Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1996, 35(23), 6694-6702, DOI:10.1021/ic960486d

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[2,6\text{-Mes}_2\text{PhAlCl}_2]_2$.

	x	y	z	U(eq)
H(3A)	2724(6)	-1249(5)	2970(4)	24
H(4A)	2600(6)	-1821(6)	3807(5)	34
H(5A)	2574(6)	-1246(5)	4645(4)	23
H(9A)	1700(7)	902(6)	1962(5)	45
H(11A)	3821(7)	462(6)	1705(5)	40
H(13A)	1329(23)	-194(8)	2971(29)	59
H(13B)	1017(9)	450(37)	2661(15)	59
H(13C)	1456(17)	525(34)	3237(17)	59
H(14A)	2345(37)	887(32)	955(16)	81
H(14B)	3210(19)	1040(41)	1008(19)	81
H(14C)	2619(52)	1551(12)	1256(6)	81
H(15A)	4258(23)	-53(29)	3002(15)	49
H(15B)	4533(11)	-111(32)	2370(18)	49
H(15C)	4074(14)	-704(7)	2647(30)	49
H(18A)	3652(7)	443(6)	5946(4)	33
H(20A)	1513(7)	860(6)	5652(5)	39
H(22A)	4124(22)	-117(31)	4670(13)	50
H(22B)	3947(14)	-732(6)	5069(30)	50
H(22C)	4385(10)	-104(30)	5307(20)	50
H(23A)	2166(35)	868(30)	6672(15)	68
H(23B)	2441(50)	1535(11)	6377(6)	68
H(23C)	3031(18)	1023(38)	6625(17)	68
H(24A)	925(15)	553(30)	4865(21)	56
H(24B)	1130(24)	-198(11)	4719(27)	56
H(24C)	1399(12)	388(38)	4319(9)	56
H(27A)	4777(7)	3913(6)	3012(5)	37
H(28A)	4786(7)	4447(7)	3863(5)	46
H(29A)	4816(6)	3841(6)	4686(5)	39
H(33A)	5999(6)	1833(6)	2011(4)	31
H(35A)	3843(7)	2080(6)	1724(4)	35
H(37A)	6238(23)	2983(7)	2991(27)	54
H(37B)	6619(8)	2330(33)	2745(16)	54
H(37C)	6152(19)	2292(32)	3311(13)	54
H(38A)	4565(21)	1515(30)	1029(16)	51
H(38B)	5046(43)	991(7)	1373(5)	51
H(38C)	5444(25)	1594(26)	1061(17)	51
H(39A)	3501(9)	3286(11)	2659(32)	57
H(39B)	3227(20)	2585(27)	2892(21)	57
H(39C)	3111(15)	2768(36)	2249(13)	57
H(42A)	5988(7)	1733(5)	5609(4)	30
H(44A)	3818(6)	1992(6)	5894(4)	32
H(46A)	6210(21)	2880(11)	4578(27)	53
H(46B)	6181(20)	2129(28)	4365(18)	53

H(46C)	6605(7)	2307(36)	4930(11)	53
H(47A)	4507(14)	1335(33)	6541(19)	60
H(47B)	5357(33)	1545(23)	6591(17)	60
H(47C)	5130(45)	910(13)	6231(6)	60
H(48A)	3033(7)	2482(22)	5236(24)	47
H(48B)	3361(18)	2724(32)	4650(5)	47
H(48C)	3412(16)	3197(12)	5184(26)	47

Table 1. Crystal data for $TriphAlBr_2 \cdot OEt_2$.

Identification code	AB104
Empirical formula	$C_{28}H_{27}AlBr_2O$
Formula weight	566.30
Crystal size	0.68 x 0.52 x 0.16 mm
Crystal habit	plate
Crystal color	colorless
Crystal system	Monoclinic
Space group	$P2_1$
Unit cell dimensions	a = 10.686(3) Å α = 90°
	b = 9.351(3) Å β = 90.45(2)°
	c = 12.930(3) Å γ = 90°
Volume	1292.0(6) $Å^3$
Z	2
Density (calculated)	1.456 $Mg \cdot m^{-3}$
Absorption coefficient	3.189 mm^{-1}
F(000)	572
Absorption correction[1]	XABS2
Max. and min. transmission	0.65 and 0.25

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* **1995**, 28, 53-56.

Table 2. Data collection for $TriphAlBr_2 \cdot OEt_2$.

Diffractometer	Siemens R3m/V
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	0.71073 Å (MoKα)
Monochromator	graphite
θ range for data collection	1.57 to 27.50°
Scan type	ω
Index ranges	$-13 \leq h \leq 13$, $0 \leq k \leq 12$, $0 \leq \ell \leq 16$
Reflections collected	3307
Independent reflections	3155 (R_{int} = 0.1453)
Standard reflections	2 (measured every 198 reflections)
Percent decay of standards	stable

Table 3. Solution and refinement of $TriphAlBr_2 \cdot OEt_2$.

System for solution	SHELXS-86 (Sheldrick, 1990)
Structure solution	direct
System for refinement	XL-SHELXTL-Vers.5.03 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding model
Data / restraints / parameters	3155 / 0 / 290
Goodness-of-fit on F^2	1.036
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.1174P)^2 + 1.1198P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0923, wR2 = 0.1856
R indices calcd from obsd data	R1 = 0.0667, wR2 = 0.1642
Observed data (>2sigma(I))	2459
Absolute structure parameter	0.02(2)
Largest diff. peak and hole	0.748 and -1.155 $eÅ^{-3}$

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{½}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{½}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for TriphAlBr$_2$•OEt$_2$.
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Br(1)	10474(1)	6933	6028(1)	52(1)
Br(2)	7743(1)	4483(2)	5568(1)	46(1)
Al(1)	9060(2)	5426(4)	6804(2)	29(1)
O(1)	9975(6)	3799(8)	7172(6)	36(2)
C(1)	8185(7)	6071(10)	8067(7)	22(2)
C(2)	8658(7)	5813(10)	9076(7)	22(2)
C(3)	7867(8)	5863(10)	9942(7)	23(2)
C(4)	6618(7)	6320(10)	9840(7)	25(2)
C(5)	6165(7)	6682(9)	8867(7)	22(2)
C(6)	6936(7)	6593(8)	8005(7)	20(2)
C(7)	10017(7)	5570(11)	9294(7)	26(2)
C(8)	10899(8)	6463(11)	8821(8)	30(2)
C(9)	12149(8)	6365(14)	9077(10)	47(3)
C(10)	12570(9)	5420(14)	9846(11)	50(3)
C(11)	11684(9)	4509(15)	10317(8)	41(2)
C(12)	10426(8)	4626(13)	10036(7)	32(2)
C(13)	5820(8)	6454(10)	10770(7)	25(2)
C(14)	5866(9)	5426(12)	11559(7)	32(2)
C(15)	5141(9)	5572(13)	12441(8)	39(2)
C(16)	4374(9)	6729(13)	12571(8)	37(2)
C(17)	4319(8)	7761(12)	11793(7)	32(2)
C(18)	5031(8)	7632(12)	10906(7)	29(2)
C(19)	6387(8)	7121(11)	6998(7)	27(2)
C(20)	5209(8)	6729(11)	6655(7)	28(2)
C(21)	4717(9)	7254(13)	5751(8)	40(2)
C(22)	5391(9)	8255(13)	5185(8)	37(2)
C(23)	6592(10)	8686(13)	5512(8)	37(2)
C(24)	7079(9)	8104(11)	6417(7)	28(2)
C(25)	11139(11)	3402(18)	6609(9)	53(3)
C(26)	12131(13)	3059(29)	7327(14)	98(7)
C(27)	9371(11)	2667(13)	7759(9)	42(2)
C(28)	9099(14)	1331(15)	7159(12)	62(4)

Table 5. Bond lengths [Å] for $TriphAlBr_2 \cdot OEt_2$.

Br(1)-Al(1)	2.302(3)	Br(2)-Al(1)	2.297(3)
Al(1)-O(1)	1.868(8)	Al(1)-C(1)	1.983(9)
O(1)-C(27)	1.457(13)	O(1)-C(25)	1.492(12)
C(1)-C(2)	1.416(12)	C(1)-C(6)	1.423(11)
C(2)-C(3)	1.409(11)	C(2)-C(7)	1.495(11)
C(3)-C(4)	1.407(11)	C(4)-C(5)	1.387(12)
C(4)-C(13)	1.485(12)	C(5)-C(6)	1.394(11)
C(6)-C(19)	1.506(12)	C(7)-C(12)	1.373(14)
C(7)-C(8)	1.403(13)	C(8)-C(9)	1.377(13)
C(9)-C(10)	1.40(2)	C(10)-C(11)	1.41(2)
C(11)-C(12)	1.395(12)	C(13)-C(18)	1.399(13)
C(13)-C(14)	1.402(13)	C(14)-C(15)	1.390(13)
C(15)-C(16)	1.37(2)	C(16)-C(17)	1.39(2)
C(17)-C(18)	1.387(12)	C(19)-C(20)	1.382(12)
C(19)-C(24)	1.401(13)	C(20)-C(21)	1.368(14)
C(21)-C(22)	1.39(2)	C(22)-C(23)	1.41(2)
C(23)-C(24)	1.388(14)	C(25)-C(26)	1.44(2)
C(27)-C(28)	1.50(2)		

Table 6. Bond angles [°] for $TriphAlBr_2 \cdot OEt_2$.

