ORGANOMETALLICS
Organometallics, 1996, 15(8), 2009-2013, DOI:10.1021/om950681k

Table 1. Crystal data for [Cp*Rh(aniline)]$(O_3SCF_3)_2$.

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Identification code	mn611
Empirical formula	$C_{18}H_{22}F_6NO_6RhS_2$
Formula weight	629.40
Crystal size	0.32 x 0.28 x 0.24 mm
Crystal habit	prism
Crystal color	yellow/orange dichroic
Crystal system	Orthorhombic
Space group	$P2_12_12_1$
Unit cell dimensions	a = 9.5272(7) Å α = 90° b = 13.9970(10) Å β = 90° c = 17.3226(6) Å γ = 90°
Volume	2310.0(2) $Å^3$
Z	4
Density (calculated)	1.810 $Mg \cdot m^3$
Absorption coefficient	8.460 mm^{-1}
F(000)	1264
Absorption correction[1]	XABS2
Max. and min. transmission	0.20 and 0.09

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

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Table 2. Data collection for [Cp*Rh(aniline)]$(O_3SCF_3)_2$.

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	4.06 to 57.06°
Scan type	2θ-ω
Index ranges	$-10 \le h \le 10$, $0 \le k \le 15$, $0 \le \ell \le 18$
Reflections collected	2072
Independent reflections	2050 (R_{int} = 0.0231)
Standard reflections	2
Percent decay of standards	no decay

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Table 3. Solution and refinement of $[Cp^*Rh(aniline)](O_3SCF_3)_2$.

System for solution	SHELXS-86 (Sheldrick, 1990)
Structure solution	direct
System for refinement	SHELXL-93 (Sheldrick, 1993)
Refinement method	Full-matrix least-squares on F^2
Hydrogen atoms	riding
Data / restraints / parameters	2050 / 0 / 196
Goodness-of-fit on F^2	1.043
Final R indices [$I>2\sigma(I)$]	R1 = 0.0594, wR2 = 0.1536
Weighting scheme	$w^{-1} = \sigma^2(Fo^2) + (0.0999P)^2 + 26.37P$, where $P = (Fo^2 + 2Fc^2)/3$
R indices (all data)	R1 = 0.0615, wR2 = 0.1558
Absolute structure parameter	0.46(3)
Largest diff. peak and hole	3.094 and -1.498 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.

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Table 4. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for [Cp*Rh(aniline)]$(O_3SCF_3)_2$.

U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Rh	410(1)	3700(1)	7937(1)	6(1)
N	-2646(12)	4980(8)	7946(8)	21(3)
C(1)	-699(16)	2425(11)	7570(9)	22(4)
C(2)	686(16)	2475(10)	7205(8)	21(3)
C(3)	1750(14)	2450(10)	7784(7)	16(3)
C(4)	1047(14)	2389(9)	8522(7)	10(3)
C(5)	-451(16)	2379(9)	8382(7)	14(3)
C(6)	-2060(19)	2451(13)	7194(11)	43(5)
C(7)	1004(21)	2528(14)	6346(10)	45(5)
C(8)	3299(17)	2516(12)	7667(9)	34(4)
C(9)	1721(14)	2346(10)	9287(7)	14(3)
C(10)	-1576(17)	2316(11)	8984(8)	29(4)
C(11)	-1270(12)	4977(8)	7973(8)	8(3)
C(12)	-428(15)	4986(9)	7282(7)	12(3)
C(13)	1042(14)	5026(9)	7311(7)	9(3)
C(14)	1722(13)	4995(8)	8041(7)	6(3)
C(15)	943(14)	4887(9)	8728(8)	11(3)
C(16)	-531(14)	4835(9)	8688(7)	8(3)
S(1)	31(3)	5094(2)	4738(2)	12(1)
O(1)	196(12)	5017(8)	5562(6)	32(3)
O(2)	1123(11)	5602(7)	4339(6)	26(2)
O(3)	-1378(9)	5324(6)	4472(5)	10
C(17)	231(16)	3858(11)	4398(8)	23(3)
F(1)	-738(10)	3295(7)	4691(6)	39(2)
F(2)	1495(9)	3507(7)	4580(5)	32(2)
F(3)	148(8)	3821(6)	3624(4)	23(2)
S(2)	-144(3)	4661(2)	11114(2)	13(1)
O(4)	937(12)	4621(8)	11685(6)	37(3)
O(5)	-1550(10)	4590(7)	11427(5)	23(2)
O(6)	65(10)	4108(7)	10422(5)	22(2)
C(18)	-93(17)	5897(12)	10771(9)	32(4)
F(4)	1131(13)	6095(8)	10447(8)	71(4)
F(5)	-296(10)	6515(6)	11345(5)	35(2)
F(6)	-1068(13)	6061(7)	10241(5)	49(3)

