Supporting Information

First preparation and isolation of a stable ferrocenylketene

Nanyan Fu, Annette D. Allen, and Thomas T. Tidwell*

Department of Chemistry, University of Toronto, Toronto, Ontario M5S 3H6 Canada
Email: ttidwell@chem.utoronto.ca

File 1 (RTF file). Crystal data and structure refinement for **6** (k0665).

Identification code	k0665	
Empirical formula	C21 H30 Fe O Si	
Formula weight	382.39	
Temperature	150(1) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 7.9843(2) Å	a= 90°.
	b = 7.7592(3) Å	b= 93.920(2)°.
	c = 31.5333(10) Å	g = 90°.
Volume	1948.97(11) $Å^3$	
Z	4	
Density (calculated)	1.303 Mg/m^3	
Absorption coefficient	0.840 mm^{-1}	
F(000)	816	
Crystal size	0.24 x 0.20 x 0.08 mm^3	
Theta range for data collection	2.59 to 27.53°.	
Index ranges	-10<=h<=10, -9<=k<=10, -36<=l<=40	
Reflections collected	13213	
Independent reflections	4308 [R(int) = 0.0704]	
Completeness to theta = 27.53°	98.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.937 and 0.657	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4308 / 0 / 223	
Goodness-of-fit on F^2	1.048	
Final R indices [I>2sigma(I)]	R1 = 0.0453, wR2 = 0.1032	
R indices (all data)	R1 = 0.0731, wR2 = 0.1153	
Largest diff. peak and hole	0.402 and -0.790 $e.Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **6** (k0665). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Fe(1)	5147(1)	2785(1)	2995(1)	21(1)
Si(1)	2219(1)	5688(1)	4141(1)	20(1)
O(1)	6342(3)	3548(3)	4299(1)	45(1)
C(1)	3832(3)	4360(3)	3376(1)	22(1)
C(2)	2719(3)	3288(3)	3119(1)	24(1)
C(3)	2971(3)	3610(3)	2690(1)	27(1)
C(4)	4237(3)	4883(3)	2669(1)	27(1)
C(5)	4770(3)	5346(3)	3093(1)	25(1)
C(6)	6749(4)	1224(4)	3357(1)	32(1)
C(7)	5594(4)	211(4)	3096(1)	34(1)
C(8)	5807(4)	664(4)	2665(1)	33(1)
C(9)	7076(3)	1944(4)	2659(1)	31(1)
C(10)	7655(3)	2284(4)	3086(1)	32(1)
C(11)	3883(3)	4563(3)	3845(1)	23(1)
C(12)	5197(3)	4013(4)	4075(1)	29(1)
C(13)	631(3)	6577(3)	3724(1)	25(1)
C(14)	1266(4)	8043(4)	3457(1)	36(1)
C(15)	-1040(3)	7091(4)	3905(1)	36(1)
C(16)	3335(3)	7309(3)	4507(1)	27(1)
C(17)	4448(4)	8603(4)	4291(1)	39(1)
C(18)	2153(4)	8245(4)	4791(1)	34(1)
C(19)	1157(3)	4038(3)	4470(1)	23(1)
C(20)	2324(4)	3295(4)	4830(1)	31(1)
C(21)	396(4)	2579(3)	4187(1)	30(1)

Table 3. Bond lengths [Å] and angles [°] for **6**

Fe(1)-C(3)	2.032(3)
Fe(1)-C(4)	2.033(3)
Fe(1)-C(8)	2.036(3)
Fe(1)-C(9)	2.036(3)
Fe(1)-C(5)	2.036(3)
Fe(1)-C(10)	2.040(3)
Fe(1)-C(2)	2.042(3)
Fe(1)-C(7)	2.050(3)
Fe(1)-C(6)	2.050(3)
Fe(1)-C(1)	2.051(3)
Si(1)-C(19)	1.885(3)
Si(1)-C(11)	1.888(3)
Si(1)-C(16)	1.888(3)
Si(1)-C(13)	1.893(3)
O(1)-C(12)	1.174(3)
C(1)-C(5)	1.425(4)
C(1)-C(2)	1.427(4)
C(1)-C(11)	1.488(4)
C(2)-C(3)	1.405(4)
C(3)-C(4)	1.418(4)
C(4)-C(5)	1.421(4)
C(6)-C(10)	1.419(4)
C(6)-C(7)	1.429(4)
C(7)-C(8)	1.425(4)
C(8)-C(9)	1.420(4)
C(9)-C(10)	1.417(4)
C(11)-C(12)	1.304(4)
C(13)-C(14)	1.523(4)
C(13)-C(15)	1.540(4)
C(16)-C(18)	1.528(4)
C(16)-C(17)	1.532(4)
C(19)-C(20)	1.532(4)
C(19)-C(21)	1.539(4)
C(3)-Fe(1)-C(4)	40.83(11)
C(3)-Fe(1)-C(8)	104.75(11)
C(4)-Fe(1)-C(8)	118.97(12)
C(3)-Fe(1)-C(9)	120.46(12)