O(1)-Al(1)-C(1)	106.7(4)	O(1)-Al(1)-Br(2)	100.5(3)
C(1)-Al(1)-Br(2)	113.5(3)	O(1)-Al(1)-Br(1)	105.4(2)
C(1)-Al(1)-Br(1)	119.2(3)	Br(2)-Al(1)-Br(1)	109.41(12)
C(27)-O(1)-C(25)	116.6(9)	C(27)-O(1)-Al(1)	119.4(6)
C(25)-O(1)-Al(1)	121.0(8)	C(2)-C(1)-C(6)	116.0(7)
C(2)-C(1)-Al(1)	122.7(6)	C(6)-C(1)-Al(1)	120.4(6)
C(3)-C(2)-C(1)	121.0(7)	C(3)-C(2)-C(7)	116.3(7)
C(1)-C(2)-C(7)	122.6(7)	C(4)-C(3)-C(2)	120.7(8)
C(5)-C(4)-C(3)	118.9(8)	C(5)-C(4)-C(13)	121.0(7)
C(3)-C(4)-C(13)	120.0(8)	C(4)-C(5)-C(6)	120.4(7)
C(5)-C(6)-C(1)	122.4(8)	C(5)-C(6)-C(19)	116.3(7)
C(1)-C(6)-C(19)	121.3(7)	C(12)-C(7)-C(8)	118.4(8)
C(12)-C(7)-C(2)	122.2(8)	C(8)-C(7)-C(2)	118.8(8)
C(9)-C(8)-C(7)	120.6(10)	C(8)-C(9)-C(10)	121.2(11)
C(9)-C(10)-C(11)	118.2(9)	C(12)-C(11)-C(10)	119.2(11)
C(7)-C(12)-C(11)	122.2(11)	C(18)-C(13)-C(14)	117.8(8)
C(18)-C(13)-C(4)	121.2(8)	C(14)-C(13)-C(4)	120.9(8)
C(15)-C(14)-C(13)	120.8(10)	C(16)-C(15)-C(14)	121.1(10)
C(15)-C(16)-C(17)	118.7(8)	C(18)-C(17)-C(16)	121.0(9)
C(17)-C(18)-C(13)	120.5(9)	C(20)-C(19)-C(24)	119.0(8)
C(20)-C(19)-C(6)	122.5(8)	C(24)-C(19)-C(6)	118.4(7)
C(21)-C(20)-C(19)	121.5(9)	C(20)-C(21)-C(22)	119.6(9)
C(21)-C(22)-C(23)	120.6(9)	C(24)-C(23)-C(22)	118.4(10)
C(23)-C(24)-C(19)	120.9(9)	C(26)-C(25)-O(1)	110.7(10)
O(1)-C(27)-C(28)	114.9(10)		

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $TriphAlBr_2 \cdot OEt_2$.

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
Br(1)	50(1)	60(1)	46(1)	11(1)	12(1)	-16(1)
Br(2)	43(1)	48(1)	46(1)	-23(1)	-11(1)	10(1)
Al(1)	28(1)	29(2)	29(1)	-1(1)	1(1)	-1(1)
O(1)	28(3)	30(4)	51(4)	-5(3)	2(3)	5(3)
C(1)	24(4)	14(4)	28(4)	2(3)	-2(3)	-2(3)
C(2)	22(3)	15(4)	30(4)	3(3)	-2(3)	1(3)
C(3)	29(4)	16(4)	26(4)	0(3)	-4(3)	-1(3)
C(4)	24(4)	18(5)	33(5)	1(4)	-1(3)	2(3)
C(5)	23(3)	13(5)	31(4)	2(3)	-3(3)	0(3)
C(6)	25(3)	3(4)	30(4)	-2(3)	-5(3)	-1(3)
C(7)	23(4)	20(5)	33(4)	3(4)	-5(3)	3(4)
C(8)	26(4)	15(5)	50(6)	3(4)	-2(4)	1(3)
C(9)	21(4)	43(7)	76(8)	-6(6)	2(4)	-3(4)
C(10)	32(5)	32(7)	85(9)	-9(6)	-24(5)	20(5)
C(11)	43(5)	30(6)	50(6)	-7(6)	-16(4)	12(6)
C(12)	39(4)	22(5)	34(4)	-4(5)	-10(4)	6(5)
C(13)	30(4)	22(5)	22(4)	2(3)	-1(3)	-5(4)
C(14)	39(4)	22(5)	35(5)	8(4)	7(4)	-4(4)
C(15)	46(5)	41(7)	30(5)	7(5)	6(4)	-6(5)
C(16)	37(4)	38(7)	35(5)	-2(5)	13(4)	-7(5)
C(17)	28(4)	26(5)	41(5)	-1(4)	4(4)	0(4)
C(18)	27(4)	30(5)	31(5)	6(4)	3(3)	-3(4)
C(19)	34(4)	12(4)	33(4)	2(4)	-4(3)	-1(4)
C(20)	32(4)	24(5)	28(4)	-8(4)	-5(3)	-4(4)
C(21)	42(5)	29(6)	48(6)	-7(5)	-20(4)	7(5)
C(22)	47(5)	33(6)	32(5)	3(4)	-11(4)	15(5)
C(23)	45(5)	33(6)	34(5)	4(4)	2(4)	3(5)
C(24)	36(4)	18(5)	29(4)	2(4)	0(3)	0(4)
C(25)	50(6)	64(9)	45(6)	-9(6)	9(5)	8(6)
C(26)	58(8)	148(22)	87(11)	-2(13)	-10(8)	44(12)
C(27)	52(6)	24(6)	50(6)	0(5)	6(5)	1(5)
C(28)	79(9)	28(7)	78(10)	-5(7)	-14(8)	-3(7)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $TriphAlBr_2 \cdot OEt_2$.

	x	y	z	U(eq)
H(3A)	8181(8)	5585(10)	10601(7)	28
H(5A)	5323(7)	6994(9)	8788(7)	27
H(8A)	10631(8)	7141(11)	8319(8)	37
H(9A)	12736(8)	6949(14)	8726(10)	56
H(10A)	13427(9)	5393(14)	10046(11)	60
H(11A)	11944(9)	3826(15)	10818(8)	49
H(12A)	9831(8)	4032(13)	10369(7)	38
H(14A)	6400(9)	4620(12)	11490(7)	38
H(15A)	5179(9)	4857(13)	12962(8)	47
H(16A)	3889(9)	6828(13)	13179(8)	44
H(17A)	3784(8)	8565(12)	11872(7)	38
H(18A)	4984(8)	8349(12)	10387(7)	35
H(20A)	4729(8)	6080(11)	7055(7)	34
H(21A)	3922(9)	6937(13)	5512(8)	48
H(22A)	5036(9)	8651(13)	4573(8)	45
H(23A)	7059(10)	9359(13)	5123(8)	44
H(24A)	7891(9)	8377(11)	6646(7)	33
H(25A)	10969(11)	2567(18)	6159(9)	63
H(25B)	11401(11)	4208(18)	6165(9)	63
H(26A)	12917(35)	2945(185)	6951(21)	146
H(26B)	11931(77)	2165(94)	7686(94)	146
H(26C)	12219(105)	3832(83)	7834(80)	146
H(27A)	8574(11)	3040(13)	8036(9)	50
H(27B)	9914(11)	2418(13)	8356(9)	50
H(28A)	8575(83)	693(50)	7574(33)	93
H(28B)	9886(16)	848(60)	6995(71)	93
H(28C)	8656(87)	1577(18)	6517(40)	93

Table 1. Crystal data for $2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

Identification code	BS20
Empirical formula	$C_{40}H_{59.93}AlCl_{0.24}O$
Formula weight	592.38
Crystal size	0.60 x 0.60 x 0.50 mm
Crystal habit	block
Crystal color	colorless
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 12.733(9) Å α = 90° b = 17.852(5) Å β = 105.86(4)° c = 16.913(3) Å γ = 90°
Volume	3698(3) Å^3
Z	4
Density (calculated)	1.064 Mg•m^{-3}
Absorption coefficient	0.830 mm^{-1}
F(000)	1300
Absorption correction[1]	XABS2
Max. and min. transmission	0.70 and 0.58

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* 1995, 28, 53-56.

Table 2. Data collection for

$2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

Diffractometer	Syntex $P2_1$
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	1.54178 Å (CuKα)
Monochromator	graphite
θ range for data collection	3.61 to 57.09°
Scan type	$2\theta-\theta$
Index ranges	$-13 \le h \le 13$, $0 \le k \le 19$, $0 \le \ell \le 18$
Reflections collected	5194
Independent reflections	4994 (R_{int} = 0.0340)
Standard reflections	2 (measured every 198 reflections)
Percent decay of standards	stable

