I. X-ray Structural Determination of *rac*-{(1-Me_2Si(0.5dioxane)-2-methyl-1-indenyl)$_2$$Sm$$Me_2$}$_n$ (*rac*-**2a**).

DATA COLLECTION

A crystal of the compound was attached to a glass fiber and mounted on the Siemens SMART system for a data collection at 173(2) K. An initial set of cell constants was calculated from reflections harvested from three sets of 30 frames. These initial sets of frames are oriented such that orthogonal wedges of reciprocal space were surveyed. This produces orientation matrices determined from 42 reflections. Final cell constants are calculated from a set of 5932 strong reflections from the actual data collection. Final cell constants reported in this manner usually are about one order of magnetude better in precision than reported from four-circle diffractometers. Please refer to Table 1 for additional crystal and refinement information.

The data collection technique used for this specimen is generally known as a hemisphere collection. Here a randomly oriented region of reciprocal space is surveyed to the extent of 1.3 hemispheres to a resolution of 0.84 Å. Three major swaths of frames are collected with 0.30° steps in ω. In the event the lattice is triclinic some additional sets of frames are collected to better model the absorption correction.

STRUCTURE SOLUTION AND REFINEMENT

The space group C2/c was determined based on systematic absences and intensity statistics.[1] A successful direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Several full-matrix least squares / difference Fourier cycles were performed which located the remainder of the non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters unless stated otherwise. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The structure was found as expected. Individual monomers are linked in infinite chains through dioxane bridges. Both dioxanes are centered over inversion centers so only half of each is found in the asymmetric unit. One dioxane is disordered in a 0.56:0.44 ratio in two chair conformations where the oxygen is mutual in both fragments. This oxygen atom appears in both fragments in order to set up appropriate constraints/restraints. The other dioxane was used as a paradigm for the disordered fragments by utilizing the SHEXTL SAME restraint. 18 restraints were used altogether.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, The University of Minnesota. All calculations were preformed using SGI INDY R4400-SC

or Pentium computers using the SHELXTL V5.0 suite of programs. All publications arising from this report MUST either 1)include Victor G. Young, Jr. as a coauthor or 2)acknowledge both Victor G. Young, Jr. and the X-Ray Crystallographic Laboratory.

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1. SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

Some equations of interest:

$$R_{int}=\sum|F_o^2-\langle F_o^2\rangle|/\sum|F_o^2|$$

$$R1=\sum||F_o|-|F_c||/\sum|F_o|$$

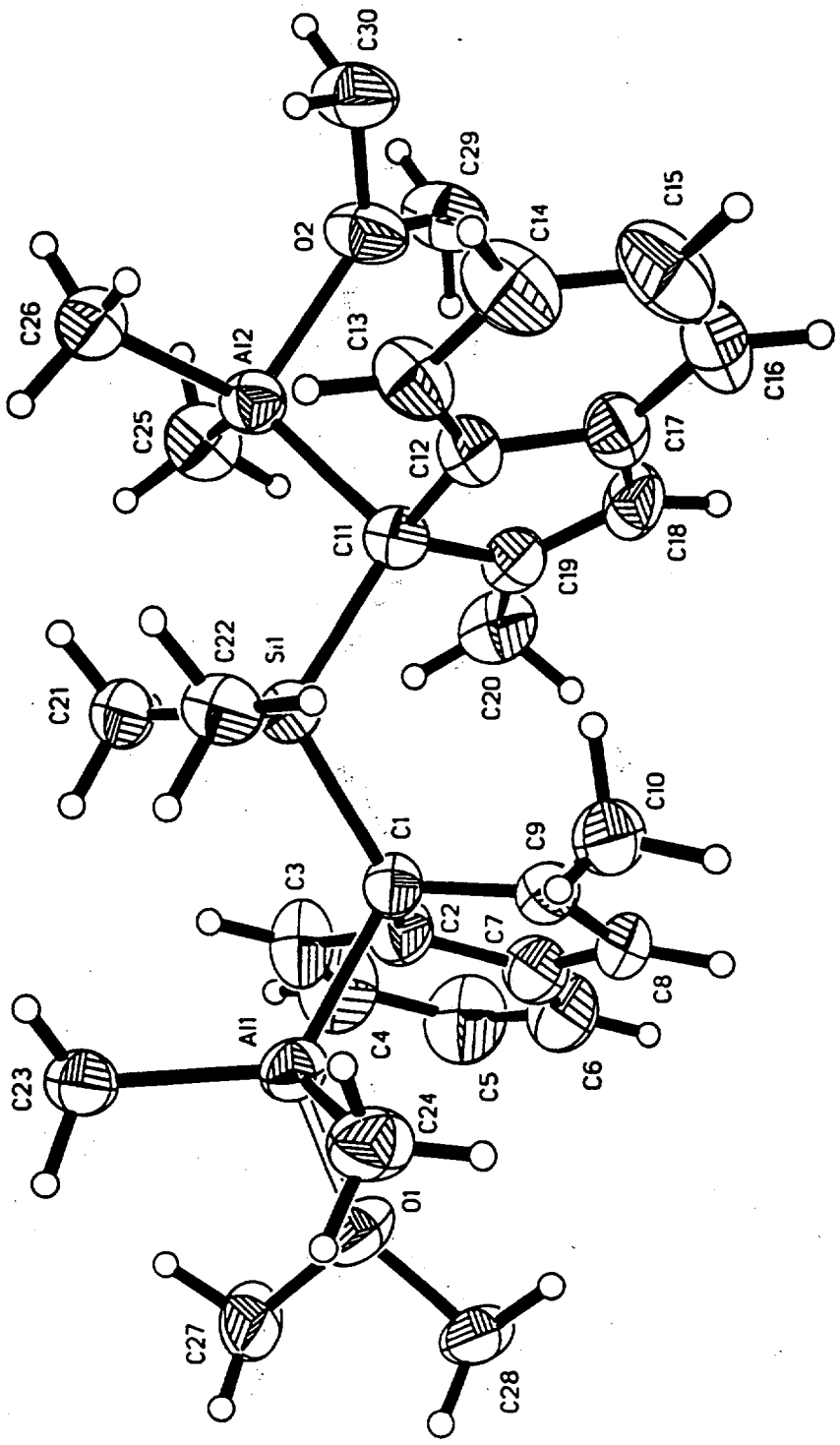
$$wR2=[\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2},$$

where $w=q/\sigma^2(F_o^2)+(a*P)^2+b*P$

$$GooF=S=[\sum[w(F_o^2-F_c^2)^2]/(n-p)^{1/2}$$

Table I.1. **Crystal data, data collection, and solution and refinement for *rac*-2a.**

Crystal Data	
Empirical formula	$C_{30}H_{42}Al_2O_2Si$
Crystal Habit, color	Block, Colorless
Crystal size	0.20 x 0.20 x 0.12 mm
Crystal system	Monoclinic
Space group	C2/c
	a = 32.701(2) Å α = 90°
	b = 10.7555(6) Å β = 91.937(1)°
	c = 16.3851(8) Å γ = 90°
Volume	5759.6(5) $Å^3$
Z	8
Formula weight	516.69
Density (calculated)	1.192 Mg/m^3
Absorption coefficient	0.167 mm^{-1}
F(000)	2224
Data Collection	
Diffractometer	Siemens SMART Platform CCD
Wavelength	0.71073 Å
Temperature	173(2) K
θ range for data collection	1.25 to 25.02°
Index ranges	$-38 \le h \le 38$, $0 \le k \le 12$, $0 \le \ell \le 19$
Reflections collected	13811
Independent reflections	4993 (R_{int} = 0.0358)
Solution and Refinement	
System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2)+(AP)^2+(BP)]^{-1}$, where $P = (Fo^2+2Fc^2))/3$, A = 0.0399, and B = 15.3394
Absorption correction	SADABS (Shedrick, 1996)
Max. and min. transmission	1.000 and 0.818
Data / restraints / parameters	4992 / 18 / 343
R indices ($I>2\sigma(I)$ = 3562)	R1 = 0.0642, wR2 = 0.1262
R indices (all data)	R1 = 0.0996, wR2 = 0.1404
Goodness-of-fit on F^2	1.040
Largest diff. peak and hole	0.694 and -0.262 $eÅ^{-3}$


