Supporting Information

Thermochemistry of the Initial Steps of MAO Formation. Aluminoxanes and Cycloaluminoxanes by Methane Elimination from Dimethylaluminum Hydroxide and Its Dimeric Aggregates

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TABLE OF CONTENTS

Table S1. Computed Energies at MP2(full)/6-31G*…….. S3
Table S2. Computed Energies at MP2(full)/6-311G**…….. S4

Cartesian Coordinates of Stationary Structures, MP2(full)/6-311G**……. S5
TMA, **1**
DMAH, **2**
MeAlO, **3**
$(TMA)_2$, cyclic, $(\mathbf{1})_2$
$(TMA)_2$, acyclic, $(\mathbf{1})_2$
$Me_2Al(OH)_2AlMe_2$, **4**
$Me_2Al(O)(OH)AlMe$, **5**
$(MeAlO)_2$, **6**
$Me_2Al(Me)(OH)AlMe_2$, **7**
$Me_2Al(O)AlMe_2$, **9**, M, TS, SOSP
$Me_2Al(O)AlMe(OH)$, **10**

Cartesian Coordinates of Stationary Structures, MP2(full)/6-31G*……. S10
TMA, **1**
DMAH, **2**
MeAlO, **3**
$(TMA)_2$, cyclic, $(\mathbf{1})_2$
$(TMA)_2$, acyclic, $(\mathbf{1})_2$
$Me_2Al(OH)_2AlMe_2$, **4**
$Me_2Al(O)(OH)AlMe$, **5**
$(MeAlO)_2$, **6**
$Me_2Al(Me)(OH)AlMe_2$, **7**

$Me_2Al(O)AlMe_2$, **9**
$Me_2Al(O)AlMe(OH)$, **10**

Cartesian Coordinates of Stationary, Donor-Coord. Structures, MP2(full)/6-31G*… S15
$TMA•OMe_2$, **1**•OMe_2
$DMAH•OMe_2$, **2**•OMe_2
$MeAlO•OMe_2$, **3**•OMe_2
$MeAlO•(OMe_2)_2$, **3**•$(OMe_2)_2$
$(TMA)_2•(OMe_2)$, cyclic, $(\mathbf{1})_2•(OMe_2)$
$(TMA)_2•(OMe_2)$, acyclic, one AlO contact, $(\mathbf{1})_2•(OMe_2)$
$(TMA)_2•(OMe_2)$, acyclic, two AlO contacts, $(\mathbf{1})_2•(OMe_2)$
$Me_2Al(O)(OH)AlMe•(OMe_2)$, **5**•$(OMe_2)$
$(MeAlO)_2•(OMe_2)_2$, **6**•$(OMe_2)_2$, trans
$(MeAlO)_2•(OMe_2)_2$, **6**•$(OMe_2)_2$, cis
$Me_3Al-O-AlMe_2•(OMe_2)$, **7**•(OMe_2)
$Me_2Al(O)AlMe_2•(OMe_2)$, **9**•(OMe_2)
$Me_2Al(O)AlMe_2•(OMe_2)_2$, **9**•$(OMe_2)_2$
$Me_2Al(O)AlMe(OH)•(OMe_2)$, **10**•$(OMe_2)$
$Me_2Al(O)AlMe(OH)•(OMe_2)_2$, **10**•$(OMe_2)_2$

Cartesian Coordinates of Stat. Struct. of Trioxanes, MP2(full)/6-31G*……. S25
Structure **11:** Addition of **10** to DMAH
Structure **12:** Methane Elimination from **11**
Structure **13:** Acyclic **12**
Structure **14:** Addition of **9** to TMA

Complete Software Reference:

Gaussian 03, Revision E.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Table S1. Computed Energies at MP2(full)/6-31G*

Molecule	Energy	VZPE	TE	S	NI	ν_1	ν_2	μ
Methane	-40.337043	29.10	30.89	44.44	0	1413.9	1413.9	0.000
Water	-76.199244	13.49	15.27	45.13	0	1734.2	3779.0	2.242
Dimethylether	-154.515545	51.63	54.29	64.21	0	222.4	269.5	1.594
TMA, **1**	-361.228480	68.70	74.02	92.08	0	28.9	29.0	0.000
DMAH, **2**	-397.158986	54.57	59.37	92.62	0	1.3	31.6	1.658
MeAlO, **3**	-356.756670	24.83	27.65	66.34	0	158.4	158.5	6.308
$(\mathbf{1})_2$, cyclic	-722.490908	139.97	150.21	124.18	0	47.0	105.0	0.000
$(\mathbf{1})_2$, acyclic	-722.465359	138.40	149.98	151.01	0	5.0	20.4	2.021
$(\mathbf{1})_2$•(OMe_2), cy.	-877.016406	192.52	206.55	159.36	0	15.6	36.0	2.989
$(\mathbf{1})_2$•(OMe_2), acy.	-877.023947	192.29	206.56	161.87	0	15.3	30.6	6.295
1•(OMe_2)•**1**	-877.027069	193.30	206.77	146.50	0	60.2	63.8	4.129
$(\mathbf{2})_2$ = **4**	-794.422321	111.65	121.07	120.38	0	46.2	84.1	0.005
2•**3** = **5**	-754.062746	81.26	89.11	111.34	0	33.8	40.4	5.566
$(\mathbf{3})_2$ = **6**	-713.725766	51.96	57.70	102.04	0	6.3	9.0	0.000
1•**2** = **7**	-758.453075	125.71	135.52	121.77	0	49.4	92.5	1.039
9	-718.128741	95.14	104.00	127.71	0	21.6	22.4	0.000
10	-754.057567	80.99	89.26	121.48	0	18.0	30.9	1.715
1•(OMe_2)	-515.781817	122.31	130.55	110.89	0	33.4	108.0	5.004
2•(OMe_2)	-551.714334	107.96	115.81	107.19	0	50.6	100.3	3.445
3•(OMe_2)	-511.315484	78.24	84.24	95.11	0	47.6	72.1	8.565
3•$(OMe_2)_2$	-665.867400	131.53	140.65	118.52	0	42.7	57.4	7.681
5•(OMe_2)	-908.630874	134.93	145.76	133.48	0	27.4	43.0	7.296
6•$(OMe_2)_2$, trans	-1022.849980	158.78	170.76	142.69	0	35.7	39.2	1.315
6•$(OMe_2)_2$, cis	-1022.844351	158.69	170.67	141.76	0	34.0	41.0	8.786
7•(OMe_2)	-912.996718	178.55	192.04	151.56	0	27.68	51.17	7.278
9•(OMe_2)	-872.683663	148.47	160.38	148.54	0	16.7	21.4	4.519
9•$(OMe_2)_2$	-1027.236688	201.66	216.73	171.94	0	7.6	12.9	4.126
10•(OMe_2)	-908.616013	134.16	145.66	145.09	0	17.5	19.2	3.050
10•$(OMe_2)_2$	-1063.169045	187.42	201.99	165.67	0	12.0	2.2	6.287
11	-1115.372671	151.74	165.27	157.55	0	24.5	31.9	0.063
12a	-1075.042910	122.57	133.50	133.84	0	33.8	40.7	0.388
12b	-1075.030386	122.55	132.93	128.18	1	-17.9	41.3	1.474
13	-1075.027249	121.43	133.89	166.11	0	14.6	15.2	0.031
14	-1115.309695	151.72	165.31	164.25	0	7.5	15.9	0.281

(a) Total energies E_{tot} (in atomic units), vibrational zero-point energies (VZPE, in kcal/mol), thermal energies (TE, in kcal/mol), molecular entropies (S, in cal K^{-1} mol^{-1}), the number of imaginary frequencies (NI), and dipole moments (μ, in Debye).

