

Exploring the structure and electronic properties of germanium doped boron clusters using density functional theory based global optimization method

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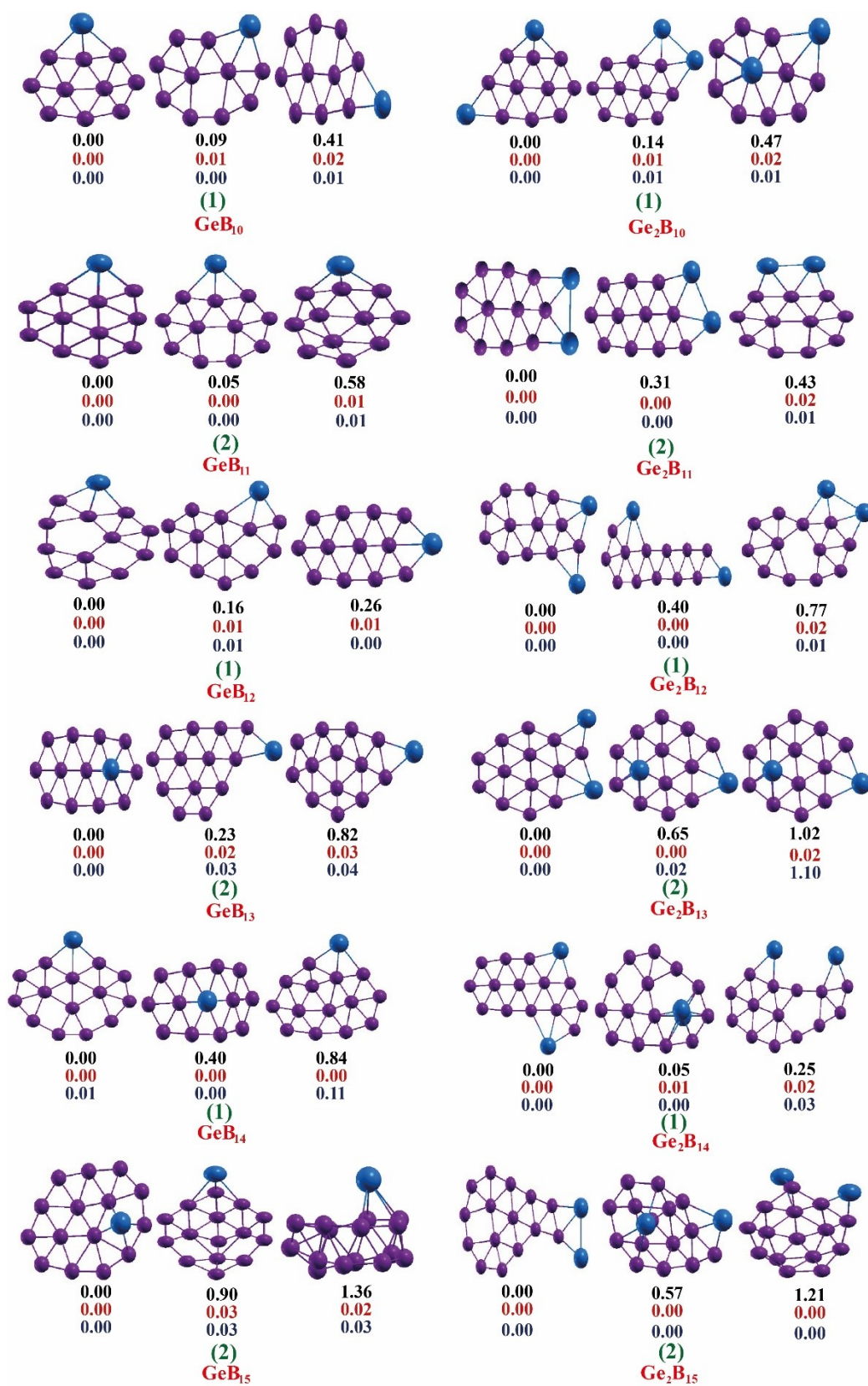


Fig. S1. Optimized geometries of GeB_n and Ge_2B_n ($n=10-15$) along with relative energies in eV computed at B3LYP (black), TPSS (red) and M06-L (light blue) functionals. Spin multiplicity is presented in round brackets. The color scheme is as follows: purple balls for B atoms and blue balls for Ge atoms.

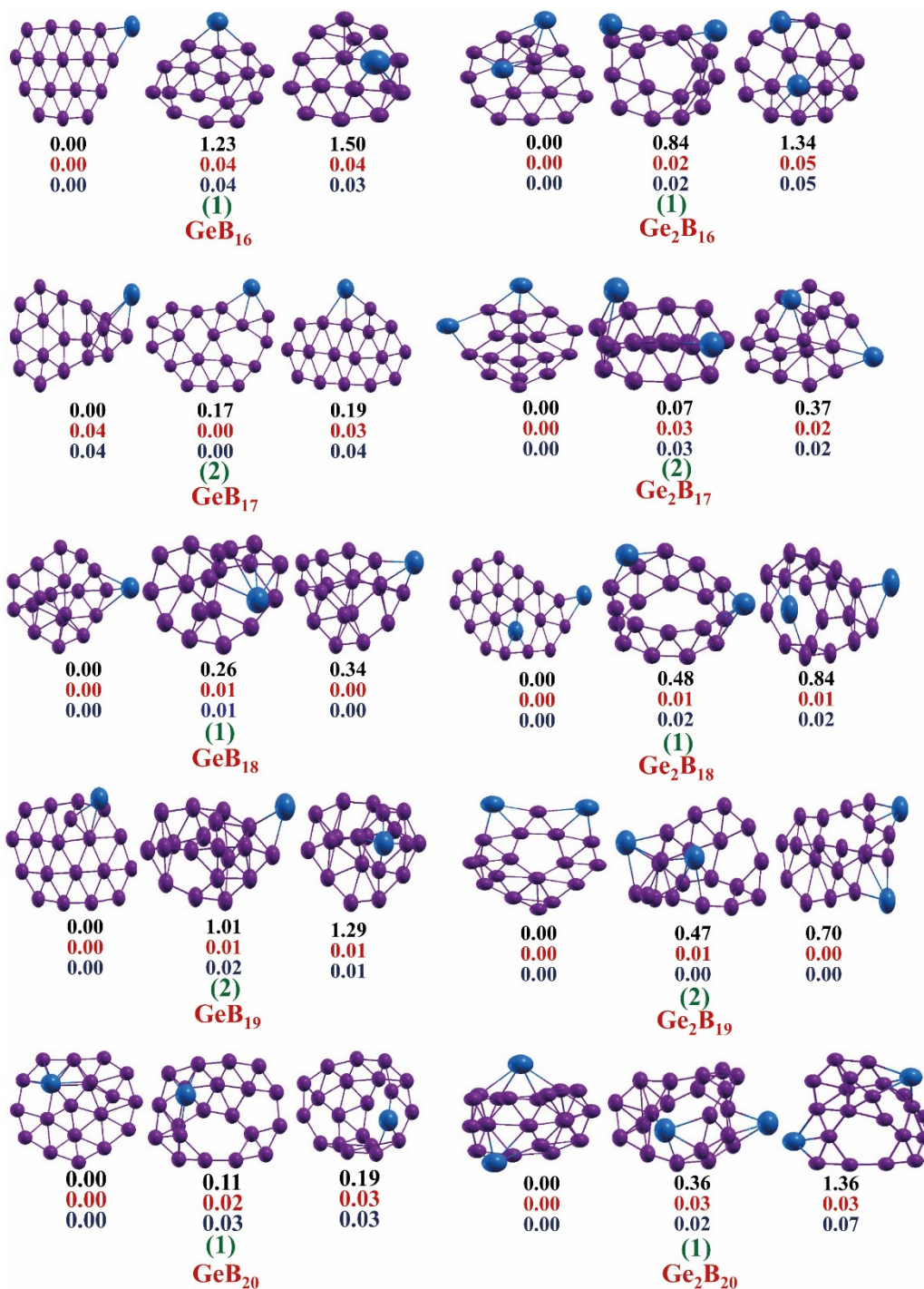


Fig. S2. Optimized geometries of GeB_n and Ge_2B_n ($n=16-20$) along with relative energies in eV computed at B3LYP (black), TPSS (red) and M06-L (light blue) functionals level. Spin multiplicity is presented in round brackets. The color scheme is as follows: purple balls for B atoms and blue balls for Ge atoms.

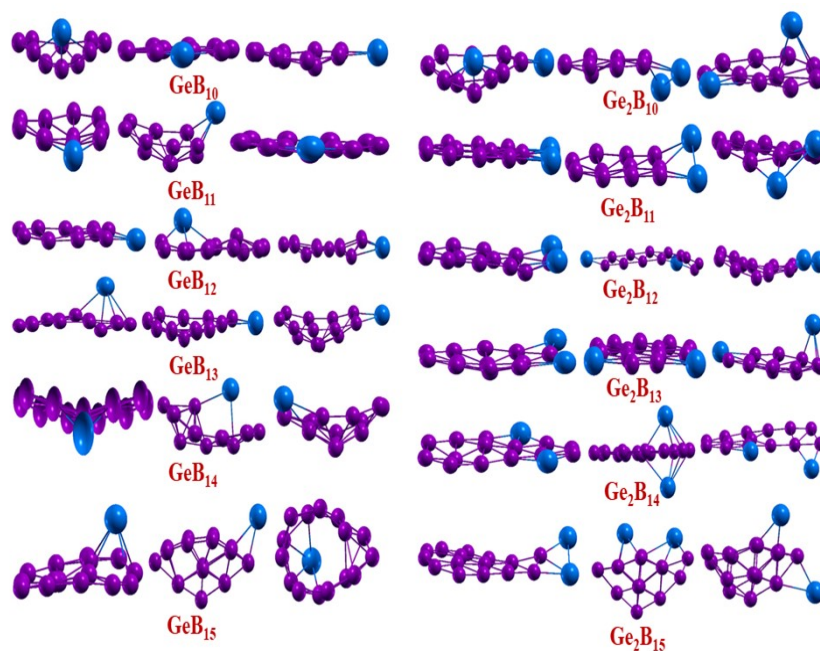


Fig. S3. Side view of low lying optimized geometrical structure of GeB_n and Ge_2B_n ($n=10-15$) computed at B3LYP level.