C30
C29
O2
C14
C15
C26
Al2
C13
C16
C25
C12
C17
C11
C18
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C22
Si1
C21
C20
C10
C1
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C3
C2
C7
C8
Al1
C4
C5
C6
C23
C24
O1
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C28

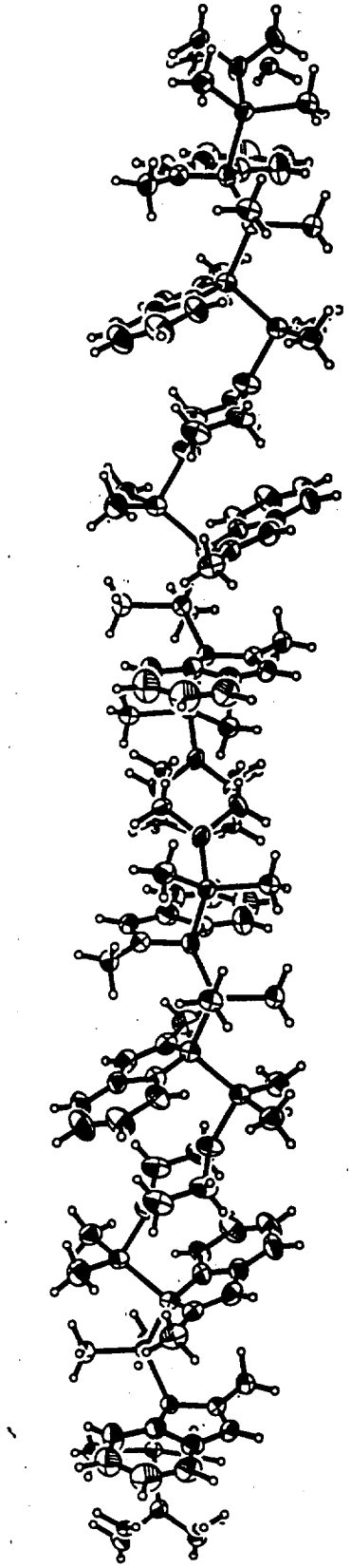

Table I.2. Atomic coordinates [$x_3 10^4$] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for *rac*-2a. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Si(1)	1087.7(3)	4481.4(9)	951.8(5)	32.0(2)	1
C(1)	947(1)	2889(3)	544(2)	34(1)	1
C(2)	777(1)	2757(3)	-310(2)	40(1)	1
C(3)	468(1)	3404(4)	-739(2)	51(1)	1
C(4)	365(1)	3089(5)	-1541(2)	68(1)	1
C(5)	566(2)	2116(5)	-1920(3)	69(1)	1
C(6)	868(1)	1462(4)	-1513(2)	59(1)	1
C(7)	976(1)	1769(4)	-705(2)	47(1)	1
C(8)	1281(1)	1278(3)	-136(2)	46(1)	1
C(9)	1280(1)	1928(3)	570(2)	41(1)	1
C(10)	1580(1)	1762(4)	1285(3)	52(1)	1
C(11)	1609(1)	5081(3)	599(2)	32(1)	1
C(12)	1969(1)	4966(3)	1190(2)	36(1)	1
C(13)	2033(1)	5412(4)	1984(2)	46(1)	1
C(14)	2407(1)	5224(5)	2388(2)	62(1)	1
C(15)	2719(1)	4588(5)	2017(3)	68(1)	1
C(16)	2668(1)	4145(4)	1235(3)	59(1)	1
C(17)	2292(1)	4352(3)	807(2)	43(1)	1
C(18)	2153(1)	4066(3)	-15(2)	47(1)	1
C(19)	1767(1)	4469(3)	-152(2)	39(1)	1
C(20)	1537(1)	4385(4)	-958(2)	51(1)	1
C(21)	672(1)	5603(3)	626(2)	44(1)	1
C(22)	1082(1)	4472(4)	2091(2)	42(1)	1
Al(1)	477.6(3)	2152(1)	1191.9(7)	37.6(3)	1
C(23)	9(1)	3252(3)	1357(2)	44(1)	1
C(24)	642(1)	1084(4)	2115(2)	51(1)	1
Al(2)	1527.1(3)	6934(1)	360.2(6)	38.7(3)	1
C(25)	1244(1)	7467(4)	-668(2)	54(1)	1
C(26)	1406(1)	7983(4)	1308(2)	51(1)	1
C(27)	-237(3)	985(8)	242(9)	64(4)	0.565(15)
O(1)	215(1)	909(2)	460(2)	50(1)	0.565(15)
C(28)	303(3)	-443(8)	536(9)	51(3)	0.565(15)
C(27')	-66(3)	1238(8)	-266(7)	34(3)	0.435(15)
O(1')	215(1)	909(2)	460(2)	50(1)	0.435(15)
C(28')	419(3)	-261(10)	200(8)	30(3)	0.435(15)
C(29)	2241(1)	7424(4)	-702(2)	58(1)	1
O(2)	2080(1)	7432(3)	122(2)	50(1)	1
C(30)	2348(1)	8136(4)	674(2)	54(1)	1

Table I.3. Bond lengths [Å] and angles [°] for *rac*-**2a**.

Si(1)-C(22)	1.868(3)	Si(1)-C(21)	1.880(4)
Si(1)-C(1)	1.889(3)	Si(1)-C(11)	1.929(3)
C(1)-C(2)	1.495(4)	C(1)-C(9)	1.501(5)
C(1)-Al(1)	2.055(3)	C(2)-C(3)	1.397(5)
C(2)-C(7)	1.413(5)	C(3)-C(4)	1.388(5)
C(4)-C(5)	1.392(6)	C(5)-C(6)	1.368(6)
C(6)-C(7)	1.399(5)	C(7)-C(8)	1.444(5)
C(8)-C(9)	1.353(5)	C(9)-C(10)	1.512(5)
C(11)-C(19)	1.503(4)	C(11)-C(12)	1.503(4)
C(11)-Al(2)	2.047(4)	C(12)-C(13)	1.397(5)
C(12)-C(17)	1.411(5)	C(13)-C(14)	1.384(5)
C(14)-C(15)	1.385(6)	C(15)-C(16)	1.372(6)
C(16)-C(17)	1.412(5)	C(17)-C(18)	1.440(5)
C(18)-C(19)	1.345(5)	C(19)-C(20)	1.500(5)
Al(1)-C(24)	1.960(4)	Al(1)-C(23)	1.963(4)
Al(1)-O(1')	1.973(3)	Al(1)-O(1)	1.973(3)
Al(2)-O(2)	1.939(3)	Al(2)-C(26)	1.970(4)
Al(2)-C(25)	1.980(4)	C(27)-C(28)#1	1.41(2)
C(27)-O(1)	1.511(7)	O(1)-C(28)	1.488(9)
C(28)-C(27)#1	1.41(2)	C(27')-O(1')	1.520(8)
C(27')-C(28')#1	1.57(2)	O(1')-C(28')	1.494(10)
C(28')-C(27')#1	1.57(2)	C(29)-O(2)	1.465(4)
C(29)-C(30)#2	1.471(5)	O(2)-C(30)	1.452(4)
C(30)-C(29)#2	1.471(5)		