C(4)-Fe(1)-C(9)	104.49(12)
C(8)-Fe(1)-C(9)	40.82(11)
C(3)-Fe(1)-C(5)	68.52(11)
C(4)-Fe(1)-C(5)	40.88(11)
C(8)-Fe(1)-C(5)	155.83(12)
C(9)-Fe(1)-C(5)	121.11(11)
C(3)-Fe(1)-C(10)	157.76(12)
C(4)-Fe(1)-C(10)	122.47(12)
C(8)-Fe(1)-C(10)	68.40(11)
C(9)-Fe(1)-C(10)	40.69(12)
C(5)-Fe(1)-C(10)	108.60(11)
C(3)-Fe(1)-C(2)	40.35(11)
C(4)-Fe(1)-C(2)	68.44(11)
C(8)-Fe(1)-C(2)	122.30(11)
C(9)-Fe(1)-C(2)	157.36(11)
C(5)-Fe(1)-C(2)	68.43(11)
C(10)-Fe(1)-C(2)	160.98(12)
C(3)-Fe(1)-C(7)	120.94(12)
C(4)-Fe(1)-C(7)	155.59(12)
C(8)-Fe(1)-C(7)	40.81(12)
C(9)-Fe(1)-C(7)	68.80(12)
C(5)-Fe(1)-C(7)	162.44(12)
C(10)-Fe(1)-C(7)	68.54(12)
C(2)-Fe(1)-C(7)	108.29(11)
C(3)-Fe(1)-C(6)	158.51(12)
C(4)-Fe(1)-C(6)	160.43(12)
C(8)-Fe(1)-C(6)	68.49(12)
C(9)-Fe(1)-C(6)	68.57(12)
C(5)-Fe(1)-C(6)	125.86(11)
C(10)-Fe(1)-C(6)	40.59(12)
C(2)-Fe(1)-C(6)	124.83(12)
C(7)-Fe(1)-C(6)	40.80(12)
C(3)-Fe(1)-C(1)	68.52(10)
C(4)-Fe(1)-C(1)	68.84(11)
C(8)-Fe(1)-C(1)	160.28(11)
C(9)-Fe(1)-C(1)	158.64(11)
C(5)-Fe(1)-C(1)	40.80(11)
C(10)-Fe(1)-C(1)	124.67(11)
C(2)-Fe(1)-C(1)	40.82(10)
C(7)-Fe(1)-C(1)	125.52(12)

C(6)-Fe(1)-C(1)	110.63(11)
C(19)-Si(1)-C(11)	108.40(12)
C(19)-Si(1)-C(16)	109.11(12)
C(11)-Si(1)-C(16)	106.93(12)
C(19)-Si(1)-C(13)	108.92(12)
C(11)-Si(1)-C(13)	106.62(12)
C(16)-Si(1)-C(13)	116.57(12)
C(5)-C(1)-C(2)	107.0(2)
C(5)-C(1)-C(11)	125.8(2)
C(2)-C(1)-C(11)	126.8(2)
C(5)-C(1)-Fe(1)	69.05(15)
C(2)-C(1)-Fe(1)	69.24(14)
C(11)-C(1)-Fe(1)	131.67(18)
C(3)-C(2)-C(1)	108.5(2)
C(3)-C(2)-Fe(1)	69.44(15)
C(1)-C(2)-Fe(1)	69.93(14)
C(2)-C(3)-C(4)	108.6(2)
C(2)-C(3)-Fe(1)	70.22(14)
C(4)-C(3)-Fe(1)	69.66(15)
C(3)-C(4)-C(5)	107.5(2)
C(3)-C(4)-Fe(1)	69.51(15)
C(5)-C(4)-Fe(1)	69.67(15)
C(4)-C(5)-C(1)	108.4(2)
C(4)-C(5)-Fe(1)	69.45(15)
C(1)-C(5)-Fe(1)	70.15(14)
C(10)-C(6)-C(7)	107.9(3)
C(10)-C(6)-Fe(1)	69.33(16)
C(7)-C(6)-Fe(1)	69.59(16)
C(8)-C(7)-C(6)	107.4(3)
C(8)-C(7)-Fe(1)	69.09(16)
C(6)-C(7)-Fe(1)	69.62(16)
C(9)-C(8)-C(7)	108.5(3)
C(9)-C(8)-Fe(1)	69.59(16)
C(7)-C(8)-Fe(1)	70.10(16)
C(10)-C(9)-C(8)	107.7(3)
C(10)-C(9)-Fe(1)	69.80(16)
C(8)-C(9)-Fe(1)	69.59(16)
C(9)-C(10)-C(6)	108.5(3)
C(9)-C(10)-Fe(1)	69.51(15)
C(6)-C(10)-Fe(1)	70.08(16)