Table 3. Solution and refinement of

$2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

System for solution	XS-SHELXTL-Vers.5.03 (Sheldrick, 1994)
Structure solution	direct
System for refinement	XL-SHELXTL-Vers.5.03 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding model
Data / restraints / parameters	4994 / 11 / 399
Goodness-of-fit on F^2	1.053
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0921P)^2 + 8.4240P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.1392, wR2 = 0.2528
R indices calcd from obsd data	R1 = 0.0982, wR2 = 0.2245
Observed data (>2sigma(I))	3385
Largest diff. peak and hole	0.700 and -0.359 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Al(1)	594(2)	1230(1)	5946(1)	64(1)
Cl(2)	880(7)	1454(5)	4841(5)	79(4)
C(1)	1067(4)	1988(3)	6829(3)	32(1)
C(2)	2108(4)	1913(3)	7400(3)	31(1)
C(3)	2451(4)	2417(3)	8051(3)	38(1)
C(4)	1795(4)	2999(3)	8152(3)	41(1)
C(5)	796(4)	3106(3)	7587(3)	36(1)
C(6)	429(4)	2608(3)	6936(3)	33(1)
C(7)	-654(4)	2782(3)	6334(3)	33(1)
C(8)	-1635(4)	2614(3)	6530(3)	46(1)
C(9)	-2610(4)	2808(4)	5970(3)	55(2)
C(10)	-2671(4)	3149(4)	5227(4)	52(2)
C(11)	-1697(4)	3308(3)	5049(3)	45(1)
C(12)	-680(4)	3147(3)	5587(3)	35(1)
C(13)	369(4)	3378(3)	5388(3)	41(1)
C(14)	733(5)	4152(4)	5762(4)	58(2)
C(15)	291(5)	3386(4)	4471(3)	61(2)
C(16)	-3790(5)	3295(5)	4631(4)	72(2)
C(17)	-4227(5)	2556(5)	4159(5)	86(2)
C(18)	-3842(7)	3899(6)	4090(5)	118(4)
C(19)	-1645(5)	2265(4)	7343(4)	56(2)
C(20)	-2432(7)	1601(5)	7239(5)	104(3)
C(21)	-1910(6)	2844(5)	7919(4)	76(2)
C(22)	2894(4)	1313(3)	7297(3)	33(1)
C(23)	3000(4)	639(3)	7750(3)	38(1)
C(24)	3724(4)	100(3)	7633(3)	41(1)
C(25)	4363(4)	191(3)	7095(4)	44(1)
C(26)	4258(4)	859(3)	6663(3)	43(1)
C(27)	3535(4)	1425(3)	6749(3)	35(1)
C(28)	3479(4)	2154(3)	6271(3)	42(1)
C(29)	3468(9)	2028(5)	5388(4)	124(4)
C(30)	4399(6)	2668(4)	6674(5)	83(2)
C(31)	5156(5)	-424(4)	7010(4)	63(2)
C(32)	6195(5)	-382(4)	7702(6)	98(3)
C(33)	5413(7)	-432(5)	6189(6)	105(3)
C(34)	2331(5)	496(3)	8360(4)	59(2)
C(35)	3041(8)	602(6)	9233(4)	110(3)
C(36)	1818(8)	-285(5)	8244(7)	119(4)
O(1)	-903(4)	968(2)	5754(3)	81(2)
C(40)	-1902(11)	1286(8)	5196(9)	42(4)
C(41)	-2577(19)	683(12)	4987(16)	119(9)

C(42)	-2222(15)	25(12)	5348(13)	99(7)
C(43)	-1128(13)	185(8)	5782(11)	59(4)
C(40A)	-1556(13)	1241(9)	4950(9)	93(5)
C(41A)	-2161(9)	777(6)	4412(6)	55(3)
C(42A)	-1254(12)	276(8)	6190(9)	87(5)
C(43A)	-771(14)	255(11)	7101(10)	132(7)

Experimental Details

Two disorder problems were encountered: During the refinement an electron density peak appeared close to H(2) and was then refined as Cl(2) with a partial occupancy of 0.241(8) (H(2): 0.759(8)).
During the refinement of the Et2O (C(40A)-C(43A)) molecule additional electron density was observed and was subsequently refined as a THF (C(40)-C(43)) molecule with a partial occupancy of 0.415(10) (Et2O: 0.585(10)). In both donor molecules C-C and O-C distances were constrained: C-C: 1.54(3), C-O: 1.45(3).
H(1) and H(2) were located in the difference map and refined with a constrained Al-H distance of 1.65(3) and fixed isotropic thermal parameter.

Table 5. Bond lengths [Å] for

$2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

Al(1)-H(1)	1.66(3)	Al(1)-H(2)	1.72(3)
Al(1)-O(1)	1.903(5)	Al(1)-C(1)	1.983(5)
Al(1)-Cl(2)	2.039(9)	C(1)-C(6)	1.413(7)
C(1)-C(2)	1.416(7)	C(2)-C(3)	1.396(7)
C(2)-C(22)	1.510(7)	C(3)-C(4)	1.373(7)
C(4)-C(5)	1.380(7)	C(5)-C(6)	1.394(7)
C(6)-C(7)	1.506(7)	C(7)-C(8)	1.410(7)
C(7)-C(12)	1.414(7)	C(8)-C(9)	1.384(8)
C(8)-C(19)	1.512(7)	C(9)-C(10)	1.380(8)
C(10)-C(11)	1.384(8)	C(10)-C(16)	1.526(8)
C(11)-C(12)	1.394(7)	C(12)-C(13)	1.520(7)
C(13)-C(15)	1.528(7)	C(13)-C(14)	1.538(8)
C(16)-C(18)	1.405(11)	C(16)-C(17)	1.563(10)
C(19)-C(21)	1.520(9)	C(19)-C(20)	1.532(9)
C(22)-C(27)	1.406(7)	C(22)-C(23)	1.413(7)
C(23)-C(24)	1.384(7)	C(23)-C(34)	1.528(7)
C(24)-C(25)	1.386(8)	C(25)-C(26)	1.385(8)
C(25)-C(31)	1.527(8)	C(26)-C(27)	1.400(7)
C(27)-C(28)	1.524(7)	C(28)-C(30)	1.497(8)
C(28)-C(29)	1.507(8)	C(31)-C(32)	1.509(9)
C(31)-C(33)	1.510(10)	C(34)-C(35)	1.518(10)
C(34)-C(36)	1.529(10)	O(1)-C(43)	1.43(2)
O(1)-C(40A)	1.469(14)	O(1)-C(40)	1.474(13)
O(1)-C(42A)	1.564(14)	C(40)-C(41)	1.36(2)
C(41)-C(42)	1.34(2)	C(42)-C(43)	1.42(2)
C(40A)-C(41A)	1.31(2)	C(42A)-C(43A)	1.50(2)

Table 6. Bond angles [°] for

$2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

H(1)-Al(1)-H(2)	115(3)	H(1)-Al(1)-O(1)	101(2)
H(2)-Al(1)-O(1)	88(3)	H(1)-Al(1)-C(1)	118(2)
H(2)-Al(1)-C(1)	116(2)	O(1)-Al(1)-C(1)	112.4(2)
H(1)-Al(1)-Cl(2)	97(2)	O(1)-Al(1)-Cl(2)	108.3(3)
C(1)-Al(1)-Cl(2)	117.6(3)	C(6)-C(1)-C(2)	116.7(4)
C(6)-C(1)-Al(1)	124.3(4)	C(2)-C(1)-Al(1)	119.0(4)
C(3)-C(2)-C(1)	120.7(4)	C(3)-C(2)-C(22)	118.3(4)
C(1)-C(2)-C(22)	120.9(4)	C(4)-C(3)-C(2)	121.0(5)
C(3)-C(4)-C(5)	119.7(5)	C(4)-C(5)-C(6)	120.4(5)
C(5)-C(6)-C(1)	121.4(4)	C(5)-C(6)-C(7)	116.7(4)
C(1)-C(6)-C(7)	121.9(4)	C(8)-C(7)-C(12)	120.1(4)
C(8)-C(7)-C(6)	120.3(4)	C(12)-C(7)-C(6)	119.5(4)
C(9)-C(8)-C(7)	118.3(5)	C(9)-C(8)-C(19)	119.7(5)
C(7)-C(8)-C(19)	122.0(5)	C(10)-C(9)-C(8)	123.3(5)
C(9)-C(10)-C(11)	117.3(5)	C(9)-C(10)-C(16)	119.1(5)
C(11)-C(10)-C(16)	123.5(6)	C(10)-C(11)-C(12)	122.9(5)
C(11)-C(12)-C(7)	118.0(5)	C(11)-C(12)-C(13)	121.0(5)
C(7)-C(12)-C(13)	121.0(4)	C(12)-C(13)-C(15)	114.2(4)
C(12)-C(13)-C(14)	109.7(5)	C(15)-C(13)-C(14)	109.8(5)
C(18)-C(16)-C(10)	115.5(7)	C(18)-C(16)-C(17)	111.6(7)
C(10)-C(16)-C(17)	109.4(6)	C(8)-C(19)-C(21)	111.2(5)
C(8)-C(19)-C(20)	112.5(5)	C(21)-C(19)-C(20)	110.2(6)
C(27)-C(22)-C(23)	119.5(5)	C(27)-C(22)-C(2)	119.9(4)
C(23)-C(22)-C(2)	120.7(4)	C(24)-C(23)-C(22)	118.9(5)
C(24)-C(23)-C(34)	119.8(5)	C(22)-C(23)-C(34)	121.3(5)
C(23)-C(24)-C(25)	123.0(5)	C(24)-C(25)-C(26)	117.3(5)
C(24)-C(25)-C(31)	119.9(5)	C(26)-C(25)-C(31)	122.8(5)
C(25)-C(26)-C(27)	122.5(5)	C(26)-C(27)-C(22)	118.8(5)
C(26)-C(27)-C(28)	119.9(4)	C(22)-C(27)-C(28)	121.3(5)
C(30)-C(28)-C(29)	109.7(6)	C(30)-C(28)-C(27)	111.4(5)
C(29)-C(28)-C(27)	112.7(5)	C(32)-C(31)-C(33)	110.4(6)
C(32)-C(31)-C(25)	110.7(6)	C(33)-C(31)-C(25)	114.1(6)
C(35)-C(34)-C(23)	110.0(6)	C(35)-C(34)-C(36)	111.0(7)
C(23)-C(34)-C(36)	111.2(6)	C(43)-O(1)-C(40)	104.7(9)
C(40A)-O(1)-C(42A)	122.4(9)	C(43)-O(1)-Al(1)	115.8(7)
C(40A)-O(1)-Al(1)	111.3(8)	C(40)-O(1)-Al(1)	131.5(7)
C(42A)-O(1)-Al(1)	121.0(6)	C(41)-C(40)-O(1)	103.5(14)
C(42)-C(41)-C(40)	118(2)	C(41)-C(42)-C(43)	103(2)
C(42)-C(43)-O(1)	110.9(14)	C(41A)-C(40A)-O(1)	120.6(12)
C(43A)-C(42A)-O(1)	114.5(12)		

