Part I Crystal Data for $(Me_2C)(Me_2Si)[(\eta^5\text{-}C_5H_3)Fe(CO)_2]_2$ (**3**) (1 of 3 structures)

Table 1.1 Crystal data and structure refinement for **3**

Empirical formula	$C_{19}H_{18}Fe_2O_4Si$	
Formula weight	450.12	
Measurement instrument	BRUKER SMART 1000	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 9.1644(10) Å	alpha = 90°
	b = 13.8521(15) Å	beta = 102.103(2)°
	c = 15.3075(17) Å	gamma = 90°
Volume, Z	1900.0(4) $Å^3$, 4	
Density (calculated)	1.574 Mg/m^3	
Absorption coefficient	1.610 mm^{-1}	
F(000)	920	
Crystal size	0.25 x 0.2 x 0.15 mm	
θ range for data collection	2.00 to 26.41°	
Limiting indices	$-11 \le h \le 11, -13 \le k \le 17, -18 \le l \le 19$	
Reflections collected	10993	
Independent reflections	3901 (R_{int} = 0.0607)	
Observed reflections	2838	
Observed Criterion	> 2sigma(I)	
Completeness to θ = 26.41°	99.7%	
Absorption correction	empirical	
Max. And min. Transmission	1.000 and 0.832	
Refinement Method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3901 / 0 / 235	
Goodness-of-fit on F^2	1.019	
Final R indices [I>2σ(I)]	R1 = 0.0375, wR2 = 0.0793	
R indices (all data)	R1 = 0.0587, wR2 = 0.0858	
Largest diff. Peak and hole	0.403 and -0.302 $eÅ^{-3}$	
Weighing scheme	calc $w=1/[s^2(Fo^2) + (0.0241P)^2 + 0.6395P]$ where $P=(Fo^2+2Fc^2)/3$	
Primary method of solution	direct	
Secondary method of solution	difmap	
Method of locating and refining H atoms	geom	
Extinction correction method	none	
Computing data collection	'BRUKER SMART'	
Computing cell refinement	'BRUKER SMART'	
Computing data reduction	'BRUKER SAINT'	
Computing structure solution	'SHELXS-97'	
Computing structure refinement	'SHELXS-97'	
Computing molecular graphics	SHELXS-97	

Computing publication material SHELXS-97; Refinement on F^2 for ALL reflections except for 3 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 $F^2 > 2sigma(F^2)$ is used only for calculating R-factors etc. 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 1.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **3**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	9293(1)	240(1)	2209(1)	39(1)
Fe(2)	9491(1)	2132(1)	2818(1)	37(1)
Si(1)	12087(1)	1494(1)	1641(1)	48(1)
C(1)	8063(4)	489(2)	1208(2)	60(1)
O(1)	7257(3)	597(2)	527(2)	96(1)
C(2)	7825(3)	33(2)	2755(2)	50(1)
O(2)	6845(3)	-153(2)	3083(2)	77(1)
C(3)	8177(4)	1931(2)	3470(2)	54(1)
O(3)	7336(3)	1857(2)	3932(2)	93(1)
C(4)	8123(3)	2456(2)	1886(2)	52(1)
O(4)	7216(3)	2716(2)	1298(2)	81(1)
C(5)	12184(3)	798(2)	3736(2)	42(1)
C(6)	11668(4)	513(2)	4585(2)	69(1)
C(7)	13911(3)	729(2)	3907(2)	66(1)
C(8)	14081(4)	1488(3)	1532(3)	74(1)
C(9)	10960(4)	1894(3)	553(2)	75(1)
C(11)	11500(3)	135(2)	2963(2)	41(1)
C(12)	10742(3)	-746(2)	3007(2)	52(1)
C(13)	10284(3)	-1121(2)	2143(2)	58(1)
C(14)	10761(3)	-481(2)	1547(2)	53(1)
C(15)	11502(3)	320(2)	2037(2)	41(1)
C(21)	11693(3)	1811(2)	3448(2)	42(1)
C(22)	11116(3)	2522(2)	3953(2)	53(1)
C(23)	10706(3)	3345(2)	3417(2)	55(1)
C(24)	11041(3)	3168(2)	2587(2)	49(1)
C(25)	11672(3)	2219(2)	2584(2)	41(1)
H(6A)	10599	554	4483	103
H(6B)	12102	943	5061	103
H(6C)	11977	-137	4746	103
H(7A)	14242	908	3374	99
H(7B)	14217	79	4069	99
H(7C)	14343	1159	4384	99
H(8A)	14181	1097	1030	111
H(8B)	14694	1228	2066	111
H(8C)	14392	2136	1443	111
H(9A)	9924	1906	583	112
H(9B)	11102	1453	94	112
H(9C)	11269	2529	418	112
H(12A)	10570	-1049	3555	63
H(13A)	9755	-1732	1984	69
H(14A)	10609	-570	900	63
H(22A)	11014	2451	4574	64
H(23A)	10281	3942	3601	66
H(24A)	10886	3622	2085	59

Table 1.3 Bond lengths (Å) and angles (°) for **3**

Fe(1)-C(1)	1.736(4)
Fe(1)-C(2)	1.750(3)
Fe(1)-C(15)	2.099(3)
Fe(1)-C(14)	2.099(3)
Fe(1)-C(13)	2.105(3)
Fe(1)-C(12)	2.107(3)
Fe(1)-C(11)	2.113(3)
Fe(1)-Fe(2)	2.7747(6)
Fe(2)-C(3)	1.740(3)
Fe(2)-C(4)	1.749(3)
Fe(2)-C(21)	2.094(3)
Fe(2)-C(24)	2.101(3)
Fe(2)-C(25)	2.107(3)
Fe(2)-C(22)	2.107(3)
Fe(2)-C(23)	2.116(3)
Si(1)-C(9)	1.851(3)
Si(1)-C(15)	1.853(3)
Si(1)-C(25)	1.861(3)
Si(1)-C(8)	1.870(3)
C(1)-O(1)	1.154(4)
C(2)-O(2)	1.147(3)
C(3)-O(3)	1.154(3)
C(4)-O(4)	1.147(3)
C(5)-C(21)	1.511(4)
C(5)-C(11)	1.525(4)
C(5)-C(6)	1.525(4)
C(5)-C(7)	1.553(4)
C(11)-C(12)	1.413(4)
C(11)-C(15)	1.442(4)
C(12)-C(13)	1.401(4)
C(13)-C(14)	1.405(4)
C(14)-C(15)	1.428(4)
C(21)-C(22)	1.421(4)
C(21)-C(25)	1.434(4)
C(22)-C(23)	1.409(4)
C(23)-C(24)	1.390(4)
C(24)-C(25)	1.436(4)

