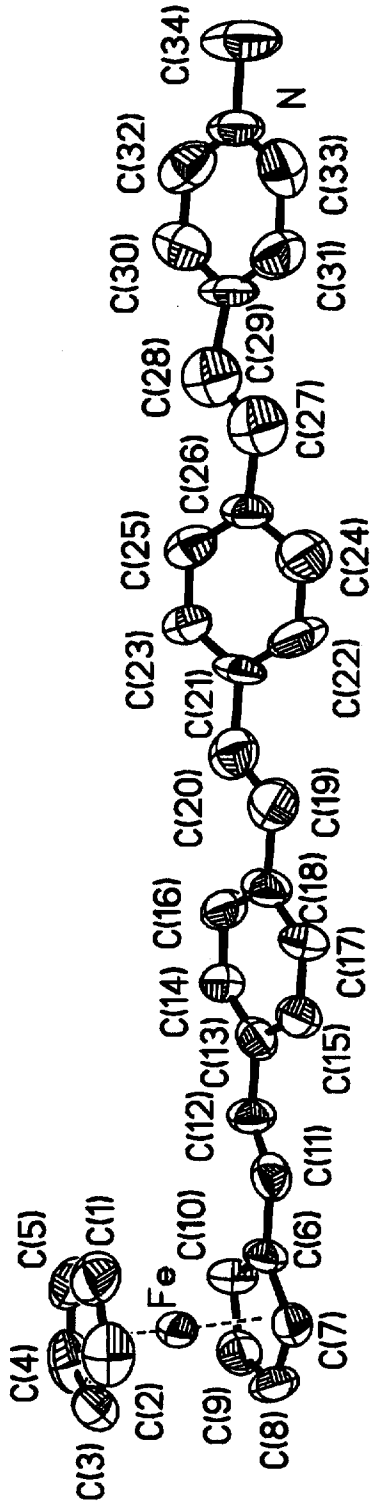
Table 1. Crystal data and structure refinement for **9-(E,E,E)**

Identification code	str62m	
Empirical formula	C34 H30 F6 Fe N P	
Formula weight	653.41	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 14.1378(9) Å	α= 90°.
	b = 17.6844(11) Å	β= 110.748(2)°.
	c = 12.6401(8) Å	γ = 90°.
Volume	2955.3(3) $Å^3$	
Z	4	
Density (calculated)	1.469 Mg/m^3	
Absorption coefficient	0.628 mm^{-1}	
F(000)	1344	
Crystal size	0.062 x 0.016 x 0.014 mm^3	
Theta range for data collection	1.54 to 23.58°.	
Index ranges	-12<=h<=12, -17<=k<=17, -11<=l<=14	
Reflections collected	11043	
Independent reflections	3103 [R(int) = 0.0769]	
Completeness to theta = 23.58°	70.3 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3103 / 0 / 348	
Goodness-of-fit on F^2	1.232	
Final R indices [I>2sigma(I)]	R1 = 0.1035, wR2 = 0.3046	
R indices (all data)	R1 = 0.1573, wR2 = 0.3432	
Largest diff. peak and hole	0.913 and -0.679 $e.Å^{-3}$	


C(34)
N
C(32)
C(33)
C(30)
C(31)
C(29)
C(28)
C(27)
C(26)
C(25)
C(24)
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C(16)
C(18)
C(14)
C(17)
C(13)
C(15)
C(12)
C(11)
C(5)
C(1)
C(10)
C(6)
Fe
C(4)
C(7)
C(2)
C(9)
C(3)
C(8)

9-(E,E,E)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **9-(E,E,E)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe	4123(1)	2859(1)	5461(1)	54(1)
N	9048(10)	5366(10)	-8013(9)	83(4)
P(1)	-82(4)	2676(3)	944(4)	95(2)
C(1)	3450(15)	2410(9)	3863(12)	87(5)
F(1)	-1274(13)	2505(10)	253(14)	205(6)
C(2)	2705(13)	2577(8)	4304(15)	91(5)
F(2)	-55(11)	1852(9)	1341(12)	195(6)
C(3)	2932(13)	2183(8)	5375(13)	85(5)
F(3)	-238(11)	3501(9)	605(12)	196(5)
C(4)	3798(13)	1746(8)	5516(15)	90(5)
F(4)	1006(14)	2797(8)	1551(15)	214(6)
C(5)	4116(13)	1894(10)	4577(16)	91(5)
F(5)	-395(16)	2925(11)	1868(18)	265(9)
C(6)	5103(10)	3694(7)	5380(9)	61(4)
F(6)	140(20)	2490(16)	-130(30)	374(14)
C(7)	4337(10)	4002(7)	5731(10)	64(4)
C(8)	4357(10)	3631(8)	6699(11)	68(4)
C(9)	5149(11)	3110(8)	6972(10)	71(4)
C(10)	5596(10)	3130(8)	6160(10)	64(4)
C(11)	5287(11)	3927(7)	4318(10)	64(4)
C(12)	6029(10)	3677(7)	4027(10)	64(4)
C(13)	6239(10)	3895(7)	3016(10)	63(4)
C(14)	6914(10)	3498(8)	2686(11)	69(4)
C(15)	5776(10)	4519(7)	2352(10)	66(4)
C(16)	7089(11)	3676(8)	1705(12)	77(4)
C(17)	5973(11)	4719(8)	1412(10)	72(4)
C(18)	6615(11)	4315(9)	1068(10)	72(4)
C(19)	6821(11)	4556(9)	12(12)	84(4)
C(20)	7240(11)	4178(9)	-504(12)	84(4)
C(21)	7485(10)	4404(8)	-1550(9)	63(4)
C(22)	7296(12)	5120(9)	-2001(11)	90(5)

C(23)	7859(10)	3885(8)	-2058(11)	72(4)
C(24)	7563(12)	5324(9)	-2942(13)	96(5)
C(25)	8098(9)	4073(9)	-3003(11)	73(4)
C(26)	7943(10)	4781(9)	-3465(9)	66(4)
C(27)	8167(13)	5049(10)	-4477(15)	109(5)
C(28)	8499(14)	4634(10)	-5076(15)	111(5)
C(29)	8671(13)	4977(12)	-6088(10)	84(5)
C(30)	9170(11)	4509(10)	-6560(13)	86(5)
C(31)	8323(13)	5634(10)	-6627(15)	96(5)
C(32)	9383(11)	4711(11)	-7486(14)	88(5)
C(33)	8536(14)	5830(9)	-7621(14)	99(5)
C(34)	9329(13)	5564(12)	-8989(12)	135(8)

Table 3. Bond lengths [Å] and angles [°] for **9-(E,E,E)**.

Fe-C(9)	1.997(13)	C(14)-C(16)	1.383(17)
Fe-C(10)	2.012(13)	C(15)-C(17)	1.361(16)
Fe-C(8)	2.014(12)	C(16)-C(18)	1.411(18)
Fe-C(4)	2.027(14)	C(17)-C(18)	1.343(18)
Fe-C(3)	2.036(14)	C(18)-C(19)	1.525(18)
Fe-C(5)	2.037(14)	C(19)-C(20)	1.223(17)
Fe-C(6)	2.053(11)	C(20)-C(21)	1.535(18)
Fe-C(7)	2.056(12)	C(21)-C(23)	1.332(17)
Fe-C(1)	2.062(14)	C(21)-C(22)	1.375(18)
Fe-C(2)	2.081(15)	C(22)-C(24)	1.416(19)
N-C(33)	1.304(19)	C(23)-C(25)	1.392(17)
N-C(32)	1.337(19)	C(24)-C(26)	1.377(18)
N-C(34)	1.466(17)	C(25)-C(26)	1.366(18)
P(1)-F(5)	1.46(2)	C(26)-C(27)	1.500(19)
P(1)-F(4)	1.471(18)	C(27)-C(28)	1.26(2)
P(1)-F(3)	1.515(16)	C(28)-C(29)	1.51(2)
P(1)-F(6)	1.53(3)	C(29)-C(31)	1.35(2)
P(1)-F(2)	1.537(16)	C(29)-C(30)	1.36(2)
P(1)-F(1)	1.628(18)	C(30)-C(32)	1.355(19)
C(1)-C(2)	1.39(2)	C(31)-C(33)	1.43(2)
C(1)-C(5)	1.39(2)	C(9)-Fe-C(10)	40.4(5)
C(2)-C(3)	1.45(2)	C(9)-Fe-C(8)	40.7(5)
C(3)-C(4)	1.40(2)	C(10)-Fe-C(8)	68.8(5)
C(4)-C(5)	1.44(2)	C(9)-Fe-C(4)	106.2(6)
C(6)-C(10)	1.403(16)	C(10)-Fe-C(4)	115.4(6)
C(6)-C(7)	1.417(16)	C(8)-Fe-C(4)	127.4(7)
C(6)-C(11)	1.512(16)	C(9)-Fe-C(3)	119.2(6)
C(7)-C(8)	1.380(16)	C(10)-Fe-C(3)	150.7(6)
C(8)-C(9)	1.396(17)	C(8)-Fe-C(3)	110.1(6)
C(9)-C(10)	1.383(17)	C(4)-Fe-C(3)	40.5(6)
C(11)-C(12)	1.305(16)	C(9)-Fe-C(5)	124.8(7)
C(12)-C(13)	1.462(16)	C(10)-Fe-C(5)	104.1(6)
C(13)-C(14)	1.365(17)	C(8)-Fe-C(5)	164.0(7)
C(13)-C(15)	1.400(16)	C(4)-Fe-C(5)	41.4(6)