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Table 5. Bond lengths [Å] for [Cp*Rh(aniline)]$(O_3SCF_3)_2$.

Rh-C(2)	2.148(14)	Rh-C(5)	2.165(14)
Rh-C(1)	2.17(2)	Rh-C(4)	2.182(13)
Rh-C(3)	2.182(13)	Rh-C(14)	2.210(12)
Rh-C(15)	2.214(13)	Rh-C(13)	2.233(13)
Rh-C(16)	2.241(12)	Rh-C(12)	2.273(13)
Rh-C(11)	2.400(12)	N-C(11)	1.31(2)
C(1)-C(5)	1.43(2)	C(1)-C(6)	1.45(2)
C(1)-C(2)	1.46(2)	C(2)-C(3)	1.43(2)
C(2)-C(7)	1.52(2)	C(3)-C(4)	1.45(2)
C(3)-C(8)	1.49(2)	C(4)-C(5)	1.45(2)
C(4)-C(9)	1.47(2)	C(5)-C(10)	1.50(2)
C(11)-C(16)	1.44(2)	C(11)-C(12)	1.44(2)
C(12)-C(13)	1.40(2)	C(13)-C(14)	1.42(2)
C(14)-C(15)	1.41(2)	C(15)-C(16)	1.41(2)
S(1)-O(2)	1.438(11)	S(1)-O(1)	1.440(11)
S(1)-O(3)	1.455(9)	S(1)-C(17)	1.84(2)
C(17)-F(1)	1.32(2)	C(17)-F(2)	1.34(2)
C(17)-F(3)	1.34(2)	S(2)-O(4)	1.429(12)
S(2)-O(6)	1.442(10)	S(2)-O(5)	1.449(11)
S(2)-C(18)	1.83(2)	C(18)-F(4)	1.32(2)
C(18)-F(6)	1.33(2)	C(18)-F(5)	1.33(2)

