Supplementary Information

The Role of Organoaluminum and Electron Donors in Propene Insertion on the Ziegler-Natta Catalyst

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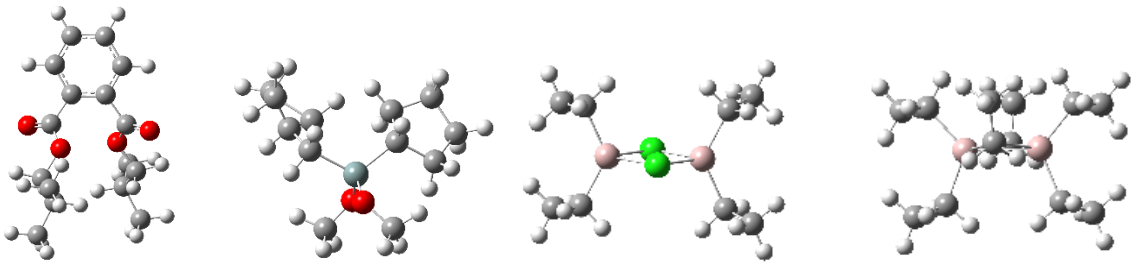


Fig. S1. Optimized geometries of DIBP, DCPDMS, $Al_2Et_4Cl_2$, and Al_2Et_6.

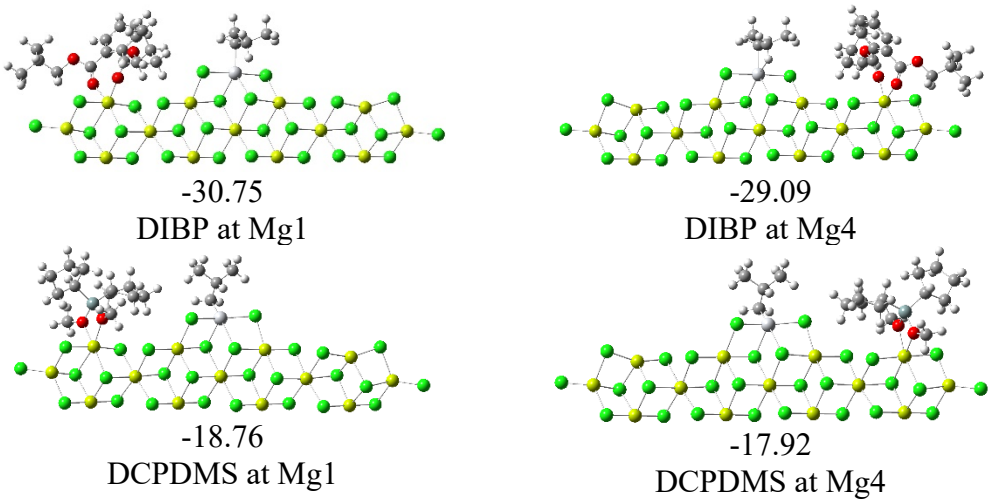


Fig. S2. Optimized geometries for DIBP and DCPDMS adsorptions onto $(MgCl_2)_{13}/TiCl_2{}^iBu$ at Mg1 (at the front of the growing chain) and at Mg4 (at the back of the growing chain). The adsorption energies (ΔE_{ads}) are shown in kcal/mol.

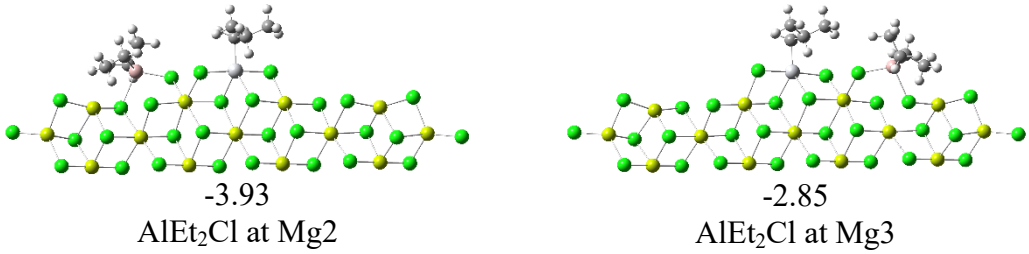


Fig. S3. Optimized geometries for $AlEt_2Cl$ adsorption onto $(MgCl_2)_{13}/TiCl_2{}^iBu$ at Mg2 (at the front of the growing chain) and at Mg3 (at the back of the growing chain). The adsorption energies (ΔE_{ads}) are shown in kcal/mol.

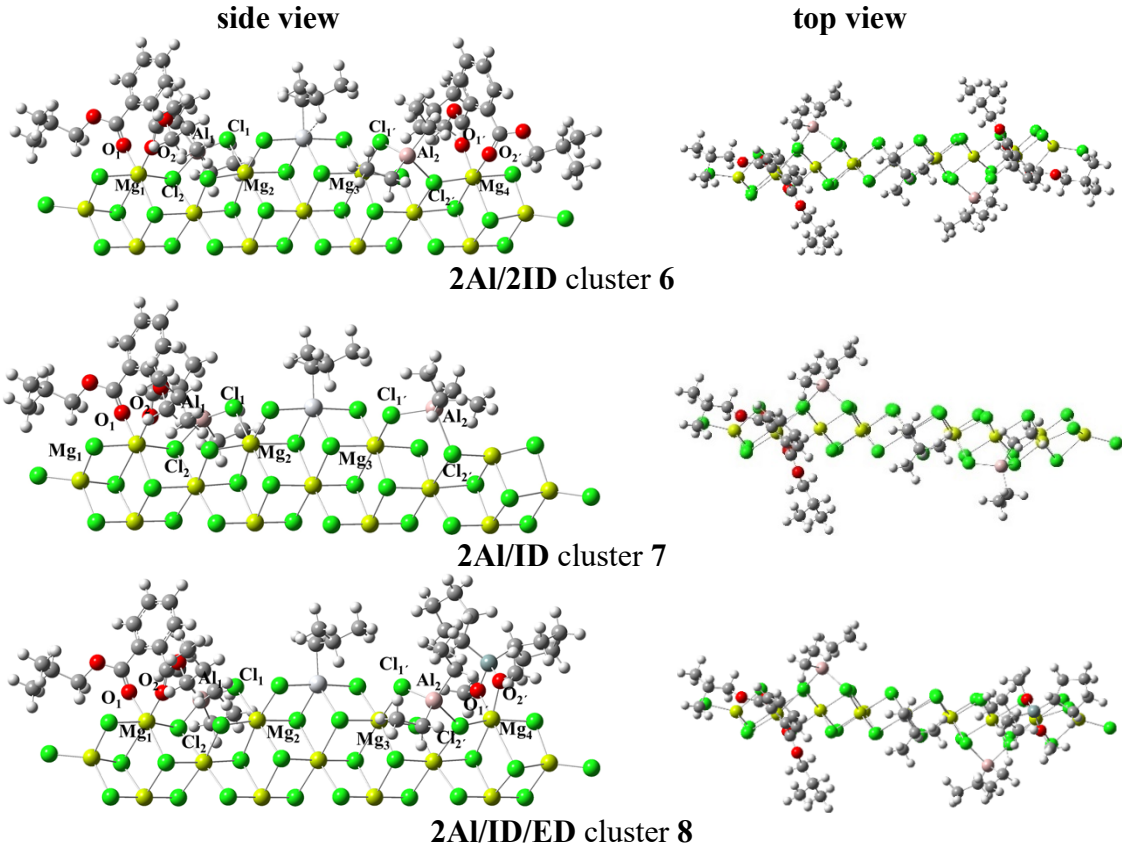
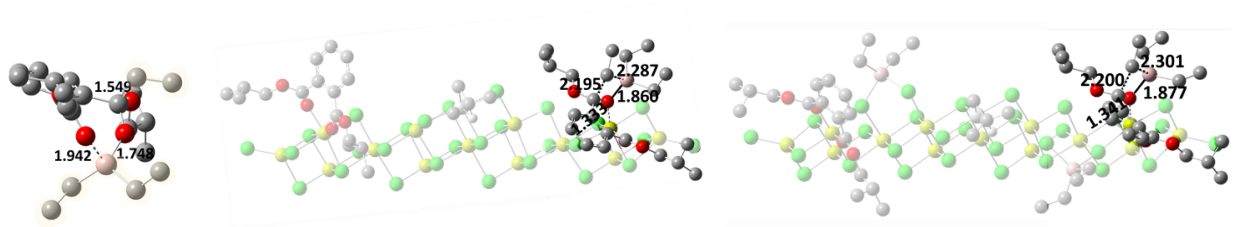


Fig. S4. Optimized geometries of 2Al/2ID/$(MgCl_2)_{13}$/$TiCl_2{}^iBu$ cluster **6**, 2Al/ID/$(MgCl_2)_{13}$/$TiCl_2{}^iBu$ cluster **7** and 2Al/ID/ED/$(MgCl_2)_{13}$/$TiCl_2{}^iBu$ cluster **8**. ID refers to DIBP, ED refers to DCPDMS, and Al refers to $AlEt_2Cl$ on the clusters.



Et-ID-$AlEt_2$ **$TS1_{Al}$** **$TS2_{Al}$**

Fig. S5. The **Et-ID-$AlEt_2$** product and the transition states for the ethyl transfer from $AlEt_3$ to DIBP on 2ID/$(MgCl_2)_{13}$/$TiCl_2{}^iBu$ cluster **2** (**$TS1_{Al}$**) and to DIBP on 2Al/2ID/$(MgCl_2)_{13}$/$TiCl_2{}^iBu$ cluster **6** (**$TS2_{Al}$**). All hydrogen atoms are omitted for clarity. The selected bond distances are shown in Å. ID refers to DIBP, ED refers to DCPDMS, and Al refers to $AlEt_2Cl$ on the clusters.

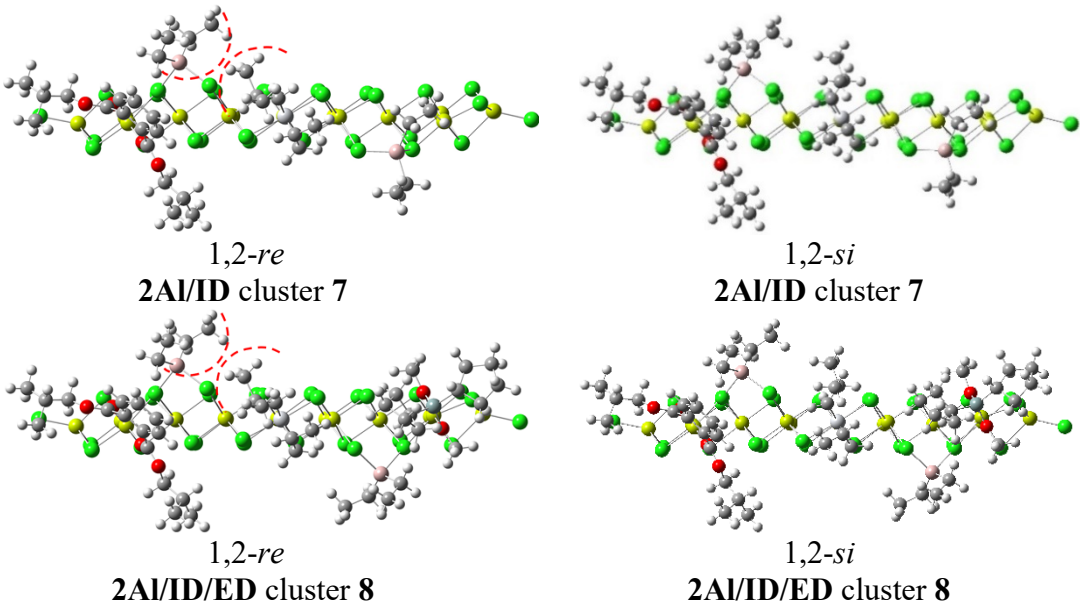


Fig. S6. Optimized geometries of 1,2-*re* and 1,2-*si* insertion transition states. ID refers to DIBP, ED refers to DCPDMS, and Al refers to $AlEt_2Cl$ on clusters **7** and **8**.

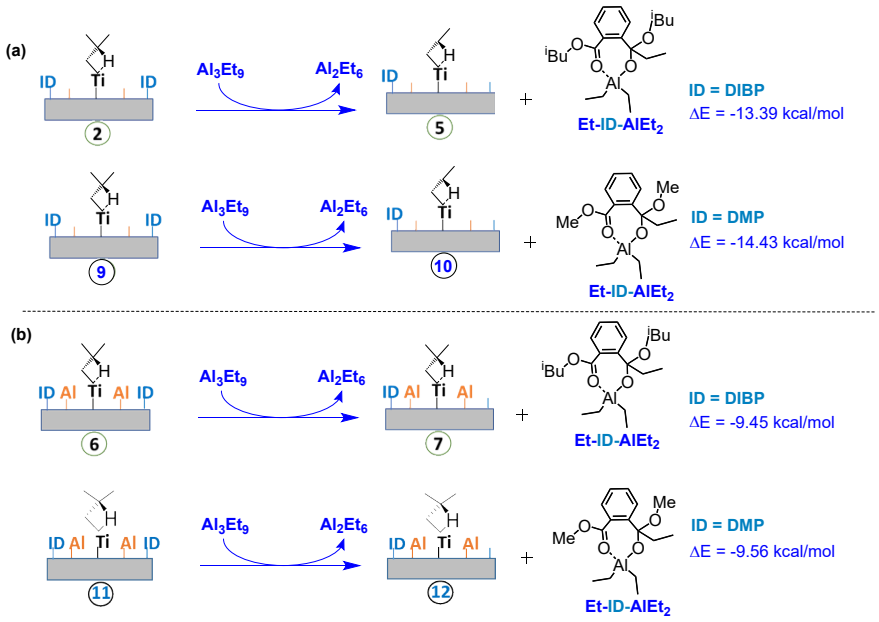


Fig. S7 The reaction energies in the extraction of diisobutyl phthalate (DIBP) and dimethyl phthalate (DMP) (shown as ID) from (a) $2ID/(MgCl_2)_{13}/TiCl_2{}^iBu$ cluster **2** and **9** and from (b) $2Al/2ID/(MgCl_2)_{13}/TiCl_2{}^iBu$ cluster **6** and **11**. ID refers to DIBP and DMP on the clusters.

Table S1. Absolute electronic energies (E) (in hartree) for the $(MgCl_2)_{13}/TiCl_2{}^iBu$ clusters with the adsorption of DIBP, DCPDMS, $AlEt_2Cl$ (referred to as Al).

		E	
		B3LYP/BS1[a]	B3LYP/def2-TZVP
1	$(MgCl_2)_{13}/TiCl_2{}^iBu$	-16492.580302	-16497.832368
2	$2ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	-18341.1932	-18346.42721
3	$2ED/(MgCl_2)_{13}/TiCl_2{}^iBu$	-18316.73343	-18321.96513
4	$2Al/(MgCl_2)_{13}/TiCl_2{}^iBu$	-18214.8994	-18220.44208
5	$ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	-17416.88832	-17422.13149
6	$2Al/2ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	-20063.52125	-20069.04829
7	$2Al/ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	-19139.21079	-19144.74628
8	$2Al/ID/ED/(MgCl_2)_{13}/TiCl_2{}^iBu$	-20051.28622	-20056.81418
	ID	-924.2501219	-924.2501219
	ED	-912.0362061	-912.0362061
	$Al_2Et_4Cl_2$	-1722.29544	-1722.600873
	$ID/ED/(MgCl_2)_{13}/TiCl_2{}^iBu$	-18328.96458	-18334.19813

[a]Basis set 1 (BS1): def2-SVP basis set was used for Mg and Cl, and def2-TZVP was used for C, H, O, Si, Al and Ti.
[b]ID refers to DIBP, ED refers to DCPDMS, and Al refers to $AlEt_2Cl$.

Table S2. Absolute electronic energies (E) (in hartree) for the intermediates and transition states in the reaction between $AlEt_3$ and DIBP on the $(MgCl_2)_{13}/TiCl_2{}^iBu$ cluster.

	imaginary frequencies (cm^{-1})	E	
		B3LYP/BS1[a]	B3LYP/def2-TZVP
Al_2Et_6	-	-960.4770347	-960.4770347
Al_3Et_9	-	-1440.703116	-1440.703116
$TS1_{Al}$	283.8i	-18821.39134	-18826.62147
$TS2_{Al}$	262.6i	-20543.71155	-20549.23425
Et-ID-$AlEt_2$	-	-1404.543139	-1404.543139

[a]Basis set 1 (BS1): def2-SVP basis set was used for Mg and Cl, and def2-TZVP was used for C, H, O, Si, Al and Ti.
[b]ID refers to DIBP.

Table S3. Absolute electronic energies (E) (in hartree) for propene insertion on the $(MgCl_2)_{13}/TiCl_2{}^iBu$ clusters.

			imaginary frequencies (cm^{-1})	E	
				B3LYP/BS1[a]	B3LYP/def2-TZVP
2	$2ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	1,2-re	90.5i	-18459.13559	-18464.36656
		1,2-si	269.7i	-18459.13577	-18464.36698
6	$2Al/2ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	1,2-re	334.8i	-20181.50023	-20186.98352
		1,2-si	315.2i	-20181.49936	-20186.98529
7	$2Al/ID/(MgCl_2)_{13}/TiCl_2{}^iBu$	1,2-re	339.2i	-19257.15036	-19262.68195
		1,2-si	295.0i	-19257.15177	-19262.68426
8	$2Al/ID/ED/(MgCl_2)_{13}/TiCl_2{}^iBu$	1,2-re	293.1i	-20169.22554	-20174.74939
		1,2-si	50.6i	-20169.22713	-20174.75172

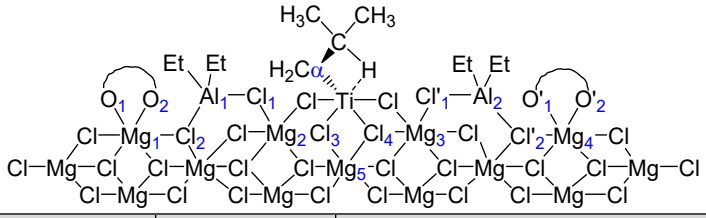
[a]Basis set 1 (BS1): def2-SVP basis set was used for Mg and Cl, and def2-TZVP was used for C, H, O, Si, Al and Ti.
[b]ID refers to DIBP, ED refers to DCPDMS, and Al refers to $AlEt_2Cl$.

Table S4. The calculated and experimental C=O frequencies (cm^{-1}) of phthalate.

	B3LYP/BS1[b]	Exp[c]
free ID[a]	1712	1725
2ID[a]/$(MgCl_2)_{13}$/$TiCl_2$[i]Bu (**2**)	1685	1707
2Al[a]/2ID[a]/$(MgCl_2)_{13}$/$TiCl_2$[i]Bu (**6**)	1676	-
Et-ID[a]-$AlEt_2$	1599	1625

[a]ID refers to DIBP and Al refers to $AlEt_2Cl$.
[b]Calculated C=O frequency of DIBP by B3LYP/BS1. For BS1, def2-SVP basis set was used for Mg and Cl, and def2-TZVP was used for C, H, O, Si, Al and Ti. The scaling factor of 0.965 cm^{-1} is applied.
[c]Experimental C=O frequency of DBP from *ACS Catal.* **2021,** *11*, 13782-13796.

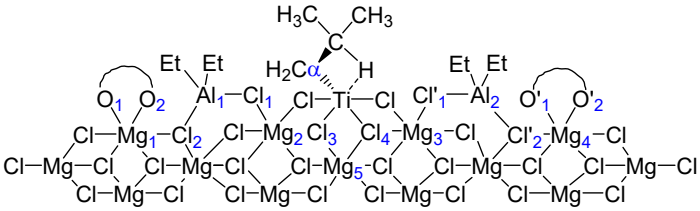
Table S5. The difference in the percent buried volume between occupied and free quadrants ($\Delta\%V_{Bur}$) from the buried volume analysis using SambVca.[a] The Ti atom is the center of the sphere with Cα-Mg_5 as the z-axis and Cl_3-Cl_4 as the xz-plane. Sphere radius used to calculate buried volume of 3.5 to 6.0 Å. Hydrogen atoms were not included in the analysis



$(MgCl_2)_{13}$/$TiCl_2$[i]Bu cluster[b]		$\Delta E_{a,re\text{-}si}$ (kcal/mol)	$\Delta\%V_{Bur}$					
			3.5	4.0	4.5	5.0	5.5	6.0
2	2ID	0.27	13.8	15.0	15.2	16.0	16.8	17.0
6	2Al/2ID	1.12	20.3	23.7	25.0	26.1	26.9	28.0
7	2Al/ID	1.45	21.2	24.2	25.2	25.8	26.0	26.7
8	2Al/ID/ED	1.46	18.3	22.2	24.4	26.2	27.3	28.7

[a](i) Poater, A.; Cosenza, B., Correa, A.; Giudice, S.; Ragone, F. Scarano, V.; Cavallo, L. *Eur. J. Inorg. Chem.* **2009**, 1759-1766. (ii) Poater, A.; Ragone, F.; Giudice, S; Costabile, C.; Dorta, R.; Nolan, S. P.; Cavallo, L. *Organometallics* **2008**, *27*, 2679-2681.
[b]ID refers to DIBP, ED refers to DCPDMS, and Al refers to $AlEt_2Cl$ on the clusters.

Table S6. The adsorption energies (ΔE_{ads} in kcal/mol) of dimethyl phthalate (DMP), diisobutyl phthalate (DIBP) and $AlEt_2Cl$ on the $(MgCl_2)_{13}/TiCl_2{}^iBu$ cluster. Selected bond distances are shown in Å.



	cluster[a]	ΔE_{ads}		bond distance (Å)							
		$AlEt_2Cl$	ID/ED	O_1-Mg_1	O_2-Mg_1	O_1'-Mg_4	O_2'-Mg_4	Cl_1-Mg_2	Cl_2-Al_1	Cl_1'-Mg_3	Cl_2'-Al_2
4	2Al	-2.77[b]	-	-	-	-	-	2.609	2.455	2.634	2.455
2	2DIBP	-	-29.68[b]	2.068	2.049	2.064	2.067	-	-	-	-
6	2Al/2DIBP	-6.34[b]	-33.25[b]	2.051	1.999	2.009	2.049	2.585	2.412	2.607	2.406
9	2DMP	-	-28.54[b]	2.077	2.057	2.077	2.071	-	-	-	-
11	2Al/2DMP	-5.90[b]	-31.66[b]	2.057	2.005	2.017	2.053	2.590	2.414	2.612	2.408

[a]DMP refers to dimethyl phthalate, DIBP refers to diisobutyl phthalate, and Al refers to $AlEt_2Cl$ on the $(MgCl_2)_{13}/TiCl_2{}^iBu$ cluster.

[b]The average adsorption energies of two adsorbed molecules.

Cartesian coordinates of optimized geometries

DIBP

Total atoms = 42

C	-3.202926185	0.748820449	1.107449042
C	-3.151084524	-1.033161613	-1.013541577
C	-1.977577344	0.374948296	0.557066184
C	-4.392155622	0.243979770	0.601130117
C	-4.366507640	-0.641997235	-0.468964201
C	-1.950551502	-0.546703496	-0.499140655
C	-0.765277632	1.058175498	1.106269776
O	-0.623198137	1.347107500	2.269028795
O	0.109564013	1.383756780	0.140261943
C	-0.695403064	-1.109035869	-1.091799383
O	-0.510795828	-1.242065066	-2.275651260
O	0.157585947	-1.530641435	-0.142267608
C	1.299468171	2.091407767	0.554623455
C	1.385311015	-2.141263353	-0.597756582
C	2.100656987	2.466636256	-0.683048770
C	1.322134584	3.407392034	-1.604760839
C	3.436597752	3.079770404	-0.253321469
C	2.063505926	-2.825175184	0.580235204
C	2.447399746	-1.837852899	1.683743576
C	3.282334041	-3.604649413	0.077565289
H	-3.206330968	1.452585854	1.928828289
H	-5.335529022	0.548828575	1.035540021
H	-5.289800012	-1.033962576	-0.875934602
H	-3.117276311	-1.732415016	-1.838296317
H	1.000280380	2.976193987	1.121383802
H	1.871078891	1.444572886	1.222622468
H	2.020648907	-1.361589397	-1.028324766
H	1.147107868	-2.851998044	-1.389549342

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H	1.903702510	3.640011099	-2.498874105
H	4.013301202	2.395455006	0.372931186
H	3.282294078	4.002296411	0.313075372
H	4.044113152	3.326671179	-1.125471905
H	1.344465510	-3.540933173	0.993418473
H	2.904570086	-2.360076513	2.526479089
H	1.579194483	-1.295206963	2.057302765
H	3.174276384	-1.108022749	1.314373764
H	3.006099398	-4.343001445	-0.678215188
H	3.766187333	-4.133473377	0.900325163
H	4.024348899	-2.933860795	-0.364549489

DCPDMS

Total atom = 39

SI	0.000000000	-0.000000000	0.468648460
O	-1.275977210	-0.462347838	1.413197156
O	1.275977210	0.462347838	1.413197156
C	-0.374455392	1.519819781	-0.570189144
C	-0.601696337	2.846778946	0.216637348
C	-0.000000000	3.983170245	-0.657136677
C	0.383211604	3.325023343	-1.991715138
C	0.717773693	1.880831792	-1.604200181
C	0.374455392	-1.519819781	-0.570189144
C	0.601696337	-2.846778946	0.216637348
C	-0.000000000	-3.983170245	-0.657136677
C	-0.383211604	-3.325023343	-1.991715138
C	-0.717773693	-1.880831792	-1.604200181
C	-1.952947875	0.303751257	2.391774247

C	1.952947875	-0.303751257	2.391774247
H	-1.290095140	1.298386322	-1.132309714
H	-0.107392385	2.824430426	1.188748647
H	-1.664561259	3.005537772	0.405528412
H	-0.693447585	4.815207916	-0.788919297
H	0.892655283	4.388577152	-0.175612747
H	1.205914472	3.837411160	-2.494493144
H	-0.470508639	3.329122454	-2.676346153
H	1.709186490	1.844282770	-1.141568978
H	0.730820811	1.202480463	-2.459498737
H	1.290095140	-1.298386322	-1.132309714
H	0.107392385	-2.824430426	1.188748647
H	1.664561259	-3.005537772	0.405528412
H	0.693447585	-4.815207916	-0.788919297
H	-0.892655283	-4.388577152	-0.175612747
H	-1.205914472	-3.837411160	-2.494493144
H	0.470508639	-3.329122454	-2.676346153
H	-1.709186490	-1.844282770	-1.141568978
H	-0.730820811	-1.202480463	-2.459498737
H	-1.255818027	0.823774572	3.055994900
H	-2.565286305	-0.371262165	2.991918624
H	-2.609739052	1.046611282	1.929419014
H	1.255818027	-0.823774572	3.055994900
H	2.565286305	0.371262165	2.991918624
H	2.609739052	-1.046611282	1.929419014