C(3)-Fe-C(5)	68.7(6)	F(4)-P(1)-F(3)	91.6(8)
C(9)-Fe-C(6)	67.3(5)	F(5)-P(1)-F(6)	172.1(15)
C(10)-Fe-C(6)	40.4(5)	F(4)-P(1)-F(6)	89.5(13)
C(8)-Fe-C(6)	67.9(5)	F(3)-P(1)-F(6)	90.7(12)
C(4)-Fe-C(6)	149.9(7)	F(5)-P(1)-F(2)	90.2(10)
C(3)-Fe-C(6)	168.5(7)	F(4)-P(1)-F(2)	93.9(8)
C(5)-Fe-C(6)	116.5(6)	F(3)-P(1)-F(2)	171.8(9)
C(9)-Fe-C(7)	66.9(5)	F(6)-P(1)-F(2)	95.5(12)
C(10)-Fe-C(7)	67.9(5)	F(5)-P(1)-F(1)	86.3(10)
C(8)-Fe-C(7)	39.6(5)	F(4)-P(1)-F(1)	177.4(9)
C(4)-Fe-C(7)	166.2(7)	F(3)-P(1)-F(1)	90.4(8)
C(3)-Fe-C(7)	131.0(6)	F(6)-P(1)-F(1)	88.9(13)
C(5)-Fe-C(7)	152.4(7)	F(2)-P(1)-F(1)	84.3(8)
C(6)-Fe-C(7)	40.3(5)	C(2)-C(1)-C(5)	108.4(14)
C(9)-Fe-C(1)	161.6(7)	C(2)-C(1)-Fe	71.2(9)
C(10)-Fe-C(1)	124.6(7)	C(5)-C(1)-Fe	69.2(8)
C(8)-Fe-C(1)	156.0(7)	C(1)-C(2)-C(3)	108.9(14)
C(4)-Fe-C(1)	68.2(6)	C(1)-C(2)-Fe	69.7(9)
C(3)-Fe-C(1)	68.7(6)	C(3)-C(2)-Fe	67.7(8)
C(5)-Fe-C(1)	39.6(6)	C(4)-C(3)-C(2)	106.1(14)
C(6)-Fe-C(1)	108.2(6)	C(4)-C(3)-Fe	69.4(8)
C(7)-Fe-C(1)	122.1(6)	C(2)-C(3)-Fe	71.0(8)
C(9)-Fe-C(2)	156.7(7)	C(3)-C(4)-C(5)	108.0(13)
C(10)-Fe-C(2)	162.9(7)	C(3)-C(4)-Fe	70.1(8)
C(8)-Fe-C(2)	124.1(7)	C(5)-C(4)-Fe	69.7(8)
C(4)-Fe-C(2)	67.5(6)	C(1)-C(5)-C(4)	108.5(14)
C(3)-Fe-C(2)	41.3(6)	C(1)-C(5)-Fe	71.1(9)
C(5)-Fe-C(2)	66.3(6)	C(4)-C(5)-Fe	68.9(8)
C(6)-Fe-C(2)	129.5(6)	C(10)-C(6)-C(7)	107.3(10)
C(7)-Fe-C(2)	113.6(6)	C(10)-C(6)-C(11)	128.2(12)
C(1)-Fe-C(2)	39.1(6)	C(7)-C(6)-C(11)	124.4(12)
C(33)-N-C(32)	120.2(13)	C(10)-C(6)-Fe	68.2(7)
C(33)-N-C(34)	121.4(17)	C(7)-C(6)-Fe	69.9(7)
C(32)-N-C(34)	118.2(17)	C(11)-C(6)-Fe	124.9(8)
F(5)-P(1)-F(4)	95.5(11)	C(8)-C(7)-C(6)	108.5(12)
F(5)-P(1)-F(3)	83.1(9)	C(8)-C(7)-Fe	68.5(7)

C(6)-C(7)-Fe	69.7(7)	C(20)-C(19)-C(18)	126.3(16)
C(7)-C(8)-C(9)	107.2(12)	C(19)-C(20)-C(21)	128.0(16)
C(7)-C(8)-Fe	71.8(7)	C(23)-C(21)-C(22)	119.1(11)
C(9)-C(8)-Fe	69.0(7)	C(23)-C(21)-C(20)	119.0(13)
C(10)-C(9)-C(8)	109.7(12)	C(22)-C(21)-C(20)	121.9(14)
C(10)-C(9)-Fe	70.4(7)	C(21)-C(22)-C(24)	120.8(14)
C(8)-C(9)-Fe	70.3(8)	C(21)-C(23)-C(25)	120.5(13)
C(9)-C(10)-C(6)	107.2(12)	C(26)-C(24)-C(22)	119.4(14)
C(9)-C(10)-Fe	69.2(7)	C(26)-C(25)-C(23)	122.3(13)
C(6)-C(10)-Fe	71.4(7)	C(25)-C(26)-C(24)	117.7(12)
C(12)-C(11)-C(6)	124.5(12)	C(25)-C(26)-C(27)	127.1(14)
C(11)-C(12)-C(13)	126.0(13)	C(24)-C(26)-C(27)	115.2(14)
C(14)-C(13)-C(15)	116.8(12)	C(28)-C(27)-C(26)	124.5(17)
C(14)-C(13)-C(12)	120.8(13)	C(27)-C(28)-C(29)	118.8(18)
C(15)-C(13)-C(12)	122.4(13)	C(31)-C(29)-C(30)	117.2(13)
C(13)-C(14)-C(16)	121.5(14)	C(31)-C(29)-C(28)	129.3(18)
C(17)-C(15)-C(13)	122.1(13)	C(30)-C(29)-C(28)	113.1(18)
C(14)-C(16)-C(18)	119.7(13)	C(32)-C(30)-C(29)	122.0(16)
C(18)-C(17)-C(15)	121.0(13)	C(29)-C(31)-C(33)	119.9(15)
C(17)-C(18)-C(16)	118.7(12)	N-C(32)-C(30)	120.7(15)
C(17)-C(18)-C(19)	119.7(14)	N-C(33)-C(31)	119.8(16)
C(16)-C(18)-C(19)	121.6(14)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **9-(E,E,E)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe	66(2)	50(1)	55(1)	5(1)	33(1)	0(1)
N	89(10)	118(12)	51(7)	-6(8)	38(7)	-40(9)
P(1)	89(4)	93(3)	109(4)	21(3)	43(3)	17(2)
C(1)	117(15)	84(11)	59(9)	-10(8)	31(10)	-14(10)
C(2)	76(11)	78(10)	101(13)	-3(10)	10(11)	6(9)
C(3)	105(13)	81(11)	82(11)	-14(9)	50(10)	-35(10)
C(4)	90(12)	48(9)	117(14)	12(8)	16(11)	7(9)
C(5)	86(12)	90(12)	106(13)	-45(10)	43(11)	-14(10)
C(6)	73(9)	72(9)	47(8)	-2(7)	34(7)	-20(7)
C(7)	83(10)	51(8)	63(9)	-2(6)	30(8)	-9(7)
C(8)	72(10)	83(10)	62(9)	-9(7)	41(8)	2(8)
C(9)	92(11)	72(9)	49(8)	1(6)	24(8)	-16(9)
C(10)	65(9)	82(9)	57(8)	8(7)	36(7)	1(7)
C(11)	82(10)	48(8)	57(8)	5(6)	18(8)	-6(7)
C(12)	73(10)	82(9)	45(7)	2(6)	32(7)	-7(8)
C(13)	74(10)	63(9)	50(8)	-2(7)	20(7)	-24(7)
C(14)	77(10)	73(9)	71(9)	-10(7)	42(8)	-14(8)
C(15)	73(9)	71(9)	58(8)	-3(7)	27(7)	-16(7)
C(16)	76(10)	92(11)	79(10)	-28(9)	46(9)	-20(9)
C(17)	95(11)	74(9)	61(9)	8(7)	45(9)	-10(8)
C(18)	81(11)	95(11)	42(8)	-1(7)	25(8)	-28(9)
C(19)	81(11)	84(11)	87(11)	-9(8)	31(9)	-2(9)
C(20)	73(11)	95(11)	81(11)	-20(9)	24(9)	-17(9)
C(21)	65(9)	93(11)	38(7)	17(7)	26(7)	-17(8)
C(22)	118(13)	107(13)	65(9)	-3(9)	60(9)	23(10)
C(23)	87(11)	80(10)	60(9)	-3(7)	38(8)	1(8)
C(24)	128(14)	79(11)	87(11)	14(9)	47(11)	19(10)
C(25)	64(9)	94(11)	65(9)	-11(8)	30(8)	3(8)
C(26)	75(10)	88(11)	40(7)	8(7)	27(7)	-9(8)
C(29)	80(12)	141(16)	38(8)	-7(9)	30(8)	-52(11)
C(30)	69(11)	113(13)	66(10)	13(9)	11(9)	-23(9)

C(31)	113(14)	104(13)	96(12)	-26(11)	67(11)	-19(11)
C(32)	61(10)	129(15)	79(11)	-31(11)	33(9)	-15(10)
C(33)	120(15)	77(11)	99(13)	-4(9)	38(12)	-28(10)
C(34)	115(14)	240(20)	63(10)	0(12)	44(10)	-73(15)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **9-(E,E,E)**.

	x	y	z	U(eq)
H(1)	3496	2610	3203	104
H(2)	2150	2889	3969	109
H(3)	2576	2215	5868	102
H(4)	4110	1418	6114	108
H(5)	4674	1681	4464	110
H(7)	3895	4390	5371	77
H(8)	3923	3712	7095	81
H(9)	5347	2796	7605	85
H(10)	6125	2826	6136	77
H(11)	4842	4273	3840	77
H(12)	6464	3327	4507	77
H(14)	7266	3098	3130	83
H(15)	5319	4806	2561	79
H(16)	7516	3377	1467	92
H(17)	5657	5142	1000	86
H(19)	6608	5037	-268	100
H(20)	7434	3693	-227	101
H(22)	6990	5474	-1684	108
H(23)	7961	3394	-1779	87
H(24)	7482	5819	-3205	115
H(25)	8374	3704	-3331	87
H(30)	9372	4035	-6240	103
H(31)	7945	5959	-6355	115
H(32)	9767	4390	-7757	105
H(33)	8309	6288	-7984	118
H(34A)	8856	5926	-9451	203
H(34B)	9319	5118	-9425	203
H(34C)	9997	5778	-8729	203

Table 6. Torsion angles [°] for **9-(E,E,E)**.

C(9)-Fe-C(1)-C(2)	156.3(16)	C(1)-Fe-C(2)-C(3)	121.7(13)
C(10)-Fe-C(1)-C(2)	-172.7(9)	C(1)-C(2)-C(3)-C(4)	-3.4(16)
C(8)-Fe-C(1)-C(2)	-54.7(18)	Fe-C(2)-C(3)-C(4)	-61.0(10)
C(4)-Fe-C(1)-C(2)	80.7(10)	C(1)-C(2)-C(3)-Fe	57.5(11)
C(3)-Fe-C(1)-C(2)	37.1(9)	C(9)-Fe-C(3)-C(4)	-80.6(11)
C(5)-Fe-C(1)-C(2)	119.0(14)	C(10)-Fe-C(3)-C(4)	-42.4(15)
C(6)-Fe-C(1)-C(2)	-131.1(10)	C(8)-Fe-C(3)-C(4)	-124.6(10)
C(7)-Fe-C(1)-C(2)	-88.9(11)	C(5)-Fe-C(3)-C(4)	38.4(9)
C(9)-Fe-C(1)-C(5)	37(2)	C(6)-Fe-C(3)-C(4)	158(2)
C(10)-Fe-C(1)-C(5)	68.2(12)	C(7)-Fe-C(3)-C(4)	-164.4(9)
C(8)-Fe-C(1)-C(5)	-173.8(13)	C(1)-Fe-C(3)-C(4)	81.0(10)
C(4)-Fe-C(1)-C(5)	-38.3(10)	C(2)-Fe-C(3)-C(4)	116.2(13)
C(3)-Fe-C(1)-C(5)	-82.0(10)	C(9)-Fe-C(3)-C(2)	163.2(10)
C(6)-Fe-C(1)-C(5)	109.9(11)	C(10)-Fe-C(3)-C(2)	-158.6(11)
C(7)-Fe-C(1)-C(5)	152.1(10)	C(8)-Fe-C(3)-C(2)	119.2(10)
C(2)-Fe-C(1)-C(5)	-119.0(14)	C(4)-Fe-C(3)-C(2)	-116.2(13)
C(5)-C(1)-C(2)-C(3)	3.2(17)	C(5)-Fe-C(3)-C(2)	-77.8(10)
Fe-C(1)-C(2)-C(3)	-56.3(10)	C(6)-Fe-C(3)-C(2)	41(3)
C(5)-C(1)-C(2)-Fe	59.5(10)	C(7)-Fe-C(3)-C(2)	79.4(11)
C(9)-Fe-C(2)-C(1)	-161.4(13)	C(1)-Fe-C(3)-C(2)	-35.2(9)
C(10)-Fe-C(2)-C(1)	21(2)	C(2)-C(3)-C(4)-C(5)	2.4(16)
C(8)-Fe-C(2)-C(1)	156.4(9)	Fe-C(3)-C(4)-C(5)	-59.6(10)
C(4)-Fe-C(2)-C(1)	-82.7(10)	C(2)-C(3)-C(4)-Fe	62.0(9)
C(3)-Fe-C(2)-C(1)	-121.7(13)	C(9)-Fe-C(4)-C(3)	116.3(10)
C(5)-Fe-C(2)-C(1)	-37.5(9)	C(10)-Fe-C(4)-C(3)	158.5(8)
C(6)-Fe-C(2)-C(1)	68.2(12)	C(8)-Fe-C(4)-C(3)	76.7(11)
C(7)-Fe-C(2)-C(1)	112.3(10)	C(5)-Fe-C(4)-C(3)	-119.0(13)
C(9)-Fe-C(2)-C(3)	-39.7(19)	C(6)-Fe-C(4)-C(3)	-171.2(9)
C(10)-Fe-C(2)-C(3)	142.5(18)	C(7)-Fe-C(4)-C(3)	58(3)
C(8)-Fe-C(2)-C(3)	-81.9(11)	C(1)-Fe-C(4)-C(3)	-82.3(10)
C(4)-Fe-C(2)-C(3)	39.1(9)	C(2)-Fe-C(4)-C(3)	-39.9(9)
C(5)-Fe-C(2)-C(3)	84.2(10)	C(9)-Fe-C(4)-C(5)	-124.7(10)
C(6)-Fe-C(2)-C(3)	-170.1(9)	C(10)-Fe-C(4)-C(5)	-82.5(10)
C(7)-Fe-C(2)-C(3)	-126.0(9)	C(8)-Fe-C(4)-C(5)	-164.3(9)