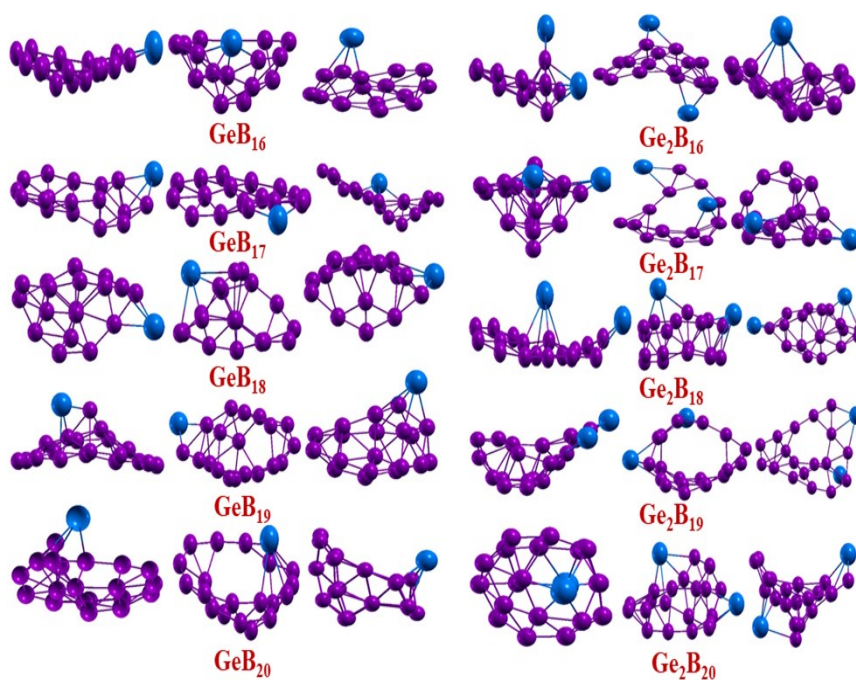


Fig. S4. Side view of low lying optimized geometrical structure of GeB_n and Ge_2B_n ($n=10-15$) computed at B3LYP level.

Table S1. Binding energy per atom (E_b) of GeB_n ($n=10-20$) obtained using B3LYP, TPSS and M06-L functionals in eV.

GeB_n	B3LYP	TPSS	M06-L
GeB_{10}	4.59	5.06	4.74
GeB_{11}	4.59	5.06	4.74
GeB_{12}	4.61	5.09	4.77
GeB_{13}	4.69	5.18	4.86
GeB_{14}	4.69	5.16	4.84
GeB_{15}	4.71	5.20	4.88
GeB_{16}	4.74	5.24	4.91
GeB_{17}	4.69	5.19	4.87
GeB_{18}	4.70	5.21	4.89
GeB_{19}	4.75	5.26	4.93
GeB_{20}	4.74	5.27	4.94

Table S2. Binding energy per atom (E_b) of Ge_2B_n ($n=10-20$) obtained using B3LYP, TPSS and M06-L functionals in eV.

Ge_2B_n	B3LYP	TPSS	M06L
Ge_2B_{10}	4.55	4.72	5.00
Ge_2B_{11}	4.59	4.75	5.00
Ge_2B_{12}	4.60	4.76	5.02
Ge_2B_{13}	4.65	4.82	5.10
Ge_2B_{14}	4.65	4.83	5.10
Ge_2B_{15}	4.68	4.83	5.09
Ge_2B_{16}	4.68	4.91	5.23
Ge_2B_{17}	4.62	4.86	5.20
Ge_2B_{18}	4.73	4.90	5.24
Ge_2B_{19}	4.68	4.87	5.21
Ge_2B_{20}	4.89	4.90	5.22

Table S3. Second difference in binding Energy (Δ^2E) of GeB_n ($n=10-20$) obtained using B3LYP, TPSS and M06-L functionals in eV.

GeB_n	B3LYP	TPSS	M06-L
GeB_{10}	1.03	1.2	1.12
GeB_{11}	-0.31	-0.46	-0.44
GeB_{12}	-0.77	-0.79	-0.86
GeB_{13}	0.91	1.39	1.57
GeB_{14}	-0.27	-0.87	-1.02
GeB_{15}	-0.23	-0.17	0.12
GeB_{16}	1.44	1.64	1.1
GeB_{17}	-1.04	-1.29	-0.92
GeB_{18}	-0.87	-0.54	-0.53
GeB_{19}	1.15	0.63	0.44
GeB_{20}	7.98	8.76	8.69

Table S4. Second difference in binding Energy (Δ^2E) of Ge_2B_n ($n=10-20$) obtained using B3LYP, TPSS and M06-L functionals in eV.

Ge_2B_n	B3LYP	TPSS	M06-L
Ge_2B_{10}	0.43	0.77	1.33
Ge_2B_{11}	0.42	0.06	-0.34
Ge_2B_{12}	-0.60	-0.67	-0.75
Ge_2B_{13}	0.68	0.78	1.08
Ge_2B_{14}	-0.58	2.50	2.46
Ge_2B_{15}	0.48	-1.21	-2.52
Ge_2B_{16}	1.16	4.70	5.17
Ge_2B_{17}	-3.07	-1.58	-1.13
Ge_2B_{18}	2.83	1.34	1.28
Ge_2B_{19}	-0.65	-1.19	-0.98
Ge_2B_{20}	-0.91	0.05	-0.76

Table S5. Vertical ionization potential (VIP)) of GeB_n ($n=10-20$) obtained using B3LYP, TPSS, and M06-L functionals in eV.

GeB_n	B3LYP	TPSS	M06L
GeB_{10}	8.36	8.233	8.234
GeB_{11}	7.22	7.24	7.23
GeB_{12}	7.85	7.92	7.94
GeB_{13}	7.62	7.59	7.57
GeB_{14}	7.81	7.88	7.84
GeB_{15}	7.45	7.55	7.52
GeB_{16}	7.75	7.76	7.72
GeB_{17}	7.38	7.5	7.47
GeB_{18}	7.69	7.737	7.745
GeB_{19}	7.36	7.34	7.30
GeB_{20}	7.61	7.64	7.61

Table S6. Vertical ionization potential (VIP)) of Ge_2B_n ($n=10-20$) obtained using B3LYP, TPSS, and M06-L functionals in eV.

Ge_2B_n	B3LYP	TPSS	M06L
Ge_2B_{10}	7.77	7.79	7.73
Ge_2B_{11}	7.34	7.44	7.36
Ge_2B_{12}	7.36	7.6.0	7.62
Ge_2B_{13}	6.94	7.05	6.95
Ge_2B_{14}	7.26	7.28	7.24
Ge_2B_{15}	6.80	6.86	6.76
Ge_2B_{16}	7.68	7.59	7.47
Ge_2B_{17}	7.32	7.32	7.32
Ge_2B_{18}	7.53	7.51	7.64
Ge_2B_{19}	6.65	6.78	6.49
Ge_2B_{20}	6.81	7.04	6.93

Table S7. Vertical electron affinity (VEA) of GeB_n ($n=10-20$) obtained using B3LYP, TPSS and M06-L functionals in eV.

GeB_n	B3LYP	TPSS	M06-L
GeB_{10}	1.90	2.01	1.96
GeB_{11}	2.45	2.51	2.47
GeB_{12}	2.63	2.49	2.39
GeB_{13}	2.76	2.85	2.79
GeB_{14}	2.85	2.95	2.88
GeB_{15}	3.15	3.24	3.18
GeB_{16}	3.02	3.01	2.98
GeB_{17}	3.15	3.34	3.27
GeB_{18}	2.41	2.61	2.56
GeB_{19}	3.28	3.28	3.21
GeB_{20}	2.64	2.65	2.58

Table S8. Vertical electron affinity (VEA) of Ge_2B_n ($n=10-20$) obtained using B3LYP, TPSS and M06-L functionals in eV.

Ge_2B_n	B3LYP	TPSS	M06-L
Ge_2B_{10}	2.14	2.14	1.92
Ge_2B_{11}	3.02	3.12	3.08
Ge_2B_{12}	2.82	2.56	2.38
Ge_2B_{13}	2.80	2.90	2.83
Ge_2B_{14}	2.60	2.58	2.41
Ge_2B_{15}	2.89	2.95	2.83
Ge_2B_{16}	2.30	2.04	1.89
Ge_2B_{17}	3.21	3.23	3.03
Ge_2B_{18}	2.89	2.94	2.55
Ge_2B_{19}	2.70	2.69	2.53
Ge_2B_{20}	2.35	2.11	1.98

Table S9. Calculated relative electrophilicity and nucleophilicity indices of GeB_n clusters to predict the most reactive sites.