C(22)-Si(1)-C(21)	104.8(2)	C(22)-Si(1)-C(1)	109.8(2)
C(21)-Si(1)-C(1)	108.5(2)	C(22)-Si(1)-C(11)	109.9(2)
C(21)-Si(1)-C(11)	109.7(2)	C(1)-Si(1)-C(11)	113.77(14)
C(2)-C(1)-C(9)	102.1(3)	C(2)-C(1)-Si(1)	119.7(3)
C(9)-C(1)-Si(1)	116.5(2)	C(2)-C(1)-Al(1)	100.7(2)
C(9)-C(1)-Al(1)	105.9(2)	Si(1)-C(1)-Al(1)	110.1(2)
C(3)-C(2)-C(7)	118.7(3)	C(3)-C(2)-C(1)	131.6(3)
C(7)-C(2)-C(1)	109.7(3)	C(4)-C(3)-C(2)	120.1(4)
C(3)-C(4)-C(5)	120.3(4)	C(6)-C(5)-C(4)	120.8(4)
C(5)-C(6)-C(7)	119.6(4)	C(6)-C(7)-C(2)	120.4(4)
C(6)-C(7)-C(8)	132.2(4)	C(2)-C(7)-C(8)	107.4(3)
C(9)-C(8)-C(7)	109.9(3)	C(8)-C(9)-C(1)	110.7(3)
C(8)-C(9)-C(10)	125.5(3)	C(1)-C(9)-C(10)	123.7(3)
C(19)-C(11)-C(12)	102.0(3)	C(19)-C(11)-Si(1)	115.6(2)
C(12)-C(11)-Si(1)	117.4(2)	C(19)-C(11)-Al(2)	108.4(2)
C(12)-C(11)-Al(2)	107.3(2)	Si(1)-C(11)-Al(2)	105.8(2)
C(13)-C(12)-C(17)	118.9(3)	C(13)-C(12)-C(11)	131.5(3)
C(17)-C(12)-C(11)	109.5(3)	C(14)-C(13)-C(12)	120.0(4)
C(13)-C(14)-C(15)	120.9(4)	C(16)-C(15)-C(14)	120.8(4)
C(15)-C(16)-C(17)	119.1(4)	C(12)-C(17)-C(16)	120.3(4)
C(12)-C(17)-C(18)	107.4(3)	C(16)-C(17)-C(18)	132.3(4)
C(19)-C(18)-C(17)	110.6(3)	C(18)-C(19)-C(20)	124.6(3)
C(18)-C(19)-C(11)	110.6(3)	C(20)-C(19)-C(11)	124.7(3)
C(24)-Al(1)-C(23)	116.3(2)	C(24)-Al(1)-O(1')	100.0(2)
C(23)-Al(1)-O(1')	99.56(13)	C(24)-Al(1)-O(1)	100.0(2)
C(23)-Al(1)-O(1)	99.56(13)	C(24)-Al(1)-C(1)	115.8(2)
C(23)-Al(1)-C(1)	116.1(2)	O(1')-Al(1)-C(1)	105.33(13)
O(1)-Al(1)-C(1)	105.33(13)	O(2)-Al(2)-C(26)	102.37(14)
O(2)-Al(2)-C(25)	99.26(14)	C(26)-Al(2)-C(25)	113.8(2)
O(2)-Al(2)-C(11)	101.03(13)	C(26)-Al(2)-C(11)	115.8(2)
C(25)-Al(2)-C(11)	119.9(2)	C(28)#1-C(27)-O(1)	108.1(10)
C(28)-O(1)-C(27)	104.9(6)	C(28)-O(1)-Al(1)	122.2(4)
C(27)-O(1)-Al(1)	120.6(4)	C(27)#1-C(28)-O(1)	107.7(10)
O(1')-C(27')-C(28')#1	102.6(9)	C(28')-O(1')-C(27')	103.7(6)

C(28')-O(1')-Al(1)	123.7(5)	C(27')-O(1')-Al(1)	123.9(3)
O(1')-C(28')-C(27')#1	102.0(8)	O(2)-C(29)-C(30)#2	109.3(3)
C(30)-O(2)-C(29)	110.5(3)	C(30)-O(2)-Al(2)	124.5(2)
C(29)-O(2)-Al(2)	123.4(2)	O(2)-C(30)-C(29)#2	109.6(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x+1/2,-y+3/2,-z

Table I.4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for rac-2a. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^*b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Si(1)	35(1)	33(1)	27(1)	-1(1)	-2(1)	-1(1)
C(1)	32(2)	36(2)	33(2)	-8(2)	-6(1)	3(2)
C(2)	42(2)	40(2)	38(2)	-10(2)	-2(2)	0(2)
C(3)	54(2)	65(3)	34(2)	-12(2)	-11(2)	17(2)
C(4)	74(3)	83(3)	44(2)	-14(2)	-20(2)	13(3)
C(5)	86(3)	82(4)	38(2)	-25(2)	-13(2)	-1(3)
C(6)	68(3)	61(3)	49(2)	-28(2)	8(2)	-1(2)
C(7)	46(2)	49(2)	47(2)	-13(2)	5(2)	-3(2)
C(8)	40(2)	32(2)	66(3)	-10(2)	7(2)	3(2)
C(9)	36(2)	31(2)	55(2)	1(2)	-2(2)	0(2)
C(10)	42(2)	42(2)	73(3)	4(2)	-13(2)	4(2)
C(11)	36(2)	38(2)	23(2)	-1(2)	2(1)	-3(2)
C(12)	35(2)	42(2)	32(2)	5(2)	3(2)	1(2)
C(13)	38(2)	67(3)	33(2)	-1(2)	-3(2)	0(2)
C(14)	50(2)	94(4)	40(2)	4(2)	-12(2)	-5(2)
C(15)	43(2)	97(4)	62(3)	24(3)	-13(2)	2(3)
C(16)	39(2)	65(3)	73(3)	19(2)	13(2)	13(2)
C(17)	40(2)	41(2)	48(2)	11(2)	7(2)	4(2)
C(18)	55(2)	40(2)	48(2)	-4(2)	21(2)	4(2)
C(19)	48(2)	36(2)	34(2)	1(2)	10(2)	-2(2)
C(20)	72(3)	55(3)	26(2)	-9(2)	6(2)	-9(2)
C(21)	41(2)	39(2)	53(2)	3(2)	1(2)	3(2)
C(22)	44(2)	52(2)	30(2)	-5(2)	3(2)	-9(2)
Al(1)	35(1)	30(1)	48(1)	2(1)	-9(1)	-1(1)
C(23)	38(2)	40(2)	53(2)	3(2)	0(2)	-4(2)
C(24)	49(2)	43(2)	61(3)	14(2)	-5(2)	-3(2)
Al(2)	40(1)	38(1)	38(1)	0(1)	3(1)	-3(1)
C(25)	55(2)	56(3)	51(2)	15(2)	-2(2)	3(2)
C(26)	51(2)	45(2)	58(2)	-7(2)	11(2)	-4(2)
C(27)	28(4)	52(5)	111(10)	-29(6)	-18(5)	7(4)
O(1)	44(1)	27(1)	78(2)	-7(1)	-27(1)	3(1)
C(28)	40(6)	28(5)	82(9)	7(5)	-19(5)	-5(4)
C(27')	28(5)	26(5)	48(6)	2(4)	-4(4)	-3(4)
O(1')	44(1)	27(1)	78(2)	-7(1)	-27(1)	3(1)
C(28')	18(5)	19(5)	54(8)	7(5)	1(4)	-9(4)
C(29)	54(2)	79(3)	40(2)	-6(2)	7(2)	-19(2)
O(2)	47(1)	62(2)	41(2)	-7(1)	9(1)	-20(1)
C(30)	53(2)	65(3)	45(2)	-13(2)	10(2)	-20(2)

Table I.5. Torsion angles [°] for *rac*-2a.

