ORGANOMETALLICS
Organometallics, 1996, 15(11), 2604-2610, DOI:10.1021/om9505468

L2610-1

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{31} H_{22} Fe_2 O_7 Si_2$
Color; Habit	red parellelepiped
Crystal size (mm)	0.3 x 0.3 x 0.3
Crystal System	Monoclinic
Space Group	C2/c
Unit Cell Dimensions	a = 29.079(6) Å
	b = 9.731(2) Å
	c = 21.113(4) Å
	β = 97.10(3)°
Volume	5928(2) $Å^3$
Z	8
Formula weight	674.4
Density(calc.)	1.511 Mg/m^3
Absorption Coefficient	1.102 mm^{-1}
F(000)	2752

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-2

Data Collection

Diffractometer Used	Syntex P21
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	136
Monochromator	Highly oriented graphite crystal
2θ Range	3.5 to 50.0°
Scan Type	ω
Scan Speed	Constant; 8.37°/min. in ω
Scan Range (ω)	1.20°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections
Index Ranges	$-1 \leq h \leq 34$, $0 \leq k \leq 11$ $-25 \leq l \leq 24$
Reflections Collected	5591
Independent Reflections	5254 (R_{int} = 6.84%)
Observed Reflections	3163 ($F > 4.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.3150 / 0.7046

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-3

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\Sigma w(F_o-F_c)^2$
Extinction Correction	Not applied
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0013F^2$
Number of Parameters Refined	379
Final R Indices (obs. data)	R = 5.95 %, wR = 6.62 %
R Indices (all data)	R = 10.75 %, wR = 7.86 %
Goodness-of-Fit	1.14
Largest and Mean Δ/σ	0.695, 0.125
Data-to-Parameter Ratio	8.3:1
Largest Difference Peak	0.50 $eÅ^{-3}$
Largest Difference Hole	-0.49 $eÅ^{-3}$

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-4

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Fe(1)	945(1)	-1217(1)	1133(1)	22(1)
Fe(2)	1012(1)	1453(1)	714(1)	21(1)
Si(1)	1400(1)	456(2)	1665(1)	22(1)
Si(2)	1012(1)	3728(2)	320(1)	25(1)
O(1)	1197(2)	-3512(6)	1994(3)	47(2)
O(2)	199(2)	-344(6)	1870(3)	43(2)
O(3)	1690(2)	-1644(5)	336(2)	33(2)
O(4)	303(2)	-2558(5)	129(3)	38(2)
O(5)	184(2)	2488(5)	1224(3)	37(2)
O(6)	442(2)	364(5)	-419(2)	33(2)
O(7)	1865(2)	1406(5)	97(2)	33(2)
C(1)	1108(2)	-2604(9)	1663(3)	30(3)
C(2)	487(3)	-648(8)	1584(3)	30(3)
C(3)	1410(2)	-1466(7)	657(3)	26(2)
C(4)	540(3)	-2011(8)	519(4)	28(2)
C(5)	505(3)	2077(8)	1032(3)	27(2)
C(6)	668(2)	755(7)	25(4)	24(2)
C(7)	1531(2)	1397(7)	344(3)	24(2)
C(8)	2045(2)	266(7)	1726(3)	23(2)
C(9)	2265(2)	-999(8)	1837(4)	32(3)
C(10)	2749(3)	-1105(8)	1910(4)	38(3)
C(11)	3008(3)	32(8)	1872(4)	32(3)
C(12)	2809(3)	1289(9)	1757(4)	42(3)
C(13)	2325(2)	1413(8)	1703(4)	36(3)
C(14)	1279(2)	1056(8)	2478(3)	27(2)
C(15)	1024(3)	2238(9)	2564(4)	41(3)
C(16)	935(3)	2617(10)	3177(4)	51(3)
C(17)	1098(3)	1862(11)	3696(4)	56(4)
C(18)	1355(3)	702(10)	3609(4)	53(4)
C(19)	1444(3)	309(8)	3011(3)	37(3)
C(20)	1590(3)	4579(8)	466(4)	31(3)
C(21)	1821(3)	5049(8)	-33(4)	35(3)
C(22)	2255(3)	5668(8)	80(4)	45(3)
C(23)	2463(3)	5861(9)	696(5)	52(4)
C(24)	2232(3)	5417(8)	1198(5)	46(3)
C(25)	1806(3)	4785(8)	1088(4)	33(3)
C(26)	806(2)	3748(8)	-552(3)	27(2)
C(27)	1037(3)	3023(9)	-986(4)	39(3)
C(28)	874(3)	2919(10)	-1625(4)	47(3)
C(29)	470(3)	3583(9)	-1851(4)	44(3)
C(30)	232(3)	4327(9)	-1440(4)	43(3)
C(31)	396(2)	4405(7)	-801(3)	26(2)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-5

Table 2. Bond lengths (Å)

Fe(1)-Fe(2)	2.759 (1)	Fe(1)-Si(1)	2.301 (2)
Fe(1)-C(1)	1.781 (8)	Fe(1)-C(2)	1.819 (8)
Fe(1)-C(3)	1.798 (7)	Fe(1)-C(4)	1.813 (7)
Fe(2)-Si(1)	2.385 (2)	Fe(2)-Si(2)	2.365 (2)
Fe(2)-C(5)	1.798 (8)	Fe(2)-C(6)	1.794 (7)
Fe(2)-C(7)	1.785 (7)	Si(1)-C(8)	1.873 (7)
Si(1)-C(14)	1.887 (7)	Si(2)-C(20)	1.866 (8)
Si(2)-C(26)	1.865 (7)	O(1)-C(1)	1.136 (10)
O(2)-C(2)	1.131 (10)	O(3)-C(3)	1.134 (9)
O(4)-C(4)	1.139 (9)	O(5)-C(5)	1.136 (9)
O(6)-C(6)	1.140 (8)	O(7)-C(7)	1.157 (9)
C(8)-C(9)	1.393 (10)	C(8)-C(13)	1.386 (10)
C(9)-C(10)	1.402 (10)	C(10)-C(11)	1.346 (11)
C(11)-C(12)	1.362 (11)	C(12)-C(13)	1.404 (10)
C(14)-C(15)	1.392 (11)	C(14)-C(19)	1.377 (10)
C(15)-C(16)	1.400 (12)	C(16)-C(17)	1.357 (13)
C(17)-C(18)	1.377 (15)	C(18)-C(19)	1.374 (12)
C(20)-C(21)	1.395 (12)	C(20)-C(25)	1.397 (10)
C(21)-C(22)	1.392 (11)	C(22)-C(23)	1.378 (13)
C(23)-C(24)	1.392 (14)	C(24)-C(25)	1.377 (11)
C(26)-C(27)	1.392 (11)	C(26)-C(31)	1.397 (9)
C(27)-C(28)	1.377 (11)	C(28)-C(29)	1.374 (12)
C(29)-C(30)	1.380 (12)	C(30)-C(31)	1.377 (10)