C(1)-Fe(1)-C(2)	91.84(15)
C(1)-Fe(1)-C(15)	110.06(13)
C(2)-Fe(1)-C(15)	158.03(13)
C(1)-Fe(1)-C(14)	91.80(14)
C(2)-Fe(1)-C(14)	141.89(12)
C(15)-Fe(1)-C(14)	39.79(10)
C(1)-Fe(1)-C(13)	109.99(14)
C(2)-Fe(1)-C(13)	104.99(13)
C(15)-Fe(1)-C(13)	66.66(11)
C(14)-Fe(1)-C(13)	39.05(12)
C(1)-Fe(1)-C(12)	148.61(14)
C(2)-Fe(1)-C(12)	94.09(12)
C(15)-Fe(1)-C(12)	66.41(11)
C(14)-Fe(1)-C(12)	65.24(13)
C(13)-Fe(1)-C(12)	38.85(12)
C(1)-Fe(1)-C(11)	149.97(13)
C(2)-Fe(1)-C(11)	118.15(13)
C(15)-Fe(1)-C(11)	40.04(10)
C(14)-Fe(1)-C(11)	66.04(11)
C(13)-Fe(1)-C(11)	65.88(11)
C(12)-Fe(1)-C(11)	39.12(10)
C(1)-Fe(1)-Fe(2)	95.38(11)
C(2)-Fe(1)-Fe(2)	89.86(9)
C(15)-Fe(1)-Fe(2)	89.76(7)
C(14)-Fe(1)-Fe(2)	127.48(8)
C(13)-Fe(1)-Fe(2)	149.78(9)
C(12)-Fe(1)-Fe(2)	115.40(9)
C(11)-Fe(1)-Fe(2)	83.92(7)
C(3)-Fe(2)-C(4)	92.59(15)
C(3)-Fe(2)-C(21)	114.73(14)
C(4)-Fe(2)-C(21)	152.46(13)
C(3)-Fe(2)-C(24)	141.27(13)
C(4)-Fe(2)-C(24)	94.70(13)
C(21)-Fe(2)-C(24)	66.54(11)
C(3)-Fe(2)-C(25)	154.43(14)
C(4)-Fe(2)-C(25)	112.95(12)
C(21)-Fe(2)-C(25)	39.92(10)
C(24)-Fe(2)-C(25)	39.92(10)
C(3)-Fe(2)-C(22)	91.33(14)
C(4)-Fe(2)-C(22)	150.30(13)
C(21)-Fe(2)-C(22)	39.53(10)
C(24)-Fe(2)-C(22)	65.02(12)
C(25)-Fe(2)-C(22)	66.03(11)
C(3)-Fe(2)-C(23)	104.12(13)
C(4)-Fe(2)-C(23)	111.85(13)
C(21)-Fe(2)-C(23)	66.44(11)
C(24)-Fe(2)-C(23)	38.50(11)
C(25)-Fe(2)-C(23)	66.19(11)
C(22)-Fe(2)-C(23)	38.97(12)
C(3)-Fe(2)-Fe(1)	92.13(10)
C(4)-Fe(2)-Fe(1)	88.99(10)
C(21)-Fe(2)-Fe(1)	86.71(7)
C(24)-Fe(2)-Fe(1)	125.94(8)
C(25)-Fe(2)-Fe(1)	89.65(7)
C(22)-Fe(2)-Fe(1)	120.27(9)
C(23)-Fe(2)-Fe(1)	152.50(9)
C(9)-Si(1)-C(15)	114.28(15)
C(9)-Si(1)-C(25)	111.76(15)
C(15)-Si(1)-C(25)	95.73(12)
C(9)-Si(1)-C(8)	106.97(17)
C(15)-Si(1)-C(8)	112.36(15)
C(25)-Si(1)-C(8)	115.74(15)
O(1)-C(1)-Fe(1)	175.8(3)
O(2)-C(2)-Fe(1)	175.9(3)
O(3)-C(3)-Fe(2)	175.3(3)
O(4)-C(4)-Fe(2)	176.1(3)
C(21)-C(5)-C(11)	106.5(2)
C(21)-C(5)-C(6)	111.3(2)
C(11)-C(5)-C(6)	110.8(2)
C(21)-C(5)-C(7)	109.7(2)
C(11)-C(5)-C(7)	109.4(2)
C(6)-C(5)-C(7)	109.2(3)
C(12)-C(11)-C(15)	107.6(3)
C(12)-C(11)-C(5)	127.6(3)
C(15)-C(11)-C(5)	124.8(2)
C(12)-C(11)-Fe(1)	70.20(16)
C(15)-C(11)-Fe(1)	69.43(16)

C(5)-C(11)-Fe(1)	124.93(18)	C(22)-C(21)-Fe(2)	70.74(16)
C(13)-C(12)-C(11)	109.2(3)	C(25)-C(21)-Fe(2)	70.54(16)
C(13)-C(12)-Fe(1)	70.50(18)	C(5)-C(21)-Fe(2)	122.07(18)
C(11)-C(12)-Fe(1)	70.68(15)	C(23)-C(22)-C(21)	109.2(3)
C(12)-C(13)-C(14)	107.8(3)	C(23)-C(22)-Fe(2)	70.84(18)
C(12)-C(13)-Fe(1)	70.65(16)	C(21)-C(22)-Fe(2)	69.73(16)
C(14)-C(13)-Fe(1)	70.23(17)	C(24)-C(23)-C(22)	107.8(3)
C(13)-C(14)-C(15)	109.2(3)	C(24)-C(23)-Fe(2)	70.17(16)
C(13)-C(14)-Fe(1)	70.72(18)	C(22)-C(23)-Fe(2)	70.18(16)
C(15)-C(14)-Fe(1)	70.10(16)	C(23)-C(24)-C(25)	109.3(3)
C(14)-C(15)-C(11)	106.2(2)	C(23)-C(24)-Fe(2)	71.33(16)
C(14)-C(15)-Si(1)	130.5(2)	C(25)-C(24)-Fe(2)	70.27(14)
C(11)-C(15)-Si(1)	122.5(2)	C(21)-C(25)-C(24)	106.6(2)
C(14)-C(15)-Fe(1)	70.11(16)	C(21)-C(25)-Si(1)	122.5(2)
C(11)-C(15)-Fe(1)	70.53(15)	C(24)-C(25)-Si(1)	130.0(2)
Si(1)-C(15)-Fe(1)	116.11(13)	C(21)-C(25)-Fe(2)	69.55(15)
C(22)-C(21)-C(25)	107.1(2)	C(24)-C(25)-Fe(2)	69.81(15)
C(22)-C(21)-C(5)	127.4(3)	Si(1)-C(25)-Fe(2)	117.16(13)
C(25)-C(21)-C(5)	125.5(2)		