C(3)-Fe-C(4)-C(5)	119.0(13)	C(10)-Fe-C(6)-C(7)	-119.2(10)
C(6)-Fe-C(4)-C(5)	-52.2(15)	C(8)-Fe-C(6)-C(7)	-36.4(7)
C(7)-Fe-C(4)-C(5)	177(2)	C(4)-Fe-C(6)-C(7)	-163.8(11)
C(1)-Fe-C(4)-C(5)	36.7(9)	C(3)-Fe-C(6)-C(7)	46(3)
C(2)-Fe-C(4)-C(5)	79.1(10)	C(5)-Fe-C(6)-C(7)	160.5(9)
C(2)-C(1)-C(5)-C(4)	-1.7(17)	C(1)-Fe-C(6)-C(7)	118.4(9)
Fe-C(1)-C(5)-C(4)	59.0(10)	C(2)-Fe-C(6)-C(7)	80.3(10)
C(2)-C(1)-C(5)-Fe	-60.7(11)	C(9)-Fe-C(6)-C(11)	160.8(14)
C(3)-C(4)-C(5)-C(1)	-0.5(17)	C(10)-Fe-C(6)-C(11)	122.2(15)
Fe-C(4)-C(5)-C(1)	-60.4(11)	C(8)-Fe-C(6)-C(11)	-155.0(14)
C(3)-C(4)-C(5)-Fe	59.9(10)	C(4)-Fe-C(6)-C(11)	77.6(17)
C(9)-Fe-C(5)-C(1)	-166.6(9)	C(3)-Fe-C(6)-C(11)	-73(3)
C(10)-Fe-C(5)-C(1)	-128.0(10)	C(5)-Fe-C(6)-C(11)	41.9(14)
C(8)-Fe-C(5)-C(1)	170.8(19)	C(7)-Fe-C(6)-C(11)	-118.6(15)
C(4)-Fe-C(5)-C(1)	119.4(14)	C(1)-Fe-C(6)-C(11)	-0.2(14)
C(3)-Fe-C(5)-C(1)	81.9(10)	C(2)-Fe-C(6)-C(11)	-38.3(15)
C(6)-Fe-C(5)-C(1)	-86.9(11)	C(10)-C(6)-C(7)-C(8)	-0.5(14)
C(7)-Fe-C(5)-C(1)	-59.0(16)	C(11)-C(6)-C(7)-C(8)	176.9(10)
C(2)-Fe-C(5)-C(1)	37.1(10)	Fe-C(6)-C(7)-C(8)	57.7(9)
C(9)-Fe-C(5)-C(4)	74.0(11)	C(10)-C(6)-C(7)-Fe	-58.1(8)
C(10)-Fe-C(5)-C(4)	112.5(10)	C(11)-C(6)-C(7)-Fe	119.2(11)
C(8)-Fe-C(5)-C(4)	51(2)	C(9)-Fe-C(7)-C(8)	-39.0(8)
C(3)-Fe-C(5)-C(4)	-37.5(9)	C(10)-Fe-C(7)-C(8)	-82.9(8)
C(6)-Fe-C(5)-C(4)	153.7(9)	C(4)-Fe-C(7)-C(8)	24(3)
C(7)-Fe-C(5)-C(4)	-178.4(11)	C(3)-Fe-C(7)-C(8)	70.4(11)
C(1)-Fe-C(5)-C(4)	-119.4(14)	C(5)-Fe-C(7)-C(8)	-160.8(13)
C(2)-Fe-C(5)-C(4)	-82.4(10)	C(6)-Fe-C(7)-C(8)	-120.5(11)
C(9)-Fe-C(6)-C(10)	38.5(8)	C(1)-Fe-C(7)-C(8)	159.1(9)
C(8)-Fe-C(6)-C(10)	82.8(8)	C(2)-Fe-C(7)-C(8)	115.5(10)
C(4)-Fe-C(6)-C(10)	-44.6(14)	C(9)-Fe-C(7)-C(6)	81.5(8)
C(3)-Fe-C(6)-C(10)	165(2)	C(10)-Fe-C(7)-C(6)	37.6(7)
C(5)-Fe-C(6)-C(10)	-80.3(10)	C(8)-Fe-C(7)-C(6)	120.5(11)
C(7)-Fe-C(6)-C(10)	119.2(10)	C(4)-Fe-C(7)-C(6)	144(2)
C(1)-Fe-C(6)-C(10)	-122.4(9)	C(3)-Fe-C(7)-C(6)	-169.0(8)
C(2)-Fe-C(6)-C(10)	-160.5(9)	C(5)-Fe-C(7)-C(6)	-40.2(16)
C(9)-Fe-C(6)-C(7)	-80.6(8)	C(1)-Fe-C(7)-C(6)	-80.4(10)

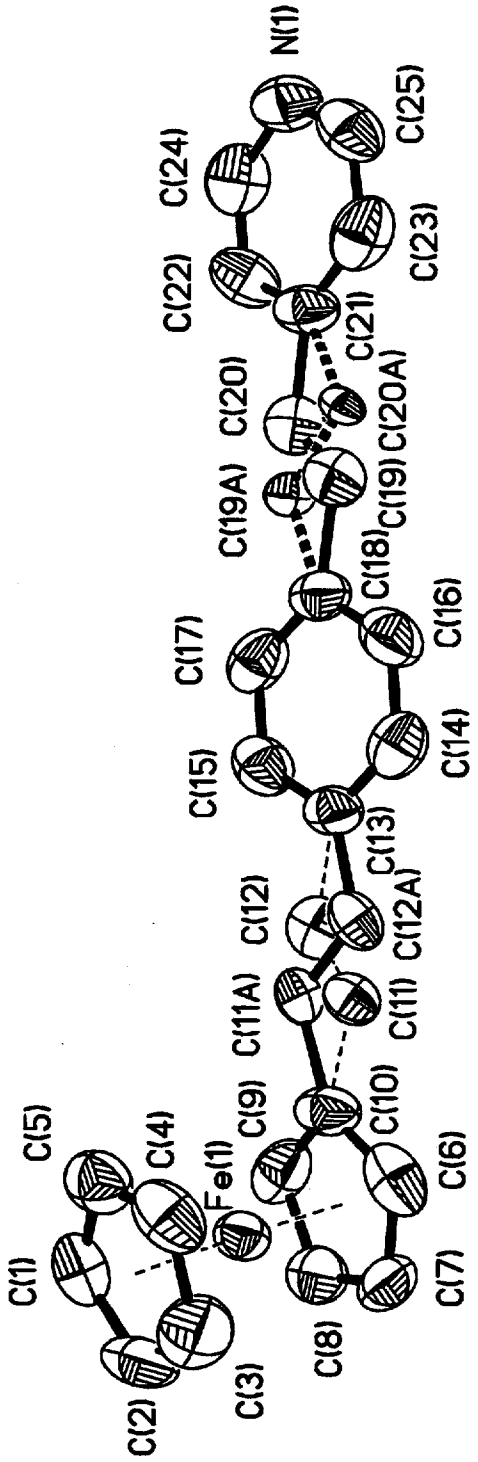
C(2)-Fe-C(7)-C(6)	-123.9(9)	C(7)-Fe-C(9)-C(8)	38.0(8)
C(6)-C(7)-C(8)-C(9)	1.8(14)	C(1)-Fe-C(9)-C(8)	161.3(16)
Fe-C(7)-C(8)-C(9)	60.2(9)	C(2)-Fe-C(9)-C(8)	-58.5(17)
C(6)-C(7)-C(8)-Fe	-58.4(8)	C(8)-C(9)-C(10)-C(6)	2.2(14)
C(9)-Fe-C(8)-C(7)	117.4(11)	Fe-C(9)-C(10)-C(6)	61.7(9)
C(10)-Fe-C(8)-C(7)	80.6(8)	C(8)-C(9)-C(10)-Fe	-59.4(9)
C(4)-Fe-C(8)-C(7)	-173.1(9)	C(7)-C(6)-C(10)-C(9)	-1.1(14)
C(3)-Fe-C(8)-C(7)	-130.8(9)	C(11)-C(6)-C(10)-C(9)	-178.3(11)
C(5)-Fe-C(8)-C(7)	146(2)	Fe-C(6)-C(10)-C(9)	-60.3(9)
C(6)-Fe-C(8)-C(7)	37.0(8)	C(7)-C(6)-C(10)-Fe	59.2(8)
C(1)-Fe-C(8)-C(7)	-48.2(18)	C(11)-C(6)-C(10)-Fe	-118.0(12)
C(2)-Fe-C(8)-C(7)	-86.7(10)	C(8)-Fe-C(10)-C(9)	37.1(8)
C(10)-Fe-C(8)-C(9)	-36.8(7)	C(4)-Fe-C(10)-C(9)	-85.4(10)
C(4)-Fe-C(8)-C(9)	69.5(11)	C(3)-Fe-C(10)-C(9)	-56.4(15)
C(3)-Fe-C(8)-C(9)	111.8(9)	C(5)-Fe-C(10)-C(9)	-127.9(10)
C(5)-Fe-C(8)-C(9)	29(2)	C(6)-Fe-C(10)-C(9)	117.5(11)
C(6)-Fe-C(8)-C(9)	-80.4(8)	C(7)-Fe-C(10)-C(9)	79.9(8)
C(7)-Fe-C(8)-C(9)	-117.4(11)	C(1)-Fe-C(10)-C(9)	-165.5(9)
C(1)-Fe-C(8)-C(9)	-165.6(14)	C(2)-Fe-C(10)-C(9)	178.7(17)
C(2)-Fe-C(8)-C(9)	155.9(9)	C(9)-Fe-C(10)-C(6)	-117.5(11)
C(7)-C(8)-C(9)-C(10)	-2.5(15)	C(8)-Fe-C(10)-C(6)	-80.4(8)
Fe-C(8)-C(9)-C(10)	59.5(9)	C(4)-Fe-C(10)-C(6)	157.1(9)
C(7)-C(8)-C(9)-Fe	-62.0(9)	C(3)-Fe-C(10)-C(6)	-173.9(10)
C(8)-Fe-C(9)-C(10)	-120.5(11)	C(5)-Fe-C(10)-C(6)	114.6(9)
C(4)-Fe-C(9)-C(10)	110.3(10)	C(7)-Fe-C(10)-C(6)	-37.6(7)
C(3)-Fe-C(9)-C(10)	152.1(9)	C(1)-Fe-C(10)-C(6)	77.0(10)
C(5)-Fe-C(9)-C(10)	68.8(10)	C(2)-Fe-C(10)-C(6)	61(2)
C(6)-Fe-C(9)-C(10)	-38.5(7)	C(10)-C(6)-C(11)-C(12)	-7(2)
C(7)-Fe-C(9)-C(10)	-82.5(8)	C(7)-C(6)-C(11)-C(12)	175.8(12)
C(1)-Fe-C(9)-C(10)	41(2)	Fe-C(6)-C(11)-C(12)	-95.9(15)
C(2)-Fe-C(9)-C(10)	-179.0(13)	C(6)-C(11)-C(12)-C(13)	-179.2(11)
C(10)-Fe-C(9)-C(8)	120.5(11)	C(11)-C(12)-C(13)-C(14)	-167.7(13)
C(4)-Fe-C(9)-C(8)	-129.2(9)	C(11)-C(12)-C(13)-C(15)	13(2)
C(3)-Fe-C(9)-C(8)	-87.4(10)	C(15)-C(13)-C(14)-C(16)	-3.7(18)
C(5)-Fe-C(9)-C(8)	-170.6(9)	C(12)-C(13)-C(14)-C(16)	177.1(11)
C(6)-Fe-C(9)-C(8)	82.0(8)	C(14)-C(13)-C(15)-C(17)	0.9(18)

