Supporting Information available for

A motif for heteronuclear C≡E (E = Si, Ge, Sn, Pb) bonding: Lewis acid-base pair strategy

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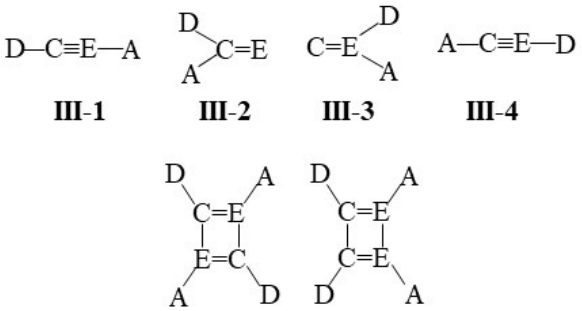
Supporting Information Available (S1-S9).

S1

In order to evaluate the effects of dispersion, B3LYP-D3BJ and BP86-D3BJ methods were employed. Here, we took the dissociation reaction $(NHC^{AR})C{\equiv}E(Al(C_6F_5)_3) \rightarrow (NHC^{AR})C{\equiv}E + Al(C_6F_5)_3$ as the test example, which has the smallest dissociation energy among the decomposition channels we considered. From the values in Table S1, the dissociation energies at B3LYP-D3BJ and BP86-D3BJ levels are very close, and a little larger than the values without dispersion correction. Clearly, the dispersion has the effect on our target compounds due to the bulky system, but the influence is favorable in the stability of our target compounds.

Table S1 The dissociation energies for the reaction $(NHC^{AR})C{\equiv}E(Al(C_6F_5)_3) \rightarrow (NHC^{AR})C{\equiv}E + Al(C_6F_5)_3$ at three kinds of levels.

	B3LYP/def2-SVP	B3LYP-D3BJ/def2-SVP	BP86-D3BJ/def2-SVP
E = Si	20.8	47.7	48.0
E = Ge	19.1	46.4	46.9
E = Sn	15.4	42.8	42.8
E = Pb	14.4	39.5	41.5



Scheme S1 The possible competitive initial structures and dimers of **III-1**.

Table S2 The Mayer, Wiberg and Fuzzy bond index values (MBI, WBI, FBI) of C≡E, C_{NHC}=C and E-Al bonds in **III-1** at the level of B3LYP/def2-SVP.

	C≡E			C_{NHC}=C	E-Al
	MBI	WBI	FBI	MBI	MBI
E=Si	2.40	2.08	2.33	1.13	0.49
E=Ge	2.30	2.06	2.31	1.07	0.64
E=Sn	2.20	1.87	2.29	1.07	0.51
E=Pb	1.92	1.73	2.20	1.36	0.42

Table S3 The dissociation energies (in kcal/mol) of **III-1** at the level of BP86-D3BJ/def2-svp.

	E=Si	E=Ge	E=Sn	E=Pb
III-1→ ^{1}EC + NHC^{AR}+ Al(C_6F_5)$_3$	202.5	204.1	195.2	191.1
III-1→ ^{3}EC + NHC^{AR}+ Al(C_6F_5)$_3$	185.9	180.6	170.6	165.3
III-1→ NHC^{AR} + CEAl(C_6F_5)$_3$	180.8	140.7	127.6	121.6
III-1→ NHC^{AR}CE + Al(C_6F_5)$_3$	48.0	46.9	42.8	41.5

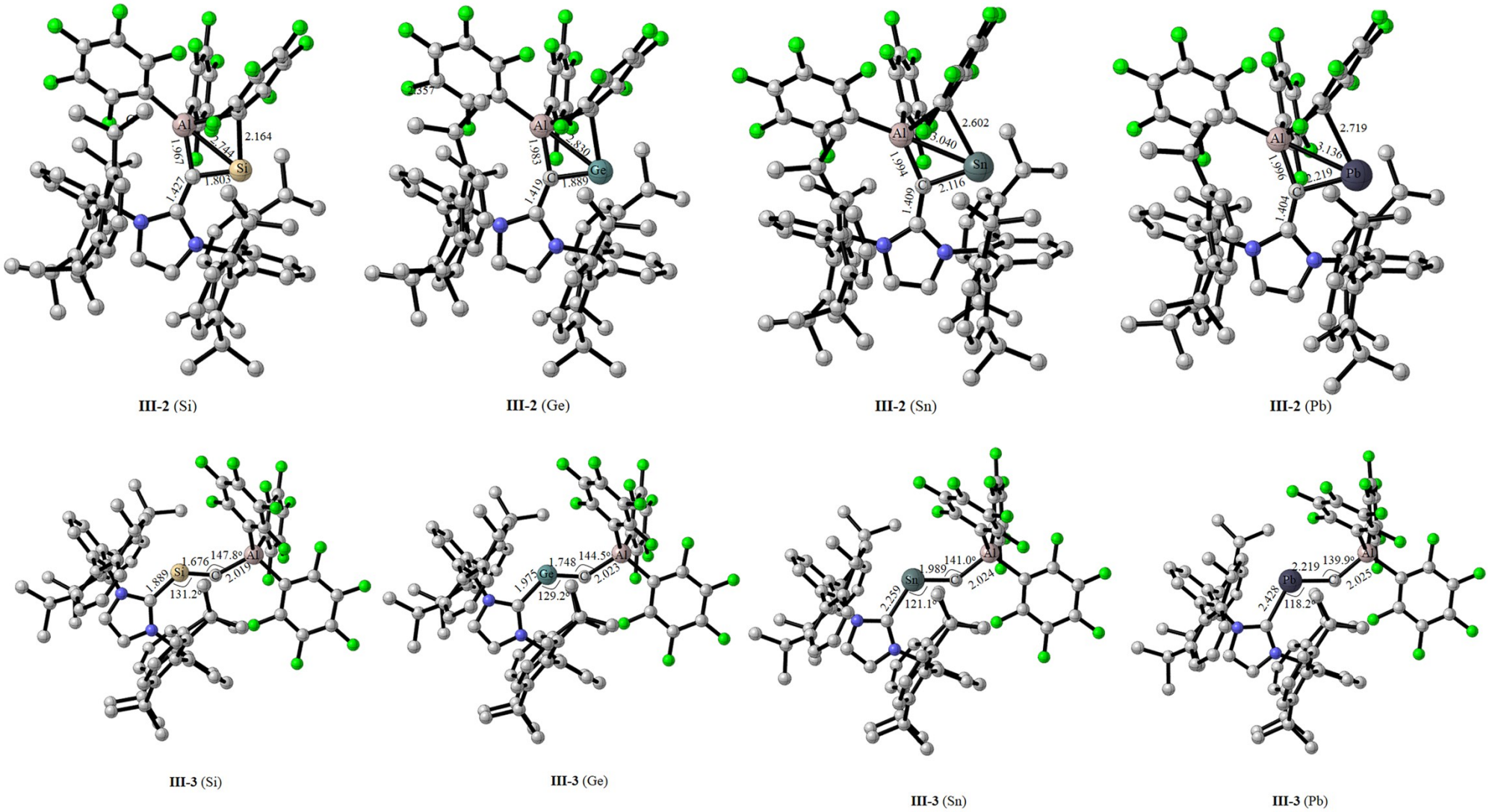


Figure S1 Structures of **III-2** and **III-3**, H atoms are omitted for clarity. Calculated bond lengths [Å] and angles [°] are at the level of B3LYP/def2-TZVPP//B3LYP/def2-SVP.