Table S2. Computed Energies at MP2(full)/6-311G**

Molecule	Energy	VZPE	TE	S	NI	ν_1	ν_1	μ
Methane	-40.398042	28.56	30.36	44.46	0	1363.9	1363.9	0.000
Water	-76.282896	13.72	15.50	45.08	0	1667.2	3909.9	2.195
TMA, **1**	-361.527843	67.36	72.78	93.53	0	27.1	27.2	0.000
DMAH, **2**	-397.471197	53.91	58.67	84.76	0	39.7	62.4	1.607
MeAlO, **3**	-356.997647	24.47	27.27	66.00	0	175.6	175.7	6.412
$(\mathbf{1})_2$, cyclic	-723.088587	137.35	147.74	125.15	0	41.6	101.9	0.000
$(\mathbf{1})_2$, acyclic	-723.065045	135.85	147.54	152.44	0	2.68	20.05	2.430
$(\mathbf{2})_2$ = **4**	-795.040601	110.00	119.67	122.31	0	46.2	77.7	0.004
2•3 = **5**	-754.610953	80.33	88.15	110.11	0	44.6	52.3	5.569
$(\mathbf{3})_2$ = **6**, C_{2h}	-714.198083	51.17	56.35	92.25	1	-10.3	14.9	0.646
$(\mathbf{3})_2$ = **6**, C_1	-714.199654	51.19	56.95	100.25	0	8.2	18.3	0.051
1•2 = **7**	-759.061773	123.61	133.59	122.84	0	49.3	90.4	0.956
9, M	-718.666498	93.26	102.29	133.94	0	7.2	12.6	0.001
9, TS	-718.666494	93.23	101.70	126.37	1	-10.7	11.6	0.004
9, SOSP	-718.666482	93.27	101.14	116.58	2	-11.4	-8.5	0.000
10	-754.608428	79.79	88.16	122.89	0	16.0	24.1	1.620
HO−Al=O	-392.920707	9.85	12.52	63.15	0	207.6	219.0	5.716

(a) Total energies E_{tot} (in atomic units), vibrational zero-point energies (VZPE, in kcal/mol), thermal energies (TE, in kcal/mol), molecular entropies (S, in cal K^{-1} mol^{-1}), the number of imaginary frequencies (NI), and dipole moments (μ, in Debye).

Cartesian Coordinates of Stationary Structures, MP2(full)/6-311G**

Trimethylaluminum (TMA), Me_3Al (de facto C_3), 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.000054	-0.000060	-0.000447
2	6	0	0.482268	1.903375	0.000143
3	1	0	0.066077	2.414790	0.876312
4	1	0	1.562227	2.076875	-0.000602
5	1	0	0.064676	2.415853	-0.874728
6	6	0	1.407421	-1.369255	0.000137
7	1	0	2.057607	-1.265198	0.876981
8	1	0	1.017985	-2.391389	-0.001893
9	1	0	2.060739	-1.262845	-0.874086
10	6	0	-1.889629	-0.534073	-0.000041
11	1	0	-2.127653	-1.137642	0.884026
12	1	0	-2.579806	0.314374	-0.014805
13	1	0	-2.121510	-1.164323	-0.866830

Dimethylaluminumhydroxide (DMAH), Me_2AlOH, 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000579	0.055680	-0.000030
2	8	0	0.057366	1.774489	-0.000025
3	6	0	-1.697082	-0.918588	0.000017
4	1	0	-1.762087	-1.574005	0.875869
5	1	0	-2.583735	-0.278615	0.001150
6	1	0	-1.763107	-1.572257	-0.877068
7	6	0	1.723723	-0.855033	-0.000006
8	1	0	1.832428	-1.500921	0.878068
9	1	0	1.830597	-1.504831	-0.875403
10	1	0	2.558618	-0.150058	-0.002371
11	1	0	-0.739014	2.302659	0.000276

Methylaluminumoxide, MeAlO (de facto C_{3v}), 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.187028	0.000287	-0.000039
2	8	0	-1.810530	-0.000253	0.000031
3	6	0	1.751349	0.000053	-0.000006
4	1	0	2.136358	1.022049	-0.029783
5	1	0	2.135466	-0.486139	0.900055
6	1	0	2.135674	-0.537935	-0.869979

$(TMA)_2$, cyclic, $(1)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.306147	-0.000052	0.000046
2	13	0	-1.306288	-0.000013	0.000029
3	6	0	2.223978	-1.729005	-0.119163
4	1	0	2.958313	-1.748639	-0.932765
5	1	0	2.768843	-1.961080	0.803204
6	1	0	1.523642	-2.553706	-0.294075
7	6	0	-2.223746	1.729157	0.118842
8	1	0	-2.962118	1.747431	0.928805
9	1	0	-1.523775	2.553030	0.299050
10	1	0	-2.763830	1.963639	-0.805729
11	6	0	2.224018	1.728890	0.119092
12	1	0	2.958793	1.748533	0.932290
13	1	0	1.523771	2.553594	0.294335
14	1	0	2.768393	1.960959	-0.803574
15	6	0	-2.224119	-1.728964	-0.118934
16	1	0	-2.765377	-1.962742	0.805130
17	1	0	-1.524221	-2.553174	-0.297864
18	1	0	-2.961541	-1.747423	-0.929757
19	6	0	-0.000018	-0.250985	1.673556
20	1	0	-0.846888	0.228419	2.187174
21	1	0	0.000013	-1.305902	1.960001
22	1	0	0.846884	0.228478	2.187062
23	6	0	0.000044	0.250943	-1.673465
24	1	0	0.846753	-0.228662	-2.187133
25	1	0	-0.847102	-0.228057	-2.187011
26	1	0	0.000340	1.305921	-1.959694

$(TMA)_2$, acyclic, $(1)_2$

Dimethylaluminum Hydroxide Cyclodimer, $(Me_2AlOH)_2$, C_1, 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000091	0.103737	-1.208879
2	1	0	0.000203	0.648402	-1.995443
3	13	0	-1.438014	0.000055	0.000141
4	13	0	1.438386	0.000068	-0.000227
5	8	0	0.000283	-0.103784	1.208923
6	1	0	0.000697	-0.649769	1.994577
7	6	0	-2.378605	-1.717040	-0.067057
8	1	0	-2.989841	-1.887681	0.826996
9	1	0	-3.063612	-1.769121	-0.920959
10	1	0	-1.689499	-2.563623	-0.157037
11	6	0	2.378365	1.717556	0.065675
12	1	0	2.993435	1.885383	-0.826284
13	1	0	1.688447	2.564106	0.149652
14	1	0	3.059532	1.772965	0.922413
15	6	0	-2.378664	1.717109	0.067093
16	1	0	-2.992537	1.885726	-0.825555
17	1	0	-1.689663	2.564143	0.153424
18	1	0	-3.061281	1.770539	0.922815

19	6	0	2.378190	-1.717557	-0.065574
20	1	0	3.063433	-1.771580	-0.919132
21	1	0	1.688239	-2.563580	-0.154496
22	1	0	2.988907	-1.887552	0.828972

Dimethylalum. Hydr. Methylaluminumoxide Cycloadd., (Me_2AlOH)(MeAlO), C_1, 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.224586	-0.001415	-1.272896
2	13	0	-1.191676	0.000328	-0.157299
3	13	0	1.466500	-0.001578	-0.130437
4	8	0	0.310176	-0.000991	1.233077
5	1	0	0.339977	-0.000272	2.188015
6	6	0	-2.148395	-1.701709	0.063712
7	1	0	-2.688629	-1.742486	1.017063
8	1	0	-2.896949	-1.847428	-0.723608
9	1	0	-1.480119	-2.568958	0.029130
10	6	0	3.389813	0.000920	0.038094
11	1	0	3.879488	-0.011596	-0.938261
12	1	0	3.734823	0.889078	0.575848
13	1	0	3.736382	-0.871649	0.599726
14	6	0	-2.145025	1.704326	0.063205
15	1	0	-2.896732	1.848866	-0.721332
16	1	0	-1.476080	2.570831	0.023807
17	1	0	-2.681343	1.747892	1.018660

Methylaluminumoxide Cyclodimer, $(MeAlO)_2$, C_1, Permethylcyclodialuminoxane, 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.211042	-0.003858	-0.003785
2	13	0	-1.211031	0.004641	0.000809
3	8	0	0.004105	1.274135	-0.002245
4	8	0	-0.004114	-1.273275	-0.002139
5	6	0	3.145338	-0.003071	0.004221
6	1	0	3.539419	0.580969	-0.832498
7	1	0	3.529376	0.454561	0.920706
8	1	0	3.550319	-1.015283	-0.064714
9	6	0	-3.145345	0.001387	0.003031
10	1	0	-3.532879	-0.575916	0.847489
11	1	0	-3.534778	-0.464822	-0.906783
12	1	0	-3.551485	1.013532	0.066040

Trimethylalum. Dimethylaluminum Hydroxide Cycloadd., $Me_2Al(Me)(OH)AlMe_2$, C_1, 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000167	-0.009440	-1.319452