Table 6. Bond angles [°] for [Cp*Rh(aniline)]$(O_3SCF_3)_2$. L2013-6

C(2)-Rh-C(5)	64.9(5)	C(2)-Rh-C(1)	39.7(6)
C(5)-Rh-C(1)	38.5(5)	C(2)-Rh-C(4)	64.5(5)
C(5)-Rh-C(4)	38.9(5)	C(1)-Rh-C(4)	65.2(5)
C(2)-Rh-C(3)	38.4(5)	C(5)-Rh-C(3)	65.2(5)
C(1)-Rh-C(3)	65.8(5)	C(4)-Rh-C(3)	38.7(5)
C(2)-Rh-C(14)	129.3(5)	C(5)-Rh-C(14)	152.4(5)
C(1)-Rh-C(14)	167.0(5)	C(4)-Rh-C(14)	119.7(5)
C(3)-Rh-C(14)	109.7(5)	C(2)-Rh-C(15)	159.5(5)
C(5)-Rh-C(15)	120.5(5)	C(1)-Rh-C(15)	155.7(5)
C(4)-Rh-C(15)	106.3(5)	C(3)-Rh-C(15)	122.9(5)
C(14)-Rh-C(15)	37.2(5)	C(2)-Rh-C(13)	110.1(5)
C(5)-Rh-C(13)	170.2(5)	C(1)-Rh-C(13)	132.3(5)
C(4)-Rh-C(13)	148.2(5)	C(3)-Rh-C(13)	116.7(5)
C(14)-Rh-C(13)	37.3(5)	C(15)-Rh-C(13)	67.3(5)
C(2)-Rh-C(16)	163.2(5)	C(5)-Rh-C(16)	104.3(5)
C(1)-Rh-C(16)	124.0(6)	C(4)-Rh-C(16)	116.0(5)
C(3)-Rh-C(16)	150.8(5)	C(14)-Rh-C(16)	66.2(5)
C(15)-Rh-C(16)	36.9(5)	C(13)-Rh-C(16)	78.5(5)
C(2)-Rh-C(12)	112.4(5)	C(5)-Rh-C(12)	136.2(6)
C(1)-Rh-C(12)	109.5(5)	C(4)-Rh-C(12)	174.6(5)
C(3)-Rh-C(12)	141.2(5)	C(14)-Rh-C(12)	65.7(5)
C(15)-Rh-C(12)	78.2(5)	C(13)-Rh-C(12)	36.2(5)
C(16)-Rh-C(12)	65.6(4)	C(2)-Rh-C(11)	133.7(5)
C(5)-Rh-C(11)	112.0(5)	C(1)-Rh-C(11)	107.2(5)
C(4)-Rh-C(11)	143.1(4)	C(3)-Rh-C(11)	172.1(5)
C(14)-Rh-C(11)	76.3(4)	C(15)-Rh-C(11)	65.0(5)
C(13)-Rh-C(11)	64.7(5)	C(16)-Rh-C(11)	35.9(4)
C(12)-Rh-C(11)	35.8(5)	C(5)-C(1)-C(6)	126(2)
C(5)-C(1)-C(2)	106.2(14)	C(6)-C(1)-C(2)	127.6(13)
C(5)-C(1)-Rh	70.6(9)	C(6)-C(1)-Rh	123.1(11)
C(2)-C(1)-Rh	69.4(8)	C(3)-C(2)-C(1)	109.7(11)
C(3)-C(2)-C(7)	123.2(14)	C(1)-C(2)-C(7)	127.2(14)
C(3)-C(2)-Rh	72.1(8)	C(1)-C(2)-Rh	70.9(8)
C(7)-C(2)-Rh	124.3(12)	C(2)-C(3)-C(4)	107.1(11)
C(2)-C(3)-C(8)	127.3(13)	C(4)-C(3)-C(8)	125.6(12)
C(2)-C(3)-Rh	69.5(8)	C(4)-C(3)-Rh	70.6(8)
C(8)-C(3)-Rh	123.1(11)	C(3)-C(4)-C(5)	108.0(12)
C(3)-C(4)-C(9)	126.6(12)	C(5)-C(4)-C(9)	125.4(12)
C(3)-C(4)-Rh	70.7(7)	C(5)-C(4)-Rh	69.9(8)
C(9)-C(4)-Rh	124.9(9)	C(1)-C(5)-C(4)	109.1(13)
C(1)-C(5)-C(10)	125(2)	C(4)-C(5)-C(10)	126.1(12)
C(1)-C(5)-Rh	70.9(9)	C(4)-C(5)-Rh	71.2(8)
C(10)-C(5)-Rh	124.7(10)	N-C(11)-C(16)	121.3(13)
N-C(11)-C(12)	121.8(13)	C(16)-C(11)-C(12)	116.4(10)
N-C(11)-Rh	131.9(9)	C(16)-C(11)-Rh	66.0(7)
C(12)-C(11)-Rh	67.3(7)	C(13)-C(12)-C(11)	121.7(12)
C(13)-C(12)-Rh	70.3(8)	C(11)-C(12)-Rh	76.9(7)
C(12)-C(13)-C(14)	119.1(12)	C(12)-C(13)-Rh	73.5(8)
C(14)-C(13)-Rh	70.5(7)	C(15)-C(14)-C(13)	120.9(11)