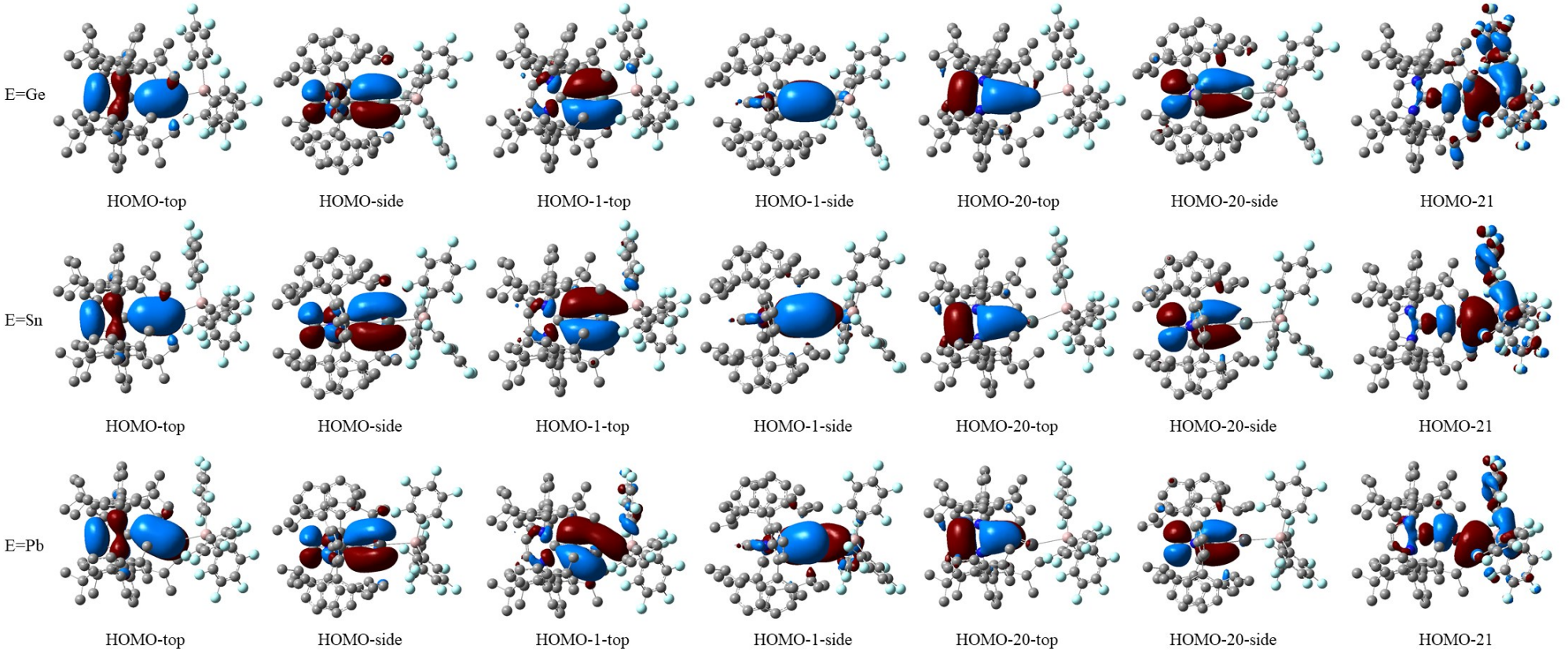


Figure S2 Molecular orbitals of **III-1** for E=Ge/Sn/Pb systems.

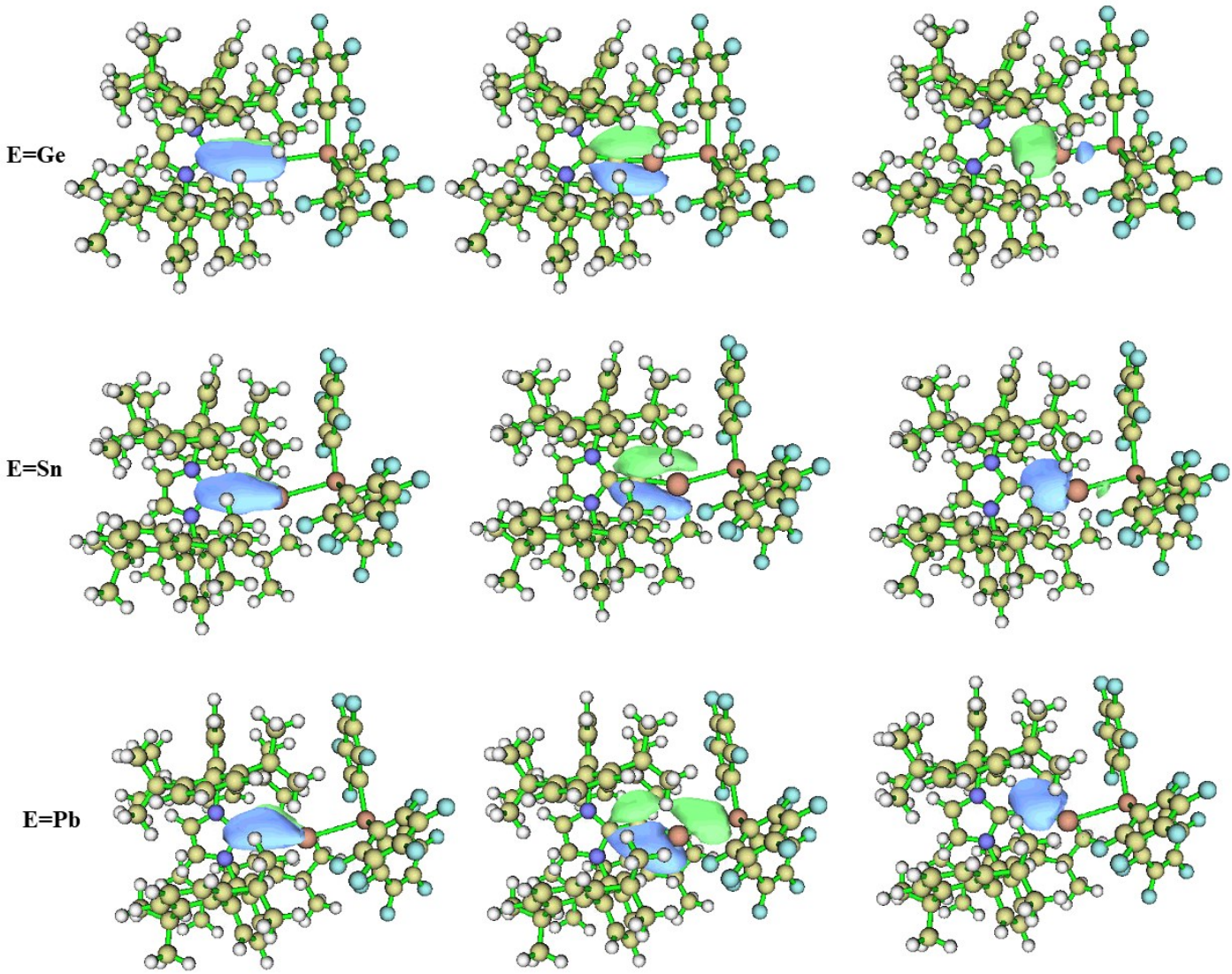


Figure S3 Isosurface map of all unique Pipek-Mezey localized molecular orbitals (LMOs) of **III-1**. Green and blue correspond to positive and negative orbital phases, respectively.