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

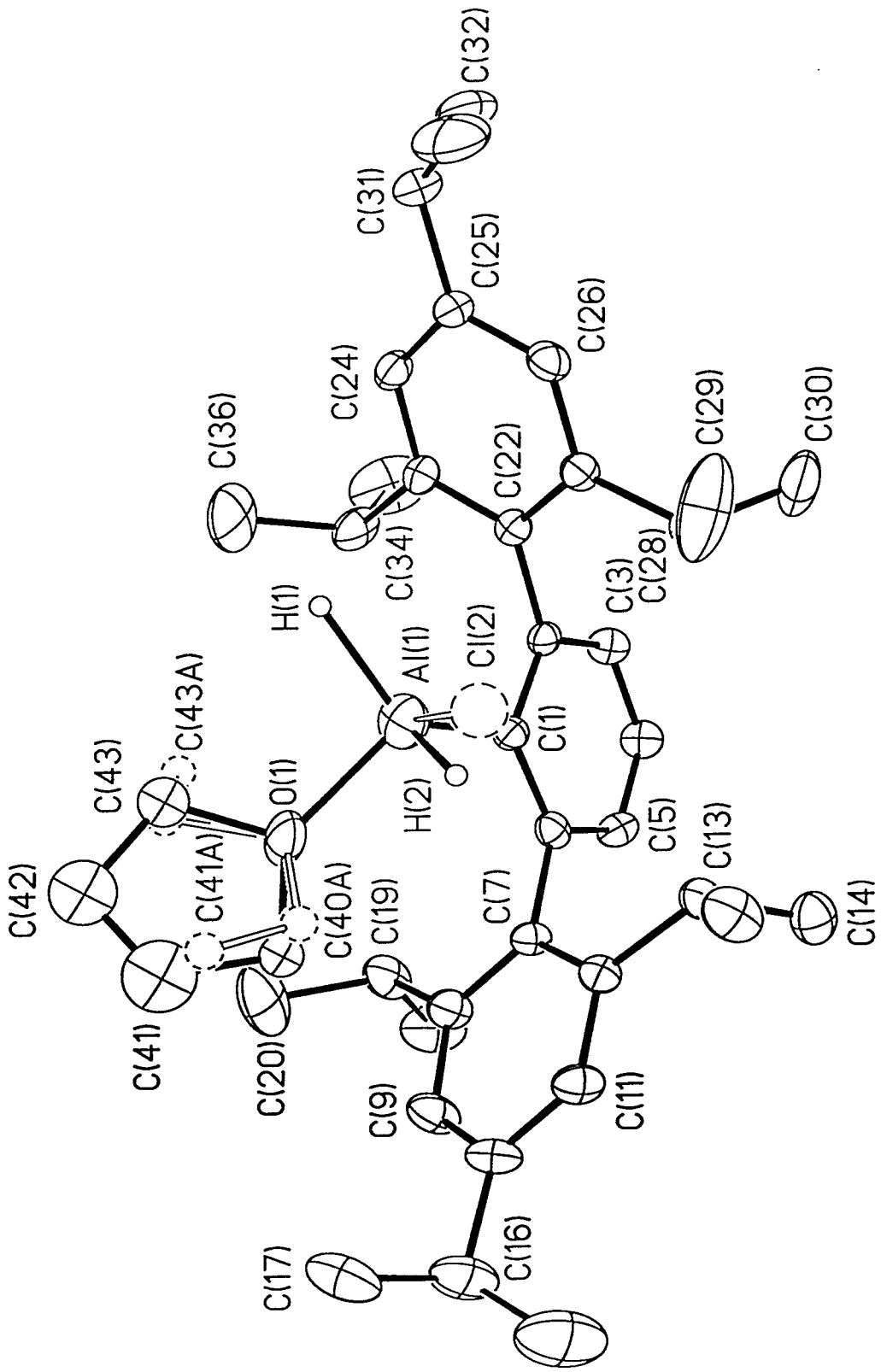
The anisotropic displacement factor exponent takes the form: $-2\pi^2 [(ha^*)^2U_{11} + \ldots + 2hka^*b^*U_{12}]$

	U11	U22	U33	U23	U13	U12
Al(1)	69(1)	54(1)	66(1)	-25(1)	16(1)	-9(1)
C(1)	32(3)	31(3)	36(3)	3(2)	16(2)	2(2)
C(2)	33(3)	28(3)	33(3)	6(2)	13(2)	1(2)
C(3)	39(3)	46(3)	28(3)	2(2)	7(2)	4(3)
C(4)	44(3)	45(3)	33(3)	-6(2)	10(2)	2(3)
C(5)	43(3)	37(3)	32(3)	5(2)	17(2)	9(3)
C(6)	32(3)	39(3)	30(3)	6(2)	10(2)	-5(2)
C(7)	32(3)	38(3)	29(3)	3(2)	9(2)	5(2)
C(8)	41(3)	55(4)	42(3)	9(3)	12(3)	2(3)
C(9)	35(3)	81(5)	50(4)	12(3)	15(3)	2(3)
C(10)	35(3)	66(4)	49(4)	1(3)	3(3)	15(3)
C(11)	44(3)	57(4)	32(3)	8(3)	9(3)	10(3)
C(12)	34(3)	39(3)	33(3)	-2(2)	11(2)	1(2)
C(13)	37(3)	50(4)	36(3)	10(3)	12(2)	-1(3)
C(14)	64(4)	61(4)	52(4)	8(3)	19(3)	-10(3)
C(15)	58(4)	90(5)	41(3)	8(3)	23(3)	-2(4)
C(16)	51(4)	106(6)	48(4)	9(4)	-3(3)	12(4)
C(17)	45(4)	125(7)	75(5)	-15(5)	-4(4)	6(4)
C(18)	94(6)	173(10)	76(6)	24(7)	7(5)	32(7)
C(19)	46(3)	77(5)	49(4)	19(3)	20(3)	-4(3)
C(20)	105(6)	130(8)	82(6)	28(5)	31(5)	-52(6)
C(21)	77(5)	116(6)	42(4)	17(4)	33(3)	23(4)
C(22)	35(3)	33(3)	31(3)	-1(2)	7(2)	0(2)
C(23)	43(3)	32(3)	39(3)	5(2)	12(2)	-1(3)
C(24)	43(3)	29(3)	47(3)	4(2)	5(3)	1(3)
C(25)	36(3)	33(3)	61(4)	-1(3)	10(3)	3(2)
C(26)	37(3)	46(4)	49(3)	-6(3)	20(3)	-2(3)
C(27)	34(3)	39(3)	32(3)	5(2)	8(2)	0(2)
C(28)	47(3)	43(3)	43(3)	12(3)	22(3)	3(3)
C(29)	251(12)	78(6)	49(4)	4(4)	51(6)	-58(7)
C(30)	100(6)	43(4)	95(6)	15(4)	8(5)	-20(4)
C(31)	50(4)	40(4)	102(5)	-4(4)	27(4)	11(3)
C(32)	52(4)	61(5)	166(9)	-8(5)	3(5)	23(4)
C(33)	105(6)	89(6)	138(8)	-10(6)	64(6)	38(5)
C(34)	75(4)	48(4)	66(4)	24(3)	40(4)	14(3)
C(35)	154(8)	140(8)	52(5)	23(5)	52(5)	51(7)
C(36)	133(8)	84(6)	177(10)	28(6)	106(8)	-26(6)
O(1)	71(3)	41(3)	99(4)	9(2)	-28(3)	-17(2)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $2,6Trip_2PhAlH_{1.76}Cl_{0.24}\cdot(OEt_2)_{0.58}(THF)_{0.42}$.

	x	y	z	U(eq)
H(1)	1183(37)	396(18)	6089(30)	50
H(2)	292(66)	1565(38)	4954(23)	50
H(3A)	3149(4)	2355(3)	8431(3)	46
H(4A)	2029(4)	3328(3)	8608(3)	49
H(5A)	355(4)	3521(3)	7643(3)	43
H(9A)	-3272(4)	2701(4)	6105(3)	66
H(11A)	-1723(4)	3536(3)	4536(3)	53
H(13A)	947(4)	3009(3)	5657(3)	49
H(14A)	825(32)	4136(7)	6356(5)	87
H(14B)	178(16)	4526(5)	5511(18)	87
H(14C)	1428(17)	4288(10)	5656(21)	87
H(15A)	7(33)	2903(9)	4227(6)	92
H(15B)	1017(8)	3470(24)	4394(3)	92
H(15C)	-202(27)	3788(15)	4202(6)	92
H(16A)	-4294(5)	3418(5)	4974(4)	86
H(17A)	-4939(21)	2651(9)	3768(24)	129
H(17B)	-4305(41)	2171(10)	4553(6)	129
H(17C)	-3712(22)	2383(17)	3861(26)	129
H(18A)	-4605(9)	3994(26)	3790(32)	176
H(18B)	-3423(48)	3778(17)	3699(28)	176
H(18C)	-3534(53)	4347(11)	4403(6)	176
H(19A)	-893(5)	2073(4)	7606(4)	67
H(20A)	-2364(38)	1289(20)	6779(26)	157
H(20B)	-3183(8)	1787(5)	7128(39)	157
H(20C)	-2253(34)	1302(21)	7745(15)	157
H(21A)	-1364(23)	3244(14)	8018(24)	113
H(21B)	-1902(39)	2604(7)	8442(11)	113
H(21C)	-2635(17)	3055(20)	7670(14)	113
H(24A)	3787(4)	-354(3)	7936(3)	49
H(26A)	4693(4)	936(3)	6295(3)	51
H(28A)	2781(4)	2410(3)	6273(3)	51
H(29A)	2853(36)	1702(34)	5122(13)	186
H(29B)	4153(26)	1790(37)	5367(4)	186
H(29C)	3389(61)	2510(7)	5100(12)	186
H(30A)	4376(27)	3112(14)	6330(17)	124
H(30B)	5095(6)	2407(11)	6742(30)	124
H(30C)	4327(25)	2820(24)	7213(15)	124
H(31A)	4802(5)	-914(4)	7065(4)	75
H(32A)	6016(6)	-385(34)	8230(6)	147
H(32B)	6586(25)	80(18)	7652(22)	147
H(32C)	6657(23)	-815(19)	7673(23)	147
H(33A)	5809(47)	-893(18)	6139(18)	157
H(33B)	5866(44)	3(20)	6151(17)	157