2	1	0	0.000115	0.471457	-2.147583
3	13	0	-1.382483	-0.005564	-0.062776
4	13	0	1.382296	-0.005767	-0.062184
5	6	0	-2.449902	-1.644998	-0.114440
6	1	0	-3.019988	-1.787330	0.810946
7	1	0	-3.179173	-1.632591	-0.932504
8	1	0	-1.824830	-2.533968	-0.250937
9	6	0	2.174757	1.785934	0.054982
10	1	0	2.735916	2.050686	-0.849079
11	1	0	1.420982	2.566640	0.206716
12	1	0	2.883827	1.857764	0.888098
13	6	0	-2.173681	1.786684	0.055301
14	1	0	-2.732234	2.054061	-0.849603
15	1	0	-1.419225	2.566078	0.210428
16	1	0	-2.884720	1.857734	0.886800
17	6	0	2.449244	-1.645510	-0.114146
18	1	0	3.165403	-1.640930	-0.943802
19	1	0	1.822553	-2.535988	-0.232098
20	1	0	3.034061	-1.778571	0.803394
21	6	0	-0.000534	-0.317466	1.548679
22	1	0	0.839880	0.147067	2.089158
23	1	0	-0.839027	0.149863	2.089433
24	1	0	-0.001752	-1.377019	1.818477

$Me_2Al–O–AlMe_2$•(Me_2O), Sinn-Monomer, Permethyldialuminoxane, 9, M

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000331	-0.017992	-0.004853
2	13	0	-1.707084	-0.007783	0.001609
3	13	0	1.707785	-0.007378	-0.005527
4	6	0	-2.627082	0.948958	1.439552
5	1	0	-2.481905	2.030974	1.341182
6	1	0	-3.705590	0.765980	1.446181
7	1	0	-2.234685	0.671839	2.423524
8	6	0	-2.688429	-0.940344	-1.411008
9	1	0	-3.227905	-1.802382	-1.001125
10	1	0	-2.042076	-1.308013	-2.212214
11	1	0	-3.447534	-0.291440	-1.861682
12	6	0	2.686697	-1.417585	0.933213
13	1	0	2.040610	-2.223760	1.290362
14	1	0	3.213431	-1.007622	1.803089
15	1	0	3.456022	-1.861614	0.291865
16	6	0	2.628078	1.435461	-0.954597
17	1	0	3.713157	1.406262	-0.819114
18	1	0	2.431448	1.382864	-2.031450
19	1	0	2.277685	2.418995	-0.623836

$Me_2Al–O–AlMe_2$•(Me_2O), Sinn-Monomer, Permethyldialuminoxane, 9, TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-0.001001	-0.005997	-0.007798
2	13	0	-1.708570	-0.003085	-0.004519
3	13	0	1.706481	-0.000678	-0.003570
4	6	0	-2.649704	-1.283355	1.137464
5	1	0	-2.712826	-0.904379	2.164634
6	1	0	-3.675771	-1.465260	0.803600
7	1	0	-2.134614	-2.247286	1.189666
8	6	0	-2.660792	1.273875	-1.140926
9	1	0	-2.872950	0.827209	-2.119934
10	1	0	-2.083403	2.184279	-1.325410
11	1	0	-3.626258	1.564352	-0.714727
12	6	0	2.682648	-1.147570	-1.252571
13	1	0	2.035847	-1.619950	-1.996514
14	1	0	3.203314	-1.947926	-0.713478
15	1	0	3.456592	-0.585734	-1.787043
16	6	0	2.630095	1.165027	1.268266
17	1	0	3.712410	1.006404	1.278152
18	1	0	2.457500	2.219983	1.026224
19	1	0	2.261834	1.017333	2.288971

$Me_2Al–O–AlMe_2$•(Me_2O), Sinn-Monomer, Permethyldialuminoxane, 9, SOSP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	0.000000	-1.708129
2	13	0	0.000000	0.000000	1.708152
3	8	0	0.000000	0.000000	0.000011
4	6	0	1.724194	0.001952	2.634037
5	1	0	2.315868	0.883250	2.362587
6	1	0	1.621164	-0.003894	3.722880
7	1	0	2.323372	-0.871344	2.353516
8	6	0	0.000000	1.724176	-2.634050
9	1	0	0.017487	1.621167	-3.722770
10	1	0	-0.887312	2.311172	-2.372014
11	1	0	0.867029	2.327971	-2.344317
12	6	0	0.000000	-1.724176	-2.634050
13	1	0	-0.017487	-1.621167	-3.722770
14	1	0	0.887312	-2.311172	-2.372014
15	1	0	-0.867029	-2.327971	-2.344317
16	6	0	-1.724194	-0.001952	2.634037
17	1	0	-1.621164	0.003894	3.722880
18	1	0	-2.323372	0.871344	2.353516
19	1	0	-2.315868	-0.883250	2.362587

$Me_2Al–O–AlMe–OH$, Hydroxytrimethyldialuminoxane, 10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.236174	-0.015373	0.000000
2	13	0	-0.092447	1.688008	0.000000

3	13	0	-0.018973	-1.703136	0.000000
4	8	0	-1.367177	-2.761323	0.000000
5	1	0	-2.264319	-2.432994	0.000000
6	6	0	-0.018973	2.608668	1.724156
7	1	0	-0.015230	3.697636	1.622856
8	1	0	-0.871684	2.335452	2.355072
9	1	0	0.881694	2.327753	2.281733
10	6	0	1.743020	-2.521427	0.000000
11	1	0	2.322299	-2.221074	-0.878676
12	1	0	2.322299	-2.221074	0.878676
13	1	0	1.674995	-3.611770	0.000000
14	6	0	-0.018973	2.608668	-1.724156
15	1	0	-0.871684	2.335452	-2.355072
16	1	0	0.881694	2.327753	-2.281733
17	1	0	-0.015230	3.697636	-1.622856

Cartesian Coordinates of Stationary Structures, MP2(full)/6-31G*

Trimethylaluminum (TMA), Me_3Al (de facto C_3), 1

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.000069	-0.000073	-0.000384
2	6	0	0.477963	1.910146	0.000130
3	1	0	0.061628	2.421647	0.875819
4	1	0	1.557134	2.087226	-0.000708
5	1	0	0.060254	2.422707	-0.874292
6	6	0	1.415494	-1.368878	0.000129
7	1	0	2.065785	-1.264791	0.876524
8	1	0	1.029622	-2.392158	-0.001989
9	1	0	2.068863	-1.262365	-0.873686
10	6	0	-1.893368	-0.541207	-0.000060
11	1	0	-2.131621	-1.144882	0.883518
12	1	0	-2.586257	0.304771	-0.014926
13	1	0	-2.125045	-1.171573	-0.866455

Dimethylaluminumhydroxide (DMAH), Me_2AlOH, 2

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.001104	0.045491	0.000199
2	8	0	-0.057981	1.773609	-0.001360
3	6	0	1.711977	-0.913670	0.000871
4	1	0	1.839706	-1.473796	-0.932168
5	1	0	2.584646	-0.263895	0.111441
6	1	0	1.745582	-1.650121	0.810897
7	6	0	-1.739016	-0.849663	-0.000833
8	1	0	-1.819734	-1.583681	-0.809130
9	1	0	-1.906852	-1.395779	0.933661
10	1	0	-2.556311	-0.133166	-0.115242

11	1	0	0.753403	2.300190	0.008607

Methylaluminumoxide, MeAlO (de facto C_{3v}), 3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.188025	0.000304	0.000021
2	8	0	1.818507	-0.000269	-0.000018
3	6	0	-1.760432	-0.000085	-0.000017
4	1	0	-2.143573	1.022611	-0.019614
5	1	0	-2.143091	-0.528934	-0.875881
6	1	0	-2.143119	-0.494965	0.895470

$(TMA)_2$, cyclic, $(1)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.294943	0.000000	0.000118
2	13	0	1.295027	-0.000015	0.000180
3	6	0	-2.220805	-1.730936	0.111032
4	1	0	-2.949036	-1.754694	0.929800
5	1	0	-2.775606	-1.955993	-0.806779
6	1	0	-1.526628	-2.562785	0.274579
7	6	0	2.219951	1.731406	-0.111022
8	1	0	2.951413	1.753881	-0.926926
9	1	0	1.525613	2.562190	-0.279286
10	1	0	2.770804	1.959257	0.808476
11	6	0	-2.219921	1.731370	-0.111287
12	1	0	-2.947842	1.754982	-0.930344
13	1	0	-1.525299	2.562801	-0.275061
14	1	0	-2.774950	1.957200	0.806186
15	6	0	2.220782	-1.731035	0.110485
16	1	0	2.777720	-1.954532	-0.806412
17	1	0	1.526252	-2.563178	0.271015
18	1	0	2.947097	-1.756139	0.930908
19	6	0	-0.000142	-0.233063	-1.687468
20	1	0	0.847119	0.247145	-2.197308
21	1	0	0.001047	-1.286780	-1.978878
22	1	0	-0.848646	0.244932	-2.197247
23	6	0	0.000076	0.232253	1.687998
24	1	0	-0.847474	-0.247808	2.197420
25	1	0	0.848470	-0.246115	2.197637
26	1	0	-0.000775	1.285855	1.979924