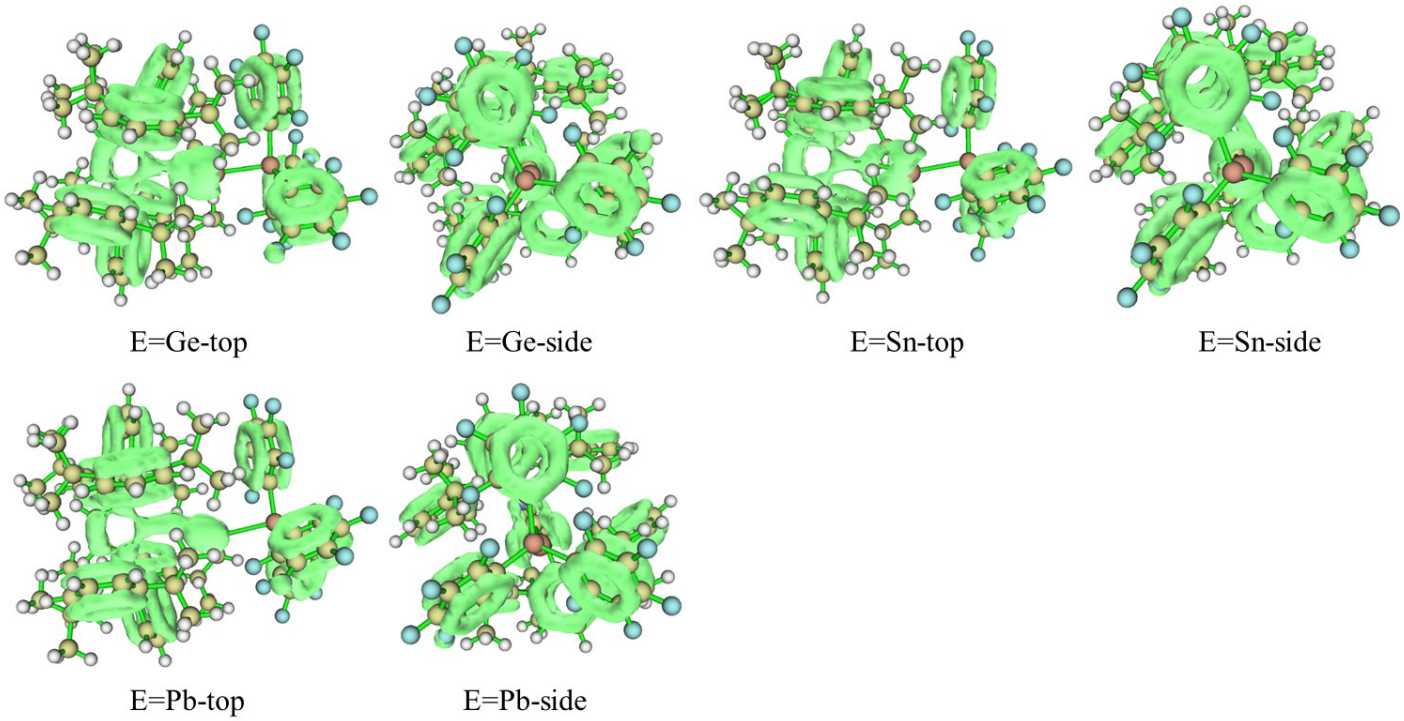


Figure S4 The localized orbital locator calculated based on π orbitals (LOL-π) of **III-1**.

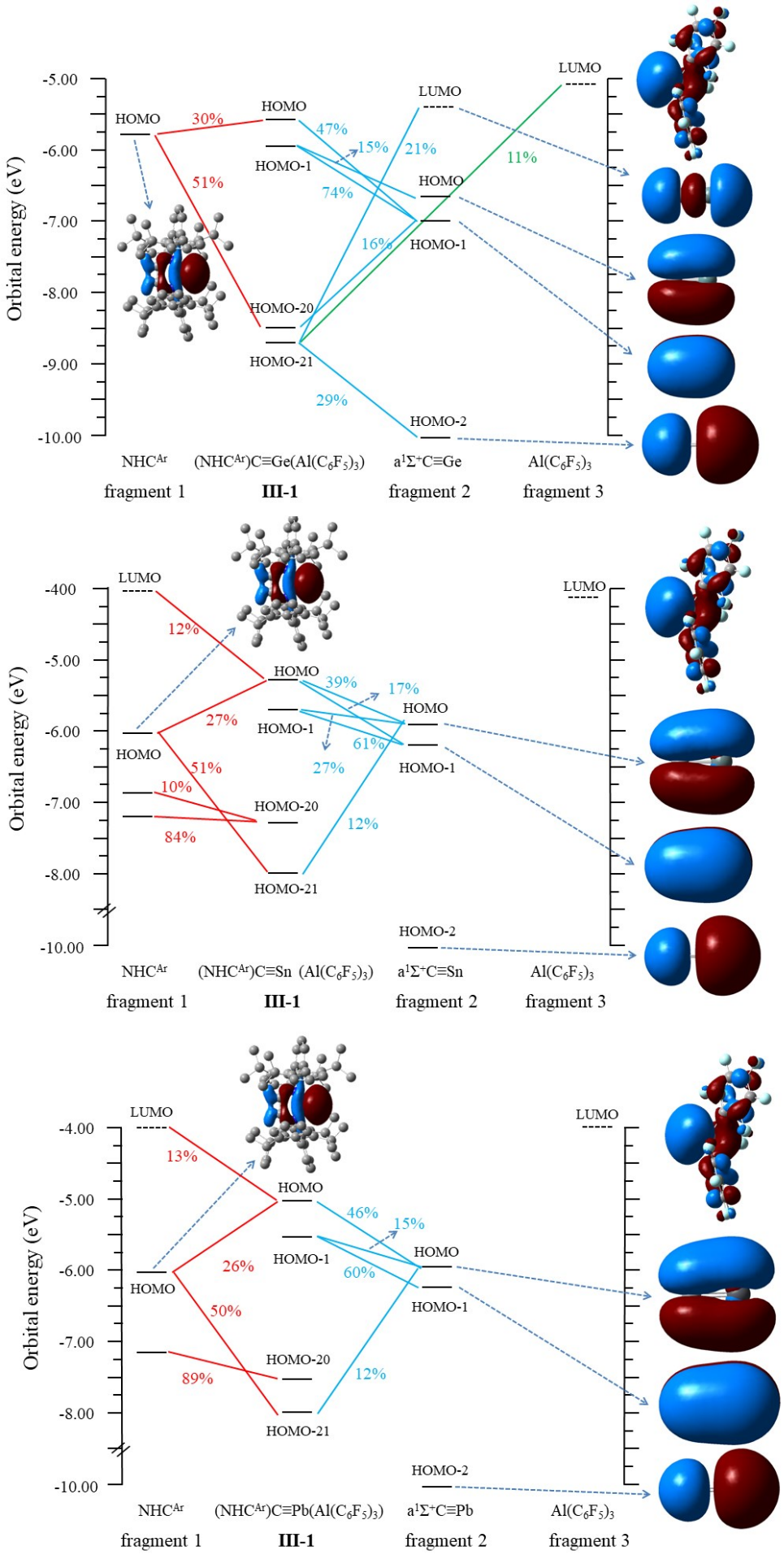


Figure S5 The orbital interaction diagram and orbital contributions of three fragments in **III-1** (E=Ge/Sn/Pb). Solid and dashed bars correspond to occupied and virtual MOs, respectively.

