Improvement of Catalytic Activity of Aluminum Complexes for the Ring-Opening Polymerization of ε-Caprolactone: Aluminum Thioamidate and Thioureidate Systems

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Supporting Information

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Table S1. ^{1}H and ^{13}C NMR peaks (in $CDCl_3$) of two methyl groups on Al atoms and carbonyl groups of ligands

L-Al	^{1}H NMR for $(CH_3)_2Al$	^{13}C NMR for $(CH_3)_2Al$	^{13}C NMR for OC or SC
	ppm		
$\mathbf{O^{H}}$	-0.65	-10.32	174.84
$\mathbf{O^{Cl}}$	-0.92	-10.29	175.30
$\mathbf{O^{Me}}$	-0.98	-9.89	174.17
$\mathbf{O^{Pr}}$	-1.14	-8.98	155.76
$\mathbf{O^{OMe}}$	-0.92	-10.39	174.73
$\mathbf{S^{H}}$	-0.48	-10.06	195.74
$\mathbf{S^{Cl}}$	-0.48	-10.01	196.67
$\mathbf{S^{Me}}$	-0.44	-8.51	195.59
$\mathbf{S^{Pr}}$	-0.49	-8.89	196.28
$\mathbf{S^{OMe}}$	-0.43	-10.04	196.20
$\mathbf{U^{H}}$	-0.88	-9.54	164.05
$\mathbf{U^{Cl}}$	-0.89	-9.54	164.16
$\mathbf{U^{OMe}}$	-0.91	-9.67	163.92
$\mathbf{US^{H}}$	-0.63	-9.61	173.77
$\mathbf{US^{Cl}}$	-0.65	-9.75	175.12
$\mathbf{US^{OMe}}$	-0.64	-9.63	174.27

Table S2. Kinetic study of CL polymerization with various Al complexes bearing amidates[a]

	[CL]:[**O^{X}-Al**]:[BnOH] = 100:0.5:2				
	X =				
Time/min	H	OMe	Pr	Cl	Me
	PCL conversion[b]				
5	0.10				0.26
10	0.30	0.25	0.32	0.07	0.49
15					0.60
20	0.62	0.48	0.56	0.37	0.74
25					0.78
30	0.78	0.62	0.72	0.56	0.85
35					0.88
40	0.86	0.74	0.82	0.72	0.90
44	0.90				
50		0.82	0.90	0.82	
60		0.88		0.90	
65		0.90			
$k_{obs}\times 10^3$/ min^{-1} (error)	55.3 (13)	36.7 (5)	47.3 (17)	43.9 (18)	57.9 (23)
I.P/ min (error)	3 (1)	3 (1)	3 (1)	10(2)	0
R^2	0.999	0.999	0.998	0.997	0.995

[a] In general, the reaction was carried out in toluene with [**CL**] = 2.0 M at 25°C.
[b] The data were determined from ^{1}H NMR analysis.

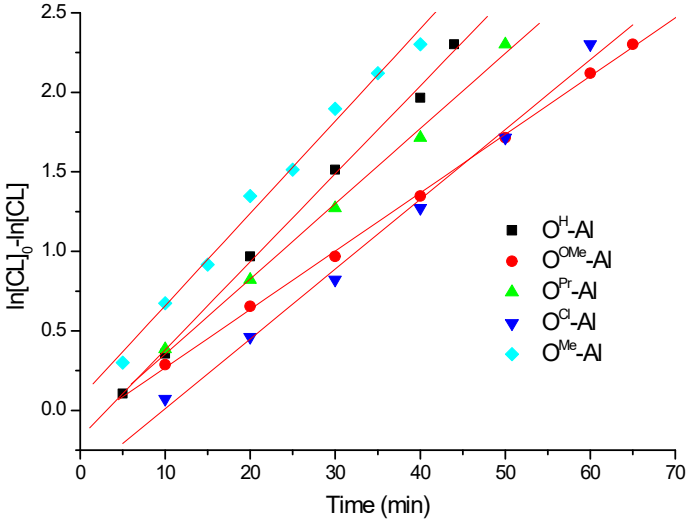


Figure S1. First-order kinetic plots of CL polymerization with various concentrations of various Al complexes bearing amide with 4 eq. BnOH plotted against time with [CL] = 2.0 M in toluene 5 mL (**Table S1**).

Table S3. Kinetic study of CL polymerization with various Al complexes bearing thioamidates[a]

	[CL]:[$\mathbf{S^X}$-**Al**]:[BnOH] = 100:0.5:2				
	X =				
Time/min	H	OMe	Pr	Cl	Me
	PCL conversion[b]				
2			0.08		
3	0.15			0.10	0.13
4		0.10	0.38		
5					0.26
6	0.37	0.20		0.26	
7			0.53		
8		0.30			
9	0.54			0.43	
10		0.40	0.71		0.57
12	0.66	0.50	0.80	0.52	
14			0.86		
15		0.63		0.61	0.78
16	0.78		0.90		
20	0.84	0.80		0.73	0.90
24	0.92				
25				0.80	
28		0.90			
35				0.90	
$k_{obs}\times 10^3$/ min^{-1} (error)	108.2 (46)	95.1 (34)	155.6 (59)	68.5 (8)	127.1 (70)
I.P/ min (error)	2 (1)	4 (1)	2 (1)	1 (1)	3 (1)
R^2	0.996	0.996	0.996	0.999	0.995

[a] In general, the reaction was carried out in toluene with [**CL**] = 2.0 M at 25°C.
[b] The data were determined from ^{1}H NMR analysis.

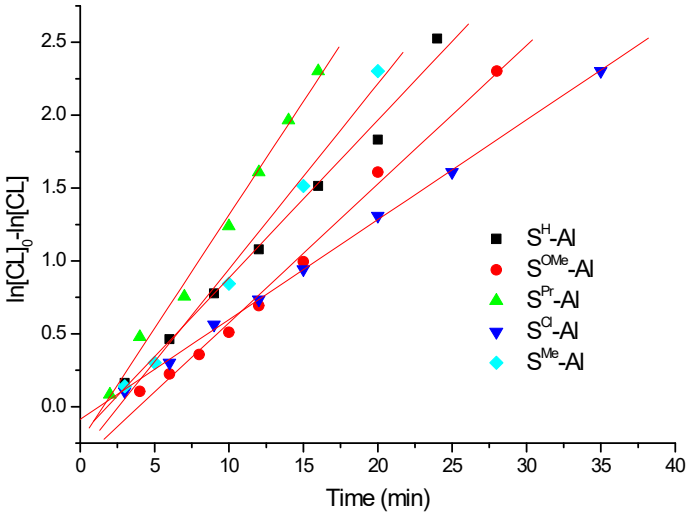


Figure S2. First-order kinetic plots of CL polymerization with various concentrations of various Al complexes bearing thioamide with 4 eq. BnOH plotted against time with [CL] = 2.0 M in toluene 5 mL (**Table S2**).

Table S4. Kinetic study of CL polymerization with various Al complexes bearing ureas and thioureas[a]

Time	[CL]:[**Al**]:[BnOH]					
min	**US^{OMe}-Al**	**US^{H}-Al**	**US^{Cl}-Al**	**U^{OMe}-Al**	**U^{H}-Al**	**U^{Cl}-Al**
	PCL conversion[b]					
3		0.23	0.20	0.17	0.05	0.09
4	0.10	0.48				
5						
6	0.34		0.47	0.44	0.15	0.21
8	0.58					
9		0.67	0.70	0.64		0.34
10	0.74				0.28	
12	0.82	0.81	0.83	0.72		0.43
14	0.90					
15		0.90	0.90	0.84		0.50
20				0.90	0.50	
25						0.68
30					0.64	
35						0.80
40					0.76	0.85
50					0.85	
$k_{obs}\times 10^3$/ min^{-1} (error)	219.4 (87)	155.5 (152)	176.5 (55)	126.2 (55)	38.3 (8)	47.6 (6)
I.P/ min (error)	4 (1)	1 (1)	2 (1)	1 (1)	2 (1)	1 (1)
R^2	0.997	0.986	0.999	0.996	0.999	0.999

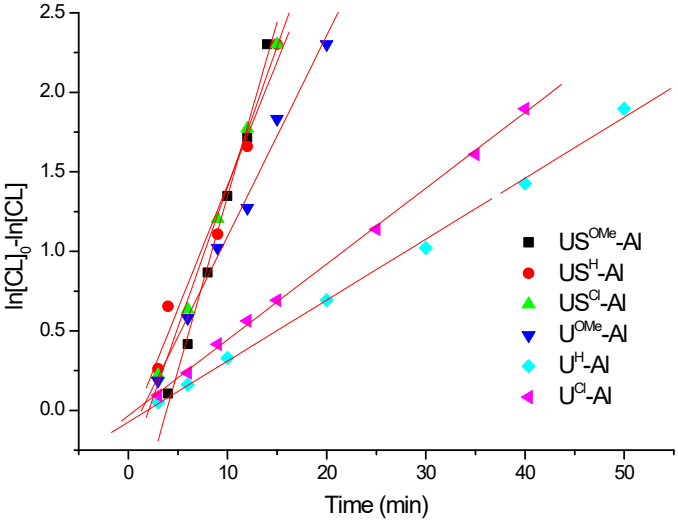


Figure S3. First-order kinetic plots of CL polymerization with various concentrations of various Al complexes bearing urea and thiourea with 4 eq. BnOH plotted against time with [CL] = 2.0 M in toluene 5 mL (**Table S3**).

Table S5. Kinetic study of CL polymerization with various concentration of **O^{Pr}-Al** and BnOH in toluene 5 mL, [CL] = 2.0 M at room temperature[a]

	[CL]:[**O^{Pr}-Al**]:[BnOH]			
time	100:0.25:1	100:0.5:2	100:1:4	100:2:8
min	PCL conversion[b]			
1				0.16
2			0.17	0.47
3				0.65
4				0.75
5			0.38	0.83
6				0.88
7				0.90
8			0.57	
10		0.32	0.66	
13			0.74	
15			0.80	
18			0.86	
20		0.56	0.90	
30		0.72		
40		0.82		
50		0.90		
60	0.15			
120	0.22			
180	0.32			

240	0.40			
300	0.48			
360	0.52			
540	0.70			
930	0.90			
$k_{obs}\times 10^2$/ min^{-1} (error)	2.47 (9)	4.72 (31)	11.52 (30)	35.99 (162)
I.P/ min (error)	28(15)	2(1)	1(1)	1(1)
R^2	0.996	0.998	0.998	0.995

[a] In general, the reaction was carried out in toluene with [CL] = 2.0 M at 25°C.

[b] The data were determined from ^{1}H NMR analysis.

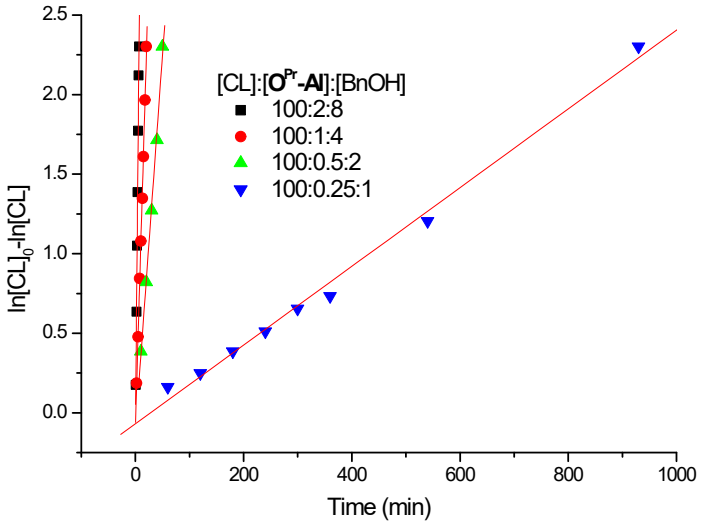


Figure S4. First-order kinetic plots of CL polymerization with various concentrations of [**O^{Pr}-Al**·4BnOH] plotted against time with [CL] = 2.0 M in toluene 5 mL

Table S6. Kinetic study of CL polymerization with various concentration of **S^{Pr}-Al** and BnOH in toluene 5 mL, [CL] = 2.0 M at room temperature[a]

	[CL]:[**S^{Pr}-Al**]:[BnOH]			
time	100:0.25:1	100:0.5:2	100:1:4	100:2:8
min	PCL conversion[b]			
1				0.23
2		0.08	0.19	0.50
3			0.36	0.70
4		0.38	0.48	0.80
5			0.63	0.90
6			0.73	
7		0.53	0.80	
8			0.84	
9			0.88	
10		0.71	0.91	
12		0.80		
14		0.86		
16		0.90		
30	0.26			
60	0.51			
90	0.68			
120	0.79			
150	0.86			
180	0.90			

$k_{obs}\times 10^2$/ min^{-1} (error)	1.35 (2)	15.56 (59)	27.97 (49)	49.99 (268)
I.P/ min (error)	7(2)	2(1)	2(1)	1(1)
R^2	0.999	0.996	0.999	0.996

[a] In general, the reaction was carried out in toluene with [CL] = 2.0 M at 25°C.

[b] The data were determined from ^{1}H NMR analysis.

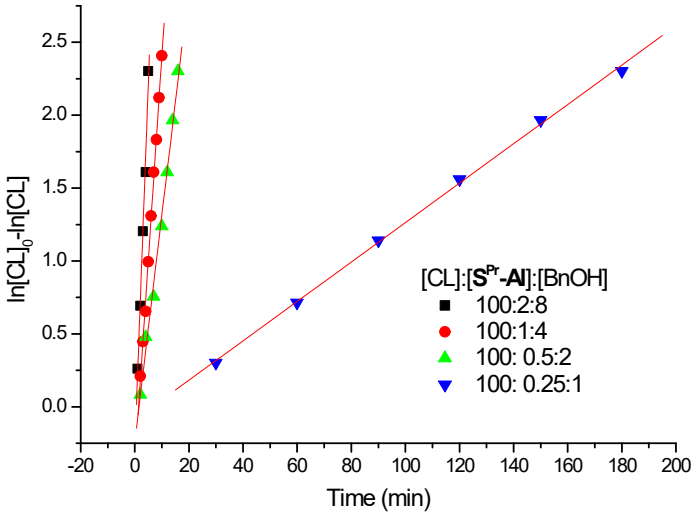


Figure S5. First-order kinetic plots of CL polymerization with various concentrations of [**S^{Pr}-Al**·4BnOH] plotted against time with [CL] = 2.0 M in toluene 5 mL