C(22)-Si(1)-C(1)-C(2)	156.8(3)	C(21)-Si(1)-C(1)-C(2)	42.8(3)
C(11)-Si(1)-C(1)-C(2)	-79.6(3)	C(22)-Si(1)-C(1)-C(9)	-79.6(3)
C(21)-Si(1)-C(1)-C(9)	166.5(3)	C(11)-Si(1)-C(1)-C(9)	44.0(3)
C(22)-Si(1)-C(1)-Al(1)	40.9(2)	C(21)-Si(1)-C(1)-Al(1)	-73.1(2)
C(11)-Si(1)-C(1)-Al(1)	164.53(14)	C(9)-C(1)-C(2)-C(3)	-177.7(4)
Si(1)-C(1)-C(2)-C(3)	-47.3(5)	Al(1)-C(1)-C(2)-C(3)	73.3(5)
C(9)-C(1)-C(2)-C(7)	3.4(4)	Si(1)-C(1)-C(2)-C(7)	133.8(3)
Al(1)-C(1)-C(2)-C(7)	-105.5(3)	C(7)-C(2)-C(3)-C(4)	-1.0(6)
C(1)-C(2)-C(3)-C(4)	-179.8(4)	C(2)-C(3)-C(4)-C(5)	0.8(7)
C(3)-C(4)-C(5)-C(6)	-0.4(8)	C(4)-C(5)-C(6)-C(7)	0.4(7)
C(5)-C(6)-C(7)-C(2)	-0.7(6)	C(5)-C(6)-C(7)-C(8)	-178.4(4)
C(3)-C(2)-C(7)-C(6)	1.0(6)	C(1)-C(2)-C(7)-C(6)	180.0(4)
C(3)-C(2)-C(7)-C(8)	179.2(3)	C(1)-C(2)-C(7)-C(8)	-1.8(4)
C(6)-C(7)-C(8)-C(9)	177.1(4)	C(2)-C(7)-C(8)-C(9)	-0.9(4)
C(7)-C(8)-C(9)-C(1)	3.2(4)	C(7)-C(8)-C(9)-C(10)	-174.5(3)
C(2)-C(1)-C(9)-C(8)	-4.1(4)	Si(1)-C(1)-C(9)-C(8)	-136.4(3)
Al(1)-C(1)-C(9)-C(8)	100.9(3)	C(2)-C(1)-C(9)-C(10)	173.7(3)
Si(1)-C(1)-C(9)-C(10)	41.4(4)	Al(1)-C(1)-C(9)-C(10)	-81.3(4)
C(22)-Si(1)-C(11)-C(19)	143.8(3)	C(21)-Si(1)-C(11)-C(19)	-101.5(3)
C(1)-Si(1)-C(11)-C(19)	20.3(3)	C(22)-Si(1)-C(11)-C(12)	23.3(3)
C(21)-Si(1)-C(11)-C(12)	138.1(3)	C(1)-Si(1)-C(11)-C(12)	-100.2(3)
C(22)-Si(1)-C(11)-Al(2)	-96.2(2)	C(21)-Si(1)-C(11)-Al(2)	18.5(2)
C(1)-Si(1)-C(11)-Al(2)	140.22(14)	C(19)-C(11)-C(12)-C(13)	175.6(4)
Si(1)-C(11)-C(12)-C(13)	-57.0(5)	Al(2)-C(11)-C(12)-C(13)	61.8(4)
C(19)-C(11)-C(12)-C(17)	-0.2(4)	Si(1)-C(11)-C(12)-C(17)	127.2(3)
Al(2)-C(11)-C(12)-C(17)	-114.1(3)	C(17)-C(12)-C(13)-C(14)	-1.3(6)
C(11)-C(12)-C(13)-C(14)	-176.9(4)	C(12)-C(13)-C(14)-C(15)	-0.5(7)
C(13)-C(14)-C(15)-C(16)	1.0(7)	C(14)-C(15)-C(16)-C(17)	0.4(7)
C(13)-C(12)-C(17)-C(16)	2.7(5)	C(11)-C(12)-C(17)-C(16)	179.2(3)
C(13)-C(12)-C(17)-C(18)	-176.3(3)	C(11)-C(12)-C(17)-C(18)	0.2(4)
C(15)-C(16)-C(17)-C(12)	-2.3(6)	C(15)-C(16)-C(17)-C(18)	176.5(4)
C(12)-C(17)-C(18)-C(19)	0.0(4)	C(16)-C(17)-C(18)-C(19)	-178.9(4)
C(17)-C(18)-C(19)-C(20)	176.6(3)	C(17)-C(18)-C(19)-C(11)	-0.1(4)
C(12)-C(11)-C(19)-C(18)	0.2(4)	Si(1)-C(11)-C(19)-C(18)	-128.3(3)
Al(2)-C(11)-C(19)-C(18)	113.2(3)	C(12)-C(11)-C(19)-C(20)	-176.5(3)
Si(1)-C(11)-C(19)-C(20)	55.0(4)	Al(2)-C(11)-C(19)-C(20)	-63.5(4)
C(2)-C(1)-Al(1)-C(24)	139.1(2)	C(9)-C(1)-Al(1)-C(24)	33.2(3)
Si(1)-C(1)-Al(1)-C(24)	-93.5(2)	C(2)-C(1)-Al(1)-C(23)	-79.3(3)
C(9)-C(1)-Al(1)-C(23)	174.8(2)	Si(1)-C(1)-Al(1)-C(23)	48.0(2)
C(2)-C(1)-Al(1)-O(1')	29.7(2)	C(9)-C(1)-Al(1)-O(1')	-76.2(2)
Si(1)-C(1)-Al(1)-O(1')	157.04(14)	C(2)-C(1)-Al(1)-O(1)	29.7(2)
C(9)-C(1)-Al(1)-O(1)	-76.2(2)	Si(1)-C(1)-Al(1)-O(1)	157.04(14)
C(19)-C(11)-Al(2)-O(2)	-60.8(2)	C(12)-C(11)-Al(2)-O(2)	48.6(2)
Si(1)-C(11)-Al(2)-O(2)	174.65(13)	C(19)-C(11)-Al(2)-C(26)	-170.5(2)
C(12)-C(11)-Al(2)-C(26)	-61.1(3)	Si(1)-C(11)-Al(2)-C(26)	65.0(2)
C(19)-C(11)-Al(2)-C(25)	46.7(3)	C(12)-C(11)-Al(2)-C(25)	156.2(2)
Si(1)-C(11)-Al(2)-C(25)	-77.8(2)	C(28)#1-C(27)-O(1)-C(28)	-65(2)
C(28)#1-C(27)-O(1)-Al(1)	151.8(7)	C(24)-Al(1)-O(1)-C(28)	-21.0(7)
C(23)-Al(1)-O(1)-C(28)	-140.0(7)	O(1')-Al(1)-O(1)-C(28)	0(0)
C(1)-Al(1)-O(1)-C(28)	99.4(7)	C(24)-Al(1)-O(1)-C(27)	115.6(7)
C(23)-Al(1)-O(1)-C(27)	-3.5(7)	O(1')-Al(1)-O(1)-C(27)	0(0)
C(1)-Al(1)-O(1)-C(27)	-124.0(7)	C(27)-O(1)-C(28)-C(27)#1	65(2)
Al(1)-O(1)-C(28)-C(27)#1	-152.8(7)	C(28')#1-C(27')-O(1')-C(28')	74.1(11)
C(28')#1-C(27')-O(1')-Al(1)	-137.5(5)	C(24)-Al(1)-O(1')-C(28')	-53.7(6)
C(23)-Al(1)-O(1')-C(28')	-172.8(6)	O(1)-Al(1)-O(1')-C(28')	0(0)
C(1)-Al(1)-O(1')-C(28')	66.7(6)	C(24)-Al(1)-O(1')-C(27')	164.0(6)
C(23)-Al(1)-O(1')-C(27')	44.9(6)	O(1)-Al(1)-O(1')-C(27')	0(0)
C(1)-Al(1)-O(1')-C(27')	-75.6(6)	C(27')-O(1')-C(28')-C(27')#1	-73.6(11)
Al(1)-O(1')-C(28')-C(27')#1	137.9(6)	C(30)#2-C(29)-O(2)-C(30)	59.3(5)