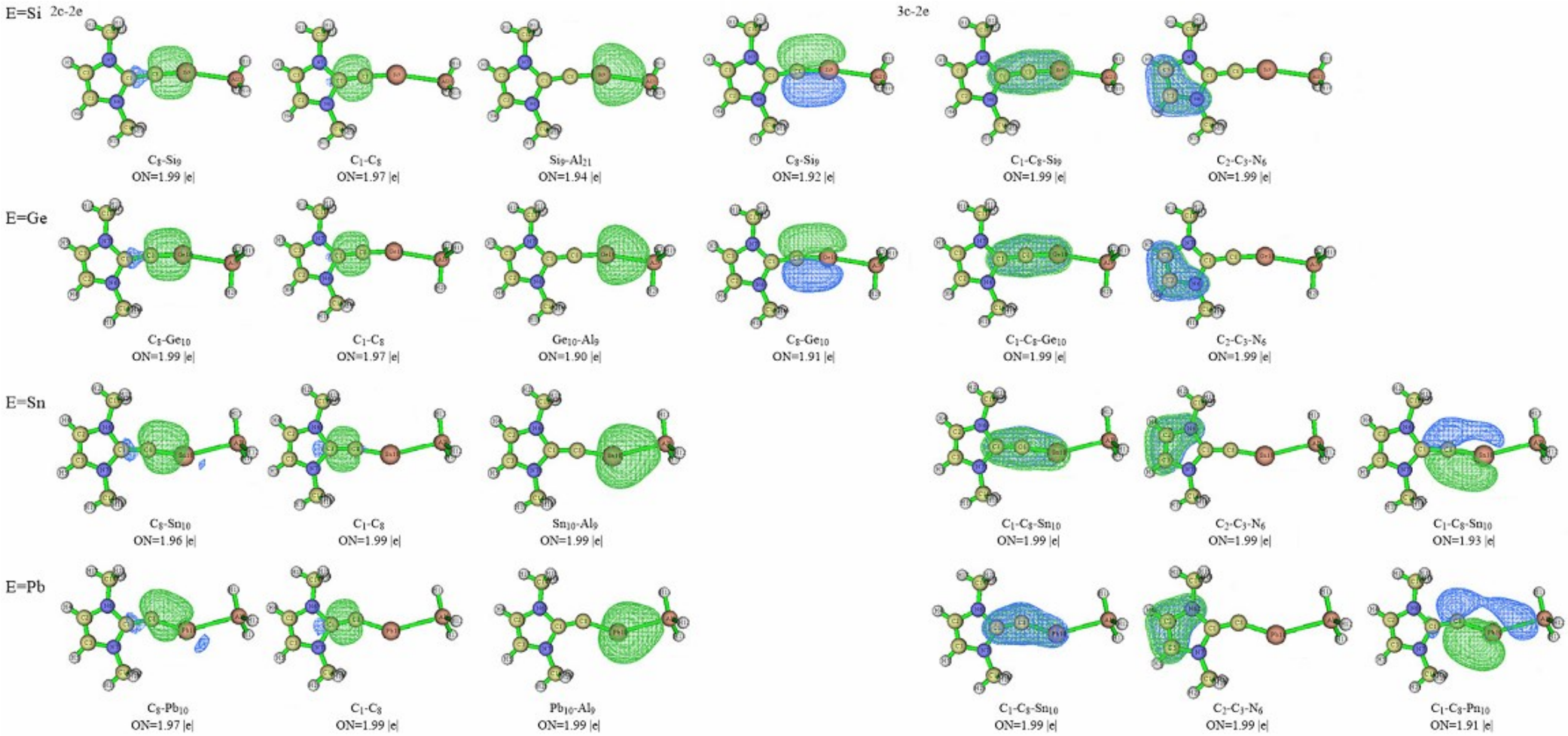


Figure S6 The AdNDP analysis of $(NHC^{ME})C{\equiv}E(AlH_3)$ calculated at the level of B3LYP/def2-SVP. Occupation numbers (ON) in |e|.

Table S4 The infrared vibrational frequency values (cm-1) and the infrared vibrational intensities (km/mol) in parenthesis of **III-1** at the level of B3LYP/def2-SVP.

system		infrared vibrational frequency values (infrared vibrational intensities)								
		1	2	3	4	5	6	7	8	9
III-1	E=Si	7.8 (0.04)	13.4 (0.003)	16.0 (0.03)	17.7 (0.02)	20.0 (0.36)	23.1 (0.06)	24.5 (0.19)	26.2 (0.28)	29.8 (0.15)
	E=Ge	12.9 (0.007)	13.8 (0.004)	16.4 (0.08)	18.1 (0.01)	20.0 (0.27)	22.9 (0.14)	24.1 (0.01)	26.3 (0.38)	30.4 (0.17)
	E=Sn	5.4 (0.01)	11.0 (0.006)	13.8 (0.05)	17.9 (0.01)	18.7 (0.16)	19.8 (0.20)	24.3 (0.04)	24.5 (0.70)	28.7 (0.34)
	E=Pb	8.9 (0.01)	11.6 (0.007)	15.7 (0.003)	16.3 (0.09)	19.7 (0.15)	22.6 (0.02)	23.2 (0.12)	25.3 (0.16)	26.9 (0.18)

S12. The geometries (in angstrom) and total energies (in a.u.) of **III-1** at the level of B3LYP/def2-SVP.

