-1.905390	-1.905390	1.217729
11.Ge	1.905390	1.905390	1.217729
12.Ge	-2.602811	0.697421	1.217729
13.Ge	-0.697421	2.602811	1.217729

D_{3d} $[Tc@Ge_{12}$3- MS=0

Bond Energy -62.57147015 eV

1.Ge	-2.455481	1.417672	1.056652
2.Ge	0.000000	2.288732	1.540832
3.Ge	-1.982100	-1.144366	1.540832
4.Ge	2.455481	1.417672	1.056652
5.Ge	0.000000	-2.835345	1.056652
6.Ge	1.982100	-1.144366	1.540832
7.Ge	-1.982100	1.144366	-1.540832
8.Ge	0.000000	2.835345	-1.056652
9.Ge	-2.455481	-1.417672	-1.056652
10.Ge	1.982100	1.144366	-1.540832
11.Ge	0.000000	-2.288732	-1.540832
12.Ge	2.455481	-1.417672	-1.056652
13.Tc	0.000000	0.000000	0.000000

D_{2d} $[Tc@Ge_{12}]^{3-}$ MS=0

Bond Energy -65.05959488 eV

1.Tc	0.000000	0.000000	0.000000
2.Ge	-0.906430	-0.906430	2.714239
3.Ge	0.562450	-2.463806	1.173995
4.Ge	-2.463806	0.562450	1.173995
5.Ge	-2.463806	-0.562450	-1.173995
6.Ge	0.562450	2.463806	-1.173995
7.Ge	-0.906430	0.906430	-2.714239
8.Ge	2.463806	-0.562450	1.173995

9.Ge	-0.562450	-2.463806	-1.173995
10.Ge	0.906430	0.906430	2.714239
11.Ge	0.906430	-0.906430	-2.714239
12.Ge	-0.562450	2.463806	1.173995
13.Ge	2.463806	0.562450	-1.173995

I_h $[Mo@Ge_{12}]^{3-}$ MS=3/2

Bond Energy -60.92326263 eV

1.Mo	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.821145
5.Ge	-2.523200	0.000000	-1.261872
6.Ge	-0.779712	-2.399706	-1.261872
7.Ge	-0.779712	2.399706	-1.261872
8.Ge	2.041311	-1.483100	-1.261872
9.Ge	2.041311	1.483100	-1.261872
10.Ge.1	0.000000	0.000000	2.821145
12.Ge	2.523200	0.000000	1.261872
13.Ge	-2.041311	1.483100	1.261872
14.Ge	-2.041311	-1.483100	1.261872
15.Ge	0.779712	2.399706	1.261872
16.Ge	0.779712	-2.399706	1.261872

D_{6h} $[Mo@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -61.79212541 eV

1.Ge	2.266699	1.308680	1.351694
2.Ge	2.266699	-1.308680	1.351694
3.Ge	0.000000	2.617359	1.351694
4.Ge	0.000000	-2.617359	1.351694
5.Ge	-2.266699	1.308680	1.351694
6.Ge	-2.266699	-1.308680	1.351694
7.Ge	2.266699	1.308680	-1.351694
8.Ge	2.266699	-1.308680	-1.351694
9.Ge	0.000000	2.617359	-1.351694
10.Ge	0.000000	-2.617359	-1.351694
11.Ge	-2.266699	1.308680	-1.351694
12.Ge	-2.266699	-1.308680	-1.351694
13.Mo	0.000000	0.000000	0.000000

D_{6d} $[Mo@Ge_{12}$3- MS=1/2

Bond Energy -62.09152785 eV

1.Mo	0.000000	0.000000	0.000000
2.Ge	-0.693942	-2.589825	-1.238957
3.Ge	1.895884	-1.895884	-1.238957
4.Ge	-2.589825	-0.693942	-1.238957
5.Ge	2.589825	0.693942	-1.238957
6.Ge	-1.895884	1.895884	-1.238957
7.Ge	0.693942	2.589825	-1.238957
8.Ge	0.693942	-2.589825	1.238957
9.Ge	2.589825	-0.693942	1.238957
10.Ge	-1.895884	-1.895884	1.238957
11.Ge	1.895884	1.895884	1.238957
12.Ge	-2.589825	0.693942	1.238957
13.Ge	-0.693942	2.589825	1.238957

D_{3d} $[Mo@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -61.65726149 eV

1.Ge	-2.270187	1.310693	1.356863
2.Ge	0.000000	2.607799	1.347349

3.Ge	-2.258420	-1.303900	1.347349
4.Ge	2.270187	1.310693	1.356863
5.Ge	0.000000	-2.621386	1.356863
6.Ge	2.258420	-1.303900	1.347349
7.Ge	-2.258420	1.303900	-1.347349
8.Ge	0.000000	2.621386	-1.356863
9.Ge	-2.270187	-1.310693	-1.356863
10.Ge	2.258420	1.303900	-1.347349
11.Ge	0.000000	-2.607799	-1.347349
12.Ge	2.270187	-1.310693	-1.356863
13.Mo	0.000000	0.000000	0.000000