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-6

Table 3. Bond angles (°)

Fe(2)-Fe(1)-Si(1)	55.4(1)	Fe(2)-Fe(1)-C(1)	153.1(2)
Si(1)-Fe(1)-C(1)	97.9(2)	Fe(2)-Fe(1)-C(2)	88.1(2)
Si(1)-Fe(1)-C(2)	86.8(2)	C(1)-Fe(1)-C(2)	93.2(3)
Fe(2)-Fe(1)-C(3)	82.0(2)	Si(1)-Fe(1)-C(3)	86.6(2)
C(1)-Fe(1)-C(3)	95.1(3)	C(2)-Fe(1)-C(3)	170.0(3)
Fe(2)-Fe(1)-C(4)	103.7(2)	Si(1)-Fe(1)-C(4)	159.1(2)
C(1)-Fe(1)-C(4)	103.0(3)	C(2)-Fe(1)-C(4)	92.9(3)
C(3)-Fe(1)-C(4)	90.6(3)	Fe(1)-Fe(2)-Si(1)	52.5(1)
Fe(1)-Fe(2)-Si(2)	175.8(1)	Si(1)-Fe(2)-Si(2)	131.0(1)
Fe(1)-Fe(2)-C(5)	96.0(2)	Si(1)-Fe(2)-C(5)	98.5(2)
Si(2)-Fe(2)-C(5)	81.4(2)	Fe(1)-Fe(2)-C(6)	81.3(2)
Si(1)-Fe(2)-C(6)	133.4(2)	Si(2)-Fe(2)-C(6)	95.4(2)
C(5)-Fe(2)-C(6)	91.8(3)	Fe(1)-Fe(2)-C(7)	102.0(2)
Si(1)-Fe(2)-C(7)	91.0(2)	Si(2)-Fe(2)-C(7)	80.6(2)
C(5)-Fe(2)-C(7)	161.8(3)	C(6)-Fe(2)-C(7)	92.9(3)
Fe(1)-Si(1)-Fe(2)	72.1(1)	Fe(1)-Si(1)-C(8)	118.3(2)
Fe(2)-Si(1)-C(8)	117.7(2)	Fe(1)-Si(1)-C(14)	120.1(2)
Fe(2)-Si(1)-C(14)	121.1(2)	C(8)-Si(1)-C(14)	105.4(3)
Fe(2)-Si(2)-C(20)	113.3(2)	Fe(2)-Si(2)-C(26)	110.1(2)
C(20)-Si(2)-C(26)	109.3(3)	Fe(1)-C(1)-O(1)	177.5(6)
Fe(1)-C(2)-O(2)	177.4(7)	Fe(1)-C(3)-O(3)	177.0(6)
Fe(1)-C(4)-O(4)	176.5(7)	Fe(2)-C(5)-O(5)	178.7(6)
Fe(2)-C(6)-O(6)	177.2(6)	Fe(2)-C(7)-O(7)	177.7(6)
Si(1)-C(8)-C(9)	122.2(5)	Si(1)-C(8)-C(13)	120.3(5)
C(9)-C(8)-C(13)	117.3(6)	C(8)-C(9)-C(10)	121.1(7)
C(9)-C(10)-C(11)	119.7(7)	C(10)-C(11)-C(12)	121.4(7)
C(11)-C(12)-C(13)	119.4(7)	C(8)-C(13)-C(12)	121.0(7)
Si(1)-C(14)-C(15)	122.5(5)	Si(1)-C(14)-C(19)	119.7(6)
C(15)-C(14)-C(19)	117.8(7)	C(14)-C(15)-C(16)	120.1(7)
C(15)-C(16)-C(17)	121.1(9)	C(16)-C(17)-C(18)	118.5(9)
C(17)-C(18)-C(19)	121.2(8)	C(14)-C(19)-C(18)	121.2(8)
Si(2)-C(20)-C(21)	121.9(6)	Si(2)-C(20)-C(25)	120.7(6)
C(21)-C(20)-C(25)	117.4(7)	C(20)-C(21)-C(22)	121.6(7)
C(21)-C(22)-C(23)	120.2(9)	C(22)-C(23)-C(24)	118.7(8)
C(23)-C(24)-C(25)	121.2(8)	C(20)-C(25)-C(24)	120.9(8)
Si(2)-C(26)-C(27)	121.5(5)	Si(2)-C(26)-C(31)	122.0(5)
C(27)-C(26)-C(31)	116.3(6)	C(26)-C(27)-C(28)	123.0(7)
C(27)-C(28)-C(29)	118.9(8)	C(28)-C(29)-C(30)	120.0(7)
C(29)-C(30)-C(31)	120.4(7)	C(26)-C(31)-C(30)	121.3(7)