III-1(Si)
E= -5311.31930702

6	0	-1.791509	0.070988	-0.132463
6	0	-3.802408	-0.286552	0.848785
6	0	-4.036243	0.198513	-0.389959
1	0	-4.500529	-0.575016	1.620817
1	0	-4.972951	0.411777	-0.883836
7	0	-2.432115	-0.380315	1.019897
7	0	-2.815160	0.425422	-1.007447
6	0	-0.419743	0.143450	-0.319819
14	0	1.211735	0.208406	-0.386142
6	0	3.776429	-0.800794	1.773611
6	0	3.158571	-0.092746	2.804198
6	0	4.293282	-2.044585	2.136438
6	0	3.028895	-0.565283	4.108859
6	0	4.200911	-2.564088	3.430990
6	0	3.554396	-1.821471	4.420416
6	0	4.448833	-1.167334	-1.559258
6	0	5.778691	-1.584588	-1.508828
6	0	3.732780	-1.579995	-2.679409
6	0	6.375810	-2.382793	-2.486253
6	0	4.274918	-2.382638	-3.684769
6	0	5.608445	-2.786381	-3.583133
6	0	4.613454	1.821987	-0.206553
6	0	5.255015	2.491511	0.838223
6	0	4.628254	2.480078	-1.436506
6	0	5.852436	3.746745	0.688710
6	0	5.204275	3.734195	-1.640064
6	0	5.823498	4.370205	-0.561256
9	0	6.147218	-3.548804	-4.529126
9	0	7.649678	-2.758474	-2.393900
9	0	6.544771	-1.197618	-0.471918
9	0	2.444044	-1.211412	-2.836774
9	0	3.538224	-2.768124	-4.728497
9	0	4.042798	1.902867	-2.505567
9	0	5.333741	1.932916	2.055272
9	0	6.452549	4.349112	1.713944
9	0	6.382741	5.564800	-0.723246
9	0	5.162514	4.327638	-2.832352
9	0	4.885606	-2.829956	1.221757
9	0	2.627759	1.117997	2.536189
9	0	2.395546	0.141055	5.047078
9	0	3.425867	-2.310471	5.650306
9	0	4.676799	-3.776174	3.717031
6	0	-1.831564	-0.815680	2.270370
6	0	-1.772911	0.103734	3.354801
6	0	-1.420598	-2.167318	2.446501
6	0	-1.153013	-0.307692	4.546043
6	0	-0.823441	-2.515870	3.671076
6	0	-0.649798	-1.594840	4.698500
1	0	-1.084911	0.404794	5.369487
1	0	-0.508363	-3.549664	3.815956
1	0	-0.158333	-1.889806	5.628536
6	0	-2.776207	0.900695	-2.384373
6	0	-3.115651	-0.009834	-3.425432
6	0	-2.602484	2.282773	-2.675193
6	0	-3.181695	0.469585	-4.744515
6	0	-2.706195	2.696953	-4.015401
6	0	-2.969711	1.808143	-5.048919
1	0	-3.441204	-0.234170	-5.536587
1	0	-2.601539	3.760102	-4.231789

1	0	-3.043889	2.162292	-6.079867
13	0	3.801652	-0.000766	-0.069330
6	0	-2.411834	1.472922	3.380615
6	0	-1.620332	2.638678	3.222026
6	0	-3.785272	1.591322	3.737850
6	0	-2.238871	3.895277	3.315089
6	0	-4.356163	2.869624	3.818590
6	0	-3.596471	4.015221	3.591990
1	0	-1.638730	4.796883	3.180438
1	0	-5.408978	2.974088	4.087947
1	0	-4.059702	5.003211	3.659105
6	0	-1.668319	-3.307898	1.486825
6	0	-0.585360	-3.984336	0.859463
6	0	-2.986995	-3.834805	1.364619
6	0	-0.864343	-5.082792	0.030287
6	0	-3.210794	-4.927499	0.516485
6	0	-2.162833	-5.538716	-0.165157
1	0	-0.039411	-5.602418	-0.460965
1	0	-4.220398	-5.327679	0.409760
1	0	-2.355208	-6.391256	-0.821515
6	0	-2.413433	3.414897	-1.694261
6	0	-1.169084	4.102324	-1.641797
6	0	-3.542248	3.939437	-1.007742
6	0	-1.065197	5.244648	-0.833960
6	0	-3.380075	5.076418	-0.202792
6	0	-2.150919	5.721512	-0.105510
1	0	-0.114281	5.778249	-0.780430
1	0	-4.239281	5.481710	0.335142
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6	0	-3.526696	-1.454019	-3.261290
6	0	-2.579326	-2.494534	-3.451043
6	0	-4.908004	-1.762026	-3.114316
6	0	-3.027577	-3.823528	-3.408168
6	0	-5.301017	-3.108129	-3.070860
6	0	-4.369663	-4.132917	-3.206415
1	0	-2.312498	-4.635438	-3.541877
1	0	-6.357291	-3.358746	-2.952146
1	0	-4.693124	-5.176724	-3.174483
6	0	-0.104036	2.578536	3.066405
6	0	0.588141	2.919464	4.401531
6	0	0.425082	3.483570	1.947741
1	0	0.170070	1.547364	2.804997
1	0	0.263473	2.256396	5.217126
1	0	1.678862	2.814926	4.304003
1	0	0.365144	3.955639	4.705638
1	0	-0.088865	3.286028	0.998329
1	0	0.294565	4.552295	2.182986
1	0	1.502334	3.311635	1.802941
6	0	-4.626156	0.389829	4.177509
6	0	-6.082060	0.428251	3.682601
6	0	-4.596562	0.247028	5.712902
1	0	-4.159242	-0.520462	3.772592
1	0	-6.151180	0.614174	2.599437
1	0	-6.585315	-0.527747	3.899672
1	0	-6.664958	1.215964	4.185354
1	0	-3.569082	0.137350	6.089326
1	0	-5.037988	1.133793	6.196175
1	0	-5.171491	-0.637179	6.034667
6	0	0.033822	3.713736	-2.505556
6	0	1.364620	3.706972	-1.741530
6	0	0.170416	4.649890	-3.725189
1	0	-0.131054	2.691116	-2.876877
1	0	1.325084	3.054424	-0.857967
1	0	2.166462	3.344661	-2.398978
1	0	1.651958	4.714538	-1.400707

1	0	-0.727474	4.658062	-4.358666
1	0	0.355705	5.687342	-3.401828
1	0	1.021111	4.338404	-4.352742
6	0	-4.960248	3.414457	-1.237573
6	0	-5.705745	4.316175	-2.242221
6	0	-5.777138	3.249986	0.053275
1	0	-4.882281	2.425678	-1.709425
1	0	-5.166358	4.386004	-3.199263
1	0	-6.714365	3.920911	-2.448867
1	0	-5.818378	5.338681	-1.846606
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1	0	-6.020900	4.222137	0.510193
1	0	-6.736314	2.750328	-0.162364
6	0	0.887312	-3.668186	1.135297
6	0	1.738169	-3.527448	-0.135202
6	0	1.499316	-4.756426	2.044216
1	0	0.939805	-2.708269	1.669235
1	0	1.368687	-2.723465	-0.785472
1	0	2.781551	-3.307134	0.128733
1	0	1.751757	-4.454603	-0.729883
1	0	0.937159	-4.884935	2.981498
1	0	1.506792	-5.733123	1.533789
1	0	2.540288	-4.514156	2.307029
6	0	-4.139408	-3.375923	2.259824
6	0	-4.222420	-4.273618	3.511629
6	0	-5.501697	-3.316949	1.550832
1	0	-3.908403	-2.366358	2.622887
1	0	-3.278412	-4.264254	4.077304
1	0	-5.025686	-3.931331	4.185300
1	0	-4.435827	-5.318232	3.232362
1	0	-5.447255	-2.757067	0.605122
1	0	-5.888148	-4.322114	1.319439
1	0	-6.249059	-2.831877	2.199912
6	0	-1.112525	-2.212201	-3.783535
6	0	-0.886494	-2.083498	-5.304544
6	0	-0.154042	-3.272878	-3.228618
1	0	-0.841354	-1.249595	-3.320665
1	0	-1.464893	-1.263994	-5.751945
1	0	0.179379	-1.894117	-5.510789
1	0	-1.169098	-3.017103	-5.818898
1	0	-0.326548	-3.451875	-2.159985
1	0	-0.259437	-4.234553	-3.756866
1	0	0.884205	-2.943865	-3.367010
6	0	-6.003242	-0.691134	-3.122622
6	0	-7.093943	-0.912595	-2.059443
6	0	-6.648252	-0.580810	-4.518833
1	0	-5.531097	0.282341	-2.920634
1	0	-6.671120	-1.080325	-1.056902
1	0	-7.763222	-0.038492	-2.009650
1	0	-7.724242	-1.784263	-2.295932
1	0	-5.903629	-0.344021	-5.292593
1	0	-7.135065	-1.528270	-4.801430
1	0	-7.414890	0.211515	-4.532807