C(12)-C(13)-C(15)-C(17)	-179.9(11)	C(23)-C(25)-C(26)-C(27)	-179.9(13)
C(13)-C(14)-C(16)-C(18)	4.5(19)	C(22)-C(24)-C(26)-C(25)	-4(2)
C(13)-C(15)-C(17)-C(18)	1(2)	C(22)-C(24)-C(26)-C(27)	178.0(14)
C(15)-C(17)-C(18)-C(16)	0(2)	C(25)-C(26)-C(27)-C(28)	3(3)
C(15)-C(17)-C(18)-C(19)	-179.9(11)	C(24)-C(26)-C(27)-C(28)	-178.6(18)
C(14)-C(16)-C(18)-C(17)	-2.5(19)	C(26)-C(27)-C(28)-C(29)	178.7(13)
C(14)-C(16)-C(18)-C(19)	177.1(11)	C(27)-C(28)-C(29)-C(31)	-16(3)
C(17)-C(18)-C(19)-C(20)	-166.4(15)	C(27)-C(28)-C(29)-C(30)	170.6(17)
C(16)-C(18)-C(19)-C(20)	14(2)	C(31)-C(29)-C(30)-C(32)	5(2)
C(18)-C(19)-C(20)-C(21)	-178.4(11)	C(28)-C(29)-C(30)-C(32)	179.1(13)
C(19)-C(20)-C(21)-C(23)	-173.6(15)	C(30)-C(29)-C(31)-C(33)	-3(2)
C(19)-C(20)-C(21)-C(22)	4(2)	C(28)-C(29)-C(31)-C(33)	-176.5(14)
C(23)-C(21)-C(22)-C(24)	-5(2)	C(33)-N-C(32)-C(30)	2(2)
C(20)-C(21)-C(22)-C(24)	177.7(13)	C(34)-N-C(32)-C(30)	178.2(12)
C(22)-C(21)-C(23)-C(25)	3(2)	C(29)-C(30)-C(32)-N	-4(2)
C(20)-C(21)-C(23)-C(25)	-179.4(11)	C(32)-N-C(33)-C(31)	-1(2)
C(21)-C(22)-C(24)-C(26)	5(2)	C(34)-N-C(33)-C(31)	-176.6(13)
C(21)-C(23)-C(25)-C(26)	-2(2)	C(29)-C(31)-C(33)-N	1(2)
C(23)-C(25)-C(26)-C(24)	2(2)		

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data and structure refinement for **5-(E,E)**.

Identification code	str55m	
Empirical formula	C25 H21 Fe N	
Formula weight	391.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 6.2814(4) Å	α= 90°.
	b = 7.7253(6) Å	β= 95.394(2)°.
	c = 19.3917(14) Å	γ = 90°.
Volume	936.83(12) $Å^3$	
Z	2	
Density (calculated)	1.387 Mg/m^3	
Absorption coefficient	0.813 mm^{-1}	
F(000)	408	
Crystal size	0.41 x 0.18 x 0.02 mm^3	
Theta range for data collection	1.05 to 23.81°.	
Index ranges	-7<=h<=5, -8<=k<=8, -22<=l<=22	
Reflections collected	4833	
Independent reflections	2602 [R(int) = 0.0346]	
Completeness to theta = 23.81°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2602 / 1 / 282	
Goodness-of-fit on F^2	0.974	
Final R indices [I>2sigma(I)]	R1 = 0.0411, wR2 = 0.0896	
R indices (all data)	R1 = 0.0593, wR2 = 0.1103	
Absolute structure parameter	-0.03(4)	
Largest diff. peak and hole	0.217 and -0.293 e.$Å^{-3}$	


N(1)
C(25)
C(24)
C(23)
C(22)
C(21)
C(20)
C(20A)
C(19)
C(19A)
C(18)
C(16)
C(17)
C(14)
C(15)
C(13)
C(12A)
C(12)
C(11)
C(11A)
C(10)
C(9)
C(6)
C(5)
C(4)
Fe(1)
C(1)
C(7)
C(8)
C(3)
C(2)

5-(E,E)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5-(E,E)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	7504(1)	8363(2)	8887(1)	48(1)
C(1)	9901(11)	7632(8)	9605(3)	66(2)
N(1)	17849(10)	9445(7)	2351(3)	72(2)
C(2)	7906(13)	7288(10)	9837(3)	75(2)
C(3)	6881(13)	6135(11)	9366(5)	86(3)
C(4)	8232(16)	5791(10)	8843(4)	71(2)
C(5)	10065(11)	6711(8)	8997(3)	67(2)
C(6)	5423(12)	9127(8)	8073(3)	71(2)
C(7)	4774(10)	9758(8)	8704(3)	65(2)
C(8)	6371(12)	10803(9)	9008(4)	64(2)
C(9)	8027(12)	10822(9)	8564(4)	67(2)
C(10)	7447(11)	9805(8)	7988(3)	64(2)
C(11)	9085(19)	9871(14)	7460(8)	47(4)
C(12)	8570(20)	9363(17)	6812(10)	53(4)
C(11A)	7850(40)	9120(30)	7246(13)	46(8)
C(12A)	9400(50)	9930(30)	7013(12)	38(6)
C(13)	10056(10)	9493(7)	6282(3)	54(2)
C(14)	9224(9)	8737(9)	5676(3)	64(2)
C(15)	12097(11)	10211(9)	6295(3)	67(2)
C(16)	10317(11)	8655(11)	5101(3)	69(2)
C(17)	13200(10)	10157(8)	5710(4)	68(2)
C(18)	12330(11)	9400(8)	5106(3)	62(2)
C(19A)	14050(30)	9770(30)	4631(13)	37(6)
C(20A)	13650(40)	9220(20)	3944(12)	35(6)
C(19)	13070(30)	9120(18)	4385(10)	57(5)
C(20)	14670(30)	9871(18)	4206(11)	60(5)
C(21)	15454(11)	9592(8)	3493(3)	61(2)
C(22)	17377(12)	10378(9)	3488(3)	74(2)
C(23)	14727(10)	8722(10)	2902(4)	76(2)
C(24)	18495(11)	10284(9)	2927(4)	77(2)
C(25)	15950(12)	8700(10)	2344(3)	73(2)

Table 3. Bond lengths [Å] and angles [°] for **5-(E,E)**.

Fe(1)-C(3)	2.012(7)
Fe(1)-C(2)	2.014(6)
Fe(1)-C(7)	2.028(6)
Fe(1)-C(1)	2.032(6)
Fe(1)-C(8)	2.036(7)
Fe(1)-C(9)	2.036(7)
Fe(1)-C(6)	2.040(6)
Fe(1)-C(4)	2.043(8)
Fe(1)-C(5)	2.049(7)
Fe(1)-C(10)	2.066(5)
C(1)-C(5)	1.390(8)
C(1)-C(2)	1.396(9)
N(1)-C(24)	1.322(8)
N(1)-C(25)	1.323(8)
C(2)-C(3)	1.390(10)
C(3)-C(4)	1.407(11)
C(4)-C(5)	1.362(11)
C(6)-C(10)	1.399(9)
C(6)-C(7)	1.412(8)
C(7)-C(8)	1.376(9)
C(8)-C(9)	1.410(11)
C(9)-C(10)	1.386(10)
C(10)-C(11)	1.520(15)
C(10)-C(11A)	1.58(2)
C(11)-C(12)	1.33(3)
C(12)-C(13)	1.456(18)
C(11A)-C(12A)	1.28(6)
C(12A)-C(13)	1.55(2)
C(13)-C(14)	1.371(8)
C(13)-C(15)	1.395(9)
C(14)-C(16)	1.366(8)
C(15)-C(17)	1.385(9)
C(16)-C(18)	1.388(9)
C(17)-C(18)	1.375(9)
C(18)-C(19A)	1.51(2)
C(18)-C(19)	1.531(19)
C(19A)-C(20A)	1.40(5)
C(20A)-C(21)	1.52(2)
C(19)-C(20)	1.24(3)
C(20)-C(21)	1.53(2)
C(21)-C(22)	1.353(9)
C(21)-C(23)	1.370(9)
C(22)-C(24)	1.351(9)
C(23)-C(25)	1.385(9)
C(3)-Fe(1)-C(2)	40.4(3)
C(3)-Fe(1)-C(7)	109.7(3)
C(2)-Fe(1)-C(7)	114.2(3)
C(3)-Fe(1)-C(1)	67.0(3)
C(2)-Fe(1)-C(1)	40.4(3)
C(7)-Fe(1)-C(1)	145.8(3)
C(3)-Fe(1)-C(8)	130.9(3)
C(2)-Fe(1)-C(8)	107.0(3)
C(7)-Fe(1)-C(8)	39.6(3)