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-7

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	19(1)	23(1)	25(1)	0(1)	4(1)	-2(1)
Fe(2)	18(1)	23(1)	22(1)	4(1)	4(1)	2(1)
Si(1)	19(1)	22(1)	24(1)	3(1)	2(1)	-1(1)
Si(2)	24(1)	25(1)	26(1)	4(1)	6(1)	3(1)
O(1)	56(4)	49(4)	39(3)	21(3)	16(3)	16(3)
O(2)	34(3)	48(4)	51(4)	-1(3)	19(3)	-2(3)
O(3)	31(3)	31(3)	39(3)	6(2)	17(3)	-8(2)
O(4)	34(3)	36(3)	43(3)	-11(3)	0(3)	-2(3)
O(5)	27(3)	40(3)	45(3)	14(3)	15(3)	7(3)
O(6)	31(3)	39(3)	27(3)	-5(3)	-4(2)	-4(3)
O(7)	30(3)	34(3)	37(3)	6(3)	13(2)	1(3)
C(1)	22(4)	49(5)	20(4)	4(4)	6(3)	-3(4)
C(2)	27(4)	31(4)	33(4)	-7(4)	4(4)	0(4)
C(3)	27(4)	24(4)	26(4)	4(3)	0(3)	-8(3)
C(4)	26(4)	21(4)	39(5)	0(3)	9(4)	1(4)
C(5)	25(4)	33(4)	25(4)	0(4)	2(3)	5(3)
C(6)	16(4)	26(4)	34(4)	6(3)	14(3)	7(3)
C(7)	30(4)	18(4)	25(4)	6(3)	3(3)	0(3)
C(8)	19(4)	29(4)	20(3)	0(3)	-1(3)	-2(3)
C(9)	22(4)	23(4)	51(5)	5(3)	-1(4)	6(4)
C(10)	29(4)	33(5)	49(5)	14(4)	-1(4)	2(4)
C(11)	18(4)	34(5)	43(5)	5(4)	-5(3)	-8(4)
C(12)	23(4)	37(5)	66(6)	-5(4)	1(4)	1(5)
C(13)	27(4)	21(4)	58(5)	-7(4)	-2(4)	-8(4)
C(14)	21(4)	34(4)	25(4)	-2(3)	4(3)	-2(3)
C(15)	43(5)	43(5)	36(5)	19(4)	4(4)	-3(4)
C(16)	42(5)	65(7)	49(5)	14(5)	11(4)	-21(5)
C(17)	58(6)	73(7)	39(5)	-12(6)	12(5)	-13(5)
C(18)	78(7)	55(6)	26(5)	-13(6)	6(5)	14(4)
C(19)	53(5)	28(4)	32(4)	-12(4)	13(4)	-1(4)
C(20)	32(4)	22(4)	39(5)	12(4)	7(4)	-1(4)
C(21)	27(4)	28(4)	52(5)	7(4)	16(4)	-1(4)
C(22)	39(5)	31(5)	68(6)	2(4)	20(5)	5(5)
C(23)	33(5)	35(5)	86(8)	-4(4)	7(5)	-4(5)
C(24)	41(5)	30(5)	65(6)	-2(4)	-6(5)	-7(5)
C(25)	36(5)	26(4)	40(5)	7(4)	9(4)	-5(4)
C(26)	25(4)	33(4)	25(4)	0(4)	15(3)	5(3)
C(27)	34(5)	55(5)	30(4)	16(4)	12(4)	11(4)
C(28)	50(6)	63(6)	30(5)	15(5)	10(4)	11(4)
C(29)	46(5)	55(6)	32(4)	5(5)	6(4)	5(4)
C(30)	34(5)	53(6)	41(5)	6(4)	0(4)	1(4)
C(31)	27(4)	23(4)	30(4)	-2(3)	8(3)	5(3)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-8

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1)	1349	2019	1349	50
H(2)	724	4403	724	50
H(9A)	2080	-1809	1868	80
H(10A)	2897	-1983	1984	80
H(11A)	3340	-43	1936	80
H(12A)	3002	2074	1710	80
H(13A)	2185	2306	1645	80
H(15A)	916	2806	2205	80
H(16A)	756	3426	3235	80
H(17A)	1037	2132	4115	80
H(18A)	1466	147	3972	80
H(19A)	1629	-492	2961	80
H(21A)	1682	4933	-466	80
H(22A)	2410	5973	-271	80
H(23A)	2764	6275	775	80
H(24A)	2375	5576	1627	80
H(25A)	1662	4465	1445	80
H(27A)	1319	2561	-825	80
H(28A)	1044	2397	-1903	80
H(29A)	352	3513	-2296	80
H(30A)	-50	4794	-1599	80
H(31A)	229	4920	-515	80

Crystal structure of $[(OC)_4Fe\text{-}Fe(CO)_3(SiHPh_2)](\mu\text{-}\eta^2\text{-}H\text{-}SiPh_2)$ (4)

L2610-9

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{30}H_{22}Fe_2O_6Si_2$
Color; Habit	clear irregular
Crystal size (mm)	0.15 x 0.15 x 0.2
Crystal System	Triclinic
Space Group	$P\bar{1}$
Unit Cell Dimensions	a = 10.018(2) Å
	b = 10.436(2) Å
	c = 14.881(3) Å
	α = 108.00(3)°
	β = 91.46(3)°
	γ = 96.97(3)°
Volume	1222.8(4) $Å^3$
Z	2
Formula weight	645.3
Density(calc.)	1.753 Mg/m^3
Absorption Coefficient	1.329 mm^{-1}
F(000)	658

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-}SiPh_2)_2$ (5)

L2610-10

Data Collection

Diffractometer Used	Syntex P21
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	129
Monochromator	Highly oriented graphite crystal
2θ Range	3.5 to 45.0°
Scan Type	ω
Scan Speed	Constant; 8.37°/min. in ω
Scan Range (ω)	2.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections
Index Ranges	$-10 \le h \le 10$, $-11 \le k \le 11$ $-15 \le l \le 15$
Reflections Collected	4471
Independent Reflections	3704 (R_{int} = 2.80%)
Observed Reflections	1947 ($F > 4.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.4796 / 0.8390

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-SiPh}_2)_2$ (5)

L2610-11

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Extinction Correction	Not Applied
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 99.0000F^2$
Number of Parameters Refined	211
Final R Indices (obs. data)	R = 9.15 %, wR = 10.58 %
R Indices (all data)	R = 16.01 %, wR = 15.90 %
Goodness-of-Fit	4.70
Largest and Mean Δ/σ	0.001, 0.000
Data-to-Parameter Ratio	9.2:1
Largest Difference Peak	1.40 $eÅ^{-3}$
Largest Difference Hole	-1.13 $eÅ^{-3}$

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-SiPh}_2)_2$ (5)