III-1(Ge)

E=-7098.86285890

6	0	-1.849110	0.058599	-0.134001
6	0	-3.847804	-0.355882	0.854979
6	0	-4.099896	0.192964	-0.353084
1	0	-4.535480	-0.687276	1.619046
1	0	-5.044407	0.428336	-0.821667
7	0	-2.475022	-0.455875	1.003380
7	0	-2.888331	0.455936	-0.975096
6	0	-0.484804	0.144726	-0.339637
6	0	3.788571	-0.856063	1.742325

6	0	3.159061	-0.195259	2.797269
6	0	4.301114	-2.115784	2.052980
6	0	3.016092	-0.727536	4.077368
6	0	4.195167	-2.694243	3.321098
6	0	3.537604	-1.997349	4.336221
6	0	4.516615	-1.083583	-1.587812
6	0	5.855372	-1.470214	-1.529416
6	0	3.826015	-1.481108	-2.729113
6	0	6.486194	-2.225189	-2.519453
6	0	4.402160	-2.242043	-3.748266
6	0	5.744183	-2.614675	-3.638794
6	0	4.590782	1.865268	-0.126121
6	0	5.230202	2.501213	0.940403
6	0	4.555050	2.585578	-1.320058
6	0	5.779967	3.783138	0.845796
6	0	5.082166	3.868567	-1.468002
6	0	5.701416	4.469280	-0.368930
9	0	6.314786	-3.335953	-4.598054
9	0	7.767310	-2.572477	-2.418685
9	0	6.594342	-1.096019	-0.467612
9	0	2.531786	-1.139502	-2.893750
9	0	3.691006	-2.614048	-4.813413
9	0	3.967522	2.041249	-2.404894
9	0	5.351922	1.881269	2.123735
9	0	6.380217	4.352943	1.889152
9	0	6.214429	5.690127	-0.478503
9	0	4.993819	4.522137	-2.625665
9	0	4.902482	-2.857887	1.108660
9	0	2.628706	1.025632	2.578995
9	0	2.372251	-0.065688	5.040135
9	0	3.394742	-2.542286	5.540555
9	0	4.667990	-3.918162	3.556118
6	0	-1.857668	-0.948687	2.223149
6	0	-1.799398	-0.085853	3.353550
6	0	-1.427933	-2.302412	2.326605
6	0	-1.166650	-0.550463	4.518145
6	0	-0.820482	-2.706868	3.528808
6	0	-0.650240	-1.838619	4.601699
1	0	-1.099335	0.120108	5.376171
1	0	-0.494000	-3.743238	3.618801
1	0	-0.149984	-2.176105	5.512424
6	0	-2.867874	0.997385	-2.326634
6	0	-3.209229	0.134322	-3.406504
6	0	-2.708132	2.393116	-2.553369
6	0	-3.296027	0.674850	-4.700429
6	0	-2.832381	2.869750	-3.870903
6	0	-3.101199	2.028722	-4.942510
1	0	-3.557102	0.007013	-5.522564
1	0	-2.739972	3.942958	-4.037713
1	0	-3.191711	2.431125	-5.954286
13	0	3.839216	0.016477	-0.064168
6	0	-2.450132	1.274303	3.453185
6	0	-1.670970	2.454059	3.344922
6	0	-3.821342	1.361959	3.827336
6	0	-2.300841	3.698596	3.502350
6	0	-4.403749	2.629144	3.973768
6	0	-3.657162	3.791741	3.795270
1	0	-1.710579	4.611586	3.406182
1	0	-5.455147	2.710137	4.256413
1	0	-4.129272	4.770782	3.912667
6	0	-1.662820	-3.395370	1.309819
6	0	-0.571755	-4.029378	0.651885
6	0	-2.975604	-3.928874	1.157938
6	0	-0.838153	-5.087766	-0.231676
6	0	-3.186658	-4.980593	0.256311

6	0	-2.131468	-5.546833	-0.452220
1	0	-0.007252	-5.573635	-0.746809
1	0	-4.192049	-5.384810	0.127357
1	0	-2.313903	-6.367752	-1.150421
6	0	-2.514384	3.478220	-1.521346
6	0	-1.272478	4.168317	-1.446763
6	0	-3.638872	3.963105	-0.799579
6	0	-1.166567	5.271188	-0.586023
6	0	-3.474551	5.060911	0.057666
6	0	-2.247716	5.707135	0.174280
1	0	-0.217798	5.806566	-0.515471
1	0	-4.330563	5.435111	0.622583
1	0	-2.139787	6.567207	0.840410
6	0	-3.595791	-1.321883	-3.303208
6	0	-2.632540	-2.336026	-3.547411
6	0	-4.969388	-1.660297	-3.153284
6	0	-3.056055	-3.673637	-3.555019
6	0	-5.337798	-3.014056	-3.161707
6	0	-4.389980	-4.015218	-3.350589
1	0	-2.328188	-4.466071	-3.730960
1	0	-6.387876	-3.288746	-3.041258
1	0	-4.694580	-5.065148	-3.358086
6	0	-0.154925	2.417595	3.177681
6	0	0.540737	2.705529	4.523455
6	0	0.357375	3.378608	2.098526
1	0	0.128956	1.402252	2.868337
1	0	0.228055	2.002060	5.309352
1	0	1.632127	2.619018	4.416253
1	0	0.306976	3.723937	4.875632
1	0	-0.159480	3.218162	1.143660
1	0	0.215349	4.433890	2.382573
1	0	1.435974	3.226851	1.940952
6	0	-4.646697	0.132333	4.215834
6	0	-6.107540	0.180211	3.736308
6	0	-4.601829	-0.083911	5.742266
1	0	-4.174814	-0.752797	3.763501
1	0	-6.188838	0.420111	2.664654
1	0	-6.598937	-0.790893	3.908977
1	0	-6.693621	0.935206	4.283605
1	0	-3.570055	-0.201597	6.104239
1	0	-5.047149	0.774220	6.271491
1	0	-5.165610	-0.988131	6.025864
6	0	-0.075114	3.826199	-2.337792
6	0	1.264159	3.803485	-1.588444
6	0	0.040378	4.810874	-3.520851
1	0	-0.234782	2.817158	-2.746842
1	0	1.239440	3.120085	-0.728162
1	0	2.062434	3.472006	-2.266490
1	0	1.546986	4.801098	-1.216051
1	0	-0.862534	4.833216	-4.146575
1	0	0.216551	5.836925	-3.158317
1	0	0.889408	4.534182	-4.166718
6	0	-5.056245	3.441141	-1.039802
6	0	-5.816788	4.384622	-1.993505
6	0	-5.859057	3.211653	0.249997
1	0	-4.977800	2.475935	-1.558120
1	0	-5.287387	4.502708	-2.951375
1	0	-6.825213	3.993467	-2.208741
1	0	-5.931088	5.386658	-1.548992
1	0	-5.307798	2.587689	0.968674
1	0	-6.103917	4.160026	0.754002
1	0	-6.817418	2.716555	0.020678
6	0	0.897931	-3.714804	0.946295
6	0	1.752525	-3.511370	-0.313430
6	0	1.516668	-4.838995	1.805757