C(30)#2-C(29)-O(2)-Al(2)	-134.8(3)	C(26)-Al(2)-O(2)-C(30)	14.9(3)
C(25)-Al(2)-O(2)-C(30)	131.9(3)	C(11)-Al(2)-O(2)-C(30)	-104.9(3)
C(26)-Al(2)-O(2)-C(29)	-149.1(3)	C(25)-Al(2)-O(2)-C(29)	-32.0(3)
C(11)-Al(2)-O(2)-C(29)	91.1(3)	C(29)-O(2)-C(30)-C(29)#2	-59.5(5)
Al(2)-O(2)-C(30)-C(29)#2	134.8(3)		

Symmetry transformations used to generate equivalent atoms:

#1 -x,-y,-z #2 -x+1/2,-y+3/2,-z

Table I.6 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for *rac*-2a.

	x	y	z	U(eq)	SOF
H(3A)	328(1)	4062(4)	-481(2)	61	1
H(4A)	157(1)	3538(5)	-1832(2)	81	1
H(5A)	492(2)	1904(5)	-2468(3)	83	1
H(6A)	1004(1)	803(4)	-1779(2)	71	1
H(8A)	1457(1)	598(3)	-242(2)	55	1
H(10A)	1757(5)	1047(15)	1183(7)	79	1
H(10B)	1430(1)	1618(24)	1783(4)	79	1
H(10C)	1748(5)	2513(10)	1350(10)	79	1
H(13A)	1821(1)	5843(4)	2248(2)	55	1
H(14A)	2450(1)	5535(5)	2927(2)	74	1
H(15A)	2971(1)	4457(5)	2308(3)	81	1
H(16A)	2882(1)	3705(4)	985(3)	70	1
H(18A)	2312(1)	3652(3)	-407(2)	56	1
H(20A)	1565(6)	3545(8)	-1181(8)	76	1
H(20B)	1648(5)	4990(17)	-1338(5)	76	1
H(20C)	1247(2)	4564(23)	-880(3)	76	1
H(21A)	406(1)	5270(11)	775(13)	66	1
H(21B)	675(5)	5722(17)	34(3)	66	1
H(21C)	719(4)	6403(7)	901(11)	66	1
H(22A)	820(3)	4138(20)	2266(2)	63	1
H(22B)	1116(7)	5322(4)	2297(2)	63	1
H(22C)	1305(4)	3950(17)	2309(2)	63	1
H(23A)	-219(3)	2766(5)	1564(13)	66	1
H(23B)	-75(5)	3638(17)	836(4)	66	1
H(23C)	86(2)	3900(13)	1752(11)	66	1
H(24A)	399(2)	681(18)	2331(10)	77	1
H(24B)	776(7)	1588(5)	2544(7)	77	1
H(24C)	833(6)	447(15)	1931(4)	77	1
H(25A)	1352(6)	8276(12)	-835(9)	81	1
H(25B)	950(2)	7539(24)	-582(5)	81	1
H(25C)	1291(7)	6852(13)	-1096(5)	81	1
H(26A)	1435(7)	8861(4)	1160(5)	76	1
H(26B)	1598(5)	7785(16)	1762(5)	76	1
H(26C)	1125(3)	7825(17)	1473(10)	76	1
H(27A)	-395(3)	534(8)	653(9)	77	0.565(15)
H(27B)	-327(3)	1864(8)	233(9)	77	0.565(15)
H(28A)	590(3)	-574(8)	728(9)	61	0.565(15)
H(28B)	121(3)	-828(8)	935(9)	61	0.565(15)
H(27C)	76(3)	1149(8)	-786(7)	41	0.435(15)
H(27D)	-171(3)	2098(8)	-221(7)	41	0.435(15)
H(28C)	655(3)	-472(10)	570(8)	37	0.435(15)
H(28D)	514(3)	-197(10)	-366(8)	37	0.435(15)
H(29A)	2256(1)	8285(4)	-913(2)	69	1
H(29B)	2057(1)	6940(4)	-1073(2)	69	1
H(30A)	2236(1)	8137(4)	1228(2)	65	1
H(30B)	2365(1)	9009(4)	485(2)	65	1

Determination of *rac*-{1-Me_2(Et_2O)-2-methyl-4,5-benz-1-indenyl}$_2$$SiMe_2$ (*rac*-**3**).

DATA COLLECTION

A crystal of the compound was attached to a glass fiber and mounted on the Siemens SMART system for a data collection at 173(2) K. An initial set of cell constants was calculated from reflections harvested from three sets of 20 frames. These initial sets of frames are oriented such that orthogonal wedges of reciprocal space were surveyed. This produces orientation matrices determined from 70 reflections. Final cell constants are calculated from a set of 8192 strong reflections from the actual data collection. Please refer to Table 1 for additional crystal and refinement information.

The data collection technique used for this specimen is generally known as a hemisphere collection. Here a randomly oriented region of reciprocal space is surveyed to the extent of 1.3 hemispheres to a resolution of 0.84 Å. Three major swaths of frames are collected with 0.30^{o} steps in ω. In the event the lattice is triclinic some additional sets of frames are collected to better model the absorption correction.

STRUCTURE SOLUTION AND REFINEMENT

The space group Pbcn was determined based on systematic absences and intensity statistics.[1] A successful direct-methods solution was calculated which provided most non-hydrogen atoms from the E-map. Several full-matrix least squares / difference Fourier cycles were performed which located the remainder of the non-hydrogen atoms. All non-hydrogen atoms were refined with anisotropic displacement parameters unless stated otherwise. All hydrogen atoms were placed in ideal positions and refined as riding atoms with relative isotropic displacement parameters.

The structure was found as expected. Halves of the molecule are related to each other by a crystallographic two-fold axis. The diethylether ligand is disordered. It was modelled by fitting one ethyl with two fragments. These refined to a 0.62:0.38 ratio. 21 restraints were applied using the SHELXTL instructions SAME and SIMU to better fit these disordered fragments. The higher than expected residual may be partly due to this disorder. There is no room for additional solvent in this structure.

Data collection and structure solution were conducted at the X-Ray Crystallographic Laboratory, 160 Kolthoff Hall, Chemistry Department, The University of Minnesota. All calculations were preformed using SGI INDY R4400-SC or Pentium computers using the SHELXTL V5.0 suite of programs. All publications arising from this report MUST either 1)include Victor G. Young, Jr. as a coauthor or 2)acknowledge both Victor G. Young, Jr. and the X-Ray

Crystallographic Laboratory.

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1. SHELXTL-Plus V5.0, Siemens Industrial Automation, Inc., Madison, WI.