$(TMA)_2$, acyclic, $(1)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.345789	-0.002142	0.001062

2	13	0	2.488801	0.004337	-0.002889
3	6	0	-2.550529	1.759364	-0.865344
4	1	0	-3.612427	1.976405	-1.037091
5	1	0	-2.159672	2.582396	-0.258041
6	1	0	-2.062551	1.808878	-1.844422
7	6	0	3.409220	-1.730682	-0.000284
8	1	0	4.046278	-1.837425	0.885292
9	1	0	2.724591	-2.583120	-0.016861
10	1	0	4.075589	-1.826044	-0.865211
11	6	0	-2.506791	-0.136937	1.963933
12	1	0	-2.022363	0.694578	2.486553
13	1	0	-2.092222	-1.067893	2.364644
14	1	0	-3.563327	-0.114879	2.259681
15	6	0	3.472197	1.704283	0.000893
16	1	0	3.210878	2.309834	0.876355
17	1	0	3.214941	2.311515	-0.874596
18	1	0	4.557874	1.574076	0.003353
19	6	0	0.509206	0.040913	-0.005757
20	1	0	0.150805	-0.474846	0.892734
21	1	0	0.138571	1.069703	-0.020582
22	1	0	0.150200	-0.501835	-0.887822
23	6	0	-2.496171	-1.638937	-1.092049
24	1	0	-3.549642	-1.926646	-1.200149
25	1	0	-2.103436	-1.514269	-2.106606
26	1	0	-1.986026	-2.496986	-0.641827

Dimethylaluminum Hydroxide Cyclodimer, $(Me_2AlOH)_2$, C_1, 4

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000142	0.122667	1.232021
2	1	0	-0.000260	0.819414	1.907799
3	13	0	1.434528	0.000049	-0.000074
4	13	0	-1.434790	0.000082	0.000093
5	8	0	-0.000139	-0.123233	-1.231975
6	1	0	-0.000453	-0.821892	-1.905810
7	6	0	2.361468	-1.728616	0.080061
8	1	0	2.927913	-1.940556	-0.834115
9	1	0	3.083034	-1.762028	0.903589
10	1	0	1.667489	-2.562317	0.231655
11	6	0	-2.360814	1.729281	-0.079034
12	1	0	-2.931789	1.938326	0.832982
13	1	0	-1.665762	2.563219	-0.224295
14	1	0	-3.078155	1.765778	-0.906110
15	6	0	2.361269	1.728788	-0.080152
16	1	0	2.930682	1.938816	0.832631
17	1	0	1.667054	2.562968	-0.227928
18	1	0	3.080216	1.763523	-0.905904
19	6	0	-2.361373	-1.728858	0.078849
20	1	0	-3.079888	-1.764875	0.904920
21	1	0	-1.666627	-2.562816	0.225492
22	1	0	-2.931094	-1.938297	-0.833864

Dimethylalum. Hydr. Methylaluminumoxide Cycloadd., (Me_2AlOH)(MeAlO), C_1, 5

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.226412	0.001463	-1.275010
2	13	0	-1.197479	0.000450	-0.148897
3	13	0	1.467081	-0.000779	-0.117756
4	8	0	0.303303	-0.001964	1.248458
5	1	0	0.332486	-0.004257	2.215235
6	6	0	-2.146884	-1.712871	0.051402
7	1	0	-2.747674	-1.747676	0.967398
8	1	0	-2.837333	-1.888271	-0.781102
9	1	0	-1.463258	-2.568239	0.078093
10	6	0	3.400780	0.000860	0.023317
11	1	0	3.861037	-0.042217	-0.966728
12	1	0	3.763118	0.904591	0.521837
13	1	0	3.761372	-0.856213	0.599222
14	6	0	-2.147379	1.713096	0.054102
15	1	0	-2.819187	1.899485	-0.791255
16	1	0	-1.464069	2.567514	0.106273
17	1	0	-2.768133	1.737049	0.956996

Methylaluminumoxide Cyclodimer, $(MeAlO)_2$, C_1, Permethylcyclodialuminoxane, 6

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.211042	-0.003858	-0.003785
2	13	0	-1.211031	0.004641	0.000809
3	8	0	0.004105	1.274135	-0.002245
4	8	0	-0.004114	-1.273275	-0.002139
5	6	0	3.145338	-0.003071	0.004221
6	1	0	3.539419	0.580969	-0.832498
7	1	0	3.529376	0.454561	0.920706
8	1	0	3.550319	-1.015283	-0.064714
9	6	0	-3.145345	0.001387	0.003031
10	1	0	-3.532879	-0.575916	0.847489
11	1	0	-3.534778	-0.464822	-0.906783
12	1	0	-3.551485	1.013532	0.066040

Trimethylalum. Dimethylaluminum Hydroxide Cycloadd., $Me_2Al(Me)(OH)AlMe_2$, C_1, 7

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000004	0.020168	-1.351135
2	1	0	-0.000028	0.720335	-2.025022
3	13	0	-1.368855	-0.008860	-0.057140
4	13	0	1.368840	-0.008939	-0.057116
5	6	0	-2.420255	-1.662110	-0.130535
6	1	0	-3.000858	-1.823614	0.784660

7	1	0	-3.136894	-1.650958	-0.959111
8	1	0	-1.783553	-2.542265	-0.268221
9	6	0	2.169330	1.784843	0.064003
10	1	0	2.702204	2.064431	-0.852342
11	1	0	1.426758	2.568133	0.253095
12	1	0	2.905169	1.843306	0.874227
13	6	0	-2.168835	1.785148	0.064230
14	1	0	-2.700316	2.065760	-0.852612
15	1	0	-1.426098	2.567899	0.254920
16	1	0	-2.905733	1.843375	0.873504
17	6	0	2.419935	-1.662399	-0.130283
18	1	0	3.134435	-1.652864	-0.960720
19	1	0	1.782847	-2.542787	-0.264632
20	1	0	3.002906	-1.822174	0.783717
21	6	0	-0.000126	-0.322554	1.567187
22	1	0	0.841048	0.139294	2.106827
23	1	0	-0.842426	0.138046	2.106139
24	1	0	0.000471	-1.383423	1.832365

$Me_2Al–O–AlMe_2$, C_2, Sinn-Monomer, Permethyldialuminoxane, 9, TS

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.000939	-0.005975	-0.007711
2	13	0	-1.708509	-0.003133	-0.004520
3	13	0	1.706542	-0.000710	-0.003541
4	6	0	-2.650009	-1.280735	1.140139
5	1	0	-2.715753	-0.898150	2.165812
6	1	0	-3.675191	-1.465084	0.804869
7	1	0	-2.133830	-2.243821	1.196816
8	6	0	-2.660788	1.271338	-1.143683
9	1	0	-2.875126	0.821814	-2.120902
10	1	0	-2.082530	2.180402	-1.331969
11	1	0	-3.625221	1.564411	-0.716911
12	6	0	2.682700	-1.150344	-1.250027
13	1	0	2.035824	-1.624985	-1.992453
14	1	0	3.204023	-1.949009	-0.709083
15	1	0	3.456129	-0.589523	-1.786291
16	6	0	2.630210	1.167755	1.265682
17	1	0	3.712453	1.008742	1.276340
18	1	0	2.458108	2.222168	1.020974
19	1	0	2.261538	1.022705	2.286610

$Me_2Al–O–AlMe_2$, C_2, Sinn-Monomer, Permethyldialuminoxane, 9, SOSP

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.000000	0.000000	-1.717991
2	13	0	0.000000	0.000000	1.718016
3	8	0	0.000000	0.000000	0.000012
4	6	0	1.732368	0.000632	2.637615
5	1	0	2.323346	0.881245	2.364300

6	1	0	1.632452	-0.005192	3.726733
7	1	0	2.329284	-0.873011	2.355135
8	6	0	0.000000	1.732349	-2.637629
9	1	0	0.017668	1.632455	-3.726622
10	1	0	-0.887045	2.318083	-2.373806
11	1	0	0.866951	2.334460	-2.345861
12	6	0	0.000000	-1.732349	-2.637629
13	1	0	-0.017668	-1.632455	-3.726622
14	1	0	0.887045	-2.318083	-2.373806
15	1	0	-0.866951	-2.334460	-2.345861
16	6	0	-1.732368	-0.000632	2.637615
17	1	0	-1.632452	0.005192	3.726733
18	1	0	-2.329284	0.873011	2.355135
19	1	0	-2.323346	-0.881245	2.364300