Symmetry transformations used to generate equivalent atoms: No

Table 1.4 Anisotropic displacement coefficients ($Å^2 \times 10^3$) for **3**
The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U11 + \ldots + 2hka^*b^*U12)$

	U11	U22	U33	U23	U13	U12
Fe(1)	34(1)	34(1)	49(1)	-1(1)	6(1)	-3(1)
Fe(2)	35(1)	34(1)	43(1)	-1(1)	9(1)	0(1)
Si(1)	44(1)	54(1)	49(1)	-3(1)	18(1)	-9(1)
C(1)	55(2)	64(2)	58(2)	-4(2)	5(2)	3(2)
O(1)	88(2)	125(2)	62(2)	0(2)	-17(2)	16(2)
C(2)	45(2)	39(2)	67(2)	2(1)	12(2)	4(1)
O(2)	62(2)	70(2)	111(2)	14(1)	44(2)	-1(1)
C(3)	55(2)	50(2)	63(2)	-8(2)	21(2)	-1(1)
O(3)	86(2)	111(2)	102(2)	-16(2)	63(2)	-13(2)
C(4)	49(2)	45(2)	60(2)	7(2)	5(2)	-9(1)
O(4)	68(2)	77(2)	82(2)	26(1)	-19(1)	-8(1)
C(5)	37(2)	47(2)	40(2)	1(1)	1(1)	4(1)
C(6)	87(3)	69(2)	48(2)	11(2)	10(2)	9(2)
C(7)	43(2)	71(2)	74(2)	-4(2)	-11(2)	10(2)
C(8)	62(2)	73(2)	97(3)	-10(2)	41(2)	-11(2)
C(9)	89(3)	90(3)	47(2)	10(2)	18(2)	-20(2)
C(11)	34(1)	38(2)	51(2)	2(1)	7(1)	5(1)
C(12)	44(2)	38(2)	74(2)	15(2)	13(2)	7(1)
C(13)	47(2)	37(2)	87(2)	-11(2)	8(2)	0(1)
C(14)	45(2)	50(2)	63(2)	-16(2)	11(2)	-1(1)
C(15)	35(1)	41(2)	49(2)	-6(1)	12(1)	0(1)
C(21)	36(2)	47(2)	43(2)	-8(1)	5(1)	-4(1)
C(22)	52(2)	60(2)	45(2)	-13(2)	6(2)	-3(2)
C(23)	54(2)	38(2)	72(2)	-15(2)	11(2)	-5(1)
C(24)	46(2)	36(2)	67(2)	0(1)	12(2)	-12(1)
C(25)	34(1)	39(2)	50(2)	0(1)	11(1)	-8(1)

#===END

Part II Crystal Data for $[Fe(CO)_2]_2(\mu\text{-}\eta^5{:}\eta^1\text{-}C_5H_4)[\mu\text{-}Me_2Si\text{-}(\eta^5\text{-}C_5H_4)\ (\mu\text{-}Me_2C)]$ (**5**) (2 of 3 structures)

Table 2.1 Crystal data and structure refinement for **5**

Empirical formula	$C_{19}H_{18}Fe_2O_4Si$	
Formula weight	450.12	
Measurement instrument	BRUKER SMART 1000	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 16.3299(17) Å	alpha = 90°
	b = 13.3165(14) Å	beta = 90°
	c = 17.2512(18) Å	gamma = 90°
Volume, Z	3751.4(7) $Å^3$, 8	
Density (calculated)	1.594 Mg/m^3	
Absorption coefficient	1.631 mm^{-1}	
F(000)	1840	
Crystal size	0.25 x 0.22 x 0.15 mm	
θ range for data collection	2.30 to 25.02°	
Limiting indices	$-19 \le h \le 19$, $-10 \le k \le 15$, $-20 \le l \le 20$	
Reflections collected	14723	
Independent reflections	3308 (R_{int} = 0.0963)	
Observed reflections	2109	
Observed Criterion	> 2sigma(I)	
Completeness to θ = 25.02°	99.9%	
Absorption correction	empirical	
Max. And min. Transmission	1.000 and 0.8076	
Refinement Method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3308 / 0 / 235	
Goodness-of-fit on F^2	1.001	
Final R indices [I>2σ(I)]	R1 = 0.0352, wR2 = 0.0492	
R indices (all data)	R1 = 0.0735, wR2 = 0.0542	
Largest diff. Peak and hole	0.316 and -0.387 $eÅ^{-3}$	
Weighing scheme	calc $w=1/[s^2(Fo^2) + (0.0241P)^2 + 0.6395P]$ where $P=(Fo^2+2Fc^2)/3$	
Primary method of solution	direct	
Secondary method of solution	difmap	
Method of locating and refining H atoms	geom	
Extinction correction method	none	
Computing data collection	'BRUKER SMART'	
Computing cell refinement	'BRUKER SMART'	
Computing data reduction	'BRUKER SAINT'	
Computing structure solution	'SHELXS-97'	
Computing structure refinement	'SHELXS-97'	
Computing molecular graphics	SHELXS-97	