L2610-12

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Fe(1)	951(3)	4975(3)	5679(2)	20(1)
Fe(2)	4101(3)	5011(3)	690(2)	18(1)
Si(1)	1423(5)	4977(5)	4135(3)	18(2)
Si(2)	3517(5)	5011(5)	-856(3)	18(2)
O(1)	1705(14)	7954(14)	6302(9)	34(6)
O(2)	826(14)	1981(14)	4983(9)	36(6)
O(3)	3590(14)	4976(12)	6550(10)	37(6)
O(4)	3448(14)	2029(13)	29(10)	40(6)
O(5)	4285(14)	8014(13)	1342(10)	37(6)
O(6)	1478(13)	5013(13)	1504(10)	37(6)
C(1)	1375(20)	6840(22)	6077(14)	26(5)
C(2)	833(18)	3127(20)	5231(13)	21(5)
C(3)	2515(22)	4996(21)	6209(14)	31(5)
C(4)	3722(20)	3170(22)	254(14)	26(5)
C(5)	4244(20)	6865(22)	1087(14)	30(5)
C(6)	2545(20)	5024(19)	1204(13)	22(4)
C(7)	2050(18)	7458(18)	3616(12)	21(4)
C(8)	2866(19)	8588(19)	3562(13)	27(5)
C(9)	4204(19)	8841(19)	3908(13)	25(5)
C(10)	4658(22)	7930(21)	4313(14)	36(5)
C(11)	3873(20)	6817(21)	4398(14)	32(5)
C(12)	2494(18)	6549(18)	4039(12)	21(4)
C(13)	3335(19)	3097(19)	3602(13)	25(5)
C(14)	3866(20)	1942(20)	2980(13)	30(5)
C(15)	3113(21)	1117(22)	2145(14)	37(5)
C(16)	1927(21)	1428(21)	1925(15)	38(5)
C(17)	1339(20)	2565(19)	2480(13)	28(5)
C(18)	2082(18)	3401(19)	3329(13)	22(4)
C(19)	1602(20)	6943(20)	-509(14)	30(5)
C(20)	1128(20)	8098(20)	-528(14)	30(5)
C(21)	1785(20)	8971(21)	-954(14)	36(5)
C(22)	3027(19)	8655(20)	-1365(14)	30(5)
C(23)	3489(20)	7470(20)	-1353(14)	31(5)
C(24)	2846(19)	6598(19)	-924(13)	25(4)
C(25)	2851(19)	2555(19)	-2464(13)	28(5)
C(26)	1968(20)	1342(20)	-2977(14)	33(5)
C(27)	700(20)	1048(21)	-2704(14)	31(5)
C(28)	254(20)	1927(20)	-1856(14)	31(5)
C(29)	1107(19)	3127(20)	-1355(14)	28(5)
C(30)	2384(18)	3456(19)	-1638(13)	23(4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-SiPh}_2)_2$ (5)

L2610-13

Table 2. Bond lengths (Å)

Fe(1)-Si(1)	2.358 (6)	Fe(1)-C(1)	1.842 (22)
Fe(1)-C(2)	1.823 (20)	Fe(1)-C(3)	1.731 (23)
Fe(1)-Fe(1A)	2.759 (6)	Fe(1)-Si(1A)	2.406 (6)
Fe(2)-Si(2)	2.359 (6)	Fe(2)-C(4)	1.816 (21)
Fe(2)-C(5)	1.827 (22)	Fe(2)-C(6)	1.753 (20)
Fe(2)-Fe(2A)	2.763 (6)	Fe(2)-Si(2A)	2.397 (6)
Si(1)-C(12)	1.894 (20)	Si(1)-C(18)	1.914 (18)
Si(1)-Fe(1A)	2.406 (6)	Si(2)-C(24)	1.891 (22)
Si(2)-C(30)	1.896 (16)	Si(2)-Fe(2A)	2.397 (6)
O(1)-C(1)	1.111 (26)	O(2)-C(2)	1.137 (24)
O(3)-C(3)	1.184 (27)	O(4)-C(4)	1.129 (25)
O(5)-C(5)	1.136 (26)	O(6)-C(6)	1.170 (24)
C(7)-C(8)	1.375 (27)	C(7)-C(12)	1.397 (30)
C(8)-C(9)	1.388 (26)	C(9)-C(10)	1.384 (34)
C(10)-C(11)	1.363 (31)	C(11)-C(12)	1.432 (26)
C(13)-C(14)	1.444 (26)	C(13)-C(18)	1.411 (28)
C(14)-C(15)	1.410 (25)	C(15)-C(16)	1.328 (32)
C(16)-C(17)	1.422 (28)	C(17)-C(18)	1.423 (23)
C(19)-C(20)	1.356 (32)	C(19)-C(24)	1.440 (27)
C(20)-C(21)	1.378 (32)	C(21)-C(22)	1.430 (29)
C(22)-C(23)	1.377 (31)	C(23)-C(24)	1.374 (31)
C(25)-C(26)	1.437 (24)	C(25)-C(30)	1.427 (25)
C(26)-C(27)	1.372 (29)	C(27)-C(28)	1.431 (26)
C(28)-C(29)	1.409 (25)	C(29)-C(30)	1.394 (27)

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-}SiPh_2)_2$ (5)

L2610-14

Table 3. Bond angles (°)