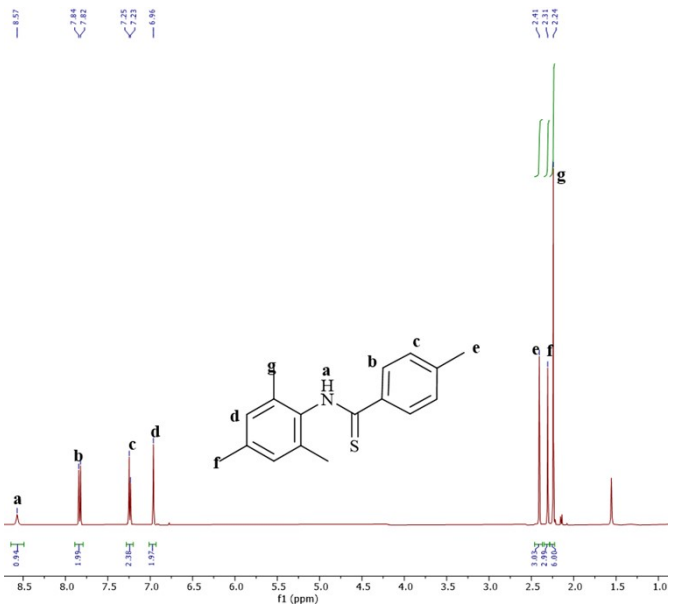


Figure S6. ^{1}H NMR spectrum of **S^{Me}-H** in $CDCl_3$

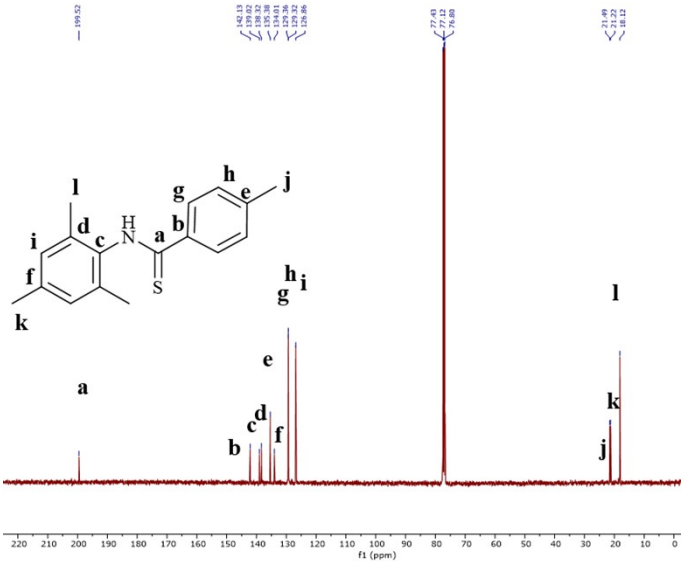


Figure S7. ^{13}C NMR spectrum of **S^{Me}-H** in $CDCl_3$

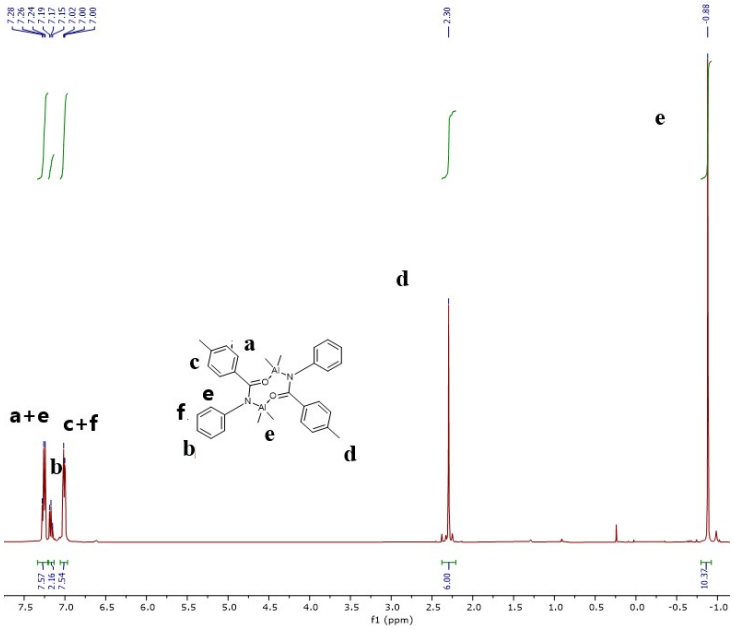


Figure S8. ^{1}H NMR spectrum of **O^{H}-Al** in $CDCl_3$

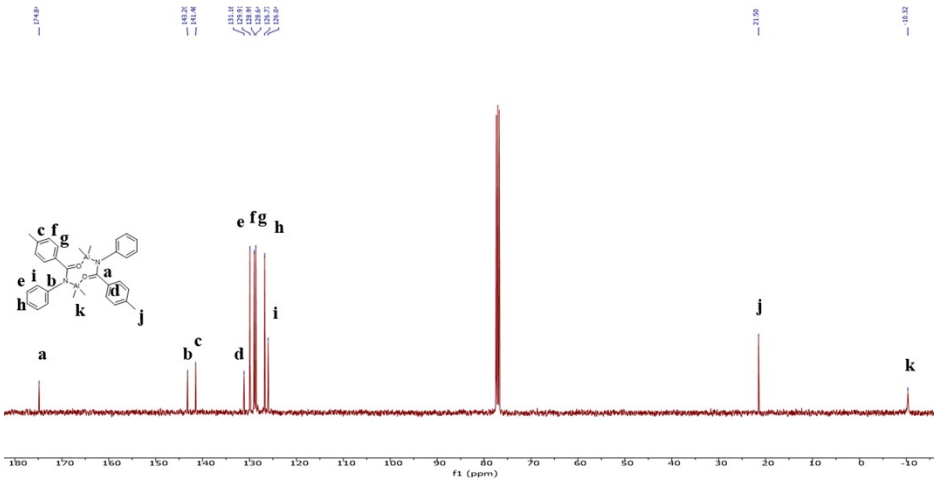


Figure S11. ^{13}C NMR spectrum of **O^{H}-Al** in $CDCl_3$

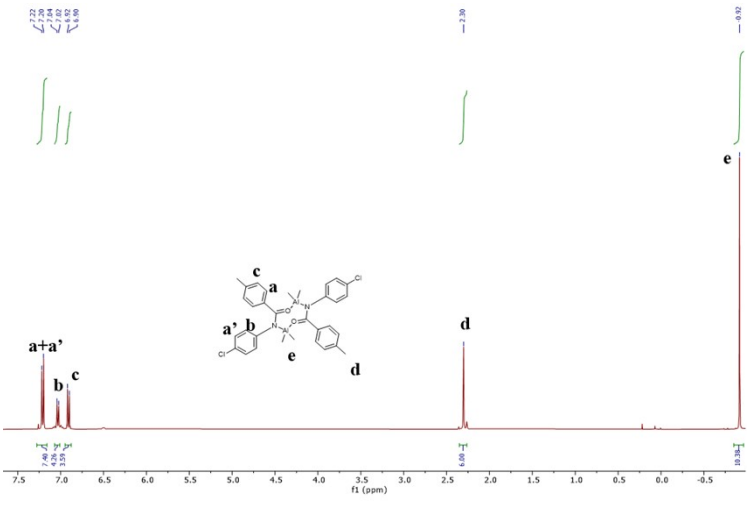


Figure S12. ^{1}H NMR spectrum of $\mathbf{O^{Cl}}$**-Al** in $CDCl_3$

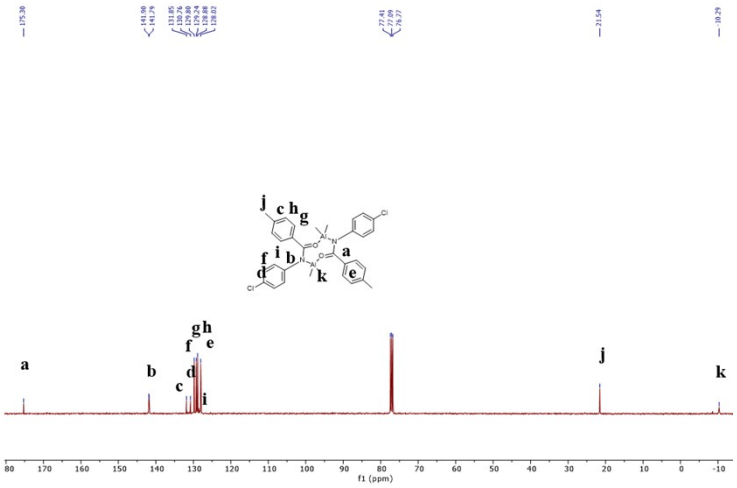


Figure S13. ^{13}C NMR spectrum of $\mathbf{O^{Cl}}$**-Al** in $CDCl_3$

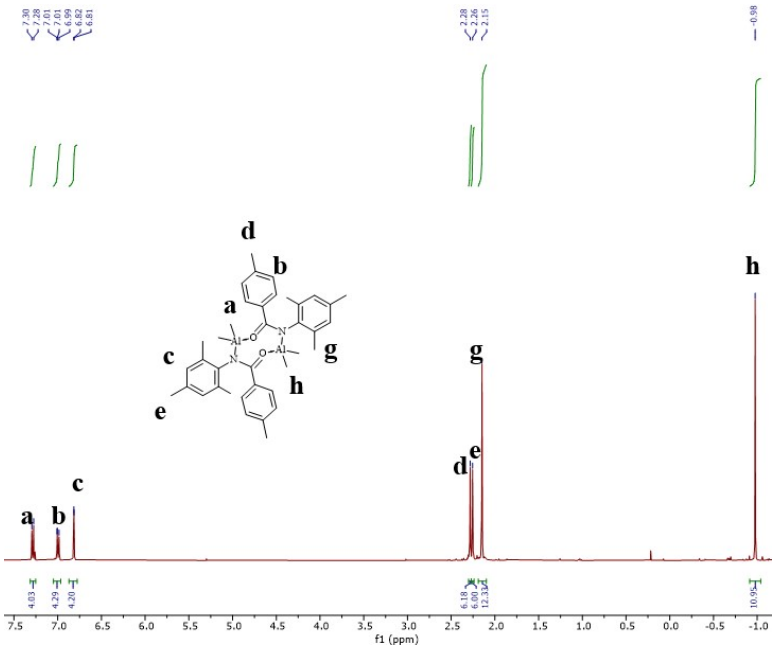


Figure S14. ^{1}H NMR spectrum of **O^{Me}-Al** in $CDCl_3$

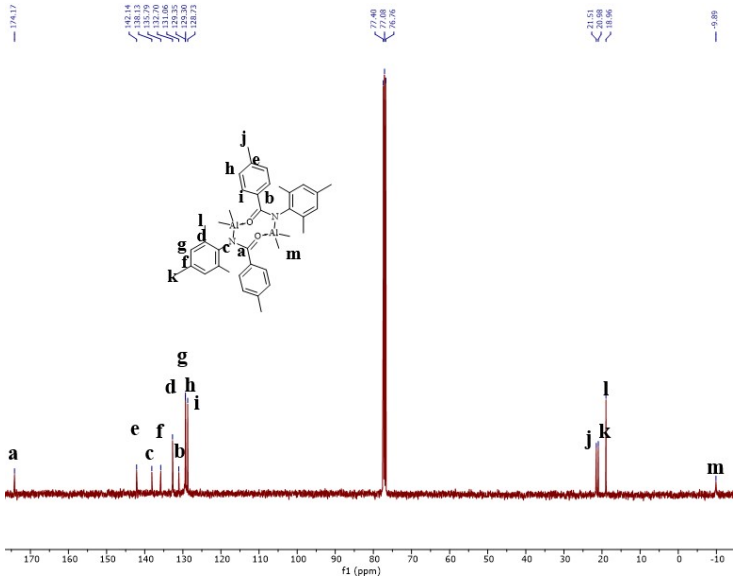


Figure S1. ^{13}C NMR spectrum of **O^{Me}-Al** in $CDCl_3$

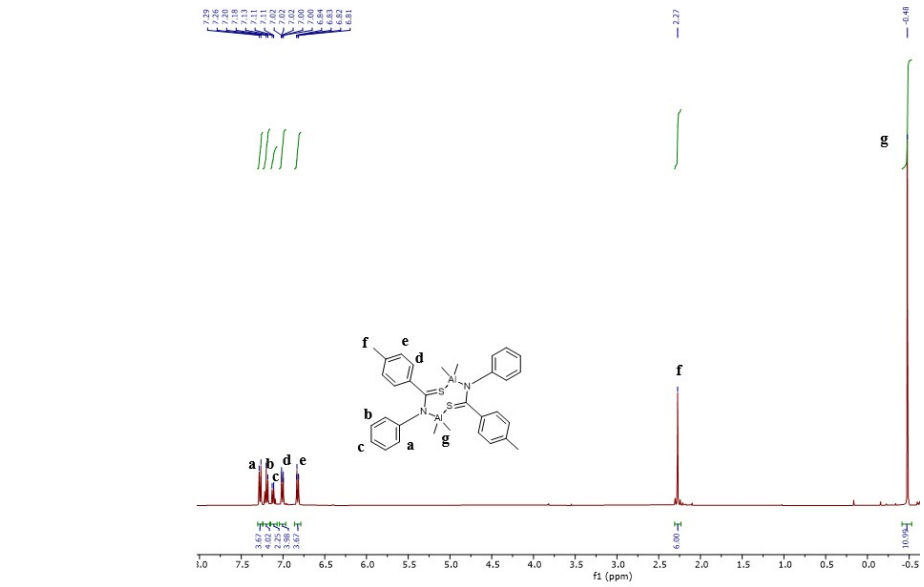


Figure S16. ^{1}H NMR spectrum of **S^{H}-Al** in $CDCl_3$

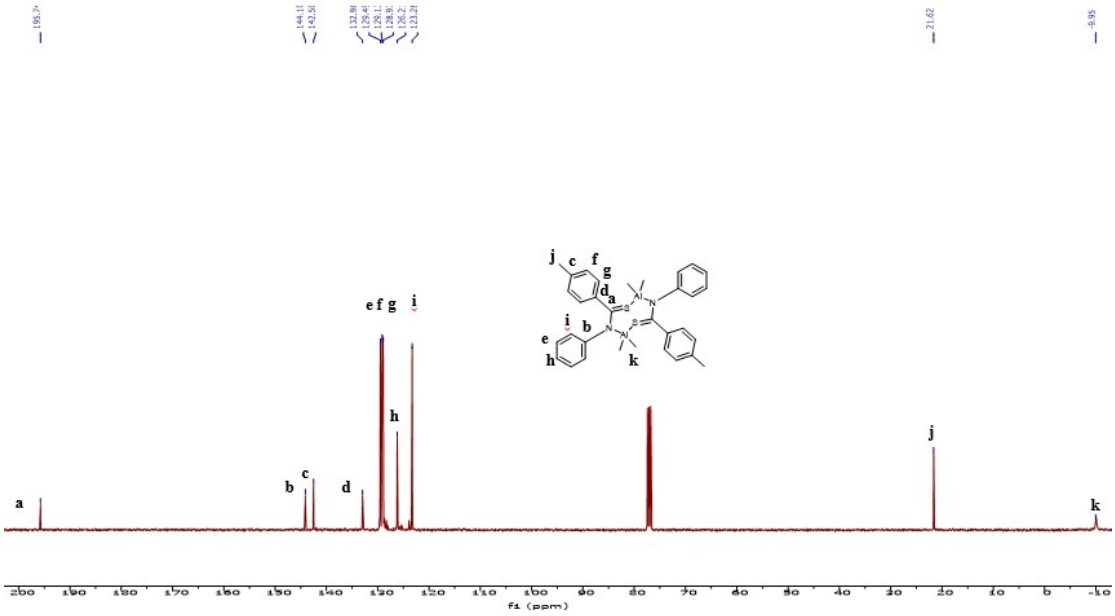


Figure S17. ^{13}C NMR spectrum of **S^{H}-Al** in $CDCl_3$

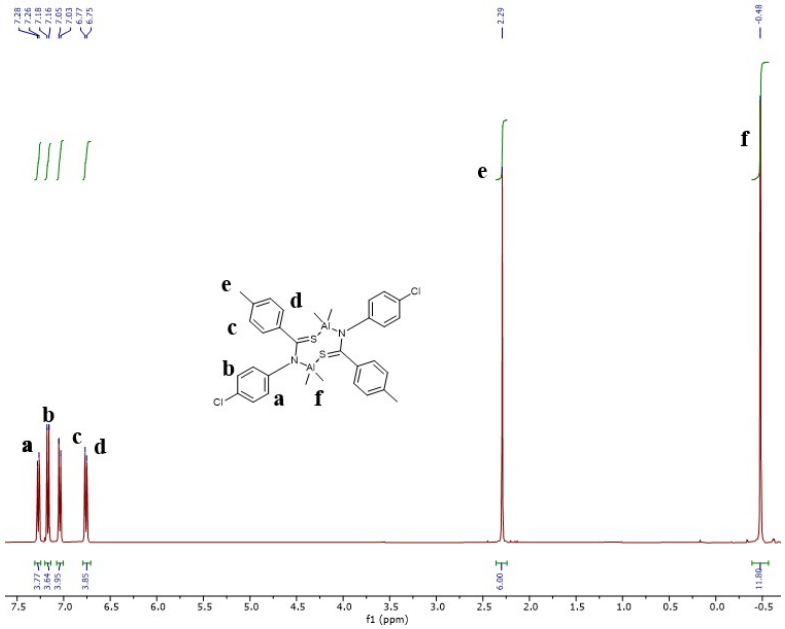


Figure S18. ^{1}H NMR spectrum of $\mathbf{S^{Cl}}$**-Al** in $CDCl_3$

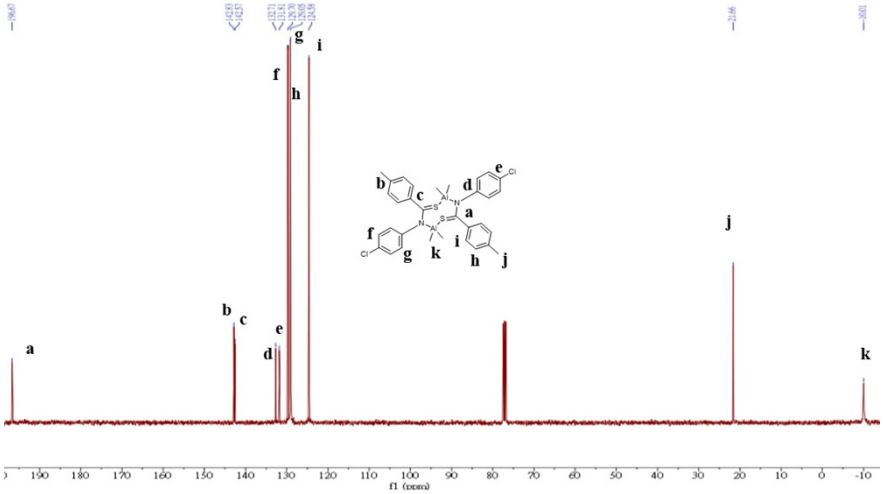


Figure S19. ^{13}C NMR spectrum of $\mathbf{S^{Cl}}$**-Al** in $CDCl_3$

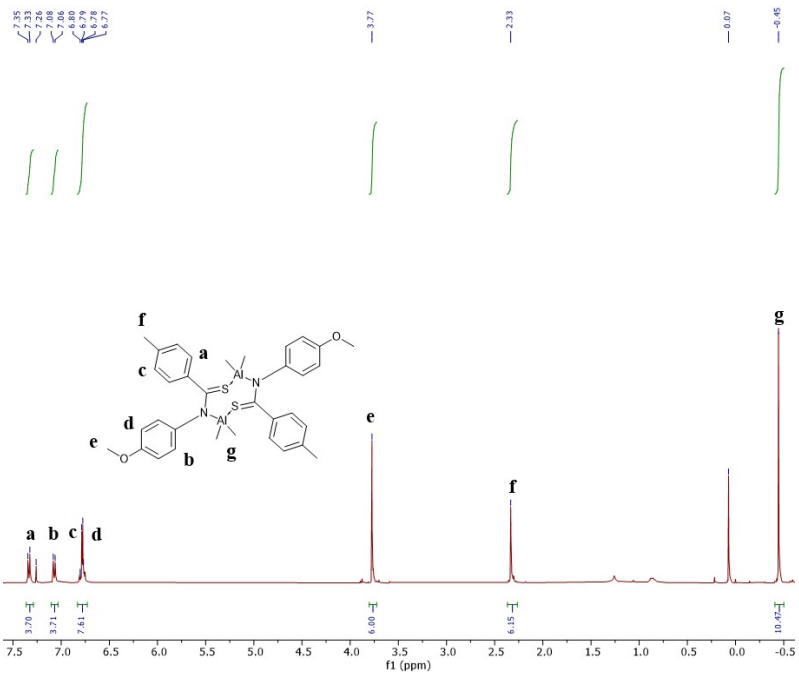


Figure S22. ^{1}H NMR spectrum of $\mathbf{S^{OMe}}$**-Al** in $CDCl_3$

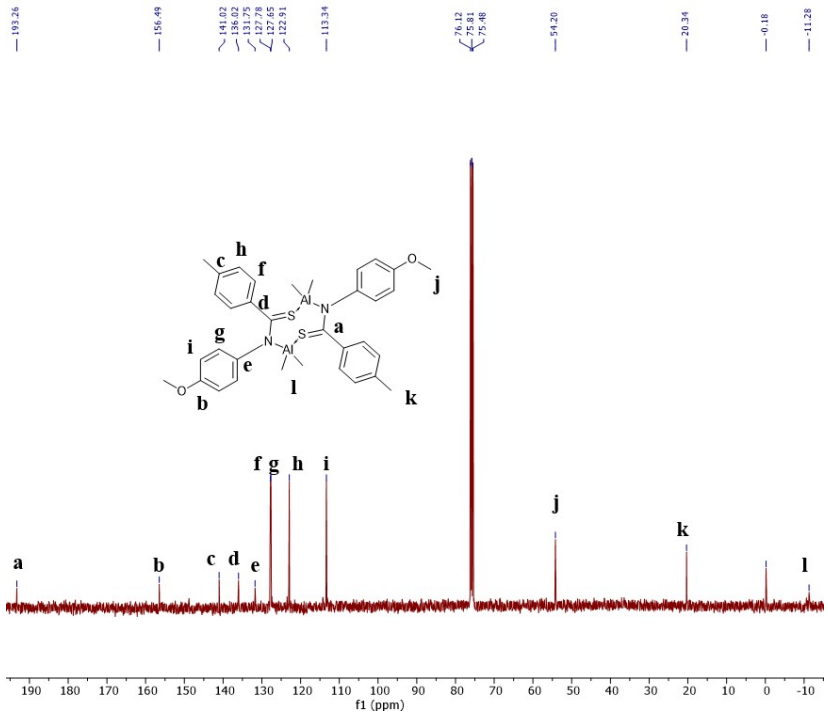


Figure S23. ^{13}C NMR spectrum of $\mathbf{S^{OMe}}$**-Al** in $CDCl_3$

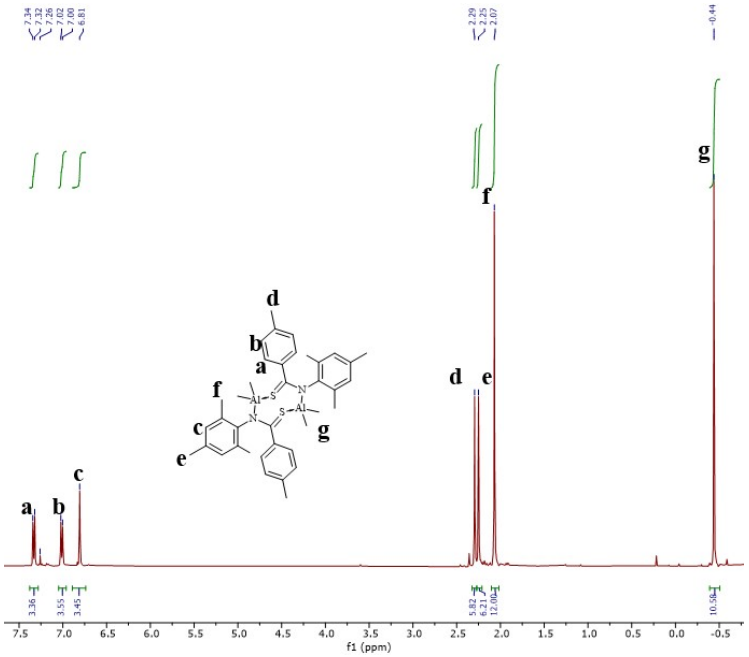


Figure S24. ^{1}H NMR spectrum of $\mathbf{S^{Me}}$**-Al** in $CDCl_3$

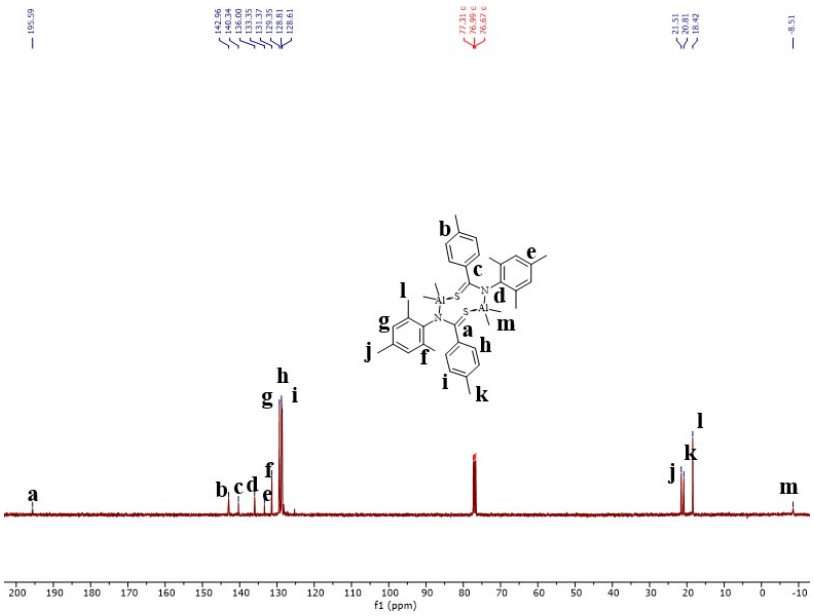


Figure S25. ^{13}C NMR spectrum of $\mathbf{S^{Me}}$**-Al** in $CDCl_3$

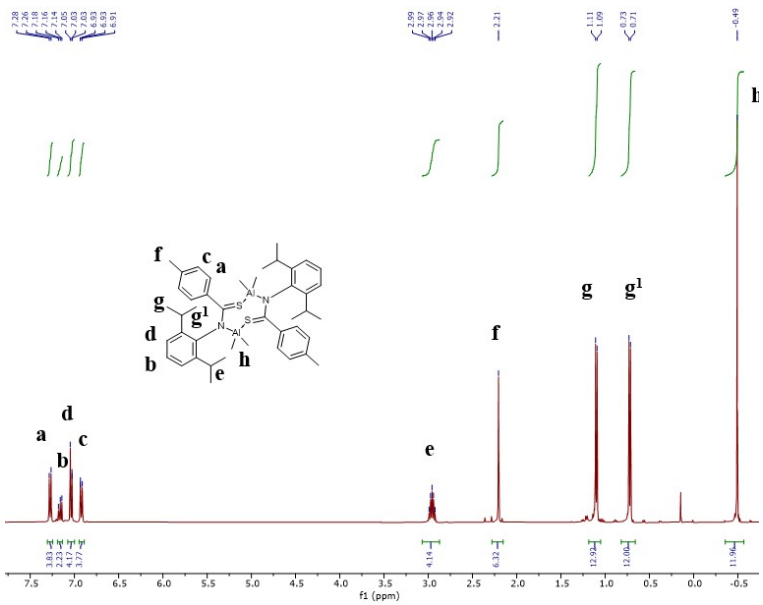


Figure S26. ^{1}H NMR spectrum of **S^{Pr}-Al** in $CDCl_3$