C(1)-Fe(1)-C(8)	115.0(3)
C(3)-Fe(1)-C(9)	169.8(4)
C(2)-Fe(1)-C(9)	131.0(3)
C(7)-Fe(1)-C(9)	67.0(3)
C(1)-Fe(1)-C(9)	109.8(3)
C(8)-Fe(1)-C(9)	40.5(3)
C(3)-Fe(1)-C(6)	117.8(3)
C(2)-Fe(1)-C(6)	147.5(3)
C(7)-Fe(1)-C(6)	40.6(2)
C(1)-Fe(1)-C(6)	171.9(3)
C(8)-Fe(1)-C(6)	67.4(3)
C(9)-Fe(1)-C(6)	66.6(3)
C(3)-Fe(1)-C(4)	40.6(3)
C(2)-Fe(1)-C(4)	68.1(3)
C(7)-Fe(1)-C(4)	134.3(4)
C(1)-Fe(1)-C(4)	66.7(3)
C(8)-Fe(1)-C(4)	170.9(4)
C(9)-Fe(1)-C(4)	148.4(3)
C(6)-Fe(1)-C(4)	112.3(3)
C(3)-Fe(1)-C(5)	66.7(3)
C(2)-Fe(1)-C(5)	67.6(3)
C(7)-Fe(1)-C(5)	172.7(3)
C(1)-Fe(1)-C(5)	39.8(2)
C(8)-Fe(1)-C(5)	147.6(3)
C(9)-Fe(1)-C(5)	117.7(3)
C(6)-Fe(1)-C(5)	134.4(3)
C(4)-Fe(1)-C(5)	38.9(3)
C(3)-Fe(1)-C(10)	149.5(3)
C(2)-Fe(1)-C(10)	169.8(3)
C(7)-Fe(1)-C(10)	67.6(2)
C(1)-Fe(1)-C(10)	132.9(3)
C(8)-Fe(1)-C(10)	67.6(3)
C(9)-Fe(1)-C(10)	39.5(3)
C(6)-Fe(1)-C(10)	39.8(3)
C(4)-Fe(1)-C(10)	118.4(3)
C(5)-Fe(1)-C(10)	112.0(2)
C(5)-C(1)-C(2)	108.4(6)
C(5)-C(1)-Fe(1)	70.7(4)
C(2)-C(1)-Fe(1)	69.1(4)
C(24)-N(1)-C(25)	115.3(5)
C(3)-C(2)-C(1)	106.6(6)
C(3)-C(2)-Fe(1)	69.7(4)
C(1)-C(2)-Fe(1)	70.5(3)
C(2)-C(3)-C(4)	108.7(8)
C(2)-C(3)-Fe(1)	69.9(4)
C(4)-C(3)-Fe(1)	70.9(4)
C(5)-C(4)-C(3)	107.4(7)
C(5)-C(4)-Fe(1)	70.8(4)
C(3)-C(4)-Fe(1)	68.5(4)
C(4)-C(5)-C(1)	108.9(6)
C(4)-C(5)-Fe(1)	70.3(5)
C(1)-C(5)-Fe(1)	69.4(4)
C(10)-C(6)-C(7)	108.2(6)
C(10)-C(6)-Fe(1)	71.1(4)
C(7)-C(6)-Fe(1)	69.2(3)
C(8)-C(7)-C(6)	108.3(6)

C(8)-C(7)-Fe(1)	70.5(4)
C(6)-C(7)-Fe(1)	70.1(3)
C(7)-C(8)-C(9)	107.2(6)
C(7)-C(8)-Fe(1)	69.9(4)
C(9)-C(8)-Fe(1)	69.8(4)
C(10)-C(9)-C(8)	109.4(7)
C(10)-C(9)-Fe(1)	71.4(4)
C(8)-C(9)-Fe(1)	69.7(4)
C(9)-C(10)-C(6)	106.9(5)
C(9)-C(10)-C(11)	112.4(8)
C(6)-C(10)-C(11)	140.6(9)
C(9)-C(10)-C(11A)	150.9(13)
C(6)-C(10)-C(11A)	102.0(13)
C(11)-C(10)-C(11A)	38.6(8)
C(9)-C(10)-Fe(1)	69.1(4)
C(6)-C(10)-Fe(1)	69.1(3)
C(11)-C(10)-Fe(1)	128.9(5)
C(11A)-C(10)-Fe(1)	126.6(8)
C(12)-C(11)-C(10)	120.5(13)
C(11)-C(12)-C(13)	122.1(15)
C(12A)-C(11A)-C(10)	111(3)
C(11A)-C(12A)-C(13)	120(3)
C(14)-C(13)-C(15)	117.4(5)
C(14)-C(13)-C(12)	110.9(9)
C(15)-C(13)-C(12)	131.6(9)
C(14)-C(13)-C(12A)	139.7(13)
C(15)-C(13)-C(12A)	102.8(13)
C(12)-C(13)-C(12A)	29.0(8)
C(16)-C(14)-C(13)	122.6(6)
C(17)-C(15)-C(13)	120.2(6)
C(14)-C(16)-C(18)	120.2(6)
C(18)-C(17)-C(15)	121.4(6)
C(17)-C(18)-C(16)	118.1(5)
C(17)-C(18)-C(19A)	101.0(12)
C(16)-C(18)-C(19A)	140.8(12)
C(17)-C(18)-C(19)	135.0(10)
C(16)-C(18)-C(19)	106.9(10)
C(19A)-C(18)-C(19)	34.1(6)
C(20A)-C(19A)-C(18)	117(2)
C(19A)-C(20A)-C(21)	114(2)
C(20)-C(19)-C(18)	121(2)
C(19)-C(20)-C(21)	122(2)
C(22)-C(21)-C(23)	116.2(5)
C(22)-C(21)-C(20A)	143.4(11)
C(23)-C(21)-C(20A)	100.4(11)
C(22)-C(21)-C(20)	108.0(10)
C(23)-C(21)-C(20)	135.8(10)
C(20A)-C(21)-C(20)	35.4(6)
C(24)-C(22)-C(21)	120.9(6)
C(21)-C(23)-C(25)	119.6(6)
N(1)-C(24)-C(22)	124.4(6)
N(1)-C(25)-C(23)	123.5(6)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5-(E,E)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

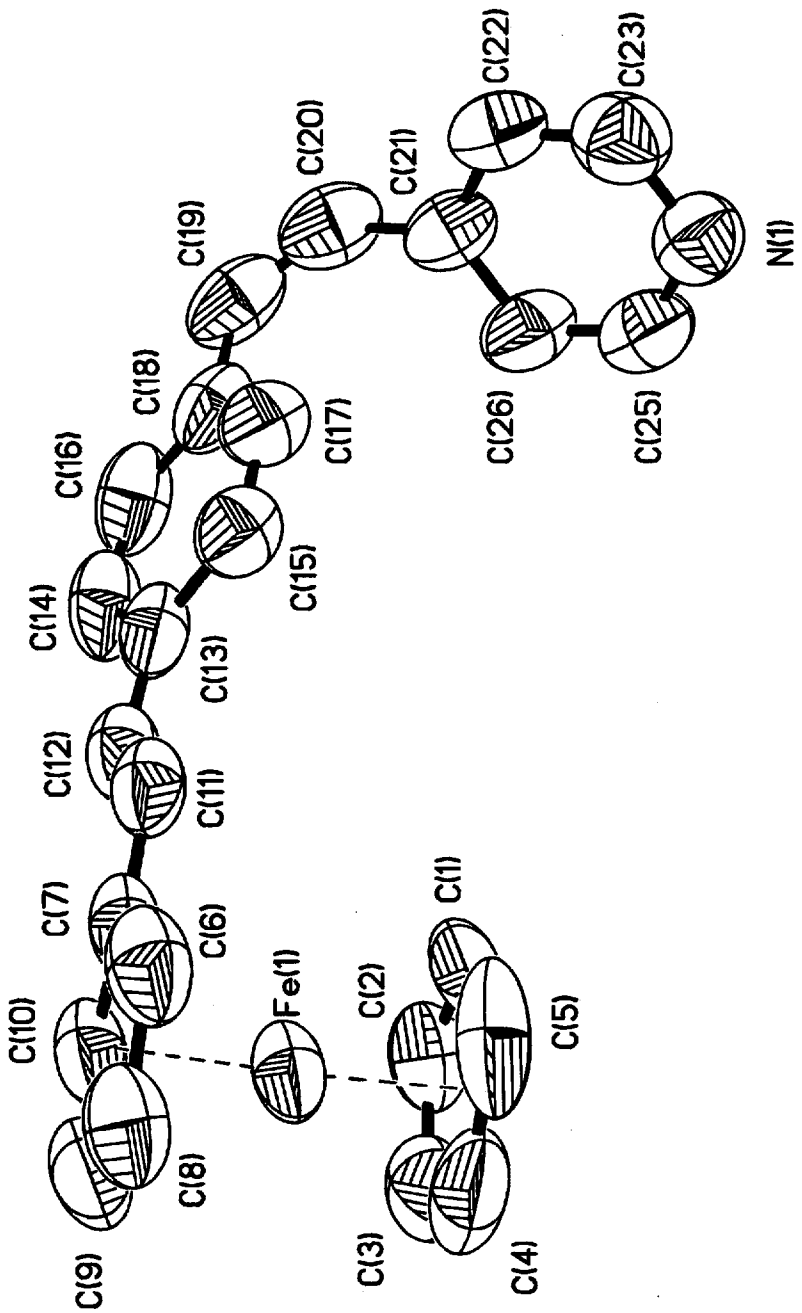
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	52(1)	50(1)	42(1)	7(1)	11(1)	1(1)
C(1)	71(4)	61(4)	61(4)	8(3)	-14(3)	2(3)
N(1)	82(4)	73(4)	65(4)	9(3)	31(3)	-4(3)
C(2)	104(6)	76(5)	48(4)	14(3)	28(4)	13(4)
C(3)	74(5)	77(6)	108(7)	38(5)	20(5)	-6(4)
C(4)	103(6)	50(4)	57(5)	4(3)	-3(4)	1(4)
C(5)	80(5)	60(4)	61(4)	12(3)	11(3)	7(4)
C(6)	91(5)	61(4)	56(4)	-3(3)	-14(4)	6(3)
C(7)	45(4)	75(5)	77(4)	18(4)	20(3)	6(3)
C(8)	72(5)	58(4)	62(4)	7(3)	14(4)	17(4)
C(9)	51(4)	55(5)	97(6)	24(5)	19(4)	3(3)
C(10)	83(5)	59(4)	54(4)	18(3)	28(4)	27(4)
C(11)	51(6)	45(6)	44(10)	6(5)	-4(5)	3(5)
C(12)	63(8)	53(7)	40(10)	-10(6)	-8(7)	-7(5)
C(11A)	59(15)	39(10)	39(13)	-8(8)	3(10)	-2(9)
C(12A)	66(15)	47(13)	1(11)	-6(8)	-4(9)	4(10)
C(13)	67(4)	49(3)	49(3)	12(3)	18(3)	14(3)
C(14)	53(3)	57(6)	81(4)	2(3)	8(3)	-2(3)
C(15)	80(5)	66(4)	54(4)	-9(3)	0(3)	2(4)
C(16)	85(4)	72(6)	48(3)	-8(4)	0(3)	11(4)
C(17)	53(4)	65(4)	89(5)	14(4)	18(4)	-2(3)
C(18)	73(5)	63(4)	54(4)	14(3)	22(3)	23(3)
C(19A)	36(10)	38(9)	38(13)	-6(8)	9(8)	-15(7)
C(20A)	40(10)	43(9)	23(12)	-8(7)	2(8)	-1(7)
C(19)	72(10)	40(6)	58(10)	-4(5)	7(8)	0(6)
C(20)	66(10)	50(7)	65(11)	-3(7)	6(9)	-3(7)
C(21)	89(5)	48(4)	48(4)	12(3)	26(3)	19(3)
C(22)	99(6)	66(5)	57(4)	-10(3)	2(4)	-17(4)
C(23)	54(4)	74(6)	101(5)	20(5)	17(3)	-8(4)
C(24)	62(4)	72(5)	96(6)	2(4)	7(4)	-23(3)
C(25)	96(5)	62(6)	58(3)	-13(4)	-5(3)	-6(4)

