Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supporting Information

Oxidation of Aromatic Alkenes and Alkynes Catalyzed by a Hexaacetonitrile Iron(II) Ionic Complex $[Fe(CH_3CN)_6][BF_4]_2$

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X-ray structural information for Complex II, $Fe(PPP)(CH_3CN)_3$

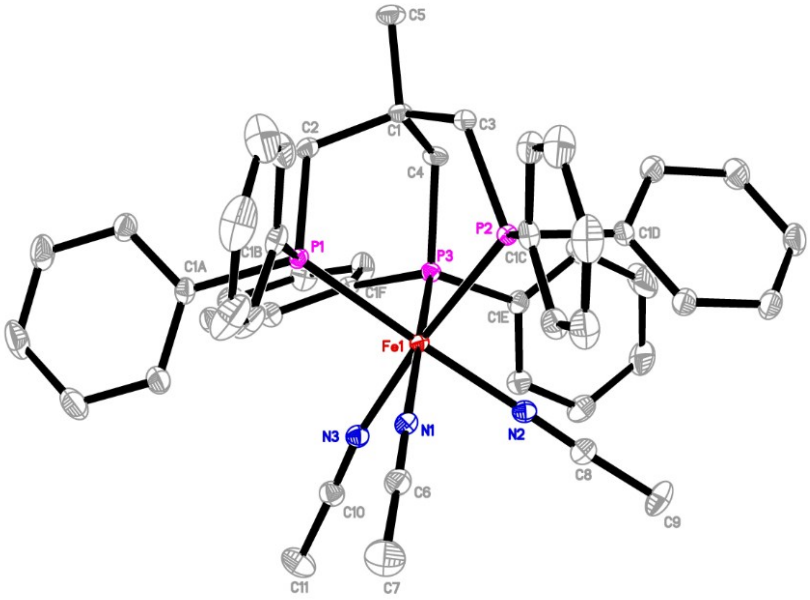

Table 1. Crystal data and structure refinement for g473.

Identification code	g473	
Empirical formula	C49 H51 B2 F8 Fe N4 O0.25 P3	
Formula weight	1022.31	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 13.2701(4) Å	α= 90°.
	b = 18.5437(7) Å	β= 91.102(2)°.
	c = 19.7957(9) Å	γ = 90°.

Volume	4870.4(3) $Å^3$
Z	4
Density (calculated)	1.394 Mg/m^3
Absorption coefficient	0.479 mm^{-1}
F(000)	2112
Crystal size	0.315 x 0.271 x 0.254 mm^3
Theta range for data collection	2.426 to 28.281°.
Index ranges	-17<=h<=17, -24<=k<=24, -26<=l<=26
Reflections collected	229324
Independent reflections	12081 [R(int) = 0.0276]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7459 and 0.7159
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	12081 / 6 / 618
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0309, wR2 = 0.0781
R indices (all data)	R1 = 0.0349, wR2 = 0.0809
Extinction coefficient	n/a
Largest diff. peak and hole	0.924 and -0.504 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for g473. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	3644(1)	7056(1)	4417(1)	9(1)
P(1)	4784(1)	7918(1)	4133(1)	10(1)
P(2)	3095(1)	7096(1)	3311(1)	10(1)
P(3)	2499(1)	7910(1)	4687(1)	10(1)
B(2)	2061(1)	5400(1)	6780(1)	23(1)
B(1)	3043(1)	3986(1)	3893(1)	24(1)
C(1)	3094(1)	8648(1)	3473(1)	12(1)
C(2)	4150(1)	8737(1)	3808(1)	12(1)
C(3)	3081(1)	8017(1)	2964(1)	13(1)
C(4)	2265(1)	8578(1)	4010(1)	14(1)
C(5)	2868(1)	9340(1)	3067(1)	17(1)
C(6)	5172(1)	5806(1)	4296(1)	16(1)
C(7)	5892(1)	5215(1)	4276(1)	29(1)
C(8)	2112(1)	5843(1)	4719(1)	16(1)
C(9)	1357(1)	5297(1)	4863(1)	24(1)
C(10)	4173(1)	6827(1)	5936(1)	16(1)
C(11)	4365(1)	6686(1)	6652(1)	25(1)
C(1A)	5695(1)	8304(1)	4748(1)	13(1)
C(2A)	6159(1)	7863(1)	5236(1)	18(1)
C(3A)	6850(1)	8152(1)	5702(1)	26(1)
C(4A)	7085(1)	8882(1)	5683(1)	28(1)
C(5A)	6644(1)	9321(1)	5193(1)	24(1)
C(6A)	5953(1)	9037(1)	4727(1)	17(1)
C(1B)	5688(1)	7633(1)	3492(1)	14(1)
C(2B)	5742(1)	7931(1)	2846(1)	20(1)
C(3B)	6448(1)	7677(1)	2389(1)	29(1)
C(4B)	7096(1)	7120(1)	2570(1)	31(1)
C(5B)	7074(1)	6835(1)	3220(1)	30(1)
C(6B)	6385(1)	7096(1)	3681(1)	21(1)
C(1C)	3776(1)	6576(1)	2675(1)	14(1)
C(2C)	3964(1)	6851(1)	2030(1)	18(1)