$Al_2Et_4Cl_2$

Total atom = 32

AL	-1.663238030	-0.000011240	0.000028654
AL	1.663218191	-0.000014644	-0.000011996
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C	-2.523859927	1.761668244	0.001394906
C	2.523796987	1.761689845	-0.000805970
C	2.523869050	-1.761680039	0.000799132
C	3.394953861	-2.061795567	1.234254954
C	-3.394894286	2.061434060	1.234971814
C	-3.394783238	-2.061491238	-1.234990642
C	3.394771480	2.061938689	-1.234304659
CL	0.000006067	-0.000265521	1.658393404
CL	-0.000017012	0.000257486	-1.658375449
H	-1.752070873	-2.531471064	0.102629263
H	-3.134222918	-1.841310774	0.906613363
H	-3.134243371	1.841219237	-0.906617882
H	-1.752148567	2.531448325	-0.102595114
H	1.752055241	2.531398905	0.103491083
H	3.134208530	1.840942626	0.907214588
H	1.752179560	-2.531453458	-0.103401554
H	3.134225300	-1.840934926	-0.907258689
H	3.859900770	-3.049678003	1.175132431
H	2.808425494	-2.038559358	2.156176550
H	4.203085337	-1.334586267	1.348372794
H	-3.859807783	3.049351395	1.176169824
H	-4.203048633	1.334218823	1.348890371
H	-2.808337598	2.037892129	2.156867661
H	-4.202961774	-1.334305126	-1.348923921
H	-2.808192196	-2.037906591	-2.156863533
H	-3.859660640	-3.049427966	-1.176227954
H	2.808180548	2.038707464	-2.156186599
H	3.859648066	3.049853224	-1.175162049
H	4.202950523	1.334797113	-1.348518656

Al_2Et_6

Total atom = 44

AL	-1.299304693	0.097418965	-0.034454716
C	-0.038392054	-0.135478430	1.732928223
C	-0.023169347	-1.527917094	2.392428257
C	0.038390528	-0.135480915	-1.732928752
C	0.023158964	-1.527920047	-2.392427542
AL	1.299303338	0.097420543	0.034453787
C	-2.016471663	1.946267502	-0.007616898
C	-2.881561105	2.347718669	-1.215946356
C	-2.576424126	-1.414372570	-0.078544206
C	-3.686120588	-1.348913364	0.987205041
C	2.016486141	1.946262390	0.007614450
C	2.881574091	2.347704392	1.215948245
C	2.576416199	-1.414376877	0.078544856
C	3.686113074	-1.348923075	-0.987204284
H	-0.905300650	0.425440147	2.116315324
H	-0.762461849	0.475473249	-2.177301026
H	0.762469311	0.475467568	2.177296062
H	0.905307206	0.425428159	-2.116312250
H	-2.619580765	2.045069489	0.904942016
H	-1.205864555	2.673042819	0.113713631
H	-2.060552377	-2.377797169	-0.012558374
H	-3.043637156	-1.413085484	-1.071877716
H	2.619601990	2.045054069	-0.904941127
H	1.205889458	2.673048079	-0.113722139
H	3.043628933	-1.413091803	1.071878521
H	2.060540497	-2.377799354	0.012558997
H	-3.729913985	1.671186375	-1.351701116
H	-2.310606819	2.332739716	-2.149221810

H	-3.291641513	3.357188711	-1.116844579
H	-4.401386252	-2.170875452	0.889374967
H	-4.256628376	-0.419090841	0.919892409
H	-3.282131451	-1.400423300	2.002181826
H	2.310613518	2.332736715	2.149220005
H	3.291669909	3.357168104	1.116845892
H	3.729916250	1.671160138	1.351710409
H	4.401375187	-2.170888232	-0.889373898
H	4.256624984	-0.419103040	-0.919892240
H	3.282123604	-1.400431851	-2.002181027
H	0.893617538	-2.070816458	2.164718636
H	-0.853859279	-2.144785597	2.050670457
H	-0.096736512	-1.453370253	3.480316138
H	-0.893636789	-2.070808473	-2.164727548
H	0.853837916	-2.144797906	-2.050659868
H	0.096738938	-1.453375238	-3.480314694

Propene

Total atom = 9

C	0.133550942	-0.451866596	0.000045504
C	1.278406053	0.219621052	0.000027258
C	-1.230849615	0.162109922	-0.000066347
H	2.234373813	-0.288325709	0.000154991
H	1.301136328	1.304014072	-0.000080241
H	0.166065670	-1.538738256	0.000187215
H	-1.803841867	-0.153834141	0.876852253
H	-1.180532878	1.251916543	-0.000307402
H	-1.803845333	-0.154218784	-0.876845305

$(MgCl_2)_{13}/TiCl_2{}^iBu$ cluster 1

Total atom = 55

CL	-10.824700511	-2.436663258	1.420414326
MG	-9.014089920	-2.544904397	0.080281518
CL	-4.767035287	-2.407867271	1.404239587
MG	-2.957715131	-2.516717133	0.065651502
CL	-7.180706514	-2.650768600	-1.228495402
CL	-1.153710537	-2.627443832	-1.285563739
CL	1.038392973	-2.367963415	1.520318382
MG	2.841776430	-2.479262927	0.171277556
CL	7.094878185	-2.341450493	1.473421510
MG	8.896634904	-2.453457997	0.126239469
CL	4.714574913	-2.581730671	-1.081650261
CL	10.679466667	-2.568505268	-1.253310369
CL	-13.909146401	-0.366000876	-0.310218694
MG	-11.745573057	-0.522250111	0.164929088
CL	-10.111296624	-0.900870433	-1.403314204
MG	-5.952961474	-0.750556288	-0.097505966
CL	-7.982068508	-0.663132940	1.441718304
CL	-3.963316349	-0.739195175	-1.516264088
MG	-0.049906152	-0.617635921	-0.059274685
CL	-2.028533073	-0.443718073	1.295556759
CL	1.925264509	-0.730961414	-1.437701708
MG	5.874931256	-0.651439224	0.113521001
MG	11.848379447	-0.717870824	-0.136243981
CL	3.827275103	-0.454874712	1.447828373
CL	8.005862952	-0.607233883	-1.312376481
CL	10.022345675	-0.882927813	1.668511734
CL	13.999415583	-0.920682867	0.405269089
CL	-10.777074899	1.695078769	0.809838680

MG	-8.835435319	0.949037600	-0.210585143
CL	-5.160333736	1.272543825	1.138154855
CL	-7.062648501	1.060932642	-1.666913276
MG	-3.148666646	1.268570241	-0.086012091
CL	0.989097997	1.552640355	1.153292492
CL	-1.117634694	1.299365056	-1.648876558
MG	2.999135487	1.237417342	-0.370430661
CL	6.990131037	1.378373352	1.488621712
CL	5.088600587	1.143654115	-1.418565064
MG	8.942802369	0.945494770	0.360673289
CL	10.963452679	1.518053817	-0.694910315
TI	-0.083688935	3.289543671	-0.443690069
CL	-2.277738731	3.385552291	0.687531667
CL	2.065082254	3.071556815	-1.657425746
C	-0.086036515	5.336054548	-0.729317922
C	0.644449118	5.484316872	0.593740732
C	2.056898061	6.073492596	0.459926147
C	-0.174000097	6.197283500	1.680898164
H	0.493338365	5.623967371	-1.617603399
H	-1.105120425	5.745932244	-0.751808215
H	0.821908964	4.430840577	1.024760071
H	2.598564379	6.031971199	1.418282023
H	2.648117677	5.539733875	-0.297367539
H	1.985249522	7.130286053	0.156947029
H	0.342143676	6.163366324	2.653288361
H	-0.307893817	7.255132877	1.403768847
H	-1.169005212	5.746901273	1.803944152

2DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 2

Total atom = 139

CL	10.779823021	-3.749063568	-1.704370927
MG	9.011532143	-3.841961384	-0.307764568
CL	4.725440980	-3.739391170	-1.502829331
MG	2.958381545	-3.832980626	-0.107789961
CL	7.219442270	-3.933090045	1.058069858
CL	1.197014096	-3.928174488	1.299676085
CL	-1.080934903	-3.719897797	-1.441352950
MG	-2.841726158	-3.815727968	-0.036038234
CL	-7.133172449	-3.711980870	-1.209061456
MG	-8.892431492	-3.808505062	0.194273481
CL	-4.674900216	-3.904450292	1.275195463
CL	-10.631693096	-3.907531166	1.629524444
CL	13.908263839	-1.641595014	-0.101788245
MG	11.731840120	-1.812294406	-0.507815082
CL	10.147637696	-2.171260328	1.115529691
MG	5.950598858	-2.054819379	-0.064246317
CL	7.931358005	-1.985139474	-1.666161580
CL	4.005374681	-2.027563742	1.414526677
MG	0.048800292	-1.941490082	0.076547145
CL	1.984346084	-1.782542938	-1.340898465
CL	-1.882809538	-2.039355436	1.516536016
MG	-5.878324815	-1.996879668	0.086147794
MG	-11.841294667	-2.078592148	0.520036966
CL	-3.873254594	-1.814852130	-1.313240056
CL	-7.964797229	-1.937064453	1.575891419
CL	-10.070639003	-2.266041067	-1.337023709
CL	-14.007049914	-2.296780228	0.048080410
CL	10.813788405	0.081112082	-1.633147830

MG	8.853169946	-0.023525563	-0.108489016
CL	5.052809727	-0.059395305	-1.362094216
CL	7.043668774	-0.369288263	1.430093095
MG	3.154376984	-0.068099948	0.001805820
CL	-1.019280137	0.210051520	-1.157939454
CL	1.136581638	0.032403986	1.603215981
MG	-3.004027591	-0.117436410	0.413573708
CL	-6.924756087	-0.194083180	-1.330828147
CL	-4.997181006	-0.182322006	1.626085021
MG	-8.987899098	-0.120136044	-0.083102329
CL	-11.019343189	-0.053092950	1.406846884
TI	0.074387162	1.974154717	0.363562941
CL	2.272147812	2.085205585	-0.756268293
CL	-2.058999761	1.805314297	1.614250210
C	0.040687484	4.044968879	0.555819903
C	-0.693214271	4.112020579	-0.770231073
O	-10.018257624	1.118062893	-1.378723206
C	-10.331659633	2.294377987	-1.451164802
C	-8.107019422	2.809398185	0.695297281
O	-8.475242951	1.655432437	0.836236431
O	9.931102436	1.214018781	1.140971129
C	10.253583006	2.364384649	1.382992564
C	8.283987323	2.933011048	-0.991917256
O	8.237870606	1.715570461	-0.989276605
O	-11.572970230	2.686697146	-1.635675481
C	-12.606354749	1.645197471	-1.735209399
O	-7.454438504	3.445754170	1.648416714
C	-7.140286334	2.691361058	2.864004404
O	11.447662122	2.677549412	1.839297340
O	8.148900500	3.640839764	-2.096520972

C	12.397993157	1.580470858	2.068207864
C	7.982630388	2.920476887	-3.363452097
C	-2.109918204	4.686446626	-0.661517320
C	0.108734089	4.789556357	-1.886670133
C	9.351881009	3.556006135	1.274391754
C	8.454299448	3.804578193	0.214731274
C	9.429144396	4.476238926	2.322455224
C	7.672597120	4.961647157	0.251701996
C	7.729964616	5.840034467	1.322721050
C	8.613901454	5.596887637	2.363051059
C	-8.329848554	3.655226462	-0.517677162
C	-9.364814835	3.441794381	-1.453317748
C	-9.515720505	4.336822742	-2.513726690
C	-7.480401780	4.750783627	-0.699027720
C	-7.618583283	5.605941009	-1.780866410
C	-8.643996438	5.400831951	-2.691225478
C	13.764861211	2.172532400	2.359931222
C	6.524474592	2.594942707	-3.657326316
C	5.671225470	3.854847997	-3.812266082
C	6.461727059	1.711222589	-4.906878914
C	14.340688551	2.885979908	1.134598325
C	14.690817613	1.049005326	2.840972494
C	-13.972713629	2.303356316	-1.686617292
C	-6.242722395	3.543752999	3.743030320
C	-15.034466109	1.236173845	-1.979102845
C	-14.221048722	2.990635687	-0.342024588
C	-5.780416593	2.698312433	4.934509896
C	-6.927678573	4.833948804	4.197579631
H	-0.543502896	4.370258193	1.413949318
H	1.033222204	4.489428388	0.549108087

H	-0.854919956	3.049277363	-1.151845749
H	-2.646875275	4.588351138	-1.607412815
H	-2.683752832	4.183515165	0.115655851
H	-2.051952314	5.748252633	-0.412602411
H	-0.403053582	4.700500276	-2.846948050
H	0.221601533	5.851738063	-1.659341695
H	1.101835326	4.354220960	-1.987753280
H	8.396387693	3.610441250	-4.098514691
H	8.593630747	2.021413446	-3.320985579
H	12.014601193	0.994093984	2.903972534
H	12.418704404	0.953618584	1.178626036
H	-8.085028889	2.450059109	3.355153543
H	-6.653036821	1.765595896	2.565806079
H	-12.437234595	1.114024685	-2.672447262
H	-12.464793075	0.954484942	-0.906430913
H	7.093575033	6.715095207	1.335070189
H	8.678838298	6.278804117	3.200678384
H	7.006623103	5.165019615	-0.573765179
H	10.136954406	4.297481009	3.118555390
H	-10.325293528	4.183859145	-3.212897542
H	-6.932709882	6.433839960	-1.903221731
H	-8.772816165	6.066032893	-3.534995559
H	-6.698893448	4.923808630	0.024792055
H	13.647416091	2.899404033	3.171768249
H	6.140824760	2.008674404	-2.819554933
H	5.997893417	4.449308923	-4.670599293
H	4.624791039	3.588156601	-3.968505808
H	5.720688491	4.490333497	-2.926261136
H	5.426867142	1.450431706	-5.131991635
H	6.874239634	2.224335574	-5.780547352

H 7.013913416 0.781099246 -4.763350162

H 14.487719216 2.177288548 0.315911534

H 13.681431218 3.681717015 0.784007534

H 15.308516083 3.332291065 1.369905832

H 15.687225307 1.443731267 3.045926132

H 14.318334474 0.588110569 3.758626627

H 14.784388384 0.266618154 2.084663068

H -14.010377961 3.058166806 -2.480340289

H -5.358997916 3.802727434 3.149649433

H -14.995323257 0.424593737 -1.248826980

H -16.031850876 1.676954113 -1.941210073

H -14.900012447 0.797636911 -2.970297341

H -13.473882707 3.759083063 -0.138391573

H -15.203150856 3.466543646 -0.331052371

H -14.191364274 2.263653103 0.473325841

H -5.102279643 3.272207165 5.567876990

H -6.628836657 2.390519960 5.551554737

H -5.256939141 1.798819253 4.607049311

H -7.806773335 4.611777851 4.809098355

H -6.248568001 5.438495965 4.801667694

H -7.252547001 5.439403557 3.350388379

$(MgCl_2)_{13}/TiCl_2{}^{i}Bu/DIBP$-Mg1 cluster 5

Total atom = 97

CL -8.703845510 -4.331694467 1.584282113

MG -6.917111332 -4.214184157 0.213241103

CL -2.693903622 -3.581096057 1.467581449

MG -0.908328674 -3.464367627 0.098098715

CL -5.107385074 -4.091761503 -1.126639582

CL 0.872000647 -3.349944754 -1.283859625

CL 3.066598162 -2.850431506 1.487349872

MG	4.846391163	-2.736797841	0.107653436
CL	9.075315222	-2.101881122	1.340267332
MG	10.853334702	-1.989134242	-0.038201028
CL	6.695705580	-2.606677440	-1.177071648
CL	12.612766628	-1.881386571	-1.448070111
CL	-12.042859245	-2.631582007	-0.076246677
MG	-9.868205517	-2.532327018	0.361636380
CL	-8.228149254	-2.702400066	-1.237110409
MG	-4.094886928	-2.066503438	0.000662204
CL	-6.092605146	-2.232215443	1.574119845
CL	-2.145980590	-1.808486168	-1.450890085
MG	1.750068218	-1.231428217	-0.058171788
CL	-0.211045774	-1.303900283	1.330882843
CL	3.700118484	-1.099109556	-1.470118869
MG	7.639226689	-0.559714588	0.014853996
MG	13.572312804	0.087340337	-0.333235807
CL	5.606157390	-0.618102750	1.385640338
CL	9.723840686	-0.252424545	-1.444917280
CL	11.811243076	-0.306229285	1.499147461
CL	15.741678096	0.138805472	0.169494991
CL	-9.203190950	-0.529991726	1.481351132
MG	-7.244582146	-0.421016805	-0.014741501
CL	-3.442339825	0.036883325	1.307903914
CL	-5.350248186	-0.529421390	-1.509645364
MG	-1.554555494	0.245462020	-0.057044822
CL	2.543529838	1.070773895	1.132219531
CL	0.457736349	0.549208514	-1.637127702
MG	4.552398662	0.973358209	-0.415625207
CL	8.529241336	1.580768129	1.395260813
CL	6.626134362	1.145665300	-1.482090419

MG	10.496359042	1.389141823	0.227825797
CL	12.414531420	2.203632736	-0.856091422
TI	1.254783947	2.651008206	-0.460653462
CL	-0.958080346	2.516373856	0.639292479
CL	3.395452642	2.684725973	-1.707800285
C	1.038496834	4.699692736	-0.722212266
C	1.767824207	4.895827142	0.592536987
O	-8.415715460	0.689200225	-1.306814259
C	-8.726201545	1.854184888	-1.490743447
C	-6.484754302	2.561463007	0.572667227
O	-6.775497904	1.398476828	0.801889780
O	-9.969207361	2.231157661	-1.689822264
O	-5.924679556	3.325972543	1.487912324
C	-11.005017204	1.185349696	-1.662892705
C	-5.613787434	2.713940110	2.781361202
C	3.102873161	5.635625722	0.453048303
C	0.896243753	5.499131235	1.699323668
C	-7.751705219	2.986885817	-1.619852787
C	-6.707081404	3.281006839	-0.718605411
C	-7.903655272	3.774530126	-2.761919265
C	-5.845189763	4.341332695	-1.013116950
C	-5.981806066	5.083813980	-2.175492775
C	-7.019636782	4.803312837	-3.051558174
C	-12.369449932	1.848971394	-1.663511001
C	-4.773247111	3.689661650	3.585485379
C	-5.519635098	4.990168691	3.888492288
C	-4.307781858	2.992529284	4.868156768
C	-12.602006025	2.662649608	-0.388477339
C	-13.436335641	0.762053764	-1.842232267
H	1.574684329	5.061234209	-1.597134255

H	-0.000211665	5.021723288	-0.720425748
H	2.061719472	3.870452421	1.001294622
H	3.656297654	5.629290150	1.394215884
H	3.728530415	5.189835725	-0.318845938
H	2.913074140	6.675599341	0.179920816
H	1.423036933	5.501660384	2.655400894
H	0.650954852	6.532327208	1.445067423
H	-0.034349579	4.946984392	1.823603903
H	-6.561964507	2.487202667	3.273128066
H	-5.083850234	1.783519782	2.591277527
H	-10.851563970	0.559457243	-2.542382138
H	-10.850507415	0.581717974	-0.770324472
H	-5.285533686	5.884467026	-2.387455004
H	-7.147728256	5.382806701	-3.956411542
H	-5.053901631	4.573945241	-0.316572497
H	-8.722282989	3.563650530	-3.435147389
H	-12.413535456	2.525019920	-2.524973792
H	-3.886904968	3.922025001	2.985258286
H	-6.404115453	4.796303295	4.501816093
H	-4.880030045	5.682130485	4.439507348
H	-5.846665320	5.489921915	2.975868934
H	-3.669681472	3.656978382	5.452700028
H	-5.157932770	2.713413002	5.496270452
H	-3.739896798	2.087118322	4.647492467
H	-12.567563641	2.016293526	0.492177093
H	-11.849880511	3.443509058	-0.265855101
H	-13.581911228	3.142555197	-0.413358597
H	-14.432915635	1.206016566	-1.824144923
H	-13.319156697	0.237985831	-2.793013944
H	-13.379676342	0.015778593	-1.047014007

$(MgCl_2)_{13}/TiCl_2{}^{i}Bu/DIBP$-Mg4

Total atom = 97

CL	12.793911588	-1.725838257	-1.609713666
MG	11.032231454	-2.051669617	-0.239891698
CL	6.776435500	-2.413150421	-1.491773062
MG	5.016036075	-2.739545815	-0.123590140
CL	9.246933144	-2.377735562	1.098718971
CL	3.261352893	-3.067114787	1.257063165
CL	1.005782440	-3.059256604	-1.510230814
MG	-0.748239646	-3.387362431	-0.131741503
CL	-5.009706626	-3.748800000	-1.361568706
MG	-6.762103164	-4.077374604	0.014957628
CL	-2.573899497	-3.714568683	1.151874097
CL	-8.494695603	-4.406860593	1.423613148
CL	15.641769638	0.689165649	0.079922520
MG	13.504109615	0.279693795	-0.359730417
CL	11.953051611	-0.294327162	1.233653936
MG	7.783882144	-0.632195691	-0.001246908
CL	9.761732194	-0.300560244	-1.573863268
CL	5.831728452	-0.860875711	1.450668508
MG	1.906883858	-1.197806814	0.060165744
CL	3.827396575	-0.786787740	-1.326720390
CL	-0.016945509	-1.548316698	1.470918270
MG	-3.974505114	-1.930957803	-0.013385175
MG	-9.893346557	-2.703832744	0.336134657
CL	-1.987805748	-1.489423182	-1.380787737
CL	-6.070834910	-2.143603204	1.448271008
CL	-8.091907185	-2.645802025	-1.499764312
CL	-12.014311627	-3.157639826	-0.170203342

CL	12.272179103	2.371117145	-0.974281136
MG	10.447990571	1.395772607	0.071562042
CL	6.743951864	1.287062765	-1.216141765
CL	8.700694631	1.290598101	1.558770484
MG	4.764952563	1.042621817	0.033653532
CL	0.619643534	0.823438756	-1.159253994
CL	2.760018869	0.870811644	1.619105288
MG	-1.339530008	0.258113052	0.385234458
CL	-5.201126081	-0.225795171	-1.401551124
CL	-3.316012422	-0.065181413	1.580402076
MG	-7.278913774	-0.416524824	-0.187695762
CL	-9.317112386	-0.618806106	1.277115724
TI	1.480356645	2.696841078	0.382377559
CL	3.657850873	3.058991925	-0.733507242
CL	-0.622046828	2.257602853	1.616718461
C	1.211761497	4.745857566	0.583913338
C	0.485612638	4.733891413	-0.747044590
O	-8.430279416	0.719760636	-1.472099488
C	-8.880841987	1.851865236	-1.526872737
C	-6.754156037	2.579902068	0.658107319
O	-6.985056388	1.387742578	0.770605476
O	-10.157323434	2.096937482	-1.723340202
C	-11.057523468	0.942525151	-1.860967160
O	-6.188474238	3.266710059	1.631436117
C	-5.798559267	2.527937040	2.834293041
C	-0.989559863	5.137371894	-0.647369381
C	1.211258064	5.504431737	-1.855468534
C	-7.065410910	3.420559508	-0.538855631
C	-8.058186227	3.106181967	-1.491787032
C	-8.304921248	4.001008066	-2.534362704

C	-6.352048987	4.614022932	-0.685862574
C	-6.581209563	5.471200797	-1.750586896
C	-7.565523763	5.165586495	-2.677998598
C	-12.492897719	1.433976667	-1.831458197
C	-5.025407095	3.463743797	3.746222279
C	-13.415320012	0.255502731	-2.166161475
C	-12.847795195	2.060532237	-0.481122384
C	-4.474609638	2.653294854	4.924424936
C	-5.872210387	4.646166027	4.220676154
H	0.588594888	4.996557059	1.439778484
H	2.148319976	5.298763444	0.587960818
H	0.451834073	3.659846892	-1.133414667
H	-1.504183792	4.980541988	-1.597616950
H	-1.506327133	4.568177815	0.124151484
H	-1.057969939	6.197695465	-0.395333991
H	0.720200324	5.359381569	-2.819595203
H	1.196949748	6.571463023	-1.624147487
H	2.249591737	5.190508129	-1.951126987
H	-6.711848653	2.159142661	3.305246866
H	-5.196070858	1.677208843	2.523096229
H	-10.808704496	0.451805672	-2.802461251
H	-10.850927688	0.258672581	-1.040152613
H	-9.083392316	3.768456878	-3.246757408
H	-5.998724013	6.378039251	-1.846159951
H	-7.765153776	5.829807275	-3.508637485
H	-5.604396871	4.863209926	0.051400396
H	-12.603090997	2.194682247	-2.612640979
H	-4.174443367	3.846330655	3.172128142
H	-13.295739821	-0.559951172	-1.449123655
H	-14.458198601	0.575373940	-2.143177476

H -13.210024683 -0.144587715 -3.161452816

H -12.200266859 2.906758884 -0.246981455

H -13.878871285 2.418228292 -0.484349079

H -12.750195218 1.325800336 0.321854163

H -3.882096956 3.291777867 5.581370898

H -5.284757558 2.225695856 5.521121397

H -3.837936728 1.835244157 4.584012961

H -6.723523727 4.300342439 4.813717155

H -5.281491361 5.315565926 4.848715726

H -6.260496868 5.227357300 3.383284296

2DCPDMS/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 3

Total atom = 133

CL -10.730853616 -3.841494687 1.550245120

MG -8.958995556 -3.831301817 0.155308630

CL -4.676879444 -3.783976232 1.362483653

MG -2.906509589 -3.774935518 -0.033423177

CL -7.165214169 -3.822340860 -1.211395269

CL -1.142766722 -3.766206484 -1.438786637

CL 1.130245431 -3.728695920 1.313723491

MG 2.894043104 -3.719491321 -0.091396299

CL 7.182634094 -3.671061073 1.094214050

MG 8.946692561 -3.661722808 -0.311293332

CL 4.728379977 -3.709008885 -1.402770544

CL 10.686177001 -3.654011080 -1.745781985

CL -13.868669176 -1.650241935 0.085246536

MG -11.691925727 -1.838334889 0.483102020

CL -10.104757108 -2.077739094 -1.158096705

MG -5.919219349 -2.022602941 0.041022835

CL -7.912051723 -2.026889348 1.617958429

CL	-3.951823921	-1.879969736	-1.411450274
MG	-0.004719125	-1.869092175	-0.055449432
CL	-1.939351799	-1.855560087	1.384090654
CL	1.921080132	-1.829896474	-1.509079197
MG	5.913084971	-1.882819206	-0.090233169
MG	11.881865503	-1.892795960	-0.511380016
CL	3.915893634	-1.813037731	1.322809481
CL	7.991065046	-1.703060293	-1.570442716
CL	10.112060491	-2.213748865	1.325140950
CL	14.047172378	-2.127374351	-0.054067347
CL	-10.758394104	0.016868205	1.680217780
MG	-8.844466307	-0.009359250	0.177909404
CL	-5.011068410	-0.029696598	1.399520101
CL	-7.040127310	-0.293836598	-1.391312301
MG	-3.036393083	-0.033397696	0.138801732
CL	0.930400774	0.152352771	1.193963576
CL	-1.122521103	0.036792169	-1.556292147
CL	6.981992877	-0.228318123	1.479438131
CL	4.987418754	0.055826168	-1.448161140
MG	8.996965858	-0.000920797	0.171240988
CL	10.998715182	0.171222109	-1.260758075
TI	-0.126749693	2.103544204	-0.520050492
CL	-2.096213874	2.137637268	0.914728663
CL	2.280139183	2.323162538	-0.833512403
C	-0.477698439	4.472895115	-1.335728909
C	0.606248280	5.309204900	-2.024166002
C	-1.690715874	5.320368630	-0.939935893
O	8.510680770	2.038623504	-0.407313653
O	9.761533964	1.458501301	1.562113306
O	-9.695119605	1.543141749	-1.067698350