Si(1)-Fe(1)-C(1)	88.3(7)	Si(1)-Fe(1)-C(2)	87.1(7)
C(1)-Fe(1)-C(2)	170.1(9)	Si(1)-Fe(1)-C(3)	103.8(8)
C(1)-Fe(1)-C(3)	84.7(10)	C(2)-Fe(1)-C(3)	87.9(9)
Si(1)-Fe(1)-Fe(1A)	55.4(2)	C(1)-Fe(1)-Fe(1A)	92.3(7)
C(2)-Fe(1)-Fe(1A)	92.3(6)	C(3)-Fe(1)-Fe(1A)	159.2(8)
Si(1)-Fe(1)-Si(1A)	109.2(2)	C(1)-Fe(1)-Si(1A)	94.3(7)
C(2)-Fe(1)-Si(1A)	95.5(6)	C(3)-Fe(1)-Si(1A)	146.9(8)
Fe(1A)-Fe(1)-Si(1A)	53.8(2)	Si(2)-Fe(2)-C(4)	87.6(7)
Si(2)-Fe(2)-C(5)	88.8(7)	C(4)-Fe(2)-C(5)	172.3(9)
Si(2)-Fe(2)-C(6)	102.8(7)	C(4)-Fe(2)-C(6)	87.4(9)
C(5)-Fe(2)-C(6)	86.8(9)	Si(2)-Fe(2)-Fe(2A)	55.1(2)
C(4)-Fe(2)-Fe(2A)	91.2(7)	C(5)-Fe(2)-Fe(2A)	92.4(7)
C(6)-Fe(2)-Fe(2A)	157.9(7)	Si(2)-Fe(2)-Si(2A)	109.0(2)
C(4)-Fe(2)-Si(2A)	93.7(7)	C(5)-Fe(2)-Si(2A)	93.9(6)
C(6)-Fe(2)-Si(2A)	148.2(7)	Fe(2A)-Fe(2)-Si(2A)	53.8(2)
Fe(1)-Si(1)-C(12)	116.3(5)	Fe(1)-Si(1)-C(18)	116.9(7)
C(12)-Si(1)-C(18)	108.7(8)	Fe(1)-Si(1)-Fe(1A)	70.8(2)
C(12)-Si(1)-Fe(1A)	118.8(6)	C(18)-Si(1)-Fe(1A)	121.1(6)
Fe(2)-Si(2)-C(24)	115.0(6)	Fe(2)-Si(2)-C(30)	116.4(7)
C(24)-Si(2)-C(30)	109.4(8)	Fe(2)-Si(2)-Fe(2A)	71.0(2)
C(24)-Si(2)-Fe(2A)	120.0(6)	C(30)-Si(2)-Fe(2A)	120.4(6)
Fe(1)-C(1)-O(1)	175.9(18)	Fe(1)-C(2)-O(2)	176.0(18)
Fe(1)-C(3)-O(3)	178.0(10)	Fe(2)-C(4)-O(4)	176.0(18)
Fe(2)-C(5)-O(5)	177.5(19)	Fe(2)-C(6)-O(6)	176.9(17)
C(8)-C(7)-C(12)	122.8(17)	C(7)-C(8)-C(9)	120.1(20)
C(8)-C(9)-C(10)	117.4(19)	C(9)-C(10)-C(11)	124.2(20)
C(10)-C(11)-C(12)	118.6(21)	Si(1)-C(12)-C(7)	124.8(13)
Si(1)-C(12)-C(11)	118.3(16)	C(7)-C(12)-C(11)	116.9(17)
C(14)-C(13)-C(18)	118.2(15)	C(13)-C(14)-C(15)	120.1(19)
C(14)-C(15)-C(16)	119.5(19)	C(15)-C(16)-C(17)	124.4(18)
C(16)-C(17)-C(18)	116.8(18)	Si(1)-C(18)-C(13)	117.8(12)
Si(1)-C(18)-C(17)	121.3(15)	C(13)-C(18)-C(17)	120.9(16)
C(20)-C(19)-C(24)	120.4(20)	C(19)-C(20)-C(21)	122.3(19)
C(20)-C(21)-C(22)	118.3(21)	C(21)-C(22)-C(23)	118.9(20)
C(22)-C(23)-C(24)	123.2(19)	Si(2)-C(24)-C(19)	119.8(16)
Si(2)-C(24)-C(23)	123.4(15)	C(19)-C(24)-C(23)	116.9(19)
C(26)-C(25)-C(30)	118.1(17)	C(25)-C(26)-C(27)	122.0(17)
C(26)-C(27)-C(28)	119.8(16)	C(27)-C(28)-C(29)	118.5(18)
C(28)-C(29)-C(30)	122.2(17)	Si(2)-C(30)-C(25)	121.5(14)
Si(2)-C(30)-C(29)	119.0(13)	C(25)-C(30)-C(29)	119.3(15)

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-}SiPh_2)_2$ (5)

L260-15

Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	19(2)	19(2)	14(1)	2(1)	0(1)	-6(1)
Fe(2)	20(2)	13(2)	14(1)	0(1)	0(1)	-8(1)
Si(1)	16(3)	20(3)	12(3)	-1(2)	0(2)	-6(2)
Si(2)	22(3)	15(3)	10(3)	-2(2)	1(2)	-6(2)
O(1)	38(9)	23(9)	33(8)	-3(7)	-1(7)	-1(7)
O(2)	45(10)	25(8)	31(8)	5(7)	-6(7)	-1(7)
O(3)	37(9)	12(7)	46(9)	5(6)	3(7)	-13(6)
O(4)	44(10)	11(8)	51(10)	-2(7)	-3(8)	-7(7)
O(5)	35(9)	17(8)	46(9)	9(6)	4(7)	-11(7)
O(6)	24(8)	28(8)	46(9)	1(6)	16(7)	-7(7)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-}SiPh_2)_2$ **(5)**

L2610-16

Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(1)	400	5049	6638	50
H(7A)	1138	7290	3350	80
H(8A)	2508	9202	3284	80
H(9A)	4792	9617	3868	80
H(10A)	5584	8092	4550	80
H(11A)	4240	6225	4692	80
H(13A)	3814	3638	4190	80
H(14A)	4740	1744	3132	80
H(15A)	3454	332	1743	80
H(16A)	1431	855	1353	80
H(17A)	484	2765	2294	80
H(19A)	1102	6344	-223	80
H(20A)	308	8316	-233	80
H(21A)	1422	9777	-966	80
H(22A)	3529	9258	-1647	80
H(23A)	4293	7233	-1663	80
H(25A)	3729	2759	-2669	80
H(26A)	2279	716	-3525	80
H(27A)	109	262	-3084	80
H(28A)	-604	1707	-1628	80
H(29A)	796	3742	-801	80

Crystal structure of $[(OC)_3Fe]_2(\mu\text{-}\eta^2\text{-H-}SiPh_2)_2$ (5)

L2610-17

STRUCTURE DETERMINATION SUMMARY

Crystal Data

Empirical Formula	$C_{32} H_{20} Fe_2 O_9 Si_2$
Color; Habit	yellow parellelepiped
Crystal size (mm)	0.3 x 0.4 x 0.4
Crystal System	Monoclinic
Space Group	$P2_1/c$
Unit Cell Dimensions	$\underline{a}$ = 17.802(4) Å
	$\underline{b}$ = 17.099(3) Å
	$\underline{c}$ = 10.919(2) Å
	β = 104.50(3)°
Volume	3217.8(11) $Å^3$
Z	4
Formula weight	716.4
Density(calc.)	1.479 Mg/m^3
Absorption Coefficient	1.024 mm^{-1}
F(000)	1456