$Me_2Al–O–AlMe–OH$, Hydroxytrimethyldialuminoxane, 10

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-0.232905	-0.012621	0.000000
2	13	0	-0.090276	1.701235	0.000000
3	13	0	-0.016028	-1.709052	0.000000
4	8	0	-1.382319	-2.758696	0.000000
5	1	0	-2.281050	-2.400637	0.000000
6	6	0	-0.016028	2.612238	1.733756
7	1	0	-0.011764	3.701703	1.638170
8	1	0	-0.867923	2.336111	2.363679
9	1	0	0.884767	2.327495	2.288254
10	6	0	1.743156	-2.544383	0.000000
11	1	0	2.325266	-2.252403	-0.879080
12	1	0	2.325266	-2.252403	0.879080
13	1	0	1.657495	-3.633569	0.000000
14	6	0	-0.016028	2.612238	-1.733756
15	1	0	-0.867923	2.336111	-2.363679
16	1	0	0.884767	2.327495	-2.288254
17	1	0	-0.011764	3.701703	-1.638170

<u>Cartesian Coordinates of Stationary, Donor-Coord. Structures, MP2(full)/6-31G*</u>

$Me_3Al•(Me_2O)$, Trimethylaluminum Monoetherate, 1•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.852346	0.000088	0.075739
2	6	0	1.430160	-1.687060	-0.794751
3	1	0	2.525479	-1.726480	-0.840914
4	1	0	1.117722	-2.597878	-0.271090
5	1	0	1.080930	-1.769179	-1.830967
6	6	0	1.429356	1.688955	-0.791932
7	1	0	2.524551	1.727513	-0.841236
8	1	0	1.077147	1.774014	-1.826916
9	1	0	1.119142	2.598710	-0.265103
10	8	0	-1.131066	0.000067	-0.435884

11	6	0	-1.878244	1.191653	-0.126402
12	1	0	-2.091417	1.234641	0.945155
13	1	0	-1.257937	2.032767	-0.424574
14	1	0	-2.808747	1.183801	-0.699142
15	6	0	-1.878020	-1.191792	-0.127015
16	1	0	-2.808806	-1.183539	-0.699289
17	1	0	-1.257807	-2.032621	-0.426203
18	1	0	-2.090635	-1.235690	0.944615
19	6	0	0.695122	-0.001925	2.057965
20	1	0	0.175943	0.878066	2.456619
21	1	0	0.181804	-0.885920	2.455262
22	1	0	1.690405	0.001126	2.519062

$Me_2AlOH•(Me_2O)$, Dimethylaluminum Hydroxide Monoetherate, 2•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.811426	0.000089	0.138203
2	8	0	0.250752	-0.000143	1.816451
3	6	0	1.542332	-1.685840	-0.586509
4	1	0	2.634204	-1.702318	-0.485226
5	1	0	1.172487	-2.586684	-0.085316
6	1	0	1.335493	-1.797256	-1.657689
7	1	0	0.895727	-0.001226	2.537154
8	6	0	1.542057	1.686169	-0.586337
9	1	0	2.633991	1.702659	-0.485905
10	1	0	1.334328	1.797985	-1.657312
11	1	0	1.172485	2.586812	-0.084573
12	8	0	-1.074170	0.000026	-0.540496
13	6	0	-1.813992	1.193145	-0.193437
14	1	0	-1.964180	1.228334	0.886847
15	1	0	-1.209162	2.034284	-0.522177
16	1	0	-2.767113	1.177509	-0.726517
17	6	0	-1.813733	-1.193370	-0.193787
18	1	0	-2.766594	-1.178052	-0.727338
19	1	0	-1.208440	-2.034283	-0.522226
20	1	0	-1.964409	-1.228608	0.886423

MeAlO•(Me_2O), Methylaluminumoxide Etherate, 3•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.999151	0.322144	0.000054
2	8	0	1.049853	1.960829	0.000167
3	6	0	1.888884	-1.423604	-0.000115
4	1	0	1.643494	-2.018868	-0.884962
5	1	0	2.971759	-1.275216	0.000434
6	1	0	1.642708	-2.019489	0.884098
7	8	0	-0.918409	-0.162826	-0.000373
8	6	0	-1.851724	0.950053	-0.000105
9	1	0	-2.469085	0.888586	0.898683
10	1	0	-1.216776	1.835832	-0.000133

11	1	0	-2.469375	0.888734	-0.898704
12	6	0	-1.547364	-1.453339	0.000272
13	1	0	-2.165371	-1.557181	-0.894828
14	1	0	-0.753107	-2.195718	-0.000577
15	1	0	-2.163541	-1.557241	0.896631

MeAlO•$(Me_2O)_2$, Methylaluminumoxide Dietherate, 3•$(OMe_2)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.113055	0.478618	0.699770
2	8	0	0.205475	-0.520240	2.009607
3	6	0	0.130807	2.381032	0.189078
4	1	0	-0.832378	2.846694	0.426087
5	1	0	0.882821	2.927280	0.767606
6	1	0	0.332701	2.574994	-0.870475
7	8	0	-1.454723	-0.234812	-0.345868
8	6	0	-2.273211	-1.164719	0.409237
9	1	0	-2.589598	-1.970809	-0.257707
10	1	0	-1.619565	-1.497885	1.217048
11	1	0	-3.142378	-0.636065	0.809212
12	6	0	-2.185457	0.502822	-1.334608
13	1	0	-2.938991	1.132903	-0.853801
14	1	0	-1.464644	1.120144	-1.865758
15	1	0	-2.665760	-0.196495	-2.023623
16	8	0	1.376987	-0.298201	-0.701207
17	6	0	1.358836	-1.748104	-0.615678
18	1	0	1.506738	-2.044736	0.423207
19	1	0	0.371445	-2.050716	-0.955432
20	1	0	2.127918	-2.142444	-1.283776
21	6	0	2.712198	0.212962	-0.484174
22	1	0	3.362022	-0.147613	-1.284688
23	1	0	2.637016	1.297871	-0.519412
24	1	0	3.081977	-0.113087	0.491115

$(TMA)_2$•(OMe_2), cyclic, $(1)_2$•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.012711	-0.100662	0.882883
2	13	0	-2.200628	0.085524	-0.484867
3	6	0	0.750773	-1.790243	1.538693
4	1	0	1.841518	-1.790051	1.456439
5	1	0	0.507857	-1.953563	2.594889
6	1	0	0.376351	-2.661790	0.990221
7	6	0	-2.665856	1.976082	-0.788150
8	1	0	-3.655640	2.221825	-0.385673
9	1	0	-1.953013	2.665323	-0.322465
10	1	0	-2.696895	2.222377	-1.856101
11	6	0	0.614891	1.706928	1.365891
12	1	0	-0.102980	2.256815	1.983989
13	1	0	0.799773	2.322985	0.478997

14	1	0	1.554934	1.661145	1.926899
15	6	0	-3.288786	-1.395276	-1.188930
16	1	0	-4.322264	-1.348578	-0.827319
17	1	0	-2.891670	-2.374666	-0.900795
18	1	0	-3.338867	-1.378043	-2.283589
19	6	0	-2.061344	-0.283152	1.599501
20	1	0	-3.026559	0.243980	1.618111
21	1	0	-2.269432	-1.340331	1.788571
22	1	0	-1.578269	0.117469	2.500363
23	6	0	-0.233324	-0.279388	-1.227701
24	1	0	0.835448	-0.036554	-1.125096
25	1	0	-0.277676	-1.313985	-1.582163
26	1	0	-0.529034	0.376217	-2.057760
27	8	0	2.936842	0.035833	-0.428801
28	6	0	3.804346	1.159730	-0.460490
29	1	0	3.261740	1.987532	-0.007207
30	1	0	4.720530	0.964523	0.111447
31	1	0	4.078707	1.417629	-1.491834
32	6	0	3.552453	-1.111530	-0.995038
33	1	0	3.824899	-0.936863	-2.044164
34	1	0	4.454481	-1.390737	-0.435632
35	1	0	2.825821	-1.921433	-0.936581