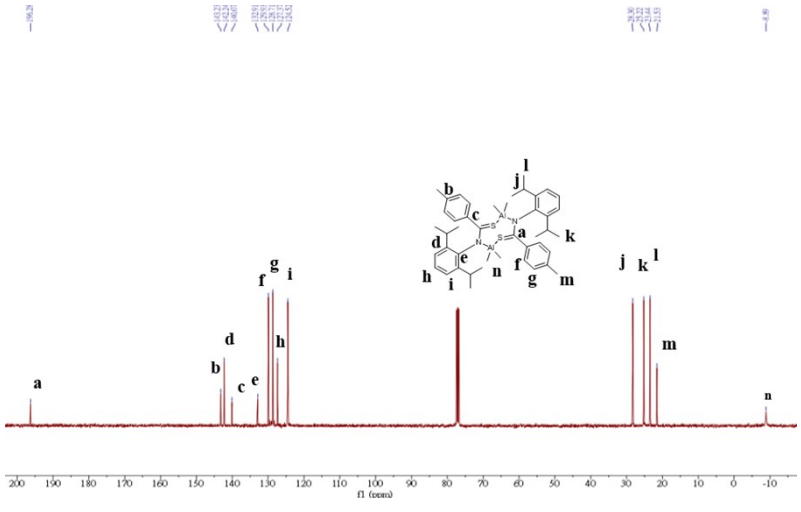


Figure S27. ^{13}C NMR spectrum of **S^{Pr}-Al** in $CDCl_3$

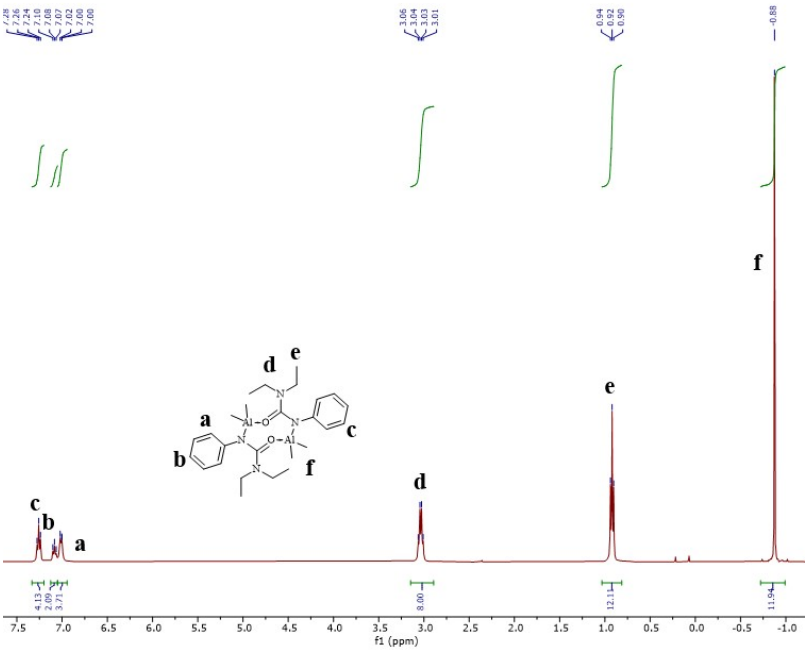


Figure S28. ^{1}H NMR spectrum of **U^{H}-Al** in $CDCl_3$

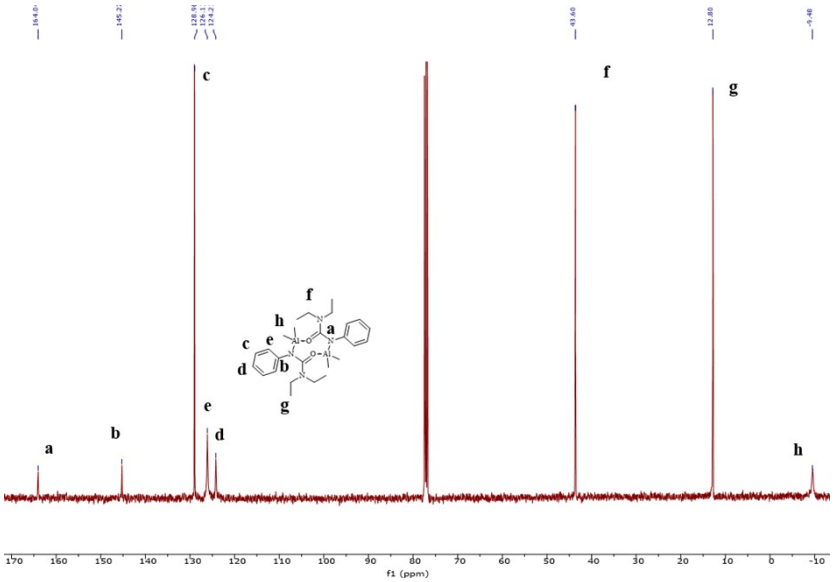


Figure S29. ^{13}C NMR spectrum of **U^{H}-Al** in $CDCl_3$

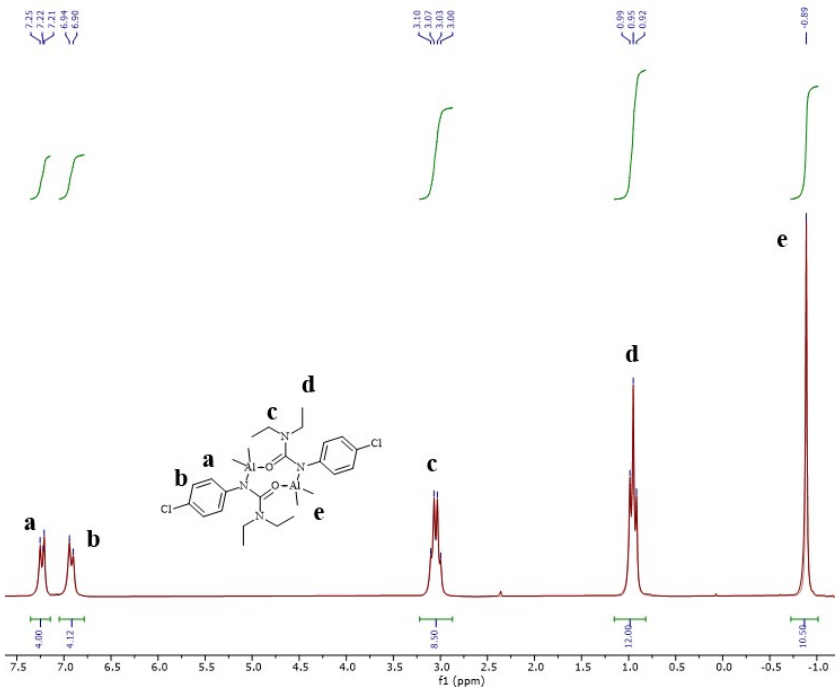


Figure S30. ^{1}H NMR spectrum of $\mathbf{U^{Cl}}$**-Al** in $CDCl_3$

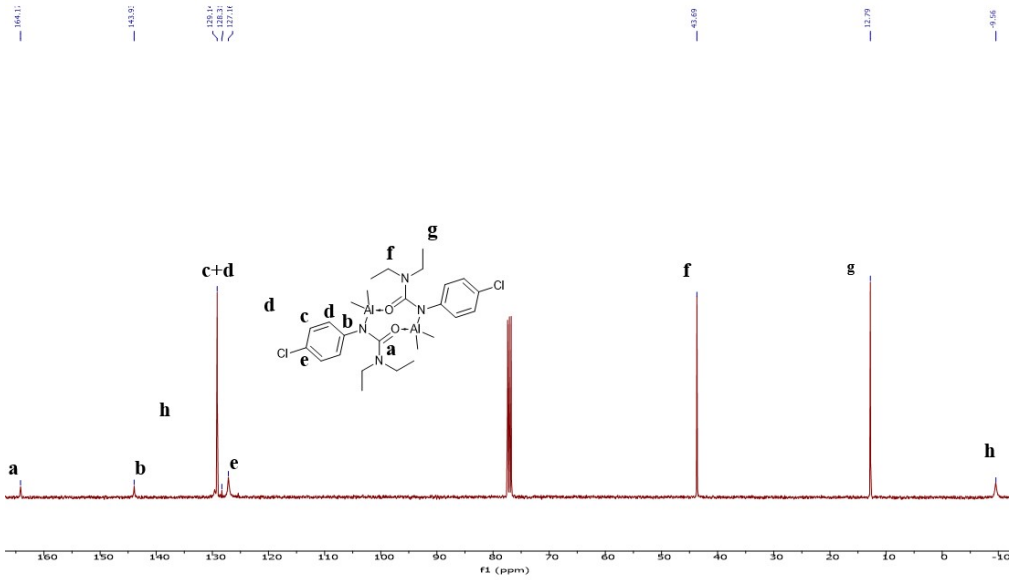


Figure S31. ^{13}C NMR spectrum of $\mathbf{U^{Cl}}$**-Al** in $CDCl_3$

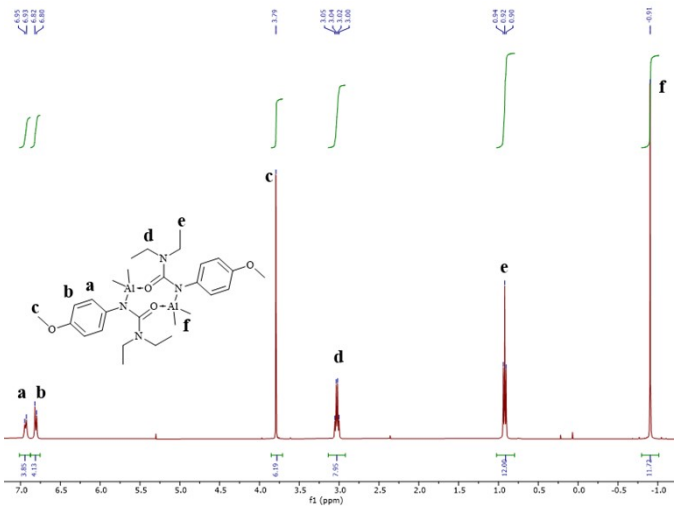


Figure S32. ^{1}H NMR spectrum of $\mathbf{U^{OMe}}$**-Al** in $CDCl_3$

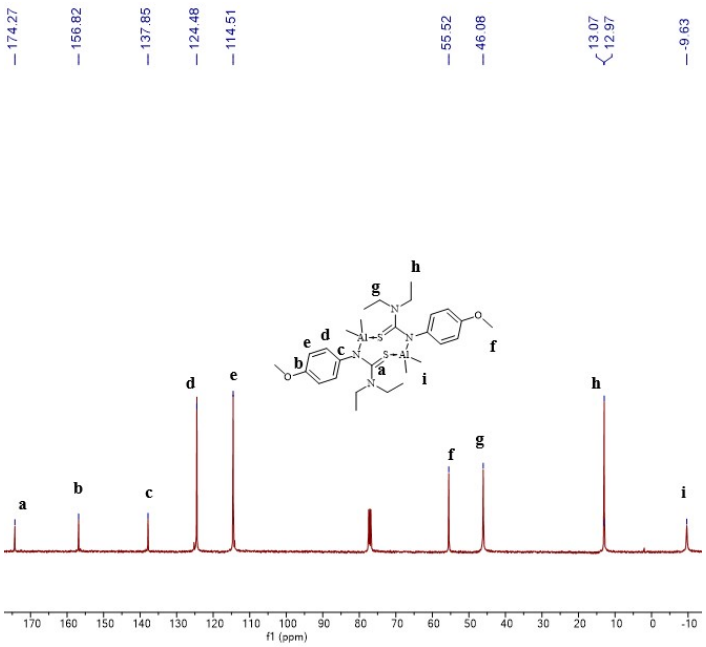


Figure S33. ^{13}C NMR spectrum of $\mathbf{U^{OMe}}$ in $CDCl_3$

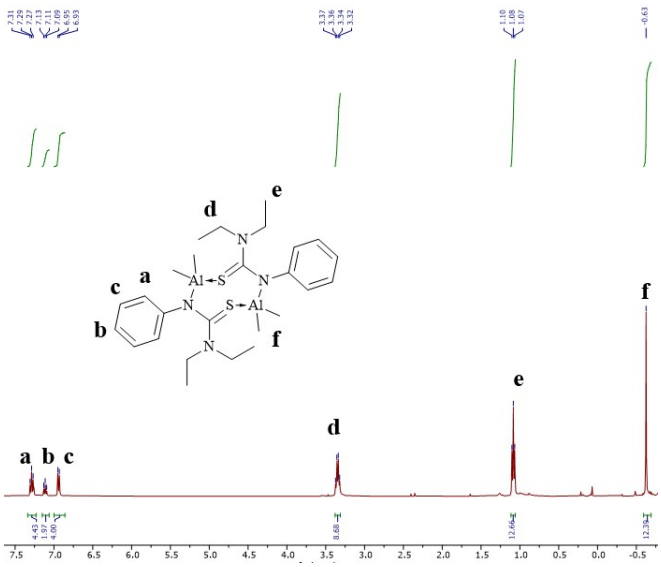


Figure S34. ^{1}H NMR spectrum of **US^{H}-Al** in $CDCl_3$

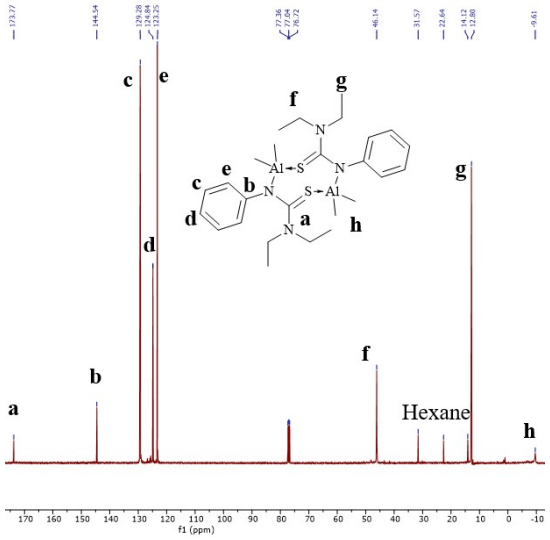


Figure S35. ^{13}C NMR spectrum of **US^{H}-Al** in $CDCl_3$

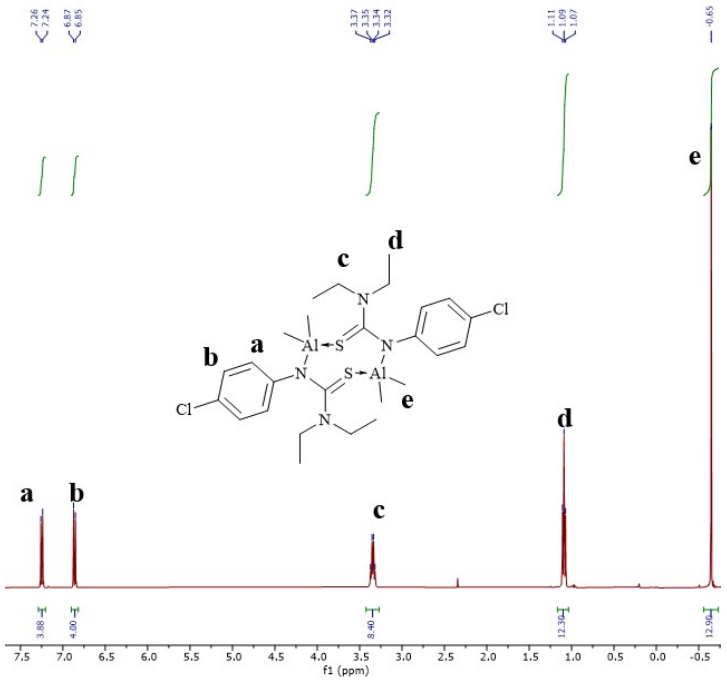


Figure S36. ^{1}H NMR spectrum of **US^{Cl}-Al** in $CDCl_3$

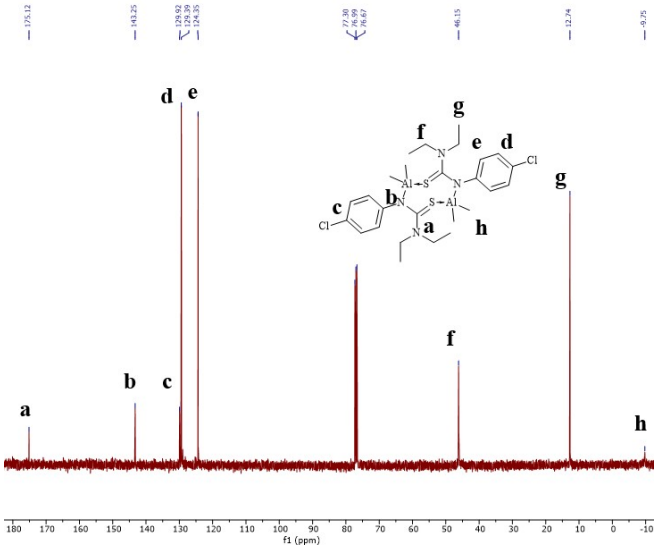


Figure S37. ^{13}C NMR spectrum of **US^{Cl}-Al** in $CDCl_3$

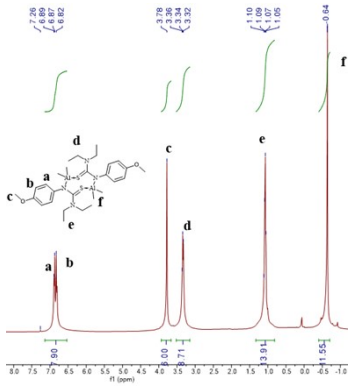


Figure S38. ^{1}H NMR spectrum of **US^{OMe}-Al** in $CDCl_3$

Figure S39. ^{13}C NMR spectrum of **US^{OMe}** in $CDCl_3$

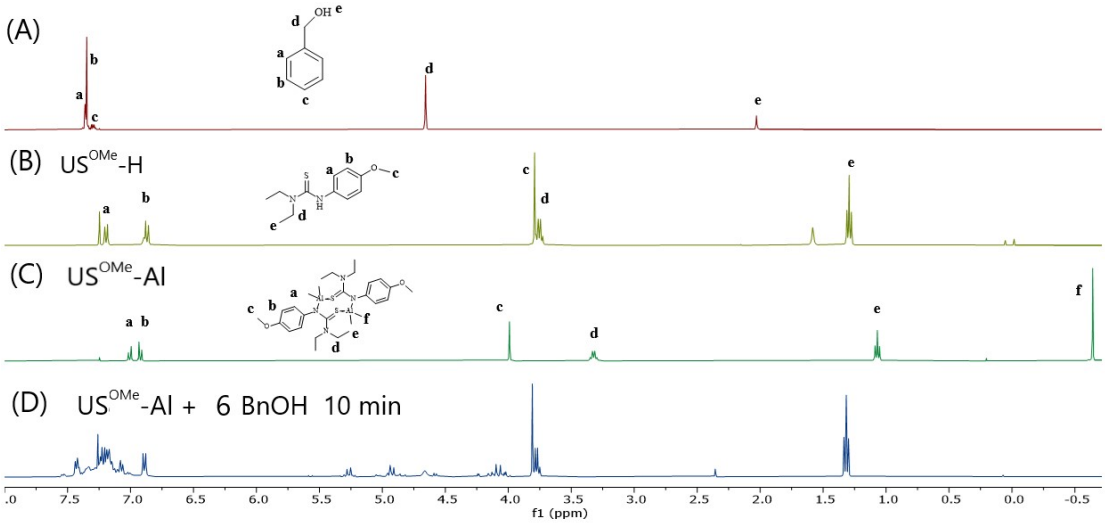


Figure S40. The ^{1}H NMR spectra of (a) BnOH; (B) **US^{OMe}-H**; (C) **US^{OMe}-Al**; and (D) the alcoholysis reactions of **US^{OMe}-Al** with 6 eq. BnOH

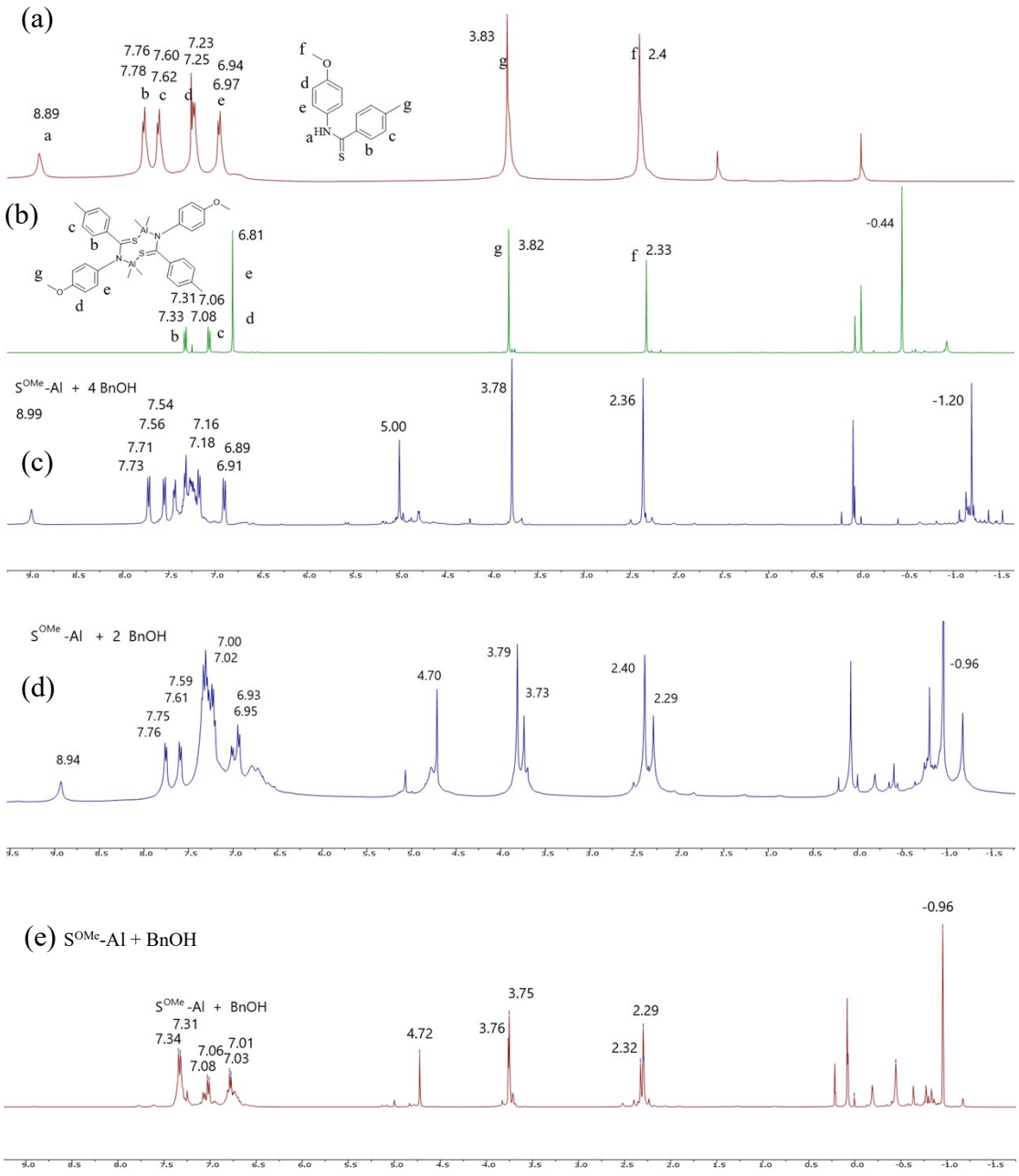
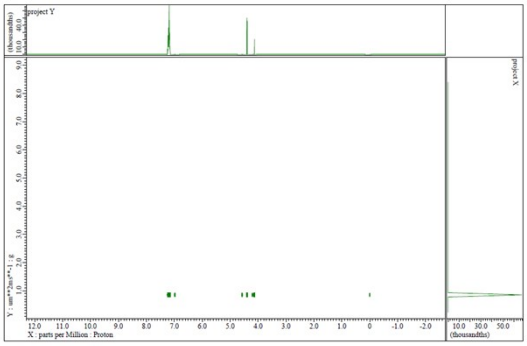
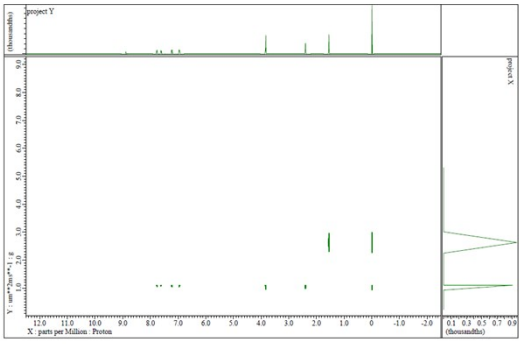


Figure S41. The ^{1}H NMR spectra of (a) **S^{OMe}-H**; (b) **S^{OMe}-Al**; (c) **S^{OMe}-Al** + 4 BnOH; and (d) **S^{OMe}-Al** + 2 BnOH; (e) **S^{OMe}-Al** + BnOH.