D_{2d} $[Mo@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -63.31548232 eV

1.Mo	0.000000	0.000000	0.000000
2.Ge	-0.908283	-0.908283	2.729709
3.Ge	0.551644	-2.491264	1.191563
4.Ge	-2.491264	0.551644	1.191563
5.Ge	-2.491264	-0.551644	-1.191563
6.Ge	0.551644	2.491264	-1.191563
7.Ge	-0.908283	0.908283	-2.729709
8.Ge	2.491264	-0.551644	1.191563
9.Ge	-0.551644	-2.491264	-1.191563
10.Ge	0.908283	0.908283	2.729709
11.Ge	0.908283	-0.908283	-2.729709
12.Ge	-0.551644	2.491264	1.191563
13.Ge	2.491264	0.551644	-1.191563

S_4 [Mo@Ge_{12}3- MS=1/2

Bond Energy -63.50884962 eV

1.Mo	0.000000	0.000000	0.000050
2.Ge	-0.663609	-1.136819	2.692804
3.Ge	0.533318	-2.646047	0.952920
4.Ge	-2.317103	0.621045	1.445523
5.Ge	-2.645874	-0.533276	-0.953460
6.Ge	0.621305	2.317192	-1.445104
7.Ge	-1.136457	0.664418	-2.692716
8.Ge	2.317103	-0.621045	1.445523
9.Ge	-0.621305	-2.317192	-1.445104
10.Ge	0.663609	1.136819	2.692804
11.Ge	1.136457	-0.664418	-2.692716
12.Ge	-0.533318	2.646047	0.952920
13.Ge	2.645874	0.533276	-0.953460

I_h $[Nb@Ge_{12}]^{3-}$ MS=2

Bond Energy -60.04616672 eV

1.Nb	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.855121
5.Ge	-2.553587	0.000000	-1.277069
6.Ge	-0.789102	-2.428606	-1.277069
7.Ge	-0.789102	2.428606	-1.277069
8.Ge	2.065895	-1.500961	-1.277069
9.Ge	2.065895	1.500961	-1.277069
10.Ge.1	0.000000	0.000000	2.855121
12.Ge	2.553587	0.000000	1.277069
13.Ge	-2.065895	1.500961	1.277069
14.Ge	-2.065895	-1.500961	1.277069
15.Ge	0.789102	2.428606	1.277069

16.Ge	0.789102	-2.428606	1.277069

D_{6h} $[Nb@Ge_{12}]^{3-}$ MS=1

Bond Energy -61.80474039 eV

1.Ge	2.278170	1.315302	1.361785
2.Ge	2.278170	-1.315302	1.361785
3.Ge	0.000000	2.630604	1.361785
4.Ge	0.000000	-2.630604	1.361785
5.Ge	-2.278170	1.315302	1.361785
6.Ge	-2.278170	-1.315302	1.361785
7.Ge	2.278170	1.315302	-1.361785
8.Ge	2.278170	-1.315302	-1.361785
9.Ge	0.000000	2.630604	-1.361785
10.Ge	0.000000	-2.630604	-1.361785
11.Ge	-2.278170	1.315302	-1.361785
12.Ge	-2.278170	-1.315302	-1.361785
13.Nb	0.000000	0.000000	0.000000

D_{6d} $[Nb@Ge_{12}]^{3-}$ MS=1

Bond Energy -62.17789737 eV

1.Nb	0.000000	0.000000	0.000000
2.Ge	-0.698746	-2.607754	-1.243400
3.Ge	1.909008	-1.909008	-1.243400
4.Ge	-2.607754	-0.698746	-1.243400
5.Ge	2.607754	0.698746	-1.243400
6.Ge	-1.909008	1.909008	-1.243400
7.Ge	0.698746	2.607754	-1.243400
8.Ge	0.698746	-2.607754	1.243400
9.Ge	2.607754	-0.698746	1.243400
10.Ge	-1.909008	-1.909008	1.243400
11.Ge	1.909008	1.909008	1.243400
12.Ge	-2.607754	0.698746	1.243400
13.Ge	-0.698746	2.607754	1.243400