Some equations of interest:

$$R_{int}=\sum|F_o^2-\langle F_o^2\rangle|/\sum|F_o^2|$$

$$R1=\sum||F_o|-|F_c||/\sum|F_o|$$

$$wR2=[\sum[w(F_o^2-F_c^2)^2]/\sum[w(F_o^2)^2]]^{1/2},$$

where $w=q/\sigma^2(F_o^2)+(a*P)^2+b*P$

$$GooF=S=[\sum[w(F_o^2-F_c^2)^2]/(n-p)^{1/2}$$

Table II.1. **Crystal data, data collection, and solution and refinement for *rac*-3.**

Crystal Data	
Empirical formula	$C_{21}H_{29}AlOSi_{0.50}$
Crystal Habit, color	Colorless, Block
Crystal size	0.40 x 0.35 x 0.15 mm
Crystal system	Orthorhombic
Space group	Pbcn
	a = 14.4047(3) Å $\alpha = 90^{o}$
	b = 11.9718(2) Å $\beta = 90^{o}$
	c = 22.6699(5) Å $\gamma = 90^{o}$
Volume	3909.43(14) $Å^3$
Z	8
Formula weight	338.47
Density (calculated)	1.150 Mg/m^3
Absorption coefficient	0.138 mm^{-1}
F(000)	1464
Data Collection	
Diffractometer	Siemens SMART Platform CCD
Wavelength	0.71073 Å
Temperature	173(2) K
θ range for data collection	1.80 to 25.04°
Index ranges	$0 \le h \le 17$, $0 \le k \le 14$, $0 \le \ell \le 26$
Reflections collected	18905
Independent reflections	3442 (R_{int} = 0.0306)
Solution and Refinement	
System used	SHELXTL-V5.0
Solution	Direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting scheme	$w = [\sigma^2(F_o^2)+(AP)^2+(BP)]^{-1}$, where P = $(Fo^2+2Fc^2))/3$, A = 0.0694, and B = 5.4316
Absorption correction	SADABS (Sheldrick, 1996)
Max. and min. transmission	1.000 and 0.852
Data / restraints / parameters	3439 / 21 / 232
R indices (I>2σ(I) = 2894)	R1 = 0.0709, wR2 = 0.1789
R indices (all data)	R1 = 0.0839, wR2 = 0.1889
Goodness-of-fit on F^2	1.121
Largest diff. peak and hole	0.568 and -0.233 $eÅ^{-3}$

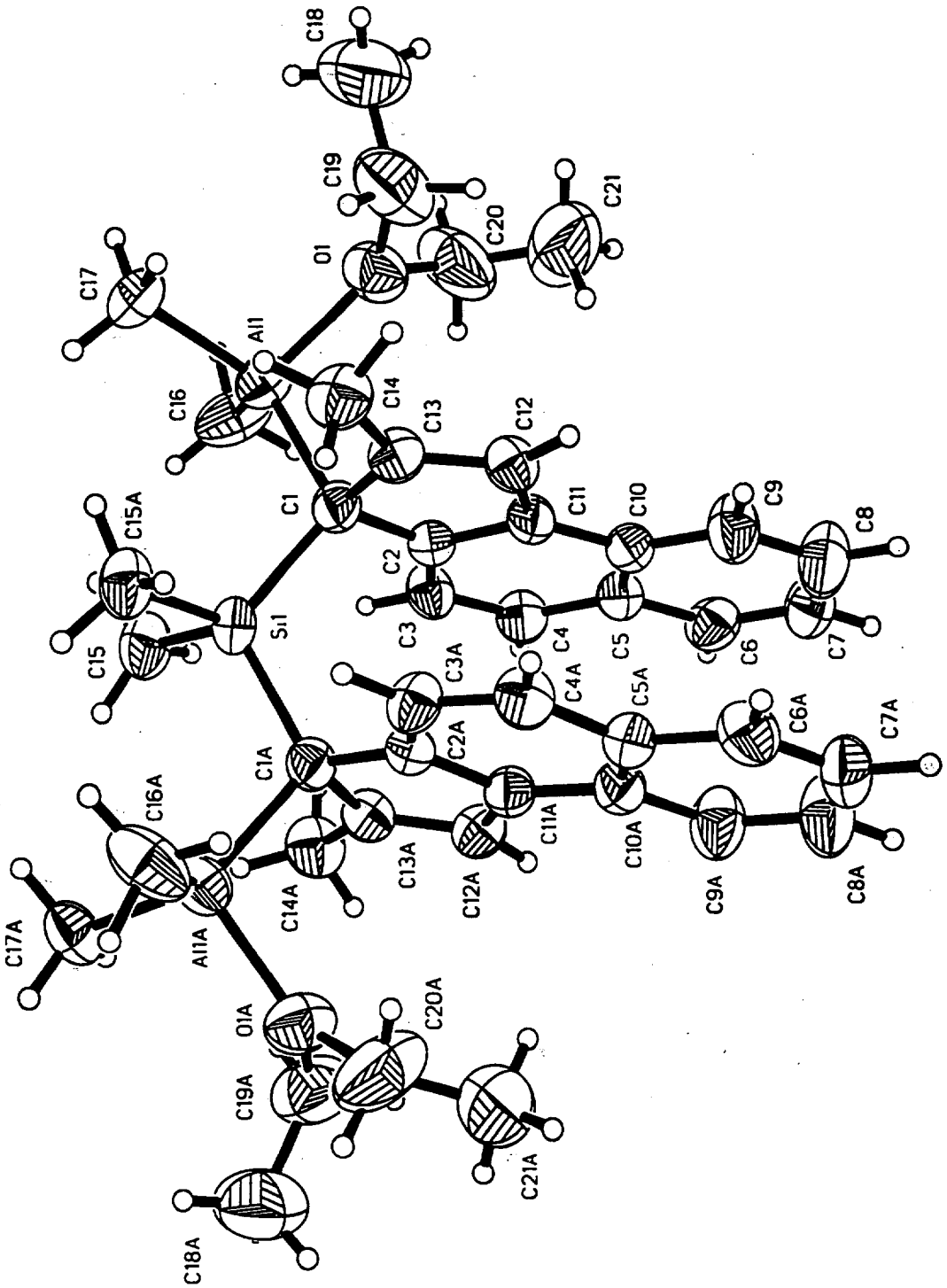
C18
C19
C21
C20
O1
C17
Al1
C16
C14
C13
C12
C1
C11
C10
C9
C8
C15A
C2
C15
Si1
C3
C4
C5
C6
C7
C3A
C4A
C5A
C6A
C7A
C1A
C2A
C16A
C11A
C10A
C13A
C14A
C12A
C9A
C8A
C17A
Al1A
O1A
C20A
C19A
C21A
C18A

Table II.2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for rac-3. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)	SOF
Al(1)	-512(1)	999(1)	6100(1)	46(1)	1
C(1)	-418(2)	1893(3)	6863(1)	38(1)	1
C(2)	196(2)	2861(2)	6731(1)	36(1)	1
C(3)	1158(2)	2879(3)	6580(2)	41(1)	1
C(4)	1584(2)	3878(3)	6477(2)	45(1)	1
C(5)	1092(2)	4901(3)	6510(1)	42(1)	1
C(6)	1543(3)	5963(3)	6414(2)	52(1)	1
C(7)	1064(3)	6925(3)	6470(2)	60(1)	1
C(8)	124(3)	6911(3)	6615(2)	70(1)	1
C(9)	-326(3)	5931(3)	6704(2)	60(1)	1
C(10)	140(2)	4908(3)	6656(1)	41(1)	1
C(11)	-297(2)	3851(3)	6756(1)	38(1)	1
C(12)	-1238(2)	3595(3)	6902(1)	42(1)	1
C(13)	-1337(2)	2471(3)	6974(1)	41(1)	1
C(14)	-2241(2)	1922(3)	7123(2)	53(1)	1
Si(1)	0	996(1)	7500	39(1)	1
C(15)	935(3)	16(3)	7242(2)	56(1)	1
C(16)	681(3)	605(4)	5709(2)	70(1)	1
C(17)	-1382(3)	-290(3)	6092(2)	54(1)	1
C(18)	-2491(4)	1784(5)	5009(2)	115(2)	1
C(19)	-2067(4)	2187(5)	5549(2)	93(2)	1
O(1)	-1074(2)	2043(2)	5564(1)	63(1)	1
C(20)	-648(14)	2858(16)	5182(9)	106(5)	0.62(3)
C(21)	-1048(24)	3968(9)	5204(7)	133(9)	0.62(3)
C(20')	-461(21)	2443(18)	5106(11)	92(6)	0.38(3)
C(21')	-371(23)	3652(18)	5089(9)	105(7)	0.38(3)

Table 2.3. Bond lengths [Å] and angles [°] for *rac*-3.