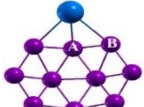
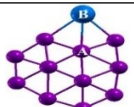
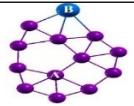
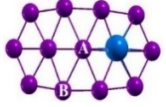
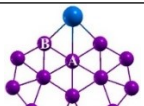
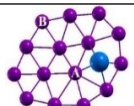
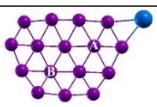
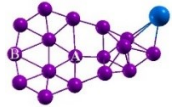
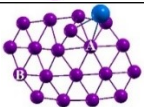
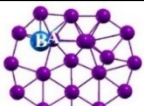
Cluster	Structure	Sites	f_k^{elc}	f_k^{nu}
GeB_{10}		A	1.70	0.59
		B	0.66	1.50
GeB_{11}		A	0.82	1.22
		B	1.09	0.91
GeB_{12}		A	0.31	3.24
		B	1.40	0.71
GeB_{13}		A	0.22	4.64
		B	1.07	0.94
GeB_{14}		A	0.04	23.42
		B	2.34	0.43
GeB_{15}		A	0.80	1.25
		B	1.06	0.94
GeB_{16}		A	1.81	0.55
		B	0.60	1.68
GeB_{17}		A	1.52	0.66
		B	0.77	1.29
GeB_{18}		A	0.38	2.60
		B	2.34	0.43
GeB_{19}		A	0.72	1.40
		B	1.22	0.82
GeB_{20}		A	0.32	3.10
		B	2.37	0.42

Table S10. Calculated relative electrophilicity and nucleophilicity indices of Ge_2B_n clusters to predict the most reactive sites using B3LYP functional.

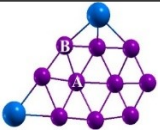
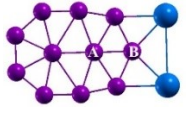
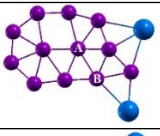
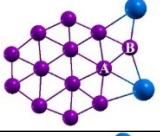
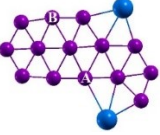
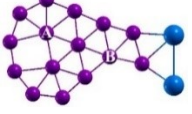
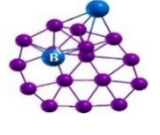
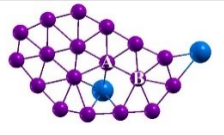
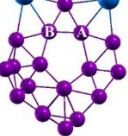
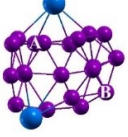
Cluster	Structure	Sites	f^{elc}	f^{nu}
Ge_2B_{10}		A	2.31	0.43
		B	0.55	1.82
Ge_2B_{11}		A	0.80	1.25
		B	1.11	0.93
Ge_2B_{12}		A	0.15	6.70
		B	1.50	0.67
Ge_2B_{13}		A	1.13	0.89
		B	0.90	1.11
Ge_2B_{14}		A	2.54	0.39
		B	0.62	1.60
Ge_2B_{15}		A	0.70	1.40
		B	1.37	0.73
Ge_2B_{16}		A	0.29	3.49
		B	2.06	0.48
Ge_2B_{17}		A	0.74	1.36
		B	1.31	0.76
Ge_2B_{18}		A	5.11	0.20
		B	0.40	2.53
Ge_2B_{19}		A	2.02	0.49
		B	0.64	1.56
Ge_2B_{20}		A	1.99	0.78
		B	0.65	1.54

Table S11. Calculated relative electrophilicity and nucleophilicity indices of B_{16} and B_{20} clusters to predict the most reactive sites using B3LYP functional.

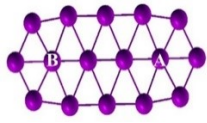
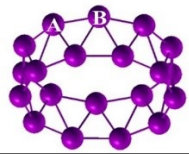
Cluster	Structure	Sites	f^{elc}	f^{nu}
B_{16}		A	1.09	0.91
		B	0.73	1.38
B_{20}		A	1.59	0.63
		B	0.56	1.77

Table S12. Calculated relative electrophilicity and nucleophilicity indices of GeB_{20} cluster to predict the most reactive sites using TPSS functional.

Cluster	Structure	Sites	TPSS		B3LYP	
			f^{elc}	f^{nu}	f^{elc}	f^{nu}
GeB_{20}		A	0.40	2.48	0.32	3.10
		B	2.10	1.45	2.37	0.42

Table S13. Minimum vibrational frequency of the first three lowest energy isomers of GeB_n and Ge_2B_n clusters ($n=10-20$).

Cluster	Minimum vibrational frequency (cm^{-1})	Cluster	Minimum vibrational frequency (cm^{-1})
GeB_{10}	119, 96, 49	Ge_2B_{10}	71, 64, 44
GeB_{11}	118, 36, 98	Ge_2B_{11}	55, 58, 57
GeB_{12}	62, 73, 66	Ge_2B_{12}	61, 37, 22
GeB_{13}	66, 57, 62	Ge_2B_{13}	58, 41, 31
GeB_{14}	62, 102, 90	Ge_2B_{14}	48, 27, 23
GeB_{15}	71, 52, 89	Ge_2B_{15}	28, 55, 42
GeB_{16}	47, 85, 50	Ge_2B_{16}	20, 35, 36
GeB_{17}	37, 49, 57	Ge_2B_{17}	83, 31, 90
GeB_{18}	73, 85, 74	Ge_2B_{18}	28, 49, 63
GeB_{19}	78, 50, 109	Ge_2B_{19}	65, 50, 43
GeB_{20}	49, 61, 57	Ge_2B_{20}	74, 63, 56

Cartesian coordinates of first three lowest energy isomers of GeB_n clusters (n=10-20)

GeB₁₀

11

scf done: -2325.416817

Ge	7.197013	8.293269	10.832114
B	8.178436	6.593898	9.777301
B	7.225148	8.613495	6.309530
B	9.343493	6.502501	7.261502
B	7.918458	6.512002	8.081143
B	6.283191	9.200953	7.390054
B	8.281340	7.425834	6.499093
B	6.769462	7.654797	7.565148
B	9.350266	6.145454	8.768942
B	6.172227	8.590820	8.875454
B	6.779532	7.118531	9.157475

11

scf done: -2325.413343

Ge	9.010889	6.039466	6.045521
B	6.947953	7.642908	10.726061
B	7.646007	6.249655	7.666299
B	6.380997	6.069847	8.509821
B	10.409561	8.072424	8.306273
B	10.313341	7.282043	7.017083
B	7.627312	7.119937	9.197137
B	8.326458	8.235796	10.497850

11

scf done: -2325.401469

Ge	6.046925	7.578340	7.050158
B	10.658517	6.777556	7.348104
B	11.222313	7.661134	6.031836
B	7.701437	6.781410	8.193632
B	8.039695	7.570117	6.621471
B	9.057758	6.547938	7.375583
B	9.655776	7.548527	6.149544
B	11.864026	6.348182	8.418042
B	12.242952	7.148806	7.115679
B	10.436264	6.011004	8.990730
B	8.876660	6.178351	9.065175
B	9.549706	8.342361	9.564433
B	8.988509	7.155809	8.013334

B 6.070081 6.692994 9.876584

GeB₁₁

12

scf done: -2350.248926

Ge	6.077197	7.713080	7.201530
B	11.101640	8.388004	6.293114
B	8.075382	8.570890	6.972085
B	9.416061	6.104404	6.526781
B	9.666872	10.806200	6.042595
B	6.810751	9.550536	6.643810
B	10.793280	6.806862	6.355979
B	9.629900	9.352920	6.776880
B	8.022231	6.843308	6.800255
B	8.175631	10.334153	6.421658
B	9.488747	7.693456	6.865747
B	10.957752	9.948758	6.007682

12

scf done: -2350.250876

Ge	9.191793	5.959453	5.578697
B	9.410750	10.235170	8.737130
B	6.676336	9.807060	7.542043
B	8.887291	7.417550	6.989428
B	10.461807	7.255877	7.047992
B	7.483592	7.451260	6.259233
B	9.661903	8.585324	7.882443
B	11.306949	8.265868	7.916928
B	6.450395	8.581121	6.621590
B	7.905398	10.335090	8.340508
B	7.922485	8.702600	7.419723

12

scf done: -2350.227751

Ge	7.776475	9.445639	9.778340
B	9.872642	7.466758	7.599833
B	9.441849	8.785874	8.310046
B	6.660786	9.446405	7.918710
B	8.910713	8.479739	6.718930
B	6.136513	6.787438	6.408405
B	8.905892	6.606654	6.715900
B	7.411978	9.259122	6.425890
B	7.475313	6.046513	6.259251
B	6.057654	8.330335	6.865409
B	7.510023	7.676476	6.050890
B	8.260945	9.737163	7.707129
B	10.802403	9.537330	8.640852

GeB₁₂

13

scf done: -2375.092384

Ge	6.996856	11.628143	6.065410
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B	6.755408	6.689216	6.780378
B	9.615651	10.226677	7.702383
B	8.735099	11.345747	7.161200
B	7.949289	9.937646	7.062085
B	9.360846	6.111422	8.335707
B	10.368931	7.292461	8.512500
B	8.003935	6.070168	7.597686
B	6.066900	7.960684	6.296612
B	9.030162	7.550136	7.519374
B	7.593127	8.241503	6.918109
B	6.527813	9.454868	6.410889
B	10.206570	8.758714	8.075903