Computing publication material SHELXS-97; Refinement on F^2 for ALL reflections except for 3 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 $F^2 > 2sigma(F^2)$ is used only for calculating R-factors etc. 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 2.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **5**
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	871(1)	4031(1)	3328(1)	35(1)
Fe(2)	1850(1)	2953(1)	5067(1)	36(1)
Si(1)	821(1)	2300(1)	3479(1)	41(1)
C(1)	761(2)	3888(3)	2332(2)	49(1)
O(1)	696(2)	3818(2)	1666(1)	78(1)
C(2)	-171(2)	4069(3)	3522(2)	50(1)
O(2)	-863(2)	4117(2)	3665(2)	80(1)
C(3)	867(2)	3106(2)	5465(2)	42(1)
O(3)	220(2)	3227(2)	5697(1)	64(1)
C(4)	2328(2)	3733(3)	5758(2)	50(1)
O(4)	2648(2)	4239(2)	6203(2)	77(1)
C(5)	2778(2)	3276(2)	3539(2)	40(1)
C(6)	2855(2)	2878(3)	2704(2)	63(1)
C(7)	3593(2)	3759(3)	3782(2)	66(1)
C(8)	-96(2)	1766(3)	3991(2)	65(1)
C(9)	873(2)	1497(2)	2580(2)	65(1)
C(11)	2114(2)	4057(2)	3632(2)	35(1)
C(12)	1909(2)	4930(2)	3194(2)	42(1)
C(13)	1308(2)	5469(2)	3602(2)	41(1)
C(14)	1142(2)	4936(2)	4294(2)	37(1)
C(15)	1651(2)	4071(2)	4340(2)	33(1)
C(21)	2520(2)	2460(2)	4115(2)	34(1)
C(22)	2939(2)	2174(2)	4797(2)	46(1)
C(23)	2434(2)	1538(2)	5237(2)	47(1)
C(24)	1697(2)	1415(2)	4830(2)	42(1)
C(25)	1724(2)	1993(2)	4124(2)	34(1)
H(6A)	2347	2574	2550	95
H(6B)	3285	2386	2681	95
H(6C)	2981	3424	2361	95
H(7D)	3548	4010	4302	99
H(7A)	3719	4303	3437	99
H(7B)	4021	3266	3759	99
H(8A)	-48	1049	4019	97
H(8B)	-584	1940	3711	97
H(8C)	-126	2037	4506	97
H(9A)	847	801	2723	97
H(9B)	1377	1626	2312	97
H(9C)	420	1657	2247	97
H(12A)	2156	5130	2699	50
H(13A)	1062	6109	3444	49
H(14A)	745	5143	4690	44
H(22A)	3493	2387	4940	55
H(23A)	2573	1234	5737	56
H(24A)	1234	1004	5001	51

Table 2.3 Bond lengths (Å) and angles (°) for **5**

Fe(1)-C(2)	1.735(4)	C(1)-O(1)	1.156(4)
Fe(1)-C(1)	1.738(4)	C(2)-O(2)	1.159(4)
Fe(1)-C(12)	2.089(3)	C(3)-O(3)	1.142(4)
Fe(1)-C(11)	2.097(3)	C(4)-O(4)	1.146(4)
Fe(1)-C(13)	2.098(3)	C(5)-C(11)	1.510(4)
Fe(1)-C(14)	2.104(3)	C(5)-C(21)	1.532(4)
Fe(1)-C(15)	2.162(3)	C(5)-C(7)	1.537(4)
Fe(1)-Si(1)	2.3222(10)	C(5)-C(6)	1.541(4)
Fe(2)-C(3)	1.757(4)	C(11)-C(12)	1.427(4)
Fe(2)-C(4)	1.764(4)	C(11)-C(15)	1.437(4)
Fe(2)-C(15)	1.974(3)	C(12)-C(13)	1.405(4)
Fe(2)-C(25)	2.080(3)	C(13)-C(14)	1.415(4)
Fe(2)-C(21)	2.080(3)	C(14)-C(15)	1.423(4)
Fe(2)-C(24)	2.104(3)	C(21)-C(22)	1.412(4)
Fe(2)-C(22)	2.111(3)	C(21)-C(25)	1.441(4)
Fe(2)-C(23)	2.132(3)	C(22)-C(23)	1.404(4)
Si(1)-C(8)	1.879(3)	C(23)-C(24)	1.403(4)
Si(1)-C(9)	1.885(3)	C(24)-C(25)	1.441(4)
Si(1)-C(25)	1.891(3)		