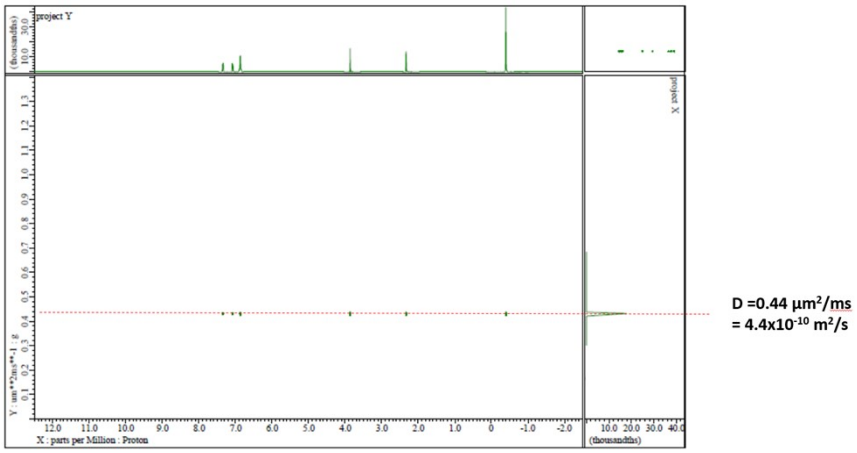
(a) BnOH (D = 7.88×10^{-10} m^2/s)



(b) **S^{OMe}-H** (D = 1.09×10^{-9} m^2/s)



(c) **S^{OMe}-Al** (D = 4.4×10^{-10} m^2/s)



(d) the mixture of **S^{OMe}-Al** with 4 BnOH (D = 5.8×10^{-10} m^2/s)

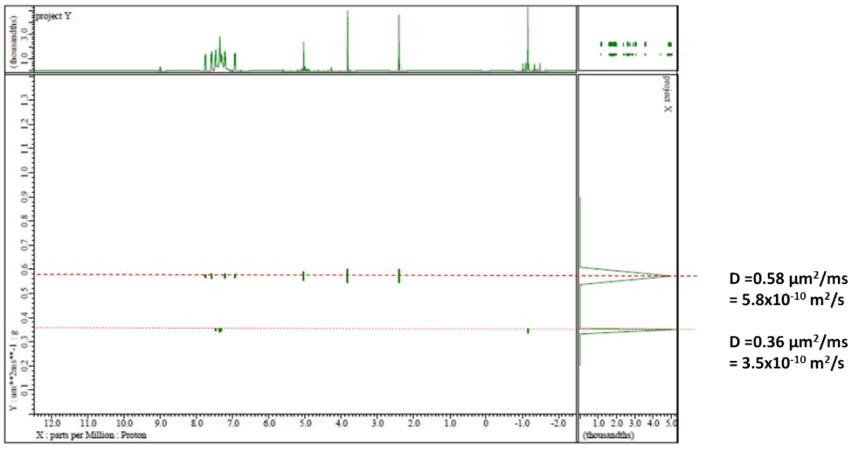


Figure S42. DOSY spectrum of (a) BnOH; (b) **S^{OMe}-H**; (c) **S^{OMe}-Al** and (d) the mixture of **S^{OMe}-Al** with 4 BnOH in $CDCl_3$

Table S7. Cartesian coordinate of CL

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-1.37346	-0.02703	0.01184
C	-0.59628	1.138495	0.608833
C	0.6242	1.564546	-0.23669
C	1.862385	0.680969	-0.04047
C	1.653483	-0.79893	-0.38556
C	0.556261	-1.48773	0.426478
H	-0.27355	0.899838	1.631561
H	0.337785	1.585549	-1.29669
H	2.184825	0.75521	1.008937
H	1.410535	-0.91919	-1.44945
H	-1.31567	1.957244	0.674562
H	0.882105	2.595484	0.03376
H	2.687581	1.078351	-0.64478
H	2.592054	-1.34185	-0.21212
H	0.655987	-2.57343	0.353959
H	0.618886	-1.21809	1.489673
O	-2.49714	0.087685	-0.41583
O	-0.7708	-1.24353	-0.07348

Table S8. Cartesian coordinate of $[S^{Pr}AlOMe_2]_2$

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	0.089082	6.105712	0.733066
N	3.653725	4.238963	0.844998
C	3.282005	5.417731	1.271547
C	3.720600	5.994089	2.569772
C	2.761114	6.422633	3.500229
H	1.705853	6.281838	3.289498
C	3.167024	6.966322	4.715473
H	2.411982	7.273276	5.435400
C	4.523883	7.132108	5.025836
C	5.470526	6.726406	4.076740
H	6.529886	6.855369	4.285084
C	5.079855	6.152457	2.870664
H	5.830619	5.843557	2.155200
C	4.951407	7.705028	6.355227
H	4.223817	8.432180	6.731299
H	5.925100	8.201247	6.285337
H	5.041361	6.913495	7.111166
C	4.529416	3.403888	1.656092
C	3.998477	2.711386	2.759080
C	4.872813	1.899169	3.491296
H	4.491376	1.349159	4.346383
C	6.211632	1.770696	3.136354

C	6.702115	2.447587	2.023090	C	-3.280389	7.716677	-3.138697
H	7.743512	2.328046	1.738629	C	-3.770790	7.039740	-2.025427
C	5.873159	3.272180	1.256481	H	-4.812182	7.159221	-1.740920
Al	2.842403	3.381690	-0.735551	C	-2.941761	6.215171	-1.258871
N	-0.722281	5.248476	-0.847495	H	-3.939765	8.353458	-3.722529
C	-0.350555	4.069713	-1.274043	H	6.870951	1.133894	3.720227
C	-0.789171	3.493302	-2.572236	C	6.425748	3.956092	0.008577
C	0.170364	3.064678	-3.502722	H	5.680172	4.676268	-0.346774
H	1.225616	3.205556	-3.292002	C	6.648520	2.920416	-1.112360
C	-0.235538	2.520881	-4.717827	H	6.968956	3.416279	-2.036819
H	0.519482	2.213853	-5.437764	H	7.429962	2.207205	-0.823366
C	-1.592482	2.354989	-5.028152	H	5.732853	2.355796	-1.305044
C	-2.539059	2.760780	-4.079159	C	7.721416	4.744224	0.275148
H	-3.598417	2.631841	-4.287464	H	8.034996	5.267828	-0.635206
C	-2.148352	3.334895	-2.873076	H	7.597050	5.490996	1.066905
H	-2.899138	3.643884	-2.157674	H	8.541632	4.080902	0.571486
C	-2.019317	1.781596	-6.357559	C	2.519202	2.748929	3.124969
H	-1.300304	1.041205	-6.724343	H	2.022875	3.538409	2.555073
H	-3.001016	1.300874	-6.292274	C	2.286614	3.061010	4.612873
H	-2.091061	2.570238	-7.118438	H	1.212525	3.149285	4.810715
C	-1.598030	6.083537	-1.658538	H	2.675511	2.267333	5.261423
C	-1.067173	6.776086	-2.761540	H	2.764364	4.002741	4.899158
C	-1.941580	7.588274	-3.493700	C	1.857291	1.415125	2.724107
H	-1.560206	8.138322	-4.348792	H	0.773330	1.464439	2.878039

H	2.051722	1.184794	1.672119	O	-0.574935	7.691619	0.551972
H	2.253158	0.588157	3.326438	O	-0.043043	5.318669	2.260632
C	-3.494260	5.531204	-0.010957	O	3.506366	1.795774	-0.554418
H	-2.748636	4.811049	0.344336	O	2.974573	4.168738	-2.263106
C	0.412086	6.738625	-3.127505	C	3.191304	0.649588	-1.309425
H	0.908511	5.949241	-2.557559	H	3.721808	0.644706	-2.274387
C	-3.717012	6.566841	1.110016	H	3.495584	-0.247831	-0.754135
H	-4.498497	7.280032	0.821085	H	2.112331	0.567506	-1.515837
H	-4.037379	6.070944	2.034482	C	3.868301	5.109120	-2.802840
H	-2.801354	7.131489	1.302663	H	3.625761	5.275797	-3.860717
C	-4.789905	4.743022	-0.277490	H	3.798158	6.075209	-2.282645
H	-4.665533	3.996269	-1.069264	H	4.912641	4.763901	-2.752493
H	-5.103430	4.219389	0.632866	C	-0.936799	4.378306	2.800361
H	-5.610161	5.406314	-0.573788	H	-0.866594	3.412186	2.280235
C	1.073913	8.072522	-2.726814	H	-0.694343	4.211711	3.858270
H	0.879497	8.302958	-1.674847	H	-1.981143	4.723500	2.749908
H	2.157872	8.023270	-2.880774	C	-0.259731	8.837811	1.306921
H	0.677966	8.899394	-3.329225	H	-0.563473	9.735258	0.751382
C	0.644610	6.426418	-4.615393	H	-0.790610	8.843021	2.271674
H	0.255586	7.219987	-5.263998	H	0.819191	8.919546	1.513740
H	1.718695	6.338236	-4.813301	S	0.619438	3.042161	-0.218862
H	0.166939	5.484607	-4.901547	S	2.312028	6.445298	0.216368

Table S9. Cartesian coordinate of $[S^{Pr}AlOMe_2]_2$ in state 1b

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	0.288008	2.617687	-0.127047
N	2.415696	-0.817615	-0.288484
C	2.715052	0.395020	-0.662248
C	4.047335	1.032617	-0.431559
C	4.099896	2.232061	0.295760
H	3.184303	2.650947	0.701468
C	5.322115	2.853224	0.533244
H	5.345161	3.770985	1.116585
C	6.519059	2.322756	0.032052
C	6.451374	1.140399	-0.714116
H	7.362594	0.711656	-1.124662
C	5.236934	0.494782	-0.935404
H	5.215868	-0.425075	-1.504717
C	7.842019	2.993402	0.314446
H	7.740440	4.083900	0.344216
H	8.591084	2.742055	-0.443876
H	8.242423	2.678170	1.287355
C	3.467203	-1.635898	0.308785
C	3.849139	-1.445311	1.650381
C	4.841354	-2.283463	2.174287
H	5.146792	-2.154390	3.208526
C	5.435390	-3.277820	1.405685
C	5.031876	-3.455663	0.085865
H	5.486359	-4.240396	-0.512736
C	4.044058	-2.648217	-0.485381
Al	0.454274	-1.638116	-0.133909
N	-1.508920	1.795529	-0.014035
C	-1.625129	0.713397	0.710875
C	-2.907145	0.078681	1.107756
C	-4.034171	0.019307	0.271846
H	-3.993162	0.417300	-0.730890
C	-5.220116	-0.558866	0.719673
H	-6.075421	-0.593614	0.048918
C	-5.334007	-1.080890	2.013294
C	-4.204677	-1.029163	2.841966
H	-4.258561	-1.437900	3.848042
C	-3.010995	-0.476388	2.397150
H	-2.144777	-0.465698	3.048106
C	-6.619524	-1.700049	2.504443
H	-7.415311	-1.628278	1.756428
H	-6.479015	-2.761619	2.745606
H	-6.971333	-1.208587	3.419374
C	-2.634412	2.493982	-0.591034
C	-2.925940	2.282779	-1.952714
C	-3.996649	2.995949	-2.501218
H	-4.244892	2.857006	-3.549590

C	-4.745310	3.882911	-1.729692	H	1.532421	-1.768206	3.035015
C	-4.422534	4.081443	-0.390969	H	2.831362	-1.779293	4.238716
H	-4.999941	4.784508	0.203099	C	-2.984905	3.676819	1.656063
C	-3.354539	3.399529	0.204495	H	-2.133556	3.045987	1.926175
H	-5.574789	4.425325	-2.175922	C	-2.113499	1.322662	-2.816701
H	6.204701	-3.915073	1.834150	H	-1.447990	0.740434	-2.172625
C	3.603586	-2.912185	-1.921400	C	-2.522378	5.136426	1.820850
H	2.929981	-2.107062	-2.220673	H	-3.340103	5.838947	1.620005
C	2.817768	-4.235095	-2.010108	H	-2.168155	5.313028	2.843364
H	2.442331	-4.392678	-3.029075	H	-1.706415	5.357320	1.125419
H	3.462207	-5.085281	-1.754161	C	-4.135238	3.325989	2.616552
H	1.976921	-4.223455	-1.312962	H	-4.429624	2.276144	2.511645
C	4.774729	-2.916528	-2.921300	H	-3.828430	3.494408	3.655627
H	4.396639	-3.057697	-3.940809	H	-5.018731	3.946662	2.425340
H	5.337624	-1.977065	-2.901270	C	-1.228933	2.110565	-3.800983
H	5.479538	-3.730353	-2.716047	H	-0.611662	2.831540	-3.260264
C	3.191064	-0.421989	2.566810	H	-0.572646	1.429490	-4.354531
H	2.579958	0.254772	1.965869	H	-1.844633	2.661389	-4.523404
C	4.211873	0.454924	3.313071	C	-3.002287	0.313493	-3.565500
H	3.688299	1.248399	3.858727	H	-3.654645	0.805056	-4.296752
H	4.787757	-0.124441	4.044533	H	-2.377358	-0.403153	-4.109573
H	4.913947	0.924404	2.618482	H	-3.637893	-0.255241	-2.878399
C	2.254601	-1.137644	3.560977	O	-0.159643	3.988259	-1.102511
H	1.702894	-0.406675	4.162973	O	1.007031	3.065896	1.394513

O	1.141048	-3.046479	0.600881	S	1.572585	1.392667	-1.578876
O	-0.168567	-1.572844	-1.760779	C	-2.307502	-3.248115	0.042407
C	0.685337	-4.082219	1.416467	C	-2.510674	-3.560227	-1.420094
H	0.085467	-3.719145	2.264640	C	-3.898998	-3.135873	-1.947903
H	0.060294	-4.804984	0.862517	C	-5.034663	-4.106463	-1.605238
H	1.547422	-4.633147	1.819150	C	-5.268719	-4.295374	-0.101530
C	0.431474	-1.548672	-3.028801	C	-4.059792	-4.829162	0.661769
H	-0.296488	-1.194718	-3.772499	H	-2.355565	-4.635190	-1.587088
H	1.293020	-0.871819	-3.080002	H	-4.133468	-2.135319	-1.567071
H	0.761533	-2.553907	-3.334549	H	-4.816311	-5.085310	-2.057308
C	1.218496	4.389183	1.830175	H	-5.568919	-3.349050	0.362449
H	0.819222	4.520229	2.846353	H	-1.720347	-3.010159	-1.933058
H	2.295960	4.619045	1.863384	H	-3.822914	-3.042365	-3.036936
H	0.738254	5.137434	1.182731	H	-5.963734	-3.752600	-2.069476
C	0.674961	4.900056	-1.769533	H	-6.093350	-5.004018	0.050835
H	0.151833	5.310119	-2.645822	H	-4.355853	-5.193076	1.647735
H	0.949683	5.748027	-1.121308	H	-3.574781	-5.655538	0.127261
H	1.609093	4.437395	-2.126466	O	-1.467541	-2.454760	0.450004
S	-0.101092	0.099567	1.353588	O	-3.076950	-3.815238	0.977715

Table S10. Cartesian coordinate of $S^{Pr}AlOMe_2$

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	0.729943	5.653129	0.562817
N	-0.251917	5.467950	-1.100037
C	0.008199	4.201404	-1.366835
C	-0.559331	3.431501	-2.490820
C	-0.823989	4.036691	-3.731528
H	-0.581799	5.080238	-3.889199
C	-1.385256	3.298231	-4.767392
H	-1.570641	3.780603	-5.723862
C	-1.719310	1.946729	-4.599265
C	-1.445015	1.347345	-3.362213
H	-1.687715	0.298675	-3.209947
C	-0.864620	2.070629	-2.325746
H	-0.660987	1.590148	-1.374414
C	-2.378316	1.167687	-5.710662
H	-2.064526	1.529219	-6.695498
H	-2.144340	0.099989	-5.646862
H	-3.470759	1.266851	-5.659582
C	-1.239929	6.294907	-1.726563
C	-0.798550	7.425721	-2.444048
C	-1.768061	8.272830	-2.991987
H	-1.451925	9.148887	-3.551434
C	-3.126191	8.012824	-2.829274
C	-3.536365	6.897464	-2.104081
H	-4.597553	6.709378	-1.967183
C	-2.609843	6.016644	-1.533750
H	-3.864961	8.682536	-3.261470
C	-3.106374	4.838008	-0.703262
H	-2.252744	4.219528	-0.419341
C	0.683007	7.733419	-2.632626
H	1.262994	6.921100	-2.187665
C	-3.738940	5.330773	0.611420
H	-4.590256	5.995226	0.421595
H	-4.096070	4.480849	1.204761
H	-2.998240	5.872273	1.208175
C	-4.064490	3.937042	-1.502959
H	-3.594120	3.587194	-2.427998
H	-4.342900	3.060247	-0.906979
H	-4.988761	4.463167	-1.768651
C	1.078265	9.018171	-1.882723
H	0.886379	8.908645	-0.811929
H	2.148607	9.216790	-2.011316
H	0.522411	9.886922	-2.256292
C	1.063764	7.815398	-4.122282
H	0.549343	8.640839	-4.628249
H	2.142053	7.981146	-4.227970
H	0.811599	6.889995	-4.653593

O	1.972799	6.818852	0.352358	C	-2.378316	1.167687	-5.710662
O	-0.279666	5.735464	1.951936	H	-2.064526	1.529219	-6.695498
C	-0.556273	6.840410	2.782046	H	-2.144340	0.099989	-5.646862
H	-0.354950	6.585594	3.831980	H	-3.470759	1.266851	-5.659582
H	0.044687	7.728972	2.531440	C	-1.239929	6.294907	-1.726563
H	-1.616200	7.123705	2.702621	C	-0.798550	7.425721	-2.444048
C	2.937121	7.354931	1.223242	C	-1.768061	8.272830	-2.991987
H	3.222823	8.358846	0.879804	H	-1.451925	9.148887	-3.551434
H	2.572537	7.449620	2.258575	C	-3.126191	8.012824	-2.829274
H	3.846666	6.735914	1.242188	C	-3.536365	6.897464	-2.104081
S	1.093357	3.469174	-0.199581	H	-4.597553	6.709378	-1.967183
Al	0.729943	5.653129	0.562817	C	-2.609843	6.016644	-1.533750
N	-0.251917	5.467950	-1.100037	H	-3.864961	8.682536	-3.261470
C	0.008199	4.201404	-1.366835	C	-3.106374	4.838008	-0.703262
C	-0.559331	3.431501	-2.490820	H	-2.252744	4.219528	-0.419341
C	-0.823989	4.036691	-3.731528	C	0.683007	7.733419	-2.632626
H	-0.581799	5.080238	-3.889199	H	1.262994	6.921100	-2.187665
C	-1.385256	3.298231	-4.767392	C	-3.738940	5.330773	0.611420
H	-1.570641	3.780603	-5.723862	H	-4.590256	5.995226	0.421595
C	-1.719310	1.946729	-4.599265	H	-4.096070	4.480849	1.204761
C	-1.445015	1.347345	-3.362213	H	-2.998240	5.872273	1.208175
H	-1.687715	0.298675	-3.209947	C	-4.064490	3.937042	-1.502959
C	-0.864620	2.070629	-2.325746	H	-3.594120	3.587194	-2.427998
H	-0.660987	1.590148	-1.374414	H	-4.342900	3.060247	-0.906979

H	-4.988761	4.463167	-1.768651	O	-0.279666	5.735464	1.951936
C	1.078265	9.018171	-1.882723	C	-0.556273	6.840410	2.782046
H	0.886379	8.908645	-0.811929	H	-0.354950	6.585594	3.831980
H	2.148607	9.216790	-2.011316	H	0.044687	7.728972	2.531440
H	0.522411	9.886922	-2.256292	H	-1.616200	7.123705	2.702621
C	1.063764	7.815398	-4.122282	C	2.937121	7.354931	1.223242
H	0.549343	8.640839	-4.628249	H	3.222823	8.358846	0.879804
H	2.142053	7.981146	-4.227970	H	2.572537	7.449620	2.258575
H	0.811599	6.889995	-4.653593	H	3.846666	6.735914	1.242188
O	1.972799	6.818852	0.352358	S	1.093357	3.469174	-0.199581

Table S11. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state 1a

	Coordinates (Angstroms)						
Atom	X	Y	Z	C	-2.730183	-1.688215	1.797539
Al	1.531112	-2.028145	-0.640476	H	-2.392061	-2.714278	1.897529
N	0.289207	-0.586500	0.048255	C	-5.491243	0.556026	3.181529
C	-0.796801	-1.285034	0.271518	H	-6.043408	1.333074	2.642006
C	-2.014807	-0.808963	0.969230	H	-6.184234	-0.261430	3.407152
C	-2.471794	0.513723	0.845729	H	-5.173073	0.988709	4.139454
H	-1.945973	1.211833	0.207530	C	0.543080	0.737499	0.525965
C	-3.600846	0.937989	1.539165	C	0.624113	1.782535	-0.418671
H	-3.941264	1.964073	1.421585	C	0.895580	3.073833	0.046431
C	-4.300943	0.071617	2.389781	H	0.952357	3.892716	-0.665975
C	-3.847043	-1.249091	2.501896	C	1.093958	3.325061	1.401402
H	-4.376179	-1.943769	3.150025	C	1.034532	2.274708	2.312580
				H	1.207118	2.471462	3.367294