13

scf done: -2375.086407

Ge	8.714926	7.787821	11.052793
B	6.990724	8.850516	6.201969
B	7.943114	10.053087	6.576714
B	8.091425	7.306255	8.658766
B	9.151080	8.492631	9.033959
B	9.807790	10.086577	9.076965
B	7.318752	6.087156	7.970563
B	6.824982	7.629346	7.504792
B	8.951093	10.275470	7.711592
B	8.051191	8.781225	7.635059
B	6.219159	7.468994	5.943488
B	9.958595	9.167415	10.272973
B	6.253545	6.202698	6.836610

13

scf done: -2375.082885

Ge	6.030081	8.966183	6.478427
B	6.088484	7.854811	8.172176
B	7.844879	8.139523	6.116335
B	10.939017	5.824764	10.237358
B	10.318328	7.145724	7.828502
B	9.161332	7.834302	6.937625
B	9.502136	5.988633	10.845971
B	11.274008	6.276535	8.772607
B	7.149204	7.507828	9.292547
B	7.695627	8.386302	7.820953
B	8.720236	7.405716	8.560878
B	8.304108	6.818428	10.185465
B	9.937037	6.925514	9.533978

GeB₁₃

14

scf done: -2399.964031

Ge	6.136114	8.746282	6.555072
B	6.561902	9.375268	9.020872
B	6.139403	10.635001	8.144745
B	7.184330	8.082281	9.895924

B	6.847888	11.073599	6.810564
B	8.512804	7.299953	9.047635
B	8.699787	8.970821	6.750521
B	9.939283	6.589943	8.578615
B	9.381503	7.666471	7.562718
B	8.034487	6.950247	10.600620
B	8.027254	10.277738	6.139353
B	7.735604	8.385310	8.125668

14

scf done: -2399.955682

Ge	12.910263	8.738707	8.412217
B	11.611999	9.648999	7.274738
B	7.112932	6.103855	8.523557
B	6.033638	8.266483	6.471202
B	9.728662	7.130027	8.478474
B	6.963661	9.419423	5.992578
B	9.245570	8.149128	7.128323
B	8.251699	6.889736	7.619389
B	6.399383	7.011375	7.403848
B	7.670587	8.077190	6.573596
B	10.108793	9.570618	6.783052
B	8.582722	6.154006	9.032690
B	10.715524	8.349250	7.939301
B	8.543965	9.529960	6.275700
B	7.684792	9.988771	7.791353
B	9.326562	6.267248	10.000862

14

scf done: -2399.933948

Ge	6.141062	6.450179	12.460983
B	9.833267	7.552760	7.678715
B	9.206094	7.087382	6.268194
B	8.565471	8.221036	8.803562
B	6.933727	8.126913	8.280889
B	7.660507	7.022774	11.283025
B	6.247059	6.406504	10.379014
B	8.957215	7.456272	10.342734
B	6.138239	6.717727	8.779487
B	10.035893	7.626147	9.233088
B	6.634063	6.818385	7.218860
B	8.072210	7.873970	7.156682
B	7.231494	7.657155	9.802695
B	7.740504	6.669359	6.049233

GeB₁₄

15

scf done: -2424.802184

Ge	6.071028	9.645652	7.741941
B	7.960648	8.914805	12.070117
B	8.755903	7.256406	9.509658
B	8.793948	7.522688	7.733413

B	8.761207	7.843081	6.089247
B	9.874541	6.078424	7.942470
B	7.781393	8.501163	8.713743
B	8.758660	7.631798	11.735931
B	8.007093	8.619083	10.410105
B	9.894801	5.962732	9.537748
B	7.269775	9.921577	11.163362
B	9.589056	6.646481	6.531542
B	7.804837	8.714781	7.005243
B	9.501867	6.509031	10.872384
B	7.041708	9.778497	9.601083

15

scf done: -2424.771131

Ge	8.509402	9.490033	8.121652
B	8.141541	7.450061	11.389589
B	8.446120	6.193482	10.069796
B	6.085582	8.824388	7.588430
B	6.335900	8.017231	8.889633
B	7.104465	7.396183	10.234148
B	6.936699	8.746700	6.265782
B	8.918415	7.882798	9.714890
B	7.184362	7.530420	7.384578
B	9.627622	7.066353	11.265762
B	9.495433	6.386610	8.608885
B	10.254037	6.559760	9.953440
B	7.776700	6.760593	8.732501
B	8.868074	6.949353	7.168611
B	8.259953	7.907650	6.110484

15

scf done: -2424.787448

Ge	6.897074	5.936389	10.724971
B	8.420101	7.423101	10.332629
B	7.238830	6.765695	7.488183
B	9.069965	8.867488	10.030920
B	8.261204	9.101897	6.811488
B	6.104780	5.622561	7.128954
B	8.761381	7.509273	7.474330
B	9.060519	10.267181	9.224071
B	8.600879	10.364437	7.753108
B	6.728314	5.594379	8.579132
B	8.069229	6.520939	8.941447
B	9.418229	7.447632	9.019721
B	7.743929	7.681943	6.110296
B	6.618820	6.570058	5.954161
B	9.197065	8.942657	8.244575

GeB₁₅

16

scf done: -2449.650133

Ge	6.659189	8.559726	8.698162
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B	8.544924	8.979271	7.401902
B	10.069241	6.103732	6.623515
B	9.776658	10.319081	8.288569
B	9.338327	7.604274	6.748870
B	6.027629	7.507942	6.231695
B	7.096200	10.182058	6.984097
B	6.150118	9.039251	6.459951
B	8.537247	6.103194	6.319518
B	8.324038	10.679494	7.745671
B	11.810767	8.391208	7.937949
B	7.631261	7.617210	6.881264
B	6.967382	6.302000	6.048854
B	11.227070	9.710233	8.461965
B	10.225265	8.693131	7.677698
B	11.053058	7.183544	7.189515

16

scf done: -2449.617128

Ge	10.897057	8.550966	5.819637
B	6.314683	6.441617	8.608361
B	7.169058	5.822702	7.434956
B	8.484012	5.943630	6.714673
B	6.010682	7.357784	9.830309
B	7.607475	7.052643	9.970647
B	8.874363	8.510193	9.328084
B	6.633287	8.771058	9.669188
B	9.055769	9.958330	8.511634
B	9.796600	6.721514	7.038567
B	9.124900	6.881025	9.905531
B	10.094927	8.899274	8.017737
B	7.749566	9.807992	9.242367
B	11.086542	7.642653	7.537745
B	8.527511	6.334305	8.351740
B	10.133495	7.228863	8.776682

16

scf done: -2449.600305

Ge	9.522122	9.856514	8.981841
B	6.764770	8.641121	10.699667
B	7.597777	10.003083	10.206427
B	8.745536	7.533912	9.312172
B	6.060872	9.662138	9.653247
B	6.636006	8.031429	7.230006
B	6.011882	9.226248	8.111616
B	7.020965	6.143331	7.498526
B	7.544706	9.550125	7.213005
B	7.383208	6.407335	9.017231
B	7.998322	8.398982	6.221671
B	7.498486	7.231539	10.398051
B	7.250599	10.263656	8.631768
B	7.565173	6.906650	6.246593
B	8.333292	7.238735	7.776031

B 8.424040 8.602605 10.489426

GeB₁₆

17

scf done: -2474.506545

Ge	6.107732	6.035588	9.208929
B	7.328316	11.039627	10.302663
B	10.021365	10.536389	6.998773
B	10.621435	12.089234	7.632182
B	6.601877	8.025085	9.444850
B	6.860575	9.615906	9.950702
B	11.431563	11.163681	6.559403
B	7.588999	8.857863	8.484708
B	11.064367	9.755158	6.079005
B	8.555912	9.836506	7.459956
B	7.425735	7.304033	8.179259
B	8.499734	8.114327	7.200693
B	9.767063	8.877629	6.555360
B	9.702901	12.623178	8.789502
B	8.473116	11.957281	9.561571
B	7.830369	10.509761	8.857843
B	8.947541	11.399264	7.981931

17

scf done: -2474.461367

Ge	6.307369	6.039630	8.540348
B	7.865699	10.550104	8.447132
B	7.858416	10.351892	6.608932
B	7.503870	8.686660	6.683679
B	7.499319	10.213246	10.174757
B	6.403770	9.118259	10.508274
B	6.514231	8.107372	7.901264
B	9.020725	9.353290	6.089785
B	10.257504	8.345973	6.411424
B	8.828671	10.947219	9.700591
B	6.037864	7.999676	9.511220
B	10.309505	9.578396	7.311888
B	8.848279	7.618962	6.381932
B	6.611874	9.948252	7.411046
B	6.292802	9.603666	8.963300
B	7.501204	7.064479	7.130108
B	9.687904	10.533830	8.531638

17

scf done: -2474.451270

Ge	7.128741	10.254240	6.303786
B	8.901947	8.607911	8.098009
B	9.218954	7.532909	6.812462
B	10.752445	7.883217	7.858517
B	10.617835	6.642993	6.882142
B	10.554039	9.161912	8.781045
B	9.440732	6.013453	6.142791