1	0	0.941637	-2.779755	1.523603
1	0	1.378032	-2.685476	-0.932535
1	0	2.792383	-3.291433	-0.034487
1	0	1.779364	-4.412870	-0.945915
1	0	0.953043	-5.016849	2.733918
1	0	1.534427	-5.790374	1.249814
1	0	2.554666	-4.600297	2.083394
6	0	-4.134924	-3.526695	2.071154
6	0	-4.214873	-4.488806	3.274327
6	0	-5.494382	-3.441627	1.359506
1	0	-3.913696	-2.535654	2.487139
1	0	-3.273174	-4.500471	3.843910
1	0	-5.023824	-4.188911	3.961300
1	0	-4.417809	-5.519439	2.940598
1	0	-5.438595	-2.834963	0.443226
1	0	-5.872737	-4.436661	1.076529
1	0	-6.248204	-2.994483	2.028161
6	0	-1.177070	-2.011157	-3.889517
6	0	-0.980685	-1.831466	-5.409373
6	0	-0.185687	-3.064143	-3.379692
1	0	-0.921329	-1.057189	-3.401140
1	0	-1.590935	-1.016683	-5.821920
1	0	0.075052	-1.604770	-5.629778
1	0	-1.245955	-2.757217	-5.946608
1	0	-0.340920	-3.280723	-2.315246
1	0	-0.273837	-4.011609	-3.936118
1	0	0.843414	-2.706048	-3.517807
6	0	-6.082251	-0.608825	-3.105184
6	0	-7.158745	-0.893185	-2.042656
6	0	-6.742696	-0.449914	-4.489495
1	0	-5.623905	0.362786	-2.865886
1	0	-6.723573	-1.092495	-1.051336
1	0	-7.843419	-0.034392	-1.952183
1	0	-7.775160	-1.766280	-2.308730
1	0	-6.009654	-0.168474	-5.259347
1	0	-7.217268	-1.392291	-4.807733
1	0	-7.521850	0.329781	-4.462731
32	0	1.215204	0.226811	-0.383234

III-1(Sn)

E= -5236.18115565

6	0	-2.009197	0.024265	-0.042677
6	0	-4.098581	-0.408175	0.750720
6	0	-4.241230	0.260698	-0.412036
1	0	-4.851535	-0.789571	1.425604
1	0	-5.141237	0.567606	-0.924345
7	0	-2.743531	-0.572333	0.992395
7	0	-2.977803	0.543368	-0.916139
6	0	-0.635509	0.061268	-0.122899
6	0	4.040484	-0.674396	1.846332
6	0	3.760475	0.188444	2.908202
6	0	4.350823	-1.985614	2.211188
6	0	3.803532	-0.195797	4.248230
6	0	4.383619	-2.429060	3.535345
6	0	4.104731	-1.524106	4.561408
6	0	4.607413	-1.273395	-1.473535
6	0	5.897769	-1.790789	-1.356917
6	0	3.900685	-1.674995	-2.603383
6	0	6.465859	-2.669606	-2.279918
6	0	4.414441	-2.555347	-3.557917
6	0	5.708557	-3.054476	-3.390876
6	0	4.837777	1.801562	-0.332425
6	0	5.745217	2.402620	0.542848
6	0	4.558825	2.518741	-1.494471
6	0	6.322829	3.652502	0.301715

6	0	5.097509	3.773063	-1.779944
6	0	5.990451	4.341563	-0.867998
9	0	6.219833	-3.890698	-4.287594
9	0	7.701711	-3.137725	-2.124550
9	0	6.650486	-1.424002	-0.301935
9	0	2.649024	-1.219040	-2.821517
9	0	3.688456	-2.922902	-4.613585
9	0	3.704091	2.001509	-2.402005
9	0	6.113648	1.773429	1.668515
9	0	7.184129	4.190575	1.162225
9	0	6.523118	5.533651	-1.112521
9	0	4.760753	4.431905	-2.888371
9	0	4.625405	-2.904741	1.269178
9	0	3.422247	1.467084	2.652077
9	0	3.533666	0.669964	5.225526
9	0	4.128409	-1.921056	5.828500
9	0	4.649915	-3.702204	3.824147
6	0	-2.265778	-1.186424	2.216862
6	0	-2.320321	-0.429791	3.420191
6	0	-1.900554	-2.560742	2.253851
6	0	-1.909929	-1.035344	4.619299
6	0	-1.517458	-3.111287	3.490186
6	0	-1.494977	-2.361196	4.659943
1	0	-1.945272	-0.446007	5.537133
1	0	-1.259373	-4.170248	3.523516
1	0	-1.189170	-2.818214	5.604203
6	0	-2.842159	1.185491	-2.213009
6	0	-3.123597	0.415645	-3.378924
6	0	-2.631264	2.590877	-2.324665
6	0	-3.092189	1.048213	-4.632949
6	0	-2.637528	3.161685	-3.610186
6	0	-2.839724	2.408150	-4.758968
1	0	-3.309996	0.450329	-5.519072
1	0	-2.511430	4.240943	-3.691645
1	0	-2.838624	2.885012	-5.742050
13	0	4.040133	-0.003323	-0.037502
6	0	-2.863064	0.972116	3.553982
6	0	-1.976549	2.079074	3.557029
6	0	-4.241017	1.158667	3.852233
6	0	-2.499582	3.361545	3.780861
6	0	-4.714668	2.461373	4.068418
6	0	-3.856225	3.557056	4.022935
1	0	-1.829233	4.222438	3.775273
1	0	-5.770669	2.620883	4.296594
1	0	-4.243539	4.564703	4.195759
6	0	-1.985891	-3.555309	1.120861
6	0	-0.800333	-4.107879	0.562104
6	0	-3.251806	-4.103712	0.774698
6	0	-0.918360	-5.136616	-0.385472
6	0	-3.314387	-5.117065	-0.192457
6	0	-2.159878	-5.628040	-0.776865
1	0	-0.016072	-5.569705	-0.821223
1	0	-4.283434	-5.535356	-0.471459
1	0	-2.225621	-6.426199	-1.520965
6	0	-2.511505	3.596826	-1.202635
6	0	-1.284424	4.285299	-0.982858
6	0	-3.685955	4.020208	-0.520969
6	0	-1.243039	5.296258	-0.010380
6	0	-3.586445	5.028123	0.449023
6	0	-2.373559	5.654171	0.717263
1	0	-0.305708	5.824450	0.173541
1	0	-4.481982	5.349187	0.984210
1	0	-2.314858	6.441738	1.473129
6	0	-3.574702	-1.026340	-3.408767
6	0	-2.640791	-2.069070	-3.646441