O	-8.287503652	1.971284731	0.838220443
MG	3.004857335	0.012734691	-0.189516861
C	-0.847834806	3.211808813	-2.097808544
C	10.715244641	1.322403184	2.623907194
C	7.905026422	2.547212111	-1.604830934
C	-7.661619766	2.420666814	2.049924757
C	-10.737264543	1.475294913	-2.050943465
C	-10.267758547	4.133103779	0.224575946
C	-11.401748768	3.625313833	1.146482503
C	-11.915774001	4.902071637	1.818179310
C	-10.632303608	5.675533182	2.141529005
C	-9.668822947	5.381182709	0.964513185
C	-7.722045165	3.718966245	-1.486668165
C	-6.220488706	3.396176810	-1.200762987
C	-5.527203176	3.312313993	-2.586319117
C	-6.550157086	3.845639344	-3.598288747
C	-7.895613581	3.425141260	-2.999413940
SI	-8.996792658	2.902369620	-0.371285458
SI	9.119191933	2.874415723	0.915566535
C	7.769383911	3.633439854	1.983956530
C	6.299953417	3.473823798	1.478839087
C	5.422067030	3.317556682	2.749641523
C	6.348048356	3.612180337	3.938160550
C	7.721508897	3.138755124	3.452060542
C	10.445706749	4.126625494	0.511356398
C	11.620246851	3.685436447	-0.391473682
C	12.212255153	5.010843404	-0.879412475
C	10.974869778	5.860746138	-1.193457534
C	9.913063533	5.449988684	-0.140739763
H	-0.008445625	4.177182207	-0.339167960

H	0.931042110	6.134570258	-1.387457749
H	1.478775882	4.706812452	-2.273882920
H	0.204739769	5.729932101	-2.948176398
H	-1.399271504	6.142773507	-0.283848382
H	-2.141949685	5.747389915	-1.837859016
H	-2.443991803	4.723943854	-0.426670413
H	-1.905167118	3.103104797	-2.324957724
H	-0.235288032	3.021166491	-2.980368050
H	10.478834710	2.001327046	3.443274040
H	10.667843611	0.298331273	2.987307968
H	11.719867014	1.526723969	2.251966366
H	7.438995743	3.515552267	-1.421119153
H	8.664546709	2.645322141	-2.380621773
H	7.137728663	1.845164887	-1.922910831
H	-6.986676887	3.252316010	1.844995471
H	-8.422288367	2.725121535	2.769031685
H	-7.080778793	1.596385412	2.454004901
H	-10.798172604	2.405161970	-2.616713102
H	-10.509600955	0.658215658	-2.732442318
H	-11.691367710	1.284951899	-1.558986219
H	-10.738492392	4.505037321	-0.696057518
H	-11.019604867	2.935879060	1.901985664
H	-12.174282681	3.084919815	0.599344489
H	-12.533361661	5.469257606	1.114776138
H	-12.524900597	4.702592181	2.700907819
H	-10.205960939	5.299380412	3.074825790
H	-10.800213428	6.744706312	2.276920295
H	-8.654101866	5.216525402	1.334180510
H	-9.607616325	6.229037137	0.281191965
H	-7.861254118	4.798205088	-1.356703813

H	-6.102095089	2.455611319	-0.666085271
H	-5.780762569	4.177762873	-0.578386662
H	-4.588163100	3.867173773	-2.613477163
H	-5.297583221	2.270002433	-2.816059936
H	-6.393669340	3.454289795	-4.604880606
H	-6.498076545	4.937121422	-3.657681780
H	-8.047624754	2.356141648	-3.166523941
H	-8.742044628	3.957230639	-3.439487355
H	7.992245376	4.706037790	2.020322093
H	6.185939110	2.598987609	0.841613219
H	6.004853947	4.344100296	0.889718139
H	4.548372281	3.970388525	2.731072252
H	5.058517886	2.290666207	2.816632712
H	6.029432102	3.114410077	4.855475115
H	6.380211099	4.686905586	4.141771169
H	7.766338497	2.048052872	3.489687138
H	8.542293275	3.531260765	4.056875419
H	10.870289851	4.401249931	1.487270257
H	11.264321924	3.101521907	-1.242811063
H	12.341181032	3.058431707	0.133447010
H	12.796905883	5.472786846	-0.077833205
H	12.873539180	4.891462660	-1.738850052
H	10.614403084	5.623379984	-2.197191631
H	11.178767391	6.932019359	-1.174099372
H	8.936678786	5.328762912	-0.615531246
H	9.785900025	6.221345549	0.619612619

$(MgCl_2)_{13}/TiCl_2{}^{i}Bu/DCPDMS$-Mg1

Total atom = 94

CL	8.923793167	-4.532349797	-0.967595858

MG	7.134576355	-4.157933478	0.352994049
CL	2.915131501	-3.768240185	-1.003634722
MG	1.127260333	-3.395012002	0.318106456
CL	5.324076785	-3.785569917	1.644913160
CL	-0.654314364	-3.021726768	1.649530282
CL	-2.845552928	-3.050594876	-1.168581786
MG	-4.627074247	-2.676866260	0.162447011
CL	-8.853615724	-2.282721975	-1.173362313
MG	-10.635023419	-1.908976129	0.158616045
CL	-6.476333720	-2.304904810	1.397696805
CL	-12.393600353	-1.535884256	1.519671903
CL	12.262249943	-2.553638162	0.348883377
MG	10.087829741	-2.539512856	-0.102303963
CL	8.447409775	-2.403345199	1.497841695
MG	4.324601458	-2.015922340	0.151759078
CL	6.337968222	-2.430900959	-1.342325333
CL	2.355392968	-1.481971561	1.507403987
MG	-1.532343924	-1.183546086	0.019064892
CL	0.422250406	-1.558279408	-1.342651655
CL	-3.472297408	-0.756335684	1.389075761
MG	-7.411440386	-0.522845791	-0.155350230
MG	-13.347043161	0.192026314	0.049981618
CL	-5.388124136	-0.846273490	-1.495674049
CL	-9.485768717	0.063138334	1.219197137
CL	-11.587171171	-0.540468277	-1.673117659
CL	-15.515193674	0.152094800	-0.453772827
CL	9.404043626	-0.747319582	-1.538973248
MG	7.465949533	-0.375925582	-0.115648329
CL	3.681799260	-0.110545311	-1.460122821
CL	5.607572038	-0.266790039	1.412849413

MG 1.698173423 0.261883693 -0.272951406
CL -2.215133266 0.780513622 -1.472035066
CL -0.232227618 0.736674557 1.342596700
CL -8.292027427 1.327707136 -1.903473905
CL -6.335059230 1.417936704 0.985573065
MG -10.265312796 1.358296609 -0.733248585
CL -12.184613116 2.363434977 0.177290537
TI -0.949648741 2.779067574 0.064877428
CL 1.024467383 2.415173253 -1.317249593
CL -3.319489797 3.286964203 0.330111553
C -0.341918879 5.171208969 0.604582410
C -1.328224729 6.196961602 1.173081288
C 0.958660916 5.826936278 0.130491411
O 8.462781362 1.214051066 0.960548078
O 7.149825596 1.555847945 -1.028388183
MG -4.303782634 1.052435314 -0.138769789
C -0.115991119 3.975663985 1.514889788
C 6.604563891 1.918064257 -2.306456621
C 9.479412507 1.150956699 1.970571289
C 9.350925051 3.544489116 -0.619698764
C 10.434128779 2.805068003 -1.440426705
C 11.098718522 3.924632288 -2.246884812
C 9.915712964 4.788890626 -2.698090846
C 8.907627710 4.749852635 -1.522288265
C 6.746124982 3.631249368 1.048902206
C 5.222024672 3.440994133 0.763427925
C 4.504701023 3.608088015 2.129018372
C 5.565986293 4.152727176 3.094371011
C 6.864943370 3.516432500 2.590865494
SI 7.938281440 2.545557010 0.081634676

H	-0.838859667	4.813062172	-0.358045449
H	-1.558736633	6.971070029	0.438692593
H	-2.262730128	5.728699172	1.479421515
H	-0.884106285	6.678036889	2.046716727
H	0.761659120	6.592294975	-0.622442091
H	1.451864644	6.305856280	0.978721402
H	1.642665724	5.094627130	-0.296658871
H	0.922440497	3.777582318	1.767599529
H	-0.747150340	3.959668012	2.404626781
H	6.004792245	2.824846899	-2.222040174
H	7.410761081	2.068318812	-3.024674003
H	5.961124453	1.108566822	-2.639043858
H	9.645557363	2.132074824	2.415775583
H	9.148893368	0.460578082	2.743912584
H	10.408720557	0.788562208	1.530598402
H	9.846417077	3.972927399	0.262495183
H	9.987928056	2.073857400	-2.117472190
H	11.132705814	2.254665227	-0.810182920
H	11.765813124	4.502876088	-1.599992679
H	11.694573253	3.551813476	-3.081116514
H	9.463735744	4.349937611	-3.591017670
H	10.205156696	5.808140282	-2.956769640
H	7.886463317	4.653316806	-1.898320600
H	8.931889893	5.677187125	-0.948767825
H	7.007190434	4.663230557	0.788581836
H	5.006240770	2.459560773	0.345253967
H	4.881327698	4.181775410	0.037699160
H	3.632044985	4.259448259	2.061247171
H	4.158849875	2.633925997	2.480309142
H	5.353019645	3.912547436	4.137336888

H 5.634051050 5.242003041 3.014782918

H 6.895801850 2.467703696 2.895776392

H 7.758800900 4.006036702 2.983938540

$(MgCl_2)_{13}$/$TiCl_2{}^{i}$Bu/DCPDMS-Mg4

Total atom = 94

CL -12.406029345 -1.871232786 1.501362818

MG -10.637884996 -2.112248001 0.122443335

CL -6.383781139 -2.507440724 1.364127891

MG -4.617484179 -2.749404748 -0.015849003

CL -8.848725917 -2.355732758 -1.228319562

CL -2.857761428 -2.991339847 -1.405190163

CL -0.607977366 -3.112852465 1.363906991

MG 1.151912001 -3.354307035 -0.025328765

CL 5.412707212 -3.749954754 1.194959937

MG 7.172858819 -3.991297377 -0.194667143

CL 2.981579310 -3.599106532 -1.320309802

CL 8.908547737 -4.232513949 -1.613411158

CL -15.267890000 0.607816084 -0.066814037

MG -13.127258437 0.187916269 0.356116350

CL -11.571216326 -0.288204437 -1.261792372

MG -7.412139164 -0.665799595 -0.028171777

CL -9.400258053 -0.385817939 1.529040489

CL -5.434359177 -0.798807281 -1.468753132

MG -1.517888682 -1.186992410 -0.079709530

CL -3.445062462 -0.902373893 1.341618918

CL 0.406564336 -1.418784451 -1.517059472

MG 4.360092645 -1.873032390 -0.062686974

MG 10.290948617 -2.575017082 -0.431464410

CL 2.377277094 -1.526411184 1.329665429

CL	6.451838381	-1.983459818	-1.530232842
CL	8.487678769	-2.626920561	1.399807243
CL	12.413428774	-3.037055671	0.052573993
CL	-11.923246087	2.273933086	1.051642120
MG	-10.090538704	1.372380692	-0.043664234
CL	-6.339546810	1.227289016	1.263970676
CL	-8.321389024	1.339160521	-1.504410369
MG	-4.331027365	1.006064179	0.062331034
CL	-0.365528288	0.747115880	1.118860262
CL	-2.424643023	0.791902421	-1.627383092
CL	5.597945991	-0.295937754	1.455076102
CL	3.663955343	0.116116872	-1.492851027
MG	7.636388025	-0.343893371	0.163293314
CL	9.653340445	-0.448667105	-1.252034311
TI	-1.201763465	2.764064459	-0.637590630
CL	-3.150862355	3.044498323	0.807178576
CL	1.210284574	2.695706999	-0.970460357
C	-1.314307575	5.134045927	-1.504428515
C	-0.151174465	5.835196467	-2.214174064
C	-2.429659753	6.112663283	-1.123886851
O	7.392456002	1.708004335	-0.504842236
O	8.528924624	1.077148192	1.517433574
MG	1.684944516	0.340527319	-0.250525649
C	-1.819458907	3.902775547	-2.236048706
C	9.423589308	0.880734269	2.620145857
C	6.883812551	2.226167606	-1.742681997
SI	8.060816343	2.527027517	0.799779417
C	6.777435962	3.473878907	1.797745759
C	5.315090513	3.462541194	1.248783535
C	4.387447121	3.456089309	2.493482331

C	5.305090655	3.690093559	3.701712466
C	6.629227984	3.045432886	3.279983622
C	9.526537465	3.608449856	0.385088226
C	10.671171394	3.000819201	-0.457961876
C	11.414479602	4.229653710	-0.989746043
C	10.283886433	5.188533140	-1.381995965
C	9.160721321	4.950438055	-0.340181995
H	-0.872807563	4.811456934	-0.502199001
H	0.262899452	6.634316709	-1.596260119
H	0.651011188	5.138422512	-2.454396169
H	-0.511046197	6.277225106	-3.145260889
H	-2.050198373	6.914617426	-0.488069713
H	-2.838803185	6.563603157	-2.030109883
H	-3.239308422	5.611481651	-0.595006185
H	-2.884070875	3.900925592	-2.455087788
H	-1.236661555	3.628466082	-3.116769190
H	9.223085095	1.602508704	3.411937506
H	9.262712620	-0.123069500	3.006808146
H	10.456918898	0.976700237	2.284867115
H	6.531560854	3.250224745	-1.617502204
H	7.669878209	2.196582585	-2.497300152
H	6.047267536	1.604724109	-2.053928055
H	7.120846911	4.514780649	1.803746436
H	5.120522544	2.582531813	0.638760259
H	5.139168974	4.337168178	0.619868450
H	3.594902406	4.202093167	2.421878153
H	3.907337186	2.480116288	2.584539871
H	4.904253387	3.268066900	4.624719489
H	5.453782407	4.761400754	3.867937963
H	6.547693926	1.959001940	3.357693524

H 7.470896914 3.365980436 3.898295567

H 9.950284415 3.880067811 1.362165422

H 10.278505761 2.414763220 -1.291394851

H 11.307044606 2.329487283 0.119554123

H 12.024494104 4.667314496 -0.193450707

H 12.081010261 3.997387098 -1.821559586

H 9.922832247 4.936971750 -2.382070003

H 10.601528843 6.231477119 -1.411720684

H 8.186749145 4.917928035 -0.833833110

H 9.106805329 5.766688948 0.380998602

2Al/$(MgCl_2)_{13}$/$TiCl_2$^{i}Bu cluster 4

Total atom = 87

CL 10.760741798 -3.049461950 -1.794679877

MG 9.002512638 -3.126133945 -0.384994630

CL 4.708548174 -3.029659464 -1.552211965

MG 2.950281544 -3.106360464 -0.143525589

CL 7.219093860 -3.200769604 0.993540427

CL 1.198467840 -3.185703585 1.277008931

CL -1.097761319 -3.001303097 -1.450363025

MG -2.848688127 -3.080731802 -0.032862663

CL -7.147786571 -2.983598797 -1.176880694

MG -8.897749033 -3.064054657 0.239612200

CL -4.673147699 -3.154019631 1.292110944

CL -10.627520906 -3.145554413 1.687413984

CL 13.902451994 -0.929551202 -0.235131899

MG 11.723533999 -1.101380387 -0.624943680

CL 10.150367508 -1.442102693 1.012721792

MG 5.945020115 -1.331956961 -0.139195284

CL 7.914691099 -1.281735095 -1.755267562

CL	4.010578142	-1.287643563	1.352675707
MG	0.044470339	-1.209515696	0.041544476
CL	1.970852145	-1.067065301	-1.391375199
CL	-1.877205908	-1.290319066	1.495523477
MG	-5.882742226	-1.256980222	0.092065023
MG	-11.841986037	-1.326230340	0.567894987
CL	-3.886677623	-1.091831510	-1.323104015
CL	-7.957905334	-1.179679099	1.595264652
CL	-10.084544663	-1.534936320	-1.299997994
CL	-14.011267190	-1.546936779	0.113066777
CL	10.817263722	1.006711183	-1.470958366
MG	8.852718399	0.499203178	-0.334526966
CL	5.191237520	0.690810860	-1.290674186
CL	7.316966786	0.482387556	1.523256569
MG	3.185599142	0.814871788	0.065317224
CL	-1.011168377	0.901240174	-1.213465129
CL	1.120207626	0.724043414	1.551146123
MG	-3.077143035	0.837783893	0.225395515
CL	-7.214882616	0.646571028	-1.549530196
CL	-5.127266746	0.608950491	1.467133109
MG	-9.010766688	0.416943515	0.040885731
CL	-11.037417600	0.883491561	1.134480160
TI	0.083553349	2.662523161	0.321318801
CL	2.093763414	2.648095542	-1.110836844
CL	-1.972709138	2.458941033	1.690941558
C	0.195745834	4.707935456	0.627144639
C	-0.653700704	4.912526026	-0.613653731
C	-1.999926976	5.583819717	-0.322974721
C	0.087577026	5.604757452	-1.762510101
CL	4.210346650	2.318731035	1.934953248

CL	-4.099445137	2.548516141	-1.496357634
AL	6.399554794	2.732980708	1.868652947
C	7.053503899	3.142675304	3.670257698
C	6.957661107	3.689891710	0.229216288
C	6.507380323	4.451073549	4.273022237
C	8.034495026	3.038759695	-0.642761985
AL	-6.297596409	2.923786059	-1.552975096
C	-6.813800582	3.535878755	-3.343363893
C	-7.011248957	3.670698714	0.132825203
C	-8.177205649	2.926857555	0.790624708
C	-6.238468764	4.904586953	-3.753444021
H	-0.278961088	5.016677876	1.556808994
H	1.214836264	5.081706316	0.548397741
H	-0.935099771	3.890336570	-1.036159994
H	-2.632283564	5.597711037	-1.212145065
H	-2.537124071	5.068058264	0.471680736
H	-1.826641866	6.615703172	-0.009455925
H	-0.518507299	5.612347649	-2.670696919
H	0.298221770	6.640255450	-1.486196573
H	1.032583742	5.111743313	-1.986540671
H	8.149431741	3.182242133	3.641590777
H	6.810157410	2.304542922	4.331658705
H	6.076540391	3.887703750	-0.386104638
H	7.324314779	4.670698884	0.554088499
H	6.911805697	4.637517545	5.271542214
H	6.760064351	5.320138438	3.659206323
H	5.419095225	4.426497749	4.365558329
H	8.936401921	2.801127196	-0.058222264
H	7.613375969	2.153105466	-1.148922173
H	8.393316562	3.673180168	-1.456241281

H	-6.512271929	2.777944401	-4.073979034
H	-7.909268147	3.569686201	-3.394715123
H	-6.199288076	3.764537349	0.857838357
H	-7.334758035	4.693742119	-0.092491245
H	-9.005002151	2.771381014	0.080875746
H	-7.819915922	1.978637926	1.221861390
H	-8.628868802	3.462317829	1.628693509
H	-6.542174187	5.698493167	-3.065399724
H	-5.146154418	4.890789510	-3.769126102
H	-6.571074554	5.202918652	-4.751369061

$(MgCl_2)_{13}/TiCl_2{}^{i}Bu/AlEt_2Cl$-Mg2

Total atom = 71

CL	10.150700678	-3.366064538	-1.357236921
MG	8.367206968	-3.217056021	0.014431862
CL	4.101533291	-3.077722764	-1.248027510
MG	2.318076639	-2.928921536	0.122665302
CL	6.559196012	-3.068437740	1.354401454
CL	0.540567768	-2.781620308	1.505431803
CL	-1.699406691	-2.806278432	-1.274366872
MG	-3.475945994	-2.659504201	0.105518089
CL	-7.747093547	-2.516706602	-1.134050060
MG	-9.522598166	-2.371191447	0.244847843
CL	-5.323903903	-2.513674746	1.391260076
CL	-11.278517044	-2.223911592	1.655593979
CL	13.352039862	-1.215007088	0.028825039
MG	11.174657909	-1.341248362	-0.386544059
CL	9.561101243	-1.436977810	1.244433176
MG	5.384103872	-1.285956303	-0.002549270
CL	7.381349265	-1.492310700	-1.571775469

CL	3.428201676	-1.000823067	1.433852490
MG	-0.508184227	-0.908561369	0.037378590
CL	1.446462244	-1.001461101	-1.360893630
CL	-2.455857788	-0.752298391	1.449992278
MG	-6.432203904	-0.713474643	-0.034448431
MG	-12.396231104	-0.491339587	0.318695518
CL	-4.407040900	-0.784207727	-1.415627677
CL	-8.527372918	-0.388228392	1.406861071
CL	-10.617714145	-0.974118594	-1.477331837
CL	-14.564840308	-0.673900787	-0.155912165
CL	10.374860161	0.701915005	-1.468079542
MG	8.371954639	0.391649327	-0.330626812
CL	4.726405374	0.615774493	-1.398886930
CL	6.785244921	0.651124162	1.469533451
MG	2.701345274	0.982082253	-0.122674654
CL	-1.568245097	1.066940945	-1.524185396
CL	0.550386229	1.192438361	1.253180466
MG	-3.482165596	1.095803719	0.124953642
CL	-7.493420487	1.162092065	-1.652796024
CL	-5.540541611	1.224884864	1.237027804
MG	-9.435123038	0.967527785	-0.445608189
CL	-11.408353214	1.757577129	0.556168430
TI	-0.366008044	2.982056839	-0.312747771
CL	1.709415460	2.671558382	-1.592967008
CL	-2.468182410	3.112094192	1.014313292
C	-0.253789450	5.049115934	-0.419274956
C	-1.031289327	4.979385762	-1.719017128
C	-2.406226505	5.652995534	-1.651503181
C	-0.231989506	5.439193579	-2.943006058
CL	3.727682181	2.643875942	1.573118356

AL	5.940754260	2.959338725	1.521559726
C	6.558246509	3.552882620	3.283454627
C	6.574369263	3.694370595	-0.201812618
C	6.051502698	4.943535539	3.709872280
C	7.654604943	2.913744195	-0.954260323
H	-0.776396509	5.540619506	0.398719411
H	0.770535900	5.402814036	-0.518323636
H	-1.269374563	3.884344313	-1.941083033
H	-2.984690193	5.457333396	-2.556637849
H	-2.980137001	5.305980043	-0.793399378
H	-2.276094826	6.733301859	-1.560688428
H	-0.782250677	5.246317665	-3.865925450
H	-0.051190265	6.513875547	-2.874253446
H	0.730600356	4.933791914	-3.007177210
H	7.655113429	3.545782467	3.285499097
H	6.262034974	2.808889058	4.030103434
H	5.718702913	3.842871753	-0.864787668
H	6.962189645	4.696188626	0.016814772
H	6.436243059	5.231767271	4.691630026
H	6.356859365	5.723225048	3.006714852
H	4.961191292	4.972652514	3.770516408
H	8.528653315	2.715609647	-0.315601314
H	7.219205463	1.989516064	-1.371002413
H	8.060727970	3.438479849	-1.821686721

$(MgCl_2)_{13}/TiCl_2{}^{i}Bu/AlEt_2Cl$-Mg3

Total atom = 71

CL	-11.421836538	-2.139071544	1.695532777
MG	-9.638446335	-2.451663849	0.351529754
CL	-5.370007708	-2.376455531	1.610390277

MG	-3.586598614	-2.688985149	0.267491820
CL	-7.830512004	-2.759390678	-0.961075567
CL	-1.809461949	-3.005267971	-1.087139033
CL	0.433583507	-2.579064201	1.657425698
MG	2.209839760	-2.895093119	0.305895052
CL	6.483881477	-2.822184339	1.541747871
MG	8.258999215	-3.139092326	0.191287143
CL	4.057706915	-3.196557477	-0.952664801
CL	10.014579261	-3.459974739	-1.190706258
CL	-14.441077926	-0.106535274	-0.188487111
MG	-12.279639758	-0.311725102	0.275897592
CL	-10.686995109	-0.906961350	-1.267472839
MG	-6.506078230	-0.817015558	-0.028075104
CL	-8.506318711	-0.497368199	1.518658418
CL	-4.539824565	-1.025449414	-1.462950897
MG	-0.603033779	-0.939053353	-0.067924075
CL	-2.552249913	-0.552066085	1.286792260
CL	1.344431664	-1.267221030	-1.451043705
MG	5.316968774	-1.215278767	0.042217210
MG	11.277472184	-1.565616600	-0.266129344
CL	3.299293275	-0.805340945	1.374841132
CL	7.425380178	-1.398463212	-1.404689842
CL	9.473510437	-1.480813425	1.566791167
CL	13.425858148	-1.811321371	0.268337877
CL	-11.211756127	1.911956644	0.696768721
MG	-9.314866030	0.990298906	-0.266075648
CL	-5.607625803	1.271436782	1.006828147
CL	-7.564108691	0.885142202	-1.748639589
MG	-3.625945871	1.063480529	-0.253248502
CL	0.427103359	1.313988397	0.848826917

CL	-1.682668336	0.811870333	-1.898498758
MG	2.581532648	0.939358180	-0.453144082
CL	6.668198695	0.823623804	1.463011175
CL	4.657823320	0.482134616	-1.581134970
MG	8.507420088	0.331670518	-0.021556227
CL	10.572648796	0.590928135	-1.109403382
TI	-0.523578783	2.863229847	-1.010957347
CL	-2.669587102	3.235129485	0.184060240
CL	1.571872690	2.333516034	-2.208327901
C	-0.484030098	4.836540707	-1.637403397
C	0.315679335	5.180354947	-0.395053747
C	1.714529770	5.723175252	-0.704481307
C	-0.434435737	6.076692529	0.595904770
CL	3.605949585	2.817106177	1.048894612
AL	5.823269082	3.110440990	1.143097617
C	6.292329405	3.926678488	2.862693214
C	6.619362960	3.611543737	-0.595052588
C	7.783039482	2.757489784	-1.105846292
C	5.751144162	5.352803370	3.074270292
H	0.059227289	4.956247652	-2.572930161
H	-1.474051352	5.285120018	-1.682840249
H	0.512645364	4.218502453	0.189372040
H	2.303879111	5.833186176	0.206999026
H	2.253987637	5.066045095	-1.384865872
H	1.622460556	6.705082914	-1.173483087
H	0.129813014	6.191104989	1.523350233
H	-0.570517995	7.067369130	0.157257443
H	-1.416579783	5.675180115	0.841409697
H	5.938812234	3.276298751	3.669436489
H	7.385659782	3.932948701	2.953097464

H	5.837584431	3.634538817	-1.357734988
H	6.967227039	4.645753962	-0.488670357
H	8.578501947	2.668088362	-0.349427796
H	7.410735046	1.773040369	-1.429191685
H	8.282804242	3.169514034	-1.985171378
H	6.107590063	6.043934515	2.305541489
H	4.659297062	5.374987581	3.047570523
H	6.057511027	5.764643361	4.039466242