C	0.764824	0.963855	1.901625	C	3.365944	-3.083521	1.283444
H	1.302637	4.334975	1.745336	H	2.790115	-4.007877	1.456134
C	0.752932	-0.155452	2.936194	H	4.219288	-3.346644	0.636514
H	0.508386	-1.092445	2.432666	H	3.772965	-2.765249	2.254685
C	0.412892	1.539244	-1.908538	C	3.042708	-1.568507	-3.010902
H	0.222651	0.474617	-2.055438	H	3.357490	-0.666034	-3.556216
C	2.155971	-0.344865	3.540719	H	3.937297	-1.974119	-2.507259
H	2.486027	0.551653	4.080059	H	2.733712	-2.308420	-3.773937
H	2.153585	-1.182156	4.249781	S	-0.656696	-2.932251	-0.305051
H	2.872149	-0.566133	2.745384	C	1.898392	-4.573742	-2.264105
C	-0.308271	0.085006	4.025770	C	2.713727	-5.780446	-2.661200
H	-1.304730	0.211941	3.590948	C	3.433542	-5.587529	-4.017034
H	-0.341794	-0.766615	4.716024	C	2.529297	-5.793157	-5.239428
H	-0.079825	0.980360	4.616652	C	1.329113	-4.839944	-5.321706
C	1.688525	1.868486	-2.702522	C	0.373223	-4.922339	-4.135695
H	2.523699	1.272398	-2.327225	H	2.068684	-6.668105	-2.702005
H	1.547726	1.629053	-3.763657	H	3.888989	-4.589491	-4.041621
H	1.949321	2.931722	-2.627600	H	2.158735	-6.828822	-5.234006
C	-0.799069	2.320009	-2.449578	H	1.662244	-3.799009	-5.418492
H	-0.664306	3.403097	-2.341260	H	3.437188	-5.929320	-1.857690
H	-0.943483	2.107449	-3.515849	H	4.257822	-6.308157	-4.060201
H	-1.722113	2.044902	-1.925828	H	3.132041	-5.686162	-6.149233
O	2.005746	-1.258136	-2.133801	H	0.749882	-5.071017	-6.224775
O	2.585053	-2.054862	0.744090	H	-0.572155	-4.425357	-4.355970

H	0.158655	-5.959596	-3.851032	O	0.847608	-4.195362	-2.973952
O	2.219153	-3.894992	-1.288615				

Table S12. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state TS1a

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	-1.134049	0.874545	0.319420
N	0.650971	0.018257	-0.128725
C	1.283775	1.060813	-0.620709
C	2.742915	1.176565	-0.862566
C	3.549654	0.078303	-1.211554
H	3.114950	-0.903006	-1.339378
C	4.920404	0.235635	-1.391022
H	5.520428	-0.628979	-1.664542
C	5.542001	1.478530	-1.213278
C	4.736915	2.569650	-0.860766
H	5.192877	3.545043	-0.708941
C	3.362682	2.428072	-0.700755
H	2.759144	3.285715	-0.424127
C	7.027327	1.642548	-1.422747
H	7.248359	1.904078	-2.466258
H	7.435382	2.440793	-0.793816
H	7.569288	0.718161	-1.196754
C	1.257823	-1.204541	0.293506
C	1.008458	-2.360110	-0.484532
C	1.594760	-3.562851	-0.078340
H	1.431989	-4.463823	-0.661077
C	2.383313	-3.626856	1.070220
C	2.583079	-2.485268	1.838529
H	3.180706	-2.547032	2.743837
C	2.025530	-1.252126	1.475183
H	2.830673	-4.571074	1.369959
C	2.247319	-0.035112	2.366027
H	1.754161	0.824530	1.909645
C	0.150028	-2.279140	-1.745475
H	-0.611502	-1.514785	-1.569908
C	1.573950	-0.236558	3.735842
H	1.998094	-1.094597	4.272227
H	1.716754	0.654420	4.359206
H	0.499963	-0.389268	3.602749
C	3.743258	0.299071	2.515395
H	4.217915	0.457711	1.542135
H	3.866339	1.212586	3.109075
H	4.285154	-0.504197	3.029524
C	-0.593077	-3.587781	-2.057941
H	-1.135102	-3.960535	-1.181955

H	-1.318354	-3.418805	-2.862027	C	-4.174850	0.367803	-1.567132
H	0.086673	-4.378807	-2.397144	C	-5.484312	1.136925	-1.840383
C	0.974941	-1.830785	-2.968027	C	-6.723520	0.458952	-1.236552
H	1.803001	-2.525555	-3.157036	C	-6.709573	0.328794	0.293236
H	0.344607	-1.803722	-3.865071	C	-5.490960	-0.397050	0.861016
H	1.393478	-0.830145	-2.828516	H	-4.338936	-0.710329	-1.661154
O	-2.211025	-0.585509	-0.141634	H	-5.387146	2.165529	-1.469878
O	-0.918143	0.954675	2.040839	H	-6.819696	-0.545211	-1.675639
C	-1.652579	1.730604	2.956106	H	-6.752395	1.319409	0.763691
H	-1.440392	2.806200	2.847185	H	-3.400665	0.642019	-2.285772
H	-2.738660	1.591979	2.845426	H	-5.619304	1.210099	-2.925875
H	-1.375376	1.441807	3.980620	H	-7.622054	1.012800	-1.535984
C	-2.347031	-1.738995	0.671071	H	-7.607257	-0.215072	0.616170
H	-2.901180	-2.513381	0.123411	H	-5.650883	-0.660058	1.909045
H	-1.358911	-2.134102	0.928586	H	-5.266783	-1.319054	0.312097
H	-2.877060	-1.499963	1.602045	O	-2.788999	1.696752	-0.097085
S	0.199563	2.403860	-0.910047	O	-4.329153	0.459806	0.900697
C	-3.596106	0.699100	-0.204111				

Table S13. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state 2a

	Coordinates (Angstroms)			C	-2.730874	-1.368700	-0.746478
Atom	X	Y	Z	C	-3.409406	-0.251500	-1.264567
Al	1.128386	-1.142564	0.400563	H	-2.865666	0.649219	-1.514180
N	-0.551529	-0.300459	-0.166177	C	-4.786891	-0.285492	-1.455190
C	-1.271207	-1.361368	-0.497008	H	-5.287652	0.590049	-1.861303

C	-5.539996	-1.420068	-1.123943	H	-1.640368	-0.582301	4.350035
C	-4.861104	-2.530588	-0.604598	H	-0.313567	0.239507	3.508925
H	-5.421676	-3.421587	-0.332412	C	-3.641848	-0.122725	2.515374
C	-3.481692	-2.513502	-0.428774	H	-4.151407	-0.272066	1.558351
H	-2.975602	-3.381837	-0.021043	H	-3.848625	-0.990544	3.152494
C	-7.031886	-1.454816	-1.346909	H	-4.082011	0.756316	3.001164
H	-7.267546	-1.831595	-2.351180	C	1.245755	2.942284	-2.053306
H	-7.529925	-2.112992	-0.627254	H	1.865449	2.976006	-1.152315
H	-7.474317	-0.456747	-1.261264	H	1.892706	2.703132	-2.904933
C	-1.048104	0.996009	0.175666	H	0.837825	3.944484	-2.227501
C	-0.693385	2.083620	-0.652540	C	-0.750601	1.864252	-3.174967
C	-1.157486	3.356600	-0.304521	H	-1.309085	2.803053	-3.275380
H	-0.917772	4.204586	-0.939149	H	-0.138258	1.735581	-4.075464
C	-1.921648	3.555723	0.842912	H	-1.472200	1.041597	-3.144212
C	-2.222991	2.476665	1.667938	O	2.127289	0.604883	0.385305
H	-2.800280	2.640985	2.573568	O	1.088175	-1.327614	2.120610
C	-1.794927	1.178952	1.360837	C	0.925403	-2.462325	2.930719
H	-2.272892	4.552158	1.097851	H	0.336946	-3.253996	2.441612
C	-2.122884	0.040669	2.321945	H	1.899084	-2.890782	3.214645
H	-1.743813	-0.893689	1.904350	H	0.400041	-2.185140	3.856519
C	0.137400	1.885609	-1.915857	C	2.339089	1.482597	1.494549
H	0.623043	0.909246	-1.840394	H	2.957151	2.331516	1.180253
C	-1.396217	0.238676	3.665193	H	1.351543	1.841268	1.790045
H	-1.691050	1.177931	4.148562	H	2.806174	0.947881	2.323764

S	-0.323799	-2.820833	-0.544723	H	6.551980	-1.253329	0.074251
C	3.302023	-0.192938	-0.212227	H	2.973085	0.635151	-2.107151
C	3.816732	0.591952	-1.416093	H	5.056367	0.240558	-3.141572
C	5.030280	-0.070482	-2.090088	H	7.191293	-0.130720	-2.035544
C	6.373193	0.296193	-1.441302	H	7.487085	0.206299	0.408310
C	6.527516	-0.157850	0.015958	H	5.701649	0.168057	1.991971
C	5.414479	0.322183	0.947754	H	5.218905	1.395205	0.816071
H	4.046678	1.625528	-1.130126	O	2.649458	-1.326706	-0.548499
H	4.883717	-1.157476	-2.088532	O	4.216482	-0.451401	0.800217
H	6.497420	1.388908	-1.487675				

Table S14. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state TS2a

	Coordinates (Angstroms)			C	-3.421700	-2.250846	-1.309137
Atom	X	Y	Z	H	-2.929827	-3.188283	-1.071673
Al	0.956422	-1.009127	0.406019	C	-6.863814	-1.040750	-2.428879
N	-0.746658	-0.143128	0.051461	H	-7.084544	-0.218836	-3.118065
C	-1.312534	-1.067361	-0.702228	H	-7.150090	-1.980189	-2.912972
C	-2.709296	-1.047065	-1.181917	H	-7.512163	-0.913725	-1.551716
C	-3.361982	0.157209	-1.497648	C	-1.391840	0.972208	0.676035
H	-2.833230	1.098353	-1.419424	C	-1.003551	2.268421	0.279460
C	-4.686728	0.149379	-1.920046	C	-1.604379	3.356839	0.921893
H	-5.169390	1.090649	-2.171129	H	-1.330600	4.365362	0.624486
C	-5.410760	-1.047006	-2.022466	C	-2.542684	3.168129	1.932886
C	-4.752663	-2.244996	-1.712835	C	-2.887584	1.877829	2.325924
H	-5.290221	-3.186740	-1.790666	H	-3.603952	1.737216	3.130521

C	-2.321907	0.753051	1.714544	C	1.914342	-1.521221	3.078515
H	-2.998149	4.025808	2.420930	H	1.988210	-0.520939	3.529749
C	-2.688807	-0.639240	2.216411	H	1.594255	-2.224563	3.859602
H	-2.215793	-1.383611	1.572996	H	2.917107	-1.809476	2.738259
C	0.016754	2.504870	-0.829568	C	4.265863	1.052150	2.221262
H	0.385533	1.534617	-1.171580	H	5.145689	1.542729	1.779255
C	-2.120961	-0.868182	3.629429	H	3.879284	1.689214	3.020538
H	-2.522983	-0.140567	4.344765	H	4.569031	0.088154	2.645986
H	-2.379988	-1.872789	3.984645	S	-0.234635	-2.403701	-1.057659
H	-1.030357	-0.783375	3.612451	C	3.463539	0.100191	0.126286
C	-4.206285	-0.889961	2.155710	C	4.309003	0.887798	-0.885222
H	-4.591530	-0.734294	1.142470	C	4.615317	0.126673	-2.184465
H	-4.429914	-1.921141	2.452880	C	5.832164	-0.804533	-2.092268
H	-4.753761	-0.224764	2.833761	C	5.691512	-1.942756	-1.074449
C	1.238659	3.283983	-0.311126	C	5.387780	-1.479531	0.351803
H	1.751502	2.725363	0.476799	H	5.238283	1.238129	-0.420496
H	1.951560	3.447433	-1.128721	H	3.722435	-0.437719	-2.478199
H	0.954098	4.268058	0.080817	H	6.717111	-0.204160	-1.830560
C	-0.624207	3.213956	-2.037557	H	4.890369	-2.629806	-1.376104
H	-1.002415	4.206587	-1.765227	H	3.709880	1.776409	-1.099779
H	0.113778	3.344408	-2.837693	H	4.800184	0.858566	-2.980942
H	-1.462304	2.637366	-2.445936	H	6.035395	-1.233768	-3.082126
O	3.207421	0.901185	1.290988	H	6.623297	-2.525370	-1.055443
O	0.977483	-1.538619	2.030164	H	5.566346	-2.298055	1.056687

H	6.048126	-0.649922	0.643274	O	4.014608	-1.144835	0.553408
O	2.240175	-0.157317	-0.416602				

Table S15. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state 3a

	Coordinates (Angstroms)						
Atom	X	Y	Z	C	-1.985338	3.389349	-1.198158
				H	-1.895246	4.060432	-2.048003
Al	1.323173	-0.068734	0.638089	C	-2.858874	3.704842	-0.161083
N	-0.536462	0.193484	0.003777	C	-2.967205	2.853221	0.934558
C	-0.948727	-1.051609	-0.041787	H	-3.638030	3.112269	1.749064
C	-2.329991	-1.504285	-0.308941	C	-2.221361	1.671634	1.018790
C	-3.176415	-0.806288	-1.187330	H	-3.448668	4.616883	-0.202772
H	-2.814411	0.071670	-1.706694	C	-2.343756	0.796951	2.261547
C	-4.483429	-1.234210	-1.393145	H	-1.716124	-0.086959	2.132415
H	-5.120936	-0.682138	-2.079430	C	-0.271376	1.899689	-2.319673
C	-4.995641	-2.355894	-0.725799	H	0.202773	0.936728	-2.116645
C	-4.146298	-3.048728	0.147244	C	-1.799463	1.533509	3.499258
H	-4.521186	-3.918737	0.680756	H	-2.367926	2.448963	3.703848
C	-2.831002	-2.641152	0.345253	H	-1.868779	0.888709	4.383930
H	-2.189649	-3.186867	1.029425	H	-0.748937	1.792860	3.342773
C	-6.411431	-2.819828	-0.965578	C	-3.789246	0.310465	2.474331
H	-6.459197	-3.499269	-1.827045	H	-4.163736	-0.222221	1.594125
H	-6.808750	-3.360916	-0.100590	H	-3.836384	-0.370400	3.332512
H	-7.078596	-1.977802	-1.178389	H	-4.468091	1.147110	2.678429
C	-1.359082	1.364339	-0.055291	C	0.858201	2.940645	-2.416580
C	-1.216496	2.220712	-1.166741	H	1.439834	2.963104	-1.491846

H	1.541554	2.680508	-3.233820	C	4.317465	-0.274498	-1.569231
H	0.460550	3.943972	-2.613629	C	3.788818	-1.637419	-2.042576
C	-1.027741	1.771803	-3.655437	C	4.376983	-2.836011	-1.280100
H	-1.509783	2.714766	-3.939414	C	3.939521	-2.960028	0.185274
H	-0.334033	1.497808	-4.459092	C	4.209011	-1.727429	1.041872
H	-1.806159	1.001125	-3.606445	H	5.386380	-0.345578	-1.335289
O	4.164493	1.501021	0.097071	H	2.694213	-1.643457	-1.978901
O	1.185691	0.634375	2.212192	H	5.475326	-2.777090	-1.323240
C	2.197420	0.927447	3.139976	H	2.871497	-3.194586	0.238976
H	2.743523	0.026547	3.467194	H	4.217668	0.473330	-2.362170
H	2.936693	1.635030	2.734713	H	4.039822	-1.753014	-3.103888
H	1.749141	1.383032	4.034278	H	4.099730	-3.761579	-1.800140
C	5.363059	1.365446	0.842715	H	4.469104	-3.803297	0.650290
H	6.149363	0.826612	0.294450	H	4.021116	-1.939920	2.098762
H	5.712823	2.381646	1.038733	H	5.250062	-1.400059	0.943985
H	5.180014	0.862082	1.800052	O	2.269786	0.645276	-0.708496
S	0.342834	-2.189951	0.309702	O	3.343018	-0.617715	0.738303
C	3.547516	0.340267	-0.399815				

Table S16. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state TS3a

	Coordinates (Angstroms)						
Atom	X	Y	Z	C	-2.466315	-1.215660	-0.650417
Al	1.325213	-0.645575	0.682580	C	-3.196871	-0.189987	-1.274726
N	-0.412243	0.033322	0.016407	H	-2.708313	0.732266	-1.557693
C	-1.026127	-1.080419	-0.331134	C	-4.556387	-0.343422	-1.526976
				H	-5.099092	0.462855	-2.014547

C	-5.239413	-1.508656	-1.153741	H	-1.719838	0.004348	4.478444
C	-4.507845	-2.527835	-0.529426	H	-0.443181	0.919066	3.655412
H	-5.014413	-3.439817	-0.222823	C	-3.642063	0.134665	2.499438
C	-3.143932	-2.393349	-0.292526	H	-4.069664	-0.138594	1.529514
H	-2.595814	-3.192081	0.195485	H	-3.811382	-0.696369	3.194397
C	-6.711710	-1.672308	-1.441595	H	-4.194564	1.002044	2.880710
H	-6.869043	-2.128566	-2.428138	C	1.314403	3.123509	-1.942578
H	-7.195337	-2.319834	-0.702648	H	1.886493	3.071013	-1.013246
H	-7.230249	-0.707741	-1.442408	H	1.986005	2.888769	-2.777950
C	-1.030570	1.308484	0.226529	H	0.963638	4.153087	-2.081083
C	-0.746647	2.344800	-0.688702	C	-0.664241	2.181212	-3.217716
C	-1.337621	3.594343	-0.474068	H	-1.146712	3.157789	-3.344477
H	-1.145177	4.401238	-1.176063	H	-0.007260	2.016859	-4.080560
C	-2.167298	3.818919	0.621487	H	-1.446267	1.414459	-3.242915
C	-2.411054	2.789664	1.525776	O	4.059277	0.686623	1.459246
H	-3.047166	2.974112	2.387075	O	1.043019	-0.693428	2.390395
C	-1.851802	1.517357	1.355206	C	1.859997	-1.217982	3.400908
H	-2.617602	4.796481	0.773394	H	2.037765	-2.300073	3.279800
C	-2.134762	0.430830	2.386965	H	2.841895	-0.719800	3.440573
H	-1.636694	-0.488429	2.074692	H	1.373476	-1.072431	4.376408
C	0.143946	2.125685	-1.907216	C	5.314996	0.076934	1.762959
H	0.573719	1.124425	-1.826465	H	6.145991	0.575938	1.251762
C	-1.525656	0.802127	3.751186	H	5.439466	0.186147	2.841176
H	-1.955758	1.730890	4.146176	H	5.289914	-0.985874	1.505160

S	0.039671	-2.459130	-0.321574	H	2.223351	-2.150297	-2.118302
C	3.506360	0.502784	0.237715	H	4.615102	1.744157	-0.983878
C	4.408023	0.664863	-0.968147	H	4.232168	0.871852	-3.089994
C	3.809740	0.224944	-2.311842	H	3.890386	-1.349222	-3.771206
C	4.098398	-1.235283	-2.699350	H	3.536672	-3.288627	-2.382756
C	3.295290	-2.306692	-1.951362	H	3.042279	-3.299344	-0.052111
C	3.540404	-2.403095	-0.445211	H	4.616146	-2.515171	-0.243152
H	5.366654	0.165257	-0.800809	O	2.281744	0.897803	0.168555
H	2.730928	0.414897	-2.306696	O	3.057165	-1.294730	0.302434
H	5.175174	-1.430860	-2.578556				

Table S17. Cartesian coordinate of $S^{Pr}AlOMe_2$ in state 4a

	Coordinates (Angstroms)			C	-3.707481	-2.424209	0.201144
Atom	X	Y	Z	H	-3.267450	-3.205884	0.811092
Al	0.997867	-1.299434	0.597963	C	-7.169075	-1.374723	-1.014994
N	-0.630455	-0.415688	0.007973	H	-7.419517	-1.929164	-1.929215
C	-1.426313	-1.465208	-0.088130	H	-7.714756	-1.842997	-0.189427
C	-2.879188	-1.434621	-0.355926	H	-7.545622	-0.354080	-1.139951
C	-3.474165	-0.424089	-1.133638	C	-1.026728	0.959926	0.018882
H	-2.867564	0.354263	-1.576357	C	-0.538858	1.787422	-1.017606
C	-4.848761	-0.413605	-1.341731	C	-0.921689	3.131884	-1.011324
H	-5.286118	0.373663	-1.950691	H	-0.575559	3.793052	-1.798489
C	-5.680224	-1.388747	-0.772853	C	-1.733154	3.643322	0.000862
C	-5.083560	-2.390600	0.004435	C	-2.155734	2.818597	1.037588
H	-5.705898	-3.155019	0.462777	H	-2.756242	3.234359	1.841601