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

	x	y	z	U(eq)
H(1)	10944	8355	9821	79
H(2)	7368	7742	10229	90
H(3)	5526	5668	9392	103
H(4)	7929	5069	8463	85
H(5)	11236	6720	8737	80
H(6)	4640	8389	7767	85
H(7)	3486	9510	8884	78
H(8)	6361	11387	9427	76
H(9)	9309	11423	8646	80
H(11)	10460	10271	7591	57
H(12)	7212	8909	6693	63
H(11A)	7074	8236	7012	55
H(12A)	10125	10783	7279	46
H(14)	7860	8261	5656	77
H(15)	12718	10728	6698	81
H(16)	9712	8099	4705	82
H(17)	14558	10644	5725	82
H(19A)	15307	10332	4787	45
H(20A)	12391	8669	3776	42
H(19)	12312	8372	4077	68
H(20)	15410	10629	4514	72
H(22)	17938	10992	3876	89
H(23)	13419	8150	2875	91
H(24)	19808	10848	2947	92
H(25)	15408	8130	1943	88

Table 1. Crystal data and structure refinement for **5-(E,Z)**.

Identification code	str53m	
Empirical formula	C25 H21 Fe N	
Formula weight	391.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 17.7672(18) Å	α= 90°.
	b = 10.0114(9) Å	β= 106.027(2)°.
	c = 11.3680(11) Å	γ = 90°.
Volume	1943.5(3) $Å^3$	
Z	4	
Density (calculated)	1.337 Mg/m^3	
Absorption coefficient	0.784 mm^{-1}	
F(000)	816	
Crystal size	0.12 x 0.04 x 0.015 mm^3	
Theta range for data collection	1.19 to 20.81°.	
Index ranges	-17<=h<=17, -10<=k<=10, -7<=l<=11	
Reflections collected	7085	
Independent reflections	2025 [R(int) = 0.0329]	
Completeness to theta = 20.81°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2025 / 0 / 244	
Goodness-of-fit on F^2	1.023	
Final R indices [I>2sigma(I)]	R1 = 0.0318, wR2 = 0.0835	
R indices (all data)	R1 = 0.0546, wR2 = 0.1071	
Largest diff. peak and hole	0.163 and -0.210 $e.Å^{-3}$	



5-(E,Z)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **5-(E,Z)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3882(1)	371(1)	6384(1)	74(1)
C(1)	3056(4)	1718(6)	6504(5)	99(2)
N(1)	827(2)	4307(4)	11420(5)	94(1)
C(2)	2742(3)	860(5)	5628(7)	95(2)
C(3)	3124(5)	889(6)	4768(6)	108(2)
C(4)	3728(4)	1817(8)	5108(9)	124(2)
C(5)	3690(4)	2350(5)	6268(8)	118(2)
C(6)	4121(3)	-777(4)	7926(4)	77(1)
C(7)	4775(3)	49(5)	7910(5)	90(2)
C(8)	5015(3)	-261(5)	6852(6)	97(2)
C(9)	4515(3)	-1279(5)	6207(5)	97(2)
C(10)	3973(3)	-1595(4)	6863(4)	85(1)
C(11)	3666(3)	-679(4)	8796(4)	78(1)
C(12)	3082(3)	-1460(4)	8884(4)	83(1)
C(13)	2583(3)	-1305(4)	9701(4)	78(1)
C(14)	2077(3)	-2313(4)	9860(5)	94(2)
C(15)	2576(3)	-130(4)	10375(5)	84(1)
C(16)	1615(3)	-2157(5)	10637(6)	98(2)
C(17)	2110(3)	9(4)	11132(5)	85(1)
C(18)	1601(3)	-990(5)	11282(4)	83(1)
C(19)	1097(3)	-882(6)	12102(5)	104(2)
C(20)	823(3)	208(7)	12496(5)	105(2)
C(21)	860(2)	1618(5)	12140(5)	84(1)
C(22)	1189(3)	2612(6)	12949(4)	93(1)
C(23)	1155(3)	3907(6)	12553(6)	104(2)
C(25)	508(3)	3344(7)	10653(5)	98(2)
C(26)	515(3)	2025(6)	10953(4)	99(2)

Table 3. Bond lengths [Å] and angles [°] for **5-(E,Z)**.

Fe(1)-C(5)	2.009(5)	C(21)-C(22)	1.372(6)
Fe(1)-C(4)	2.014(5)	C(21)-C(26)	1.381(6)
Fe(1)-C(3)	2.023(5)	C(22)-C(23)	1.368(6)
Fe(1)-C(1)	2.025(4)	C(25)-C(26)	1.362(6)
Fe(1)-C(7)	2.027(4)	C(5)-Fe(1)-C(4)	42.0(2)
Fe(1)-C(2)	2.030(4)	C(5)-Fe(1)-C(3)	68.2(2)
Fe(1)-C(10)	2.036(4)	C(4)-Fe(1)-C(3)	40.3(2)
Fe(1)-C(8)	2.036(4)	C(5)-Fe(1)-C(1)	40.0(2)
Fe(1)-C(9)	2.039(4)	C(4)-Fe(1)-C(1)	67.2(2)
Fe(1)-C(6)	2.040(5)	C(3)-Fe(1)-C(1)	65.0(2)
C(1)-C(2)	1.316(6)	C(5)-Fe(1)-C(7)	106.9(2)
C(1)-C(5)	1.381(8)	C(4)-Fe(1)-C(7)	130.5(3)
N(1)-C(25)	1.319(6)	C(3)-Fe(1)-C(7)	170.2(3)
N(1)-C(23)	1.320(6)	C(1)-Fe(1)-C(7)	117.3(2)
C(2)-C(3)	1.336(7)	C(5)-Fe(1)-C(2)	66.6(2)
C(3)-C(4)	1.391(8)	C(4)-Fe(1)-C(2)	66.4(2)
C(4)-C(5)	1.442(8)	C(3)-Fe(1)-C(2)	38.5(2)
C(6)-C(10)	1.422(6)	C(1)-Fe(1)-C(2)	37.89(18)
C(6)-C(7)	1.430(6)	C(7)-Fe(1)-C(2)	148.7(3)
C(6)-C(11)	1.444(6)	C(5)-Fe(1)-C(10)	166.0(4)
C(7)-C(8)	1.418(7)	C(4)-Fe(1)-C(10)	150.7(4)
C(8)-C(9)	1.416(6)	C(3)-Fe(1)-C(10)	118.3(2)
C(9)-C(10)	1.408(6)	C(1)-Fe(1)-C(10)	129.2(3)
C(11)-C(12)	1.325(6)	C(7)-Fe(1)-C(10)	68.42(18)
C(12)-C(13)	1.458(6)	C(2)-Fe(1)-C(10)	110.1(2)
C(13)-C(14)	1.395(6)	C(5)-Fe(1)-C(8)	117.5(3)
C(13)-C(15)	1.405(6)	C(4)-Fe(1)-C(8)	109.8(2)
C(14)-C(16)	1.372(7)	C(3)-Fe(1)-C(8)	132.8(3)
C(15)-C(17)	1.357(6)	C(1)-Fe(1)-C(8)	150.7(3)
C(16)-C(18)	1.383(7)	C(7)-Fe(1)-C(8)	40.85(19)
C(17)-C(18)	1.391(6)	C(2)-Fe(1)-C(8)	170.0(3)
C(18)-C(19)	1.464(7)	C(10)-Fe(1)-C(8)	68.3(2)
C(19)-C(20)	1.322(7)	C(5)-Fe(1)-C(9)	151.7(4)
C(20)-C(21)	1.475(7)	C(4)-Fe(1)-C(9)	118.7(3)

C(3)-Fe(1)-C(9)	111.4(2)	C(7)-C(6)-Fe(1)	68.9(3)
C(1)-Fe(1)-C(9)	167.4(3)	C(11)-C(6)-Fe(1)	121.8(3)
C(7)-Fe(1)-C(9)	68.48(19)	C(8)-C(7)-C(6)	108.7(5)
C(2)-Fe(1)-C(9)	131.8(3)	C(8)-C(7)-Fe(1)	69.9(3)
C(10)-Fe(1)-C(9)	40.42(17)	C(6)-C(7)-Fe(1)	69.9(3)
C(8)-Fe(1)-C(9)	40.66(18)	C(9)-C(8)-C(7)	107.7(5)
C(5)-Fe(1)-C(6)	127.1(3)	C(9)-C(8)-Fe(1)	69.8(3)
C(4)-Fe(1)-C(6)	168.1(4)	C(7)-C(8)-Fe(1)	69.2(3)
C(3)-Fe(1)-C(6)	148.6(3)	C(10)-C(9)-C(8)	108.1(5)
C(1)-Fe(1)-C(6)	107.5(2)	C(10)-C(9)-Fe(1)	69.7(3)
C(7)-Fe(1)-C(6)	41.16(18)	C(8)-C(9)-Fe(1)	69.6(3)
C(2)-Fe(1)-C(6)	116.5(2)	C(9)-C(10)-C(6)	109.1(5)
C(10)-Fe(1)-C(6)	40.85(16)	C(9)-C(10)-Fe(1)	69.9(3)
C(8)-Fe(1)-C(6)	69.2(2)	C(6)-C(10)-Fe(1)	69.7(2)
C(9)-Fe(1)-C(6)	68.8(2)	C(12)-C(11)-C(6)	127.6(4)
C(2)-C(1)-C(5)	110.5(6)	C(11)-C(12)-C(13)	127.7(4)
C(2)-C(1)-Fe(1)	71.2(3)	C(14)-C(13)-C(15)	115.6(5)
C(5)-C(1)-Fe(1)	69.4(3)	C(14)-C(13)-C(12)	122.1(5)
C(25)-N(1)-C(23)	114.6(4)	C(15)-C(13)-C(12)	122.3(4)
C(1)-C(2)-C(3)	110.1(5)	C(16)-C(14)-C(13)	121.5(5)
C(1)-C(2)-Fe(1)	70.9(3)	C(17)-C(15)-C(13)	122.0(5)
C(3)-C(2)-Fe(1)	70.5(3)	C(14)-C(16)-C(18)	122.6(5)
C(2)-C(3)-C(4)	108.7(6)	C(15)-C(17)-C(18)	122.4(5)
C(2)-C(3)-Fe(1)	71.0(3)	C(16)-C(18)-C(17)	115.8(5)
C(4)-C(3)-Fe(1)	69.5(3)	C(16)-C(18)-C(19)	120.2(5)
C(3)-C(4)-C(5)	105.9(5)	C(17)-C(18)-C(19)	123.9(5)
C(3)-C(4)-Fe(1)	70.2(3)	C(20)-C(19)-C(18)	128.6(5)
C(5)-C(4)-Fe(1)	68.8(3)	C(19)-C(20)-C(21)	130.4(5)
C(1)-C(5)-C(4)	104.7(5)	C(22)-C(21)-C(26)	115.7(5)
C(1)-C(5)-Fe(1)	70.6(3)	C(22)-C(21)-C(20)	123.6(5)
C(4)-C(5)-Fe(1)	69.2(3)	C(26)-C(21)-C(20)	120.6(5)
C(10)-C(6)-C(7)	106.4(5)	C(23)-C(22)-C(21)	119.7(5)
C(10)-C(6)-C(11)	127.9(5)	N(1)-C(23)-C(22)	125.2(5)
C(7)-C(6)-C(11)	125.4(5)	N(1)-C(25)-C(26)	124.8(5)
C(10)-C(6)-Fe(1)	69.4(3)	C(25)-C(26)-C(21)	120.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **5-(E,Z)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