2Al/2DIBP/$(MgCl_2)_{13}TiCl_2{}^{i}Bu$ cluster 6

Total atom = 171

CL	10.815819228	-3.902748438	-1.937793061
MG	9.063198075	-4.034634930	-0.525862144
CL	4.764681069	-3.885310235	-1.670452221
MG	3.011872756	-4.017122405	-0.258798554
CL	7.285027039	-4.163504987	0.856149515
CL	1.265644675	-4.152325980	1.164106489
CL	-1.041118097	-3.853658222	-1.544171745
MG	-2.786593307	-3.988668854	-0.124128169
CL	-7.089890691	-3.839438109	-1.245651003
MG	-8.834698123	-3.975349601	0.172567483
CL	-4.605781588	-4.113692847	1.204165473
CL	-10.558681064	-4.113899501	1.623413381
CL	13.966647355	-1.852385523	-0.305250175
MG	11.786417742	-2.005040731	-0.693909028
CL	10.218777130	-2.410724874	0.935516561
MG	6.009566797	-2.247320065	-0.194611637
CL	7.971930165	-2.134934502	-1.813959435
CL	4.080754812	-2.262691096	1.305798922
MG	0.109561358	-2.125787349	0.015040309

CL 2.030462690 -1.927425695 -1.418400326

CL -1.806432078 -2.263478575 1.472300126

MG -5.817485547 -2.168556239 0.087557744

MG -11.774599844 -2.249198114 0.584543826

CL -3.826751059 -1.947420462 -1.327812357

CL -7.886573862 -2.149061167 1.600762155

CL -10.025034000 -2.383328423 -1.297811704

CL -13.946316111 -2.448083516 0.129085660

CL 10.925570061 -0.102687360 -1.854715293

MG 8.964762580 -0.156106295 -0.412101088

CL 5.149480358 -0.239711652 -1.358851970

CL 7.293288867 -0.639761224 1.440907875

MG 3.265556188 -0.096379430 0.114748890

CL -0.955680089 0.052865926 -1.145625151

CL 1.199448982 -0.238687780 1.598899955

MG -3.022299025 -0.080512002 0.296250795

CL -7.022640285 -0.357995066 -1.447198001

CL -4.964562567 -0.453203741 1.636214310

MG -9.000360581 -0.255709874 0.133066668

CL -10.984016867 -0.286267635 1.624150768

TI 0.147976592 1.732540262 0.452668824

CL 2.146472894 1.794765064 -0.987452299

CL -1.892876231 1.485119116 1.831589782

C 0.249131455 3.772349700 0.826333524

C -0.624162811 4.017477874 -0.391208179

O -9.973858192 1.136262745 -1.013691366

C -10.528843419 2.213654073 -0.839719818

C -8.306433054 2.529813899 1.417358906

O -8.323040586 1.336425411 1.154693795

O 9.866509981 1.243100523 0.785385405

C	10.239530287	2.406088114	0.700133435
C	7.920367422	2.610337831	-1.448728857
O	8.152651466	1.414537234	-1.345536019
O	-11.804512103	2.393337166	-1.092398729
C	-12.577400300	1.262710055	-1.620102628
O	-7.777989123	2.974175616	2.534680046
C	-7.170677075	1.989603632	3.439471104
O	11.486007081	2.761312410	0.900371652
O	7.314659892	3.101921997	-2.504836035
C	12.457854400	1.721797858	1.269962045
C	6.886108280	2.167846321	-3.553154961
C	-1.965688642	4.675328908	-0.052543003
C	0.095434202	4.752559381	-1.526835954
C	9.340412738	3.585640650	0.474809398
C	8.265800039	3.660937626	-0.441693520
C	9.593720401	4.681121100	1.304126342
C	7.480002040	4.817284734	-0.457964546
C	7.718896456	5.873377698	0.406985816
C	8.787412189	5.808903302	1.286848046
C	-8.836419377	3.628567107	0.549267078
C	-9.850521691	3.487318478	-0.428426014
C	-10.268084202	4.621518957	-1.129955961
C	-8.284970058	4.896611621	0.759128272
C	-8.686264398	6.000580313	0.023766581
C	-9.686963876	5.863266766	-0.924023487
C	13.836697942	2.353540161	1.335748255
C	5.934595328	2.894697696	-4.486027118
C	6.600566488	4.071831015	-5.200689642
C	5.359454437	1.880060437	-5.480279464
C	14.317031693	2.800073663	-0.047004486

C	14.806855334	1.349737319	1.969969377
C	-14.025573913	1.693031262	-1.769932502
C	-6.493483711	2.734227052	4.575323684
C	-14.786222723	0.596193981	-2.524592403
C	-14.671866356	1.988217495	-0.414348817
C	-5.705583451	1.724938825	5.417832185
C	-7.487659654	3.527787432	5.425268816
CL	4.386034901	1.442335738	1.863379842
CL	-4.134757240	1.775786443	-1.157257298
AL	6.110237641	0.651451754	3.099778735
AL	-5.719344910	1.240017442	-2.686194460
C	7.297445182	2.171104252	3.497110407
C	6.772807674	3.120115589	4.590163707
C	5.545310819	-0.685178480	4.422739793
C	4.344437356	-0.287255425	5.299925570
C	-6.896984137	2.805807454	-2.895387389
C	-4.994776124	0.209104179	-4.192654501
C	-3.728249808	0.787470760	-4.849479884
C	-6.298816586	3.944481553	-3.741460395
H	-0.211381403	4.043742755	1.774451038
H	1.263442902	4.157651067	0.745053180
H	-0.912024251	3.012988960	-0.844429430
H	-2.615587209	4.718142831	-0.927890247
H	-2.487567746	4.127672724	0.730713002
H	-1.788246894	5.695452039	0.296214957
H	-0.526899052	4.793629480	-2.423163677
H	0.312922893	5.777326728	-1.216991623
H	1.035075737	4.266157483	-1.785308432
H	7.787129385	1.827660690	-4.067792034
H	6.409450086	1.319242870	-3.070048026

H	12.142592017	1.316244754	2.231823815
H	12.414548354	0.936154918	0.518651239
H	-7.969861823	1.336858146	3.795430204
H	-6.466351325	1.395795832	2.861022015
H	-12.128356838	0.978780855	-2.572168861
H	-12.480601550	0.435286803	-0.920396905
H	7.075948730	6.743181224	0.383402386
H	8.997180333	6.628934555	1.960860939
H	6.664310302	4.877624591	-1.161715900
H	10.428240627	4.631913676	1.987406262
H	-11.055390038	4.517305924	-1.861152155
H	-8.220412475	6.961156585	0.199338688
H	-10.020066774	6.714585821	-1.502886112
H	-7.519886586	5.007969142	1.511484074
H	13.768159148	3.231073904	1.988794621
H	5.108929599	3.272103177	-3.873314264
H	7.419517479	3.726291912	-5.837924374
H	5.882164365	4.591270512	-5.837341803
H	7.007534452	4.796741152	-4.494445816
H	4.641141899	2.363955767	-6.143492447
H	6.147234363	1.448446594	-6.103592236
H	4.847906233	1.063985375	-4.967667175
H	14.419683882	1.938647322	-0.711062496
H	13.623479934	3.505612683	-0.507200561
H	15.291353602	3.286524848	0.024870873
H	15.809028411	1.777962620	2.022579101
H	14.502989624	1.085022388	2.985325227
H	14.861317755	0.430716967	1.382631470
H	-14.037895588	2.605563533	-2.376856335
H	-5.778028046	3.431762619	4.126215731

H	-14.767598603	-0.345228842	-1.971046353
H	-15.829612444	0.886002580	-2.657353795
H	-14.360443046	0.418861414	-3.514842186
H	-14.123233052	2.752982773	0.137310724
H	-15.695681979	2.341482053	-0.548950328
H	-14.707498754	1.083244152	0.196612770
H	-5.180078759	2.234878595	6.226485816
H	-6.371331774	0.985040622	5.869955140
H	-4.967020997	1.191412091	4.817974950
H	-8.207859391	2.859362987	5.905359304
H	-6.968163101	4.075855062	6.213302059
H	-8.046011928	4.249647208	4.827526436
H	8.273819187	1.770934022	3.796047177
H	7.476118198	2.737423715	2.578403238
H	7.463578396	3.945882978	4.788344372
H	5.814066958	3.564536854	4.311021495
H	6.620245733	2.599852909	5.539138551
H	5.327705458	-1.628076023	3.914890774
H	6.415389093	-0.889920464	5.059712079
H	4.107373415	-1.059054022	6.037891208
H	4.527686297	0.638027434	5.853180653
H	3.446597372	-0.129655927	4.698909157
H	-7.833065971	2.463404402	-3.353077974
H	-7.172603544	3.190640521	-1.909002043
H	-4.799270554	-0.815647779	-3.867423068
H	-5.794809466	0.131618902	-4.940205624
H	-2.895898336	0.827020840	-4.143899974
H	-3.400514077	0.183714633	-5.700730421
H	-3.884842877	1.804190997	-5.220747155
H	-6.046051011	3.609018107	-4.750473317

H -6.988914036 4.787230851 -3.849608520

H -5.381251238 4.337565389 -3.296186228

2Al/DIBP/$(MgCl_2)_{13}TiCl_2{}^{i}Bu$ cluster 7

Total atom = 129

CL -8.993778889 -4.178545288 2.208706808

MG -7.230491909 -4.262965000 0.805541636

CL -2.966287529 -3.645144100 1.924829399

MG -1.203706984 -3.730683705 0.522011674

CL -5.442400974 -4.338723456 -0.566181411

CL 0.553974583 -3.818443636 -0.890583983

CL 2.813913742 -3.110352638 1.780573198

MG 4.570306567 -3.198809866 0.370315113

CL 8.838949848 -2.583649239 1.465883072

MG 10.594477348 -2.673115094 0.056865948

CL 6.398970530 -3.263707260 -0.949212408

CL 12.330083979 -2.768982619 -1.383101675

CL -12.307113834 -2.546456208 0.432594631

MG -10.121446927 -2.475391161 0.825780163

CL -8.519178242 -2.865459053 -0.771974319

MG -4.345059419 -2.243125644 0.330850608

CL -6.321761012 -2.182270019 1.942758958

CL -2.417645144 -2.201354767 -1.169744938

MG 1.521384558 -1.615658853 0.096765915

CL -0.415652507 -1.479125514 1.516282249

CL 3.448133551 -1.694472740 -1.350887956

MG 7.429076638 -1.138225267 0.011777917

MG 13.372254212 -0.729285182 -0.493130280

CL 5.420965654 -0.987225176 1.411192121

CL 9.494597876 -1.052769495 -1.504260771

CL	11.633515699	-0.873569593	1.398236322
CL	15.550858616	-0.700162439	-0.030170101
CL	-9.437769293	-0.417604335	1.825073491
MG	-7.476174079	-0.417941555	0.378284818
CL	-3.671793967	-0.081989105	1.334087894
CL	-5.756236432	-0.889731230	-1.426722862
MG	-1.807427999	0.111052161	-0.156432799
CL	2.385798002	0.726041062	1.073489192
CL	0.280731204	0.021779268	-1.631506567
MG	4.443844986	0.657071799	-0.361942821
CL	8.582560152	1.062365633	1.408117369
CL	6.521338266	0.477439949	-1.568955363
MG	10.394403938	0.803658570	-0.156789310
CL	12.376816341	1.316452372	-1.311406722
TI	1.139724240	2.171095045	-0.663427506
CL	-0.846585202	2.168772164	0.783960215
CL	3.219042493	1.986559282	-2.009668886
CL	5.309826419	2.655738154	1.143436237
AL	7.462001237	3.230710185	1.136126207
C	7.920562689	4.105682065	2.831061379
C	8.113859087	3.826525650	-0.633021292
C	9.346977443	3.118491566	-1.200563402
C	7.219973828	5.454890451	3.076062948
C	0.855434951	4.144893250	-1.230716082
C	1.681745932	4.585933471	-0.036197583
O	-8.498367668	0.799700077	-0.916730153
C	-9.000337245	1.916624128	-0.913053992
C	-6.754404539	2.501861002	1.246326836
O	-6.811401188	1.282385094	1.187841241
O	-10.272678146	2.116263550	-1.159795739

O	-6.252875767	3.112098197	2.295456767
C	-11.113885740	0.954329396	-1.481917600
C	-5.731758820	2.278582302	3.385860177
C	2.963099946	5.329251395	-0.426564191
C	0.879004865	5.356631278	1.017101076
C	-8.246502647	3.202785551	-0.742536441
C	-7.209822044	3.453613031	0.186537279
C	-8.608599312	4.216539011	-1.633305049
C	-6.571389361	4.697203836	0.158084833
C	-6.914824970	5.672151265	-0.765057171
C	-7.944343162	5.433233670	-1.661111289
C	-12.550591453	1.424405549	-1.622086332
C	-5.061216350	3.183384600	4.403309747
C	-6.041833417	4.166874601	5.044729803
C	-4.370671433	2.306372932	5.453417010
C	-13.119536157	1.899771238	-0.283224679
C	-13.385564601	0.281831517	-2.212437950
CL	-3.035364484	1.408236117	-2.014466955
AL	-4.698696878	0.395453321	-3.172971904
C	-6.013248969	1.783228439	-3.643274513
C	-5.568171742	2.728144887	-4.774491259
C	-4.020629695	-0.972021307	-4.407703858
C	-2.912390989	-0.505908967	-5.369419105
H	7.693032560	3.419641386	3.653549310
H	9.008080215	4.247013515	2.863346695
H	7.300936533	3.754914429	-1.359276772
H	8.339735909	4.895039759	-0.537091456
H	10.181467082	3.126432369	-0.481869089
H	9.080872957	2.096030980	-1.511349076
H	9.753301875	3.585869836	-2.100272228

H	7.447648952	6.182295514	2.291911012
H	6.133775593	5.342069438	3.105924702
H	7.522928454	5.904860237	4.025405544
H	1.302497429	4.368147629	-2.197655232
H	-0.192488618	4.435757695	-1.192981614
H	2.051219806	3.658978311	0.515171549
H	3.590243617	5.517706883	0.446321754
H	3.545497203	4.761264840	-1.150463051
H	2.700079107	6.290602806	-0.873483718
H	1.479713351	5.540760055	1.910162644
H	0.575371115	6.322525991	0.607247848
H	-0.017046196	4.813197784	1.313814615
H	-6.577058752	1.735960508	3.813373263
H	-5.036388455	1.563331561	2.952498637
H	-10.726654861	0.525167548	-2.406498962
H	-11.009713226	0.228155426	-0.678580357
H	-6.383395104	6.614484266	-0.774338730
H	-8.234484667	6.186653816	-2.381460185
H	-5.786964311	4.891703552	0.873125106
H	-9.415141632	4.033017665	-2.327154427
H	-12.557517639	2.261552540	-2.329437387
H	-4.288008709	3.750461627	3.873703489
H	-6.820893935	3.633868281	5.596921663
H	-5.524860350	4.820909216	5.749125986
H	-6.529146061	4.796416655	4.299104762
H	-3.844208391	2.926996639	6.179819972
H	-5.097851982	1.700654136	6.000622436
H	-3.644669968	1.631316925	4.997337817
H	-13.150135076	1.074276857	0.431699216
H	-12.520554519	2.703628397	0.147633274

H -14.137580681 2.271870121 -0.410547526
H -14.425719145 0.593392777 -2.319468692
H -13.021889930 -0.012478883 -3.199626095
H -13.360608084 -0.597381830 -1.565234095
H -6.948256150 1.285277385 -3.927001466
H -6.247367352 2.369495006 -2.749652138
H -6.327536239 3.481307604 -5.007417475
H -4.653193889 3.265800933 -4.513400349
H -5.366653467 2.184208273 -5.700707296
H -3.665526088 -1.831567911 -3.833418885
H -4.879001087 -1.339762994 -4.984165194
H -2.602370310 -1.304718660 -6.049257083
H -3.233055608 0.335040725 -5.990389581
H -2.022338225 -0.182732682 -4.825435346

2Al/DIBP/DCPDMS/$(MgCl_2)_{13}TiCl_2{}^{i}Bu$ cluster 8

Total atom = 168

CL -10.546788552 -4.067125668 1.315571456
MG -8.745133117 -4.074532913 -0.041085307
CL -4.489057874 -4.043406568 1.259770085
MG -2.689394933 -4.052071016 -0.095135466
CL -6.921360147 -4.082725891 -1.366333072
CL -0.894823352 -4.060529974 -1.464008785
CL 1.316691808 -4.018357324 1.338296380
MG 3.111265416 -4.028151740 -0.027722605
CL 7.373233277 -3.994184281 1.251458741
MG 9.165847670 -4.005157671 -0.112612262
CL 4.975470673 -4.037347434 -1.297909676
CL 10.938176539 -4.017635352 -1.508767417
CL -13.639255547 -1.867099670 -0.230256956

MG -11.473494321 -2.061123259 0.216675321
CL -9.849675855 -2.321308397 -1.387199267
MG -5.682493394 -2.274945682 -0.102744421
CL -7.700934495 -2.303030433 1.452685302
CL -3.702400121 -2.157684668 -1.530196101
MG 0.220678845 -2.151999888 -0.095242812
CL -1.748741947 -2.079664763 1.282737611
CL 2.186016635 -2.161705952 -1.492495870
MG 6.146747785 -2.204365165 0.033742447
MG 12.117684767 -2.258276929 -0.262141520
CL 4.108112665 -2.108320947 1.392839119
CL 8.267921033 -2.054029535 -1.399613611
CL 10.303826245 -2.558426028 1.537654004
CL 14.272032174 -2.504206098 0.246891780
CL -10.654766695 -0.273148023 1.571803066
MG -8.638840825 -0.201952326 0.203793897
CL -4.869196940 -0.385577437 1.270998359
CL -6.907825069 -0.519792389 -1.629082015
MG -2.935005564 -0.115817877 -0.115364071
CL 1.245304281 -0.100736670 1.310283189
CL -0.805502535 -0.116790593 -1.525422718
MG 3.347581095 -0.102502894 -0.072074073
CL 7.424941279 -0.387516771 1.601819197
CL 5.341233920 -0.357423497 -1.372355540
MG 9.138092337 -0.027784728 -0.234807364
CL 11.400534254 -0.133686281 -1.090638740
TI 0.189286495 1.732989724 -0.150013934
CL -1.856258003 1.651382576 1.210743630
CL 2.291409992 1.629285473 -1.463245981
C 0.094323750 3.799559621 -0.321792789

C	0.904064534	3.921837657	0.956678238
O	-9.495213362	1.308207730	-0.887063088
C	-9.890459949	2.452259781	-0.702233125
C	-7.677996736	2.448889585	1.567894379
O	-7.866636060	1.268027035	1.314806266
O	-11.129784969	2.813852167	-0.933085046
O	-7.142604023	2.826054470	2.706110423
C	-12.064256040	1.809597117	-1.461762317
C	-6.744720229	1.779672597	3.655650243
C	2.258779187	4.606850700	0.751752244
C	0.126975754	4.543948102	2.121594182
C	-9.025019330	3.611546314	-0.304331917
C	-8.000406872	3.601283820	0.670855426
C	-9.258401363	4.788742403	-1.019885859
C	-7.243787904	4.761922840	0.859121421
C	-7.461150585	5.904420438	0.105470281
C	-8.479560665	5.920617382	-0.833947857
C	-13.446686343	2.432026376	-1.540039492
C	-5.974714723	2.428914984	4.791140813
C	-6.826370653	3.426376878	5.578583140
C	-5.416634340	1.323769487	5.694327856
C	-14.009155615	2.729403932	-0.148141343
C	-14.365319994	1.489424992	-2.326656027
O	9.534293771	1.926189759	0.493271811
O	8.498802652	1.438360391	-1.600186559
C	7.899579551	1.332023320	-2.909362932
C	10.260904329	2.315429029	1.669977951
SI	9.027499265	2.845610301	-0.831308719
C	10.417914108	3.722831121	-1.744382428
C	11.729680072	3.942767851	-0.950329040

C	12.712705091	4.411048209	-2.027399184
C	12.397614161	3.513453520	-3.236000028
C	10.909595478	3.090238711	-3.081272939
C	7.613624577	3.974646579	-0.388902922
C	8.028536969	5.249886424	0.419220756
C	7.227685736	6.428169088	-0.192329381
C	6.136246109	5.776684784	-1.048003954
C	6.812210511	4.517682661	-1.601580792
CL	-3.980289416	1.585810815	-1.749348797
CL	4.434766372	1.592503734	1.602305913
AL	-5.674093450	0.933364070	-3.105100943
AL	6.005923572	0.905624929	3.081531362
C	5.354408946	-0.397754396	4.396288970
C	7.058142294	2.495312209	3.582315862
C	-5.066535875	-0.264422952	-4.537319864
C	-6.846128270	2.492314432	-3.373494056
C	-3.859185751	0.232530039	-5.352946618
C	-6.284657661	3.553529840	-4.337369139
C	3.996160730	-0.069823044	5.042880583
C	6.286842474	3.498194770	4.461197864
H	0.599568516	4.166335761	-1.213312314
H	-0.925433199	4.172711873	-0.253117743
H	1.171391277	2.876897743	1.323214322
H	2.865411671	4.558858553	1.657535682
H	2.817601439	4.139860787	-0.057876269
H	2.096775903	5.657606941	0.500405560
H	0.704224613	4.496664396	3.047301929
H	-0.077878484	5.594311974	1.902325739
H	-0.822709545	4.036468709	2.284878424
H	-7.657942833	1.293204896	4.004022612

H	-6.141218891	1.053884301	3.115862011
H	-11.690234689	1.508253311	-2.440705704
H	-12.051637762	0.951084530	-0.793684801
H	-6.840924449	6.777074640	0.261340245
H	-8.672219776	6.807282497	-1.423396461
H	-6.467904407	4.756730624	1.608998256
H	-10.055312979	4.803140717	-1.748132817
H	-13.355557513	3.372451974	-2.095493421
H	-5.127903717	2.961615721	4.345013968
H	-7.674251380	2.923876865	6.052544277
H	-6.236726343	3.896571699	6.367563346
H	-7.219524927	4.216906069	4.938043465
H	-4.823412995	1.756172381	6.501263725
H	-6.222801262	0.743048970	6.150446997
H	-4.778154090	0.635832238	5.137732825
H	-14.136801997	1.803073661	0.416786832
H	-13.352081931	3.389194976	0.420636613
H	-14.984551806	3.212929758	-0.224963339
H	-15.368834270	1.912438751	-2.393537438
H	-14.001186579	1.331070542	-3.344364439
H	-14.440339353	0.515787491	-1.837817375
H	8.349849328	2.055481290	-3.586982891
H	8.084054251	0.326831146	-3.278909906
H	6.827921618	1.492043783	-2.832292546
H	11.313395524	2.065940875	1.544233431
H	10.153759216	3.383019179	1.854927408
H	9.850640597	1.769448511	2.516200508
H	10.022953805	4.719742379	-1.976563515
H	12.078913185	2.998144767	-0.527150064
H	11.622574118	4.657818812	-0.132024658

H	12.518347746	5.460303243	-2.267304747
H	13.753114170	4.337388565	-1.708117193
H	13.034968804	2.628391165	-3.222831797
H	12.580438411	4.023605755	-4.182018096
H	10.838047202	2.003756127	-3.055223386
H	10.302021593	3.434018787	-3.919810761
H	6.918913709	3.389343987	0.220552673
H	9.100068905	5.458878540	0.366882030
H	7.792546782	5.112781881	1.474742003
H	6.824928645	7.091331693	0.573847487
H	7.880266760	7.033294312	-0.826502977
H	5.759930140	6.436603217	-1.831210309
H	5.286471509	5.486004788	-0.424907942
H	7.473574762	4.796939651	-2.429668379
H	6.099764276	3.786274955	-1.983310008
H	6.125747713	-0.461881702	5.174699035
H	5.312452830	-1.391693821	3.945675895
H	7.951618288	2.157883278	4.121496393
H	7.423874193	3.003188814	2.684901950
H	-4.839445931	-1.245935726	-4.113409616
H	-5.922202743	-0.425365260	-5.205472249
H	-7.812110508	2.131415221	-3.746812819
H	-7.055026447	2.954303135	-2.403985488
H	-4.051679007	1.199839451	-5.825211161
H	-2.975091018	0.352587023	-4.723368940
H	-3.593876570	-0.465767193	-6.151959596
H	-6.101089758	3.140022693	-5.332229815
H	-6.967789343	4.399103134	-4.466043024
H	-5.335350954	3.960221489	-3.979669077
H	3.194992430	-0.044527286	4.301912189

H	3.717012507	-0.813019023	5.795068922
H	4.003238240	0.902848168	5.542702294
H	5.938284221	3.036916375	5.388548800
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MG	-9.789928702	-3.819985033	0.306868981
CL	-5.498159984	-3.812096825	1.485828769
MG	-3.739159025	-3.961096875	0.085435226
CL	-8.005733886	-3.966866836	-1.064446335
CL	-1.985937102	-4.111651827	-1.327352000
CL	0.306673521	-3.935451656	1.403669711
MG	2.059319188	-4.086620586	-0.006951427
CL	6.356378872	-4.077892679	1.149940949
MG	8.107483298	-4.229697410	-0.258701956
CL	3.884840395	-4.231636986	-1.323840011
CL	9.838403115	-4.383794805	-1.699158607
CL	-14.632059439	-1.502144968	0.098869096
MG	-12.458941700	-1.722577717	0.498699935
CL	-10.890107529	-2.134381549	-1.127032650
MG	-6.687101850	-2.110575214	0.036841858
CL	-8.659543394	-1.978470648	1.645084164
CL	-4.747323143	-2.143865702	-1.448974797
MG	-0.784861097	-2.143122680	-0.125785784
CL	-2.710618714	-1.924512999	1.297041313
CL	1.138343326	-2.300884504	-1.571671713
MG	5.139026832	-2.343889343	-0.155844431

MG 11.096549955 -2.575469147 -0.610052618
CL 3.144286129 -2.100593232 1.248978933
CL 7.220743622 -2.348164125 -1.653406498
CL 9.328793810 -2.703321512 1.254821037
CL 13.258071203 -2.842570841 -0.143860381
CL -11.489930453 0.163878301 1.596992653
MG -9.558214106 -0.022519965 0.070638848
CL -5.723110322 -0.128403528 1.327955515
CL -7.731580406 -0.409913404 -1.460462897
MG -3.842965375 -0.200353545 -0.062398491
CL 0.336949062 -0.013949414 1.093540916
CL -1.828828579 -0.149312917 -1.659419087
MG 2.305652675 -0.400957931 -0.495209422
CL 6.247350630 -0.431934944 1.126239921
CL 4.269720786 -0.572372168 -1.742632964
MG 8.347374102 -0.465970944 -0.024663090
CL 10.266853707 -0.589511513 -1.612290038
TI -0.724759142 1.772584652 -0.423264240
CL -2.933185274 1.954637849 0.669139363
CL 1.391538460 1.539436325 -1.688039064
C -0.631758634 3.842611118 -0.609061158
C 0.098879543 3.882734710 0.719645614
O 9.501930047 0.376239682 1.425316749
C 9.709619584 1.404518537 2.049063294
C 7.734254813 2.662494914 -0.161220741
O 8.425945774 1.635932190 -0.654610655
O -10.570415246 1.255936240 -1.201837804
C -10.710522477 2.454840445 -1.375265283
C -8.360396937 2.814394616 0.656766073
O -8.811179539 1.703380662 0.883637979