Al(1)-O(1)	1.922(3)	Al(1)-C(17)	1.988(3)
Al(1)-C(16)	1.991(4)	Al(1)-C(1)	2.039(3)
C(1)-C(2)	1.488(4)	C(1)-C(13)	1.514(4)
C(1)-Si(1)	1.899(3)	C(2)-C(11)	1.384(4)
C(2)-C(3)	1.427(4)	C(3)-C(4)	1.365(4)
C(4)-C(5)	1.417(4)	C(5)-C(10)	1.411(5)
C(5)-C(6)	1.444(5)	C(6)-C(7)	1.349(5)
C(7)-C(8)	1.394(6)	C(8)-C(9)	1.355(5)
C(9)-C(10)	1.400(5)	C(10)-C(11)	1.431(4)
C(11)-C(12)	1.428(4)	C(12)-C(13)	1.362(5)
C(13)-C(14)	1.499(4)	Si(1)-C(15)#1	1.879(4)
Si(1)-C(15)	1.879(3)	Si(1)-C(1)#1	1.899(3)
C(18)-C(19)	1.450(6)	C(19)-O(1)	1.440(5)
O(1)-C(20)	1.441(7)	O(1)-C(20')	1.444(8)
C(20)-C(21)	1.450(10)	C(20')-C(21')	1.454(10)

O(1)-Al(1)-C(17)	103.6(2)	O(1)-Al(1)-C(16)	103.7(2)
C(17)-Al(1)-C(16)	110.9(2)	O(1)-Al(1)-C(1)	102.84(13)
C(17)-Al(1)-C(1)	117.2(2)	C(16)-Al(1)-C(1)	116.4(2)
C(2)-C(1)-C(13)	101.4(2)	C(2)-C(1)-Si(1)	113.8(2)
C(13)-C(1)-Si(1)	114.2(2)	C(2)-C(1)-Al(1)	106.2(2)
C(13)-C(1)-Al(1)	108.8(2)	Si(1)-C(1)-Al(1)	111.7(2)
C(11)-C(2)-C(3)	119.7(3)	C(11)-C(2)-C(1)	110.7(3)
C(3)-C(2)-C(1)	129.6(3)	C(4)-C(3)-C(2)	119.4(3)
C(3)-C(4)-C(5)	121.6(3)	C(10)-C(5)-C(4)	120.2(3)
C(10)-C(5)-C(6)	117.9(3)	C(4)-C(5)-C(6)	121.9(3)
C(7)-C(6)-C(5)	120.5(3)	C(6)-C(7)-C(8)	120.6(3)
C(9)-C(8)-C(7)	120.7(4)	C(8)-C(9)-C(10)	121.1(4)
C(9)-C(10)-C(5)	119.3(3)	C(9)-C(10)-C(11)	123.4(3)
C(5)-C(10)-C(11)	117.3(3)	C(2)-C(11)-C(12)	108.2(3)
C(2)-C(11)-C(10)	121.7(3)	C(12)-C(11)-C(10)	130.1(3)
C(13)-C(12)-C(11)	109.8(3)	C(12)-C(13)-C(14)	123.5(3)
C(12)-C(13)-C(1)	109.9(3)	C(14)-C(13)-C(1)	126.6(3)
C(15)#1-Si(1)-C(15)	102.8(2)	C(15)#1-Si(1)-C(1)#1	110.1(2)
C(15)-Si(1)-C(1)#1	111.2(2)	C(15)#1-Si(1)-C(1)	111.2(2)
C(15)-Si(1)-C(1)	110.1(2)	C(1)#1-Si(1)-C(1)	111.0(2)
O(1)-C(19)-C(18)	113.5(4)	C(20)-O(1)-C(19)	109.2(9)
C(19)-O(1)-C(20')	123.4(14)	C(20)-O(1)-Al(1)	129.8(9)
C(19)-O(1)-Al(1)	120.7(3)	C(20')-O(1)-Al(1)	114.3(13)
O(1)-C(20)-C(21)	115.5(8)	O(1)-C(20')-C(21')	113.8(10)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2

Table II.4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for rac-3. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Al(1)	43(1)	48(1)	48(1)	-5(1)	1(1)	-5(1)
C(1)	34(2)	35(2)	45(2)	1(1)	-2(1)	-4(1)
C(2)	36(2)	34(2)	38(2)	0(1)	-4(1)	0(1)
C(3)	30(2)	38(2)	54(2)	5(1)	3(1)	5(1)
C(4)	32(2)	49(2)	53(2)	1(2)	3(1)	-2(1)
C(5)	46(2)	37(2)	43(2)	2(1)	-5(1)	-2(1)
C(6)	45(2)	53(2)	59(2)	0(2)	-5(2)	-11(2)
C(7)	66(3)	36(2)	77(3)	5(2)	-8(2)	-12(2)
C(8)	67(3)	39(2)	104(3)	-6(2)	2(2)	1(2)
C(9)	49(2)	43(2)	86(3)	-1(2)	2(2)	6(2)
C(10)	38(2)	37(2)	47(2)	2(1)	-5(1)	-2(1)
C(11)	34(2)	38(2)	42(2)	1(1)	-3(1)	1(1)
C(12)	33(2)	45(2)	47(2)	2(2)	3(1)	6(1)
C(13)	34(2)	45(2)	44(2)	-1(2)	2(1)	-3(1)
C(14)	38(2)	58(2)	64(2)	0(2)	4(2)	-8(2)
Si(1)	45(1)	28(1)	45(1)	0	3(1)	0
C(15)	58(2)	41(2)	68(2)	-6(2)	5(2)	7(2)
C(16)	51(2)	97(3)	62(2)	-36(2)	8(2)	-7(2)
C(17)	56(2)	48(2)	57(2)	-10(2)	-3(2)	-14(2)
C(18)	112(5)	134(5)	99(4)	-5(4)	-40(4)	12(4)
C(19)	104(4)	101(4)	75(3)	1(3)	-10(3)	42(3)
O(1)	67(2)	71(2)	51(2)	12(1)	-3(1)	-1(1)
C(20)	87(9)	106(11)	126(10)	66(10)	-27(7)	-20(10)
C(21)	226(26)	85(7)	89(8)	18(7)	-40(12)	-41(10)
C(20')	104(15)	79(11)	94(12)	64(10)	-9(9)	-7(10)
C(21')	124(20)	83(13)	107(14)	3(10)	-8(12)	-16(13)

Table 11.5 · Torsion angles [°] for *rac-3*.