Crystal structure of $[(OC)_4Fe]_2(\mu\text{-}\eta^2\text{-}Ph_2Si\text{-}O\text{-}SiPh_2)$ (6)

Data Collection

Diffractometer Used	Syntex P21
Radiation	MoKα (λ = 0.71073 Å)
Temperature (K)	291
Monochromator	Highly oriented graphite crystal
2θ Range	3.5 to 45.0°
Scan Type	ω
Scan Speed	Constant; 4.19°/min. in ω
Scan Range (ω)	1.00°
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 25.0% of total scan time
Standard Reflections	3 measured every 97 reflections
Index Ranges	$-18 \leq h \leq 19$, $-18 \leq k \leq 1$ $-11 \leq l \leq 1$
Reflections Collected	5303
Independent Reflections	4176 (R_{int} = 1.53%)
Observed Reflections	2438 ($F > 4.0\sigma(F)$)
Absorption Correction	Semi-empirical
Min./Max. Transmission	0.5779 / 0.6422

Crystal structure of $[(OC)_4Fe]_2(\mu\text{-}\eta^2\text{-}Ph_2Si\text{-}O\text{-}SiPh_2)$ (6)

L2610-19

Solution and Refinement

System Used	Siemens SHELXTL PLUS (PC Version)
Solution	Direct Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Extinction Correction	Not Applied
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 99.0000F^2$
Number of Parameters Refined	406
Final R Indices (obs. data)	R = 4.41 %, wR = 4.78 %
R Indices (all data)	R = 9.45 %, wR = 8.99 %
Goodness-of-Fit	2.47
Largest and Mean Δ/σ	0.025, 0.004
Data-to-Parameter Ratio	6.0:1
Largest Difference Peak	0.29 $eÅ^{-3}$
Largest Difference Hole	-0.28 $eÅ^{-3}$

Crystal structure of $[(OC)_4Fe]_2(\mu\text{-}\eta^2\text{-}Ph_2Si\text{-}O\text{-}SiPh_2)$ (6)

L2610-20

Table 1. Atomic coordinates ($x10^4$) and equivalent isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U(eq)
Fe(1)	8524(1)	6101(1)	713(1)	44(1)
Fe(2)	8461(1)	5700(1)	3243(1)	51(1)
Si(1)	7617(1)	5075(1)	-153(2)	41(1)
Si(2)	7186(1)	5149(1)	2348(2)	45(1)
O(1)	9461(4)	7504(4)	1653(8)	112(4)
O(2)	9748(4)	4913(4)	1355(6)	85(3)
O(3)	7100(3)	7050(3)	192(6)	64(3)
O(4)	8880(4)	6252(4)	-1739(6)	79(3)
O(5)	10091(4)	6217(5)	4198(7)	117(4)
O(6)	7818(4)	7280(4)	2983(7)	82(3)
O(7)	8183(5)	5576(6)	5749(7)	139(5)
O(8)	8882(4)	4044(4)	3139(7)	87(3)
O(9)	7204(3)	4796(3)	958(4)	45(2)
C(1)	9118(5)	6947(6)	1347(9)	63(4)
C(2)	9256(5)	5354(5)	1160(8)	54(3)
C(3)	7636(5)	6664(5)	397(8)	49(3)
C(4)	8716(5)	6190(5)	-791(8)	51(3)
C(5)	9458(6)	6015(6)	3800(8)	76(4)
C(6)	8052(6)	6657(6)	3022(9)	65(4)
C(7)	8298(6)	5599(6)	4780(10)	76(4)
C(8)	8704(5)	4689(6)	3143(8)	60(4)
C(9)	8080(4)	4214(4)	-695(8)	48(3)
C(10)	8353(6)	3572(6)	57(10)	78(4)
C(11)	8703(7)	2959(6)	-379(13)	98(6)
C(12)	8783(5)	2954(7)	-1599(14)	92(6)
C(13)	8500(6)	3567(7)	-2358(11)	91(6)
C(14)	8156(6)	4186(5)	-1925(9)	74(4)
C(15)	6819(4)	5366(4)	-1542(7)	42(3)
C(16)	6152(5)	4909(6)	-1831(8)	67(4)
C(17)	5526(5)	5072(7)	-2826(9)	84(5)
C(18)	5550(5)	5690(6)	-3595(9)	75(4)
C(19)	6195(5)	6161(5)	-3360(8)	64(4)
C(20)	6819(5)	5988(4)	-2350(7)	50(3)
C(21)	6380(4)	5877(5)	2172(8)	51(3)
C(22)	6302(5)	6366(5)	3150(9)	66(4)
C(23)	5708(6)	6894(6)	3002(12)	85(5)
C(24)	5172(6)	6949(6)	1884(13)	87(5)
C(25)	5234(5)	6480(7)	886(10)	82(5)
C(26)	5827(5)	5942(5)	1036(9)	64(4)
C(27)	6962(4)	4293(5)	3277(7)	50(3)
C(28)	7022(5)	3541(5)	2869(8)	63(4)
C(29)	6872(6)	2907(6)	3542(11)	82(5)
C(30)	6668(6)	2995(7)	4649(11)	87(5)
C(31)	6604(6)	3752(8)	5076(9)	84(5)
C(32)	6746(5)	4373(6)	4399(8)	69(4)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor

Crystal structure of $[(OC)_4Fe]_2(\mu\text{-}\eta^2\text{-}Ph_2Si\text{-}O\text{-}SiPh_2)$ (6)

L2610-21

Table 2. Bond lengths (Å)