B	7.935350	10.102692	8.854910
B	7.716034	8.259629	6.544166
B	6.038669	8.373938	7.151691
B	6.706065	9.198399	8.390356
B	9.481850	10.271475	8.886613
B	7.890938	6.364964	6.210887
B	9.186668	8.700545	9.780790
B	6.514979	6.911385	6.790793
B	7.907282	7.913799	9.422563
B	6.799061	7.440511	8.366975

GeB₁₇

18

scf done: -2499.309826

Ge	12.415521	8.250874	5.406088
B	9.356909	6.504188	8.785841
B	6.054077	7.020028	8.633539
B	10.761774	6.064041	8.046631
B	10.037095	7.463513	6.974895
B	13.007627	7.431323	7.103754
B	12.298053	6.680467	8.279504
B	11.397638	8.176805	7.666257
B	11.496957	6.619624	6.702377
B	11.110404	7.587357	9.185975
B	8.419706	7.266099	7.175443
B	8.917247	7.477340	11.540012
B	6.844146	7.215710	7.331373
B	7.413732	7.185835	11.408574
B	6.484783	6.955594	10.153578
B	9.995198	7.433047	10.372437
B	7.698404	6.646409	8.608966
B	8.452985	6.707170	10.167626

18

scf done: -2499.316159

Ge	11.810131	6.884289	7.484953
B	10.191762	11.049815	9.707035
B	5.946151	10.668392	7.578490
B	10.517916	8.570529	7.922568
B	6.177883	7.778583	6.387225
B	9.336922	12.302021	9.672772
B	6.986067	11.554857	8.282895
B	10.130589	9.747508	8.877952
B	6.007299	9.226780	6.986670
B	9.670921	7.527254	7.024506
B	7.354847	6.855032	6.226736
B	10.319047	6.198995	6.281297
B	8.829099	6.270728	6.086446
B	8.735825	10.931722	8.729361
B	7.488815	9.991439	7.726061
B	8.935352	8.997243	7.874455
B	7.513447	8.330297	7.192322

B 7.958898 12.486972 9.078063

18

scf done: -2499.316870

Ge	8.056472	10.727843	6.975782
B	7.498506	9.507003	12.513292
B	8.737196	11.050251	10.558059
B	8.073108	10.859552	12.026628
B	9.412748	9.639884	9.871218
B	5.992098	5.678232	7.896617
B	6.198230	6.247767	6.449967
B	6.667492	6.250855	9.219354
B	6.997506	7.571361	6.163412
B	7.156085	6.844456	7.636861
B	7.617076	7.732484	8.924892
B	7.432564	8.167880	11.669693
B	8.776887	10.827053	8.941958
B	8.582899	8.220949	10.136881
B	8.594500	9.167518	8.502758
B	7.338741	7.070626	10.459783
B	7.832358	8.424025	7.238556
B	8.570259	9.461985	11.290723

GeB₁₈

19

scf done: -2524.151321

Ge	8.526963	5.707536	6.734549
B	10.875725	6.864928	10.708274
B	8.014299	7.598823	7.133705
B	7.649218	8.317599	12.883381
B	7.514555	8.901149	11.288688
B	10.252087	6.830647	9.308660
B	9.251452	7.242473	8.157307
B	6.624002	7.312687	12.126657
B	5.869715	6.651440	10.908579
B	7.594376	6.276365	10.710574
B	6.327532	6.283788	9.491522
B	10.127930	7.184167	12.049941
B	7.933899	8.506299	8.455602
B	9.185126	8.046942	13.084443
B	7.760762	9.278592	9.814895
B	9.266601	6.374645	10.722177
B	7.026411	6.935737	8.227607
B	8.386437	7.153951	11.897192
B	6.849217	7.877820	9.923089

19

scf done: -2524.1387405

Ge	6.138892	11.051992	8.160698
B	8.031772	10.918023	6.984916
B	9.229996	7.804784	9.155750
B	7.490928	9.472939	7.513466

B	10.236691	8.545036	6.010869
B	10.356146	7.419743	8.161100
B	8.877583	9.558471	6.565926
B	8.618017	6.940097	7.898037
B	10.232218	6.670394	6.296839
B	6.530196	7.744311	7.545543
B	10.701744	10.214638	6.125827
B	7.393519	6.775802	6.624994
B	8.748906	7.845523	6.277912
B	9.446841	11.142395	6.355595
B	11.721664	9.080134	6.552247
B	6.330456	8.927318	8.545369
B	7.722341	8.179985	8.992423
B	8.735639	6.097639	6.298406
B	11.439464	7.549028	6.874589

19

scf done: -2524.141576

Ge	6.082620	8.516674	7.617853
B	8.471779	9.532561	10.664906
B	9.053793	5.796603	10.000507
B	8.358413	9.991484	9.129881
B	9.090213	8.491505	9.300163
B	10.152825	7.341786	11.971647
B	8.622361	6.913297	7.421989
B	9.472020	8.686289	11.572624
B	7.566710	7.177939	6.161033
B	6.407081	7.357200	9.738271
B	8.336800	8.450863	6.474263
B	8.566243	9.430191	7.715378
B	9.759040	5.987608	11.406543
B	7.240271	8.585448	10.243717
B	9.943103	7.278080	10.303058
B	6.969205	6.252448	7.339772
B	6.065018	6.348681	8.641669
B	7.798336	6.330508	8.957057
B	9.450042	6.910870	8.758512

GeB₁₉

20

scf done: -2549.024926

Ge	7.569464	8.854053	11.515729
B	6.714851	8.169081	9.349673
B	7.051643	11.613804	7.030760
B	10.611782	7.573821	7.960160
B	11.078545	9.412545	5.932948
B	8.040745	7.356914	9.496878
B	8.590037	11.207269	6.836024
B	9.398505	6.669153	8.886409
B	9.958989	10.405539	6.389351
B	9.813837	8.711352	8.902308
B	10.638119	9.270603	7.540511

B	9.178357	8.644746	10.390083
B	9.155939	9.986150	7.890565
B	8.093986	9.246196	9.126691
B	7.683743	10.636129	8.188092
B	6.244235	9.604360	8.845321
B	6.051662	10.934904	7.987144
B	10.635122	5.945240	8.174681
B	11.550659	8.016817	6.476947
B	11.580249	6.554894	7.125298

20

scf done: -2548.987783

Ge	-3.291583	-0.425461	-0.182191
B	-1.119937	-0.156642	-0.736937
B	3.007131	-0.524961	-1.045071
B	2.158582	1.718809	-0.085037
B	3.005790	-0.478421	1.198214
B	-0.722860	1.741220	-0.479669
B	0.412418	0.693719	-1.381485
B	4.150483	-0.607888	0.061392
B	1.534200	-0.000432	1.683228
B	1.482104	-1.603016	-0.293210
B	0.644595	1.327831	0.813886
B	3.060766	-1.815164	0.137414
B	3.521133	0.822065	0.053164
B	0.791989	2.237879	-0.609496
B	-2.191866	1.178110	-0.151039
B	0.133183	-1.084261	-1.086381
B	0.233317	-0.765550	0.632667
B	-1.113948	0.537273	0.983439
B	0.049626	0.236990	1.999067
B	1.541120	-0.424146	-1.697905

20

scf done: -2548.977379

Ge	-2.387111	-0.962082	-0.070298
B	-1.038100	0.123961	-1.335899
B	2.926684	0.125807	-0.305289
B	0.008883	-0.777062	-0.347833
B	2.410045	-0.958001	1.340957
B	-0.831311	2.570796	0.098782
B	0.502323	0.726685	-1.693681
B	0.192218	0.612913	2.360365
B	2.882488	-1.214611	-1.376417
B	0.682917	2.211944	-0.509444
B	1.986365	1.392490	-0.289649
B	1.542642	-1.371061	-0.249064
B	3.228505	-1.529069	0.127669
B	-0.739382	-0.054576	1.086674
B	1.473494	-0.233007	2.454139
B	-0.732873	1.744914	-1.305142
B	1.899382	-0.134115	-1.857298

B	-0.541271	1.681326	1.383846
B	1.010685	0.230728	0.822286
B	-1.633015	1.124876	0.042243

GeB₂₀

21

scf done: -2573.856363

B	1.536197	1.747109	0.494364
B	0.821088	-0.993463	0.835554
B	-0.610608	0.023251	1.421558
B	2.066632	0.041625	0.279944
B	0.882972	0.594893	1.451319
B	0.006430	-1.526288	-0.834856
B	0.482353	3.003915	-0.327975
B	0.639295	-2.676772	0.654505
B	-2.368886	0.478091	1.239951
B	3.422008	-0.078272	-0.718771
B	-1.041581	2.966323	0.076602
B	2.168146	-2.517009	0.499424
B	-1.986993	-0.985912	1.330692
B	2.787751	1.405533	-0.776401
B	-0.752583	-1.849763	0.727330
B	1.947120	2.697259	-0.811787
B	-1.969657	1.953274	0.716819
B	3.191089	-1.470373	-0.128859
B	-0.216655	1.661232	0.725678
B	1.554369	-1.321804	-0.805637
Ge	-1.962264	-0.492633	-0.945227