O(1)-Al(1)-C(1)-C(2)	-61.7(2)	C(17)-Al(1)-C(1)-C(2)	-174.5(2)
C(16)-Al(1)-C(1)-C(2)	50.9(3)	O(1)-Al(1)-C(1)-C(13)	46.8(2)
C(17)-Al(1)-C(1)-C(13)	-66.0(3)	C(16)-Al(1)-C(1)-C(13)	159.4(2)
O(1)-Al(1)-C(1)-Si(1)	173.72(14)	C(17)-Al(1)-C(1)-Si(1)	60.9(2)
C(16)-Al(1)-C(1)-Si(1)	-73.7(2)	C(13)-C(1)-C(2)-C(11)	-0.6(3)
Si(1)-C(1)-C(2)-C(11)	-123.7(2)	Al(1)-C(1)-C(2)-C(11)	113.1(2)
C(13)-C(1)-C(2)-C(3)	-179.0(3)	Si(1)-C(1)-C(2)-C(3)	57.9(4)
Al(1)-C(1)-C(2)-C(3)	-65.4(4)	C(11)-C(2)-C(3)-C(4)	1.6(5)
C(1)-C(2)-C(3)-C(4)	180.0(3)	C(2)-C(3)-C(4)-C(5)	-0.6(5)
C(3)-C(4)-C(5)-C(10)	0.3(5)	C(3)-C(4)-C(5)-C(6)	178.6(3)
C(10)-C(5)-C(6)-C(7)	0.8(5)	C(4)-C(5)-C(6)-C(7)	-177.6(4)
C(5)-C(6)-C(7)-C(8)	-0.8(6)	C(6)-C(7)-C(8)-C(9)	0.3(7)
C(7)-C(8)-C(9)-C(10)	0.3(7)	C(8)-C(9)-C(10)-C(5)	-0.3(6)
C(8)-C(9)-C(10)-C(11)	178.8(4)	C(4)-C(5)-C(10)-C(9)	178.1(3)
C(6)-C(5)-C(10)-C(9)	-0.3(5)	C(4)-C(5)-C(10)-C(11)	-1.0(5)
C(6)-C(5)-C(10)-C(11)	-179.4(3)	C(3)-C(2)-C(11)-C(12)	178.7(3)
C(1)-C(2)-C(11)-C(12)	0.1(4)	C(3)-C(2)-C(11)-C(10)	-2.5(5)
C(1)-C(2)-C(11)-C(10)	178.9(3)	C(9)-C(10)-C(11)-C(2)	-177.0(3)
C(5)-C(10)-C(11)-C(2)	2.1(5)	C(9)-C(10)-C(11)-C(12)	1.6(6)
C(5)-C(10)-C(11)-C(12)	-179.3(3)	C(2)-C(11)-C(12)-C(13)	0.6(4)
C(10)-C(11)-C(12)-C(13)	-178.2(3)	C(11)-C(12)-C(13)-C(14)	-179.3(3)
C(11)-C(12)-C(13)-C(1)	-1.0(4)	C(2)-C(1)-C(13)-C(12)	0.9(3)
Si(1)-C(1)-C(13)-C(12)	123.8(3)	Al(1)-C(1)-C(13)-C(12)	-110.7(3)
C(2)-C(1)-C(13)-C(14)	179.2(3)	Si(1)-C(1)-C(13)-C(14)	-57.9(4)
Al(1)-C(1)-C(13)-C(14)	67.6(4)	C(2)-C(1)-Si(1)-C(15)#1	166.3(2)
C(13)-C(1)-Si(1)-C(15)#1	50.5(3)	Al(1)-C(1)-Si(1)-C(15)#1	-73.5(2)
C(2)-C(1)-Si(1)-C(15)	-80.5(3)	C(13)-C(1)-Si(1)-C(15)	163.7(2)
Al(1)-C(1)-Si(1)-C(15)	39.7(2)	C(2)-C(1)-Si(1)-C(1)#1	43.2(2)
C(13)-C(1)-Si(1)-C(1)#1	-72.6(2)	Al(1)-C(1)-Si(1)-C(1)#1	163.4(2)
C(18)-C(19)-O(1)-C(20)	74.4(12)	C(18)-C(19)-O(1)-C(20')	53.2(14)
C(18)-C(19)-O(1)-Al(1)	-111.7(5)	C(17)-Al(1)-O(1)-C(20)	-148.8(13)
C(16)-Al(1)-O(1)-C(20)	-32.9(13)	C(1)-Al(1)-O(1)-C(20)	88.7(13)
C(17)-Al(1)-O(1)-C(19)	38.6(3)	C(16)-Al(1)-O(1)-C(19)	154.5(3)
C(1)-Al(1)-O(1)-C(19)	-83.8(3)	C(17)-Al(1)-O(1)-C(20')	-127.5(13)
C(16)-Al(1)-O(1)-C(20')	-11.7(13)	C(1)-Al(1)-O(1)-C(20')	110.0(13)
C(19)-O(1)-C(20)-C(21)	41(2)	C(20')-O(1)-C(20)-C(21)	172(7)
Al(1)-O(1)-C(20)-C(21)	-132.3(11)	C(20)-O(1)-C(20')-C(21')	12(4)
C(19)-O(1)-C(20')-C(21')	71(3)	Al(1)-O(1)-C(20')-C(21')	-124(2)

Symmetry transformations used to generate equivalent atoms:

#1 -x,y,-z+3/2

Table II.6 Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for rac-3.

	x	y	z	U(eq)	SOF
H(3A)	1498(2)	2201(3)	6552(2)	49	1
H(4A)	2226(2)	3888(3)	6380(2)	53	1
H(6A)	2182(3)	5984(3)	6310(2)	62	1
H(7A)	1370(3)	7619(3)	6411(2)	72	1
H(8A)	-206(3)	7595(3)	6651(2)	84	1
H(9A)	-968(3)	5938(3)	6800(2)	72	1
H(12A)	-1722(2)	4128(3)	6943(1)	50	1
H(14A)	-2754(2)	2368(3)	6964(2)	80	1
H(14B)	-2303(2)	1867(3)	7552(2)	80	1
H(14C)	-2258(2)	1172(3)	6950(2)	80	1
H(15A)	1212(3)	-360(3)	7584(2)	84	1
H(15B)	1415(3)	439(3)	7033(2)	84	1
H(15C)	666(3)	-542(3)	6976(2)	84	1
H(16A)	558(3)	342(4)	5307(2)	105	1
H(16B)	991(3)	13(4)	5934(2)	105	1
H(16C)	1082(3)	1265(4)	5694(2)	105	1
H(17A)	-1408(3)	-608(3)	5694(2)	81	1
H(17B)	-2003(3)	-37(3)	6209(2)	81	1
H(17C)	-1165(3)	-860(3)	6370(2)	81	1
H(18A)	-3164(4)	1728(5)	5064(2)	173	1
H(18B)	-2239(4)	1047(5)	4911(2)	173	1
H(18C)	-2357(4)	2307(5)	4688(2)	173	1
H(19A)	-2212(4)	2990(5)	5596(2)	112	1
H(19B)	-2343(4)	1785(5)	5888(2)	112	1
H(20A)	-687(14)	2582(16)	4771(9)	127	0.62(3)
H(20B)	18(14)	2913(16)	5286(9)	127	0.62(3)
H(21A)	-683(24)	4504(9)	4974(7)	200	0.62(3)
H(21B)	-1094(24)	4228(9)	5613(7)	200	0.62(3)
H(21C)	-1672(24)	3905(9)	5035(7)	200	0.62(3)
H(20C)	-696(21)	2181(18)	4720(11)	110	0.38(3)
H(20D)	161(21)	2111(18)	5166(11)	110	0.38(3)
H(21D)	28(23)	3889(18)	4762(9)	157	0.38(3)
H(21E)	-104(23)	3907(18)	5463(9)	157	0.38(3)
H(21F)	-991(23)	3978(18)	5040(9)	157	0.38(3)