H(33C)	4732(7)	-412(37)	5746(6)	157
H(34A)	1729(5)	874(3)	8256(4)	71
H(35A)	2603(16)	517(38)	9619(5)	166
H(35B)	3333(45)	1113(13)	9299(13)	166
H(35C)	3647(33)	243(26)	9344(14)	166
H(36A)	1333(46)	-341(15)	8600(33)	178
H(36B)	2396(8)	-664(5)	8387(42)	178
H(36C)	1398(48)	-350(15)	7669(12)	178
H(40A)	-2225(11)	1673(8)	5479(9)	50
H(40B)	-1747(11)	1511(8)	4705(9)	50
H(41A)	-3273(19)	806(12)	5112(16)	143
H(41B)	-2743(19)	613(12)	4385(16)	143
H(42A)	-2260(15)	-373(12)	4934(13)	118
H(42B)	-2653(15)	-131(12)	5727(13)	118
H(43A)	-628(13)	-101(8)	5538(11)	71
H(43B)	-995(13)	25(8)	6362(11)	71
H(40C)	-2046(13)	1636(9)	5055(9)	111
H(40D)	-1047(13)	1487(9)	4682(9)	111
H(41C)	-2534(9)	1054(6)	3914(6)	83
H(41D)	-2703(9)	542(6)	4646(6)	83
H(41E)	-1696(9)	390(6)	4273(6)	83
H(42C)	-2060(12)	276(8)	6072(9)	104
H(42D)	-1042(12)	-186(8)	5950(9)	104
H(43C)	-1029(14)	-192(11)	7326(10)	198
H(43D)	-993(14)	704(11)	7348(10)	198
H(43E)	27(14)	241(11)	7225(10)	198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C(19)
C(7)
C(14)
C(41)
C(20)
C(9)
C(11)
C(16)
C(17)

Table 1. Crystal data for $[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene$.

Identification code	RW44
Empirical formula	$C_{96}H_{126}Al_2O_{0.52}$
Formula weight	1341.42
Crystal size	0.62 x 0.50 x 0.42 mm
Crystal habit	parallelepiped
Crystal color	colorless
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 13.075(7) Å α = 93.66(4)°
	b = 13.337(7) Å β = 97.58(4)°
	c = 13.400(6) Å γ = 115.41(4)°
Volume	2073(2) $Å^3$
Z	1 (2/2)
Density (calculated)	1.074 $Mg \cdot m^{-3}$
Absorption coefficient	0.642 mm^{-1}
F(000)	732
Absorption correction[1]	XABS2
Max. and min. transmission	0.79 and 0.70

1) XABS2: an empirical absorption correction program. Parkin,S.; Moezzi, B.; Hope, H. *J. Appl. Cryst.* 1995, 28, 53-56.

Table 2. Data collection for

$[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene.$

Diffractometer	Syntex $P2_1$
Temperature	130(2) K
Radiation source	normal-focus sealed tube
Wavelength	1.54178 Å (CuKα)
Monochromator	graphite
θ range for data collection	3.36 to 56.86°
Scan type	2θ–θ
Index ranges	$-14 \le h \le 13$, $-14 \le k \le 14$, $0 \le \ell \le 14$
Reflections collected	5863
Independent reflections	5568 (R_{int} = 0.0887)
Standard reflections	2 (measured every 198 reflections)
Percent decay of standards	stable (+2.8)

Table 3. Solution and refinement of

$[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene$.

System for solution	XS-SHELXTL-Vers. 5.03 (Sheldrick, 1994)
Structure solution	direct
System for refinement	XL-SHELXTL-Vers. 5.03 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding model
Data / restraints / parameters	5568 / 1 / 465
Goodness-of-fit on F^2	1.041
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.1412P)^2 + 1.6995P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.1055, wR2 = 0.2338
R indices calcd from obsd data	R1 = 0.0803, wR2 = 0.2059
Observed data (>2sigma(I))	4156
Largest diff. peak and hole	0.849 and -0.472 eÅ^{-3}

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) $Goodness\text{-}of\text{-}Fit = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$

where M is the number of reflections
and N is the number of parameters refined.

3) Refinement is based on F^2 for ALL reflections except for those with very negative F^2 or flagged by the user for potential systematic errors. Weighted R-factors wR and all goodnesses of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The observed criterion of $F^2 > 2\sigma(F^2)$ is used only for calculating R indices for observed data and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R-factors based on ALL data will be even larger.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for $[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene$. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Al(1)	4033(1)	4393(1)	5313(1)	25(1)
O(1)	5534(13)	4902(14)	5782(13)	42(5)
C(1)	3291(3)	2772(3)	4864(3)	21(1)
C(2)	3570(3)	2042(3)	5418(3)	21(1)
C(3)	3113(3)	900(3)	5048(3)	26(1)
C(4)	2351(4)	484(3)	4129(3)	27(1)
C(5)	2016(3)	1178(3)	3594(3)	25(1)
C(6)	2463(3)	2321(3)	3961(3)	22(1)
C(7)	4321(3)	2417(3)	6460(3)	23(1)
C(8)	5463(3)	2603(3)	6592(3)	21(1)
C(9)	6072(4)	2752(3)	7579(3)	23(1)
C(10)	5555(4)	2750(3)	8434(3)	26(1)
C(11)	4442(4)	2642(3)	8272(3)	30(1)
C(12)	3805(4)	2489(3)	7313(3)	26(1)
C(13)	6064(3)	2575(3)	5694(3)	24(1)
C(14)	7207(4)	3616(4)	5779(3)	36(1)
C(15)	6237(4)	1538(4)	5552(4)	40(1)
C(16)	6185(4)	2802(3)	9482(3)	31(1)
C(17)	5493(4)	1777(4)	9980(3)	39(1)
C(18)	6462(4)	3886(4)	10171(3)	41(1)
C(19)	2573(4)	2323(4)	7206(3)	33(1)
C(20)	2450(4)	3220(4)	7861(4)	46(1)
C(21)	1784(4)	1156(4)	7434(4)	51(1)
C(22)	1996(3)	3001(3)	3391(3)	24(1)
C(23)	2386(4)	3396(3)	2496(3)	26(1)
C(24)	1848(4)	3931(3)	1935(3)	29(1)
C(25)	948(4)	4106(3)	2215(3)	28(1)
C(26)	605(4)	3741(3)	3118(3)	28(1)
C(27)	1118(3)	3208(3)	3718(3)	24(1)
C(28)	3365(4)	3235(4)	2140(3)	35(1)
C(29)	4264(4)	4312(4)	1835(4)	45(1)
C(30)	2922(5)	2281(4)	1269(4)	51(1)
C(31)	367(4)	4629(4)	1523(3)	34(1)
C(32)	-23(5)	5404(4)	2073(4)	53(1)
C(33)	-645(5)	3733(4)	796(4)	48(1)
C(34)	699(4)	2819(3)	4700(3)	32(1)
C(35)	318(5)	3597(5)	5252(4)	57(2)
C(36)	-248(5)	1630(4)	4521(4)	57(2)
C(37)	4718(5)	-461(4)	7391(3)	42(1)
C(38)	3634(5)	-643(4)	7494(3)	43(1)
C(39)	2773(4)	-1710(4)	7384(4)	45(1)

C(40)	3001(4)	-2606(4)	7155(3)	43(1)
C(41)	4091(5)	-2433(4)	7054(3)	41(1)
C(42)	4957(4)	-1352(4)	7174(3)	39(1)
C(43)	-654(7)	952(6)	10253(5)	79(2)
C(44)	-176(5)	1353(5)	9408(5)	66(2)
C(45)	-860(5)	1395(4)	8586(4)	55(1)
C(46)	-1993(5)	1066(4)	8563(4)	52(1)
C(47)	-2486(5)	657(4)	9364(5)	58(2)
C(48)	-1825(7)	614(5)	10221(5)	67(2)

Experimental Details

H(1) and H(2) were located in the difference map and refined freely with fixed thermal parameters.
During the refinement a peak close to H(1) was observed and was then refined as O(1) with a partial occupancy of 0.260(13) (H(1): 0.740(13)).

Table 5. Bond lengths [Å] for

$[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene.$

Al(1)-H(2)	1.46(4)	Al(1)-O(1)	1.78(2)
Al(1)-H(1)	1.74(5)	Al(1)-O(1)#1	1.82(2)
Al(1)-C(1)	1.963(4)	Al(1)-Al(1)#1	2.635(3)
O(1)-Al(1)#1	1.82(2)	C(1)-C(2)	1.399(5)
C(1)-C(6)	1.414(6)	C(2)-C(3)	1.403(5)
C(2)-C(7)	1.514(5)	C(3)-C(4)	1.390(6)
C(4)-C(5)	1.383(6)	C(5)-C(6)	1.405(5)
C(6)-C(22)	1.490(5)	C(7)-C(8)	1.388(6)
C(7)-C(12)	1.420(5)	C(8)-C(9)	1.407(5)
C(8)-C(13)	1.528(5)	C(9)-C(10)	1.404(5)
C(10)-C(11)	1.386(6)	C(10)-C(16)	1.513(6)
C(11)-C(12)	1.387(6)	C(12)-C(19)	1.515(6)
C(13)-C(15)	1.499(6)	C(13)-C(14)	1.526(6)
C(16)-C(17)	1.531(6)	C(16)-C(18)	1.538(6)
C(19)-C(20)	1.515(6)	C(19)-C(21)	1.531(6)
C(22)-C(27)	1.407(6)	C(22)-C(23)	1.410(5)
C(23)-C(24)	1.389(6)	C(23)-C(28)	1.515(6)
C(24)-C(25)	1.386(6)	C(25)-C(26)	1.391(6)
C(25)-C(31)	1.508(6)	C(26)-C(27)	1.394(6)
C(27)-C(34)	1.527(5)	C(28)-C(30)	1.522(7)
C(28)-C(29)	1.537(6)	C(31)-C(33)	1.511(7)
C(31)-C(32)	1.525(7)	C(34)-C(36)	1.515(6)
C(34)-C(35)	1.521(6)	C(37)-C(38)	1.359(7)
C(37)-C(42)	1.376(7)	C(38)-C(39)	1.367(7)
C(39)-C(40)	1.377(7)	C(40)-C(41)	1.369(7)
C(41)-C(42)	1.382(7)	C(43)-C(48)	1.392(10)
C(43)-C(44)	1.391(9)	C(44)-C(45)	1.344(8)
C(45)-C(46)	1.347(8)	C(46)-C(47)	1.349(8)
C(47)-C(48)	1.364(9)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 6. Bond angles [°] for

$[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene$.