Fe(1)-Fe(2)	2.875 (2)	Fe(1)-Si(1)	2.412 (2)
Fe(1)-C(1)	1.822 (9)	Fe(1)-C(2)	1.804 (9)
Fe(1)-C(3)	1.809 (9)	Fe(1)-C(4)	1.766 (10)
Fe(2)-Si(2)	2.426 (2)	Fe(2)-C(5)	1.807 (10)
Fe(2)-C(6)	1.782 (10)	Fe(2)-C(7)	1.782 (11)
Fe(2)-C(8)	1.793 (10)	Si(1)-O(9)	1.638 (6)
Si(1)-C(9)	1.854 (8)	Si(1)-C(15)	1.869 (7)
Si(2)-O(9)	1.641 (5)	Si(2)-C(21)	1.873 (8)
Si(2)-C(27)	1.879 (9)	O(1)-C(1)	1.135 (12)
O(2)-C(2)	1.134 (11)	O(3)-C(3)	1.134 (10)
O(4)-C(4)	1.149 (12)	O(5)-C(5)	1.155 (12)
O(6)-C(6)	1.142 (12)	O(7)-C(7)	1.128 (14)
O(8)-C(8)	1.147 (12)	C(9)-C(10)	1.385 (12)
C(9)-C(14)	1.384 (13)	C(10)-C(11)	1.366 (16)
C(11)-C(12)	1.375 (22)	C(12)-C(13)	1.353 (16)
C(13)-C(14)	1.363 (16)	C(15)-C(16)	1.390 (12)
C(15)-C(20)	1.382 (11)	C(16)-C(17)	1.376 (11)
C(17)-C(18)	1.357 (15)	C(18)-C(19)	1.373 (14)
C(19)-C(20)	1.388 (10)	C(21)-C(22)	1.389 (13)
C(21)-C(26)	1.382 (11)	C(22)-C(23)	1.369 (14)
C(23)-C(24)	1.352 (16)	C(24)-C(25)	1.379 (18)
C(25)-C(26)	1.378 (14)	C(27)-C(28)	1.375 (13)
C(27)-C(32)	1.378 (13)	C(28)-C(29)	1.372 (15)
C(29)-C(30)	1.354 (18)	C(30)-C(31)	1.392 (18)
C(31)-C(32)	1.353 (16)		

Crystal structure of $[(OC)_4Fe]_2(\mu\text{-}\eta^2\text{-}Ph_2Si\text{-}O\text{-}SiPh_2)$ (**6**)

L2610-22

Table 3. Bond angles (°)

Fe(2)-Fe(1)-Si(1)	91.1(1)	Fe(2)-Fe(1)-C(1)	89.0(3)
Si(1)-Fe(1)-C(1)	173.8(3)	Fe(2)-Fe(1)-C(2)	76.7(3)
Si(1)-Fe(1)-C(2)	87.6(3)	C(1)-Fe(1)-C(2)	98.5(4)
Fe(2)-Fe(1)-C(3)	93.9(3)	Si(1)-Fe(1)-C(3)	81.1(3)
C(1)-Fe(1)-C(3)	92.7(4)	C(2)-Fe(1)-C(3)	165.2(4)
Fe(2)-Fe(1)-C(4)	167.7(3)	Si(1)-Fe(1)-C(4)	87.9(3)
C(1)-Fe(1)-C(4)	93.2(4)	C(2)-Fe(1)-C(4)	91.0(4)
C(3)-Fe(1)-C(4)	98.1(4)	Fe(1)-Fe(2)-Si(2)	87.9(1)
Fe(1)-Fe(2)-C(5)	88.9(3)	Si(2)-Fe(2)-C(5)	172.7(4)
Fe(1)-Fe(2)-C(6)	76.4(3)	Si(2)-Fe(2)-C(6)	89.6(3)
C(5)-Fe(2)-C(6)	96.1(5)	Fe(1)-Fe(2)-C(7)	169.3(3)
Si(2)-Fe(2)-C(7)	89.1(3)	C(5)-Fe(2)-C(7)	95.2(4)
C(6)-Fe(2)-C(7)	93.4(5)	Fe(1)-Fe(2)-C(8)	95.9(3)
Si(2)-Fe(2)-C(8)	79.4(3)	C(5)-Fe(2)-C(8)	94.3(4)
C(6)-Fe(2)-C(8)	166.9(4)	C(7)-Fe(2)-C(8)	93.6(5)
Fe(1)-Si(1)-O(9)	107.5(2)	Fe(1)-Si(1)-C(9)	113.3(3)
O(9)-Si(1)-C(9)	108.9(3)	Fe(1)-Si(1)-C(15)	115.0(2)
O(9)-Si(1)-C(15)	106.7(3)	C(9)-Si(1)-C(15)	105.1(3)
Fe(2)-Si(2)-O(9)	106.4(2)	Fe(2)-Si(2)-C(21)	113.5(3)
O(9)-Si(2)-C(21)	110.0(3)	Fe(2)-Si(2)-C(27)	112.9(2)
O(9)-Si(2)-C(27)	105.6(3)	C(21)-Si(2)-C(27)	108.2(4)
Si(1)-O(9)-Si(2)	134.0(3)	Fe(1)-C(1)-O(1)	174.4(8)
Fe(1)-C(2)-O(2)	173.4(9)	Fe(1)-C(3)-O(3)	176.5(8)
Fe(1)-C(4)-O(4)	176.5(7)	Fe(2)-C(5)-O(5)	177.6(9)
Fe(2)-C(6)-O(6)	174.4(8)	Fe(2)-C(7)-O(7)	176.3(10)
Fe(2)-C(8)-O(8)	176.6(8)	Si(1)-C(9)-C(10)	123.9(7)
Si(1)-C(9)-C(14)	119.8(6)	C(10)-C(9)-C(14)	116.2(8)
C(9)-C(10)-C(11)	121.7(10)	C(10)-C(11)-C(12)	120.6(10)
C(11)-C(12)-C(13)	118.4(11)	C(12)-C(13)-C(14)	121.3(12)
C(9)-C(14)-C(13)	121.7(9)	Si(1)-C(15)-C(16)	117.8(6)
Si(1)-C(15)-C(20)	127.0(6)	C(16)-C(15)-C(20)	115.2(7)
C(15)-C(16)-C(17)	122.8(9)	C(16)-C(17)-C(18)	120.1(9)
C(17)-C(18)-C(19)	119.7(8)	C(18)-C(19)-C(20)	119.3(8)
C(15)-C(20)-C(19)	122.8(8)	Si(2)-C(21)-C(22)	122.8(6)
Si(2)-C(21)-C(26)	120.1(7)	C(22)-C(21)-C(26)	117.1(8)
C(21)-C(22)-C(23)	121.9(8)	C(22)-C(23)-C(24)	120.2(11)
C(23)-C(24)-C(25)	119.6(10)	C(24)-C(25)-C(26)	120.4(9)
C(21)-C(26)-C(25)	120.8(9)	Si(2)-C(27)-C(28)	120.6(7)
Si(2)-C(27)-C(32)	123.2(7)	C(28)-C(27)-C(32)	116.2(9)
C(27)-C(28)-C(29)	121.6(9)	C(28)-C(29)-C(30)	121.5(10)
C(29)-C(30)-C(31)	117.7(11)	C(30)-C(31)-C(32)	120.3(10)
C(27)-C(32)-C(31)	122.7(10)		