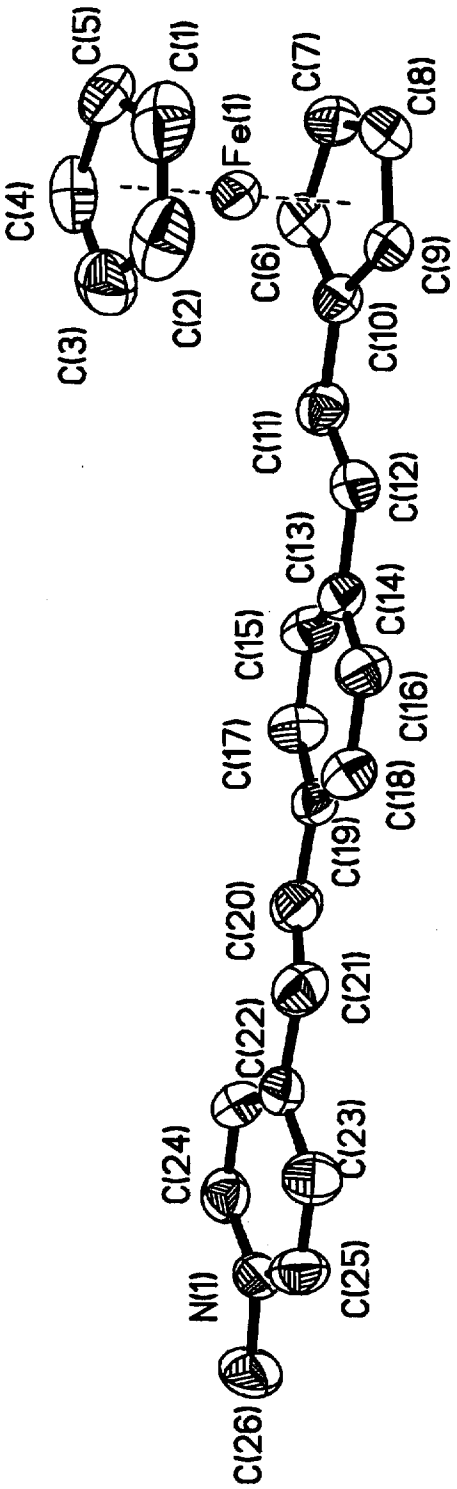
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	70(1)	59(1)	84(1)	-2(1)	4(1)	17(1)
C(1)	128(5)	70(3)	92(4)	-5(3)	20(4)	46(3)
N(1)	86(3)	103(3)	93(3)	8(3)	26(3)	9(2)
C(2)	81(3)	79(4)	119(5)	9(4)	17(4)	22(3)
C(3)	126(5)	96(4)	84(4)	-1(3)	1(4)	39(4)
C(4)	106(5)	113(5)	171(7)	81(5)	69(5)	53(4)
C(5)	92(4)	49(3)	170(7)	5(4)	-35(4)	3(3)
C(6)	79(3)	57(3)	79(3)	-2(3)	-4(3)	19(2)
C(7)	75(3)	77(3)	101(4)	-4(3)	-6(3)	17(3)
C(8)	72(3)	90(4)	119(4)	11(3)	11(3)	29(3)
C(9)	101(4)	77(3)	104(4)	-9(3)	13(4)	34(3)
C(10)	93(3)	54(3)	90(3)	-9(3)	-4(3)	19(2)
C(11)	92(3)	52(3)	73(3)	-4(2)	-7(3)	8(3)
C(12)	98(4)	50(3)	84(3)	-5(2)	-5(3)	6(3)
C(13)	83(3)	55(3)	76(3)	6(3)	-8(3)	4(3)
C(14)	91(3)	49(3)	121(4)	1(3)	-7(3)	-7(3)
C(15)	101(4)	61(3)	82(3)	1(2)	15(3)	-21(2)
C(16)	81(3)	65(4)	132(5)	26(3)	2(3)	-16(3)
C(17)	103(4)	69(3)	79(3)	-1(2)	18(3)	-26(3)
C(18)	90(3)	68(3)	77(3)	22(3)	-1(3)	-18(3)
C(19)	112(4)	108(5)	83(4)	30(3)	13(3)	-39(4)
C(20)	108(4)	127(5)	86(4)	14(4)	34(3)	-29(4)
C(21)	77(3)	107(4)	73(3)	13(3)	29(3)	-15(3)
C(22)	92(3)	116(4)	66(3)	-1(3)	14(3)	-6(3)
C(23)	100(4)	111(5)	95(4)	-15(4)	17(3)	0(3)
C(25)	95(4)	123(4)	74(3)	9(4)	20(3)	5(3)
C(26)	110(4)	111(5)	68(4)	4(3)	11(3)	-16(3)

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

	x	y	z	U(eq)
H(1)	2876	1877	7186	118
H(2)	2316	313	5611	114
H(3)	3005	375	4060	129
H(4)	4083	2046	4675	149
H(5)	4019	2981	6751	142
H(7)	5004	684	8497	108
H(8)	5427	133	6623	117
H(9)	4541	-1670	5477	117
H(10)	3580	-2235	6638	102
H(11)	3798	14	9361	94
H(12)	2978	-2194	8363	100
H(14)	2053	-3108	9428	113
H(15)	2902	573	10299	100
H(16)	1298	-2864	10735	118
H(17)	2132	802	11566	102
H(19)	951	-1687	12383	125
H(20)	566	61	13094	126
H(22)	1433	2408	13763	112
H(23)	1382	4557	13126	125
H(25)	260	3582	9848	117
H(26)	286	1399	10357	119

Table 1. Crystal data and structure refinement for **8-(E,E)**.

Identification code	str57m	
Empirical formula	C26 H24 F6 Fe N P	
Formula weight	551.28	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 12.0649(9) Å	α= 90°.
	b = 15.7470(12) Å	β= 95.150(2)°.
	c = 12.5267(9) Å	γ = 90°.
Volume	2370.3(3) $Å^3$	
Z	4	
Density (calculated)	1.545 Mg/m^3	
Absorption coefficient	0.767 mm^{-1}	
F(000)	1128	
Crystal size	0.14 x 0.09 x 0.09 mm^3	
Theta range for data collection	1.69 to 23.26°.	
Index ranges	-13<=h<=12, -17<=k<=17, -13<=l<=13	
Reflections collected	11387	
Independent reflections	3400 [R(int) = 0.0571]	
Completeness to theta = 23.26°	100.0 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3400 / 0 / 316	
Goodness-of-fit on F^2	1.060	
Final R indices [I>2sigma(I)]	R1 = 0.0548, wR2 = 0.1356	
R indices (all data)	R1 = 0.0882, wR2 = 0.1502	
Largest diff. peak and hole	0.746 and -0.414 e.$Å^{-3}$	


C(5)
C(1)
C(7)
C(8)
Fe(1)
C(4)
C(6)
C(9)
C(3)
C(2)
C(10)
C(11)
C(12)
C(13)
C(14)
C(15)
C(16)
C(17)
C(18)
C(19)
C(20)
C(21)
C(22)
C(24)
C(23)
N(1)
C(25)
C(26)

8-(E,E)

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **8-(E,E)**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	14906(1)	2042(1)	18423(1)	39(1)
N(1)	11400(4)	-387(3)	7551(3)	48(1)
C(1)	15260(6)	3288(4)	18668(6)	74(2)
P(1)	9597(1)	2743(1)	11160(1)	65(1)
F(2)	9621(5)	3692(3)	10797(3)	129(2)
C(2)	14916(5)	3145(4)	17601(6)	72(2)
C(3)	15643(6)	2582(4)	17180(5)	67(2)
F(3)	8359(4)	2646(4)	10770(6)	179(3)
C(4)	16460(5)	2370(4)	18005(5)	61(2)
F(4)	9195(6)	3019(5)	12234(5)	201(3)
C(5)	16221(5)	2812(4)	18926(5)	63(2)
F(5)	10776(4)	2866(4)	11684(7)	191(3)
C(6)	14730(4)	754(3)	18618(4)	46(1)
F(6)	9646(4)	1777(3)	11486(5)	134(2)
C(7)	14599(4)	1182(4)	19586(4)	53(1)
C(8)	13715(4)	1755(3)	19420(4)	49(1)
C(9)	13278(4)	1691(3)	18340(4)	45(1)
C(10)	13894(4)	1059(3)	17834(4)	42(1)
C(11)	13749(4)	770(3)	16724(4)	48(1)
C(12)	12985(4)	1033(3)	15992(4)	46(1)
C(13)	12804(4)	752(3)	14871(4)	41(1)
C(14)	12100(4)	1212(3)	14154(4)	48(1)
C(15)	13306(4)	40(3)	14482(4)	51(1)
C(16)	11931(4)	998(4)	13097(4)	51(1)
C(17)	13128(4)	-192(3)	13418(4)	51(1)
C(18)	12450(4)	288(3)	12701(4)	42(1)
C(19)	12324(4)	37(4)	11567(4)	52(1)
C(20)	11804(4)	444(4)	10767(4)	53(1)
C(21)	11702(4)	156(3)	9646(4)	46(1)
C(22)	12351(4)	-476(4)	9263(4)	52(1)
C(23)	10905(5)	519(4)	8921(4)	55(2)

C(24)	12200(5)	-729(4)	8215(4)	54(2)
C(25)	10765(5)	232(4)	7887(4)	56(2)
C(26)	11181(5)	-705(4)	6441(4)	72(2)
F(1)	9925(9)	2494(4)	10078(5)	230(4)

Table 3. Bond lengths [Å] and angles [°] for **8-(E,E)**.