H(2)-Al(1)-O(1)	106(2)	H(2)-Al(1)-H(1)	116(3)
H(2)-Al(1)-O(1)#1	110(2)	O(1)-Al(1)-O(1)#1	85.9(8)
H(2)-Al(1)-C(1)	127(2)	O(1)-Al(1)-C(1)	111.7(6)
H(1)-Al(1)-C(1)	104(3)	O(1)#1-Al(1)-C(1)	107.8(5)
Al(1)-O(1)-Al(1)#1	94.1(8)	C(2)-C(1)-C(6)	118.6(3)
C(2)-C(1)-Al(1)	121.3(3)	C(6)-C(1)-Al(1)	120.1(3)
C(1)-C(2)-C(3)	121.0(4)	C(1)-C(2)-C(7)	122.5(3)
C(3)-C(2)-C(7)	116.4(3)	C(4)-C(3)-C(2)	119.4(4)
C(5)-C(4)-C(3)	120.7(4)	C(4)-C(5)-C(6)	120.3(4)
C(5)-C(6)-C(1)	119.8(3)	C(5)-C(6)-C(22)	117.5(3)
C(1)-C(6)-C(22)	122.7(3)	C(8)-C(7)-C(12)	120.5(4)
C(8)-C(7)-C(2)	121.1(3)	C(12)-C(7)-C(2)	118.3(4)
C(7)-C(8)-C(9)	119.4(3)	C(7)-C(8)-C(13)	122.2(3)
C(9)-C(8)-C(13)	118.3(4)	C(10)-C(9)-C(8)	121.0(4)
C(11)-C(10)-C(9)	117.7(4)	C(11)-C(10)-C(16)	122.0(4)
C(9)-C(10)-C(16)	120.2(4)	C(10)-C(11)-C(12)	123.3(4)
C(11)-C(12)-C(7)	117.8(4)	C(11)-C(12)-C(19)	119.7(4)
C(7)-C(12)-C(19)	122.4(4)	C(15)-C(13)-C(8)	112.5(3)
C(15)-C(13)-C(14)	110.2(4)	C(8)-C(13)-C(14)	112.0(3)
C(10)-C(16)-C(17)	110.8(4)	C(10)-C(16)-C(18)	112.0(3)
C(17)-C(16)-C(18)	110.3(4)	C(20)-C(19)-C(12)	112.7(4)
C(20)-C(19)-C(21)	110.6(4)	C(12)-C(19)-C(21)	110.8(4)
C(27)-C(22)-C(23)	119.3(4)	C(27)-C(22)-C(6)	119.8(3)
C(23)-C(22)-C(6)	120.8(4)	C(24)-C(23)-C(22)	118.7(4)
C(24)-C(23)-C(28)	120.2(4)	C(22)-C(23)-C(28)	121.1(4)
C(25)-C(24)-C(23)	123.2(4)	C(24)-C(25)-C(26)	116.9(4)
C(24)-C(25)-C(31)	119.4(4)	C(26)-C(25)-C(31)	123.6(4)
C(25)-C(26)-C(27)	122.5(4)	C(26)-C(27)-C(22)	119.2(4)
C(26)-C(27)-C(34)	120.2(4)	C(22)-C(27)-C(34)	120.6(3)
C(23)-C(28)-C(30)	111.4(4)	C(23)-C(28)-C(29)	112.5(4)
C(30)-C(28)-C(29)	110.2(4)	C(25)-C(31)-C(33)	110.4(4)
C(25)-C(31)-C(32)	114.5(4)	C(33)-C(31)-C(32)	109.5(4)
C(36)-C(34)-C(35)	110.2(4)	C(36)-C(34)-C(27)	111.9(4)
C(35)-C(34)-C(27)	113.3(3)	C(38)-C(37)-C(42)	120.1(4)
C(37)-C(38)-C(39)	120.5(5)	C(38)-C(39)-C(40)	119.8(5)
C(41)-C(40)-C(39)	120.3(4)	C(40)-C(41)-C(42)	119.4(5)
C(37)-C(42)-C(41)	119.9(5)	C(48)-C(43)-C(44)	118.8(6)
C(45)-C(44)-C(43)	119.0(6)	C(44)-C(45)-C(46)	121.7(6)
C(45)-C(46)-C(47)	120.8(6)	C(46)-C(47)-C(48)	119.7(6)
C(47)-C(48)-C(43)	119.9(6)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1

Table 7. Anisotropic displacement parameters [$Å^2 \times 10^3$] for $[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene$.
The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + \ldots + 2hka^* b^* U_{12}]$

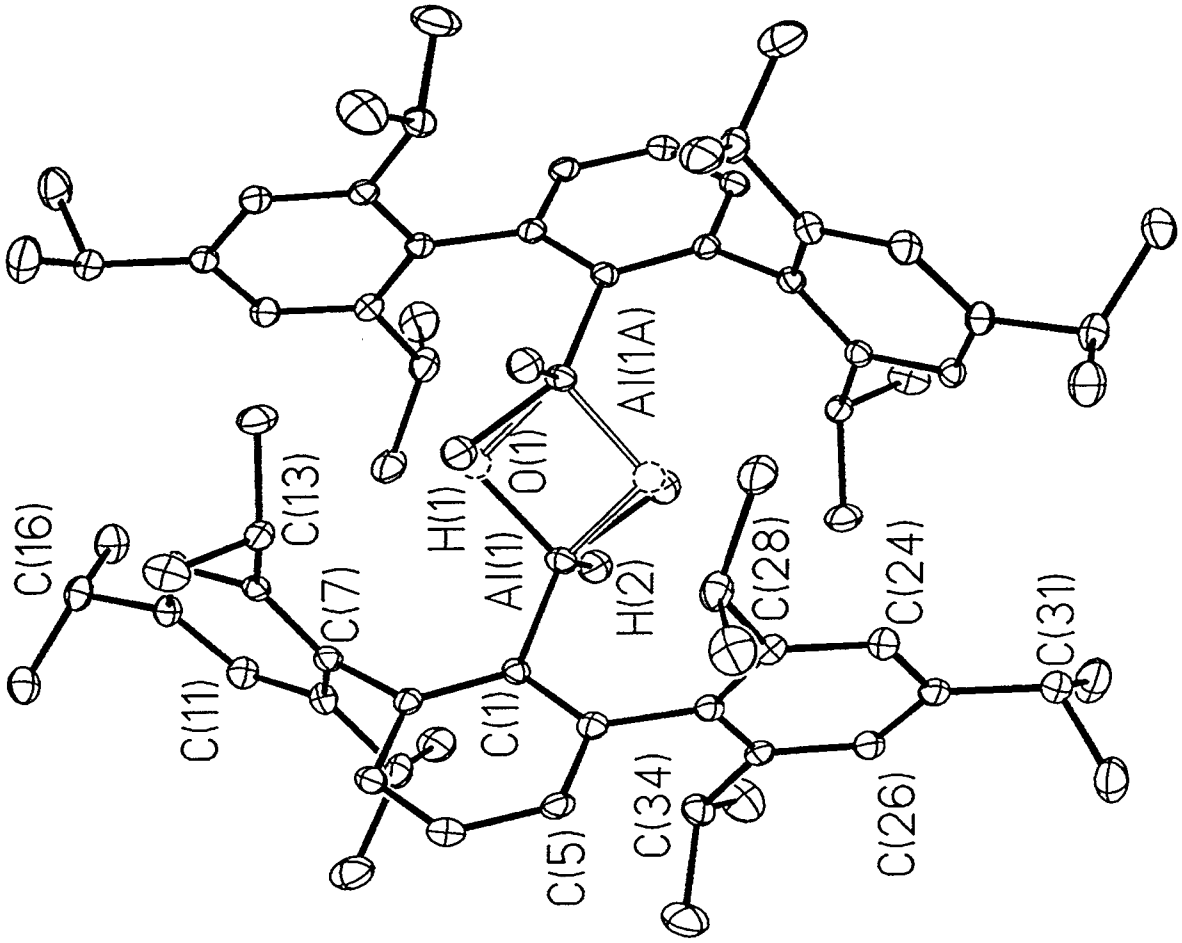
	U11	U22	U33	U23	U13	U12
Al(1)	26(1)	18(1)	29(1)	3(1)	5(1)	7(1)
C(1)	22(2)	21(2)	20(2)	5(2)	6(2)	9(2)
C(2)	18(2)	25(2)	20(2)	4(2)	5(2)	9(2)
C(3)	25(2)	22(2)	30(2)	5(2)	7(2)	9(2)
C(4)	26(2)	24(2)	26(2)	1(2)	8(2)	6(2)
C(5)	20(2)	23(2)	24(2)	-1(2)	-1(2)	3(2)
C(6)	20(2)	26(2)	23(2)	4(2)	8(2)	10(2)
C(7)	24(2)	21(2)	20(2)	4(2)	2(2)	6(2)
C(8)	23(2)	18(2)	22(2)	3(2)	3(2)	8(2)
C(9)	24(2)	24(2)	26(2)	4(2)	4(2)	14(2)
C(10)	30(3)	29(2)	20(2)	2(2)	3(2)	16(2)
C(11)	33(3)	36(2)	23(2)	6(2)	8(2)	18(2)
C(12)	32(3)	28(2)	23(2)	6(2)	7(2)	17(2)
C(13)	22(2)	30(2)	22(2)	4(2)	3(2)	13(2)
C(14)	24(3)	40(2)	36(2)	7(2)	9(2)	7(2)
C(15)	46(3)	35(2)	37(3)	1(2)	18(2)	15(2)
C(16)	34(3)	42(2)	22(2)	4(2)	1(2)	21(2)
C(17)	47(3)	47(3)	28(2)	10(2)	6(2)	24(2)
C(18)	50(3)	49(3)	26(2)	1(2)	0(2)	26(2)
C(19)	32(3)	46(3)	25(2)	10(2)	5(2)	21(2)
C(20)	35(3)	49(3)	64(3)	12(2)	21(3)	23(2)
C(21)	31(3)	43(3)	76(4)	-1(3)	11(3)	15(2)
C(22)	21(2)	20(2)	27(2)	2(2)	2(2)	7(2)
C(23)	22(2)	28(2)	27(2)	2(2)	2(2)	10(2)
C(24)	28(3)	31(2)	26(2)	6(2)	1(2)	13(2)
C(25)	24(2)	20(2)	36(2)	3(2)	0(2)	8(2)
C(26)	24(2)	25(2)	33(2)	4(2)	3(2)	9(2)
C(27)	20(2)	22(2)	23(2)	1(2)	-2(2)	3(2)
C(28)	34(3)	53(3)	27(2)	12(2)	9(2)	25(2)
C(29)	31(3)	68(3)	40(3)	21(2)	14(2)	22(2)
C(30)	57(4)	60(3)	52(3)	9(3)	23(3)	38(3)
C(31)	28(3)	36(2)	38(2)	13(2)	4(2)	14(2)
C(32)	54(4)	46(3)	57(3)	-4(2)	-15(3)	29(3)
C(33)	60(4)	47(3)	37(3)	5(2)	-7(2)	27(3)
C(34)	31(3)	36(2)	32(2)	13(2)	13(2)	15(2)
C(35)	73(4)	61(3)	50(3)	15(3)	33(3)	34(3)
C(36)	50(4)	52(3)	57(3)	23(3)	21(3)	5(3)
C(37)	51(3)	30(2)	34(3)	6(2)	5(2)	8(2)
C(38)	55(4)	49(3)	33(3)	5(2)	3(2)	32(3)
C(39)	33(3)	68(3)	39(3)	9(2)	7(2)	25(3)
C(40)	37(3)	37(3)	34(3)	3(2)	1(2)	0(2)
C(41)	58(4)	36(3)	30(2)	0(2)	8(2)	21(2)
C(42)	32(3)	46(3)	35(3)	8(2)	9(2)	13(2)
C(43)	107(6)	81(5)	67(4)	-4(4)	-13(4)	70(5)
C(44)	46(4)	73(4)	79(5)	-6(3)	6(3)	29(3)
C(45)	50(4)	48(3)	61(4)	0(3)	17(3)	15(3)