C(2)-Fe(1)-C(1)	95.36(16)	C(25)-Fe(2)-C(24)	40.30(11)
C(2)-Fe(1)-C(12)	143.24(15)	C(21)-Fe(2)-C(24)	66.48(12)
C(1)-Fe(1)-C(12)	92.14(14)	C(3)-Fe(2)-C(22)	155.85(14)
C(2)-Fe(1)-C(11)	154.23(14)	C(4)-Fe(2)-C(22)	93.79(15)
C(1)-Fe(1)-C(11)	110.41(15)	C(15)-Fe(2)-C(22)	111.66(13)
C(12)-Fe(1)-C(11)	39.85(11)	C(25)-Fe(2)-C(22)	66.94(12)
C(2)-Fe(1)-C(13)	105.31(15)	C(21)-Fe(2)-C(22)	39.37(11)
C(1)-Fe(1)-C(13)	111.01(14)	C(24)-Fe(2)-C(22)	65.05(13)
C(12)-Fe(1)-C(13)	39.21(11)	C(3)-Fe(2)-C(23)	117.23(14)
C(11)-Fe(1)-C(13)	66.36(12)	C(4)-Fe(2)-C(23)	103.28(15)
C(2)-Fe(1)-C(14)	92.09(14)	C(15)-Fe(2)-C(23)	145.84(13)
C(1)-Fe(1)-C(14)	150.22(14)	C(25)-Fe(2)-C(23)	66.96(12)
C(12)-Fe(1)-C(14)	65.71(12)	C(21)-Fe(2)-C(23)	66.02(12)
C(11)-Fe(1)-C(14)	65.74(12)	C(24)-Fe(2)-C(23)	38.69(11)
C(13)-Fe(1)-C(14)	39.37(11)	C(22)-Fe(2)-C(23)	38.64(11)
C(2)-Fe(1)-C(15)	114.89(14)	C(8)-Si(1)-C(9)	102.01(17)
C(1)-Fe(1)-C(15)	149.52(14)	C(8)-Si(1)-C(25)	105.27(15)
C(12)-Fe(1)-C(15)	66.23(11)	C(9)-Si(1)-C(25)	109.07(15)
C(11)-Fe(1)-C(15)	39.41(10)	C(8)-Si(1)-Fe(1)	117.13(12)
C(13)-Fe(1)-C(15)	66.10(12)	C(9)-Si(1)-Fe(1)	117.95(12)
C(14)-Fe(1)-C(15)	38.94(10)	C(25)-Si(1)-Fe(1)	104.69(10)
C(2)-Fe(1)-Si(1)	88.44(12)	O(1)-C(1)-Fe(1)	178.2(3)
C(1)-Fe(1)-Si(1)	89.91(11)	O(2)-C(2)-Fe(1)	178.1(3)
C(12)-Fe(1)-Si(1)	127.58(10)	O(3)-C(3)-Fe(2)	177.2(3)
C(11)-Fe(1)-Si(1)	91.25(9)	O(4)-C(4)-Fe(2)	179.2(4)
C(13)-Fe(1)-Si(1)	153.23(9)	C(11)-C(5)-C(21)	102.9(2)
C(14)-Fe(1)-Si(1)	119.13(9)	C(11)-C(5)-C(7)	107.7(3)
C(15)-Fe(1)-Si(1)	87.36(8)	C(21)-C(5)-C(7)	111.0(3)
C(3)-Fe(2)-C(4)	94.15(16)	C(11)-C(5)-C(6)	113.2(3)
C(3)-Fe(2)-C(15)	90.59(14)	C(21)-C(5)-C(6)	112.6(3)
C(4)-Fe(2)-C(15)	93.33(14)	C(7)-C(5)-C(6)	109.2(3)
C(3)-Fe(2)-C(25)	106.63(13)	C(12)-C(11)-C(15)	108.4(3)
C(4)-Fe(2)-C(25)	159.21(14)	C(12)-C(11)-C(5)	132.4(3)
C(15)-Fe(2)-C(25)	87.14(12)	C(15)-C(11)-C(5)	118.4(3)
C(3)-Fe(2)-C(21)	145.63(13)	C(12)-C(11)-Fe(1)	69.75(18)
C(4)-Fe(2)-C(21)	119.12(15)	C(15)-C(11)-Fe(1)	72.75(17)
C(15)-Fe(2)-C(21)	79.83(12)	C(5)-C(11)-Fe(1)	131.1(2)
C(25)-Fe(2)-C(21)	40.55(10)	C(13)-C(12)-C(11)	108.3(3)
C(3)-Fe(2)-C(24)	94.61(14)	C(13)-C(12)-Fe(1)	70.73(18)
C(4)-Fe(2)-C(24)	139.28(14)	C(11)-C(12)-Fe(1)	70.40(17)
C(15)-Fe(2)-C(24)	126.23(12)	C(12)-C(13)-C(14)	107.5(3)

C(12)-C(13)-Fe(1)	70.05(18)	C(5)-C(21)-Fe(2)	115.6(2)
C(14)-C(13)-Fe(1)	70.56(17)	C(23)-C(22)-C(21)	109.2(3)
C(13)-C(14)-C(15)	109.9(3)	C(23)-C(22)-Fe(2)	71.48(19)
C(13)-C(14)-Fe(1)	70.07(18)	C(21)-C(22)-Fe(2)	69.13(17)
C(15)-C(14)-Fe(1)	72.75(17)	C(24)-C(23)-C(22)	107.7(3)
C(14)-C(15)-C(11)	105.7(3)	C(24)-C(23)-Fe(2)	69.57(18)
C(14)-C(15)-Fe(2)	137.9(2)	C(22)-C(23)-Fe(2)	69.88(18)
C(11)-C(15)-Fe(2)	116.3(2)	C(23)-C(24)-C(25)	109.5(3)
C(14)-C(15)-Fe(1)	68.31(17)	C(23)-C(24)-Fe(2)	71.73(18)
C(11)-C(15)-Fe(1)	67.85(17)	C(25)-C(24)-Fe(2)	68.97(16)
Fe(2)-C(15)-Fe(1)	126.29(14)	C(24)-C(25)-C(21)	105.4(3)
C(22)-C(21)-C(25)	108.2(3)	C(24)-C(25)-Si(1)	126.1(2)
C(22)-C(21)-C(5)	126.8(3)	C(21)-C(25)-Si(1)	127.2(2)
C(25)-C(21)-C(5)	124.1(3)	C(24)-C(25)-Fe(2)	70.73(17)
C(22)-C(21)-Fe(2)	71.50(18)	C(21)-C(25)-Fe(2)	69.72(17)
C(25)-C(21)-Fe(2)	69.73(16)	Si(1)-C(25)-Fe(2)	113.87(14)

Symmetry transformations used to generate equivalent atoms: No

Table 2.4 Anisotropic displacement coefficients ($Å^2 \times 10^3$) for **5**
The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U11 + \ldots + 2hka^*b^*U12)$

	U11	U22	U33	U23	U13	U12
Fe(1)	34(1)	39(1)	31(1)	0(1)	-3(1)	1(1)
Fe(2)	39(1)	39(1)	28(1)	0(1)	-2(1)	5(1)
Si(1)	45(1)	42(1)	35(1)	-3(1)	-4(1)	-6(1)
C(1)	51(2)	50(2)	46(2)	0(2)	-3(2)	1(2)
O(1)	97(2)	104(2)	33(2)	-3(2)	-9(2)	-1(2)
C(2)	46(3)	55(2)	49(2)	-11(2)	-4(2)	-4(2)
O(2)	37(2)	110(2)	93(2)	-19(2)	2(2)	0(2)
C(3)	57(2)	38(2)	31(2)	-3(2)	-5(2)	3(2)
O(3)	50(2)	82(2)	59(2)	2(1)	14(1)	18(2)
C(4)	55(3)	54(3)	41(2)	4(2)	-4(2)	11(2)
O(4)	91(2)	80(2)	60(2)	-19(2)	-27(2)	-12(2)
C(5)	34(2)	42(2)	44(2)	7(2)	7(2)	4(2)
C(6)	69(3)	73(3)	47(2)	10(2)	24(2)	22(2)
C(7)	37(2)	68(3)	94(3)	19(2)	3(2)	-3(2)
C(8)	50(3)	66(3)	78(3)	10(2)	-2(2)	-17(2)
C(9)	94(3)	47(2)	54(3)	-12(2)	-13(2)	-8(2)
C(11)	31(2)	35(2)	38(2)	2(2)	-1(2)	-4(2)
C(12)	43(2)	43(2)	39(2)	12(2)	-1(2)	-9(2)
C(13)	43(2)	32(2)	48(2)	2(2)	-6(2)	-2(2)
C(14)	38(2)	36(2)	37(2)	-10(2)	-2(2)	1(2)
C(15)	32(2)	31(2)	37(2)	-7(2)	-3(2)	-5(2)
C(21)	35(2)	37(2)	32(2)	-3(2)	5(2)	11(2)
C(22)	37(2)	51(2)	49(2)	-1(2)	-5(2)	11(2)
C(23)	63(3)	39(2)	38(2)	6(2)	0(2)	14(2)
C(24)	55(3)	31(2)	41(2)	3(2)	6(2)	1(2)
C(25)	42(2)	30(2)	30(2)	-3(2)	5(2)	2(2)