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C(15)-C(14)-Rh	71.6(7)	C(13)-C(14)-Rh	72.2(7)
C(16)-C(15)-C(14)	119.2(12)	C(16)-C(15)-Rh	72.6(8)
C(14)-C(15)-Rh	71.2(7)	C(15)-C(16)-C(11)	121.5(12)
C(15)-C(16)-Rh	70.5(8)	C(11)-C(16)-Rh	78.1(7)
O(2)-S(1)-O(1)	115.7(6)	O(2)-S(1)-O(3)	113.9(6)
O(1)-S(1)-O(3)	115.5(6)	O(2)-S(1)-C(17)	103.7(6)
O(1)-S(1)-C(17)	103.7(6)	O(3)-S(1)-C(17)	101.7(6)
F(1)-C(17)-F(2)	108.6(12)	F(1)-C(17)-F(3)	108.6(13)
F(2)-C(17)-F(3)	105.9(12)	F(1)-C(17)-S(1)	111.6(10)
F(2)-C(17)-S(1)	111.3(10)	F(3)-C(17)-S(1)	110.5(10)
O(4)-S(2)-O(6)	117.1(6)	O(4)-S(2)-O(5)	113.9(6)
O(6)-S(2)-O(5)	113.7(6)	O(4)-S(2)-C(18)	104.1(7)
O(6)-S(2)-C(18)	103.5(6)	O(5)-S(2)-C(18)	102.2(7)
F(4)-C(18)-F(6)	106.8(14)	F(4)-C(18)-F(5)	108.0(13)
F(6)-C(18)-F(5)	107.6(13)	F(4)-C(18)-S(2)	111.0(12)
F(6)-C(18)-S(2)	111.7(11)	F(5)-C(18)-S(2)	111.5(11)

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Table 7. Anisotropic displacement parameters [$Å^2$ x 10^3] for [Cp*Rh(aniline)]$(O_3SCF_3)_2$.

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
Rh	7(1)	3(1)	6(1)	0(1)	-1(1)	1(1)
S(1)	2(2)	25(2)	7(1)	-6(1)	3(1)	-2(1)
C(17)	20(8)	35(9)	15(7)	1(7)	-4(7)	3(8)
F(1)	39(6)	27(5)	52(6)	1(5)	13(5)	-15(5)
F(2)	19(5)	47(6)	29(5)	-5(4)	-12(4)	24(5)
F(3)	21(4)	29(4)	19(4)	-11(4)	-6(3)	5(4)
S(2)	2(2)	27(2)	11(1)	-3(1)	1(1)	2(1)
C(18)	33(10)	37(9)	25(8)	-11(7)	19(8)	-13(8)
F(4)	66(8)	36(6)	112(10)	-16(7)	76(8)	-21(6)
F(5)	33(5)	34(5)	38(5)	-21(4)	8(5)	-6(5)
F(6)	92(9)	31(6)	25(5)	1(4)	-22(6)	10(6)

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Table 8. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for [Cp*Rh(aniline)]$(O_3SCF_3)_2$.

	x	y	z	U(eq)
H(1A)	-3136(12)	4895(8)	8371(8)	25
H(1B)	-3079(12)	5068(8)	7503(8)	25
H(6A)	-1931(19)	2500(89)	6634(12)	65
H(6B)	-2590(55)	3006(55)	7379(55)	65
H(6C)	-2578(56)	1865(45)	7315(60)	65
H(7A)	256(73)	2883(80)	6084(15)	67
H(7B)	1060(134)	1880(14)	6133(18)	67
H(7C)	1902(70)	2856(82)	6267(11)	67
H(8A)	3731(22)	1896(25)	7779(59)	50
H(8B)	3688(23)	3001(56)	8014(46)	50
H(8C)	3496(18)	2694(74)	7130(19)	50
H(9A)	1940(81)	1681(11)	9415(22)	21
H(9B)	1081(39)	2608(56)	9677(10)	21
H(9C)	2588(49)	2722(51)	9280(16)	21
H(10A)	-1260(45)	2638(62)	9456(21)	43
H(10B)	-1774(74)	1644(11)	9098(41)	43
H(10C)	-2430(37)	2627(63)	8793(24)	43
H(12)	-880(15)	4965(9)	6793(7)	14
H(13)	1575(14)	5073(9)	6850(7)	11
H(14)	2715(13)	5048(8)	8066(7)	7
H(15)	1408(14)	4851(9)	9213(8)	13
H(16)	-1050(14)	4703(9)	9144(7)	10