Crystal structure of $[(OC)_4Fe]_2(\mu\text{-}\eta^2\text{-}Ph_2Si\text{-}O\text{-}SiPh_2)$ (6)

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Table 4. Anisotropic displacement coefficients ($Å^2 x 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe(1)	44(1)	42(1)	46(1)	-2(1)	12(1)	-2(1)
Fe(2)	52(1)	59(1)	40(1)	-8(1)	7(1)	-3(1)
Si(1)	47(1)	36(1)	40(1)	-1(1)	9(1)	1(1)
Si(2)	48(1)	47(1)	39(1)	-4(1)	9(1)	3(1)
O(1)	91(6)	78(6)	177(9)	-41(5)	55(5)	-54(6)
O(2)	69(5)	90(5)	95(5)	34(4)	19(4)	12(4)
O(3)	64(4)	56(4)	76(4)	18(3)	26(3)	11(3)
O(4)	86(5)	94(5)	64(4)	13(4)	31(4)	21(4)
O(5)	68(5)	173(8)	93(5)	-47(5)	-11(4)	-6(6)
O(6)	98(5)	56(4)	104(6)	-12(4)	47(4)	-22(4)
O(7)	167(9)	209(10)	47(5)	-62(7)	40(5)	-15(6)
O(8)	83(5)	63(5)	105(6)	11(4)	2(4)	16(4)
O(9)	52(3)	41(3)	41(3)	-10(3)	8(2)	0(3)
C(1)	51(6)	65(7)	83(7)	-3(5)	36(5)	2(5)
C(2)	47(5)	65(6)	48(5)	-9(5)	6(4)	0(5)
C(3)	58(6)	35(5)	56(5)	-5(4)	20(4)	0(4)
C(4)	57(5)	37(5)	61(6)	9(4)	15(5)	6(5)
C(5)	77(7)	96(8)	49(6)	-11(6)	3(5)	-3(5)
C(6)	77(7)	55(6)	66(6)	-23(5)	23(5)	-19(5)
C(7)	80(7)	88(8)	59(7)	-33(6)	14(6)	-14(6)
C(8)	53(6)	72(7)	49(5)	-2(5)	0(4)	7(5)
C(9)	50(5)	37(5)	54(5)	1(4)	5(4)	-6(4)
C(10)	96(8)	62(7)	73(7)	23(6)	14(6)	2(6)
C(11)	113(10)	55(8)	126(11)	22(7)	28(9)	3(7)
C(12)	57(7)	60(8)	167(13)	14(5)	45(8)	-32(8)
C(13)	110(9)	79(8)	105(9)	-1(7)	67(8)	-29(7)
C(14)	110(8)	62(6)	69(7)	21(6)	57(6)	3(5)
C(15)	52(5)	31(4)	41(5)	2(4)	11(4)	3(4)
C(16)	73(6)	76(7)	47(5)	-16(6)	9(5)	8(5)
C(17)	59(6)	119(9)	60(6)	-29(6)	-12(5)	14(7)
C(18)	63(6)	98(8)	55(6)	9(6)	-1(5)	2(6)
C(19)	75(7)	60(6)	50(5)	8(5)	2(5)	16(5)
C(20)	52(5)	44(5)	52(5)	4(4)	8(4)	-2(4)
C(21)	51(5)	48(5)	55(6)	-2(4)	13(4)	2(4)
C(22)	46(5)	73(7)	74(7)	8(5)	9(5)	-9(5)
C(23)	64(7)	82(8)	110(9)	16(6)	23(6)	-10(7)
C(24)	61(7)	64(7)	142(11)	24(6)	36(8)	21(7)
C(25)	49(6)	111(9)	82(8)	11(6)	8(5)	30(7)
C(26)	53(6)	71(7)	72(7)	9(5)	21(5)	15(5)
C(27)	48(5)	58(6)	42(5)	-12(4)	7(4)	7(4)
C(28)	69(6)	64(6)	56(6)	-10(5)	17(5)	8(5)
C(29)	83(7)	58(7)	105(9)	-19(6)	22(7)	24(6)
C(30)	67(7)	93(9)	93(9)	-30(6)	9(6)	56(7)
C(31)	77(7)	123(10)	55(7)	-21(7)	20(5)	24(7)
C(32)	85(7)	72(7)	58(6)	-14(5)	30(5)	-3(5)

The anisotropic displacement exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$

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Table 5. H-Atom coordinates ($x10^4$) and isotropic displacement coefficients ($Å^2 x10^3$)

	x	y	z	U
H(10A)	8285	3551	901	80
H(11A)	8913	2528	162	80
H(12A)	9028	2521	-1906	80
H(13A)	8548	3562	-3214	80
H(14A)	7959	4615	-2478	80
H(16A)	6136	4466	-1296	80
H(17A)	5073	4745	-2987	80
H(18A)	5118	5806	-4297	80
H(19A)	6214	6602	-3895	80
H(20A)	7273	6313	-2199	80
H(22A)	6684	6332	3944	80
H(23A)	5662	7219	3697	80
H(24A)	4759	7324	1778	80
H(25A)	4855	6530	92	80
H(26A)	5855	5606	345	80
H(28A)	7177	3460	2098	80
H(29A)	6903	2387	3230	80
H(30A)	6589	2549	5135	80
H(31A)	6442	3824	5844	80
H(32A)	6700	4892	4706	80

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