#===END

Part III Crystal Data for $(Me_2C)(Me_2Ge)[(\eta^5\text{-}C_5H_3)Fe(CO)]_2(\mu\text{-}CO)_2$ (7) (3 of 3 structures)

Table 3.1 Crystal data and structure refinement for **7**

Empirical formula	C19 H18 Fe2 Ge O4	
Formula weight	494.62	
Measurement instrument	ENRAF-NONIUS CAD-4	
Temperature	298(2) K	
Wavelength	0.71073 Å	
Crystal system, space group	Monoclinic, P2(1)/n	
Unit cell dimensions	a = 9.162(4) Å	alpha = 90 deg.
	b = 15.227(6) Å	beta = 91.098(8) deg.
	c = 12.986(5) Å	gamma = 90 deg.
Volume	1811.4(12) $Å^3$	
Z, Calculated density	4, 1.814 Mg/m^3	
Absorption coefficient	3.250 mm^{-1}	
F(000)	992	
Crystal size	0.30 x 0.20 x 0.15 mm	
Theta range for data collection	2.06 to 25.02 deg.	
Limiting indices	-8<=h<=10, -14<=k<=18, -15<=l<=11	
Reflections collected / unique	6628 / 2925 [R(int) = 0.0560]	
Completeness to theta = 25.02	91.5 %	
Absorption correction	None	
Max. and min. transmission	0.6413 and 0.4422	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2925 / 5 / 244	
Goodness-of-fit on F^2	1.083	
Final R indices [I>2sigma(I)]	R1 = 0.0744, wR2 = 0.1770	
R indices (all data)	R1 = 0.0983, wR2 = 0.1904	
Largest diff. peak and hole	1.480 and -0.946 $eÅ^{-3}$	

Table 3.2 Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **7**

U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Fe(1)	5090(1)	7214(1)	7495(1)	32(1)
Fe(2)	5104(1)	5599(1)	7238(1)	35(1)
Ge(1)	2293(1)	6234(1)	8849(1)	40(1)
O(1)	6269(9)	6208(4)	9239(6)	50(2)
O(2)	6226(9)	6631(5)	5504(6)	58(2)
O(3)	8035(8)	7887(5)	7665(6)	54(2)
O(4)	8013(8)	4902(5)	7178(9)	76(3)
C(1)	5725(10)	6295(5)	8423(8)	38(2)
C(2)	5728(10)	6521(6)	6310(10)	46(3)
C(3)	6887(10)	7636(5)	7612(7)	34(2)
C(4)	6865(10)	5186(6)	7205(9)	45(2)
C(5)	3186(17)	6122(10)	10194(9)	73(4)
C(6)	213(14)	6148(10)	9026(11)	73(4)
C(11)	2928(10)	7246(6)	8085(7)	35(2)
C(12)	3705(11)	7999(7)	8401(10)	54(3)
C(13)	4114(12)	8440(7)	7475(10)	53(3)
C(14)	3591(11)	8023(6)	6652(10)	48(3)
C(15)	2879(10)	7245(6)	6980(8)	39(2)
C(21)	2956(9)	5446(5)	7821(7)	33(2)
C(22)	3795(11)	4603(6)	7897(9)	50(3)
C(23)	4143(12)	4380(7)	6879(11)	62(3)
C(24)	3584(11)	4986(7)	6180(9)	48(3)
C(25)	2843(9)	5654(6)	6747(7)	33(2)
C(7)	2190(5)	6480(3)	6260(3)	78(1)
C(8)	518(10)	6493(10)	6439(11)	41(3)
C(9)	2506(14)	6638(10)	5120(7)	38(3)
Ge(2)	2190(5)	6480(3)	6260(3)	78(1)
C(8')	250(40)	6100(70)	5890(40)	180(40)
C(9')	3110(60)	6560(40)	4950(20)	80(17)
H(5A)	4227	6161	10140	109
H(5B)	2930	5564	10485	109
H(5C)	2845	6585	10630	109
H(6A)	-275	6190	8367	109
H(6B)	-107	6617	9462	109
H(6C)	-15	5594	9338	109
H(12A)	3889	8196	9110	65
H(13A)	4647	8998	7456	63
H(14A)	3696	8213	5936	58
H(22A)	4013	4263	8522	60
H(23A)	4692	3855	6687	74
H(24A)	3672	4961	5430	58

Table 3.3 Bond lengths (Å) and angles (°) for **7**

Fe(1)-C(3)	1.771(9)	Fe(2)-C(22)	2.124(9)
Fe(1)-C(1)	1.929(10)	Fe(2)-C(21)	2.135(9)
Fe(1)-C(2)	1.964(11)	Fe(2)-C(24)	2.150(10)
Fe(1)-C(13)	2.071(10)	Fe(2)-C(25)	2.158(9)
Fe(1)-C(12)	2.117(9)	Ge(1)-C(21)	1.903(9)
Fe(1)-C(15)	2.121(10)	Ge(1)-C(5)	1.923(12)
Fe(1)-C(14)	2.132(10)	Ge(1)-C(11)	1.929(10)
Fe(1)-C(11)	2.138(9)	Ge(1)-C(6)	1.928(13)
Fe(1)-Fe(2)	2.4816(18)	O(1)-C(1)	1.171(12)
Fe(2)-C(4)	1.733(9)	O(2)-C(2)	1.162(13)
Fe(2)-C(2)	1.943(12)	O(3)-C(3)	1.120(11)
Fe(2)-C(1)	1.944(10)	O(4)-C(4)	1.139(12)
Fe(2)-C(23)	2.103(10)	C(11)-C(12)	1.406(13)