(TMA)$_2$•(OMe$_2$), acyclic, one AlO contact, (1)$_2$•(OMe$_2$)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-2.879314	0.102183	-0.060118
2	13	0	1.585214	-0.896606	0.163641
3	6	0	-2.496119	2.044420	0.084090
4	1	0	-3.427147	2.623515	0.041984
5	1	0	-2.012127	2.318052	1.029272
6	1	0	-1.868957	2.419447	-0.733383
7	6	0	2.374055	-1.980164	-1.289127
8	1	0	1.948721	-2.990910	-1.274472
9	1	0	2.157193	-1.573093	-2.283588
10	1	0	3.459938	-2.108265	-1.217126
11	6	0	-3.558360	-0.831087	1.544033
12	1	0	-3.065443	-0.507648	2.467376
13	1	0	-3.443983	-1.918439	1.477285
14	1	0	-4.630139	-0.638854	1.678548
15	6	0	2.365064	-0.977567	1.981966
16	1	0	2.127363	-1.936537	2.457680
17	1	0	1.981998	-0.201844	2.655528
18	1	0	3.458572	-0.898711	1.988523
19	6	0	-0.404991	-0.677083	0.078686
20	1	0	-0.868337	-1.668342	0.065007
21	1	0	-0.729238	-0.123151	0.964755
22	1	0	-0.627117	-0.146535	-0.853231
23	6	0	-3.314632	-0.625408	-1.845547
24	1	0	-4.365589	-0.433388	-2.095333
25	1	0	-2.716991	-0.178404	-2.647569
26	1	0	-3.175479	-1.710496	-1.901557
27	8	0	2.114501	0.975014	-0.416225

28	6	0	3.522349	1.186029	-0.653358
29	1	0	4.052845	1.279643	0.297875
30	1	0	3.878240	0.320208	-1.205820
31	1	0	3.645159	2.092694	-1.249542
32	6	0	1.517449	2.096101	0.271518
33	1	0	1.705081	3.001203	-0.310030
34	1	0	0.449178	1.904760	0.324986
35	1	0	1.944670	2.191034	1.273266

$(TMA)_2$•(OMe_2), acyclic, two AlO contacts, $(1)_2$•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.911621	0.362246	0.005703
2	13	0	1.911712	0.361802	-0.006001
3	6	0	-1.520603	1.760574	1.341726
4	1	0	-1.307687	1.375330	2.344735
5	1	0	-0.701168	2.429172	1.063617
6	1	0	-2.414155	2.391179	1.443710
7	6	0	2.037943	0.835099	1.908794
8	1	0	2.855588	1.558095	2.027731
9	1	0	1.146053	1.316309	2.318745
10	1	0	2.289642	-0.013235	2.554767
11	6	0	-3.110313	-1.106409	0.599773
12	1	0	-2.999698	-1.384965	1.653195
13	1	0	-3.066989	-2.029160	0.008875
14	1	0	-4.141010	-0.742473	0.493001
15	6	0	3.109455	-1.107450	-0.600453
16	1	0	4.140316	-0.743524	-0.495209
17	1	0	2.997547	-1.386487	-1.653613
18	1	0	3.066754	-2.029867	-0.009014
19	6	0	1.521173	1.761158	-1.341146
20	1	0	2.413826	2.393554	-1.439927
21	1	0	1.311193	1.377249	-2.345274
22	1	0	0.699996	2.427881	-1.063713
23	6	0	-2.037088	0.835476	-1.909156
24	1	0	-2.850593	1.563150	-2.027847
25	1	0	-1.142835	1.311384	-2.320187
26	1	0	-2.294074	-0.011875	-2.554335
27	8	0	-0.000073	-0.798793	0.000145
28	6	0	0.023019	-1.644027	1.200945
29	1	0	0.986260	-2.152684	1.242619
30	1	0	-0.098360	-0.974155	2.047269
31	1	0	-0.800380	-2.353683	1.142289
32	6	0	-0.023721	-1.644581	-1.200280
33	1	0	-0.987244	-2.152720	-1.241612
34	1	0	0.097931	-0.975167	-2.046939
35	1	0	0.799313	-2.354636	-1.141402

$Me_2Al(OH)(O)AlMe$•(Me_2O), DMAH Methyaluminumoxide Cycloadduct Etherate, 5•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.661659	0.850142	-0.262857
2	13	0	1.771594	-0.175471	-0.082180
3	8	0	0.348173	0.414821	1.228520
4	8	0	0.524508	0.196212	-1.326323
5	6	0	-1.704703	2.500627	-0.232493
6	1	0	-2.297132	2.634293	0.678707
7	1	0	-1.043331	3.369383	-0.312920
8	1	0	-2.396760	2.551753	-1.079005
9	6	0	2.145984	-2.092583	0.229922
10	1	0	2.578438	-2.565890	-0.659371
11	1	0	1.252561	-2.671201	0.490358
12	1	0	2.865718	-2.238639	1.043338
13	8	0	-1.992805	-0.591067	-0.169961
14	6	0	-2.737055	-0.751783	1.055977
15	1	0	-3.626802	-1.349056	0.849481
16	1	0	-2.107441	-1.234699	1.806073
17	1	0	-3.025275	0.245599	1.382095
18	6	0	-1.646120	-1.862574	-0.783494
19	1	0	-2.572393	-2.350276	-1.092413
20	1	0	-1.004078	-1.621323	-1.625566
21	1	0	-1.101977	-2.474177	-0.061790
22	6	0	3.236894	1.127883	0.170514
23	1	0	4.028422	0.991626	-0.575250
24	1	0	3.718542	1.029802	1.151025
25	1	0	2.899534	2.166569	0.075676
26	1	0	0.593811	1.056369	1.914592

$(MeAlO)_2$•$(Me_2O)_2$, Permethylcyclodialuminoxane Dietherate, trans 6•$(OMe_2)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-0.910293	0.820803	-0.099332
2	13	0	0.910155	-0.820614	-0.099455
3	8	0	-0.000072	-0.000020	1.195021
4	8	0	-0.000022	0.000237	-1.394614
5	6	0	-1.498861	2.692008	-0.064769
6	1	0	-2.029025	2.953987	0.857112
7	1	0	-0.641658	3.370439	-0.135041
8	1	0	-2.162034	2.929754	-0.902751
9	6	0	1.498557	-2.691886	-0.065045
10	1	0	2.162862	-2.929403	-0.902192
11	1	0	0.641336	-3.370144	-0.136842
12	1	0	2.027330	-2.954360	0.857494
13	8	0	2.645143	0.172118	-0.121091
14	8	0	-2.645144	-0.172159	-0.120994
15	6	0	2.632869	1.435803	-0.826452
16	1	0	2.042965	1.270610	-1.723454
17	1	0	2.160422	2.199939	-0.203299
18	1	0	3.664793	1.711756	-1.054174
19	6	0	3.257442	0.281629	1.182476

20	1	0	2.642418	0.916496	1.823049
21	1	0	3.305929	-0.727343	1.587760
22	1	0	4.264305	0.687462	1.064139
23	6	0	-3.256952	-0.282376	1.182759
24	1	0	-4.263600	-0.688803	1.064644
25	1	0	-2.641282	-0.916989	1.822953
26	1	0	-3.305950	0.726474	1.588300
27	6	0	-2.632786	-1.435572	-0.826884
28	1	0	-3.664703	-1.711534	-1.054612
29	1	0	-2.042968	-1.269932	-1.723867
30	1	0	-2.160200	-2.199911	-0.204086

$(MeAlO)_2$•$(Me_2O)_2$, Permethylcyclodialuminoxane Dietherate, cis 6•$(OMe_2)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	1.404955	-0.837511	-0.049798
2	13	0	-1.032086	-0.970655	-0.006710
3	8	0	0.193693	-0.737708	1.261314
4	8	0	0.157187	-0.940363	-1.323670
5	6	0	3.121342	-1.775019	0.064622
6	1	0	3.694825	-1.500227	0.956500
7	1	0	2.960520	-2.856709	0.115571
8	1	0	3.757023	-1.584792	-0.806029
9	6	0	-2.661130	-2.065070	0.063818
10	1	0	-3.323918	-1.807396	0.897695
11	1	0	-2.389534	-3.117678	0.193352
12	1	0	-3.252834	-2.005747	-0.856065
13	8	0	-1.829930	0.889694	0.035350
14	8	0	2.019787	1.058477	-0.294142
15	6	0	-2.858524	1.203389	-0.919742
16	1	0	-2.509407	0.824416	-1.879159
17	1	0	-3.798311	0.721556	-0.638190
18	1	0	-2.984896	2.288025	-0.963713
19	6	0	-2.121027	1.361210	1.368703
20	1	0	-3.069103	0.940217	1.715624
21	1	0	-1.293111	1.006073	1.979646
22	1	0	-2.176504	2.452681	1.353123
23	6	0	2.378770	1.745958	0.918476
24	1	0	2.927904	2.654697	0.661650
25	1	0	1.479145	1.978697	1.492350
26	1	0	3.016807	1.069340	1.483792
27	6	0	1.243510	1.879750	-1.193535
28	1	0	1.872019	2.704583	-1.537622
29	1	0	0.940737	1.222889	-2.004122
30	1	0	0.357796	2.253428	-0.674682