C	-1.809909	1.461792	1.077454	C	2.441169	-0.789656	2.985268
H	-2.018237	4.691967	-0.010735	H	3.354943	-0.824632	2.374028
C	-2.231194	0.613469	2.272363	H	2.486342	0.113680	3.608359
H	-1.956545	-0.426244	2.083376	H	2.445083	-1.660955	3.656708
C	0.355650	1.211483	-2.112809	C	8.057030	-3.448299	-3.656661
H	1.025199	0.484765	-1.639353	H	7.894985	-2.743014	-4.480198
C	-1.451870	1.044160	3.529656	H	8.903071	-4.092775	-3.902427
H	-1.646939	2.094213	3.778717	H	7.161771	-4.068488	-3.529944
H	-1.749870	0.430729	4.388423	S	-0.582076	-2.981979	0.192439
H	-0.377745	0.910320	3.369568	C	7.586890	-1.878987	-1.854964
C	-3.753209	0.644160	2.498913	C	6.253934	-1.589606	-2.529212
H	-4.294692	0.328895	1.600926	C	5.415671	-0.576963	-1.745406
H	-4.024303	-0.031953	3.317888	C	4.111596	-0.180900	-2.452100
H	-4.101596	1.647198	2.771588	C	3.140870	-1.337427	-2.742298
C	1.249712	2.259283	-2.791353	C	2.773479	-2.155706	-1.500899
H	1.808144	2.848063	-2.055765	H	5.710755	-2.535488	-2.653354
H	1.973259	1.758464	-3.443340	H	5.194538	-0.982316	-0.752426
H	0.671461	2.950960	-3.415845	H	4.346099	0.330392	-3.397273
C	-0.468920	0.450903	-3.170685	H	2.223318	-0.925249	-3.181208
H	-1.199021	1.118226	-3.645334	H	6.442973	-1.223677	-3.549009
H	0.185606	0.055613	-3.956399	H	6.023224	0.317519	-1.570253
H	-1.009905	-0.394186	-2.735248	H	3.594674	0.548943	-1.820127
O	8.420745	-2.783196	-2.446406	H	3.560035	-2.021727	-3.494171
O	1.267140	-0.762411	2.203048	H	1.993754	-2.887141	-1.766313

H	3.649825	-2.733544	-1.167799	O	2.359781	-1.315803	-0.447039
O	7.949101	-1.354839	-0.829615				

Table S18. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$

	Coordinates (Angstroms)						
Atom	X	Y	Z	C	4.337723	1.342381	3.305595
				H	3.891293	0.633210	3.996995
Al	0.473616	6.140570	0.692281	C	5.720863	1.361247	3.138262
N	3.268837	3.999714	0.939598	C	6.299269	2.262791	2.249541
C	3.064569	5.264583	1.240045	H	7.377881	2.270341	2.118954
C	3.728605	6.037743	2.319074	C	5.514605	3.158792	1.513106
C	4.134136	5.503999	3.553119	Al	2.457551	3.347005	-0.694621
H	3.957341	4.464164	3.788088	N	-0.337817	5.487805	-0.941853
C	4.750477	6.318281	4.498702	C	-0.133334	4.222973	-1.242261
H	5.041552	5.890108	5.454454	C	-0.796986	3.449601	-2.321362
C	5.002232	7.673698	4.244773	C	-1.203057	3.983310	-3.555252
C	4.587527	8.202088	3.013889	H	-1.027079	5.023324	-3.790022
H	4.761170	9.252667	2.795178	C	-1.818880	3.168778	-4.500955
C	3.949676	7.404706	2.070484	H	-2.110376	3.596954	-5.456577
H	3.624627	7.828263	1.126702	C	-2.069565	1.813106	-4.247324
C	5.717200	8.533231	5.257457	C	-1.654332	1.284753	-3.016602
H	5.522367	8.194370	6.280135	H	-1.827137	0.233989	-2.798115
H	5.414549	9.582403	5.178235	C	-1.017009	2.082406	-2.073073
H	6.803358	8.493259	5.101280	H	-0.691544	1.658866	-1.129428
C	4.122042	3.126298	1.708270	C	-2.783959	0.953263	-5.260146
C	3.509826	2.221165	2.598633	H	-2.589398	1.292457	-6.282766

H	-2.480570	-0.095711	-5.181133	C	1.627572	2.420913	4.286530
H	-3.870140	0.992447	-5.103925	H	0.539072	2.397794	4.408879
C	-1.191099	6.361135	-1.710536	H	2.050690	1.648601	4.939486
C	-0.578966	7.266245	-2.600984	H	1.982548	3.396311	4.637174
C	-1.406930	8.145006	-3.307896	C	1.400755	0.871370	2.282360
H	-0.960563	8.854168	-3.999345	H	0.307504	0.890257	2.371348
C	-2.790054	8.126133	-3.140445	H	1.669337	0.729036	1.231724
C	-3.368379	7.224586	-2.251676	H	1.770779	0.011062	2.854015
H	-4.446981	7.217026	-2.121006	C	-3.246988	5.370582	-0.534573
C	-2.583645	6.328615	-1.515278	H	-2.473271	4.736634	-0.094936
H	-3.415767	8.815967	-3.700546	C	0.931666	7.298922	-2.813126
H	6.346520	0.671407	3.698416	H	1.379977	6.480093	-2.244491
C	6.178048	4.116815	0.532443	C	-3.906472	6.144440	0.621891
H	5.404403	4.750877	0.092846	H	-4.716814	6.787058	0.258176
C	6.837416	3.342932	-0.624073	H	-4.331306	5.449403	1.355946
H	7.262293	4.037945	-1.358125	H	-3.175846	6.782403	1.131645
H	7.647706	2.700223	-0.260403	C	-4.249671	4.435808	-1.235415
H	6.106703	2.705056	-1.133811	H	-3.765785	3.873958	-2.041211
C	7.180854	5.051435	1.233310	H	-4.665916	3.719313	-0.517426
H	7.597183	5.767899	0.515338	H	-5.085933	4.997451	-1.667879
H	6.697045	5.613325	2.039121	C	1.530213	8.616067	-2.285278
H	8.017052	4.489677	1.665750	H	1.261821	8.758576	-1.234620
C	1.999170	2.188437	2.810571	H	2.623449	8.597125	-2.374455
H	1.550908	3.007375	2.242052	H	1.160124	9.476291	-2.857015

C	1.303035	7.066094	-4.289096	H	3.806428	5.595336	-3.344978
H	0.879897	7.838307	-4.942155	H	3.943032	5.978931	-1.618909
H	2.391519	7.089080	-4.411610	H	4.874152	4.627160	-2.315920
H	0.947915	6.090655	-4.639479	C	-0.975044	4.336223	2.343313
O	0.046292	7.814365	0.700035	H	-0.875207	3.892269	3.342673
O	0.107753	5.196950	2.098544	H	-1.943019	4.860418	2.313686
O	2.885006	1.673276	-0.702693	H	-1.011760	3.508794	1.616575
O	2.823348	4.290865	-2.100724	C	0.286020	8.732039	1.742266
C	2.646654	0.755860	-1.745447	H	-0.056463	9.730643	1.437643
H	3.181917	1.029324	-2.667958	H	-0.251389	8.461015	2.664246
H	2.992559	-0.241988	-1.442228	H	1.356447	8.809135	1.993097
H	1.576100	0.675822	-1.994802	O	0.665873	3.548590	-0.460694
C	3.906226	5.151453	-2.345584	O	2.265381	5.939218	0.458703

Table S19. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state 1c

	Coordinates (Angstroms)						
Atom	X	Y	Z	C	-5.542932	2.761907	0.495321
				H	-5.881569	3.579739	1.127123
Al	-0.591994	2.213912	-0.138348	C	-4.340028	2.127018	0.786275
N	-2.245864	-0.813644	0.337384	H	-3.739591	2.455985	1.627070
C	-2.574263	0.448516	0.397631	C	-7.633873	3.044830	-0.908439
C	-3.881821	1.055321	0.000065	H	-7.855761	3.028392	-1.980777
C	-4.650206	0.665681	-1.107684	H	-7.638420	4.087879	-0.574392
H	-4.320398	-0.139044	-1.748441	H	-8.460747	2.534549	-0.396575
C	-5.840623	1.325175	-1.404461	C	-3.124946	-1.772363	-0.285015
H	-6.410481	1.015915	-2.277396	C	-2.850830	-2.159874	-1.612541
C	-6.317275	2.371968	-0.605458	C	-3.685472	-3.116150	-2.199695

H	-3.493678	-3.431228	-3.221942	C	3.262952	4.029374	2.232177
C	-4.753313	-3.672167	-1.497480	H	3.413245	4.346943	3.259889
C	-4.996919	-3.278052	-0.185079	C	3.991163	4.641261	1.212270
H	-5.823427	-3.721555	0.363832	C	3.795925	4.255990	-0.110388
C	-4.188714	-2.325246	0.446183	H	4.356373	4.746548	-0.901616
Al	-0.478066	-1.490963	1.115006	C	2.878395	3.251706	-0.443153
N	1.189495	1.629087	0.308438	H	4.705469	5.425178	1.450700
C	1.472434	0.354001	0.122796	H	-5.390968	-4.414029	-1.971675
C	2.847415	-0.214320	0.018520	C	-4.439942	-1.949636	1.899614
C	3.966238	0.252514	0.724687	H	-3.788472	-1.109571	2.151489
H	3.878037	1.080527	1.414124	C	-4.040326	-3.116784	2.821242
C	5.207260	-0.361686	0.560111	H	-4.148550	-2.834353	3.876132
H	6.058620	0.008583	1.126555	H	-4.671906	-3.995045	2.639054
C	5.377553	-1.438541	-0.318454	H	-2.999850	-3.400657	2.633359
C	4.253903	-1.901282	-1.018004	C	-5.884965	-1.484472	2.145424
H	4.353900	-2.747222	-1.693578	H	-6.008523	-1.160929	3.186066
C	3.008657	-1.310458	-0.846750	H	-6.140874	-0.643505	1.491382
H	2.140653	-1.698104	-1.366926	H	-6.607906	-2.288216	1.962580
C	6.729960	-2.078469	-0.517709	C	-1.681684	-1.570673	-2.396201
H	7.396945	-1.884486	0.328931	H	-1.263815	-0.736821	-1.830523
H	6.643348	-3.163494	-0.643747	C	-2.113261	-0.989642	-3.753628
H	7.220728	-1.686439	-1.418154	H	-1.254874	-0.515501	-4.243070
C	2.173268	2.636492	0.604812	H	-2.502701	-1.759973	-4.430489
C	2.338451	3.017871	1.953138	H	-2.886070	-0.223185	-3.629961

C	-0.566646	-2.618799	-2.572099	O	-0.606473	3.904014	0.225085
H	0.301837	-2.170104	-3.070893	O	-0.921295	1.759232	-1.780916
H	-0.253166	-3.012309	-1.601167	O	-1.025477	-3.115106	0.833667
H	-0.909806	-3.463034	-3.183795	O	-0.343964	-0.802869	2.720083
C	2.643551	2.876684	-1.901024	C	-0.500357	-4.394219	1.007208
H	1.930757	2.048982	-1.936980	H	-0.159670	-4.579268	2.041808
C	1.527704	2.364576	3.069016	H	-1.276054	-5.140579	0.781176
H	1.111837	1.423818	2.694764	H	0.358836	-4.586807	0.345589
C	1.990218	4.049064	-2.656661	C	-1.332783	-0.325816	3.594186
H	2.658839	4.917648	-2.698657	H	-0.859299	0.027890	4.523396
H	1.750679	3.754206	-3.685200	H	-1.889606	0.519473	3.168257
H	1.064477	4.356836	-2.159318	H	-2.055093	-1.109804	3.874298
C	3.935295	2.397919	-2.586424	C	-1.602722	2.522171	-2.744945
H	4.370522	1.546303	-2.051885	H	-1.262330	2.241458	-3.751875
H	3.725266	2.086201	-3.616384	H	-2.690067	2.345749	-2.700852
H	4.689146	3.193290	-2.627551	H	-1.435449	3.605034	-2.626487
C	0.337187	3.260531	3.465333	C	-1.719188	4.738854	0.419895
H	-0.269203	3.508319	2.591139	H	-1.474879	5.764468	0.109105
H	-0.293969	2.750782	4.203026	H	-2.607539	4.421621	-0.150670
H	0.692822	4.201102	3.904948	H	-2.010244	4.775547	1.482979
C	2.380471	2.023214	4.302491	C	2.223934	-2.813391	2.268571
H	2.708205	2.922583	4.837273	C	2.199432	-2.331117	3.697817
H	1.792730	1.420767	5.005217	C	3.448409	-1.500171	4.066903
H	3.274490	1.452404	4.029663	C	4.704982	-2.328601	4.358295

C	5.169868	-3.210535	3.192245	H	5.521260	-1.652774	4.642797
C	4.141536	-4.244204	2.739869	H	6.076772	-3.753248	3.489464
H	2.104087	-3.190533	4.375374	H	4.611388	-5.016384	2.127455
H	3.648479	-0.785964	3.259959	H	3.656291	-4.735603	3.592627
H	4.515212	-2.969239	5.232364	O	1.450825	-2.404859	1.413135
H	5.433169	-2.595645	2.322848	O	3.135938	-3.700360	1.854585
H	1.294549	-1.723226	3.771641	O	-1.720611	1.293550	0.926795
H	3.199382	-0.904517	4.951471	O	0.483204	-0.455343	-0.084981

Table S20. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state TS1c

	Coordinates (Angstroms)			C	-7.549560	2.755457	-0.031884
Atom	X	Y	Z	H	-7.437980	3.692050	-0.594382
Al	-0.498307	2.159200	0.314779	H	-7.975394	3.010652	0.944293
N	-1.970548	-1.043373	0.246786	H	-8.275498	2.137238	-0.570596
C	-2.348120	0.169188	0.557865	C	-2.786818	-1.897571	-0.582076
C	-3.699414	0.772174	0.337335	C	-2.535486	-1.910780	-1.970209
C	-4.539387	0.515037	-0.758566	C	-3.308054	-2.761313	-2.767665
H	-4.234226	-0.166824	-1.538047	H	-3.131021	-2.786234	-3.839543
C	-5.772501	1.153914	-0.865824	C	-4.291724	-3.577619	-2.213735
H	-6.398300	0.946084	-1.730481	C	-4.512759	-3.555205	-0.840118
C	-6.221500	2.052666	0.109734	H	-5.272359	-4.201357	-0.409100
C	-5.383014	2.303063	1.203563	C	-3.767806	-2.718290	-0.001251
H	-5.704007	2.994464	1.979252	Al	-0.139910	-1.709073	0.849662
C	-4.140739	1.687062	1.309999	N	1.378689	1.669465	0.300107
H	-3.497232	1.907514	2.153736	C	1.647528	0.410160	-0.004987

C	2.988980	-0.166765	-0.272672	C	-3.987562	-2.747488	1.503115
C	4.186684	0.342847	0.251219	H	-3.483137	-1.878059	1.928634
H	4.181285	1.218101	0.884755	C	-3.324724	-4.003386	2.100871
C	5.399372	-0.275822	-0.037139	H	-3.414189	-4.010784	3.195011
H	6.314446	0.128340	0.388978	H	-3.804804	-4.912105	1.717554
C	5.463446	-1.402030	-0.868050	H	-2.265630	-4.041096	1.826030
C	4.263079	-1.907260	-1.386537	C	-5.469222	-2.634239	1.896254
H	4.282660	-2.786280	-2.026108	H	-5.567880	-2.569610	2.986678
C	3.045133	-1.309584	-1.087945	H	-5.922917	-1.739105	1.456169
H	2.125713	-1.720769	-1.486053	H	-6.048698	-3.504685	1.567667
C	6.786382	-2.038620	-1.216463	C	-1.453813	-1.044122	-2.605323
H	6.688328	-3.122156	-1.342961	H	-1.063773	-0.360883	-1.852237
H	7.176986	-1.635015	-2.160170	C	-1.991983	-0.158424	-3.741372
H	7.539646	-1.850498	-0.444299	H	-1.194300	0.499270	-4.105176
C	2.351939	2.729004	0.212752	H	-2.357736	-0.748459	-4.590737
C	2.803639	3.346744	1.396969	H	-2.809648	0.480438	-3.391208
C	3.741296	4.378686	1.283835	C	-0.283314	-1.922368	-3.085062
H	4.111870	4.860535	2.184490	H	0.545031	-1.295353	-3.438259
C	4.205520	4.798222	0.039880	H	0.071019	-2.555897	-2.266596
C	3.720947	4.196412	-1.117193	H	-0.589862	-2.576610	-3.911159
H	4.072106	4.539186	-2.086538	C	2.250639	2.560840	-2.360903
C	2.781312	3.159955	-1.061190	H	1.523806	1.781983	-2.123482
H	4.936432	5.599851	-0.027244	C	2.331311	2.905500	2.777379
H	-4.880326	-4.232884	-2.850772	H	1.571979	2.130030	2.640439

C	1.481984	3.619023	-3.172892	C	-1.413394	-1.201717	3.596858
H	2.137341	4.437809	-3.493584	H	-1.022281	-0.740115	4.513685
H	1.046393	3.162841	-4.069820	H	-2.189291	-0.540608	3.199984
H	0.667493	4.040718	-2.577629	H	-1.852743	-2.176142	3.844769
C	3.374296	1.918648	-3.195300	C	-1.928127	3.015385	-1.966633
H	3.907563	1.152945	-2.623450	H	-1.754927	3.006728	-3.051671
H	2.955526	1.446518	-4.092050	H	-2.974991	2.719028	-1.793882
H	4.105800	2.666485	-3.524590	H	-1.813193	4.055361	-1.619879
C	1.668335	4.062560	3.544218	C	-1.671392	4.312549	1.698753
H	0.852321	4.479065	2.951226	H	-1.422980	5.359003	1.927436
H	1.264683	3.702471	4.498742	H	-2.528322	4.320251	1.005279
H	2.388194	4.859157	3.768003	H	-2.012034	3.842752	2.636720
C	3.484728	2.296163	3.597524	C	1.262258	-2.034550	2.956049
H	4.272183	3.036190	3.782330	C	1.921855	-0.949757	3.790260
H	3.119154	1.947477	4.571140	C	3.293344	-1.398508	4.331588
H	3.942881	1.443481	3.084943	C	3.198775	-2.211808	5.631547
O	-0.543962	3.663803	1.170542	C	2.432395	-3.536990	5.515447
O	-1.031505	2.133804	-1.337464	C	1.015125	-3.406938	4.957842
O	-0.428051	-3.253486	0.117969	H	1.275654	-0.634271	4.616814
O	-0.373776	-1.327846	2.657048	H	3.819413	-1.966447	3.553492
C	0.362137	-4.412074	0.090965	H	2.711856	-1.587586	6.395864
H	1.146490	-4.408741	0.859657	H	2.975382	-4.237621	4.868281
H	-0.271373	-5.298070	0.248871	H	2.026147	-0.096815	3.119297
H	0.850118	-4.529130	-0.891208	H	3.895140	-0.503419	4.524127

H	4.210064	-2.419077	6.003847	O	1.552072	-2.098194	1.705919
H	2.368383	-4.003812	6.507608	O	1.019950	-3.242669	3.528062
H	0.455410	-4.332546	5.113429	O	-1.503763	0.935383	1.213835
H	0.458568	-2.594718	5.441170	O	0.626860	-0.370346	-0.148889

Table S21. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state 2c

Coordinates (Angstroms)				C	-2.629219	-1.918640	-0.679904
Atom	X	Y	Z	C	-2.513070	-1.925478	-2.088132
Al	-0.225571	2.239826	-0.080206	C	-3.214862	-2.911401	-2.791507
N	-1.846088	-0.950926	0.040468	H	-3.141618	-2.943664	-3.875062
C	-2.260324	0.266617	0.333545	C	-4.005061	-3.847344	-2.126458
C	-3.674937	0.725449	0.351190	C	-4.104688	-3.812714	-0.738340
C	-4.676059	0.305520	-0.537803	H	-4.723786	-4.543512	-0.225418
H	-4.449838	-0.383245	-1.339474	C	-3.415977	-2.853555	0.014349
C	-5.976614	0.787414	-0.403193	Al	-0.087571	-1.402723	0.667538
H	-6.736032	0.459296	-1.108645	N	1.621418	1.638772	-0.266660
C	-6.325259	1.677054	0.620387	C	1.916856	0.364717	-0.413380
C	-5.319351	2.088038	1.506871	C	3.283064	-0.228274	-0.469289
H	-5.563998	2.775511	2.313183	C	4.422218	0.441487	-0.946079
C	-4.012482	1.635715	1.369044	H	4.350163	1.450960	-1.323241
H	-3.239452	1.962046	2.054806	C	5.664552	-0.186078	-0.937769
C	-7.733159	2.205242	0.747694	H	6.529860	0.352497	-1.316235
H	-7.838469	3.165521	0.225522	C	5.822593	-1.487437	-0.444446
H	-8.004123	2.374462	1.795362	C	4.682008	-2.155153	0.021184
H	-8.462996	1.514583	0.312919	H	4.772202	-3.167827	0.406621

C	3.431321	-1.548907	-0.005370	H	-5.326712	-1.599330	1.587212
H	2.567568	-2.105756	0.341797	H	-5.657469	-3.339486	1.670480
C	7.171777	-2.162771	-0.447962	C	-1.677465	-0.893680	-2.843614
H	7.263315	-2.879466	0.374931	H	-1.306375	-0.146303	-2.140482
H	7.327532	-2.717649	-1.382773	C	-2.515667	-0.133212	-3.887189
H	7.985457	-1.435221	-0.361025	H	-1.907039	0.652846	-4.347183
C	2.619039	2.679375	-0.147433	H	-2.875386	-0.792981	-4.685782
C	3.284968	2.868588	1.079371	H	-3.386290	0.346057	-3.425958
C	4.201054	3.922793	1.168188	C	-0.441292	-1.538959	-3.494981
H	4.725350	4.089697	2.104840	H	0.144137	-0.777762	-4.023698
C	4.450141	4.760785	0.085712	H	0.206738	-1.995138	-2.741744
C	3.780201	4.553424	-1.116056	H	-0.727317	-2.313535	-4.217347
H	3.977963	5.207072	-1.961036	C	2.158617	3.310650	-2.603923
C	2.851837	3.515603	-1.259928	H	1.484746	2.456017	-2.524961
H	5.165124	5.574116	0.178806	C	3.056908	1.975287	2.292723
H	-4.543426	-4.603519	-2.691984	H	2.338048	1.194788	2.030635
C	-3.525384	-2.840474	1.531571	C	1.284445	4.524328	-2.965805
H	-2.893099	-2.038545	1.917671	H	1.888855	5.429156	-3.104577
C	-2.988799	-4.153396	2.125498	H	0.740821	4.332963	-3.898312
H	-3.000903	-4.103155	3.219581	H	0.548820	4.717225	-2.180356
H	-3.594531	-5.013962	1.815377	C	3.171434	3.000900	-3.722567
H	-1.956369	-4.314656	1.801843	H	3.757229	2.102538	-3.496237
C	-4.965739	-2.551017	1.991859	H	2.646555	2.829054	-4.669762
H	-5.007273	-2.496234	3.086361	H	3.873365	3.829199	-3.876301