O	10.842844826	1.585146735	2.699680605
C	11.813257017	0.487120517	2.649368794
O	6.517068442	2.875120222	-0.660372515
C	6.259249863	2.560068630	-2.051331981
O	-11.888102701	3.010672181	-1.552697522
O	-7.684786024	3.484233625	1.568475125
C	-13.065156659	2.127395206	-1.513418597
C	-7.450055490	2.823878187	2.854192393
C	1.530257178	4.420596340	0.619380702
C	-0.688451048	4.574056189	1.838099199
C	-9.583333027	3.434526977	-1.514304762
C	-8.494491606	3.567772639	-0.627419689
C	-9.635150356	4.243371550	-2.650469504
C	-7.491931647	4.493667593	-0.929719364
C	-7.535360992	5.255645319	-2.086658827
C	-8.615021775	5.134574691	-2.948608132
C	7.783444832	2.991202965	1.312500208
C	8.724364295	2.509480315	2.255206744
C	8.694728901	3.006820031	3.564311811
C	6.841173903	3.924561934	1.758773810
C	6.808279573	4.381975415	3.065353331
C	7.748696265	3.928836456	3.976733494
C	-14.317450484	2.983273385	-1.477568522
C	-6.473484208	3.665399848	3.656105669
C	-7.027195811	5.055154765	3.975938729
C	-6.098822711	2.899239967	4.929124933
C	-14.401752666	3.805960901	-0.189902682
C	-15.535380454	2.066197018	-1.642334787
C	13.030746077	0.857285372	3.476160072
C	4.905606175	3.125938483	-2.447739096

C	13.950934609	-0.367663034	3.546356724
C	13.760724159	2.079017209	2.914934986
C	4.582493577	2.674033703	-3.875288602
C	4.847401404	4.649315609	-2.320535968
AL	9.737709463	2.560438107	-1.594598519
C	8.801920582	4.479983684	-0.774957184
C	9.170056744	5.270955087	-2.051498005
C	9.503027031	2.318827732	-3.547221145
C	11.516565942	2.702228354	-0.734934374
C	10.817088565	2.213319517	-4.341774632
C	12.406543282	3.897749324	-1.116605143
H	-0.034513502	4.152319514	-1.463917332
H	-1.609811638	4.317742678	-0.605196065
H	0.231656790	2.813763731	1.095215808
H	2.062769279	4.297698490	1.564801223
H	2.093140118	3.912718905	-0.162197548
H	1.501331321	5.486100199	0.382118244
H	-0.180706054	4.467313742	2.798684351
H	-0.774365046	5.639871997	1.616288563
H	-1.692067874	4.162772035	1.935533057
H	-8.415749856	2.727803425	3.354668579
H	-7.057497545	1.830131799	2.651843845
H	-13.022707403	1.497263077	-2.402228641
H	-12.983053312	1.496313929	-0.630377328
H	7.055222031	2.998252825	-2.656251276
H	6.276592792	1.478585198	-2.170842262
H	11.318722749	-0.406922947	3.028065244
H	12.075592970	0.319465643	1.604487149
H	-6.733061084	5.947921275	-2.305412709
H	-8.670051737	5.732291331	-3.848994575

H	-6.665634938	4.604188903	-0.243832322
H	-10.485146839	4.158113150	-3.312367413
H	9.419627942	2.633779341	4.272079561
H	6.052276091	5.096754215	3.363594425
H	7.745419178	4.279475984	5.000272664
H	6.113966646	4.295412520	1.054041155
H	-14.280048200	3.669302189	-2.331428235
H	-5.568931798	3.776038365	3.048351308
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H	-6.291796682	5.645967428	4.525248913
H	-7.289391690	5.603418899	3.070268978
H	-5.368597557	3.462710785	5.511954094
H	-6.974137086	2.737008486	5.563697127
H	-5.665769390	1.924937928	4.696487701
H	-14.441952973	3.150274545	0.683573275
H	-13.541895605	4.468183725	-0.077706251
H	-15.302108649	4.422818990	-0.187355956
H	-16.455677731	2.650799446	-1.598579300
H	-15.515612729	1.542030525	-2.600072417
H	-15.572365322	1.310333625	-0.855041334
H	12.686836485	1.090272427	4.490241420
H	4.160609960	2.686795229	-1.779645635
H	14.252069607	-0.695046859	2.548443458
H	14.854183179	-0.131694212	4.110852638
H	13.459704944	-1.211491712	4.034738300
H	13.107270946	2.950629599	2.861739944
H	14.614092663	2.336737553	3.544716651
H	14.137543004	1.876835537	1.909079017
H	3.596793775	3.034047098	-4.173011372
H	5.311163490	3.069126665	-4.588727430

H 4.578269570 1.586773092 -3.956513848

H 5.568271915 5.127050133 -2.990259294

H 3.855721647 5.017722408 -2.589884786

H 5.061469899 4.981816749 -1.303969652

H 9.549428339 4.632665267 0.005569905

H 7.878493858 4.911051448 -0.408906550

H 9.260682856 6.330881113 -1.790613633

H 10.117364326 4.979297840 -2.507518777

H 8.400363135 5.187298300 -2.817887422

H 8.930742108 1.394947466 -3.683678426

H 8.885875360 3.110810350 -3.982845827

H 12.038519094 1.773922433 -0.989543575

H 11.409711612 2.684102041 0.353772281

H 11.454266357 1.412691792 -3.960535725

H 10.636525752 2.003396043 -5.399968122

H 11.398164652 3.138100706 -4.295018648

H 11.962233149 4.852481275 -0.823327238

H 13.385806117 3.843911475 -0.631895632

H 12.588937417 3.943513641 -2.192710745

$TS2_{Al}$

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MG -3.624861937 -4.099086668 -0.033385886

CL -7.868772506 -4.046609264 -1.262544327

CL -1.844632900 -4.161583932 -1.418700343

CL 0.394831553 -4.142912027 1.361507607

MG 2.174234048 -4.205432797 -0.020964399

CL 6.448136894 -4.256376725 1.215716306

MG 8.226765615 -4.319944631 -0.165028518
CL 4.025073274 -4.267347612 -1.309375984
CL 9.985489026 -4.382875969 -1.579018844
CL -14.524233964 -1.670814511 -0.081660330
MG -12.359328152 -1.909414351 0.347283377
CL -10.758238896 -2.220048124 -1.270510373
MG -6.578249241 -2.255186779 -0.026394907
CL -8.580281463 -2.226028729 1.547384542
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MG -0.673515393 -2.265233712 -0.078523299
CL -2.627141810 -2.136285221 1.318138483
CL 1.277241504 -2.331672302 -1.494051169
MG 5.250760217 -2.450842312 -0.006872825
MG 11.215314366 -2.640229807 -0.360263413
CL 3.228381446 -2.295978668 1.371949048
CL 7.359641313 -2.359985325 -1.461258303
CL 9.413368572 -2.883599214 1.460436946
CL 13.369024644 -2.930154968 0.131273862
CL -11.486456194 -0.128000117 1.676765583
MG -9.486889672 -0.116951243 0.282891971
CL -5.715269665 -0.377184155 1.328129075
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MG -3.787963014 -0.161575794 -0.075604176
CL 0.395499199 -0.245399800 1.309524640
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MG 2.495043271 -0.295333660 -0.094378670
CL 6.512512811 -0.597637983 1.440198005
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MG 8.448515226 -0.369348565 -0.178446347
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TI	-0.635431720	1.614958032	-0.125980889
CL	-2.671443678	1.586225949	1.246494209
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C	-0.675550285	3.684696271	-0.290511234
C	0.152946131	3.781041787	0.978281773
O	9.458872343	0.681451095	1.202225606
C	9.981966348	1.773337819	1.401390318
C	7.938888776	2.689797092	-0.914443013
O	8.512859974	1.509513784	-1.187802791
O	-10.324268459	1.401258473	-0.812658061
C	-10.695441568	2.554513754	-0.635723815
C	-8.461468474	2.527033894	1.613199799
O	-8.670005170	1.347710873	1.369365420
O	11.209516226	1.870922783	1.857460145
C	11.935542784	0.631024189	2.157811797
O	6.656242840	2.835123638	-1.230208491
C	6.180800854	2.332702589	-2.507873448
O	-11.929357552	2.938299638	-0.860037119
O	-7.912156712	2.903696907	2.745045742
C	-12.887575018	1.948054871	-1.372134349
C	-7.523180766	1.857474787	3.698640212
C	1.519728932	4.437885828	0.760903016
C	-0.595597498	4.413268165	2.156451421
C	-9.804367561	3.700319783	-0.255748963
C	-8.771270544	3.678337331	0.710204112
C	-10.021835442	4.875939221	-0.978874784
C	-7.991109603	4.825834324	0.882201058
C	-8.193521023	5.966114803	0.121072122
C	-9.219901249	5.994157004	-0.809348789
C	8.277391502	3.430576840	0.352287523

C	9.284922444	3.088875471	1.287956989
C	9.584188018	3.984729041	2.322219169
C	7.579069054	4.625743790	0.557436126
C	7.865861027	5.481973253	1.607615162
C	8.890963185	5.171615510	2.486540793
C	-14.257436573	2.598084410	-1.447810756
C	-6.733208354	2.502062073	4.822957300
C	-7.561973832	3.518643915	5.610308624
C	-6.185311400	1.394357730	5.729262058
C	-14.804742383	2.919932719	-0.055297477
C	-15.200403951	1.667566989	-2.219837385
C	13.299656207	0.987523383	2.720582048
C	4.764465689	2.824968096	-2.748679691
C	13.963994909	-0.293674385	3.239036917
C	14.176174671	1.693200196	1.683809918
C	4.247588477	2.203705958	-4.050139139
C	4.669651643	4.351142224	-2.785643853
CL	-4.814212555	1.559530324	-1.705604290
CL	3.571144761	1.374781330	1.584625781
AL	-6.525501460	0.934137367	-3.050365118
AL	5.174963443	0.661188844	3.017271240
C	-7.668980671	2.513887528	-3.321320506
C	-7.092048834	3.559856358	-4.292699805
C	-5.950834923	-0.282715898	-4.480017181
C	-4.740631890	0.188232476	-5.306920443
C	6.267735851	2.214788369	3.526808958
C	4.553415724	-0.662744397	4.328436165
C	3.188868826	-0.370911460	4.978469334
C	5.607160762	3.123029608	4.580264922
AL	9.745402797	2.061382031	-2.491781334

C	8.881715817	4.178150479	-2.231475590
C	9.212019686	1.232315520	-4.208317664
C	11.574454625	2.548086772	-1.884745977
C	10.329150170	0.970964176	-5.232415894
C	12.760689697	1.913113944	-2.632209230
C	9.286581996	4.496037094	-3.691201074
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H	-1.683209848	4.086839972	-0.208714857
H	0.401758552	2.728327358	1.335124631
H	2.137075340	4.370261564	1.657927183
H	2.059847894	3.965473634	-0.058008849
H	1.377060659	5.493570326	0.518336245
H	-0.008104584	4.346854673	3.074513634
H	-0.778937320	5.469492402	1.946197021
H	-1.554667182	3.926787160	2.328666974
H	-8.441226554	1.388449988	4.058053399
H	-6.936269709	1.118135025	3.158990381
H	-12.526439550	1.629048105	-2.350320770
H	-12.888220825	1.096319724	-0.695331603
H	6.862147728	2.704759952	-3.276860917
H	6.216443994	1.245972716	-2.494254294
H	11.332812668	0.060884563	2.864323635
H	12.024756100	0.063321364	1.232288659
H	-7.555334513	6.827956014	0.264111187
H	-9.400858510	6.879478962	-1.404501170
H	-7.208596576	4.811815568	1.625046755
H	-10.824947478	4.899626326	-1.700028998
H	10.356132111	3.717226792	3.027675246
H	7.291916288	6.391291431	1.728780211
H	9.139658330	5.833126961	3.305625317

H	6.793294391	4.886302644	-0.133444945
H	-14.150359988	3.531221437	-2.012640004
H	-5.881735785	3.017835517	4.365984221
H	-8.413689453	3.033206855	6.095035233
H	-6.958145145	3.984902442	6.390849409
H	-7.947910979	4.310776073	4.967360697
H	-5.578461059	1.822753965	6.528155653
H	-6.996819517	0.829843068	6.196117935
H	-5.562679043	0.692440789	5.172222708
H	-14.948157447	2.001627661	0.518863161
H	-14.130317462	3.570881072	0.503278285
H	-15.770232487	3.423207044	-0.130564423
H	-16.195332701	2.110744360	-2.284568077
H	-14.846063593	1.492158329	-3.238207829
H	-15.292519856	0.700387805	-1.721222515
H	13.139903227	1.663365313	3.568401127
H	4.145946381	2.454577598	-1.928973558
H	14.091396018	-1.025508878	2.438193627
H	14.949542197	-0.066309922	3.648055495
H	13.373122168	-0.760740357	4.029915375
H	13.705657524	2.601935675	1.305993479
H	15.137366482	1.969442549	2.120554826
H	14.372551780	1.032531962	0.835743651
H	3.211221717	2.495868845	-4.220945050
H	4.836351908	2.537685999	-4.909663909
H	4.281316980	1.114575696	-4.012058636
H	5.281315817	4.766553424	-3.592331267
H	3.638378842	4.661673855	-2.961355800
H	4.992731516	4.801364285	-1.846170614
H	-8.643369945	2.169692667	-3.688561015

H	-7.864681121	2.984315859	-2.353129620
H	-7.759396489	4.417915651	-4.421772473
H	-6.133271234	3.949699021	-3.941547526
H	-6.921493288	3.138585745	-5.286621812
H	-5.738282726	-1.265947163	-4.052617566
H	-6.814089037	-0.431538014	-5.141180614
H	-4.493628767	-0.518855158	-6.104064897
H	-4.919154334	1.156383679	-5.782964739
H	-3.849977420	0.295596360	-4.684336506
H	7.222959498	1.842284724	3.916278832
H	6.514015197	2.803610311	2.639851832
H	4.537282165	-1.657707702	3.878746313
H	5.327837011	-0.705575052	5.105625249
H	2.386028570	-0.364918007	4.239104293
H	2.929917416	-1.121519620	5.730762116
H	3.172394747	0.601429912	5.478847458
H	5.375617514	2.577732236	5.498841405
H	6.249326947	3.963436557	4.862117933
H	4.668230676	3.546845218	4.214655643
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H	9.612350818	4.598143040	-1.543443100
H	8.423649781	1.823481578	-4.684692335
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H	11.666151315	2.316307431	-0.818919362
H	11.668849588	3.638234610	-1.939838880
H	11.102449167	0.316632386	-4.826416646
H	9.943557146	0.491308833	-6.136529906
H	10.821858884	1.894761556	-5.547392019
H	12.761438959	2.178822055	-3.691368431
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H 8.537774633 4.172418688 -4.412065144

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Et-DIBP-AlEt$_2$

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C 3.940663811 0.096586761 0.356358401

C -3.562529384 0.148735275 0.023486570

O 2.832440266 -0.842031491 0.222365560

C -5.020790132 -0.014566774 0.443556462

O -2.724765473 -0.370039528 1.050763506

O 1.529285964 0.835812777 -0.382386007

C 1.662973929 -0.372956687 -0.161207732

C -0.716139399 -1.335910400 0.053751309

C 0.636338735 -1.427489529 -0.351614086

C -1.529896026 -2.433364538 -0.227249275

C 1.102903866 -2.574052598 -1.012379266

C -1.070170649 -3.549923547 -0.911975683

C 0.255274221 -3.624105960 -1.313878931

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C -0.769818743 -0.334828694 2.357851567

AL -0.071533818 1.851217322 -0.806122508

C -1.275783892 0.731859819 3.322258552

C -0.492596949 1.414109193 -2.696402083

C 0.391847555 3.717872293 -0.350511709

C 0.517248425 1.904912261 -3.749528132

C 0.882402785 3.998118537 1.079335402

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C	-5.408985510	-1.480060792	0.649164186
H	3.632806222	0.884428993	1.043254008
H	-3.337681796	1.204209183	-0.136995368
H	4.125867294	0.546071568	-0.621439216
H	-3.384546484	-0.375814932	-0.926793369
H	-2.550455019	-2.404976721	0.120412294
H	2.141785476	-2.623246496	-1.306046550
H	-1.750409410	-4.366488992	-1.120091006
H	0.629217933	-4.489369628	-1.845119192
H	0.322758521	-0.304109526	2.310176381
H	-1.041170326	-1.331608482	2.714960389
H	-0.826699841	0.594571101	4.308383204
H	-1.020915553	1.729821282	2.966888324
H	-2.358402255	0.675775359	3.430345753
H	-1.477181667	1.844778778	-2.922820041
H	-0.633582722	0.331708846	-2.805705810
H	-0.488868625	4.341107774	-0.555063381
H	1.145696495	4.068458495	-1.067923796
H	0.647029068	2.989713242	-3.708518237
H	0.215054263	1.657918098	-4.772691025
H	1.507853645	1.464439260	-3.597923970
H	0.133551737	3.712217714	1.821735839
H	1.789808458	3.432470537	1.312249632
H	1.115441705	5.055078711	1.246781457
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H	-5.133968757	0.505351831	1.401200814
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H	5.958762101	1.093950118	1.899034872

H -5.688539083 1.720827326 -0.700253764

H -5.842628493 0.188244148 -1.564012956

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H 6.477861136 -2.279264131 0.298925469

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H -4.777554067 -1.953842724 1.401134519

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12re-TS for 2DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 2

Total atom = 148

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MG 8.977798432 -4.092016969 -0.119804150

CL 4.695792331 -4.023748881 -1.331870092

MG 2.924457669 -4.020272119 0.060864381

CL 7.181522822 -4.087562378 1.243576242

CL 1.158762028 -4.017711374 1.466124371

CL -1.110329125 -3.951734649 -1.289328849

MG -2.875462282 -3.949931981 0.113811620

CL -7.162845678 -3.879125648 -1.076345309

MG -8.926440164 -3.878156514 0.324881264

CL -4.712646026 -3.945946606 1.422421569

CL -10.670130291 -3.877982404 1.758167685

CL 13.892710533 -1.924717287 -0.028566202

MG 11.715920518 -2.100611669 -0.430505185

CL 10.124579919 -2.350178532 1.206321457

MG 5.931688823 -2.267901426 0.008962379

CL 7.917057262 -2.309244411 -1.588259693

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CL	1.971169122	-2.037756527	-1.293545464
CL	-1.905211029	-2.093572366	1.562236445
MG	-5.896552000	-2.101505475	0.119666497
MG	-11.861130126	-2.107287416	0.539439039
CL	-3.886457639	-2.018957244	-1.281912645
CL	-7.986237788	-1.936622653	1.596954341
CL	-10.087421693	-2.418509931	-1.297991958
CL	-14.027477363	-2.334586358	0.074535275
CL	10.820127893	-0.264589526	-1.666436784
MG	8.869050548	-0.280306596	-0.149790628
CL	5.015295867	-0.353044406	-1.415063839
CL	7.028802022	-0.499308117	1.391661854
MG	3.127329668	-0.258590585	-0.018336491
CL	-0.957626751	-0.029684764	-1.162312097
CL	1.088344175	-0.113189759	1.546905240
MG	-2.974426837	-0.231765174	0.320787950
CL	-6.928865993	-0.374674626	-1.404398134
CL	-4.979760467	-0.199912584	1.534178528
MG	-8.993043280	-0.215446110	-0.171680208
CL	-11.025598749	-0.040017935	1.308612625
TI	0.091312697	1.968498244	0.311546590
CL	2.444214576	2.002694207	-0.626565343
CL	-2.121157468	1.859051877	1.363946119
C	0.521181140	3.767845319	1.453907415
C	1.771674293	4.637248326	1.604680378
O	-10.013486035	0.951105507	-1.542127386
C	-10.319009815	2.122738136	-1.685164823
C	-8.087488345	2.749965157	0.424284310

O	-8.473202762	1.613221660	0.636969429
O	9.916006287	1.064355555	1.029629431
C	10.118341187	2.265395635	1.085160794
C	7.782282283	2.544856422	-0.982837807
O	8.185747412	1.399753362	-1.100773384
O	-11.557481272	2.512152357	-1.893789982
C	-12.598135889	1.474122252	-1.933297681
O	-7.417874120	3.431825406	1.333667515
C	-7.109045364	2.745483848	2.590028129
O	11.321825049	2.776454186	1.218115055
O	7.123568997	3.149188086	-1.950763337
C	12.454938794	1.839033403	1.280976282
C	6.843670983	2.376692829	-3.163222924
C	1.459099605	6.137162431	1.639603991
C	2.539022388	4.236228586	2.876310717
C	9.044638567	3.313169386	1.118715982
C	7.962815091	3.415999564	0.219190064
C	9.144001233	4.229666040	2.166882023
C	7.015240115	4.423450404	0.422062656
C	7.105987250	5.298008838	1.493270961
C	8.178202671	5.204403592	2.367761475
C	-8.306644777	3.524177620	-0.836271008
C	-9.344435541	3.261828957	-1.756207116
C	-9.490952164	4.092595375	-2.868371532
C	-7.450864601	4.601711772	-1.083901988
C	-7.585383035	5.391708834	-2.214596252
C	-8.613109593	5.138661631	-3.110262594
C	13.746279161	2.630130972	1.184880395
C	5.847313985	3.150398632	-4.008061778
C	6.396764761	4.502008581	-4.468104629

C	5.430674517	2.275465185	-5.195017383
C	13.886542711	3.316920108	-0.175528553
C	14.919031597	1.681874395	1.461806472
C	-13.959714237	2.144011734	-1.925653401
C	-6.197314563	3.635637981	3.415422803
C	-15.029083374	1.069901468	-2.159166829
C	-14.205444880	2.908728724	-0.623032870
C	-5.741850067	2.854496120	4.652623082
C	-6.863311758	4.959266003	3.796091067
C	-0.546091640	3.195421884	-1.428334847
C	-0.316587945	4.305535856	-0.619500889
C	-1.471292229	5.148060566	-0.152220588
H	-0.330215800	4.172780597	1.999176174
H	0.740429046	2.783604494	1.960974490
H	2.434182857	4.440308162	0.756965806
H	2.377335055	6.710597256	1.780580120
H	0.994302130	6.495099765	0.720574675
H	0.790129493	6.377993160	2.470440372
H	3.440416399	4.842934631	2.988111047
H	1.925443514	4.381944781	3.769084000
H	2.844245776	3.189180358	2.843378174
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H	6.450536394	1.409540983	-2.859987866
H	12.372180221	1.299018895	2.224613345
H	12.353033221	1.131925537	0.459921581
H	-8.054806215	2.545594989	3.097493844
H	-6.634213837	1.797846414	2.345257953
H	-12.431997383	0.887531955	-2.837431140
H	-12.462586142	0.832382049	-1.065160084
H	6.347092557	6.056226661	1.634725137

H	8.270271214	5.887970865	3.201615663
H	6.194993011	4.508776575	-0.274396868
H	9.989059859	4.164379061	2.837198027
H	-10.302219770	3.902944614	-3.556471519
H	-6.895033432	6.206916056	-2.387005156
H	-8.739015777	5.752780694	-3.992317947
H	-6.667728468	4.812753661	-0.372023569
H	13.727638637	3.398246056	1.966487435
H	4.962206052	3.320705978	-3.385603261
H	7.274332001	4.367493053	-5.106746035
H	5.647439016	5.046156099	-5.046181320
H	6.689113516	5.127696359	-3.623826396
H	4.685438057	2.789338027	-5.804171666
H	6.285423433	2.050515345	-5.838486042
H	5.000769143	1.329398354	-4.862086240
H	13.910146069	2.576718232	-0.979192470
H	13.058955921	4.001208280	-0.368828744
H	14.813626895	3.891046202	-0.221374138
H	15.865023222	2.219709673	1.380965488
H	14.860380582	1.254575345	2.465058091
H	14.934776942	0.852587064	0.751574736
H	-13.989996814	2.852492888	-2.761258122
H	-5.312320483	3.847226002	2.805360326
H	-14.997571360	0.301406257	-1.383407561
H	-16.023085905	1.519725302	-2.149106084
H	-14.895970858	0.574229558	-3.123223646
H	-13.452483372	3.681497142	-0.461436214
H	-15.183654600	3.392329360	-0.641820177
H	-14.183510017	2.229118969	0.232393711
H	-5.054733270	3.455235959	5.250554055

H	-6.592049225	2.593526555	5.288427464
H	-5.231032424	1.931066157	4.375953672
H	-7.743501970	4.784976023	4.421289758
H	-6.174538256	5.588470072	4.363063386
H	-7.182776389	5.519101317	2.916085687
H	-1.566187709	2.896615820	-1.636475718
H	0.634677002	4.807849455	-0.729702988
H	-1.227608073	5.788490987	0.691555534
H	-1.764066262	5.795719069	-0.984901576
H	-2.329247608	4.529934918	0.108747629
H	0.204035225	2.884338723	-2.144893623

12si-TS for 2DIBP/$(MgCl_2)_{13}$/$TiCl_2$^{i}Bu cluster 2

Total atom = 148

CL	-10.798239597	-4.080177506	1.473075783
MG	-9.023418358	-4.069006262	0.081705028
CL	-4.743212607	-4.021953690	1.301062497
MG	-2.969600552	-4.011586071	-0.088838168
CL	-7.224929571	-4.058030930	-1.278742234
CL	-1.201681490	-4.002024895	-1.491203979
CL	1.063130992	-3.964755081	1.268293211
MG	2.830471436	-3.955969827	-0.131977823
CL	7.116122472	-3.906253013	1.065450570
MG	8.881979188	-3.898270627	-0.332901234
CL	4.669805004	-3.946005752	-1.437628618
CL	10.627967214	-3.890819476	-1.763380798
CL	-13.932539358	-1.888190025	0.000609304
MG	-11.756868287	-2.073092311	0.404517147
CL	-10.163554652	-2.313278554	-1.231801636
MG	-5.972590237	-2.251867331	-0.027134833

CL	-7.960436758	-2.301205413	1.566500776
CL	-4.020993822	-2.114338488	-1.491649091
MG	-0.070885300	-2.095138195	-0.132353457
CL	-2.013536228	-2.042772072	1.283507373
CL	1.867530214	-2.085124198	-1.566582788
MG	5.856543255	-2.115486744	-0.117808293
MG	11.821616321	-2.133380404	-0.528173152
CL	3.844348490	-2.039265370	1.281196070
CL	7.948880167	-1.943846226	-1.590364478
CL	10.044166870	-2.455113178	1.303808687
CL	13.986610611	-2.370156096	-0.061748605
CL	-10.857204891	-0.249801462	1.656647480
MG	-8.904259339	-0.265255080	0.143529833
CL	-5.054563293	-0.346361989	1.411293368
CL	-7.062098262	-0.473184597	-1.399750404
MG	-3.161061368	-0.249692062	0.022658370
CL	0.927116083	-0.035810404	1.176114975
CL	-1.121740541	-0.093905154	-1.529719037
MG	2.936103034	-0.236190940	-0.313627772
CL	6.892299757	-0.406992466	1.425066824
CL	4.948905210	-0.192294812	-1.512856182
MG	8.958616136	-0.241215151	0.197396119
CL	10.991698348	-0.057317339	-1.280481830
TI	-0.124381861	1.982151169	-0.269367004
CL	-2.457995346	1.997114797	0.681404803
CL	2.068079407	1.844357558	-1.370330433
C	-0.612838656	3.794945245	-1.365533602
C	0.217246505	4.619948736	-2.353072220
O	9.982816153	0.906486429	1.580984107
C	10.284816250	2.076572369	1.742760522