Trimethylaluminum Dimethylaluminum Hydroxide Cycloadduct Etherate, $Me_2Al(Me)(OH)AlMe_2$•(OMe_2), 7•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	-0.416767	-0.516246	-0.768668
2	1	0	-0.586537	-0.781929	-1.688487
3	13	0	1.231906	-0.940140	-0.113337
4	13	0	-2.097924	0.116461	0.026078
5	6	0	1.206355	-1.562676	1.741708
6	1	0	0.767997	-2.566317	1.778897
7	1	0	2.204818	-1.644380	2.186034
8	1	0	0.597132	-0.937723	2.401820
9	6	0	-2.866744	-1.484866	0.915281
10	1	0	-3.051786	-2.309924	0.216695
11	1	0	-2.215726	-1.877688	1.705531
12	1	0	-3.830148	-1.260624	1.389585
13	6	0	2.302918	-1.765666	-1.540818
14	1	0	3.362113	-1.813785	-1.265827
15	1	0	2.250099	-1.246361	-2.504461
16	1	0	1.983621	-2.797938	-1.724513
17	6	0	-3.008997	0.741349	-1.634747
18	1	0	-3.134731	-0.050029	-2.385479
19	1	0	-2.483091	1.568490	-2.128310
20	1	0	-4.019428	1.108119	-1.417573
21	6	0	-1.492441	1.555055	1.273728
22	1	0	-2.355033	1.959706	1.818058
23	1	0	-0.799828	1.194310	2.044196
24	1	0	-1.024400	2.414232	0.776206
25	8	0	1.955432	0.901107	-0.003382
26	6	0	2.178205	1.595043	1.248031
27	1	0	2.419094	0.836783	1.987499
28	1	0	3.019390	2.277884	1.113494
29	1	0	1.274850	2.134740	1.533043
30	6	0	1.650221	1.814037	-1.083760
31	1	0	2.456700	2.546377	-1.154159
32	1	0	1.604440	1.222193	-1.994508
33	1	0	0.692282	2.299150	-0.893521

$Me_2Al–O–AlMe_2$•(OMe_2), Sinn-Monomer Monoetherate, 9•(OMe_2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	0.787461	-0.699123	0.137744
2	13	0	-2.384730	0.207629	-0.005422
3	8	0	-0.678576	0.262962	0.128815
4	6	0	-3.305266	-1.530793	-0.004407
5	1	0	-3.193707	-2.033721	0.962860
6	1	0	-4.377541	-1.442860	-0.203859
7	1	0	-2.881832	-2.206975	-0.754782
8	6	0	1.516429	-1.135061	1.924424
9	1	0	2.535289	-1.539110	1.888127
10	1	0	1.535131	-0.268267	2.595465
11	1	0	0.904154	-1.895697	2.422642
12	6	0	1.030943	-1.969268	-1.355697
13	1	0	1.975942	-2.523730	-1.321956
14	1	0	0.235817	-2.724404	-1.351149
15	1	0	0.979412	-1.469854	-2.329911
16	6	0	-3.380001	1.895525	-0.157302

17	1	0	-4.246732	1.915915	0.512076
18	1	0	-2.762647	2.769725	0.066584
19	1	0	-3.771876	2.024690	-1.173023
20	8	0	2.027272	0.794149	-0.426492
21	6	0	1.802662	2.086331	0.174411
22	1	0	2.257530	2.850987	-0.459544
23	1	0	0.723561	2.201774	0.222728
24	1	0	2.241180	2.111242	1.176040
25	6	0	3.425100	0.481149	-0.551168
26	1	0	3.891209	0.433184	0.436696
27	1	0	3.484001	-0.485454	-1.046804
28	1	0	3.906830	1.247784	-1.162528

$Me_2Al–O–AlMe_2$•$(Me_2O)_2$, Sinn-Monomer Dietherate, 9•$(OMe_2)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	-1.544263	-0.759920	0.249852
2	13	0	1.491736	0.525222	0.539008
3	8	0	0.015793	-0.098277	-0.136660
4	6	0	2.215031	-0.381602	2.146269
5	1	0	2.275432	-1.470291	2.024935
6	1	0	3.213264	-0.032981	2.437109
7	1	0	1.563569	-0.209175	3.011005
8	6	0	-2.251863	-2.061365	-1.070337
9	1	0	-3.308659	-2.308690	-0.912466
10	1	0	-2.154451	-1.707955	-2.104170
11	1	0	-1.706972	-3.011644	-1.017689
12	6	0	-2.034373	-0.977527	2.154174
13	1	0	-3.033064	-1.399888	2.316872
14	1	0	-1.330097	-1.653659	2.653344
15	1	0	-1.988984	-0.028136	2.700466
16	6	0	1.810666	2.467315	0.317554
17	1	0	2.790620	2.804607	0.675322
18	1	0	1.722791	2.780500	-0.729344
19	1	0	1.067212	3.044690	0.880565
20	8	0	2.735179	-0.211536	-0.892173
21	8	0	-2.649766	0.879050	-0.224492
22	6	0	-2.220447	1.653853	-1.361680
23	1	0	-2.629186	2.663452	-1.273362
24	1	0	-1.135043	1.659072	-1.318376
25	1	0	-2.568972	1.181889	-2.285158
26	6	0	-4.078945	0.761105	-0.145639
27	1	0	-4.464245	0.234697	-1.023274
28	1	0	-4.294468	0.197267	0.759543
29	1	0	-4.516143	1.760457	-0.079445
30	6	0	2.406239	-1.503830	-1.440933
31	1	0	2.721146	-2.291697	-0.750219
32	1	0	1.326242	-1.505736	-1.556205
33	1	0	2.914651	-1.616006	-2.401799
34	6	0	4.145294	-0.054745	-0.666031
35	1	0	4.674509	-0.182896	-1.613529
36	1	0	4.289886	0.956235	-0.290659
37	1	0	4.494548	-0.786162	0.067705

$Me_2Al–O–AlMe–OH•(OMe_2)$, Hydroxytrimethyldialuminoxane Etherate, $10•(OMe_2)$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.688747	0.270029	0.222352
2	13	0	2.386412	0.214507	0.009099
3	13	0	-0.791872	-0.647868	0.198671
4	8	0	-1.677225	-0.773188	1.713164
5	1	0	-1.367929	-1.371909	2.406668
6	6	0	3.322420	-1.513648	0.088019
7	1	0	4.365629	-1.441616	-0.234116
8	1	0	3.326247	-1.910220	1.109844
9	1	0	2.831533	-2.267653	-0.535997
10	6	0	-0.911250	-2.116700	-1.103212
11	1	0	-0.780464	-1.759178	-2.130791
12	1	0	-0.119034	-2.853772	-0.927866
13	1	0	-1.858092	-2.665205	-1.064124
14	6	0	3.350001	1.897359	-0.304634
15	1	0	2.806958	2.764205	0.082183
16	1	0	3.495785	2.063695	-1.378548
17	1	0	4.346668	1.892560	0.148271
18	8	0	-2.012319	0.742023	-0.502364
19	6	0	-3.390673	0.329774	-0.626054
20	1	0	-3.380623	-0.610341	-1.172954
21	1	0	-3.822091	0.189438	0.366354
22	1	0	-3.931990	1.091864	-1.190688
23	6	0	-1.886693	2.015949	0.174307
24	1	0	-2.323399	1.940628	1.171964
25	1	0	-0.819347	2.208614	0.236339
26	1	0	-2.395317	2.775275	-0.423337

$Me_2Al–O–AlMe–OH•(OMe_2)_2$, Hydroxytrimethyldialuminoxane Dietherate, $10•(OMe_2)_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.031799	-0.016934	-0.320077
2	13	0	1.490421	0.435649	0.518498
3	13	0	-1.572826	0.594307	-0.542205
4	8	0	-2.264577	0.619266	-2.153745
5	1	0	-1.765307	0.169353	-2.850004
6	6	0	2.086743	2.318136	0.460563
7	1	0	3.031468	2.504892	0.984702
8	1	0	2.205349	2.678122	-0.567700
9	1	0	1.341632	2.969154	0.933010
10	6	0	-2.252591	2.030913	0.618420
11	1	0	-2.152387	1.816041	1.688960
12	1	0	-1.704554	2.962066	0.437510
13	1	0	-3.308748	2.251438	0.427712
14	6	0	1.874180	-0.636332	2.146303
15	1	0	1.760567	-1.715154	1.980182
16	1	0	1.187646	-0.376045	2.961250