C(11)-C(15)	1.435(14)
C(12)-C(13)	1.434(17)
C(13)-C(14)	1.326(17)
C(14)-C(15)	1.422(13)
C(15)-C(7)	1.614(11)
C(21)-C(25)	1.432(13)
C(21)-C(22)	1.498(13)
C(22)-C(23)	1.408(17)
C(23)-C(24)	1.385(17)
C(24)-C(25)	1.433(13)
C(25)-C(7)	1.525(10)
C(7)-C(9)	1.533(9)
C(7)-C(8)	1.554(8)
C(7)-C(9')	1.921(10)
C(7)-C(8')	1.922(10)
C(8)-C(8')	0.95(6)
C(9)-C(9')	0.62(4)

C(3)-Fe(1)-C(1)	86.6(4)
C(3)-Fe(1)-C(2)	88.4(4)
C(1)-Fe(1)-C(2)	90.5(4)
C(3)-Fe(1)-C(13)	94.3(4)
C(1)-Fe(1)-C(13)	141.9(5)
C(2)-Fe(1)-C(13)	127.6(5)
C(3)-Fe(1)-C(12)	108.3(4)
C(1)-Fe(1)-C(12)	103.8(5)
C(2)-Fe(1)-C(12)	158.4(4)
C(13)-Fe(1)-C(12)	40.0(5)
C(3)-Fe(1)-C(15)	154.1(4)
C(1)-Fe(1)-C(15)	119.2(4)
C(2)-Fe(1)-C(15)	93.5(4)
C(13)-Fe(1)-C(15)	64.3(4)
C(12)-Fe(1)-C(15)	65.4(4)
C(3)-Fe(1)-C(14)	115.0(4)
C(1)-Fe(1)-C(14)	157.5(4)
C(2)-Fe(1)-C(14)	96.1(4)
C(13)-Fe(1)-C(14)	36.7(5)
C(12)-Fe(1)-C(14)	64.7(5)
C(15)-Fe(1)-C(14)	39.1(4)
C(3)-Fe(1)-C(11)	145.8(4)
C(1)-Fe(1)-C(11)	93.6(4)
C(2)-Fe(1)-C(11)	125.8(4)
C(13)-Fe(1)-C(11)	65.2(4)
C(12)-Fe(1)-C(11)	38.6(4)
C(15)-Fe(1)-C(11)	39.4(4)
C(14)-Fe(1)-C(11)	65.1(4)
C(3)-Fe(1)-Fe(2)	111.3(3)
C(1)-Fe(1)-Fe(2)	50.4(3)
C(2)-Fe(1)-Fe(2)	50.2(3)
C(13)-Fe(1)-Fe(2)	153.6(3)
C(12)-Fe(1)-Fe(2)	129.7(3)
C(15)-Fe(1)-Fe(2)	89.3(3)
C(14)-Fe(1)-Fe(2)	120.6(3)
C(11)-Fe(1)-Fe(2)	94.5(2)
C(4)-Fe(2)-C(2)	87.8(4)
C(4)-Fe(2)-C(1)	87.6(4)
C(2)-Fe(2)-C(1)	90.7(4)
C(4)-Fe(2)-C(23)	93.5(4)
C(2)-Fe(2)-C(23)	128.8(5)
C(1)-Fe(2)-C(23)	140.5(5)
C(4)-Fe(2)-C(22)	106.5(4)
C(2)-Fe(2)-C(22)	160.2(4)
C(1)-Fe(2)-C(22)	103.2(4)
C(23)-Fe(2)-C(22)	38.9(5)
C(4)-Fe(2)-C(21)	146.5(4)
C(2)-Fe(2)-C(21)	125.7(3)
C(1)-Fe(2)-C(21)	92.1(4)
C(23)-Fe(2)-C(21)	66.3(4)
C(22)-Fe(2)-C(21)	41.2(4)
C(4)-Fe(2)-C(24)	114.8(4)
C(2)-Fe(2)-C(24)	96.4(4)
C(1)-Fe(2)-C(24)	156.7(4)
C(23)-Fe(2)-C(24)	38.0(5)
C(22)-Fe(2)-C(24)	65.4(4)
C(21)-Fe(2)-C(24)	65.7(4)
C(4)-Fe(2)-C(25)	153.6(4)
C(2)-Fe(2)-C(25)	94.7(4)
C(1)-Fe(2)-C(25)	118.5(4)
C(23)-Fe(2)-C(25)	64.7(4)
C(22)-Fe(2)-C(25)	66.4(4)
C(21)-Fe(2)-C(25)	39.0(3)
C(24)-Fe(2)-C(25)	38.9(3)
C(4)-Fe(2)-Fe(1)	111.7(3)
C(2)-Fe(2)-Fe(1)	50.9(3)
C(1)-Fe(2)-Fe(1)	49.9(3)
C(23)-Fe(2)-Fe(1)	154.3(3)
C(22)-Fe(2)-Fe(1)	130.5(3)
C(21)-Fe(2)-Fe(1)	93.0(2)
C(24)-Fe(2)-Fe(1)	120.7(3)
C(25)-Fe(2)-Fe(1)	89.7(2)
C(21)-Ge(1)-C(5)	116.5(5)
C(21)-Ge(1)-C(11)	92.3(4)
C(5)-Ge(1)-C(11)	114.3(5)
C(21)-Ge(1)-C(6)	111.7(5)
C(5)-Ge(1)-C(6)	106.8(6)
C(11)-Ge(1)-C(6)	115.1(5)
O(1)-C(1)-Fe(1)	139.9(7)
O(1)-C(1)-Fe(2)	140.2(7)
Fe(1)-C(1)-Fe(2)	79.7(4)
O(2)-C(2)-Fe(2)	142.0(8)
O(2)-C(2)-Fe(1)	139.1(8)
Fe(2)-C(2)-Fe(1)	78.9(5)
O(3)-C(3)-Fe(1)	178.0(9)
O(4)-C(4)-Fe(2)	178.9(9)
C(12)-C(11)-C(15)	107.4(9)
C(12)-C(11)-Ge(1)	131.1(8)
C(15)-C(11)-Ge(1)	120.7(6)
C(12)-C(11)-Fe(1)	69.9(5)
C(15)-C(11)-Fe(1)	69.7(5)
Ge(1)-C(11)-Fe(1)	117.2(4)
C(11)-C(12)-C(13)	106.0(10)
C(11)-C(12)-Fe(1)	71.5(5)
C(13)-C(12)-Fe(1)	68.2(6)
C(14)-C(13)-C(12)	110.8(10)
C(14)-C(13)-Fe(1)	74.2(6)
C(12)-C(13)-Fe(1)	71.7(6)
C(13)-C(14)-C(15)	108.6(10)
C(13)-C(14)-Fe(1)	69.1(6)
C(15)-C(14)-Fe(1)	70.1(5)
C(14)-C(15)-C(11)	107.0(9)
C(14)-C(15)-C(7)	127.2(9)
C(11)-C(15)-C(7)	125.7(7)