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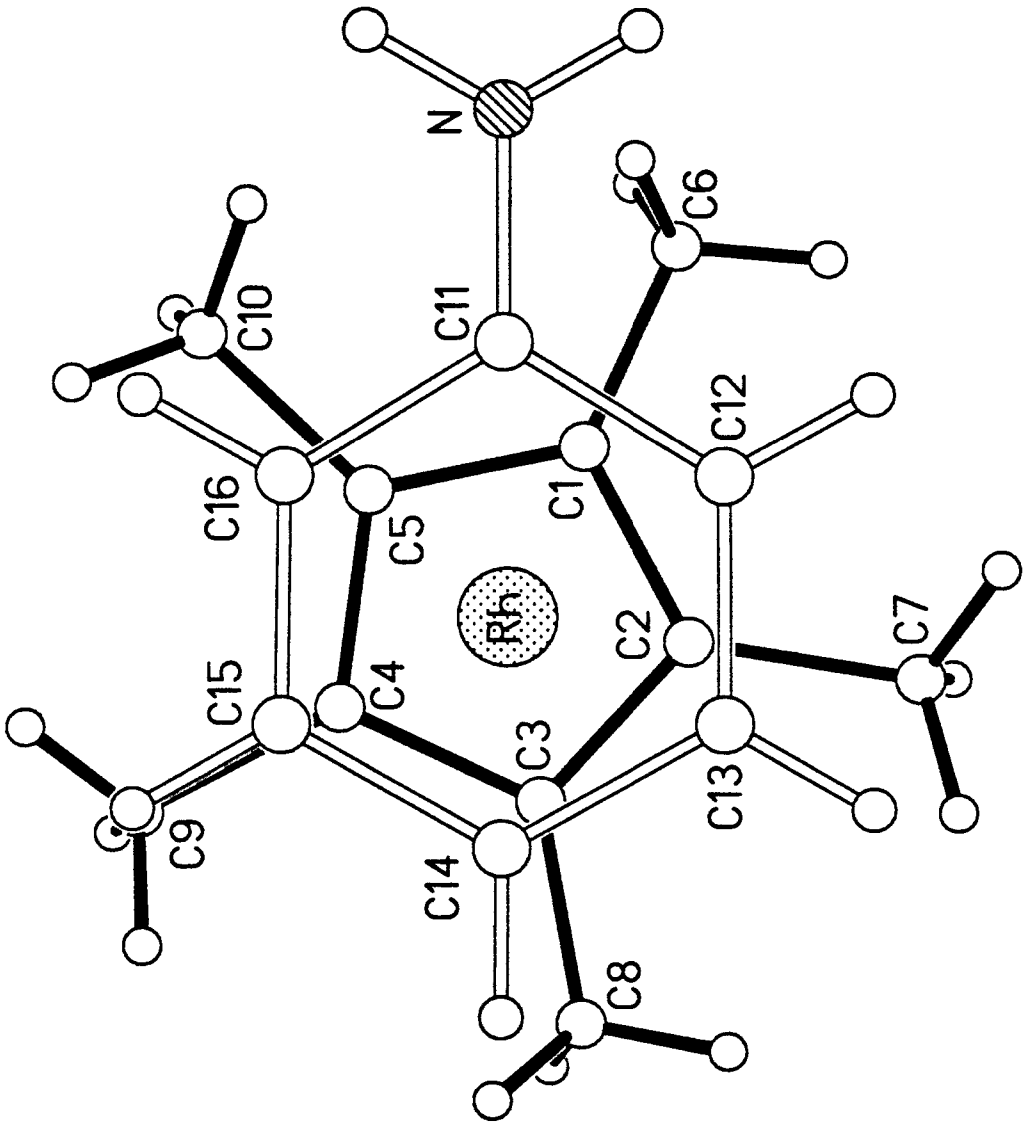