C(46)	51(4)	47(3)	59(3)	-1(3)	4(3)	26(3)
C(47)	53(4)	48(3)	76(4)	7(3)	22(3)	24(3)
C(48)	101(6)	47(3)	67(4)	13(3)	45(4)	37(3)

Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for $[Trip_2PhAl(H)(\mu\text{-}H)_{0.74}(\mu\text{-}OH)_{0.26}]_2 \cdot 4benzene$.

	x	y	z	U(eq)
H(1)	5486(42)	4727(72)	5598(65)	35
H(2)	3630(37)	5022(34)	5960(31)	35
H(3A)	3323(3)	415(3)	5423(3)	31
H(4A)	2058(4)	-284(3)	3866(3)	33
H(5A)	1480(3)	879(3)	2975(3)	30
H(9A)	6846(4)	2856(3)	7669(3)	28
H(11A)	4097(4)	2675(3)	8847(3)	36
H(13A)	5552(3)	2570(3)	5067(3)	29
H(14A)	7102(7)	4286(4)	5954(21)	53
H(14B)	7478(13)	3653(13)	5128(7)	53
H(14C)	7777(8)	3578(12)	6310(15)	53
H(15A)	5500(6)	876(4)	5509(24)	60
H(15B)	6785(21)	1545(13)	6130(12)	60
H(15C)	6540(26)	1516(14)	4924(13)	60
H(16A)	6930(4)	2789(3)	9405(3)	38
H(17A)	5287(23)	1093(4)	9518(10)	59
H(17B)	4791(13)	1808(14)	10125(21)	59
H(17C)	5959(10)	1774(14)	10615(12)	59
H(18A)	6951(22)	4533(4)	9867(12)	61
H(18B)	6867(24)	3886(13)	10841(8)	61
H(18C)	5746(5)	3928(13)	10243(19)	61
H(19A)	2315(4)	2370(4)	6482(3)	39
H(20A)	2970(21)	3960(4)	7714(18)	69
H(20B)	2645(27)	3161(18)	8579(4)	69
H(20C)	1655(8)	3118(17)	7713(18)	69
H(21A)	1839(23)	586(4)	6976(18)	76
H(21B)	988(6)	1055(11)	7333(25)	76
H(21C)	2020(19)	1081(11)	8140(9)	76
H(24A)	2110(4)	4190(3)	1329(3)	34
H(26A)	-3(4)	3860(3)	3334(3)	34
H(28A)	3761(4)	3025(4)	2721(3)	42
H(29A)	4468(21)	4941(7)	2364(12)	67
H(29B)	3943(11)	4464(16)	1191(13)	67
H(29C)	4953(12)	4218(11)	1754(24)	67
H(30A)	2369(23)	1594(8)	1480(10)	76
H(30B)	3568(6)	2165(19)	1086(18)	76
H(30C)	2543(26)	2470(13)	680(9)	76
H(31A)	936(4)	5088(4)	1107(3)	41
H(32A)	634(8)	5984(18)	2545(20)	80
H(32B)	-622(22)	4969(6)	2451(22)	80
H(32C)	-331(29)	5757(23)	1575(5)	80
H(33A)	-381(6)	3276(18)	399(18)	72
H(33B)	-998(18)	4085(4)	337(17)	72
H(33C)	-1213(13)	3255(17)	1181(4)	72
H(34A)	1365(4)	2820(3)	5163(3)	38
H(35A)	163(33)	3364(21)	5917(13)	86
H(35B)	-383(19)	3560(25)	4850(15)	86

H(35C)	928(14)	4366(7)	5345(26)	86
H(36A)	-6(13)	1143(7)	4138(25)	86
H(36B)	-947(10)	1610(7)	4133(24)	86
H(36C)	-403(23)	1366(12)	5176(4)	86
H(37A)	5312(5)	283(4)	7469(3)	50
H(38A)	3474(5)	-25(4)	7643(3)	52
H(39A)	2019(4)	-1832(4)	7466(4)	54
H(40A)	2400(4)	-3347(4)	7066(3)	52
H(41A)	4250(5)	-3052(4)	6903(3)	49
H(42A)	5716(4)	-1224(4)	7106(3)	46
H(43A)	-189(7)	911(6)	10842(5)	94
H(44A)	622(5)	1593(5)	9411(5)	79
H(45A)	-537(5)	1663(4)	8007(4)	66
H(46A)	-2449(5)	1122(4)	7976(4)	63
H(47A)	-3291(5)	401(4)	9331(5)	69
H(48A)	-2163(7)	352(5)	10796(5)	80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H(1)
O(1)
Al(1A)
Al(1)
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C(28)
C(24)
C(31)
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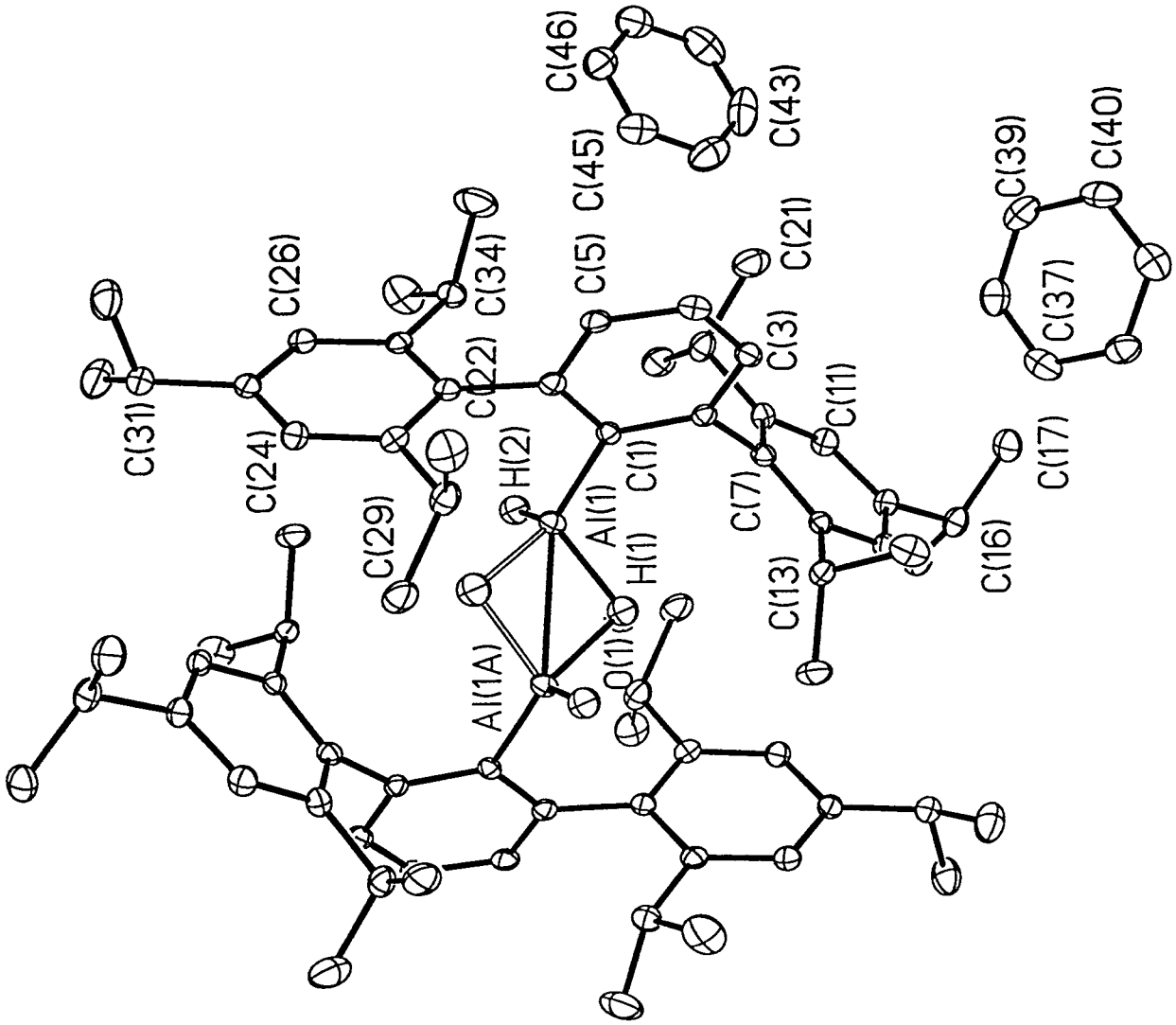
C(34)
C(26)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C(17)
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Al(1)
C(7)
H(1)
C(13)
C(16)
Al(1A)
O(1)