C	2.432670	2.773680	3.451053	C	-0.965944	3.876211	2.071728
H	1.500049	3.242371	3.126324	H	-0.532293	4.687491	2.673430
H	2.219381	2.109784	4.296967	H	-1.969040	4.203101	1.751489
H	3.107883	3.562255	3.804691	H	-1.092844	3.000599	2.728644
C	4.365016	1.283395	2.723292	C	-0.376301	-0.975405	3.380798
H	5.124089	2.016387	3.020640	C	0.452979	-0.534440	4.602374
H	4.186102	0.627544	3.581286	C	1.933979	-0.927253	4.533290
H	4.780385	0.679406	1.910123	C	2.224423	-2.417952	4.740559
O	-0.124072	3.601532	0.978571	C	1.445434	-3.357831	3.810085
O	-0.785171	2.378186	-1.715560	C	-0.066161	-3.354571	4.056404
O	0.223132	-3.092654	0.514917	H	-0.011058	-0.913788	5.520972
O	-1.582984	-0.214869	3.281586	H	2.315329	-0.617942	3.557109
C	0.354186	-3.921019	-0.612787	H	1.993068	-2.692165	5.781392
H	1.186485	-3.603032	-1.262319	H	1.627780	-3.131601	2.754499
H	0.562627	-4.949801	-0.287592	H	0.372687	0.557496	4.623950
H	-0.561447	-3.940710	-1.221892	H	2.483924	-0.350728	5.288992
C	-2.521330	-0.363485	4.336477	H	3.301866	-2.587760	4.611822
H	-2.181080	0.123775	5.261600	H	1.795591	-4.385390	3.980405
H	-3.437226	0.127927	3.996529	H	-0.504889	-4.274292	3.662256
H	-2.732533	-1.419405	4.539697	H	-0.263180	-3.332977	5.141209
C	-1.969091	2.999824	-2.152282	O	0.324362	-0.734727	2.232497
H	-2.011542	2.979321	-3.249841	O	-0.823725	-2.328176	3.416060
H	-2.870985	2.488721	-1.778088	O	-1.381767	1.117264	0.747346
H	-2.027190	4.054004	-1.837374	O	0.929996	-0.474998	-0.499880

Table S22. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state TS2c

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	-0.423249	2.166327	0.108043
N	-1.781177	-1.128852	0.256471
C	-2.226632	0.087818	0.482455
C	-3.593768	0.621114	0.254964
C	-4.542734	0.068756	-0.622995
H	-4.313993	-0.814209	-1.200471
C	-5.789839	0.668178	-0.778113
H	-6.501443	0.229505	-1.473214
C	-6.144060	1.819828	-0.063981
C	-5.202917	2.354055	0.826555
H	-5.453406	3.240215	1.404610
C	-3.950470	1.773250	0.980393
H	-3.237634	2.200845	1.674938
C	-7.484265	2.481519	-0.267778
H	-7.420369	3.256071	-1.043548
H	-7.835151	2.967790	0.648580
H	-8.244588	1.761285	-0.587139
C	-2.432881	-2.123209	-0.554304
C	-2.249714	-2.069674	-1.956234
C	-2.845060	-3.074639	-2.728018
H	-2.718451	-3.053951	-3.806758
C	-3.594681	-4.091665	-2.142945
C	-3.752867	-4.126052	-0.760655
H	-4.340162	-4.920060	-0.309059
C	-3.167034	-3.154793	0.059552
Al	0.040219	-1.368872	0.902648
N	1.439826	1.681738	-0.185499
C	1.799312	0.431941	-0.403225
C	3.194037	-0.066000	-0.573119
C	4.239084	0.670731	-1.152911
H	4.066843	1.668811	-1.528350
C	5.515046	0.123839	-1.256943
H	6.304521	0.710884	-1.719836
C	5.801373	-1.158412	-0.772491
C	4.752236	-1.894842	-0.205954
H	4.941666	-2.897647	0.169357
C	3.468480	-1.369181	-0.118607
H	2.678200	-1.969819	0.316871
C	7.200032	-1.720974	-0.835849
H	7.755080	-1.487461	0.082504
H	7.190025	-2.811086	-0.941256
H	7.765353	-1.300651	-1.674233
C	2.395461	2.766141	-0.093849
C	3.130674	2.949927	1.094139
C	4.040949	4.012362	1.140198
H	4.624454	4.166755	2.043584

C	4.207459	4.872903	0.059697	H	0.455290	-2.013616	-2.581349
C	3.449926	4.687390	-1.093186	H	-0.431973	-2.246801	-4.103657
H	3.572979	5.367264	-1.931765	C	1.720731	3.471390	-2.478618
C	2.528902	3.638329	-1.194917	H	1.083008	2.590720	-2.381056
H	4.920392	5.691406	0.118123	C	2.966346	2.048371	2.309978
H	-4.052844	-4.857532	-2.763275	H	2.199400	1.303347	2.099118
C	-3.361156	-3.205268	1.566887	C	0.782624	4.674501	-2.685695
H	-2.659654	-2.496645	2.012592	H	1.348769	5.601333	-2.839436
C	-3.045126	-4.598348	2.136413	H	0.148015	4.515124	-3.565230
H	-3.110576	-4.589374	3.230255	H	0.133056	4.814247	-1.816495
H	-3.751574	-5.355204	1.776865	C	2.623574	3.252835	-3.706737
H	-2.035046	-4.911318	1.856191	H	3.252420	2.362975	-3.588976
C	-4.783026	-2.753435	1.952076	H	2.010871	3.113484	-4.605360
H	-4.905286	-2.752413	3.042278	H	3.284192	4.109783	-3.884326
H	-4.991571	-1.743864	1.583010	C	2.475215	2.850354	3.528746
H	-5.536145	-3.429390	1.528602	H	1.559457	3.394475	3.283497
C	-1.458561	-0.964535	-2.648645	H	2.248794	2.171273	4.357303
H	-1.132300	-0.236262	-1.909267	H	3.226500	3.574467	3.868173
C	-2.320215	-0.189516	-3.661615	C	4.269119	1.290883	2.629572
H	-1.743770	0.650431	-4.063360	H	5.078896	1.980615	2.898529
H	-2.636678	-0.820360	-4.501363	H	4.115010	0.613423	3.477787
H	-3.217004	0.222188	-3.187237	H	4.602927	0.692624	1.776348
C	-0.188955	-1.523029	-3.315666	O	-0.425635	3.615536	1.037592
H	0.383251	-0.705644	-3.769862	O	-1.138606	2.193174	-1.471782

O	0.390099	-3.063906	0.824663	C	1.455660	-1.147439	4.454604
O	-0.035404	0.662621	3.831450	C	2.005385	-2.549928	4.152257
C	0.547092	-3.925444	-0.275037	C	1.157001	-3.689818	4.731899
H	1.350382	-3.588797	-0.950975	C	-0.259026	-3.774574	4.150823
H	0.816075	-4.929433	0.082894	C	-1.084471	-2.499790	4.328021
H	-0.373736	-4.016947	-0.869292	H	1.096588	-1.090474	5.489256
C	-0.942721	0.774952	4.911166	H	2.096628	-2.669966	3.066865
H	-0.541202	0.364073	5.850128	H	1.092889	-3.568628	5.824545
H	-1.117462	1.844680	5.051546	H	-0.209256	-3.987948	3.077419
H	-1.896626	0.281623	4.686517	H	2.251925	-0.404055	4.359524
C	-2.200772	2.982410	-1.947369	H	3.018776	-2.621932	4.567243
H	-2.037702	3.225883	-3.006788	H	1.669096	-4.645187	4.557678
H	-3.160651	2.450151	-1.869855	H	-0.800196	-4.602313	4.630030
H	-2.300377	3.932127	-1.399294	H	-2.147532	-2.708431	4.181724
C	-1.020313	3.867928	2.284008	H	-0.973711	-2.087332	5.339491
H	-0.444022	4.631380	2.825941	O	0.896495	-0.565588	2.219729
H	-2.046896	4.255716	2.169276	O	-0.783864	-1.496252	3.347769
H	-1.061236	2.967850	2.914983	O	-1.362799	0.895512	1.039126
C	0.384086	-0.649572	3.470886	O	0.868276	-0.472167	-0.456646

Table S23. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state 3c

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	-0.550790	2.309673	-0.416870
N	-1.947026	-0.957001	0.320541
C	-2.309617	0.302898	0.486940
C	-3.685218	0.873227	0.466306
C	-4.833837	0.216288	-0.014789
H	-4.776470	-0.786233	-0.408832

C	-6.071095	0.852246	0.003029	H	4.060160	1.756252	0.759703
H	-6.940104	0.322240	-0.379191	C	5.374085	0.088276	0.560824
C	-6.219249	2.153070	0.500449	H	6.190977	0.608758	1.054478
C	-5.076155	2.802922	0.983101	C	5.558083	-1.230077	0.126301
H	-5.158675	3.812728	1.377438	C	4.483536	-1.867100	-0.509223
C	-3.831987	2.184308	0.963419	H	4.598659	-2.888676	-0.863096
H	-2.963294	2.719561	1.328090	C	3.264681	-1.223534	-0.682699
C	-7.559777	2.844474	0.486134	H	2.441750	-1.752558	-1.149659
H	-7.658209	3.545744	1.321512	C	6.854974	-1.959676	0.371941
H	-8.384320	2.126028	0.541411	H	7.694256	-1.266096	0.486094
H	-7.688789	3.420705	-0.439767	H	6.792176	-2.554563	1.293205
C	-2.832282	-2.029387	-0.059539	H	7.088070	-2.650884	-0.445050
C	-3.015438	-2.278025	-1.437519	C	2.192909	3.029474	0.158721
C	-3.814743	-3.366412	-1.804056	C	2.252552	3.434995	1.508807
H	-3.967118	-3.580565	-2.858122	C	2.975463	4.595782	1.805447
C	-4.422273	-4.170766	-0.843432	H	3.030036	4.935266	2.835890
C	-4.227736	-3.903221	0.508402	C	3.624007	5.322006	0.808712
H	-4.708874	-4.533052	1.250266	C	3.561438	4.892113	-0.513356
C	-3.417894	-2.841804	0.932361	H	4.072733	5.457588	-1.287570
Al	-0.047959	-1.345438	0.389692	C	2.840153	3.745324	-0.867017
N	1.343363	1.922714	-0.187533	H	4.179155	6.220850	1.063796
C	1.712600	0.672815	-0.361763	H	-5.047057	-5.006193	-1.148602
C	3.075964	0.095545	-0.225361	C	-3.229680	-2.568325	2.420221
C	4.159596	0.746936	0.390046	H	-2.367730	-1.909016	2.545291

C	-2.932724	-3.849804	3.216928	H	2.035595	4.018355	-4.242081
H	-2.727933	-3.596266	4.262066	H	1.082034	4.569765	-2.850275
H	-3.779730	-4.545963	3.210297	C	4.184809	2.947521	-2.854211
H	-2.053684	-4.364281	2.820246	H	4.651139	2.172005	-2.236839
C	-4.460687	-1.845372	3.003004	H	4.120324	2.574888	-3.883331
H	-4.307484	-1.632630	4.068131	H	4.846653	3.821676	-2.856041
H	-4.651545	-0.897778	2.491544	C	0.472499	3.448980	3.312807
H	-5.360245	-2.466771	2.908009	H	-0.264264	3.773549	2.573673
C	-2.407390	-1.390753	-2.519936	H	-0.029717	2.825696	4.062051
H	-1.899506	-0.549926	-2.042616	H	0.873887	4.334984	3.821440
C	-3.498755	-0.789898	-3.425661	C	2.639404	2.172500	3.660049
H	-3.048648	-0.116074	-4.162553	H	3.180094	3.017273	4.102821
H	-4.043558	-1.566938	-3.974845	H	2.145053	1.636104	4.476927
H	-4.223522	-0.212349	-2.842127	H	3.373984	1.498260	3.205518
C	-1.349894	-2.154417	-3.337916	O	-0.860314	3.856473	0.285862
H	-0.908046	-1.491907	-4.091464	O	-1.076979	2.075556	-2.041309
H	-0.551314	-2.517700	-2.684528	O	0.226931	-2.857670	-0.395398
H	-1.793551	-3.010884	-3.860637	O	-0.486501	-0.924834	3.706833
C	2.783737	3.304249	-2.324014	C	-0.300560	-4.150861	-0.253619
H	2.176806	2.397802	-2.384789	H	-0.914810	-4.264606	0.649375
C	1.592100	2.640620	2.631818	H	-0.934031	-4.405777	-1.114928
H	1.134495	1.740903	2.210902	H	0.516667	-4.885866	-0.200537
C	2.098283	4.364848	-3.203851	C	-0.833543	-1.388489	5.001982
H	2.654040	5.309820	-3.198711	H	-0.153084	-0.998352	5.772566

H	-1.841783	-1.016606	5.204450	C	1.039996	-4.035728	2.920905
H	-0.841315	-2.483674	5.047660	H	1.802847	-2.139977	4.803157
C	-0.458701	1.572101	-3.194838	H	3.168406	-1.154422	2.246207
H	0.210797	0.726149	-2.980135	H	3.676445	-3.745591	3.794771
H	-1.222361	1.218280	-3.901151	H	2.124539	-3.445656	1.157455
H	0.125213	2.349658	-3.711318	H	1.886230	-0.453899	4.310084
C	-0.532762	5.140103	-0.183284	H	4.024050	-1.335462	3.770861
H	-0.717148	5.252553	-1.264014	H	4.393805	-3.268645	2.258788
H	-1.148521	5.889843	0.333591	H	2.669673	-4.952194	1.890447
H	0.523379	5.383134	0.008352	H	0.439345	-4.866222	2.539881
C	0.607282	-1.579752	3.074097	H	1.268216	-4.256846	3.975757
C	1.884496	-1.478752	3.932090	O	0.780906	-0.945348	1.884016
C	3.193099	-1.732420	3.172864	O	0.147431	-2.922383	2.841458
C	3.474861	-3.205513	2.856792	O	-1.343742	1.141726	0.720733
C	2.341744	-3.927774	2.116027	O	0.763250	-0.151611	-0.719172

Table S24. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state TS3c

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	-0.550655	2.288664	-0.319023
N	-1.892413	-0.958009	0.555041
C	-2.308407	0.294755	0.638666
C	-3.719658	0.798235	0.548040
C	-4.871259	0.008057	0.362951
H	-4.803097	-1.063383	0.268305
C	-6.134075	0.589434	0.294004
H	-6.999505	-0.053165	0.150491
C	-6.311079	1.973664	0.400699
C	-5.169307	2.759784	0.595944
H	-5.269325	3.838371	0.691100
C	-3.902961	2.191608	0.670848
H	-3.048304	2.840117	0.824831
C	-7.678688	2.598612	0.280859
H	-7.757587	3.509581	0.883757
H	-8.466899	1.907431	0.597677
H	-7.887898	2.878449	-0.760282
C	-2.737994	-2.045739	0.128138
C	-2.961483	-2.218485	-1.257293
C	-3.719317	-3.323214	-1.661488
H	-3.905596	-3.475128	-2.720886
C	-4.242899	-4.222396	-0.737662
C	-4.012889	-4.030271	0.621997
H	-4.435105	-4.730109	1.336580
C	-3.250864	-2.949958	1.084155
Al	0.010812	-1.489552	0.634459
N	1.341494	1.943141	-0.081382
C	1.699884	0.680519	-0.206726
C	3.079250	0.123403	-0.108481
C	4.144775	0.734724	0.572865
H	4.022494	1.705366	1.031096
C	5.369518	0.082156	0.692332
H	6.175434	0.567643	1.237414
C	5.579819	-1.185498	0.134844
C	4.519203	-1.781227	-0.561550
H	4.656135	-2.762450	-1.009980
C	3.287887	-1.146095	-0.680581
H	2.465923	-1.639574	-1.189343
C	6.893852	-1.906920	0.308352
H	7.714029	-1.210085	0.509088
H	6.843786	-2.607795	1.152563
H	7.150635	-2.491215	-0.581849
C	2.221295	3.041090	0.202691
C	2.239995	3.554387	1.518253
C	3.061440	4.656246	1.778440
H	3.099132	5.062028	2.785657

C	3.828382	5.241190	0.772653	H	-0.591671	-2.200556	-2.806614
C	3.778090	4.730145	-0.520587	H	-1.961693	-2.761433	-3.801948
H	4.369561	5.194746	-1.304827	C	2.927601	3.107762	-2.264613
C	2.972990	3.627846	-0.833837	H	2.264926	2.239916	-2.292731
H	4.459553	6.097249	0.996541	C	1.430591	2.923792	2.646791
H	-4.832439	-5.070806	-1.075572	H	0.806465	2.133432	2.227236
C	-3.063679	-2.731063	2.581994	C	2.329726	4.163269	-3.212841
H	-2.201190	-2.077837	2.711557	H	2.952240	5.065160	-3.249108
C	-2.766802	-4.038645	3.334100	H	2.254868	3.765292	-4.231698
H	-2.514183	-3.823985	4.379301	H	1.326936	4.459782	-2.886404
H	-3.633461	-4.709887	3.351220	C	4.312871	2.638096	-2.745006
H	-1.928951	-4.575348	2.882214	H	4.720989	1.872170	-2.077271
C	-4.288450	-2.028189	3.200359	H	4.241987	2.212970	-3.753163
H	-4.146800	-1.893245	4.280630	H	5.027021	3.469316	-2.783574
H	-4.456080	-1.043006	2.757316	C	0.490744	3.939382	3.317784
H	-5.198088	-2.624070	3.054078	H	-0.194071	4.355680	2.574962
C	-2.467910	-1.230020	-2.311061	H	-0.102442	3.440097	4.093730
H	-1.909208	-0.433579	-1.817998	H	1.044297	4.756888	3.796247
C	-3.656593	-0.564958	-3.033095	C	2.356621	2.250082	3.676907
H	-3.292779	0.211697	-3.714535	H	3.036097	2.973821	4.143425
H	-4.225395	-1.293476	-3.624180	H	1.756739	1.793601	4.474241
H	-4.342640	-0.093029	-2.323286	H	2.962577	1.464155	3.212753
C	-1.506267	-1.889744	-3.316147	O	-0.847232	3.885923	0.292534
H	-1.239418	-1.174605	-4.101916	O	-1.061638	2.030658	-1.947948

O	0.265668	-2.678476	-0.644433	C	1.829785	-1.411954	3.950399
O	-0.490958	-0.614105	3.840061	C	3.037881	-1.821001	3.089261
C	-0.139219	-4.008665	-0.806706	C	3.165610	-3.327624	2.807499
H	-1.017038	-4.276602	-0.199450	C	2.145868	-3.955652	1.845982
H	-0.414196	-4.193231	-1.855532	C	0.677363	-3.882107	2.281737
H	0.673341	-4.710836	-0.555138	H	1.519153	-2.237604	4.596947
C	-0.808911	-1.316613	5.047597	H	3.022112	-1.261601	2.151840
H	-0.134094	-1.036086	5.862979	H	3.137297	-3.871454	3.764612
H	-1.827573	-1.016476	5.294934	H	2.227631	-3.495702	0.853877
H	-0.776991	-2.395374	4.874700	H	2.106716	-0.586092	4.621465
C	-0.406608	1.522425	-3.078425	H	3.945496	-1.502960	3.615728
H	0.226520	0.653937	-2.843233	H	4.168098	-3.497861	2.392073
H	-1.147957	1.198828	-3.821990	H	2.409652	-5.015938	1.722218
H	0.222126	2.286963	-3.560976	H	0.097792	-4.620944	1.715256
C	-0.532383	5.096586	-0.350461	H	0.594854	-4.174944	3.342184
H	-0.724773	5.060194	-1.435364	O	0.762120	-0.303870	2.070465
H	-1.146840	5.908558	0.064761	O	0.097498	-2.605102	2.132626
H	0.524720	5.368884	-0.202963	O	-1.411674	1.209865	0.843304
C	0.641481	-0.882661	3.180519	O	0.756289	-0.161597	-0.475891

Table S25. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state 4c

	Coordinates (Angstroms)		
Atom	X	Y	Z
Al	-0.370808	2.123759	-0.474937
N	-1.900924	-1.048554	0.332132
C	-2.258714	0.207376	0.565097
C	-3.653623	0.709106	0.753008
C	-4.753967	-0.087314	1.117874
H	-4.640350	-1.148501	1.277249

C	-6.015619	0.476582	1.277375	H	3.923682	1.403315	1.574654
H	-6.846287	-0.162598	1.566616	C	5.441015	0.002786	0.996247
C	-6.236014	1.843876	1.066430	H	6.173269	0.414533	1.686384
C	-5.135309	2.637716	0.718757	C	5.788145	-1.098130	0.198521
H	-5.271568	3.705063	0.562902	C	4.816982	-1.625395	-0.662157
C	-3.865030	2.090965	0.574567	H	5.060454	-2.481307	-1.286674
H	-3.033088	2.742770	0.328669	C	3.541059	-1.073646	-0.725327
C	-7.617082	2.438337	1.187298	H	2.795446	-1.492886	-1.393465
H	-8.126430	2.436313	0.214432	C	7.178490	-1.681971	0.256008
H	-7.577864	3.477388	1.530958	H	7.197349	-2.713855	-0.109174
H	-8.241550	1.869017	1.883741	H	7.872799	-1.100139	-0.364705
C	-2.865257	-2.073395	-0.007238	H	7.573358	-1.673423	1.277856
C	-3.475168	-2.047391	-1.281442	C	2.367234	2.953200	0.234009
C	-4.383757	-3.066754	-1.589332	C	2.331998	3.651404	1.459517
H	-4.871870	-3.061146	-2.559595	C	3.122064	4.800091	1.581391
C	-4.669591	-4.086177	-0.685750	H	3.106959	5.352995	2.516458
C	-4.034341	-4.108146	0.551903	C	3.920974	5.245328	0.531877
H	-4.253359	-4.907668	1.254063	C	3.942804	4.538198	-0.666334
C	-3.119316	-3.112437	0.914321	H	4.563589	4.890185	-1.485588
Al	-0.074037	-1.663749	0.025554	C	3.168985	3.385172	-0.843903
N	1.475353	1.839203	0.044607	H	4.524907	6.141634	0.647167
C	1.840030	0.580251	-0.057783	H	-5.380222	-4.865230	-0.948780
C	3.209291	0.036211	0.067221	C	-2.471415	-3.160451	2.293811
C	4.174613	0.571519	0.931966	H	-1.721765	-2.369864	2.339029