17	1	0	2.885150	-0.478459	2.541196
18	8	0	-2.580742	-1.003324	0.160645
19	8	0	2.783924	-0.417418	-0.786824
20	6	0	4.184308	-0.366687	-0.470011
21	1	0	4.427405	-1.115057	0.289338
22	1	0	4.761769	-0.546573	-1.380027
23	1	0	4.381160	0.634606	-0.092989
24	6	0	2.388942	-1.682884	-1.352458
25	1	0	2.618089	-2.490795	-0.651235
26	1	0	1.317249	-1.604872	-1.513665
27	1	0	2.927395	-1.831475	-2.291675
28	6	0	-4.012922	-0.939152	0.018696
29	1	0	-4.421793	-1.948306	0.110219
30	1	0	-4.436575	-0.285436	0.786082
31	1	0	-4.193032	-0.535281	-0.974670
32	6	0	-2.165514	-1.539696	1.429601
33	1	0	-2.526424	-0.903108	2.242813
34	1	0	-2.567834	-2.550368	1.534217
35	1	0	-1.079067	-1.552684	1.406292

Cartesian Coordinates of Stationary Structures of Trioxanes, MP2(full)/6-31G*

Structure 11: Addition of 9 to DMAH

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.001432	-2.228248	0.154295
2	1	0	0.002132	-3.003822	-0.429421
3	13	0	-1.411157	-0.967772	0.044625
4	13	0	1.412465	-0.966005	0.045458
5	8	0	-0.000140	0.273011	0.015565
6	6	0	-2.414683	-0.844562	1.727942
7	1	0	-3.050875	0.047110	1.768481
8	1	0	-3.077375	-1.705003	1.873367
9	1	0	-1.746799	-0.805942	2.595267
10	6	0	2.297632	-1.109839	-1.707585
11	1	0	2.906825	-2.017198	-1.794249
12	1	0	1.580598	-1.124144	-2.536249
13	1	0	2.977602	-0.269446	-1.889439
14	6	0	-2.295147	-1.112907	-1.708914
15	1	0	-2.905446	-2.019588	-1.794786
16	1	0	-1.577566	-1.129175	-2.537070
17	1	0	-2.973918	-0.271887	-1.892397
18	6	0	2.414747	-0.841428	1.729430
19	1	0	3.080275	-1.699768	1.874292
20	1	0	1.746274	-0.805962	2.596435
21	1	0	3.047930	0.052328	1.771284
22	13	0	-0.001326	2.025245	-0.052833
23	6	0	-1.762244	2.869725	-0.090925
24	1	0	-2.315251	2.669396	0.833170
25	1	0	-1.705041	3.955060	-0.212608
26	1	0	-2.372934	2.474998	-0.910076
27	6	0	1.758421	2.872039	-0.093279
28	1	0	2.364632	2.485217	-0.919531
29	1	0	1.699344	3.958315	-0.205268

30	1	0	2.317141	2.664150	0.825663

Structure 12a: Methane Elimination from 11, Minimum

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.066220	1.581963	0.856541
2	13	0	-0.566016	1.360560	0.154358
3	13	0	1.754089	0.359366	-0.153598
4	8	0	0.180868	-0.013612	-0.962099
5	6	0	-1.625621	2.822247	-0.581094
6	1	0	-2.495232	2.461700	-1.139283
7	1	0	-1.995849	3.491905	0.202328
8	1	0	-1.026074	3.432251	-1.264053
9	6	0	3.514376	-0.360923	-0.518137
10	1	0	3.464665	-1.194177	-1.223239
11	1	0	4.173163	0.402428	-0.942200
12	1	0	3.982524	-0.720944	0.402247
13	6	0	-1.814735	0.109222	1.272298
14	1	0	-1.620334	0.815303	2.096667
15	1	0	-1.805570	-0.840864	1.825785
16	1	0	-2.846605	0.275635	0.948929
17	13	0	-0.778185	-1.313087	-0.082990
18	6	0	-2.236758	-2.168750	-1.068048
19	1	0	-2.923466	-2.711588	-0.409374
20	1	0	-2.831377	-1.437718	-1.625560
21	1	0	-1.855628	-2.893463	-1.795616
22	6	0	0.518330	-2.294935	1.052162
23	1	0	1.056527	-1.668626	1.777714
24	1	0	0.010609	-3.059394	1.652910
25	1	0	1.273847	-2.829328	0.463121

Structure 12b: Methane Elimination from 11, Transition State Structure for Methyl Rotation of AlMe group

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.168417	1.528104	0.864192
2	13	0	-0.477377	1.381332	0.171033
3	13	0	1.794895	0.277562	-0.150136
4	8	0	0.201011	-0.038440	-0.937254
5	6	0	-1.449541	2.893418	-0.584298
6	1	0	-2.333595	2.575620	-1.145887
7	1	0	-1.788929	3.588304	0.191159
8	1	0	-0.813489	3.465089	-1.267373
9	6	0	3.511711	-0.537182	-0.523891
10	1	0	4.326987	0.040135	-0.080944
11	1	0	3.556017	-1.550401	-0.114304
12	1	0	3.689079	-0.610633	-1.600342
13	6	0	-1.791678	0.212024	1.291287
14	1	0	-1.546448	0.888724	2.126758
15	1	0	-1.841146	-0.746774	1.826923

16	1	0	-2.812223	0.451257	0.977989
17	13	0	-0.863153	-1.274622	-0.090393
18	6	0	-2.387436	-1.961835	-1.108169
19	1	0	-3.127880	-2.455067	-0.468938
20	1	0	-2.905933	-1.163731	-1.649493
21	1	0	-2.069586	-2.699799	-1.852686
22	6	0	0.310582	-2.398235	1.040979
23	1	0	0.901587	-1.833904	1.775581
24	1	0	-0.274496	-3.117944	1.626002
25	1	0	1.016054	-2.992864	0.448052

Structure 13: Acyclic 12

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	13	0	2.944616	-0.526467	0.000227
2	13	0	-2.930513	-0.546967	0.000268
3	13	0	0.001830	1.227740	-0.000227
4	8	0	1.491141	0.388806	0.000307
5	8	0	-1.462586	0.344462	0.000502
6	6	0	-0.051123	3.179366	-0.001630
7	1	0	0.948052	3.621269	-0.001457
8	1	0	-0.584844	3.554307	-0.880406
9	1	0	-0.585734	3.555566	0.876062
10	6	0	3.723146	-1.012985	-1.732397
11	1	0	4.645766	-1.591911	-1.633485
12	1	0	3.021237	-1.606967	-2.327265
13	1	0	3.953594	-0.121206	-2.324859
14	6	0	3.724591	-1.010960	1.732763
15	1	0	4.647370	-1.589618	1.633764
16	1	0	3.955087	-0.118513	2.324197
17	1	0	3.023340	-1.604649	2.328700
18	6	0	-3.718669	-1.019311	1.732530
19	1	0	-3.959932	-0.122048	2.312438
20	1	0	-4.637046	-1.604902	1.633293
21	1	0	-3.017618	-1.601297	2.339988
22	6	0	-3.717206	-1.020837	-1.732248
23	1	0	-3.957947	-0.124092	-2.313174
24	1	0	-3.015658	-1.603397	-2.338584
25	1	0	-4.635685	-1.606311	-1.633267

Structure 14: Addition of 10 to TMA

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.221221	0.283532	-1.294109
2	13	0	-2.384011	-0.681575	-0.173678
3	13	0	-0.230189	0.976249	0.132368
4	6	0	-2.208553	-2.619255	-0.414565
5	1	0	-2.647897	-3.180238	0.417860
6	1	0	-2.712199	-2.962766	-1.324847
7	1	0	-1.160083	-2.925078	-0.492378

8	6	0	-0.639978	2.873413	0.392223
9	1	0	-0.300913	3.485627	-0.450814
10	1	0	-1.712182	3.061004	0.517058
11	1	0	-0.139391	3.268987	1.282607
12	6	0	-4.114079	0.249908	-0.074972
13	1	0	-4.645540	0.238954	-1.033713
14	1	0	-4.012190	1.300014	0.220991
15	1	0	-4.785876	-0.221256	0.651601
16	1	0	-1.555585	0.869531	-1.992802
17	8	0	1.395359	0.420005	0.128412
18	13	0	2.982586	-0.204631	-0.038212
19	6	0	3.890493	-0.008546	-1.767070
20	1	0	3.988878	1.046811	-2.043101
21	1	0	4.892792	-0.446446	-1.771628
22	1	0	3.316125	-0.485599	-2.568344
23	6	0	3.792771	-1.082845	1.519074
24	1	0	4.833278	-1.373456	1.347861
25	1	0	3.768777	-0.431196	2.398735
26	1	0	3.239230	-1.988635	1.790278
27	6	0	-1.206844	-0.252404	1.573198
28	1	0	-0.552196	-1.100226	1.791161
29	1	0	-0.892217	0.567971	2.235621
30	1	0	-2.187788	-0.484477	2.015901