D_{3d} $[Nb@Ge_{12}]^{3-}$ MS=1

Bond Energy -61.81645844 eV

1.Ge	-2.280252	1.316504	1.366696
2.Ge	0.000000	2.632760	1.360209
3.Ge	-2.280037	-1.316380	1.360209
4.Ge	2.280252	1.316504	1.366696
5.Ge	0.000000	-2.633008	1.366696
6.Ge	2.280037	-1.316380	1.360209
7.Ge	-2.280037	1.316380	-1.360209
8.Ge	0.000000	2.633008	-1.366696
9.Ge	-2.280252	-1.316504	-1.366696
10.Ge	2.280037	1.316380	-1.360209
11.Ge	0.000000	-2.632760	-1.360209
12.Ge	2.280252	-1.316504	-1.366696
13.Nb	0.000000	0.000000	0.000000

D_{2d} $[Nb@Ge_{12}]^{3-}$ MS=0

Bond Energy -62.54317810 eV

1.Nb	0.000000	0.000000	0.000000
2.Ge	-0.914348	-0.914348	2.744659
3.Ge	0.538348	-2.522110	1.208460
4.Ge	-2.522110	0.538348	1.208460
5.Ge	-2.522110	-0.538348	-1.208460
6.Ge	0.538348	2.522110	-1.208460

7.Ge	-0.914348	0.914348	-2.744659
8.Ge	2.522110	-0.538348	1.208460
9.Ge	-0.538348	-2.522110	-1.208460
10.Ge	0.914348	0.914348	2.744659
11.Ge	0.914348	-0.914348	-2.744659
12.Ge	-0.538348	2.522110	1.208460
13.Ge	2.522110	0.538348	-1.208460

S_4 $[Nb@Ge_{12}]^{3-}$ MS=0

Bond Energy -63.01781248 eV

1.Nb	0.000000	0.000000	-0.000401
2.Ge	-0.600356	-1.182446	2.720575
3.Ge	0.513171	-2.707649	0.925545
4.Ge	-2.308897	0.630722	1.498310
5.Ge	-2.706325	-0.517831	-0.924198
6.Ge	0.626851	2.309398	-1.499049
7.Ge	-1.184220	0.599081	-2.720931
8.Ge	2.308897	-0.630722	1.498310
9.Ge	-0.626851	-2.309398	-1.499049
10.Ge	0.600356	1.182446	2.720575
11.Ge	1.184220	-0.599081	-2.720931
12.Ge	-0.513171	2.707649	0.925545
13.Ge	2.706325	0.517831	-0.924198

I_h $[Zr@Ge_{12}]^{3-}$ MS=5/2

Bond Energy -57.61095778 eV

1.Zr	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.901588
5.Ge	-2.595147	0.000000	-1.297854
6.Ge	-0.801945	-2.468132	-1.297854
7.Ge	-0.801945	2.468132	-1.297854
8.Ge	2.099518	-1.525389	-1.297854
9.Ge	2.099518	1.525389	-1.297854
10.Ge.1	0.000000	0.000000	2.901588
12.Ge	2.595147	0.000000	1.297854
13.Ge	-2.099518	1.525389	1.297854
14.Ge	-2.099518	-1.525389	1.297854
15.Ge	0.801945	2.468132	1.297854
16.Ge	0.801945	-2.468132	1.297854

D_{6h} $[Zr@Ge_{12}]^{3-}$ MS=0

Bond Energy -60.54278908 eV

1.Ge	2.302297	1.329232	1.360940
2.Ge	2.302297	-1.329232	1.360940
3.Ge	0.000000	2.658464	1.360940
4.Ge	0.000000	-2.658464	1.360940
5.Ge	-2.302297	1.329232	1.360940
6.Ge	-2.302297	-1.329232	1.360940
7.Ge	2.302297	1.329232	-1.360940
8.Ge	2.302297	-1.329232	-1.360940
9.Ge	0.000000	2.658464	-1.360940
10.Ge	0.000000	-2.658464	-1.360940
11.Ge	-2.302297	1.329232	-1.360940
12.Ge	-2.302297	-1.329232	-1.360940
13.Zr	0.000000	0.000000	0.000000

D_{6d} $[Zr@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -60.89265685 eV

1.Zr	0.000000	0.000000	0.000000
2.Ge	-0.706957	-2.638400	-1.259546
3.Ge	1.931443	-1.931443	-1.259546
4.Ge	-2.638400	-0.706957	-1.259546
5.Ge	2.638400	0.706957	-1.259546
6.Ge	-1.931443	1.931443	-1.259546
7.Ge	0.706957	2.638400	-1.259546
8.Ge	0.706957	-2.638400	1.259546
9.Ge	2.638400	-0.706957	1.259546
10.Ge	-1.931443	-1.931443	1.259546
11.Ge	1.931443	1.931443	1.259546
12.Ge	-2.638400	0.706957	1.259546
13.Ge	-0.706957	2.638400	1.259546