6	0	-4.969168	-1.309574	-3.383250
6	0	-3.118081	-3.383463	-3.763209
6	0	-5.392681	-2.641769	-3.502300
6	0	-4.476645	-3.674206	-3.678565
1	0	-2.412798	-4.197558	-3.930977
1	0	-6.459665	-2.872948	-3.477942
1	0	-4.823417	-4.706876	-3.770259
6	0	-0.464979	1.902087	3.428346
6	0	0.202197	1.876295	4.818175
6	0	0.198744	2.967190	2.546963
1	0	-0.283157	0.928018	2.948955
1	0	-0.202340	1.077829	5.457270
1	0	1.286856	1.714683	4.725832
1	0	0.047621	2.832986	5.344481
1	0	-0.296802	3.043280	1.570010
1	0	0.176753	3.964544	3.015515
1	0	1.257919	2.713450	2.388175
6	0	-5.205213	-0.012691	4.061745
6	0	-6.585872	0.196999	3.415882
6	0	-5.366683	-0.322369	5.563507
1	0	-4.757332	-0.908534	3.604954
1	0	-6.508489	0.493666	2.358643
1	0	-7.178636	-0.730441	3.471349
1	0	-7.165756	0.978131	3.932355
1	0	-4.400864	-0.557506	6.033873
1	0	-5.798284	0.539716	6.097650
1	0	-6.036570	-1.184974	5.714809
6	0	-0.027584	4.055161	-1.828072
6	0	1.270042	4.009969	-1.007526
6	0	0.129287	5.145661	-2.910153
1	0	-0.130582	3.083243	-2.334570
1	0	1.216005	3.280892	-0.186404
1	0	2.108217	3.735714	-1.662470
1	0	1.512759	4.988044	-0.562757
1	0	-0.730616	5.200433	-3.591219
1	0	0.246251	6.138477	-2.445663
1	0	1.027727	4.953079	-3.518737
6	0	-5.083549	3.545982	-0.921580
6	0	-5.744787	4.579625	-1.856029
6	0	-5.999390	3.231175	0.271058
1	0	-4.972833	2.625687	-1.509604
1	0	-5.134326	4.760844	-2.753906
1	0	-6.737580	4.229948	-2.185201
1	0	-5.879826	5.545490	-1.342567
1	0	-5.516443	2.549416	0.985998
1	0	-6.284569	4.142356	0.820381
1	0	-6.935590	2.764967	-0.078519
6	0	0.606942	-3.698358	1.006914
6	0	1.567493	-3.467253	-0.169169
6	0	1.222705	-4.747336	1.957473
1	0	0.523954	-2.747047	1.554056
1	0	1.175921	-2.726929	-0.878938
1	0	2.541581	-3.119439	0.200213
1	0	1.761335	-4.394194	-0.732292
1	0	0.617323	-4.903261	2.861648
1	0	1.319353	-5.722679	1.452914
1	0	2.231459	-4.440006	2.277259
6	0	-4.536344	-3.747383	1.524529
6	0	-4.846408	-4.819285	2.588716
6	0	-5.748981	-3.529025	0.605526
1	0	-4.361537	-2.811466	2.071824
1	0	-4.011150	-4.937583	3.295855
1	0	-5.745515	-4.548550	3.167266
1	0	-5.029076	-5.799605	2.119282
1	0	-5.524692	-2.817637	-0.203143

1	0	-6.083611	-4.468699	0.137979
1	0	-6.602993	-3.140350	1.184889
6	0	-1.152144	-1.794280	-3.868532
6	0	-0.843821	-1.521033	-5.355608
6	0	-0.246062	-2.928317	-3.373309
1	0	-0.890663	-0.889142	-3.297071
1	0	-1.385895	-0.650140	-5.748033
1	0	0.233942	-1.333767	-5.489976
1	0	-1.113806	-2.393480	-5.973594
1	0	-0.476569	-3.206956	-2.337233
1	0	-0.345197	-3.831660	-3.997049
1	0	0.806607	-2.619275	-3.429414
6	0	-6.038291	-0.212767	-3.352666
6	0	-7.210131	-0.513540	-2.401511
6	0	-6.574786	0.064125	-4.771552
1	0	-5.561756	0.718863	-3.011992
1	0	-6.867826	-0.797902	-1.394727
1	0	-7.861962	0.370047	-2.307093
1	0	-7.840055	-1.336230	-2.775147
1	0	-5.770085	0.361343	-5.459558
1	0	-7.057798	-0.834070	-5.189400
1	0	-7.322531	0.874292	-4.754620
50	0	1.227423	0.319727	-0.439532

III-1(Pb)
E= -5214.73698316

6	0	-2.023413	-0.014799	-0.009468
6	0	-4.258278	-0.312375	0.318193
6	0	-4.106761	0.273887	-0.886298
1	0	-5.160866	-0.622443	0.825804
1	0	-4.856373	0.569127	-1.605133
7	0	-2.999354	-0.505798	0.871820
7	0	-2.749406	0.483383	-1.107611
6	0	-0.663433	-0.047510	0.217819
6	0	3.842816	-0.280686	2.169435
6	0	3.424845	0.806952	2.938601
6	0	4.001718	-1.479020	2.867437
6	0	3.177757	0.736518	4.308655
6	0	3.748568	-1.609493	4.235080
6	0	3.328082	-0.491205	4.958737
6	0	4.663418	-1.625971	-0.895563
6	0	5.876835	-2.221587	-0.548602
6	0	4.028926	-2.165126	-2.011564
6	0	6.428714	-3.304556	-1.234960
6	0	4.530046	-3.249662	-2.733409
6	0	5.741935	-3.821551	-2.338167
6	0	4.870026	1.644189	-0.441357
6	0	5.836613	2.317426	0.307302
6	0	4.531758	2.232286	-1.658979
6	0	6.434824	3.509436	-0.109940
6	0	5.092408	3.423562	-2.120357
6	0	6.052246	4.066032	-1.333658
9	0	6.242811	-4.851251	-3.011016
9	0	7.588424	-3.841702	-0.865655
9	0	6.569040	-1.730123	0.494697
9	0	2.861064	-1.643659	-2.447884
9	0	3.869735	-3.739281	-3.782905
9	0	3.594617	1.656121	-2.440916
9	0	6.235331	1.814521	1.486036
9	0	7.354558	4.117996	0.634659
9	0	6.600044	5.202434	-1.748759
9	0	4.704766	3.966796	-3.275558
9	0	4.384843	-2.592362	2.220295
9	0	3.211043	1.995910	2.340314
9	0	2.757075	1.802720	4.991375

9	0	3.070207	-0.592742	6.257317
9	0	3.871053	-2.787829	4.845366
6	0	-2.842653	-1.051330	2.206465
6	0	-3.154917	-0.221665	3.319762
6	0	-2.545058	-2.427044	2.408950
6	0	-3.090280	-0.766596	4.612727
6	0	-2.502354	-2.911964	3.729227
6	0	-2.753557	-2.097647	4.826426
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6	0	-1.463051	2.855440	-3.742109
6	0	-1.402248	2.026423	-4.855476
1	0	-1.871937	0.071177	-5.623074
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6	0	-2.691751	2.266456	3.408794
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6	0	-3.168424	3.585749	3.434061
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6	0	-4.527797	3.866707	3.326996
1	0	-2.462347	4.409503	3.546989
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6	0	-1.095867	-4.097510	1.164858
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6	0	-0.291443	3.027724	2.972426
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1	0	-1.454171	1.151559	5.674042
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1	0	-1.135827	2.900096	5.645748
1	0	-0.544627	3.146331	1.911162

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6	0	-6.619650	0.192166	4.659712
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6	0	0.178234	-3.588248	1.845994
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1	0	1.117277	-2.850220	0.009265
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1	0	0.791131	-5.506220	2.714433
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6	0	-4.946068	-3.631975	1.109572
6	0	-5.589391	-4.594926	2.127351
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6	0	-6.604645	-0.187571	-3.566824
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1	0	-7.136313	0.773411	-3.657772
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