C(12)-C(11)-C(1)	118.9(2)
C(12)-C(11)-Si(1)	116.4(2)
C(1)-C(11)-Si(1)	124.62(18)
O(1)-C(12)-C(11)	176.6(3)
C(14)-C(13)-C(15)	110.0(2)
C(14)-C(13)-Si(1)	115.09(19)
C(15)-C(13)-Si(1)	113.16(19)
C(18)-C(16)-C(17)	110.5(2)
C(18)-C(16)-Si(1)	112.99(19)
C(17)-C(16)-Si(1)	115.3(2)
C(20)-C(19)-C(21)	110.4(2)
C(20)-C(19)-Si(1)	112.94(18)
C(21)-C(19)-Si(1)	110.86(18)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for k0665. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	20(1)	18(1)	26(1)	-2(1)	3(1)	1(1)
Si(1)	19(1)	20(1)	22(1)	-1(1)	1(1)	1(1)
O(1)	31(1)	69(2)	35(1)	0(1)	-5(1)	16(1)
C(1)	22(1)	20(1)	23(1)	-3(1)	2(1)	6(1)
C(2)	17(1)	24(1)	32(2)	-3(1)	2(1)	3(1)
C(3)	25(1)	29(1)	26(2)	-4(1)	-2(1)	5(1)
C(4)	33(2)	26(1)	23(1)	2(1)	4(1)	7(1)
C(5)	27(1)	18(1)	32(2)	1(1)	5(1)	1(1)
C(6)	32(2)	30(2)	33(2)	4(1)	0(1)	11(1)
C(7)	32(2)	19(1)	53(2)	3(1)	11(1)	7(1)
C(8)	30(2)	25(1)	45(2)	-13(1)	2(1)	6(1)
C(9)	24(1)	29(2)	41(2)	-6(1)	11(1)	5(1)
C(10)	19(1)	32(2)	44(2)	-6(1)	0(1)	1(1)
C(11)	22(1)	24(1)	24(1)	-2(1)	3(1)	2(1)
C(12)	26(1)	35(2)	28(2)	-6(1)	5(1)	4(1)
C(13)	25(1)	25(1)	25(1)	1(1)	1(1)	3(1)
C(14)	36(2)	38(2)	35(2)	12(1)	2(1)	5(1)
C(15)	26(2)	45(2)	37(2)	7(1)	2(1)	7(1)
C(16)	25(1)	25(1)	30(2)	-3(1)	-2(1)	0(1)
C(17)	37(2)	33(2)	45(2)	-7(2)	3(1)	-11(1)
C(18)	41(2)	28(2)	33(2)	-7(1)	3(1)	3(1)
C(19)	21(1)	22(1)	25(1)	-1(1)	5(1)	2(1)
C(20)	34(2)	30(2)	29(2)	4(1)	1(1)	2(1)
C(21)	31(2)	27(2)	31(2)	0(1)	2(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **6**.

	x	y	z	U(eq)
H(2A)	1908	2437	3227	29
H(3A)	2365	3033	2441	32
H(4A)	4673	5369	2404	33
H(5A)	5659	6209	3179	30
H(6A)	6886	1200	3674	38
H(7A)	4781	-652	3197	41
H(8A)	5164	171	2410	40
H(9A)	7490	2503	2400	37
H(10A)	8542	3137	3180	38
H(13A)	359	5608	3522	30
H(14A)	449	8274	3217	54
H(14B)	2344	7718	3349	54
H(14C)	1414	9081	3632	54
H(15A)	-1840	7450	3672	53
H(15B)	-848	8047	4105	53
H(15C)	-1497	6103	4052	53
H(16A)	4111	6623	4704	32
H(17A)	5131	9242	4507	58
H(17B)	3740	9410	4119	58
H(17C)	5185	7985	4106	58
H(18A)	2810	8983	4992	51
H(18B)	1528	7397	4948	51
H(18C)	1364	8954	4615	51
H(19A)	210	4629	4603	27
H(20A)	1699	2476	4996	47
H(20B)	2753	4232	5015	47
H(20C)	3266	2702	4710	47
H(21A)	-180	1757	4363	44
H(21B)	1293	1985	4048	44
H(21C)	-409	3065	3971	44