Fe(1)-C(2)	2.020(6)
Fe(1)-C(1)	2.026(6)
Fe(1)-C(9)	2.033(5)
Fe(1)-C(8)	2.037(5)
Fe(1)-C(3)	2.046(6)
Fe(1)-C(7)	2.046(5)
Fe(1)-C(5)	2.051(5)
Fe(1)-C(6)	2.055(5)
Fe(1)-C(4)	2.058(5)
Fe(1)-C(10)	2.066(5)
N(1)-C(25)	1.330(7)
N(1)-C(24)	1.331(7)
N(1)-C(26)	1.479(6)
C(1)-C(2)	1.381(9)
C(1)-C(5)	1.394(9)
P(1)-F(1)	1.498(6)
P(1)-F(5)	1.525(5)
P(1)-F(4)	1.533(6)
P(1)-F(3)	1.536(5)
P(1)-F(2)	1.564(4)
P(1)-F(6)	1.575(4)
C(2)-C(3)	1.385(9)
C(3)-C(4)	1.402(8)
C(4)-C(5)	1.399(8)
C(6)-C(7)	1.408(7)
C(6)-C(10)	1.426(7)
C(7)-C(8)	1.398(7)
C(8)-C(9)	1.411(7)
C(9)-C(10)	1.425(7)
C(10)-C(11)	1.458(7)
C(11)-C(12)	1.308(6)
C(12)-C(13)	1.470(7)
C(13)-C(15)	1.383(7)
C(13)-C(14)	1.384(7)

C(14)-C(16)	1.364(7)
C(15)-C(17)	1.380(7)
C(16)-C(18)	1.394(7)
C(17)-C(18)	1.385(7)
C(18)-C(19)	1.469(7)
C(19)-C(20)	1.302(7)
C(20)-C(21)	1.470(7)
C(21)-C(22)	1.380(7)
C(21)-C(23)	1.386(7)
C(22)-C(24)	1.368(7)
C(23)-C(25)	1.368(7)

C(2)-Fe(1)-C(1)	39.9(3)
C(2)-Fe(1)-C(9)	104.9(2)
C(1)-Fe(1)-C(9)	117.4(3)
C(2)-Fe(1)-C(8)	122.7(3)
C(1)-Fe(1)-C(8)	105.8(2)
C(9)-Fe(1)-C(8)	40.56(19)
C(2)-Fe(1)-C(3)	39.8(3)
C(1)-Fe(1)-C(3)	67.2(3)
C(9)-Fe(1)-C(3)	123.9(2)
C(8)-Fe(1)-C(3)	159.6(3)
C(2)-Fe(1)-C(7)	160.3(3)
C(1)-Fe(1)-C(7)	125.6(3)
C(9)-Fe(1)-C(7)	67.7(2)
C(8)-Fe(1)-C(7)	40.0(2)
C(3)-Fe(1)-C(7)	159.3(3)
C(2)-Fe(1)-C(5)	66.9(3)
C(1)-Fe(1)-C(5)	40.0(2)
C(9)-Fe(1)-C(5)	153.3(2)
C(8)-Fe(1)-C(5)	120.7(2)
C(3)-Fe(1)-C(5)	67.1(3)
C(7)-Fe(1)-C(5)	110.9(2)
C(2)-Fe(1)-C(6)	156.1(3)
C(1)-Fe(1)-C(6)	163.8(3)
C(9)-Fe(1)-C(6)	68.2(2)

C(8)-Fe(1)-C(6)	67.8(2)
C(3)-Fe(1)-C(6)	123.8(2)
C(7)-Fe(1)-C(6)	40.17(19)
C(5)-Fe(1)-C(6)	129.2(2)
C(2)-Fe(1)-C(4)	66.8(3)
C(1)-Fe(1)-C(4)	67.1(2)
C(9)-Fe(1)-C(4)	162.4(2)
C(8)-Fe(1)-C(4)	157.0(2)
C(3)-Fe(1)-C(4)	40.0(2)
C(7)-Fe(1)-C(4)	125.0(2)
C(5)-Fe(1)-C(4)	39.8(2)
C(6)-Fe(1)-C(4)	112.6(2)
C(2)-Fe(1)-C(10)	119.5(3)
C(1)-Fe(1)-C(10)	152.8(3)
C(9)-Fe(1)-C(10)	40.7(2)
C(8)-Fe(1)-C(10)	68.1(2)
C(3)-Fe(1)-C(10)	108.8(2)
C(7)-Fe(1)-C(10)	67.7(2)
C(5)-Fe(1)-C(10)	165.6(2)
C(6)-Fe(1)-C(10)	40.50(19)
C(4)-Fe(1)-C(10)	128.3(2)
C(25)-N(1)-C(24)	120.3(5)
C(25)-N(1)-C(26)	119.1(5)
C(24)-N(1)-C(26)	120.5(5)
C(2)-C(1)-C(5)	107.9(6)
C(2)-C(1)-Fe(1)	69.8(3)
C(5)-C(1)-Fe(1)	70.9(3)
F(1)-P(1)-F(5)	96.4(5)
F(1)-P(1)-F(4)	176.5(5)
F(5)-P(1)-F(4)	86.7(4)
F(1)-P(1)-F(3)	90.8(5)
F(5)-P(1)-F(3)	172.8(5)
F(4)-P(1)-F(3)	86.1(4)
F(1)-P(1)-F(2)	88.5(3)
F(5)-P(1)-F(2)	87.8(3)
F(4)-P(1)-F(2)	89.9(4)

F(3)-P(1)-F(2)	92.6(3)
F(1)-P(1)-F(6)	88.6(4)
F(5)-P(1)-F(6)	89.9(3)
F(4)-P(1)-F(6)	93.1(4)
F(3)-P(1)-F(6)	90.0(3)
F(2)-P(1)-F(6)	176.1(3)
C(1)-C(2)-C(3)	109.1(6)
C(1)-C(2)-Fe(1)	70.3(4)
C(3)-C(2)-Fe(1)	71.1(4)
C(2)-C(3)-C(4)	107.4(6)
C(2)-C(3)-Fe(1)	69.1(4)
C(4)-C(3)-Fe(1)	70.5(3)
C(5)-C(4)-C(3)	107.8(5)
C(5)-C(4)-Fe(1)	69.8(3)
C(3)-C(4)-Fe(1)	69.6(3)
C(1)-C(5)-C(4)	107.8(6)
C(1)-C(5)-Fe(1)	69.1(3)
C(4)-C(5)-Fe(1)	70.4(3)
C(7)-C(6)-C(10)	107.8(5)
C(7)-C(6)-Fe(1)	69.6(3)
C(10)-C(6)-Fe(1)	70.2(3)
C(8)-C(7)-C(6)	108.9(5)
C(8)-C(7)-Fe(1)	69.6(3)
C(6)-C(7)-Fe(1)	70.3(3)
C(7)-C(8)-C(9)	108.1(5)
C(7)-C(8)-Fe(1)	70.3(3)
C(9)-C(8)-Fe(1)	69.6(3)
C(8)-C(9)-C(10)	108.2(5)
C(8)-C(9)-Fe(1)	69.9(3)
C(10)-C(9)-Fe(1)	70.9(3)
C(9)-C(10)-C(6)	107.0(4)
C(9)-C(10)-C(11)	128.3(5)
C(6)-C(10)-C(11)	124.7(5)
C(9)-C(10)-Fe(1)	68.4(3)
C(6)-C(10)-Fe(1)	69.4(3)
C(11)-C(10)-Fe(1)	126.2(4)

C(12)-C(11)-C(10)	126.0(5)
C(11)-C(12)-C(13)	127.6(5)
C(15)-C(13)-C(14)	117.3(4)
C(15)-C(13)-C(12)	123.2(5)
C(14)-C(13)-C(12)	119.5(5)
C(16)-C(14)-C(13)	122.0(5)
C(17)-C(15)-C(13)	121.3(5)
C(14)-C(16)-C(18)	120.7(5)
C(15)-C(17)-C(18)	120.9(5)
C(17)-C(18)-C(16)	117.7(5)
C(17)-C(18)-C(19)	119.0(5)
C(16)-C(18)-C(19)	123.3(5)
C(20)-C(19)-C(18)	127.8(5)
C(19)-C(20)-C(21)	125.2(5)
C(22)-C(21)-C(23)	116.8(5)
C(22)-C(21)-C(20)	123.6(5)
C(23)-C(21)-C(20)	119.6(5)
C(24)-C(22)-C(21)	120.9(5)
C(25)-C(23)-C(21)	120.3(5)
N(1)-C(24)-C(22)	120.5(5)
N(1)-C(25)-C(23)	121.1(5)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **8-(E,E)**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	38(1)	39(1)	40(1)	-3(1)	1(1)	-2(1)
N(1)	52(3)	54(3)	38(3)	-2(2)	5(2)	-15(2)
C(1)	71(5)	45(4)	110(6)	-25(4)	28(4)	-12(3)
P(1)	62(1)	65(1)	65(1)	20(1)	-9(1)	-10(1)
F(2)	227(6)	63(3)	89(3)	20(2)	-28(3)	-4(3)
C(2)	61(4)	54(4)	99(5)	28(4)	-1(4)	-6(3)
C(3)	81(5)	61(4)	61(4)	5(3)	16(4)	-17(4)
F(3)	97(4)	142(5)	277(8)	30(5)	-87(5)	-4(3)
C(4)	45(4)	49(4)	93(5)	6(3)	25(4)	-2(3)
F(4)	223(8)	281(9)	110(4)	-1(5)	71(5)	-40(6)
C(5)	49(4)	71(4)	67(4)	-3(3)	-5(3)	-22(3)
F(5)	80(4)	141(5)	335(9)	92(5)	-78(5)	-45(3)
C(6)	49(3)	42(3)	47(3)	3(2)	5(3)	3(2)
F(6)	89(3)	86(3)	218(5)	69(3)	-36(3)	-28(2)
C(7)	53(4)	66(4)	38(3)	6(3)	-3(3)	-4(3)
C(8)	51(3)	58(4)	40(3)	-4(3)	11(3)	-3(3)
C(9)	35(3)	59(3)	42(3)	1(3)	1(2)	-3(2)
C(10)	43(3)	42(3)	41(3)	-3(2)	3(2)	-8(2)
C(11)	46(3)	44(3)	53(3)	-6(3)	4(3)	-3(2)
C(12)	42(3)	50(3)	46(3)	0(3)	7(3)	1(2)
C(13)	40(3)	42(3)	40(3)	-5(2)	3(2)	-6(2)
C(14)	44(3)	51(3)	47(3)	-9(3)	2(3)	7(3)
C(15)	57(4)	48(3)	46(3)	4(3)	-9(3)	-2(3)
C(16)	44(3)	60(4)	49(3)	2(3)	-5(3)	2(3)
C(17)	61(4)	41(3)	50(3)	-5(3)	-1(3)	6(3)
C(18)	38(3)	46(3)	41(3)	-7(2)	3(2)	-3(2)
C(19)	47(3)	57(4)	52(3)	-6(3)	1(3)	-2(3)
C(20)	48(3)	54(4)	55(4)	-5(3)	-1(3)	4(3)
C(21)	41(3)	53(3)	42(3)	-2(3)	5(2)	-11(3)
C(22)	43(3)	63(4)	47(3)	0(3)	-6(3)	-1(3)
C(23)	61(4)	51(4)	52(4)	3(3)	1(3)	5(3)