C	8.056765652	2.731235487	-0.359867464
O	8.443916837	1.598361353	-0.590185832
O	-9.938950502	1.093523410	-1.027331289
C	-10.104264127	2.299811825	-1.091355219
C	-7.769886364	2.533060341	0.975497677
O	-8.208440163	1.402476274	1.109302828
O	11.522242900	2.466129151	1.957692412
C	12.565402059	1.430083306	1.980090062
O	7.391836442	3.428446521	-1.261072099
C	7.087484682	2.762498418	-2.529139727
O	-11.293121059	2.845384496	-1.219438559
O	-7.106739634	3.135997180	1.941290349
C	-12.451187299	1.937221041	-1.261485598
C	-6.867502734	2.377020962	3.170696454
C	-0.091481125	4.189926477	-3.796933268
C	-0.005068969	6.128332796	-2.197537136
C	-8.996312007	3.309953244	-1.141437414
C	-7.911033058	3.386419649	-0.243831723
C	-9.060859218	4.210613483	-2.205584119
C	-6.922270119	4.348886406	-0.465922417
C	-6.977927104	5.205023004	-1.554407991
C	-8.055613951	5.140681251	-2.424965699
C	8.269013360	3.484119836	0.914515680
C	9.306334744	3.210805631	1.831652272
C	9.447285430	4.022984517	2.958092530
C	7.407044301	4.552552044	1.179339928
C	7.535626162	5.323175385	2.324033278
C	8.563632602	5.060204648	3.216552927
C	-13.721414298	2.757573685	-1.137105724
C	-5.873580479	3.143711374	4.024600337

C	-6.405232228	4.512913094	4.452374927
C	-5.499181984	2.279332786	5.233156921
C	-13.814937654	3.449602822	0.224632458
C	-14.919837640	1.833267860	-1.384263626
C	13.925569832	2.102815500	1.977963024
C	6.182947513	3.668638691	-3.344983407
C	14.997564110	1.027495424	2.193353743
C	14.166037121	2.886207845	0.685516677
C	5.727203242	2.907104548	-4.594193294
C	6.857286813	4.993805095	-3.705086382
C	0.626183071	3.194126004	1.435908105
C	0.234351046	4.314975061	0.708567611
C	-0.903810656	5.174184167	1.183690419
H	-1.576313522	4.253446482	-1.150584783
H	-0.873771252	2.820369204	-1.870550793
H	1.276801049	4.409555094	-2.180330829
H	0.503835812	4.770497036	-4.504995907
H	0.138780711	3.134922543	-3.952893171
H	-1.146064913	4.347956764	-4.037855480
H	0.592742397	6.676003897	-2.928428243
H	-1.053811762	6.387722820	-2.367583598
H	0.274332088	6.497347550	-1.209893370
H	-7.830030135	2.254720531	3.671736017
H	-6.487609423	1.397818976	2.889906703
H	-12.400705084	1.398021995	-2.207869946
H	-12.350053425	1.224991795	-0.444682569
H	8.035014678	2.567048380	-3.035037522
H	6.608213783	1.812827393	-2.301321419
H	12.403030975	0.830829253	2.876574718
H	12.428965993	0.799804912	1.103706824

H	-6.186889300	5.926098597	-1.713058230
H	-8.120355952	5.811825629	-3.271380575
H	-6.096732144	4.411281417	0.226921425
H	-9.908572408	4.167075704	-2.874473657
H	10.258395500	3.825426619	3.644182073
H	6.840296739	6.131164528	2.509850807
H	8.684975799	5.659581829	4.109325142
H	6.623362110	4.771463642	0.470395255
H	-13.705131045	3.523696534	-1.920643466
H	-4.972651313	3.286546296	3.418185160
H	-7.298423683	4.405576762	5.074257282
H	-5.657506715	5.051146720	5.038054341
H	-6.667291474	5.130866425	3.592622611
H	-4.757438112	2.788211340	5.850733580
H	-6.371603665	2.080289817	5.861235097
H	-5.080360968	1.320382119	4.923718983
H	-13.833848059	2.711814549	1.030690934
H	-12.969389486	4.117554257	0.396060231
H	-14.728916664	4.042369731	0.291455473
H	-15.852621642	2.389688464	-1.279690006
H	-14.895007808	1.404848643	-2.388382561
H	-14.934799484	1.004060054	-0.673767662
H	13.957047503	2.799553990	2.823326351
H	5.297628201	3.876586488	-2.734126307
H	14.964773710	0.269409064	1.407470705
H	15.990778644	1.479103940	2.186104473
H	14.868462120	0.518541758	3.151002772
H	13.411522532	3.660156741	0.537361183
H	15.143651676	3.370855918	0.707939531
H	14.142170233	2.218787963	-0.179420794

H	5.046923379	3.520413049	-5.187202762
H	6.578174469	2.648509067	-5.229930243
H	5.208961388	1.983650645	-4.331739584
H	7.738160774	4.823487842	-4.330408614
H	6.173656118	5.635028599	-4.264810674
H	7.177415138	5.539139821	-2.816276501
H	1.665763707	2.892839264	1.426801847
H	0.998866700	4.813679462	0.127972554
H	-1.302132614	5.828305682	0.411939509
H	-1.712846427	4.571957737	1.593527713
H	-0.519422669	5.809284415	1.988356214
H	0.037546332	2.874521125	2.287966923

12re-TS for 2Al/2DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 6

Total atom = 180

CL	-10.766164698	-4.175079438	1.747042643
MG	-9.020107668	-4.192449350	0.320955713
CL	-4.716470668	-4.118745265	1.453589464
MG	-2.970229802	-4.136065927	0.027794861
CL	-7.248359359	-4.209092310	-1.075166959
CL	-1.230611935	-4.155961881	-1.409436936
CL	1.088532398	-4.059816554	1.303029416
MG	2.827405522	-4.079705444	-0.131336158
CL	7.135695088	-4.004239755	0.978255335
MG	8.873924797	-4.025189560	-0.454348681
CL	4.640407729	-4.096554365	-1.473809349
CL	10.591176977	-4.046367382	-1.919608046
CL	-13.930385343	-2.014611786	0.292042249
MG	-11.747878363	-2.190114211	0.657608284
CL	-10.187140336	-2.464320858	-1.005558773

MG -5.972848898 -2.375695209 0.114182957
CL -7.927616195 -2.394376083 1.746496178
CL -4.051322199 -2.269545351 -1.391939074
MG -0.074348437 -2.220456876 -0.113039201
CL -1.988736274 -2.138942636 1.340371786
CL 1.834846866 -2.239664964 -1.585510258
MG 5.852289148 -2.239510476 -0.216342015
MG 11.807150262 -2.263520438 -0.745847380
CL 3.867887458 -2.134064947 1.221184562
CL 7.913933847 -2.097248913 -1.733187869
CL 10.067196495 -2.547563210 1.128727228
CL 13.981599146 -2.490311455 -0.317195994
CL -10.886653750 -0.382715913 1.962799971
MG -8.939137766 -0.324267133 0.506551248
CL -5.101417233 -0.441359706 1.387919212
CL -7.295210150 -0.684291728 -1.395420249
MG -3.215185703 -0.183009297 -0.083625169
CL 0.943117580 -0.193265727 1.177249144
CL -1.121662122 -0.191464061 -1.492113206
MG 3.018126586 -0.164048257 -0.215170425
CL 7.080431282 -0.568469535 1.462320424
CL 4.966087560 -0.402522473 -1.599733065
MG 9.035880952 -0.325534621 -0.121416336
CL 11.006748988 -0.227926852 -1.625903979
TI -0.080779022 1.847625618 -0.203069043
CL -2.271781145 1.805876627 1.025646088
CL 1.984431631 1.672525145 -1.522819919
C -0.542973486 3.700109689 -1.234977143
C -1.763066716 4.622305129 -1.297077974
O 10.011201842 0.983675912 1.119831461

C	10.553781943	2.076892506	1.025191615
C	8.306177038	2.545293797	-1.178229223
O	8.336195344	1.335618898	-1.009146974
O	-9.852273267	1.154456925	-0.582279452
C	-10.174744841	2.325318363	-0.428702461
C	-7.798973795	2.356355367	1.658710725
O	-8.108565836	1.179848330	1.534898151
O	11.830755419	2.249884055	1.276440082
C	12.621257485	1.089031756	1.703022526
O	7.765393810	3.070060350	-2.254194408
C	7.165185858	2.151271598	-3.230465969
O	-11.413101572	2.737602423	-0.556479268
O	-7.137162284	2.788726769	2.706365079
C	-12.442672207	1.752059363	-0.920272702
C	-6.727060852	1.818317912	3.728576030
C	-1.440876812	6.104340016	-1.068760456
C	-2.444862157	4.471389686	-2.669294960
C	-9.217448355	3.455841326	-0.194555810
C	-8.112998910	3.450531681	0.688054134
C	-9.444746175	4.587432719	-0.981522379
C	-7.270133405	4.565638803	0.711629250
C	-7.485697730	5.658924168	-0.112244044
C	-8.584667970	5.674591300	-0.956324409
C	8.832510294	3.578287074	-0.230645971
C	9.858049022	3.371737448	0.723041883
C	10.271393358	4.451605350	1.507858439
C	8.265757440	4.852616083	-0.334491139
C	8.663369502	5.899538622	0.481799705
C	9.675368655	5.699136963	1.406156456
C	-13.800003115	2.428918287	-0.861169807

C	-5.597192919	2.423527703	4.542469947
C	-6.026458656	3.685451830	5.292992081
C	-5.057671271	1.352434074	5.496513820
C	-14.169778138	2.823336590	0.570514931
C	-14.843899788	1.486648972	-1.472343259
C	14.068395551	1.519527792	1.861895452
C	6.452897846	2.971942912	-4.289854230
C	14.849913779	0.375205113	2.518337600
C	14.689473662	1.922657672	0.522430644
C	5.682367979	2.016404659	-5.207827827
C	7.412630399	3.864425979	-5.078959400
CL	-4.428470917	1.363281382	-1.809281664
CL	4.218215766	1.570351951	1.375607497
AL	-6.154552140	0.612767688	-3.061701915
AL	5.795892850	0.903879492	2.856085275
C	-7.352886739	2.134159178	-3.423694491
C	-6.877688069	3.066968459	-4.552474567
C	-5.607431171	-0.691329327	-4.425186882
C	-4.356591842	-0.319545431	-5.241714814
C	6.970942497	2.447556578	3.202586480
C	5.080757819	-0.262112596	4.265709931
C	3.785299428	0.219908500	4.942979221
C	6.363436082	3.513411799	4.132827575
C	0.751954924	2.993766171	1.527867468
C	0.468287848	4.131738465	0.785200532
C	1.592817780	4.971050410	0.242102973
H	0.286755456	4.090331106	-1.823667648
H	-0.846494046	2.749708919	-1.762699250
H	-2.478810936	4.296791968	-0.536257568
H	-2.349335617	6.700735513	-1.175786049

H	-1.033683334	6.314494407	-0.080148781
H	-0.724806106	6.466943315	-1.811643339
H	-3.334934749	5.102967065	-2.724854766
H	-1.768196679	4.774706041	-3.472936919
H	-2.755554097	3.443441069	-2.851882065
H	-7.608667405	1.610854947	4.338974386
H	-6.415666276	0.908776972	3.223942180
H	-12.202856652	1.394449802	-1.922096798
H	-12.378714657	0.922418054	-0.219491260
H	7.973565904	1.550568796	-3.651504903
H	6.483261017	1.494614515	-2.694909846
H	12.190538575	0.729109072	2.637712962
H	12.518886818	0.317009532	0.943424175
H	-6.801123353	6.496231939	-0.083938594
H	-8.776273490	6.525416263	-1.596760588
H	-6.429921616	4.563622533	1.388568296
H	-10.302042443	4.599146634	-1.637925822
H	11.067472155	4.298730608	2.220798285
H	8.186318500	6.865986378	0.386933019
H	10.005843872	6.505920694	2.046988533
H	7.492274025	5.014159555	-1.068993130
H	-13.746717320	3.334780456	-1.475806220
H	-4.798132586	2.681024903	3.839364098
H	-6.810895718	3.457597935	6.020359521
H	-5.183530073	4.113391486	5.838605795
H	-6.409310542	4.449750363	4.615231726
H	-4.222145731	1.747277408	6.076220662
H	-5.826864786	1.028219502	6.202884521
H	-4.704367723	0.475586524	4.951998757
H	-14.249341382	1.935922293	1.202901825

H	-13.426418653	3.489889210	1.010571185
H	-15.132893402	3.336265671	0.589636859
H	-15.832987852	1.945616387	-1.432792861
H	-14.620015212	1.264684086	-2.518193902
H	-14.886420536	0.539901841	-0.929718152
H	14.084069192	2.383350231	2.536271827
H	5.724045748	3.606473047	-3.773721713
H	14.828423477	-0.521913874	1.895623946
H	15.893332181	0.662989464	2.655275045
H	14.442591054	0.119886515	3.499265014
H	14.126174324	2.722661799	0.039853859
H	15.712943838	2.273051122	0.666782700
H	14.721019544	1.067235940	-0.156390658
H	5.128112477	2.578569087	-5.960796310
H	6.363152126	1.341273710	-5.733015563
H	4.971053204	1.408219977	-4.647426199
H	8.145115350	3.260926535	-5.622252731
H	6.867483260	4.462192912	-5.811639676
H	7.958239668	4.548582158	-4.427529427
H	-8.341833090	1.731439965	-3.674322978
H	-7.491011779	2.712890032	-2.505538523
H	-7.578540248	3.887812523	-4.735466487
H	-5.909420156	3.518564338	-4.321378156
H	-6.762891109	2.531582122	-5.498406210
H	-5.456718069	-1.665552439	-3.953490882
H	-6.462649520	-0.821995124	-5.100696494
H	-4.131226815	-1.070704938	-6.004280213
H	-4.473293781	0.636369183	-5.760086935
H	-3.474862451	-0.233581392	-4.603647401
H	7.904285733	2.070833995	3.638394792

H	7.253258479	2.911415848	2.252707246
H	4.925575912	-1.264247939	3.858367834
H	5.871838323	-0.371060515	5.018964873
H	2.960668971	0.275413435	4.229639481
H	3.471803596	-0.453918786	5.745634371
H	3.897125085	1.213783583	5.385621023
H	6.104171632	3.097759602	5.109901771
H	7.049996408	4.346630064	4.313646176
H	5.447743915	3.938208160	3.713346776
H	0.059400546	2.659054284	2.289046058
H	-0.459263945	4.642384057	0.999881862
H	1.779240609	2.666739913	1.623984411
H	1.287126943	5.644844832	-0.554063792
H	1.974156040	5.583196982	1.065711640
H	2.411226233	4.345804702	-0.112639830

12si-TS for 2Al/2DIBP/$(MgCl_2)_{13}$/$TiCl_2$^{i}Bu cluster 6

Total atom = 180

CL	-10.785822142	-4.193430936	1.646601933
MG	-9.035111000	-4.186673579	0.226180271
CL	-4.735152865	-4.137502775	1.374024866
MG	-2.984254083	-4.130696966	-0.046113290
CL	-7.258810340	-4.179708244	-1.164204926
CL	-1.239946231	-4.126217943	-1.477763810
CL	1.070367985	-4.081367917	1.243551805
MG	2.813926569	-4.076965169	-0.185232325
CL	7.118629448	-4.025681689	0.939634775
MG	8.861525756	-4.022352034	-0.487416844
CL	4.631319030	-4.071190520	-1.521832363
CL	10.583552489	-4.018596883	-1.947172395

CL	-13.943328060	-2.004000776	0.220609734
MG	-11.762196729	-2.188175264	0.590075017
CL	-10.196243027	-2.433701644	-1.072639980
MG	-5.985639847	-2.369330813	0.062267337
CL	-7.945732252	-2.415672764	1.687590370
CL	-4.059110457	-2.237791387	-1.435390639
MG	-0.086226363	-2.215592448	-0.142780582
CL	-2.005317437	-2.158583697	1.305596819
CL	1.827795985	-2.209952522	-1.609094688
MG	5.840772510	-2.238389378	-0.226977578
MG	11.797267458	-2.258467861	-0.737352787
CL	3.851776728	-2.157140975	1.205670373
CL	7.907486090	-2.070624907	-1.734240047
CL	10.050880857	-2.574748741	1.126064065
CL	13.970082773	-2.495031952	-0.305775567
CL	-10.902731364	-0.403121744	1.924865695
MG	-8.943905121	-0.319568604	0.480131346
CL	-5.118909840	-0.462571097	1.379283652
CL	-7.281429958	-0.622462676	-1.416680199
MG	-3.214538080	-0.196263875	-0.068196656
CL	0.953016206	-0.195329215	1.202951546
CL	-1.132711068	-0.213982495	-1.482004317
MG	3.003435272	-0.158023383	-0.224865278
CL	7.057805473	-0.591658278	1.477902031
CL	4.957258343	-0.384861158	-1.598636615
MG	9.023647227	-0.328023901	-0.089040187
CL	11.001980574	-0.207298511	-1.583974497
TI	-0.086724409	1.825365650	-0.114158617
CL	-2.235576754	1.713346980	1.145572228
CL	1.929584425	1.679432947	-1.520690907

C	-0.781154572	3.652960939	-1.191554185
C	-0.106746896	4.456544652	-2.304420613
O	9.997570084	0.956206339	1.178803967
C	10.545045178	2.048585934	1.104644213
C	8.306514071	2.563576905	-1.098273541
O	8.334903200	1.350819952	-0.952675702
O	-9.847570471	1.191750044	-0.573216745
C	-10.190206811	2.350610722	-0.378005917
C	-7.842136911	2.328552127	1.743312829
O	-8.125155799	1.153648512	1.559266556
O	11.821746604	2.211907233	1.363762034
C	12.605638190	1.040921539	1.774243077
O	7.766833384	3.109210251	-2.164519465
C	7.163802907	2.209771327	-3.156505165
O	-11.432138027	2.750202387	-0.511760464
O	-7.202379487	2.722304001	2.819922198
C	-12.439814915	1.767513459	-0.938193773
C	-6.790462871	1.708194538	3.798317595
C	-0.613847976	3.982798990	-3.676773798
C	-0.321241913	5.966808660	-2.159666896
C	-9.255188570	3.485223117	-0.079627413
C	-8.164792321	3.460619890	0.820225070
C	-9.489661607	4.646225755	-0.820434163
C	-7.343755896	4.588801399	0.907599352
C	-7.565306748	5.713138140	0.128334856
C	-8.649895121	5.746004900	-0.733602335
C	8.834086024	3.577974891	-0.131564740
C	9.855978935	3.351209656	0.821484331
C	10.270916093	4.415892174	1.625946192
C	8.272211759	4.855985888	-0.214878003

C	8.671195554	5.887213454	0.620471669
C	9.679840571	5.667234787	1.543991518
C	-13.807576908	2.423232407	-0.879131143
C	-5.700368940	2.297757708	4.675179061
C	-6.184085403	3.505654043	5.479528350
C	-5.157592806	1.190877426	5.585580395
C	-14.215120670	2.744409349	0.560611537
C	-14.824367759	1.497596591	-1.557698673
C	14.053033278	1.463768253	1.950611468
C	6.467072382	3.052450483	-4.209012532
C	14.826611628	0.305324101	2.591503925
C	14.684393722	1.888979536	0.622823025
C	5.687826440	2.118846679	-5.141987138
C	7.442567000	3.941366833	-4.982716656
CL	-4.360771420	1.457905337	-1.740321984
CL	4.200038378	1.559530869	1.376448518
AL	-6.103161222	0.761621029	-3.000733628
AL	5.757001833	0.876264295	2.868778125
C	-7.288974170	2.308261671	-3.287778590
C	-6.769278328	3.326839065	-4.318536745
C	-5.568339279	-0.489507395	-4.417432894
C	-4.340467454	-0.072807138	-5.246953772
C	6.934644553	2.411933742	3.241146105
C	5.027346788	-0.297546811	4.264208487
C	3.732296737	0.188760051	4.939372536
C	6.322021209	3.470706014	4.176200827
C	0.781179538	3.099747979	1.395368781
C	0.255479748	4.195571484	0.671498837
C	-0.825513479	5.041026062	1.295243952
H	-1.743857696	4.067847735	-0.900772604

H	-1.032758301	2.645082334	-1.617621724
H	0.968112155	4.255216145	-2.273646674
H	-0.136516383	4.551073471	-4.478368578
H	-0.392181380	2.926610409	-3.836503643
H	-1.694730481	4.118859805	-3.765463213
H	0.163204906	6.497706121	-2.981539749
H	-1.386432738	6.213206066	-2.189435594
H	0.088193414	6.364261599	-1.230176110
H	-7.680765814	1.441583841	4.371939648
H	-6.439630427	0.837295880	3.252733939
H	-12.174280459	1.455874789	-1.948875969
H	-12.379114239	0.910038048	-0.271579150
H	7.968106543	1.605945968	-3.580793701
H	6.471866196	1.553017595	-2.633891256
H	12.167531758	0.665097885	2.699175219
H	12.506087561	0.283421011	0.999781038
H	-6.896886081	6.560428677	0.205042299
H	-8.846291597	6.620343155	-1.340013448
H	-6.515224419	4.571999193	1.598589455
H	-10.336269823	4.671992706	-1.490121389
H	11.064119871	4.247751971	2.338641579
H	8.197546260	6.856727050	0.541206812
H	10.011280742	6.461568094	2.199708306
H	7.500920512	5.032898850	-0.948104798
H	-13.752768935	3.357573544	-1.449407924
H	-4.889967851	2.613462648	4.009706429
H	-6.981783693	3.218393251	6.170480103
H	-5.368504475	3.924642411	6.071682916
H	-6.568822429	4.295619518	4.833004821
H	-4.348082332	1.574737506	6.208001081

H	-5.936192278	0.810460399	6.252435756
H	-4.767573476	0.353262455	5.005517570
H	-14.300604398	1.826393195	1.146740662
H	-13.489142637	3.395442699	1.050171987
H	-15.183571360	3.247163552	0.581218510
H	-15.820120226	1.942140197	-1.520731813
H	-14.573383923	1.326995816	-2.607077138
H	-14.867328835	0.526908186	-1.059153137
H	14.066781932	2.315229477	2.640579371
H	5.744824201	3.690755163	-3.688258257
H	14.806769502	-0.580237987	1.952415385
H	15.869908479	0.587370002	2.740785428
H	14.411758609	0.033505690	3.564813709
H	14.126925649	2.699479015	0.151106693
H	15.708019687	2.233242465	0.780270709
H	14.717625138	1.045831714	-0.071104833
H	5.147138216	2.697512101	-5.892366210
H	6.361362185	1.438866204	-5.670218710
H	4.963870970	1.515618444	-4.592515750
H	8.168830312	3.334608453	-5.530696802
H	6.909118166	4.556220638	-5.709869149
H	7.994873639	4.609261488	-4.320157048
H	-8.267688248	1.930406289	-3.607445409
H	-7.461742734	2.812459378	-2.332360783
H	-7.460873191	4.163475644	-4.460826053
H	-5.809649547	3.752749492	-4.014259504
H	-6.619349043	2.869372195	-5.299809363
H	-5.392777930	-1.475479913	-3.979959654
H	-6.435810986	-0.612573073	-5.078518220
H	-4.119904776	-0.795725550	-6.037732878

H	-4.481531035	0.897400773	-5.731698388
H	-3.447441091	0.005739299	-4.623725985
H	7.862470008	2.027502749	3.682013455
H	7.227470044	2.884455015	2.298883898
H	4.866995098	-1.295351365	3.848504107
H	5.814327525	-0.417605849	5.020118575
H	2.911767497	0.257634650	4.222542132
H	3.409551082	-0.489785163	5.734386449
H	3.850084759	1.177652107	5.391559077
H	6.052602222	3.046412441	5.146798124
H	7.009706353	4.299785459	4.371349155
H	5.411605201	3.902613355	3.752576049
H	0.311642803	2.829662743	2.334952607
H	0.960124731	4.728629536	0.046224852
H	1.841926117	2.891801691	1.323345198
H	-1.295245212	5.725333659	0.591712026
H	-1.595022405	4.420544222	1.752406233
H	-0.364645188	5.640508227	2.086520939

12re-TS for 2Al/DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 7

Total atom = 138

CL	-8.979763213	-4.511457275	1.928758866
MG	-7.226028513	-4.451625650	0.512410713
CL	-2.954268961	-3.948439808	1.659954228
MG	-1.201243972	-3.889750914	0.243844157
CL	-5.447276123	-4.386367484	-0.871937765
CL	0.546825624	-3.832291616	-1.182172163
CL	2.824871220	-3.398359676	1.531875328
MG	4.571661716	-3.341838995	0.108116000
CL	8.847682962	-2.838826474	1.231761662

MG 10.593631776 -2.783443027 -0.190851179
CL 6.391337099 -3.271088607 -1.223484646
CL 12.319439742 -2.731288257 -1.644785475
CL -12.304871129 -2.709041132 0.350337098
MG -10.116583632 -2.677062505 0.733952777
CL -8.525215358 -2.901610066 -0.905978324
MG -4.343610189 -2.392299519 0.226271984
CL -6.309384462 -2.496947334 1.849298172
CL -2.426381745 -2.196851327 -1.275258837
MG 1.521130442 -1.740844922 0.017655539
CL -0.406231676 -1.750585637 1.456729564
CL 3.438016560 -1.670822269 -1.443471844
MG 7.428090728 -1.253812865 -0.058203512
MG 13.367812776 -0.792110319 -0.558947614
CL 5.429502232 -1.247107218 1.362864158
CL 9.483352177 -1.013347237 -1.571572207
CL 11.641902149 -1.129091979 1.319602769
CL 15.549507998 -0.808982641 -0.110134406
CL -9.426286576 -0.731169581 1.937538145
MG -7.485793141 -0.592030104 0.478861993
CL -3.650695411 -0.324416316 1.399260761
CL -5.788910307 -0.908882527 -1.379573409
MG -1.789604826 0.017880804 -0.084085400
CL 2.351840021 0.432668372 1.201373726
CL 0.325913918 0.098492382 -1.477623128
MG 4.412020630 0.558057422 -0.184299891
CL 8.620968613 0.790685843 1.566949968
CL 6.491880464 0.527832091 -1.428720759
MG 10.397611280 0.696258124 -0.050584336
CL 12.369767650 1.325041364 -1.163901321