File 2. CIF file

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not relevant to the choice of reflections for refinement. R-factors based
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H3A H 0.2365 0.3033 0.2441 0.032 Uiso 1 1 calc R . .
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H4A H 0.4673 0.5369 0.2404 0.033 Uiso 1 1 calc R . .
C5 C 0.4770(3) 0.5346(3) 0.30932(9) 0.0253(6) Uani 1 1 d . . .
H5A H 0.5659 0.6209 0.3179 0.030 Uiso 1 1 calc R . .
C6 C 0.6749(4) 0.1224(4) 0.33567(10) 0.0317(7) Uani 1 1 d . . .
H6A H 0.6886 0.1200 0.3674 0.038 Uiso 1 1 calc R . .
C7 C 0.5594(4) 0.0211(4) 0.30958(10) 0.0344(7) Uani 1 1 d . . .
H7A H 0.4781 -0.0652 0.3197 0.041 Uiso 1 1 calc R . .
C8 C 0.5807(4) 0.0664(4) 0.26650(10) 0.0334(7) Uani 1 1 d . . .
H8A H 0.5164 0.0171 0.2410 0.040 Uiso 1 1 calc R . .
C9 C 0.7076(3) 0.1944(4) 0.26590(10) 0.0310(7) Uani 1 1 d . . .
H9A H 0.7490 0.2503 0.2400 0.037 Uiso 1 1 calc R . .
C10 C 0.7655(3) 0.2284(4) 0.30858(10) 0.0320(7) Uani 1 1 d . . .
H10A H 0.8542 0.3137 0.3180 0.038 Uiso 1 1 calc R . .
C11 C 0.3883(3) 0.4563(3) 0.38454(8) 0.0232(6) Uani 1 1 d . . .
C12 C 0.5197(3) 0.4013(4) 0.40746(9) 0.0292(6) Uani 1 1 d . . .
C13 C 0.0631(3) 0.6577(3) 0.37239(9) 0.0252(6) Uani 1 1 d . . .
H13A H 0.0359 0.5608 0.3522 0.030 Uiso 1 1 calc R . .
C14 C 0.1266(4) 0.8043(4) 0.34567(10) 0.0362(7) Uani 1 1 d . . .
H14A H 0.0449 0.8274 0.3217 0.054 Uiso 1 1 calc R . .
H14B H 0.2344 0.7718 0.3349 0.054 Uiso 1 1 calc R . .
H14C H 0.1414 0.9081 0.3632 0.054 Uiso 1 1 calc R . .
C15 C -0.1040(3) 0.7091(4) 0.39048(10) 0.0356(7) Uani 1 1 d . . .
H15A H -0.1840 0.7450 0.3672 0.053 Uiso 1 1 calc R . .
H15B H -0.0848 0.8047 0.4105 0.053 Uiso 1 1 calc R . .
H15C H -0.1497 0.6103 0.4052 0.053 Uiso 1 1 calc R . .
C16 C 0.3335(3) 0.7309(3) 0.45069(9) 0.0267(6) Uani 1 1 d . . .
H16A H 0.4111 0.6623 0.4704 0.032 Uiso 1 1 calc R . .
C17 C 0.4448(4) 0.8603(4) 0.42905(10) 0.0385(7) Uani 1 1 d . . .
H17A H 0.5131 0.9242 0.4507 0.058 Uiso 1 1 calc R . .

H17B H 0.3740 0.9410 0.4119 0.058 Uiso 1 1 calc R . .
H17C H 0.5185 0.7985 0.4106 0.058 Uiso 1 1 calc R . .
C18 C 0.2153(4) 0.8245(4) 0.47909(10) 0.0340(7) Uani 1 1 d . . .
H18A H 0.2810 0.8983 0.4992 0.051 Uiso 1 1 calc R . .
H18B H 0.1528 0.7397 0.4948 0.051 Uiso 1 1 calc R . .
H18C H 0.1364 0.8954 0.4615 0.051 Uiso 1 1 calc R . .
C19 C 0.1157(3) 0.4038(3) 0.44697(8) 0.0225(6) Uani 1 1 d . . .
H19A H 0.0210 0.4629 0.4603 0.027 Uiso 1 1 calc R . .
C20 C 0.2324(4) 0.3295(4) 0.48301(9) 0.0312(7) Uani 1 1 d . . .
H20A H 0.1699 0.2476 0.4996 0.047 Uiso 1 1 calc R . .
H20B H 0.2753 0.4232 0.5015 0.047 Uiso 1 1 calc R . .
H20C H 0.3266 0.2702 0.4710 0.047 Uiso 1 1 calc R . .
C21 C 0.0396(4) 0.2579(3) 0.41873(9) 0.0297(6) Uani 1 1 d . . .
H21A H -0.0180 0.1757 0.4363 0.044 Uiso 1 1 calc R . .
H21B H 0.1293 0.1985 0.4048 0.044 Uiso 1 1 calc R . .
H21C H -0.0409 0.3065 0.3971 0.044 Uiso 1 1 calc R . .