D_{3d} $[Zr@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -60.53178205 eV

1.Ge	-2.315984	1.337134	1.368234
2.Ge	0.000000	2.648147	1.354191
3.Ge	-2.293363	-1.324074	1.354191
4.Ge	2.315984	1.337134	1.368234
5.Ge	0.000000	-2.674268	1.368234
6.Ge	2.293363	-1.324074	1.354191
7.Ge	-2.293363	1.324074	-1.354191
8.Ge	0.000000	2.674268	-1.368234
9.Ge	-2.315984	-1.337134	-1.368234
10.Ge	2.293363	1.324074	-1.354191
11.Ge	0.000000	-2.648147	-1.354191
12.Ge	2.315984	-1.337134	-1.368234
13.Zr	0.000000	0.000000	0.000000

D_{2d} $[Zr@Ge_{12}]^{3-}$ MS=1/2

Bond Energy -59.52238210 eV

1.Zr	0.000000	0.000000	0.000000
2.Ge	-0.920129	-0.920129	2.666372
3.Ge	0.589527	-2.653585	1.189050
4.Ge	-2.653585	0.589527	1.189050
5.Ge	-2.653585	-0.589527	-1.189050
6.Ge	0.589527	2.653585	-1.189050
7.Ge	-0.920129	0.920129	-2.666372
8.Ge	2.653585	-0.589527	1.189050
9.Ge	-0.589527	-2.653585	-1.189050
10.Ge	0.920129	0.920129	2.666372
11.Ge	0.920129	-0.920129	-2.666372
12.Ge	-0.589527	2.653585	1.189050
13.Ge	2.653585	0.589527	-1.189050

I_h $[Y@Ge_{12}]^{3-}$ MS=2

Bond Energy -53.84275076 eV

1.Y	0.000000	0.000000	0.000000
3.Ge	0.000000	0.000000	-2.958534
5.Ge	-2.646079	0.000000	-1.323325
6.Ge	-0.817683	-2.516570	-1.323325
7.Ge	-0.817683	2.516570	-1.323325
8.Ge	2.140723	-1.555326	-1.323325
9.Ge	2.140723	1.555326	-1.323325
10.Ge.1	0.000000	0.000000	2.958534
12.Ge	2.646079	0.000000	1.323325
13.Ge	-2.140723	1.555326	1.323325

14.Ge	-2.140723	-1.555326	1.323325
15.Ge	0.817683	2.516570	1.323325
16.Ge	0.817683	-2.516570	1.323325

D_{6h} $[Y@Ge_{12}]^{3-}$ MS=0

Bond Energy -57.68544841 eV

1.Ge	2.342898	1.352673	1.361605
2.Ge	2.342898	-1.352673	1.361605
3.Ge	0.000000	2.705346	1.361605
4.Ge	0.000000	-2.705346	1.361605
5.Ge	-2.342898	1.352673	1.361605
6.Ge	-2.342898	-1.352673	1.361605
7.Ge	2.342898	1.352673	-1.361605
8.Ge	2.342898	-1.352673	-1.361605
9.Ge	0.000000	2.705346	-1.361605
10.Ge	0.000000	-2.705346	-1.361605
11.Ge	-2.342898	1.352673	-1.361605
12.Ge	-2.342898	-1.352673	-1.361605
13.Y	0.000000	0.000000	0.000000

D_{6d} $[Y@Ge_{12}]^{3-}$ MS=0

Bond Energy -58.30489319 eV

1.Y	0.000000	0.000000	0.000000
2.Ge	-0.722101	-2.694916	-1.271954
3.Ge	1.972816	-1.972816	-1.271954
4.Ge	-2.694916	-0.722101	-1.271954
5.Ge	2.694916	0.722101	-1.271954
6.Ge	-1.972816	1.972816	-1.271954
7.Ge	0.722101	2.694916	-1.271954
8.Ge	0.722101	-2.694916	1.271954
9.Ge	2.694916	-0.722101	1.271954
10.Ge	-1.972816	-1.972816	1.271954
11.Ge	1.972816	1.972816	1.271954
12.Ge	-2.694916	0.722101	1.271954
13.Ge	-0.722101	2.694916	1.271954

D_{3d} $[Y@Ge_{12}]^{3-}$ MS=0

Bond Energy -57.66147779 eV

1.Ge	-2.370037	1.368341	1.402361
2.Ge	0.000000	2.671035	1.317548
3.Ge	-2.313184	-1.335518	1.317548
4.Ge	2.370037	1.368341	1.402361
5.Ge	0.000000	-2.736682	1.402361
6.Ge	2.313184	-1.335518	1.317548
7.Ge	-2.313184	1.335518	-1.317548
8.Ge	0.000000	2.736682	-1.402361
9.Ge	-2.370037	-1.368341	-1.402361
10.Ge	2.313184	1.335518	-1.317548
11.Ge	0.000000	-2.671035	-1.317548
12.Ge	2.370037	-1.368341	-1.402361
13.Y	0.000000	0.000000	0.000000