Figure 5

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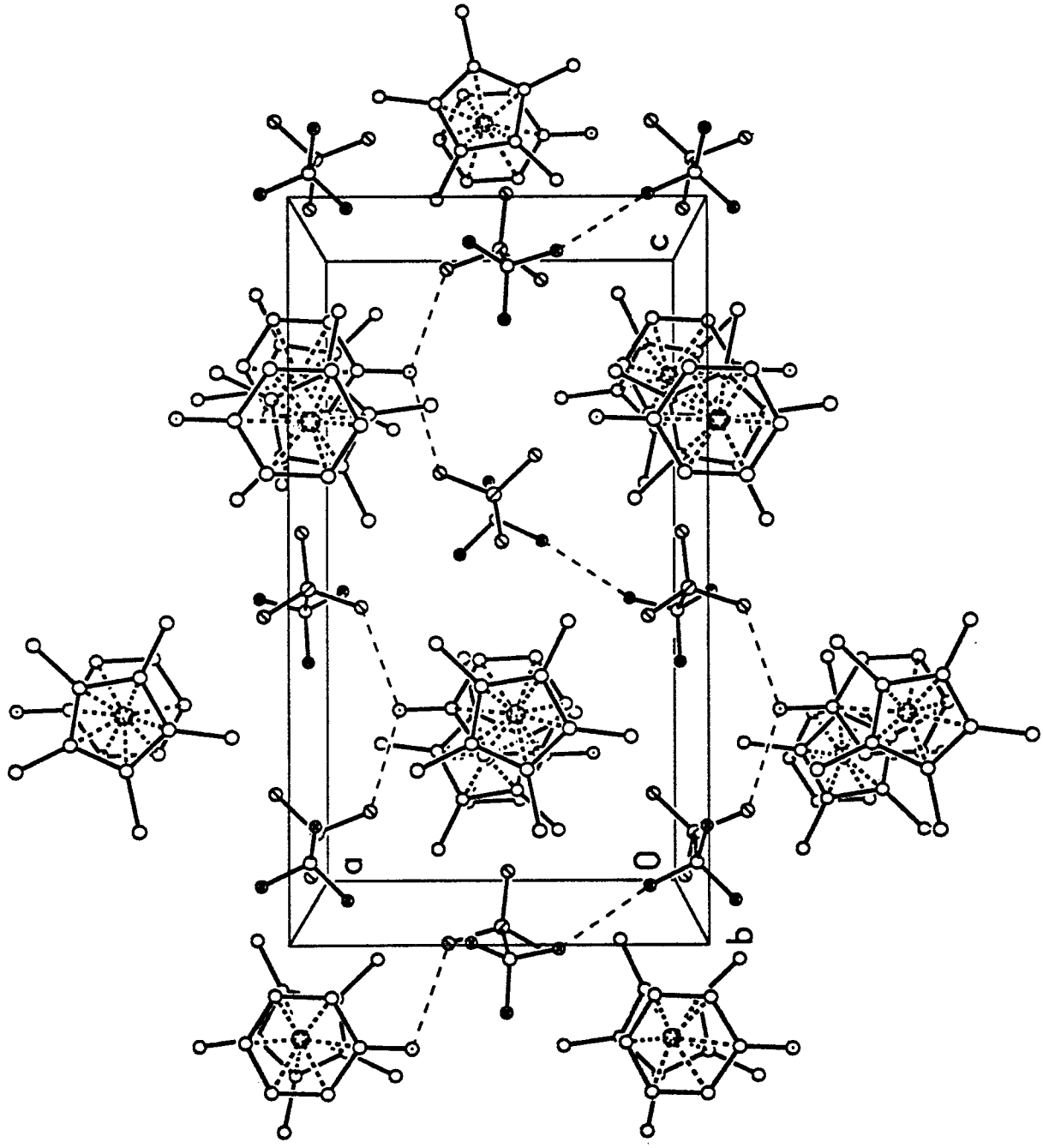

Figure 6