C(14)-C(15)-Fe(1)	70.9(6)	C(24)-C(25)-Fe(2)	70.3(6)
C(11)-C(15)-Fe(1)	70.9(5)	C(7)-C(25)-Fe(2)	121.4(5)
C(7)-C(15)-Fe(1)	121.8(5)	C(25)-C(7)-C(9)	116.7(7)
C(25)-C(21)-C(22)	106.3(8)	C(25)-C(7)-C(8)	109.2(7)
C(25)-C(21)-Ge(1)	121.8(6)	C(9)-C(7)-C(8)	110.3(7)
C(22)-C(21)-Ge(1)	131.6(7)	C(25)-C(7)-C(15)	102.1(5)
C(25)-C(21)-Fe(2)	71.4(5)	C(9)-C(7)-C(15)	111.5(7)
C(22)-C(21)-Fe(2)	69.0(5)	C(8)-C(7)-C(15)	106.3(7)
Ge(1)-C(21)-Fe(2)	119.2(4)	C(25)-C(7)-C(9')	104.0(19)
C(23)-C(22)-C(21)	105.6(9)	C(9)-C(7)-C(9')	16.0(17)
C(23)-C(22)-Fe(2)	69.7(6)	C(8)-C(7)-C(9')	125.7(18)
C(21)-C(22)-Fe(2)	69.8(5)	C(15)-C(7)-C(9')	107.3(18)
C(24)-C(23)-C(22)	111.5(9)	C(25)-C(7)-C(8')	102(3)
C(24)-C(23)-Fe(2)	72.8(6)	C(9)-C(7)-C(8')	89.9(19)
C(22)-C(23)-Fe(2)	71.3(6)	C(8)-C(7)-C(8')	29(2)
C(23)-C(24)-C(25)	108.0(9)	C(15)-C(7)-C(8')	135(3)
C(23)-C(24)-Fe(2)	69.2(6)	C(9')-C(7)-C(8')	102.6(7)
C(25)-C(24)-Fe(2)	70.9(5)	C(8')-C(8)-C(7)	97(3)
C(21)-C(25)-C(24)	108.5(8)	C(9')-C(9)-C(7)	121(4)
C(21)-C(25)-C(7)	127.3(7)	C(8)-C(8')-C(7)	53.4(8)
C(24)-C(25)-C(7)	124.0(8)	C(9)-C(9')-C(7)	43(3)
C(21)-C(25)-Fe(2)	69.7(5)		

Table 3.4 Anisotropic displacement coefficients ($Å^2 \times 10^3$) for **7**
The anisotropic displacement factor exponent takes the form: $-2\pi^2(h^2a^{*2}U11 + \ldots + 2hka^*b^*U12)$

	U11	U22	U33	U23	U13	U12
Fe(1)	23(1)	18(1)	54(1)	-4(1)	4(1)	2(1)
Fe(2)	21(1)	19(1)	64(1)	-7(1)	0(1)	0(1)
Ge(1)	39(1)	45(1)	37(1)	1(1)	4(1)	-2(1)
O(1)	55(4)	42(4)	53(4)	7(3)	-10(4)	-7(3)
O(2)	57(5)	57(5)	61(5)	-15(4)	23(4)	-7(4)
O(3)	30(4)	42(4)	89(6)	-1(4)	-3(3)	-11(3)
O(4)	29(4)	49(5)	150(9)	-8(5)	2(4)	9(3)
C(1)	33(5)	16(4)	63(7)	-2(4)	4(4)	-6(3)
C(2)	18(4)	36(5)	83(8)	-10(5)	1(5)	9(4)
C(3)	30(5)	19(4)	54(6)	3(4)	7(4)	5(3)
C(4)	28(5)	25(4)	81(7)	-14(5)	2(4)	0(4)
C(5)	74(9)	96(10)	49(7)	6(7)	-7(6)	-10(7)
C(6)	44(7)	96(10)	78(9)	3(7)	11(6)	12(6)
C(11)	30(5)	29(4)	46(5)	-16(4)	2(4)	7(4)
C(12)	28(5)	50(6)	84(8)	-32(6)	1(5)	11(4)
C(13)	43(6)	29(5)	87(9)	6(5)	15(6)	6(4)
C(14)	36(5)	31(5)	78(8)	16(5)	8(5)	13(4)
C(15)	29(5)	37(5)	51(6)	15(4)	10(4)	7(4)
C(21)	25(4)	25(4)	49(5)	1(4)	-3(4)	0(3)
C(22)	39(5)	32(5)	79(8)	15(5)	-13(5)	-19(4)
C(23)	36(6)	32(5)	117(11)	-29(6)	8(6)	-8(4)
C(24)	42(6)	47(6)	56(6)	-24(5)	7(5)	3(5)
C(25)	23(4)	39(5)	38(5)	-5(4)	2(3)	-8(4)
C(7)	65(2)	92(3)	77(3)	4(2)	-1(2)	0(2)
C(8)	31(7)	51(8)	40(8)	-3(6)	-3(5)	6(6)
C(9)	17(6)	51(9)	46(8)	17(6)	-6(6)	9(6)
Ge(2)	65(2)	92(3)	77(3)	4(2)	-1(2)	0(2)

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