21

scf done: -2573.852249

B	2.413951	1.086733	0.117498
B	0.561159	-0.660594	1.637990
B	-1.173864	1.542140	1.460686
B	1.493092	0.696989	1.380418
B	0.105443	0.849508	2.162155
B	-1.057664	-0.277332	1.718561
B	0.069703	2.323348	-0.865413
B	0.847872	-2.197331	0.674017
B	-2.407549	0.368618	0.744739
B	3.658530	0.225368	-0.826835
B	-1.131006	2.710395	0.053273
B	2.313960	-2.314442	0.104057
B	-2.135055	-1.210657	0.856660
B	3.073708	1.549579	-1.296282
B	-0.689029	-1.824704	0.875819
B	1.608053	2.066018	-1.145133
B	-2.413969	1.902250	0.447276
B	3.342987	-1.224319	-0.233020
B	-1.361412	1.249740	-0.757586
B	2.049405	-0.876252	0.881267
Ge	-1.432549	-0.935165	-1.248460

21

scf done: -2573.849434

B	2.234147	1.205044	-0.004746
B	2.406365	0.839161	-1.620464
B	1.438122	-2.464577	-0.139414
B	2.528563	-0.114055	1.098412
B	1.651641	1.208750	1.560141
B	0.808185	2.100316	0.491744
B	-1.300417	1.246874	-0.421164
B	2.386683	-1.896879	-1.309363
B	-0.127978	-0.874486	1.620786
B	1.242551	1.908666	-1.245678
B	-1.421147	-1.563270	0.871187
B	2.779516	-0.648773	-2.102421
B	2.926404	-0.369638	-0.484391
B	-0.179628	2.468064	-0.832701
B	1.309814	-0.239678	2.165897
B	-0.895902	2.523472	0.591081
B	-1.670023	1.387336	1.323511
B	-0.039931	-2.178885	0.381759
B	-1.677824	-0.170841	1.555332
B	1.522215	-1.532625	1.212793
Ge	-2.487712	-0.442809	-0.736297

Cartesian coordinates of first three lowest energy isomers of Ge_2B_n clusters (n=10-20)

Ge_2B_{10}

12

scf done: -4402.489924

B	11.106521	7.900160	8.189681
B	8.356104	6.864002	6.575576
B	8.770640	9.723061	8.314022
B	7.323136	9.463056	7.616346
B	10.921819	6.414729	7.617197
B	9.633366	5.967134	6.887802
B	10.110323	9.073407	7.701622
B	7.152630	7.950617	6.599183
B	9.981133	7.569710	6.935076
B	8.630866	8.632628	6.988576
Ge	10.321321	9.302613	9.773603
Ge	5.730883	9.390318	6.315758

12

scf done: -4402.484905

B	2.908223	1.559704	-0.297406
B	4.119657	0.483807	-0.208002
B	0.091238	1.760392	0.022605
B	2.607745	-1.671256	0.531289
B	1.391087	0.783658	0.235841
B	2.610040	-0.200731	-0.265934
B	1.522173	2.327436	-0.304372

B	3.980997	-1.047693	0.063150
B	-0.124252	0.139397	0.503387
B	1.185413	-0.934119	0.440098
Ge	-1.983796	0.969301	0.078871
Ge	-1.186880	-1.469393	-0.191474

12

scf done: -4402.472520

B	10.872111	9.728379	6.552607
B	6.202157	7.211724	7.603213
B	6.068177	8.606004	7.045140
B	9.193243	7.714387	7.595316
B	8.275980	10.697625	6.253736
B	7.621030	8.020872	7.274762
B	10.512644	8.340267	7.137633
B	7.107926	9.751458	6.609701
B	9.807786	10.731542	6.086069
B	8.907720	9.114641	6.680873
Ge	9.607129	10.272454	8.466149
Ge	7.636524	6.064363	8.403703

Ge₂B₁₁

13

scf done: -4427.342316

B	7.606447	7.824440	9.169845
B	7.088826	6.277425	9.760224
B	8.116023	9.595383	8.931328
B	8.171241	7.595671	5.806455
B	8.502039	9.071503	6.114349
B	7.993494	8.096219	7.467926
B	7.704065	6.476055	6.731440
B	8.458079	9.836786	7.433452
B	7.361917	6.239375	8.230126
B	7.251844	7.576742	10.735921
B	7.722965	9.091708	10.349271
Ge	6.615581	5.948161	11.853481
Ge	7.247001	8.759668	12.441052

13

scf done: -4427.330847

B	-3.853513	1.353989	-0.259409
B	-1.533506	-0.219541	-0.100589
B	-0.649174	1.170094	-0.291737
B	-4.099190	-1.341157	0.325953
B	-0.926863	-1.830898	0.338105
B	-4.724352	0.072725	0.021464
B	-3.135992	-0.152859	-0.314070
B	-2.248422	1.362146	-0.374770
B	-2.533315	-1.679862	0.241988
B	0.631600	-1.897630	0.392579
B	0.086770	-0.369628	-0.111521
Ge	1.300205	1.536528	0.212449

Ge 2.291351 -0.984556 -0.191823

Ge₂B₁₂

14

scf done: -4452.179373

B	-2.950214	-0.382524	0.109192
B	-4.277755	-1.491695	-0.096845
B	-4.660110	-0.010075	-0.058842
B	-1.306985	0.195240	0.094461
B	-0.777159	1.833335	0.150767
B	0.039806	-0.937171	0.143724
B	0.207924	0.647955	0.579855
B	1.577411	-0.082917	0.284166
B	-2.310086	1.758446	-0.018351
B	-1.464038	-1.490153	-0.041348
B	-3.792412	1.236975	-0.080209
B	-2.873994	-2.132887	-0.144960
Ge	1.500733	2.112613	-0.102296
Ge	2.028581	-1.978946	-0.041705

14

scf done: -4452.164727

B	3.273112	2.558910	0.125008
B	4.507132	1.641819	0.346541
B	0.339966	1.511931	-0.320611
B	0.014403	-0.096497	0.065657
B	-2.712779	0.605298	-0.053165
B	-3.032597	-1.008259	0.253963
B	-1.229991	1.107714	-0.162454
B	-1.519859	-0.587004	0.162887
B	1.806917	2.120840	-0.208985
B	1.535160	0.338963	-0.045372
B	3.097472	0.893589	-0.221571
B	4.403405	0.093561	0.520663
Ge	3.125332	-1.356718	-0.090157
Ge	-4.763197	-0.077792	0.017881

14

scf done: -4452.151030

B	4.427446	0.469025	-0.325978
B	3.477731	1.644959	-0.194591
B	1.994512	-1.837477	0.381434
B	-0.594525	1.819988	0.076228
B	3.486814	-2.081220	0.186555
B	0.693253	2.756786	0.111122
B	1.101816	-0.609100	0.236495
B	-0.352717	0.184318	0.079361
B	2.893004	-0.402687	0.001060
B	1.095745	1.099101	0.125631
B	4.576071	-1.021999	-0.131127
B	2.161936	2.475637	0.025034
Ge	-1.517502	-1.516876	-0.092361

Ge -2.382668 0.814168 0.003107

Ge₂B₁₃

15

scf done: -4477.038364

B	-0.181922	0.521886	0.210637
B	1.401522	0.101235	0.083455
B	-3.842911	-2.011142	-0.193709
B	-2.904884	-0.732032	0.111268
B	-1.057501	1.950418	-0.024072
B	0.348132	-1.179990	0.129129
B	-4.468229	-0.604329	-0.264619
B	-3.730095	0.823666	-0.169823
B	-2.628181	1.977320	-0.160412
B	-1.281489	-0.940080	0.452427
B	-2.267770	-2.377243	0.009871
B	-0.672241	-2.387787	0.085970
B	-1.907785	0.598583	0.375619
Ge	1.122681	2.218398	-0.020863
Ge	2.501280	-1.552851	-0.080034

15

scf done: -4477.014464

B	3.112454	2.665326	0.006511
B	0.259707	3.415920	-0.012622
B	1.769528	1.513333	0.002828
B	-0.061427	1.519035	-0.005122
B	3.457686	1.189463	0.014315
B	-1.144616	2.812860	-0.005591
B	0.881514	-0.055949	0.001773
B	-0.961539	-0.026695	0.003533
B	2.525335	-0.047347	0.010189
B	-1.744137	1.408101	0.001032
B	-0.106406	-1.492226	0.003653
B	-1.636544	-1.534900	0.006861
B	1.818379	3.447322	-0.004653
Ge	1.890427	-2.036527	-0.004700
Ge	-3.166979	-0.278199	0.001152

15

scf done: -4477.000929

Ge₂B₁₄

B	2.909164	1.048878	0.676111
B	2.810443	-0.415831	1.307821
B	1.677571	2.049404	0.308190
B	1.595740	-1.421753	1.120618
B	0.312750	2.771167	-0.174144
B	0.078414	-1.928476	0.873457
B	0.100121	1.339209	0.568296
B	-1.295511	-1.248495	0.498825
B	-1.178373	2.229632	-0.267716
B	-0.063590	-0.278224	0.934434

B	-1.426852	0.430847	0.241158
B	1.427583	0.468505	1.117228
B	-2.534518	1.424879	-0.395068
Ge	-3.277031	-0.463286	-0.206173
Ge	2.587509	-0.547612	-0.857766

16

scf done: -4501.872458

B	-2.643681	3.270772	-0.267743
B	1.264526	-2.622727	0.115856
B	-2.199449	0.130719	-0.080241
B	-1.474662	4.283077	0.035513
B	-1.207692	2.675994	0.300680
B	1.117573	-0.933219	0.181402
B	-0.619474	-0.510592	0.107481
B	0.803337	0.701835	0.130206
B	2.547317	-1.808277	-0.034257
B	-2.528622	1.674274	-0.198265
B	-0.836891	1.136047	-0.197681
B	0.447667	2.252937	0.225587
B	0.001954	3.795274	0.143192
B	-0.227188	-2.145601	0.105691
Ge	3.103452	0.106702	-0.081398
Ge	-2.235438	-1.966157	-0.007262