C	-1.723689	-4.484240	2.523304	H	2.567027	3.001324	-4.246994
H	-1.169686	-4.447119	3.468739	H	1.500555	3.740184	-3.038053
H	-2.411325	-5.336848	2.572108	C	4.627135	2.233227	-2.571750
H	-1.004758	-4.663009	1.720766	H	5.069648	1.609627	-1.787736
C	-3.500652	-2.908687	3.412328	H	4.608144	1.653494	-3.502064
H	-3.012553	-2.938965	4.394585	H	5.283859	3.096179	-2.732028
H	-3.983598	-1.931107	3.305844	C	0.379846	4.202317	2.977793
H	-4.287019	-3.672578	3.408431	H	-0.276678	4.355473	2.117824
C	-3.185778	-0.974966	-2.326867	H	-0.223936	3.828258	3.814676
H	-2.444030	-0.277286	-1.932904	H	0.803392	5.168634	3.280120
C	-4.445917	-0.153878	-2.661289	C	2.353137	2.883622	3.871076
H	-4.189138	0.653716	-3.355955	H	2.858606	3.783743	4.241799
H	-5.213575	-0.776217	-3.137355	H	1.722204	2.498939	4.681616
H	-4.882391	0.294974	-1.763886	H	3.107133	2.121922	3.654574
C	-2.575610	-1.599129	-3.595976	O	-0.820009	3.745233	-0.061488
H	-2.362558	-0.816207	-4.331946	O	-0.681980	1.755075	-2.128689
H	-1.640076	-2.110025	-3.353716	O	-0.100597	-2.620769	-1.418959
H	-3.260898	-2.317923	-4.061042	O	-0.058064	0.310151	3.086453
C	3.201013	2.666607	-2.187809	C	-0.456043	-3.973332	-1.571762
H	2.607897	1.753999	-2.110366	H	-0.051626	-4.609274	-0.767424
C	1.484474	3.185831	2.636011	H	-1.547555	-4.108095	-1.587239
H	0.999906	2.251019	2.355289	H	-0.057145	-4.352998	-2.523019
C	2.546230	3.526337	-3.284626	C	-1.310063	0.246435	3.772893
H	3.070837	4.481009	-3.407915	H	-1.200802	0.555742	4.818617

H	-1.955237	0.953529	3.251559	C	1.604844	-3.396681	1.293023
H	-1.752612	-0.751367	3.729026	H	-0.015648	-2.214639	4.025463
C	-0.136212	0.909711	-3.106247	H	2.898948	-1.721712	4.763469
H	-0.138159	-0.145443	-2.803793	H	1.453563	-4.237314	3.766194
H	-0.721346	0.998580	-4.032299	H	3.100197	-2.190044	2.262239
H	0.902291	1.181003	-3.351343	H	0.380419	-1.131035	5.353705
C	-0.438488	4.913998	-0.749390	H	1.925645	-2.812274	5.745226
H	0.600909	5.196502	-0.520448	H	3.139374	-4.145736	4.231228
H	-0.529165	4.804149	-1.841672	H	3.537403	-3.875460	2.008711
H	-1.086008	5.748364	-0.444631	H	2.049921	-3.323290	0.288139
C	1.008838	-0.446709	3.445955	H	1.208011	-4.422321	1.381612
C	0.776295	-1.574955	4.429583	O	2.084489	-0.153439	2.971869
C	2.035842	-2.396385	4.735363	O	0.535438	-2.471795	1.444679
C	2.324949	-3.565536	3.777736	O	-1.338602	1.104953	0.665657
C	2.718649	-3.213022	2.323460	O	0.903822	-0.239277	-0.430863

Table S26. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state TS_{rb}

	Coordinates (Angstroms)			C	3.736386	2.812839	1.849656
Atom	X	Y	Z	H	4.159029	2.724063	2.847730
Al	-0.767763	1.285789	0.252698	C	3.831307	4.032934	1.165679
N	2.240543	-0.510906	-0.814887	C	3.246413	4.127505	-0.104370
C	1.758554	0.698199	-0.606254	H	3.289890	5.069563	-0.645511
C	2.542338	1.813995	0.000330	C	2.589547	3.040133	-0.674176
C	3.109730	1.711761	1.273464	H	2.108027	3.133476	-1.642305
H	3.022885	0.783543	1.820294	C	4.557635	5.207820	1.774735

H	4.486657	5.200971	2.867679	C	-5.676266	-4.514989	-3.563472
H	4.155842	6.160178	1.412975	H	-5.163377	-5.435904	-3.861754
H	5.624899	5.184260	1.517214	H	-6.525575	-4.786802	-2.927607
C	3.689749	-0.664380	-0.715383	H	-6.084109	-4.061110	-4.476489
C	4.267440	-1.309287	0.394399	C	-3.554134	1.048331	-0.622091
C	5.659365	-1.442721	0.431033	C	-3.951444	1.494560	-1.900207
H	6.123302	-1.938883	1.278665	C	-5.198686	2.114601	-2.028198
C	6.458132	-0.962815	-0.601776	H	-5.520462	2.464132	-3.005148
C	5.866020	-0.346016	-1.698597	C	-6.027244	2.305639	-0.925416
H	6.490838	0.008789	-2.512975	C	-5.598999	1.901891	0.336038
C	4.478445	-0.186446	-1.783022	H	-6.234458	2.077629	1.200312
Al	1.269122	-2.001984	-1.689374	C	-4.357895	1.280317	0.513452
N	-2.289159	0.393570	-0.450561	H	-6.995482	2.784587	-1.046356
C	-1.995692	-0.831571	-0.928110	H	7.538123	-1.076798	-0.555818
C	-2.995394	-1.723179	-1.602979	C	3.878908	0.425450	-3.046753
C	-2.519277	-2.596157	-2.595545	H	2.822627	0.643436	-2.869252
H	-1.470317	-2.561618	-2.872342	C	3.931373	-0.592953	-4.202759
C	-3.385322	-3.488215	-3.220593	H	3.452565	-0.179253	-5.098850
H	-3.000892	-4.145000	-3.997807	H	4.970682	-0.838419	-4.453464
C	-4.738782	-3.561881	-2.862126	H	3.418639	-1.515874	-3.921869
C	-5.198703	-2.708511	-1.851247	C	4.549404	1.753870	-3.438816
H	-6.240750	-2.755070	-1.543211	H	4.018698	2.205985	-4.285227
C	-4.347509	-1.793210	-1.234889	H	4.540935	2.465227	-2.606361
H	-4.740960	-1.141979	-0.465172	H	5.590506	1.608248	-3.748777

C	3.425628	-1.909708	1.512444	H	-1.618295	2.686941	-4.160661
H	2.414513	-1.505184	1.420974	H	-3.104698	3.510313	-3.640188
C	3.941104	-1.569149	2.923395	C	-3.706185	0.837806	-4.357732
H	3.226954	-1.920690	3.678275	H	-4.483311	1.512224	-4.736273
H	4.899685	-2.057142	3.132922	H	-2.968830	0.705604	-5.158325
H	4.083826	-0.492939	3.066735	H	-4.166672	-0.135190	-4.154153
C	3.343061	-3.440142	1.339531	O	-1.262342	2.942196	0.351613
H	2.679078	-3.880274	2.095173	O	-0.144123	0.611982	1.747325
H	2.982788	-3.695292	0.340277	O	2.716512	-2.957223	-1.943110
H	4.336010	-3.889513	1.462064	O	0.558702	-1.704232	-3.236187
C	-3.901655	0.893284	1.915037	C	2.784433	-4.136803	-2.695947
H	-2.909547	0.443320	1.835622	H	2.509891	-3.972527	-3.751013
C	-3.020857	1.392319	-3.099907	H	3.811773	-4.530490	-2.677332
H	-2.217960	0.699289	-2.852068	H	2.122223	-4.927874	-2.301503
C	-3.754124	2.140688	2.804899	C	0.080169	-0.549734	-3.871417
H	-4.719112	2.635731	2.966741	H	-0.916923	-0.732624	-4.302165
H	-3.347800	1.866277	3.786327	H	-0.000799	0.308012	-3.191206
H	-3.074413	2.856026	2.331515	H	0.748368	-0.263636	-4.698758
C	-4.825250	-0.157542	2.555496	C	-0.082125	1.304065	2.970148
H	-4.883167	-1.062989	1.939527	H	-0.359464	0.635137	3.802026
H	-4.452680	-0.444686	3.546753	H	0.938053	1.671465	3.166144
H	-5.844844	0.225287	2.680981	H	-0.758632	2.170186	3.009160
C	-2.357435	2.760176	-3.353132	C	-0.503530	4.083511	0.655230
H	-1.854600	3.114224	-2.446145	H	-1.161521	4.873831	1.045173

H	0.276269	3.897052	1.412344	H	-1.904435	-1.481602	1.738866
H	0.003934	4.481469	-0.237084	H	-0.833772	-5.437459	0.028169
C	0.011799	-3.564593	0.416994	H	-2.979762	-5.122923	1.028578
C	-0.885292	-4.697038	0.828487	H	-3.630531	-3.190777	2.418569
C	-2.345832	-4.229229	1.040975	H	-1.992255	-1.717594	3.472881
C	-2.572445	-3.471370	2.355644	H	0.301968	-1.560064	2.930466
C	-1.717529	-2.209501	2.531348	H	0.059486	-3.313012	3.197206
C	-0.215469	-2.449697	2.578546	O	0.440588	-3.489736	-0.745209
H	-0.498091	-5.153568	1.748707	O	0.364726	-2.625384	1.255469
H	-2.652126	-3.616652	0.187261	O	0.560127	1.016522	-0.976464
H	-2.381110	-4.152470	3.198521	O	-0.822057	-1.261928	-0.774883

Table S27. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$ in state 1d

	Coordinates (Angstroms)			H	2.168740	4.794367	-1.128262
Atom	X	Y	Z	C	1.880861	2.686871	-0.852281
Al	-0.899979	0.832704	0.586250	H	1.230879	2.582040	-1.714555
N	2.350124	-0.791792	-0.822136	C	3.781543	5.440306	0.979339
C	1.608825	0.254992	-0.501006	H	4.031646	5.505157	2.043238
C	2.188158	1.561393	-0.076525	H	3.078600	6.247066	0.744732
C	2.976514	1.707887	1.067612	H	4.701650	5.635587	0.412795
H	3.185211	0.848293	1.691051	C	3.798910	-0.688960	-0.788326
C	3.468011	2.963593	1.417205	C	4.496103	-1.218185	0.316599
H	4.069051	3.068702	2.317062	C	5.892360	-1.143762	0.312838
C	3.207418	4.089792	0.625512	H	6.450456	-1.546987	1.152662
C	2.404633	3.930058	-0.512486	C	6.579205	-0.565936	-0.751407

C	5.871912	-0.058765	-1.836068	C	-5.621278	2.886958	-1.225204
H	6.413130	0.377920	-2.670364	C	-5.560319	2.366815	0.065074
C	4.473748	-0.111848	-1.881162	H	-6.305059	2.664679	0.798405
Al	1.555592	-2.337487	-1.676257	C	-4.548022	1.474801	0.434412
N	-2.535831	0.210918	-0.133399	H	-6.414255	3.578688	-1.498272
C	-2.517080	-1.107201	-0.452010	H	7.664869	-0.516628	-0.737068
C	-3.471209	-1.710886	-1.439272	C	3.744179	0.389387	-3.122005
C	-2.900284	-2.533896	-2.423917	H	2.672431	0.418885	-2.907561
H	-1.823498	-2.680506	-2.428860	C	3.947008	-0.601387	-4.285665
C	-3.703206	-3.111718	-3.403178	H	3.364922	-0.291079	-5.161799
H	-3.244341	-3.728641	-4.173056	H	5.003509	-0.643058	-4.577271
C	-5.091502	-2.913332	-3.414873	H	3.639310	-1.609651	-3.992033
C	-5.652631	-2.115180	-2.410357	C	4.158275	1.816425	-3.519937
H	-6.728573	-1.956371	-2.391370	H	3.547434	2.162745	-4.362110
C	-4.856249	-1.508241	-1.439492	H	4.023117	2.514259	-2.687440
H	-5.317916	-0.878556	-0.687692	H	5.206591	1.861468	-3.836508
C	-5.950912	-3.518356	-4.499735	C	3.765060	-1.894972	1.469413
H	-5.569676	-4.495851	-4.815614	H	2.720067	-1.580281	1.429731
H	-6.986815	-3.647884	-4.168371	C	4.309735	-1.509831	2.855971
H	-5.970763	-2.875501	-5.390008	H	3.664675	-1.925776	3.639362
C	-3.585327	1.106555	-0.529569	H	5.318197	-1.904638	3.023609
C	-3.624283	1.638062	-1.833981	H	4.353092	-0.423893	2.994822
C	-4.655240	2.526417	-2.160079	C	3.793237	-3.426537	1.290835
H	-4.696043	2.949353	-3.160156	H	3.185429	-3.916510	2.062965

H	3.423282	-3.714529	0.303307	O	2.975882	-3.234122	-2.089560
H	4.819712	-3.802167	1.381201	O	0.388331	-2.028789	-2.896348
C	-4.460033	0.968337	1.868739	C	3.036983	-4.484994	-2.727884
H	-3.727973	0.155396	1.888308	H	2.542958	-4.476284	-3.712419
C	-2.548719	1.311311	-2.859815	H	4.087654	-4.766277	-2.884514
H	-1.951195	0.485120	-2.470829	H	2.566941	-5.281019	-2.126312
C	-3.927108	2.089640	2.781296	C	0.192059	-0.947165	-3.766413
H	-4.641814	2.920130	2.834660	H	-0.802737	-1.025883	-4.223732
H	-3.755423	1.720850	3.800401	H	0.237119	0.019596	-3.243518
H	-2.987294	2.484589	2.383541	H	0.936356	-0.933550	-4.578131
C	-5.788435	0.399053	2.392736	C	-0.193528	0.986947	3.321493
H	-6.158010	-0.405837	1.746524	H	-0.264548	0.288451	4.171894
H	-5.655262	-0.009039	3.402075	H	0.757297	1.535444	3.423420
H	-6.568970	1.166539	2.450606	H	-1.007474	1.717929	3.437741
C	-1.600233	2.514560	-3.027425	C	-0.535172	3.620691	1.207534
H	-1.193990	2.814298	-2.055523	H	-1.204294	3.956969	2.016843
H	-0.770995	2.260321	-3.700926	H	0.438525	3.377675	1.660002
H	-2.129585	3.375323	-3.454783	H	-0.373958	4.477602	0.537363
C	-3.136659	0.849838	-4.203034	C	0.260770	-3.584283	0.632778
H	-3.729706	1.637936	-4.681848	C	-0.538444	-4.784714	1.061359
H	-2.331901	0.581040	-4.897072	C	-1.961781	-4.478443	1.576724
H	-3.778135	-0.027189	-4.066616	C	-1.994872	-3.867329	2.982088
O	-1.097841	2.553435	0.498801	C	-1.242237	-2.538331	3.114777
O	-0.248241	0.277256	2.112235	C	0.257085	-2.624985	2.872406

H	0.037610	-5.301464	1.843515	H	-1.363834	-2.155010	4.136584
H	-2.450164	-3.815080	0.859239	H	0.752170	-1.717384	3.207805
H	-1.580433	-4.591687	3.700743	H	0.714918	-3.498582	3.354047
H	-1.637361	-1.781111	2.435337	O	0.663122	-3.510107	-0.546481
H	-0.581027	-5.441506	0.190711	O	0.634118	-2.654980	1.460178
H	-2.508457	-5.428669	1.585167	O	0.332442	0.184189	-0.641131
H	-3.041498	-3.711713	3.271042	O	-1.614148	-1.825188	0.024433

Table S28. Cartesian coordinate of $[O^{Pr}AlOMe_2]_2$in state TS1d

	Coordinates (Angstroms)						
Atom	X	Y	Z	H	4.122482	6.584096	-0.049068
Al	-0.832287	0.540067	0.921575	H	2.835911	6.740274	1.152570
N	2.353469	-0.247769	-0.655932	H	2.481353	7.040231	-0.551117
C	1.615246	0.820363	-0.478413	C	3.771860	-0.379340	-0.567909
C	2.016041	2.219098	-0.284413	C	4.309729	-0.861220	0.646759
C	3.322733	2.599711	0.076602	C	5.695419	-1.042421	0.708494
H	4.079402	1.853006	0.272402	H	6.147761	-1.401711	1.627268
C	3.650731	3.944358	0.199368	C	6.507856	-0.781123	-0.394889
H	4.662511	4.219039	0.486402	C	5.945985	-0.330181	-1.585541
C	2.701906	4.949891	-0.038114	H	6.584729	-0.139475	-2.443338
C	1.405900	4.563807	-0.405727	C	4.566094	-0.116691	-1.699524
H	0.651838	5.322868	-0.595615	Al	0.956135	-1.358905	-1.410562
C	1.059968	3.223860	-0.523702	N	-2.504850	0.219930	0.133338
H	0.047222	2.952852	-0.784318	C	-3.056850	-1.032781	0.206685
C	3.057228	6.405638	0.130382	C	-4.109579	-1.453347	-0.791736
				C	-3.823872	-2.602865	-1.542492

H	-2.871488	-3.096357	-1.392057	C	4.055722	-0.728361	-4.089377
C	-4.725588	-3.081502	-2.487734	H	3.595259	-0.383633	-5.021977
H	-4.473861	-3.965586	-3.070382	H	5.097798	-0.999013	-4.299669
C	-5.953326	-2.440169	-2.703555	H	3.520164	-1.627709	-3.768364
C	-6.239819	-1.302613	-1.940992	C	4.612672	1.683974	-3.484824
H	-7.186682	-0.786874	-2.085179	H	4.112667	2.044353	-4.391033
C	-5.330620	-0.804833	-1.006172	H	4.527448	2.460148	-2.716176
H	-5.579000	0.093402	-0.455428	H	5.675662	1.555639	-3.721232
C	-6.917016	-2.941439	-3.753090	C	3.410689	-1.140440	1.848773
H	-6.895128	-4.034420	-3.829695	H	2.412899	-1.396848	1.481291
H	-7.945909	-2.637588	-3.532615	C	3.241358	0.118128	2.722705
H	-6.663535	-2.541677	-4.744199	H	2.592084	-0.102992	3.575966
C	-3.200382	1.319076	-0.490147	H	4.212246	0.463545	3.100652
C	-3.074844	1.579442	-1.872824	H	2.774817	0.935392	2.169713
C	-3.791075	2.654417	-2.416962	C	3.904257	-2.312102	2.713342
H	-3.709706	2.858249	-3.481268	H	3.146213	-2.553167	3.466983
C	-4.608943	3.455145	-1.628327	H	4.094111	-3.212023	2.117161
C	-4.709761	3.199508	-0.263340	H	4.827295	-2.069023	3.253193
H	-5.344113	3.830247	0.353921	C	-4.151442	1.913652	1.831540
C	-4.008375	2.145039	0.330006	H	-3.449969	1.127707	2.118201
H	-5.163187	4.277935	-2.073408	C	-2.207169	0.735665	-2.797449
H	7.581459	-0.935454	-0.325295	H	-1.740169	-0.049322	-2.199422
C	3.966619	0.369043	-3.013669	C	-3.774936	3.173086	2.630864
H	2.902995	0.565363	-2.864897	H	-4.489417	3.988766	2.464974

H	-3.770492	2.952896	3.705653	H	0.125171	-1.275126	-4.998121
H	-2.779421	3.514198	2.338329	H	1.050625	-2.639636	-4.332947
C	-5.564176	1.423911	2.201558	C	-0.188936	-1.241890	3.056525
H	-5.798661	0.469095	1.718667	H	-1.082820	-1.855727	2.890320
H	-5.646959	1.278919	3.285630	H	0.648345	-1.912458	3.302728
H	-6.328502	2.151114	1.900767	H	-0.364127	-0.600108	3.937263
C	-1.083748	1.577206	-3.429858	C	-0.058358	2.653656	2.579430
H	-0.473659	2.058784	-2.662062	H	-0.701259	3.141951	3.327228
H	-0.419215	0.940376	-4.018661	H	0.498746	1.850729	3.085552
H	-1.493641	2.359935	-4.079914	H	0.673662	3.399794	2.232290
C	-3.042634	0.051137	-3.896160	C	0.173915	-3.375628	-0.230708
H	-3.480157	0.790455	-4.578518	C	-0.439284	-4.650344	-0.764302
H	-2.405847	-0.613749	-4.491462	C	-1.635651	-5.096080	0.109813
H	-3.856869	-0.540818	-3.472518	C	-1.215095	-5.919212	1.335286
O	-0.833284	2.179173	1.505167	C	-0.343502	-5.154302	2.340195
O	0.135732	-0.488821	1.920615	C	0.938352	-4.574398	1.748723
O	1.637999	-3.110244	-1.291190	H	0.313791	-5.443604	-0.826804
O	0.816840	-0.983808	-3.087273	H	-2.203559	-4.213557	0.427343
C	2.901786	-3.647026	-0.954999	H	-0.671269	-6.815279	0.999041
H	3.683919	-3.126261	-1.517590	H	-0.907660	-4.323681	2.780469
H	3.107858	-3.522373	0.114340	H	-0.755557	-4.421883	-1.784062
H	2.931870	-4.714359	-1.210255	H	-2.304480	-5.702023	-0.512731
C	0.326262	-1.848679	-4.082736	H	-2.114508	-6.277853	1.850520
H	-0.617334	-2.336179	-3.788146	H	-0.059920	-5.825823	3.161723

H	1.619493	-4.249708	2.537225	O	0.685765	-3.358336	1.010835
H	1.469220	-5.300115	1.120481	O	0.325718	0.518717	-0.620970
O	-0.381314	-2.249395	-0.594313	O	-2.638237	-1.872486	1.012747