TI	1.165032644	2.298376491	-0.316222582
CL	-1.020468261	2.138664310	0.904530390
CL	3.275922348	2.224682249	-1.589563855
CL	5.373242885	2.364060380	1.562944177
AL.	7.512953838	2.969953545	1.545529195
C	8.020487235	3.688906266	3.299299879
C	8.111347878	3.743844559	-0.173665541
C	9.329996418	3.099875553	-0.840466370
C	7.337269773	5.015956582	3.678188616
C	0.556336110	4.023761915	-1.479608822
C	-0.745012603	4.815477743	-1.627517218
O	-8.518719922	0.727767365	-0.702765233
C	-8.969493422	1.862938227	-0.619832667
C	-6.644949727	2.249369901	1.496379595
O	-6.800077065	1.039739665	1.410073673
O	-10.240739298	2.129877543	-0.799419264
O	-6.061431541	2.795112618	2.538062027
C	-11.145452842	1.021686553	-1.140939680
C	-5.555657817	1.912690941	3.596573145
C	-0.577788004	6.332977871	-1.482478623
C	-1.364160620	4.516774482	-3.005411045
C	-8.149164877	3.103010075	-0.420737611
C	-7.071383890	3.261941296	0.480927938
C	-8.487019838	4.168379522	-1.259040345
C	-6.366994745	4.469714121	0.475027616
C	-6.689203423	5.497254668	-0.397225352
C	-7.760660005	5.349312337	-1.263417681
C	-12.567142098	1.553006688	-1.170638755
C	-4.557559969	2.689168287	4.436737170
C	-5.191700364	3.891443931	5.138371706

C	-3.911868401	1.724812653	5.437639810
C	-13.040266130	1.970619450	0.223564810
C	-13.479729901	0.479653310	-1.775725016
CL	-3.100521980	1.351599625	-1.903761846
AL	-4.761311767	0.399403950	-3.109296041
C	-6.082164590	1.796606451	-3.537124358
C	-5.691025103	2.705572366	-4.716482315
C	-4.099713626	-0.920336008	-4.405004521
C	-2.886334959	-0.480858713	-5.244091121
C	1.868355349	3.629463940	1.335045207
C	1.483996546	4.684922527	0.518500344
C	2.525782432	5.594485174	-0.073390406
H	7.806764286	2.934950720	4.063981261
H	9.109567315	3.820508590	3.317677355
H	7.279109623	3.738798222	-0.881344177
H	8.338222198	4.798751246	0.020313930
H	10.183043394	3.039780514	-0.146497072
H	9.056447205	2.112316990	-1.243747003
H	9.712356805	3.654970012	-1.700022431
H	7.554557364	5.807942316	2.955951559
H	6.250909028	4.908716211	3.722394195
H	7.664740747	5.378743785	4.656322257
H	1.358504650	4.450684646	-2.081015048
H	0.356878020	3.013738010	-1.943891598
H	-1.448844144	4.464878380	-0.866809257
H	-1.536963867	6.827158174	-1.649782149
H	-0.226310601	6.640548350	-0.498015588
H	0.122215744	6.722345038	-2.226929965
H	-2.310548567	5.050448074	-3.121324155
H	-0.696206651	4.840349453	-3.808293831

H	-1.564949186	3.453786876	-3.133012955
H	-6.420333458	1.588627820	4.179709149
H	-5.097166407	1.049114898	3.123689163
H	-10.827653689	0.636904647	-2.110464664
H	-11.025265579	0.243266370	-0.390445673
H	-6.109164946	6.410512409	-0.389394537
H	-8.034951177	6.145551316	-1.942777627
H	-5.549332035	4.593768677	1.168022377
H	-9.324427994	4.053965316	-1.930941838
H	-12.579409744	2.430398966	-1.827326346
H	-3.774852072	3.044307814	3.757970998
H	-5.965843547	3.567992158	5.839987953
H	-4.441447988	4.445161075	5.705674310
H	-5.649942553	4.580474238	4.427587520
H	-3.162651640	2.244917681	6.036161804
H	-4.655895422	1.312042126	6.124344918
H	-3.419875997	0.893608886	4.930343898
H	-13.060898636	1.107860646	0.893540950
H	-12.387822693	2.727585791	0.661669289
H	-14.049242201	2.384022666	0.177637987
H	-14.511430579	0.833924520	-1.799532933
H	-13.186766984	0.234935600	-2.799231462
H	-13.449820606	-0.439790172	-1.187341582
H	-7.035763769	1.301697499	-3.757760750
H	-6.262714279	2.408103633	-2.647878246
H	-6.457210692	3.456694360	-4.933362868
H	-4.761123333	3.245038625	-4.518925825
H	-5.539271163	2.133219741	-5.635138615
H	-3.862098516	-1.850411311	-3.882517377
H	-4.938644118	-1.163846462	-5.069469643

H -2.592664621 -1.247792720 -5.966606515

H -3.087901251 0.431872230 -5.811808060

H -2.017208330 -0.282011737 -4.613849955

H 1.206189829 3.282532668 2.117480281

H 0.507738577 5.112877789 0.694849147

H 2.921584735 3.413021874 1.455528898

H 2.849593184 6.281982883 0.714434687

H 3.398129886 5.030422344 -0.401222463

H 2.158980363 6.194208347 -0.902044343

12-si-TS for 2Al/DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 7

Total atom = 138

CL -8.986723690 -4.539752348 1.789370051

MG -7.224950579 -4.451377153 0.384536827

CL -2.959608648 -3.974130086 1.566475058

MG -1.198542687 -3.886909154 0.161851880

CL -5.438340228 -4.358266153 -0.988055926

CL 0.557616454 -3.800715286 -1.252739133

CL 2.820371977 -3.424274162 1.482589983

MG 4.575242058 -3.339040670 0.070232198

CL 8.844996701 -2.861527215 1.228299135

MG 10.599005568 -2.777451764 -0.182948359

CL 6.402481354 -3.241529452 -1.249271790

CL 12.333060388 -2.695957971 -1.625678222

CL -12.302174178 -2.703391797 0.229863317

MG -10.116089804 -2.680437385 0.626463821

CL -8.515511363 -2.871647328 -1.008732385

MG -4.340270203 -2.387918505 0.157519588

CL -6.315222078 -2.525268596 1.766861968

CL -2.414495557 -2.162348045 -1.328741163

MG 1.525841773 -1.735073199 -0.004270807

CL -0.409663417 -1.773760727 1.423347793

CL 3.451022493 -1.635661035 -1.452741913

MG 7.433377207 -1.249366846 -0.036495522

MG 13.375960356 -0.780241995 -0.493892206

CL 5.426784431 -1.271251109 1.373021568

CL 9.497240586 -0.978516410 -1.532877705

CL 11.639297963 -1.155325119 1.367450731

CL 15.555060335 -0.807455081 -0.033171636

CL -9.429410625 -0.758487820 1.865944239

MG -7.474286875 -0.590003261 0.418910422

CL -3.659796990 -0.346236593 1.381506079

CL -5.759586546 -0.841825001 -1.429173809

MG -1.769546859 0.009217030 -0.063350889

CL 2.368231273 0.430124267 1.238885554

CL 0.335866169 0.080760401 -1.461419887

MG 4.412349313 0.564270516 -0.171105343

CL 8.605646081 0.768998270 1.622572619

CL 6.502128453 0.551817531 -1.392584537

MG 10.401923120 0.699743696 0.026874067

CL 12.382792442 1.350192798 -1.058610651

TI 1.179419405 2.282485988 -0.214208861

CL -0.954840158 2.054753486 1.041269928

CL 3.244158620 2.226722036 -1.572730988

CL 5.350295812 2.350063272 1.602589991

AL. 7.489556701 2.952185761 1.618745654

C 7.980066526 3.639040240 3.390175250

C 8.111989135 3.750632382 -0.080317326

C 9.339573357 3.116878915 -0.740211724

C 7.294708120 4.960386292 3.784954960

C	0.349993376	3.962362836	-1.423716216
C	0.971636135	4.747521007	-2.579531559
O	-8.505148648	0.766612523	-0.723930937
C	-9.003970680	1.877111794	-0.595737857
C	-6.744227830	2.215603498	1.603989542
O	-6.810282719	1.010555347	1.412705551
O	-10.276849384	2.105286265	-0.815104758
O	-6.226366698	2.704729419	2.707384300
C	-11.120261847	0.986835363	-1.261153036
C	-5.695855537	1.754359362	3.692907426
C	0.538017076	4.137060462	-3.922691431
C	0.617525376	6.237783586	-2.541694642
C	-8.247006582	3.135484429	-0.286308773
C	-7.205756059	3.280474000	0.660191176
C	-8.612373508	4.242599041	-1.056530689
C	-6.567843346	4.520004420	0.768690183
C	-6.916003023	5.592632260	-0.036744316
C	-7.948809522	5.455229441	-0.950171779
C	-12.555892377	1.472426001	-1.350445908
C	-4.963512834	2.535679275	4.768341677
C	-5.888844643	3.482274644	5.535152578
C	-4.269680039	1.540175839	5.704479323
C	-13.125300006	1.800628096	0.031681045
C	-13.392667426	0.402882492	-2.062476131
CL	-3.012118067	1.468927400	-1.832420410
AL	-4.703649577	0.594411395	-3.051216373
C	-6.013010840	2.032567412	-3.362855921
C	-5.573088325	3.086134345	-4.395438647
C	-4.066397118	-0.654105143	-4.426780774
C	-2.910602508	-0.143836562	-5.306079528

C	1.910351688	3.726928189	1.211468497
C	1.298043754	4.720639191	0.411004967
C	0.134200496	5.501401987	0.965528062
H	7.756654082	2.871990849	4.138909507
H	9.069097498	3.768278741	3.422723350
H	7.289017351	3.756917210	-0.798749326
H	8.335975947	4.802400208	0.133224920
H	10.182957350	3.046061041	-0.035521054
H	9.071963786	2.135410290	-1.161704491
H	9.733544258	3.685039998	-1.585885117
H	7.521759132	5.764820741	3.079701299
H	6.207738556	4.854590702	3.814300868
H	7.611412458	5.304790453	4.773260113
H	-0.651820040	4.305516472	-1.174224279
H	0.199344608	2.908820981	-1.782755884
H	2.059612755	4.648971575	-2.520017155
H	0.979755308	4.690696732	-4.754100228
H	0.857295406	3.097104772	-4.005582266
H	-0.548545439	4.167989297	-4.036955678
H	1.069673784	6.754873495	-3.390106584
H	-0.464752191	6.382187893	-2.604584381
H	0.969301560	6.732452001	-1.635574673
H	-6.544159394	1.197458975	4.095614129
H	-5.037270175	1.065968640	3.168753972
H	-10.733511461	0.659213268	-2.226585587
H	-11.017971668	0.177573223	-0.541201484
H	-6.385896471	6.530947750	0.058843099
H	-8.242529692	6.284705658	-1.579820113
H	-5.780342984	4.633056286	1.497669019
H	-9.421956744	4.137715292	-1.763023112

H	-12.560285129	2.381684519	-1.962401061
H	-4.188502663	3.126423225	4.268004173
H	-6.666824793	2.922471064	6.061792545
H	-5.327438011	4.049455257	6.279743036
H	-6.379295993	4.195076454	4.870910579
H	-3.699735688	2.070910207	6.468388762
H	-4.999056610	0.906574416	6.216045048
H	-3.581823310	0.891170528	5.160138809
H	-13.158830301	0.902281827	0.652443093
H	-12.524822861	2.551183124	0.548124664
H	-14.142288981	2.187002947	-0.055256733
H	-14.432389210	0.725805790	-2.134421438
H	-13.029404984	0.218290122	-3.076072018
H	-13.368639562	-0.542233680	-1.515991244
H	-6.953823356	1.571518713	-3.687025576
H	-6.235013768	2.524921911	-2.411089731
H	-6.331369068	3.861003045	-4.546858184
H	-4.654988699	3.592468367	-4.086579167
H	-5.378076070	2.638151549	-5.373139378
H	-3.771440013	-1.591657670	-3.948291860
H	-4.927746797	-0.906215692	-5.058360852
H	-2.625119835	-0.875672463	-6.067297468
H	-3.170259253	0.779039494	-5.832313140
H	-2.020018504	0.065237332	-4.709870535
H	1.457068290	3.480517067	2.165392564
H	1.961320757	5.273509303	-0.241614612
H	2.986302892	3.614570153	1.159519402
H	-0.384425176	6.090948610	0.212417045
H	-0.582692400	4.844470657	1.456128508
H	0.525757057	6.192365700	1.718564750

12re-TS for 2Al/DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 8

Total atom = 177

CL	-10.511801961	-4.261009691	1.248122857
MG	-8.719813320	-4.200347846	-0.119961086
CL	-4.454698956	-4.216470879	1.151275200
MG	-2.664675874	-4.157150286	-0.215119059
CL	-6.905479280	-4.141864442	-1.456848803
CL	-0.879860994	-4.096991058	-1.595377435
CL	1.351366428	-4.177508154	1.190407141
MG	3.136213936	-4.118827901	-0.187078293
CL	7.407043719	-4.131030199	1.062581838
MG	9.189954540	-4.073636588	-0.312996069
CL	4.991378845	-4.063776665	-1.469297692
CL	10.952355308	-4.016331672	-1.720570178
CL	-13.621078582	-2.001344154	-0.172903069
MG	-11.451679687	-2.209226253	0.249496013
CL	-9.838599757	-2.390226230	-1.375965734
MG	-5.662477909	-2.390651153	-0.119755856
CL	-7.669804388	-2.496554045	1.446699421
CL	-3.692913580	-2.201584890	-1.554061825
MG	0.240174089	-2.250303909	-0.147761112
CL	-1.719601773	-2.247593343	1.245779624
CL	2.195555447	-2.189580388	-1.557641474
MG	6.167087285	-2.290641188	-0.062655715
MG	12.135926715	-2.312805460	-0.402297065
CL	4.137876167	-2.263559830	1.313591979
CL	8.277646301	-2.067945202	-1.502287168
CL	10.335719426	-2.701177191	1.394315973
CL	14.294491451	-2.575456209	0.079817862

CL	-10.628926665	-0.485123629	1.685342928
MG	-8.634256618	-0.350835769	0.299958649
CL	-4.829293581	-0.543828980	1.299708005
CL	-6.928039207	-0.602819356	-1.565033797
MG	-2.895911433	-0.206206139	-0.091025774
CL	1.223839184	-0.324800248	1.313428681
CL	-0.744101466	-0.123878932	-1.417851004
MG	3.329597676	-0.209282311	-0.013837365
CL	7.466679479	-0.576062013	1.601661063
CL	5.326941167	-0.368994140	-1.345591101
MG	9.162023202	-0.116304136	-0.222573807
CL	11.409222282	-0.155078737	-1.123503441
TI	0.243290553	1.814964660	0.052731812
CL	-1.987409643	1.693338041	1.191718495
CL	2.364115001	1.735949755	-1.197656459
C	-0.181176890	3.741394517	-0.850493507
C	-1.401674444	4.664072387	-0.892336660
O	-9.503327021	1.195358883	-0.729088968
C	-9.838202345	2.352809690	-0.512755070
C	-7.546382002	2.250828329	1.665417128
O	-7.837441312	1.083739356	1.445765699
O	-11.072264699	2.769268719	-0.664542445
O	-6.932136201	2.611109033	2.768077240
C	-12.080907971	1.808075178	-1.136323421
C	-6.559031226	1.569219386	3.732519912
C	-1.097635825	6.124281681	-0.535663805
C	-2.023995168	4.618576617	-2.299977188
C	-8.898280909	3.468557656	-0.163979609
C	-7.831914005	3.408821331	0.762497987
C	-9.101360997	4.650298783	-0.880778878

C	-7.001789494	4.525317648	0.900098919
C	-7.191900406	5.671736125	0.145083442
C	-8.253046767	5.738364802	-0.743705700
C	-13.442928763	2.476388586	-1.088113528
C	-5.503449955	2.132542378	4.667049791
C	-6.017994946	3.317916998	5.485659659
C	-4.997110557	0.999848482	5.566581141
C	-13.875435603	2.767674404	0.350685039
C	-14.455158161	1.577703654	-1.808446617
O	9.565728684	1.792853279	0.616956717
O	8.498184679	1.429091242	-1.486550249
C	7.886350337	1.398909981	-2.793831623
C	10.309818222	2.108487002	1.804513494
SI	9.026796571	2.788272756	-0.637004164
C	10.391851135	3.738365985	-1.514922687
C	11.706827352	3.938463059	-0.720619485
C	12.673461166	4.476696347	-1.779581293
C	12.363782023	3.634522613	-3.028446781
C	10.881698378	3.186647256	-2.888076967
C	7.607715786	3.867766869	-0.097334630
C	8.020729227	5.095521836	0.782092871
C	7.194638527	6.298616768	0.259252914
C	6.093394202	5.685935373	-0.612250497
C	6.772864772	4.472936735	-1.256703621
CL	-4.035408026	1.450425796	-1.755548026
CL	4.504512636	1.396656671	1.749723184
AL	-5.730621513	0.795508027	-3.103705027
AL	6.067390920	0.607586786	3.182799880
C	5.417827105	-0.782781177	4.406784482
C	7.127957886	2.154385979	3.790757349

C	-5.143458150	-0.419769035	-4.530945525
C	-6.907864810	2.347400533	-3.397602709
C	-3.863916757	-0.003205176	-5.278387802
C	-6.396728354	3.346279362	-4.451662634
C	4.028074168	-0.538868930	5.022235129
C	6.352065180	3.114062444	4.712743246
C	1.011651611	2.822425083	1.896320570
C	0.742982812	4.014756539	1.237866957
C	1.877996361	4.903212040	0.807019987
H	0.671031827	4.176319125	-1.372080881
H	-0.459043568	2.834067998	-1.461958631
H	-2.147050099	4.278764754	-0.190360803
H	-2.004127694	6.724883976	-0.635029582
H	-0.734887679	6.257510987	0.483171095
H	-0.352615486	6.545902239	-1.216286664
H	-2.913800145	5.251300522	-2.344219290
H	-1.315521248	4.983914105	-3.048466621
H	-2.322170062	3.607385845	-2.574220490
H	-7.470706622	1.287323607	4.263691386
H	-6.187891244	0.713657051	3.176054096
H	-11.797832566	1.519611450	-2.149104496
H	-12.042070559	0.933206545	-0.490924312
H	-6.517753356	6.509875498	0.261641673
H	-8.424799947	6.630157430	-1.331908896
H	-6.191949185	4.481920721	1.611778520
H	-9.930121871	4.702421786	-1.570976343
H	-13.367745465	3.423428039	-1.634603575
H	-4.667834698	2.466119731	4.042721268
H	-6.842306448	3.012411257	6.136355860
H	-5.226167435	3.718866569	6.120947019

H	-6.376667730	4.126369949	4.847090486
H	-4.211875046	1.364719394	6.230164654
H	-5.801142445	0.602723178	6.192196310
H	-4.586012318	0.177556717	4.979125444
H	-13.979519745	1.837253727	0.913846461
H	-13.153862546	3.401147751	0.868960975
H	-14.840033039	3.277957795	0.364570984
H	-15.447139924	2.031149483	-1.779525586
H	-14.185578517	1.430269417	-2.856699941
H	-14.516759233	0.595376820	-1.335345218
H	8.325183118	2.165630758	-3.430187476
H	8.073846797	0.419569923	-3.225954397
H	6.814481951	1.545480839	-2.696533102
H	11.356116406	1.846229263	1.654709719
H	10.225823016	3.167239721	2.044037387
H	9.897601934	1.528059353	2.626580332
H	9.977678744	4.739214780	-1.689615927
H	12.074585470	2.979266039	-0.348970189
H	11.595552594	4.608811439	0.134148774
H	12.459305933	5.533002479	-1.965822529
H	13.717462880	4.405337596	-1.471659171
H	13.011510176	2.757439470	-3.059487674
H	12.536643723	4.191033352	-3.949887017
H	10.821838775	2.099777887	-2.922789031
H	10.264656035	3.570241948	-3.702058494
H	6.934703609	3.233614816	0.487021790
H	9.088365468	5.322344154	0.725712994
H	7.804480993	4.889667221	1.830624039
H	6.800908666	6.909853087	1.071976201
H	7.826824910	6.948636205	-0.350682753

H	5.691151630	6.387622382	-1.344740703
H	5.261877633	5.344660871	0.010162220
H	7.411606918	4.812106462	-2.080131302
H	6.061213149	3.756515348	-1.667163635
H	6.165494092	-0.860276212	5.206877399
H	5.427849506	-1.752629435	3.904435512
H	8.008202496	1.775452929	4.324388173
H	7.515856533	2.709607478	2.931538983
H	-5.012468199	-1.423339596	-4.118468442
H	-5.975418211	-0.501744395	-5.242140013
H	-7.892905306	1.970538427	-3.698626713
H	-7.065382176	2.866868558	-2.447566966
H	-3.959918546	0.984126078	-5.738833652
H	-3.004934505	0.038083758	-4.605721976
H	-3.614000817	-0.705712162	-6.078709910
H	-6.262540497	2.871705030	-5.427028382
H	-7.086125597	4.183867020	-4.598419233
H	-5.430971862	3.772764601	-4.168313201
H	3.250443671	-0.513511037	4.256847862
H	3.757077059	-1.325692072	5.731847669
H	3.979136815	0.410111891	5.563591609
H	5.981773680	2.604748383	5.606001071
H	6.970432423	3.948645271	5.056913442
H	5.483688951	3.542518371	4.206095137
H	2.038238369	2.495536686	2.001129213
H	-0.197225536	4.499246828	1.458406748
H	0.297731304	2.423439966	2.604846673
H	1.595845291	5.638645629	0.058375846
H	2.224735574	5.447291204	1.691377748
H	2.713092638	4.313330781	0.431251895

12si-TS for 2Al/DIBP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$ cluster 8

Total atom = 177

CL	-10.473893256	-4.316151469	1.022415283
MG	-8.670023532	-4.196694551	-0.326038319
CL	-4.416231493	-4.263354930	0.980931500
MG	-2.614352263	-4.145311813	-0.365890241
CL	-6.844085911	-4.080703847	-1.643231023
CL	-0.817541989	-4.025859975	-1.726615898
CL	1.389225952	-4.222081235	1.072876681
MG	3.186039581	-4.104205635	-0.285125201
CL	7.445743809	-4.166095769	1.000518970
MG	9.240600642	-4.049576688	-0.355649907
CL	5.052325520	-3.993911178	-1.547479106
CL	11.015229420	-3.931812537	-1.743953885
CL	-13.572978139	-2.000793958	-0.329561543
MG	-11.407156639	-2.224795990	0.102819355
CL	-9.779668489	-2.336047718	-1.514527789
MG	-5.614802078	-2.386436867	-0.222722845
CL	-7.635630931	-2.559637716	1.320166284
CL	-3.632903422	-2.135841813	-1.630348976
MG	0.287781365	-2.240998030	-0.192705911
CL	-1.684155725	-2.298328590	1.182376912
CL	2.255405027	-2.119600481	-1.581473887
MG	6.213796151	-2.280803565	-0.057090815
MG	12.185377776	-2.284514001	-0.344731935
CL	4.172580299	-2.313129104	1.301138032
CL	8.336648372	-1.996184747	-1.467400762
CL	10.369868911	-2.749442219	1.417990204
CL	14.339900712	-2.565739990	0.144907116
CL	-10.595178507	-0.556783799	1.605875704

MG -8.588033377 -0.369589375 0.234340876

CL -4.806108214 -0.604041168 1.290077999

CL -6.848125595 -0.516622868 -1.606011205

MG -2.850976204 -0.223917607 -0.055058201

CL 1.268227636 -0.341546122 1.352546302

CL -0.704324702 -0.121742605 -1.393015065

MG 3.367166639 -0.195279435 0.027757294

CL 7.520878899 -0.574423761 1.640317480

CL 5.380483296 -0.309943952 -1.283127371

MG 9.181725944 -0.035779456 -0.200269846

CL 11.472902383 -0.072324872 -0.948875423

TI 0.237964200 1.791296250 0.127502220

CL -1.879847877 1.519700616 1.388409601

CL 2.373421616 1.754926307 -1.138481145

C -0.353155724 3.636247841 -0.760225928

C 0.401956728 4.575644524 -1.713038396

O -9.462022163 1.217807101 -0.729111903

C -9.864000623 2.341077677 -0.454996156

C -7.647353207 2.172878985 1.805573546

O -7.822434910 1.015573733 1.454830104

O -11.105748480 2.712471517 -0.656109999

O -7.115831900 2.460759115 2.971542505

C -12.034908625 1.747951161 -1.262456865

C -6.704097269 1.343064069 3.830163017

C 0.099612944 4.215876444 -3.175937809

C 0.084207176 6.053638404 -1.460010371

C -9.006274981 3.471579590 0.033524081

C -7.982517515 3.391959190 1.006235368

C -9.249643060 4.700394080 -0.585483057

C -7.238240436 4.541113709 1.290111756

C	-7.466225234	5.738922342	0.631569850
C	-8.482465741	5.821039500	-0.306790079
C	-13.420146106	2.368484029	-1.293174870
C	-5.928753161	1.902952629	5.008629168
C	-6.780217105	2.825657439	5.882568339
C	-5.354335338	0.731717846	5.813051150
C	-13.986912506	2.547782114	0.117093053
C	-14.332787568	1.490053369	-2.157189765
O	9.475032139	1.913696462	0.588595359
O	8.499364532	1.434059171	-1.534918439
C	8.039915704	1.333333118	-2.899304076
C	10.186035837	2.298988717	1.775655778
SI	8.852973674	2.843181548	-0.677415327
C	10.110688600	3.927531538	-1.553608796
C	11.229885572	4.535218121	-0.668434309
C	12.241319300	5.055288715	-1.694002820
C	12.297561766	3.936738810	-2.743725901
C	10.884396016	3.293595304	-2.753302248
C	7.295425525	3.727252569	-0.166161119
C	7.485528288	5.027863085	0.667162808
C	6.278674627	5.944332185	0.314136841
C	5.399499113	5.131216042	-0.650809402
C	6.372148400	4.160433903	-1.330550594
CL	-3.913112528	1.584616801	-1.598619370
CL	4.513215264	1.336522129	1.850764479
AL	-5.618437947	1.035133136	-2.979072678
AL	6.102291784	0.539031011	3.253420075
C	5.481815347	-0.899238636	4.435875845
C	7.122042692	2.098574406	3.896782771
C	-5.025799528	-0.054771417	-4.501714481

C	-6.792220162	2.610380261	-3.123233997
C	-3.791976166	0.472026829	-5.256509561
C	-6.227631801	3.750334174	-3.990261931
C	4.095693092	-0.690715217	5.072254595
C	6.335992169	2.985950815	4.880767120
C	1.121302684	2.917346012	1.900706214
C	0.619355063	4.045233647	1.283523835
C	-0.527575678	4.804944591	1.893719279
H	-1.299948008	4.056229162	-0.427155052
H	-0.662916411	2.729288158	-1.355831459
H	1.476884386	4.428937768	-1.568561650
H	0.644836253	4.876313492	-3.854370865
H	0.394961705	3.189391023	-3.396832900
H	-0.966856354	4.316904546	-3.392859257
H	0.632862153	6.685355830	-2.161638683
H	-0.982250293	6.251015551	-1.600474246
H	0.353991833	6.376883423	-0.453644183
H	-7.611886230	0.824551118	4.144825849
H	-6.100746587	0.667494835	3.228706678
H	-11.658797871	1.525781442	-2.261554958
H	-12.018957695	0.839899029	-0.663511238
H	-6.856256929	6.602739182	0.860369162
H	-8.683097432	6.750620182	-0.822919792
H	-6.463988179	4.482431726	2.039402649
H	-10.045987663	4.766046377	-1.311517055
H	-13.331886209	3.351822993	-1.769109361
H	-5.089714875	2.476755438	4.600317396
H	-7.619479285	2.278878536	6.321466631
H	-6.186769018	3.234812121	6.702150691
H	-7.185928803	3.662406532	5.312366680