16

scf done: -4501.870572

B	-2.618684	0.088020	2.068112
B	0.331730	-0.126778	-1.836693
B	1.735999	0.163369	1.350381
B	-1.294362	-0.010556	0.989592
B	-1.191895	0.153326	2.614424
B	-3.491733	-0.010035	0.758899
B	2.558183	0.118999	0.050835
B	-2.225162	-0.155290	-0.541581
B	0.274353	0.146781	2.006017
B	-1.318782	-0.199371	-2.056712
B	1.853197	-0.008238	-1.339193
B	-0.597855	-0.141970	-0.501819
B	-2.927372	-0.185233	-2.031510
B	-3.834812	-0.105210	-0.777310
Ge	0.898487	1.719176	-0.166406
Ge	1.093262	-1.676647	0.048681

16

scf done: -4501.863096

B	2.254632	2.489410	0.875935
B	-4.091750	-0.754762	-0.315276
B	0.760518	2.738184	0.590064
B	-4.455943	0.733228	-0.493432
B	1.544507	1.081160	0.238176
B	-2.893176	0.347944	-0.209707

B	3.206350	1.344215	0.496195
B	-2.627694	-1.357856	-0.014551
B	-2.274784	2.969829	-0.220746
B	-1.535905	1.409397	-0.083237
B	0.029179	0.485274	0.095325
B	-1.361706	-0.228927	0.030815
B	-0.802504	2.912742	0.165729
B	-3.515358	1.999759	-0.421583
Ge	3.160355	-0.379540	-0.444233
Ge	-0.697287	-2.146959	0.329591

Ge₂B₁₅

17

scf done: -4526.727713

B	3.824579	-2.381178	-0.409804
B	1.477092	1.348315	0.509588
B	0.820431	-1.448697	-0.000614
B	-0.738181	-1.143265	0.156189
B	2.339904	-1.941406	-0.190063
B	0.328451	0.183965	0.219789
B	3.656865	-0.698136	-0.231901
B	3.166077	0.999456	0.170857
B	-1.352328	0.359694	0.015115
B	1.993848	-0.254005	0.061389
B	5.449457	-0.063515	-0.308452
B	2.512658	2.491956	0.641020
B	5.072686	1.407781	0.024432
B	4.034650	2.464802	0.410950
B	5.105172	-1.548318	-0.490039
Ge	-3.076833	1.268834	-0.396668
Ge	-2.812442	-1.234061	0.306284

17

scf done: -4526.683116

B	-2.804467	0.368602	-0.752888
B	-1.628973	1.557527	-0.216462
B	0.633476	-0.588869	0.978047
B	-0.258103	0.795906	1.315007
B	1.080477	2.208580	-0.839272
B	-0.095045	2.354793	0.319744
B	-0.335474	1.606571	-1.462387
B	-1.678920	0.832231	-1.726440
B	2.343166	1.286139	-0.733362
B	-2.067088	0.719462	1.313993
B	-3.220916	-0.519997	0.509952
B	-2.323994	-1.032406	1.624717
B	1.061946	0.797785	0.216695
B	-1.320959	2.107604	1.351839
B	-0.735239	-0.855498	1.697048
Ge	2.857603	-0.514820	0.141165
Ge	-1.084148	-1.303684	-0.703076

17

scf done: -4526.675794

B	-0.716281	-0.851934	-0.453840
B	0.173078	-2.087794	0.544617
B	2.608157	0.104391	-0.968984
B	3.544960	-1.020053	-0.409343
B	-0.027097	0.817254	-0.192865
B	0.417192	-1.843036	2.162634
B	0.891799	-0.229825	-1.154373
B	1.636999	-2.461797	1.372694
B	2.034811	-1.473231	-1.016955
B	2.873753	-2.270298	0.280238
B	-1.373971	0.355309	0.618261
B	-0.614023	-0.891185	1.504674
B	0.369842	-1.878678	-1.146156
B	1.385524	-2.861600	-0.351453
B	1.443707	1.296662	-0.777893
Ge	-2.962207	-0.432851	-0.279905
Ge	0.673387	2.822822	0.278146

Ge₂B₁₆

18

scf done: -4551.565415

B	-0.476857	-0.190557	-0.500001
B	0.345211	0.600116	0.968357
B	3.521823	1.112701	0.433335
B	3.734923	-0.370362	-0.091609
B	2.347230	-1.479277	0.092533
B	0.877674	-0.977160	0.682212
B	3.705593	-1.822497	-0.767848
B	0.994161	-2.558465	-0.557005
B	-0.610020	-0.906003	1.284112
B	-0.656628	1.939863	1.349586
B	2.338771	1.952820	0.891490
B	2.172686	0.188781	0.638921
B	2.502927	-2.769545	-0.939076
B	-0.431648	-1.853379	-0.202502
B	-1.426534	0.520821	1.018142
B	0.802901	2.317531	1.224488
Ge	-2.476106	-1.185160	0.134505
Ge	-0.608614	1.856193	-0.997807

18

scf done: -4551.534439

B	-1.325069	1.656045	2.524171
B	-1.348076	1.724470	0.876622
B	-1.369198	0.226401	1.766131
B	-0.927723	2.983609	1.817740
B	0.609722	-0.496275	-1.637671
B	2.155434	-0.673632	-1.063971
B	-0.630536	3.108395	0.251917
B	0.098410	2.836821	-1.246205

B	1.411725	2.276049	-1.904371
B	0.884922	-0.883224	0.028107
B	-0.522148	-0.833965	0.881608
B	-1.728052	0.350565	-0.035085
B	0.151527	1.210433	-1.633824
B	1.783259	0.744466	-1.833294
B	-0.672938	-1.041158	-0.762688
B	-1.105233	1.775126	-0.746310
Ge	-2.654734	-1.483573	-0.250784
Ge	3.050668	-0.854572	0.675335

18

scf done: -4551.516264

B	-1.668516	0.641064	-0.490463
B	-0.527669	-0.778425	1.463059
B	-2.349236	-0.660892	0.791278
B	-2.919456	0.801482	0.787477
B	-0.566686	1.875879	0.385706
B	0.301034	0.887297	1.428143
B	-2.560938	2.094390	-0.041000
B	0.191532	2.747274	-0.842085
B	1.987942	1.258247	1.218516
B	1.049307	-1.556918	1.803520
B	-1.544874	-2.051237	0.758032
B	-1.303681	0.785303	1.441508
B	-1.372075	2.677850	-0.868878
B	1.273147	2.035986	0.054916
B	1.788887	-0.173837	1.775194
B	-0.161657	-2.411173	1.364568
Ge	2.099582	-0.074844	-0.553522
Ge	-0.789748	-1.202076	-1.169836

Ge₂B₁₇

19

scf done: -4576.360269

B	3.689858	-0.032624	-1.028574
B	-0.885398	-2.113099	-0.281974
B	1.904236	0.798574	0.975805
B	0.873291	-0.690919	1.446796
B	-0.763556	-0.555381	-0.934618
B	1.406811	1.846304	-0.109625
B	-0.692184	-0.750837	0.969418
B	3.332203	-0.296271	0.525192
B	0.335524	0.477900	-0.152679
B	2.158620	-1.652946	0.663166
B	1.913604	-2.600497	-0.678579
B	2.741418	1.166140	-0.677209
B	-1.347536	0.622226	0.112499
B	3.019363	-1.452223	-0.974972
B	0.417681	-3.052932	-0.572848
B	2.418288	-0.516308	1.820582
B	0.641142	-1.345567	-0.474107

Ge	-2.740504	-1.029233	0.040211
Ge	-0.566272	2.614929	-0.138378

19

scf done: -4576.357560

B	1.367193	-1.250563	1.450684
B	2.266511	0.512607	-0.671542
B	1.137147	1.305070	-1.521666
B	-0.141932	-1.642957	1.143715
B	0.369210	2.667139	-0.638818
B	-1.071994	2.977319	0.323656
B	1.945558	0.155942	2.080572
B	2.608040	-0.503025	0.641980
B	-1.265562	2.694694	-1.202974
B	-1.625815	-1.712780	0.771439
B	2.652043	1.099922	0.904174
B	0.112495	2.476701	1.194243
B	-0.947462	-0.278325	0.351427
B	1.679540	2.031561	0.075613
B	-0.894393	1.249452	-0.181626
B	1.361766	1.648183	1.814862
B	-0.283502	1.801276	-1.993256
Ge	1.680997	-1.704739	-0.770361
Ge	-3.129254	-0.675295	0.060598

19

scf done: -4576.346777

B	-1.027685	1.731981	-0.352920
B	1.322447	2.670700	-0.051659
B	-2.734582	2.022383	-0.270256
B	-0.832067	-1.302762	2.202693
B	1.045937	-0.060271	-0.646062
B	-2.165383	0.677968	-1.072455
B	-0.087668	0.123185	1.685350
B	0.420533	1.322493	0.676339
B	-0.546479	0.193362	-0.993633
B	0.614473	-1.552368	1.733150
B	-0.153895	3.090373	0.249742
B	-2.571417	0.714436	0.694160
B	-0.139831	-1.167279	0.154447
B	-1.738752	3.185441	0.145154
B	1.520482	-1.324410	0.458515
B	-1.911381	-0.291656	1.731751
B	2.031187	1.278243	-0.221511
Ge	3.284084	-0.386805	-0.310315
Ge	-2.197509	-1.380667	-0.646373