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Si1 0.0192(4) 0.0200(4) 0.0219(4) -0.0009(3) 0.0005(3) 0.0008(3)
O1 0.0309(11) 0.0693(16) 0.0354(12) -0.0003(11) -0.0053(10) 0.0162(11)
C1 0.0217(13) 0.0204(13) 0.0231(14) -0.0026(10) 0.0023(11) 0.0059(11)
C2 0.0165(12) 0.0244(13) 0.0320(16) -0.0026(11) 0.0021(11) 0.0028(11)
C3 0.0246(14) 0.0293(14) 0.0258(15) -0.0043(12) -0.0021(11) 0.0048(12)
C4 0.0333(15) 0.0262(14) 0.0225(14) 0.0022(11) 0.0038(12) 0.0068(12)
C5 0.0267(14) 0.0177(13) 0.0319(16) 0.0013(11) 0.0046(12) 0.0005(11)
C6 0.0323(15) 0.0299(15) 0.0325(16) 0.0038(13) -0.0003(13) 0.0106(13)
C7 0.0318(15) 0.0192(14) 0.053(2) 0.0030(13) 0.0110(14) 0.0067(12)
C8 0.0303(15) 0.0250(14) 0.0447(19) -0.0128(13) 0.0018(13) 0.0064(12)
C9 0.0238(14) 0.0293(15) 0.0410(18) -0.0060(13) 0.0112(12) 0.0046(12)
C10 0.0192(13) 0.0321(15) 0.0442(19) -0.0058(13) -0.0004(12) 0.0012(12)
C11 0.0218(13) 0.0244(13) 0.0237(14) -0.0020(11) 0.0027(11) 0.0020(11)
C12 0.0258(14) 0.0348(15) 0.0276(15) -0.0059(12) 0.0053(12) 0.0039(13)

C13 0.0251(14) 0.0253(13) 0.0250(14) 0.0007(11) 0.0007(11) 0.0033(11)
C14 0.0363(17) 0.0375(17) 0.0347(17) 0.0116(14) 0.0023(13) 0.0053(14)
C15 0.0258(15) 0.0445(18) 0.0366(18) 0.0068(14) 0.0019(13) 0.0074(14)
C16 0.0247(14) 0.0252(14) 0.0295(15) -0.0028(12) -0.0022(11) -0.0003(11)
C17 0.0369(17) 0.0333(16) 0.0454(19) -0.0074(15) 0.0033(14) -0.0113(14)
C18 0.0411(17) 0.0284(15) 0.0325(17) -0.0072(13) 0.0025(13) 0.0031(13)
C19 0.0207(13) 0.0217(13) 0.0254(14) -0.0010(11) 0.0045(11) 0.0016(11)
C20 0.0339(16) 0.0304(15) 0.0292(16) 0.0042(12) 0.0011(12) 0.0023(13)
C21 0.0312(15) 0.0272(15) 0.0305(16) 0.0002(12) 0.0017(12) -0.0024(12)

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;
All esds (except the esd in the dihedral angle between two l.s. planes)
are estimated using the full covariance matrix. The cell esds are taken
into account individually in the estimation of esds in distances, angles
and torsion angles; correlations between esds in cell parameters are only
used when they are defined by crystal symmetry. An approximate (isotropic)
treatment of cell esds is used for estimating esds involving l.s. planes.
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Fe1 C5 2.036(3) . ?
Fe1 C10 2.040(3) . ?
Fe1 C2 2.042(3) . ?
Fe1 C7 2.050(3) . ?
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Fe1 C1 2.051(3) . ?
Si1 C19 1.885(3) . ?
Si1 C11 1.888(3) . ?
Si1 C16 1.888(3) . ?
Si1 C13 1.893(3) . ?

O1 C12 1.174(3) . ?
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C1 C11 1.488(4) . ?
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