Table 1. Crystal data for

$[2,6\text{-Trip}_2\text{PhAlH}_{1.19}(\text{OH})_{0.81}]_2 \cdot 2C_6H_6$

Identification code	RW36
Empirical formula	$C_{84}H_{114}Al_2O_{1.62}$
Formula weight	1204.12
Crystal size	0.56 x 0.49 x 0.26 mm
Crystal habit	plate
Crystal color	colorless
Crystal system	Monoclinic
Space group	$P2_1/c$
Unit cell dimensions	a = 13.849(3) Å α = 90° b = 15.957(5) Å β = 108.55(2)° c = 17.689(5) Å γ = 90°
Volume	3706(2) Å^3
Z	2
Density (calculated)	1.079 Mg•m^3
Absorption coefficient	0.678 mm^{-1}
F(000)	1314
Absorption correction[1]	XABS2
Max. and min. transmission	0.86 and 0.72

1) Parkin, S. R., Moezzi, B. Hope, H. (1995). XABS2: an empirical absorption correction program. J. Appl. Cryst., 28, 53-56.

Table 2. Data collection for $[2,6\text{-Trip}_2\text{PhAlH}_{1.19}(\text{OH})_{0.81}]_2 \cdot 2C_6H_6$

Diffractometer	Siemens P4-RA
Temperature	130(2) K
Radiation source	Siemens rotating anode
Wavelength	1.54178 Å (CuKα)
Monochromator	nickel foil
θ range for data collection	3.37 to 56.10°
Scan type	$2\theta-\theta$
Index ranges	$-14 \le h \le 14$, $0 \le k \le 17$, $0 \le \ell \le 19$
Reflections collected	5293
Independent reflections	4833 (R_{int} = 0.027)
Observed [I>2σ(I)] reflections	4328
Standard reflections	2 (measured every 198 reflections)
Percent decay of standards	stable

Table 3. Solution and refinement of

$[2,6\text{-Trip}_2\text{PhAlH}_{1.19}(\text{OH})_{0.81}]_2 \cdot 2C_6H_6$

System for solution	SHELXTL-Vers. 5.03 (Sheldrick, 1994)
Structure solution	direct
System for refinement	SHELXTL-Vers. 5.03 (Sheldrick, 1994)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding model, fixed thermal parameters
Extinction correction	none
Data / restraints / parameters	4832 / 0 / 439
Goodness-of-fit on F^2	1.050
Final R indices [$I>2\sigma(I)$]	R1 = 0.0426, wR2 = 0.1026
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0452P)^2 + 2.5248P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0478, wR2 = 0.1072
Largest diff. peak and hole	0.402 and -0.252 $e\text{Å}^{-3}$

1) $R1 = \sum||Fo-Fc||/\sum|Fo|$

$wR2 = [\sum[w(Fo^2-Fc^2)^2]/\sum[w(Fo^2)^2]]^{1/2}$

2) $\text{Goodness-of-Fit} = [\sum[w(Fo^2-Fc^2)^2]/(M-N)]^{1/2}$

where M is the number of reflections

and N is the number of parameters refined.

Experimental Details

Several disorder problems were observed during the structure refinement. The Fourier difference map showed electron density close to the aluminum higher than to be expected for a hydride. These were refined as oxygens and hydrogens with partial occupancies: H(1) 47.7(7)%, O(1) 52.3(7)%, H(2) 71.5(5)%, O(2) 28.5(5)%. The hydroxyl hydrogen H(1A) was located in the difference map and refined freely with fixed thermal parameters and a partial (52.3(7)%) occupancy. H(2A) was

calculated using a riding model. The ortho trip group C(7)-C(21) was also disordered. The aromatic rings C(7)-C(12) and C(7A)-C(12A) were treated as rigid hexagons. The disorder could be modelled with split occupancies of 71.5(5)% for C(7)-C(14), C(16), C(17), C(19), C(20) and 28.5(5)% for C(7A)-C(14A), C(16A), C(17A), C(19A), C(20A). As the occupancies of O(2) and the "A" trip group independently reached ca. 29% each during the refinement they were refined as one group in the last least squares calculations.

Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [2,6-$Trip_2PhAlH_{1.19}(OH)_{0.81}]_2 \cdot 2C_6H_6$
U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Al(1)	928(1)	4851(1)	535(1)	26(1)
O(1)	-27(3)	4295(2)	-215(2)	32(1)
O(2)	1032(4)	4371(4)	1587(3)	39(2)
C(1)	2141(1)	5064(1)	215(1)	21(1)
C(2)	2649(1)	5844(1)	360(1)	21(1)
C(3)	3445(1)	6010(1)	56(1)	24(1)
C(4)	3766(1)	5409(1)	-372(1)	26(1)
C(5)	3317(1)	4622(1)	-477(1)	25(1)
C(6)	2517(1)	4444(1)	-189(1)	21(1)
C(7)	2403(3)	6486(2)	920(2)	21(1)
C(8)	2862(3)	6401(2)	1738(2)	19(1)
C(9)	2798(2)	7047(2)	2248(1)	26(1)
C(10)	2276(2)	7778(1)	1939(2)	24(1)
C(11)	1817(2)	7863(1)	1120(2)	23(1)
C(12)	1880(3)	7217(2)	611(1)	22(1)
C(7A)	2391(11)	6561(6)	803(6)	25
C(8A)	2761(9)	6561(5)	1631(6)	48(3)
C(9A)	2567(7)	7237(6)	2057(4)	23(2)
C(10A)	2002(6)	7914(4)	1653(5)	31(3)
C(11A)	1631(6)	7915(5)	825(5)	35(3)
C(12A)	1825(9)	7238(6)	400(4)	25
C(13)	3496(3)	5612(3)	2125(2)	30(1)
C(14)	3277(5)	5334(4)	2868(3)	55(1)
C(13A)	3287(9)	5826(8)	2065(8)	22(3)
C(14A)	3137(14)	5608(10)	2906(11)	67(6)
C(15)	4577(2)	5799(2)	2259(2)	70(1)
C(16)	2305(2)	8512(2)	2519(2)	28(1)
C(17)	1240(3)	8792(2)	2504(3)	41(1)
C(16A)	1936(7)	8741(5)	2125(6)	29(2)
C(17A)	1554(9)	8611(7)	2798(7)	46(4)
C(18)	2926(2)	9237(1)	2376(1)	39(1)
C(19)	1389(5)	7337(4)	-298(4)	29(1)
C(20)	287(3)	7629(2)	-521(3)	36(1)
C(19A)	1382(16)	7260(13)	-482(11)	30(5)
C(20A)	231(8)	7526(7)	-831(6)	32(3)
C(21)	2003(2)	7921(2)	-686(2)	48(1)
C(22)	2121(1)	3558(1)	-253(1)	22(1)
C(23)	2498(2)	3018(1)	400(1)	28(1)
C(24)	2184(2)	2181(1)	326(1)	29(1)
C(25)	1510(1)	1865(1)	-370(1)	25(1)
C(26)	1130(1)	2421(1)	-1004(1)	26(1)

C(27)	1419(1)	3255(1)	-965(1)	23(1)
C(28)	3263(2)	3310(1)	1182(1)	44(1)
C(29)	4325(2)	2977(2)	1280(2)	70(1)
C(30)	2935(2)	3081(2)	1899(1)	68(1)
C(31)	1170(2)	953(1)	-472(1)	33(1)
C(32)	1461(2)	451(1)	299(1)	44(1)
C(33)	1562(2)	516(1)	-1083(2)	49(1)
C(34)	995(2)	3819(1)	-1687(1)	32(1)
C(35)	-145(2)	3696(1)	-2107(1)	43(1)
C(36)	1581(2)	3682(2)	-2280(1)	50(1)
C(37)	5430(2)	3025(2)	3763(1)	46(1)
C(38)	4556(2)	2655(2)	3819(1)	45(1)
C(39)	4093(2)	2971(2)	4333(2)	58(1)
C(40)	4514(2)	3640(2)	4811(2)	67(1)
C(41)	5400(2)	4009(2)	4770(2)	58(1)
C(42)	5846(2)	3696(2)	4233(2)	50(1)