Ge₂B₁₈

20

scf done: -4601.267973

B	-2.033758	-0.161764	0.464091
B	2.715263	-0.703696	0.623543

B	1.063666	-0.128640	0.870676
B	-3.288946	0.901877	-0.003706
B	-1.650197	3.119417	-0.066247
B	0.149272	-1.640761	1.456825
B	1.661484	-1.739508	1.209590
B	-4.524006	1.908489	-0.416138
B	-3.834043	-0.789432	0.002887
B	-1.767739	1.500043	0.445439
B	-3.156410	2.683458	-0.178429
B	-1.443111	-1.692878	1.417473
B	2.407950	0.913449	0.814486
B	-0.417801	0.444635	0.222233
B	-4.793196	0.400153	-0.433588
B	-0.332738	2.399854	0.234154
B	-2.776410	-1.750944	0.690104
B	1.017417	1.575618	0.518938
Ge	4.056145	0.513853	-0.394712
Ge	-0.774379	-1.645004	-0.835340

20

scf done: -4601.250362

B	-3.060547	0.374918	0.640910
B	2.412399	1.252972	0.825170
B	-2.348504	1.735053	1.324204
B	2.146054	-0.130433	1.591054
B	-2.416764	-1.068630	1.139454
B	2.029747	1.140920	-0.831383
B	0.203187	-1.963823	0.760441
B	-0.917566	2.029447	-1.017803
B	0.072669	2.923314	0.047112
B	-0.858849	-0.968690	1.808442
B	-1.345501	-2.035774	0.531430
B	0.704672	1.939163	-1.193372
B	-1.470214	2.736246	0.397031
B	0.829340	-0.929821	1.958315
B	1.592361	2.423222	0.137156
B	-1.991519	0.317904	1.947286
B	1.697473	-1.415656	0.633456
B	-2.240766	1.443512	-0.331763
Ge	-2.487891	-0.920761	-1.107283
Ge	3.263255	-0.611089	-0.512583

20

scf done: -4601.236960

B	0.484453	-1.155328	0.511774
B	1.510695	0.498171	-1.599803
B	-0.927687	-1.705416	0.844811
B	-0.044882	0.647414	-1.884386
B	-0.597468	1.447281	1.674073
B	0.359271	2.165890	0.573169
B	-3.466958	-0.116187	1.380856
B	-3.365325	1.176331	0.573092

B	-2.051042	0.749418	1.670844
B	-2.401259	1.610721	-0.630585
B	0.759086	0.586034	1.203273
B	1.792186	1.474039	0.131791
B	-0.604638	-0.262024	1.650390
B	-0.705542	1.847264	-0.686168
B	2.871283	0.824660	-0.929110
B	1.835447	-0.302468	0.167641
B	-2.152184	-1.022936	1.595254
B	-1.553568	0.856692	-1.724136
Ge	3.998365	-0.525647	0.058764
Ge	-2.708032	-0.930534	-0.765448

Ge₂B₁₉

21

scf done: -4626.071530

B	2.053817	-0.493349	-1.011181
B	2.081160	-2.244695	-1.125213
B	3.419283	-1.479195	-0.543400
B	-0.676011	-0.879000	0.216923
B	-1.891530	0.183549	0.221613
B	0.235516	2.209991	-0.425802
B	2.457010	1.032420	1.470158
B	1.687080	2.496387	-1.068973
B	-0.555509	-2.450930	-0.148434
B	4.071034	-1.114098	0.844702
B	-0.471459	0.720202	-0.379023
B	0.753995	-2.943004	-0.857976
B	3.633511	0.046674	1.741144
B	0.963893	-1.617554	0.234077
B	3.532151	0.187930	-0.187330
B	2.884548	1.627352	-0.663101
B	1.110313	0.895888	-1.164034
B	2.182535	-0.663633	0.882372
B	1.608012	2.023709	0.558270
Ge	-2.568971	-1.853805	0.171689
Ge	-1.974678	2.238392	0.047876

21

scf done: -4626.054095

B	-2.732462	-1.467833	-0.700161
B	-3.985386	-0.678238	0.415170
B	-3.165049	-0.675376	1.788655
B	1.637655	0.289705	-1.623302
B	0.240026	1.105893	-1.673043
B	0.975631	1.024275	-0.170349
B	-0.129815	-1.497529	0.584666
B	0.222836	-2.558343	-0.692102
B	-2.718715	0.081473	-1.693557
B	-0.374676	-0.494002	2.036884
B	1.579565	-2.372736	-1.492154
B	-1.311678	0.821579	-1.834412

B	0.963251	-0.206915	1.122837
B	1.403598	-1.388554	-0.081988
B	-1.693493	-1.323032	1.142275
B	-1.297666	-2.065640	-0.419948
B	-4.004528	-0.575989	-1.104745
B	-1.864683	-0.424578	2.534486
B	2.415710	-1.088884	-1.488452
Ge	-0.841458	1.996337	0.031354

21

scf done: -4626.045655

B	4.615018	-1.469224	-0.407371
B	3.984650	-0.494823	0.834108
B	4.607048	0.044930	-0.714882
B	-0.170603	0.495141	0.559917
B	-1.435019	1.428970	1.496033
B	-1.857152	0.037285	0.874875
B	1.583663	0.820478	0.344913
B	1.867235	-2.062525	-0.161331
B	1.405453	0.818261	2.035382
B	1.972289	1.025724	-1.367189
B	0.289395	-2.327593	-0.353490
B	-0.030561	1.406935	2.177617
B	0.492880	1.257858	-0.888211
B	-0.859266	-1.078239	0.157009
B	2.682450	-0.466733	-0.506558
B	3.359637	-2.105351	0.267046
B	2.686488	0.086331	1.524622
B	3.527175	0.960365	-1.361021
B	-1.206745	-2.501691	-0.552125
Ge	-1.343770	2.246782	-0.499483
Ge	-2.955298	-1.602423	-0.119165
Ge	3.003939	0.112214	0.491965

Ge₂B₂₀

22

scf done: -4650.898873

B	0.844612	1.914514	-1.644485
B	-0.546412	0.627458	2.223286
B	-1.902406	0.583265	-1.385383
B	0.162273	1.762638	1.076011
B	1.394408	0.463954	-1.924278
B	0.064651	-0.839813	1.962752
B	-1.431905	-0.981218	-1.488968
B	1.496753	-1.266359	1.255267
B	1.072218	-1.703372	-0.349519
B	-1.113185	2.713570	0.412663
B	1.030558	0.424240	1.320532
B	-1.483422	1.780682	1.660926
B	-1.057360	1.913524	-1.143342
B	0.292545	2.765234	-0.478856

B	-1.973970	1.195321	0.166023
B	0.132622	-2.138011	0.955935
B	0.171017	-1.027290	-1.627042
B	1.783509	-1.016529	-1.635795
B	-0.810640	-1.890090	-0.303184
B	1.297505	1.283016	-0.087959
Ge	-2.980837	-0.756690	0.018263
Ge	3.070935	-0.269050	0.143520

22

scf done: -4650.890456

B	0.045724	-1.777806	0.552890
B	-0.364233	1.333272	-1.348755
B	1.146976	-1.042777	1.530721
B	-0.307907	2.645469	0.056749
B	2.254605	0.491354	-0.116677
B	1.246077	1.383173	-1.126634
B	3.785093	0.635019	1.096580
B	2.498466	1.743750	1.168772
B	-1.377874	-1.021736	0.300133
B	-2.036924	1.085920	-1.376661
B	2.497771	-0.172345	1.490601
B	1.219393	2.381902	0.550175
B	-0.472244	-0.642391	1.712619
B	-1.505012	2.519221	-0.871788
B	-0.390551	-1.463475	-0.999339
B	-1.283000	-0.288088	-1.550928
B	-1.793045	0.211036	1.487423
B	-1.658698	1.405282	0.396784
B	3.893761	1.708691	-0.014474
B	2.623848	2.152871	-0.800061
Ge	1.877620	-1.805553	-0.564040
Ge	-3.443593	-0.270751	0.229957

22

scf done: -4650.885610

B	1.115671	-0.745152	-1.775586
B	-3.249499	1.052205	-0.934451
B	1.499377	-0.537439	1.424040
B	-2.057784	1.926671	-1.231874
B	0.783923	2.048744	-0.545338
B	1.875150	1.159445	0.770507
B	1.772062	0.669557	2.405054
B	-0.723850	2.867583	-1.020242
B	-0.365361	-0.572323	-0.974451
B	0.685029	-3.085315	0.277386
B	0.738137	0.707859	-1.392436
B	0.780069	-2.057742	-1.003553
B	-1.932012	0.120368	-0.889261
B	1.740160	-2.041984	0.780700
B	0.344362	3.601371	-0.215308

B	1.836516	2.158377	2.115579
B	-0.819281	-2.708186	0.033645
B	-1.581625	-1.309583	0.031547
B	1.308246	2.956150	0.845684
B	0.077645	-1.353680	0.666034
Ge	-3.566450	-0.336279	0.485949
Ge	2.968492	-0.422616	-0.387149