H	-4.757463280	1.100958591	6.648206970
H	-6.152026537	0.108724682	6.226239695
H	-4.715752025	0.097357563	5.196284466
H	-14.112209343	1.577354365	0.602946226
H	-13.333443312	3.160457159	0.740180815
H	-14.963898928	3.032650261	0.078206713
H	-15.338424267	1.912033634	-2.190449709
H	-13.966329796	1.418890820	-3.183861991
H	-14.403175888	0.478786984	-1.751161429
H	8.176812470	2.283154064	-3.414388558
H	8.626946249	0.566754414	-3.400345302
H	6.990266506	1.053481984	-2.898007058
H	11.249695895	2.113940351	1.631356788
H	10.020455402	3.350949005	2.002566442
H	9.816970176	1.698150128	2.603432505
H	9.531842253	4.775092896	-1.941716548
H	11.705032013	3.761226659	-0.061241128
H	10.866611488	5.310961345	0.008283513
H	11.867598574	5.982378476	-2.138644101
H	13.215763661	5.272906269	-1.254260289
H	13.038048244	3.190429168	-2.450665286
H	12.588166565	4.304822377	-3.727938965
H	10.966732041	2.211751073	-2.659599855
H	10.360097763	3.492591674	-3.688944139
H	6.725833690	3.011635135	0.436094362
H	8.418830989	5.538509995	0.417969115
H	7.527788099	4.803253987	1.733318433
H	5.731234988	6.253629844	1.204841179
H	6.631914827	6.855891903	-0.172043803
H	4.861475787	5.759466105	-1.362423306

H	4.657766248	4.551814900	-0.096498361
H	6.935257711	4.687087602	-2.109844738
H	5.864194361	3.316753031	-1.797836470
H	6.238274503	-0.996272235	5.225451168
H	5.496823865	-1.851288142	3.900520814
H	8.033731318	1.736463104	4.387424817
H	7.457737235	2.705221776	3.050172804
H	-4.832763966	-1.074440282	-4.158493792
H	-5.875202354	-0.134065438	-5.192097570
H	-7.755100259	2.281032598	-3.532106543
H	-7.008458924	2.988487552	-2.119443962
H	-3.949426643	1.480551191	-5.649143072
H	-2.915691529	0.512951182	-4.606329440
H	-3.533413886	-0.164986838	-6.107321664
H	-6.033647896	3.422009501	-5.014560819
H	-6.912867914	4.601650044	-4.054232784
H	-5.283032092	4.128733486	-3.591184472
H	3.310885173	-0.644778462	4.315178879
H	3.838523956	-1.505089785	5.755451292
H	4.043411410	0.237722426	5.647787638
H	6.016046887	2.425378537	5.762672335
H	6.929708549	3.831851272	5.240137978
H	5.435082826	3.396948102	4.418437938
H	2.158322432	2.642295248	1.767455943
H	1.300816588	4.617875420	0.669215232
H	0.605909824	2.494750011	2.754281431
H	-1.023414348	5.475771140	1.196170683
H	-1.265895817	4.128997598	2.322163505
H	-0.120098602	5.415646896	2.705604154

DIBP/DCPDMS/(MgCl2)13/TiCl2iBu

Total atom = 136

CL	-10.598079191	-3.674954509	1.891122470
MG	-8.828219039	-3.865738142	0.506512230
CL	-4.543847527	-3.630584811	1.689081389
MG	-2.775254970	-3.821869872	0.306080040
CL	-7.034571904	-4.052096660	-0.847538239
CL	-1.012236172	-4.015847443	-1.089186323
CL	1.262159706	-3.566956384	1.625794492
MG	3.024529215	-3.761372457	0.232726761
CL	7.314196809	-3.526770666	1.393223106
MG	9.075121649	-3.721859176	0.002233077
CL	4.859223006	-3.940566744	-1.067093475
CL	10.816062702	-3.922097779	-1.420411432
CL	-13.743189455	-1.730711569	0.123344849
MG	-11.565670181	-1.849601221	0.541675579
CL	-9.977474693	-2.325409667	-1.047357596
MG	-5.782303850	-2.078374640	0.118819591
CL	-7.764554165	-1.895970752	1.710011705
CL	-3.836530784	-2.154595893	-1.357400368
MG	0.118266490	-1.927004163	-0.030918977
CL	-1.819301927	-1.670089359	1.368994176
CL	2.051672882	-2.124739933	-1.458524574
MG	6.045814416	-1.932939386	-0.036548309
MG	12.009620579	-1.999290762	-0.462640473
CL	4.038410148	-1.654991415	1.343597061
CL	8.132607881	-1.976372715	-1.526379200
CL	10.239341054	-2.050551323	1.403504761

CL	14.176841963	-2.160150733	0.025244943
CL	-10.663218763	0.140259922	1.505896124
MG	-8.723317636	-0.089594909	-0.003232711
CL	-4.881667355	0.024888296	1.262564606
CL	-6.876488742	-0.523658666	-1.497239793
MG	-2.997033956	-0.085188525	-0.120275119
CL	1.165146470	0.340631675	1.006321386
CL	-0.985010438	-0.113124219	-1.725088185
MG	3.151562070	-0.107926937	-0.528308009
CL	7.108506662	-0.059242735	1.272246153
CL	5.181010142	-0.220278583	-1.678634710
MG	9.126963374	-0.026986279	-0.028054597
CL	11.124965437	-0.069994239	-1.508455091
TI	0.058894520	1.948576169	-0.680364165
CL	-2.153085289	2.150777230	0.413242507
CL	2.182680968	1.668573203	-1.913621430
C	0.076449362	3.992339713	-1.063681907
C	0.826610564	4.184334082	0.240443803
O	-9.779482431	1.050830108	-1.366827916
C	-9.953256220	2.226337107	-1.640548963
C	-7.617239067	2.819000937	0.353487997
O	-8.039639314	1.719344419	0.672257036
O	-11.146314077	2.729982333	-1.865382771
O	-6.958931925	3.578993610	1.205046653
C	-12.295778704	1.817195760	-1.752034280
C	-6.706034745	3.033800930	2.540490928
C	2.236231484	4.758447533	0.060701234
C	0.032649348	4.951396416	1.303439989

C	-8.854765732	3.223721550	-1.859859486
C	-7.771109663	3.460223907	-0.988108240
C	-8.928471410	3.935283049	-3.058213855
C	-6.795231338	4.386666098	-1.366381851
C	-6.859320547	5.050168377	-2.581573066
C	-7.934159839	4.828239582	-3.429327479
C	-13.574358920	2.632773259	-1.797412478
C	-5.734954097	3.952993953	3.259531095
C	-6.303897161	5.358469956	3.462717696
C	-5.342247718	3.303847055	4.590824839
C	-13.692398518	3.565065804	-0.589568256
C	-14.761866399	1.666262250	-1.882894423
O	9.976803009	1.563185646	1.177499228
O	8.772303921	1.935230796	-0.866018883
C	8.063894883	2.322593599	-2.052691357
C	10.508874819	1.530311604	2.508928071
SI	9.616370976	2.899507434	0.220282337
C	11.142808809	3.734009741	-0.491550248
C	12.526646934	3.158151630	-0.064259108
C	13.493856493	3.438497275	-1.248255120
C	12.679612531	4.233543627	-2.283002391
C	11.231951426	3.795987333	-2.036149470
C	8.498079902	4.150106136	1.043135081
C	7.176506859	3.639273300	1.663875482
C	6.798766399	4.736738407	2.663682604
C	8.138835766	5.101681896	3.312420162
C	9.184793159	4.992784810	2.175839736
H	0.648391820	4.238401345	-1.955864646

H	-0.918084185	4.431514791	-1.085591010
H	1.003640432	3.160895059	0.713072882
H	2.787671643	4.749152238	1.003194616
H	2.803997383	4.194720837	-0.678226042
H	2.164786509	5.793675228	-0.279422884
H	0.559124714	4.954398051	2.259842891
H	-0.095593234	5.987664849	0.983725014
H	-0.953809924	4.516570728	1.458462380
H	-7.667031289	2.969018325	3.054948849
H	-6.301647735	2.031564849	2.420550294
H	-12.228174543	1.111863537	-2.580744147
H	-12.199617718	1.270009332	-0.815954103
H	-6.076929494	5.744969618	-2.857109413
H	-8.005373992	5.348615040	-4.375454642
H	-5.973016383	4.576279483	-0.693003823
H	-9.774816730	3.771724980	-3.709990879
H	-13.553280371	3.240037554	-2.709521106
H	-4.835913516	4.021432419	2.637545382
H	-7.196225105	5.328576853	4.094372584
H	-5.572365628	6.003044373	3.953648529
H	-6.578596858	5.823544942	2.515153246
H	-4.615240849	3.924141640	5.117247452
H	-6.211214985	3.186473400	5.243786616
H	-4.898443743	2.318456017	4.439362555
H	-13.718321576	2.989879795	0.339443170
H	-12.853980057	4.261122734	-0.534382191
H	-14.611264900	4.151307870	-0.646133340
H	-15.700375937	2.222785610	-1.894139937

H	-14.720125658	1.059346159	-2.789695867
H	-14.779292727	0.982845464	-1.031322374
H	7.900735432	3.400936498	-2.070528374
H	8.642491511	2.031118526	-2.928580550
H	7.102689366	1.812718351	-2.059270821
H	11.427284204	2.115129957	2.566773107
H	9.775317649	1.915457537	3.217524062
H	10.729266879	0.494172434	2.753740173
H	11.093422730	4.771657400	-0.139029261
H	12.470724567	2.085993477	0.116428930
H	12.870442595	3.625120006	0.860442569
H	14.386330226	3.977431992	-0.928831928
H	13.829043820	2.493934079	-1.678232181
H	13.006732396	4.049124056	-3.307470261
H	12.772265920	5.308103471	-2.099555987
H	11.070210857	2.804992844	-2.465847851
H	10.501556248	4.477310144	-2.478558084
H	8.233226496	4.852299487	0.240866856
H	7.323388614	2.692426667	2.187322765
H	6.410499497	3.457397541	0.909361205
H	6.388963634	5.601368496	2.131660071
H	6.051355534	4.413561255	3.390282138
H	8.368316388	4.381201690	4.101562131
H	8.135813001	6.089405583	3.775131001
H	10.109108424	4.544994560	2.547681724
H	9.458660037	5.977923547	1.796522778

DMP

Total atom = 24

C	0.080360581	1.382803695	1.997948166
C	-0.080360581	-1.382803695	1.997948166
C	0.027723899	0.700843347	0.783151188
C	0.045122815	0.693232766	3.201747020
C	-0.045122815	-0.693232766	3.201747020
C	-0.027723899	-0.700843347	0.783151188
C	-0.027723899	1.547174560	-0.448976262
C	0.027723899	-1.547174560	-0.448976262
O	0.606999087	2.560541111	-0.602176041
O	-0.606999087	-2.560541111	-0.602176041
O	0.931297502	-1.091493244	-1.335117238
O	-0.931297502	1.091493244	-1.335117238
C	1.056762257	-1.851409673	-2.547056517
C	-1.056762257	1.851409673	-2.547056517
H	0.135482631	2.462936605	1.982404692
H	0.080596625	1.238536885	4.136082315
H	-0.080596625	-1.238536885	4.136082315
H	-0.135482631	-2.462936605	1.982404692
H	0.111262195	-1.861984566	-3.088612142
H	1.350525396	-2.876624413	-2.325317209
H	1.826498020	-1.350000818	-3.127092994
H	-0.111262195	1.861984566	-3.088612142
H	-1.350525396	2.876624413	-2.325317209
H	-1.826498020	1.350000818	-3.127092994

Et-DMP-AlEt$_2$

Total atom = 46

C	-1.146218242	-3.102528053	-2.224480405
C	1.102534850	2.980027228	1.524553920
O	0.081191039	-2.519470176	-1.731292923
O	1.377920291	2.643015665	0.173624115
O	-1.133221660	-1.200370756	-0.443977422
C	-0.015773669	-1.570922351	-0.817617889
C	1.632985166	0.227577603	-0.004840176
C	1.295288774	-1.114930419	-0.300048694
C	2.916109166	0.455749710	0.492286928
C	2.225037263	-2.144629823	-0.085964873
C	3.817217660	-0.571704849	0.736082127
C	3.472976739	-1.884417273	0.448971698
C	0.737702557	1.467692878	-0.333498481
O	-0.528962157	1.369267041	0.162572538
C	0.741892903	1.663980079	-1.868829444
AL	-1.634116785	0.189032687	0.824029323
C	-0.077103400	2.863271917	-2.332644014
C	-1.172022506	-0.549611593	2.607894917
C	-3.532273821	0.565057005	0.423549908
C	-2.001841062	-1.756180657	3.082364213
C	-3.892968696	0.961572670	-1.017415333
H	-1.757978113	-2.338761200	-2.699927323
H	0.054973183	3.248616211	1.664277249
H	-1.700400596	-3.558948184	-1.406473497
H	1.349339399	2.167105944	2.216230927
H	3.210734748	1.477995404	0.672569235

H 1.947574760 -3.160319330 -0.329023955

H 4.794778752 -0.339856486 1.140378441

H 4.167073307 -2.694732091 0.628552027

H 0.353618668 0.749071581 -2.326073255

H 1.780294930 1.763017687 -2.195390884

H -0.068740395 2.928790618 -3.422796027

H -1.112461613 2.778821237 -2.003965491

H 0.332190612 3.790022232 -1.932039753

H -1.280226634 0.263324349 3.338361074

H -0.106095528 -0.807546110 2.638746344

H -3.867334108 1.356844934 1.106721820

H -4.122421108 -0.313601481 0.716256410

H -3.069205073 -1.522293287 3.117266039

H -1.716950300 -2.098437884 4.082745068

H -1.890593462 -2.614310829 2.411770179

H -3.368946955 1.869418037 -1.325303566

H -3.617524284 0.180143286 -1.732318315

H -4.964163314 1.148007130 -1.148294992

H -0.831697542 -3.850486944 -2.945287102

H 1.730996605 3.841131666 1.751041242

2DMP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$

Total atom = 103

CL 10.845327725 -3.374349825 -1.789782291

MG 9.081835159 -3.493581415 -0.389118902

CL 4.791630159 -3.381456191 -1.568470981

MG 3.029360357 -3.501356015 -0.169391288

CL 7.294433583 -3.610592054 0.980895685

CL 1.272830994 -3.623031090 1.242070406

CL	-1.014535266	-3.375950803	-1.487858385
MG	-2.770502945	-3.498235564	-0.078566006
CL	-7.065983110	-3.385311690	-1.235846358
MG	-8.820423626	-3.508252445	0.171463488
CL	-4.599164992	-3.612063865	1.237031418
CL	-10.554742717	-3.634165916	1.610570382
CL	13.974381912	-1.285843996	-0.163757830
MG	11.796999113	-1.454865633	-0.565421037
CL	10.218928633	-1.843372686	1.057104682
MG	6.017815238	-1.717421146	-0.107037888
CL	7.993151432	-1.617661100	-1.714058877
CL	4.077367984	-1.718231750	1.378282095
MG	0.116267409	-1.619545288	0.054690636
CL	2.046812175	-1.433610651	-1.366298543
CL	-1.810371859	-1.744874986	1.499179550
MG	-5.810633023	-1.688398158	0.082628160
MG	-11.771965072	-1.790384314	0.534477697
CL	-3.810578536	-1.479452244	-1.320168718
CL	-7.892338557	-1.657123321	1.579888975
CL	-10.006987318	-1.944085912	-1.331077538
CL	-13.938776238	-2.005837550	0.066117758
CL	10.874275241	0.480614790	-1.623590116
MG	8.917493315	0.297705838	-0.172126946
CL	5.092884058	0.313725139	-1.363731199
CL	7.113581946	-0.071102871	1.410596669
MG	3.206717426	0.251526654	0.019518431
CL	-0.949431826	0.560724040	-1.130174823
CL	1.195884329	0.316713609	1.625454030

MG	-2.940349997	0.188975410	0.431939107
CL	-6.874789819	0.113769028	-1.325819836
CL	-4.944857185	0.132500147	1.624357930
MG	-8.913974076	0.162281064	-0.020070040
CL	-10.948335732	0.235782917	1.432264621
TI	0.131917738	2.290400603	0.438397861
CL	2.359689039	2.455816062	-0.633716874
CL	-1.995039116	2.087106548	1.676833032
C	0.083666903	4.359820028	0.659839062
C	-0.647078345	4.438080237	-0.667260679
O	-9.891700975	1.517719980	-1.243963246
C	-9.935711198	2.718564847	-1.437707889
C	-7.805145269	2.972828077	0.824461603
O	-8.303921474	1.873054986	0.986937304
O	9.810055896	1.708223288	1.064573819
C	9.630067294	2.852537408	1.439116283
C	7.478150396	2.970577355	-0.811072906
O	8.090607420	1.950199885	-1.076307483
O	-11.063833163	3.334289862	-1.739248840
C	-12.262317678	2.511884837	-1.784119531
O	-7.216497559	3.615449063	1.817876726
C	-7.138394050	2.920402104	3.089429604
O	10.627470422	3.604149356	1.870112746
O	6.868887802	3.671634728	-1.748942558
C	11.948521697	2.998134702	1.854058135
C	6.901097060	3.129428226	-3.094021342
C	-2.067337469	5.003058691	-0.554170887
C	0.153151665	5.132631029	-1.774557974

C	8.306200957	3.542525070	1.548666860
C	7.315742853	3.571093696	0.545653974
C	8.058482408	4.183291481	2.763372867
C	6.109881452	4.226126111	0.805147341
C	5.862531105	4.816979166	2.034700572
C	6.842143990	4.799891289	3.016291289
C	-7.776208442	3.744991461	-0.453306752
C	-8.760885657	3.647225089	-1.457797104
C	-8.660206241	4.457849681	-2.589260764
C	-6.722122096	4.644511074	-0.632204820
C	-6.613332671	5.411188527	-1.781756110
C	-7.587891863	5.319814158	-2.764140565
H	-0.506249095	4.668009088	1.520342312
H	1.070566574	4.816076385	0.661564173
H	-0.802478315	3.379420336	-1.061552399
H	-2.602798858	4.908462550	-1.501377624
H	-2.637483098	4.490100887	0.219321713
H	-2.015887372	6.063105116	-0.296639996
H	-0.358558768	5.055235512	-2.735831278
H	0.264293057	6.191882508	-1.533396923
H	1.146940929	4.700361875	-1.882562942
H	7.932150130	3.025607556	-3.425238920
H	6.404670348	2.162096866	-3.107872867
H	11.975574019	2.153361667	2.539333010
H	12.189257491	2.660793636	0.848611193
H	-8.139766482	2.675626891	3.437010849
H	-6.549918322	2.013061482	2.974961428
H	-12.165876546	1.760546066	-2.565122191

H -12.410305836 2.027169675 -0.821955770

H 4.910241321 5.296677587 2.218524073

H 6.666741659 5.266987276 3.976455084

H 5.357194798 4.254855156 0.031369092

H 8.828952107 4.183211719 3.520940639

H -9.431017471 4.399337713 -3.344384246

H -5.774823351 6.084404278 -1.901701946

H -7.522308577 5.919993694 -3.662113436

H -5.978694664 4.732261268 0.145574274

H -13.067728459 3.204239290 -2.005313537

H -6.652733074 3.621685208 3.760327968

H 12.621042004 3.785315431 2.178255947

H 6.367356279 3.854762599 -3.699587460

2Al/2DMP/$(MgCl_2)_{13}$/$TiCl_2{}^{i}Bu$

Total atom = 135

CL 10.761512121 -3.657791505 -2.055207144

MG 9.027943668 -3.781077659 -0.617782736

CL 4.714142591 -3.660623835 -1.709098377

MG 2.980602481 -3.783224044 -0.273810846

CL 7.268169470 -3.900767982 0.786728557

CL 1.253652990 -3.909815448 1.174176743

CL -1.089524049 -3.650371501 -1.506866608

MG -2.815584348 -3.776320369 -0.062557183

CL -7.133948434 -3.656481691 -1.129426683

MG -8.859058416 -3.783291720 0.313976254

CL -4.616834577 -3.893674936 1.290702106

CL -10.563693481 -3.912425143 1.787884059

CL 13.925144480 -1.576515731 -0.487619560

MG 11.739087516 -1.743493109 -0.845440550

CL 10.195990927 -2.134801414 0.807969965

MG 5.971765514 -2.003294854 -0.267909389

CL 7.914483398 -1.897818882 -1.914732855

CL 4.064543215 -2.006813003 1.258749911

MG 0.074413321 -1.900674951 0.018000449

CL 1.975329067 -1.710765078 -1.442894702

CL -1.821826054 -2.029621166 1.501632772

MG -5.851265085 -1.965395785 0.168163015

MG -11.800447759 -2.064010443 0.744073853

CL -3.879857156 -1.752661175 -1.275048658

CL -7.900244144 -1.937632349 1.708460036

CL -10.075352171 -2.212403173 -1.159032718

CL -13.977366153 -2.276534932 0.320016659

CL 10.842232145 0.128660686 -2.036012709

MG 8.931566301 0.062023158 -0.522665663

CL 5.103763112 -0.000217924 -1.432580873

CL 7.274886896 -0.377117501 1.350810972

MG 3.226509323 0.141513733 0.051936683

CL -1.013537460 0.256535004 -1.157328557

CL 1.177063567 0.009106112 1.563812207

MG -3.063170762 0.138170176 0.311769310

CL -7.089741622 -0.181871996 -1.382647017

CL -4.996073946 -0.214214964 1.672961303

MG -9.033500026 -0.084820654 0.245625388

CL -10.999661879 -0.085643400 1.755816986

TI 0.104243816 1.961889114 0.403593519

CL 2.087189041 2.013992178 -1.054224070

CL	-1.920574318	1.728725245	1.806140882
C	0.199208583	4.007982650	0.745105971
C	-0.684748921	4.229845357	-0.469225665
O	-10.017435547	1.333952361	-0.865435555
C	-10.493432428	2.449852592	-0.716426107
C	-8.256216379	2.690398475	1.509425697
O	-8.309671987	1.495025352	1.269361032
O	9.916976374	1.444251914	0.639950045
C	10.288589440	2.606945717	0.570901585
C	7.921372541	2.863158811	-1.499289608
O	8.100611670	1.659093098	-1.405275879
O	-11.765217589	2.703143206	-0.943660463
C	-12.618891905	1.600824466	-1.354127594
O	-7.756204017	3.136012039	2.642876867
C	-7.253004580	2.145971668	3.582053698
O	11.547002457	2.952843824	0.730323978
O	7.341347505	3.384468425	-2.559664011
C	12.522765156	1.897694388	0.965450622
C	6.903280127	2.466612157	-3.598938212
C	-2.027067999	4.885954832	-0.130107293
C	0.022102993	4.950926634	-1.621764439
C	9.392277111	3.795554503	0.403500479
C	8.299443843	3.895680432	-0.487899822
C	9.674442119	4.873396266	1.245677043
C	7.525140361	5.059461704	-0.471468215
C	7.792321300	6.097720435	0.406927571
C	8.877519920	6.007944711	1.264131795
C	-8.705627143	3.794104087	0.606794433

C	-9.730035391	3.689448080	-0.363160213
C	-10.075664491	4.824312903	-1.100850236
C	-8.066944054	5.026413124	0.774539124
C	-8.395112959	6.128756984	0.001116772
C	-9.408503265	6.028776610	-0.938320702
CL	4.361746254	1.701028169	1.779549902
CL	-4.204152877	1.959904393	-1.172962409
AL	6.095826035	0.923621048	3.007717611
AL	-5.789301951	1.373880517	-2.681587117
C	7.284676035	2.447987788	3.383035536
C	6.764152032	3.409499815	4.467082185
C	5.548627912	-0.404099498	4.346712902
C	4.354800509	-0.002835962	5.232022355
C	-6.968367204	2.931617878	-2.940553974
C	-5.076715319	0.301460502	-4.164364360
C	-3.802639167	0.850559162	-4.831750994
C	-6.383934706	4.024299749	-3.854207846
H	-0.255195110	4.292172560	1.692399636
H	1.210899399	4.396829181	0.649606382
H	-0.971053564	3.217085136	-0.904674882
H	-2.684332376	4.910856357	-1.000692006
H	-2.539309313	4.348494445	0.666521117
H	-1.852351904	5.912626439	0.200369569
H	-0.607583717	4.975342607	-2.513554565
H	0.236951192	5.981328219	-1.329232763
H	0.962049284	4.465393189	-1.880792061
H	7.763204658	1.930754117	-3.995353074
H	6.180013068	1.765361243	-3.190627472

H	12.193101909	1.263102001	1.784538390
H	12.652225399	1.310985598	0.060072132
H	-8.063530968	1.484601279	3.880642529
H	-6.452864773	1.571531439	3.121709682
H	-12.161135702	1.060271192	-2.179106165
H	-12.782172008	0.936538603	-0.509362210
H	7.158159552	6.974196406	0.411076980
H	9.108126472	6.814474595	1.947479952
H	6.696632433	5.139961613	-1.158381407
H	10.523978271	4.805981164	1.908831066
H	-10.872893190	4.750062247	-1.825185100
H	-7.863545296	7.060509514	0.141471475
H	-9.684884263	6.881375162	-1.544398068
H	-7.293613623	5.110447231	1.522386369
H	8.262212272	2.051426095	3.683262090
H	7.459887546	3.003931582	2.457332334
H	7.455571525	4.237519699	4.653351632
H	5.804285809	3.850488272	4.186465967
H	6.615205375	2.900059016	5.422445233
H	5.329493494	-1.351980458	3.848986177
H	6.425584852	-0.600277878	4.976928042
H	4.127765315	-0.769073424	5.978844897
H	4.539966924	0.927828058	5.775529537
H	3.450617323	0.146328066	4.638433137
H	-7.914856679	2.571380694	-3.361918198
H	-7.220920473	3.365785948	-1.968808611
H	-4.895427942	-0.719543515	-3.820386816
H	-5.877831517	0.221516457	-4.910610305

H	-2.969311823	0.891745675	-4.127544621
H	-3.483856555	0.227053847	-5.672044107
H	-3.945635302	1.862431345	-5.221327678
H	-6.153143736	3.638032343	-4.850162893
H	-7.073102974	4.863863402	-3.990282754
H	-5.456031885	4.434984393	-3.447905783
H	-13.549889564	2.067096741	-1.658777587
H	-6.891757297	2.725277002	4.425252839
H	6.457090833	3.101929786	-4.356829051
H	13.439699302	2.418669086	1.219369136