C(3C)	4398(1)	6414(1)	1541(1)	23(1)
C(4C)	4634(1)	5702(1)	1688(1)	24(1)
C(5C)	4454(1)	5423(1)	2325(1)	22(1)
C(6C)	4028(1)	5857(1)	2818(1)	17(1)
C(1D)	1811(1)	6751(1)	3154(1)	13(1)
C(2D)	1640(1)	6006(1)	3191(1)	16(1)
C(3D)	678(1)	5725(1)	3099(1)	19(1)
C(4D)	-135(1)	6182(1)	2967(1)	21(1)
C(5D)	28(1)	6918(1)	2922(1)	25(1)
C(6D)	995(1)	7203(1)	3010(1)	20(1)
C(1E)	1262(1)	7565(1)	4924(1)	14(1)
C(2E)	371(1)	7686(1)	4562(1)	28(1)
C(3E)	-530(1)	7377(1)	4774(1)	36(1)
C(4E)	-555(1)	6950(1)	5345(1)	26(1)
C(5E)	330(1)	6833(1)	5713(1)	21(1)
C(6E)	1229(1)	7139(1)	5507(1)	16(1)
C(1F)	2784(1)	8492(1)	5423(1)	13(1)
C(2F)	2016(1)	8890(1)	5726(1)	19(1)
C(3F)	2236(1)	9350(1)	6265(1)	23(1)
C(4F)	3219(1)	9432(1)	6507(1)	19(1)
C(5F)	3983(1)	9039(1)	6214(1)	18(1)
C(6F)	3762(1)	8570(1)	5680(1)	15(1)
C(1S)	3951(1)	6214(1)	8394(1)	23(1)
C(2S)	2915(1)	6277(1)	8596(1)	38(1)
F(4)	2960(1)	3784(1)	4569(1)	32(1)
F(2)	3251(1)	3385(1)	3501(1)	35(1)
F(6)	1897(1)	4770(1)	6409(1)	38(1)
F(7)	1187(1)	5572(1)	7120(1)	38(1)
F(5)	2315(1)	5950(1)	6331(1)	29(1)
F(8)	2854(1)	5289(1)	7234(1)	44(1)
F(3)	2144(1)	4290(1)	3675(1)	57(1)
F(1)	3825(1)	4476(1)	3841(1)	63(1)
N(1)	4625(1)	6280(1)	4292(1)	12(1)
N(2)	2678(1)	6285(1)	4596(1)	12(1)
N(3)	4021(1)	6958(1)	5379(1)	13(1)
N(1S)	4781(1)	6173(1)	8242(1)	30(1)

O(1W)	4476(9)	5326(7)	9950(5)	123(4)

Table 3. Bond lengths [Å] and angles [°] for g473.

Fe(1)-N(2)	1.9575(11)
Fe(1)-N(1)	1.9587(11)
Fe(1)-N(3)	1.9687(11)
Fe(1)-P(3)	2.2667(3)
Fe(1)-P(1)	2.2798(3)
Fe(1)-P(2)	2.2946(4)
P(1)-C(1B)	1.8401(13)
P(1)-C(1A)	1.8430(13)
P(1)-C(2)	1.8465(12)
P(2)-C(1C)	1.8363(13)
P(2)-C(1D)	1.8406(12)
P(2)-C(3)	1.8411(12)
P(3)-C(1E)	1.8310(13)
P(3)-C(1F)	1.8467(13)
P(3)-C(4)	1.8479(12)
B(2)-F(8)	1.387(2)
B(2)-F(7)	1.3886(19)
B(2)-F(6)	1.394(2)
B(2)-F(5)	1.3972(17)
B(1)-F(3)	1.381(2)
B(1)-F(1)	1.385(2)
B(1)-F(2)	1.3896(19)
B(1)-F(4)	1.3944(19)
C(1)-C(5)	1.5418(16)
C(1)-C(3)	1.5441(17)
C(1)-C(2)	1.5472(17)
C(1)-C(4)	1.5493(17)
C(2)-H(2A)	0.9900
C(2)-H(2B)	0.9900
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-H(5A)	0.9800

C(5)-H(5B)	0.9800
C(5)-H(5C)	0.9800
C(6)-N(1)	1.1404(17)
C(6)-C(7)	1.4541(18)
C(7)-H(7A)	0.9800
C(7)-H(7B)	0.9800
C(7)-H(7C)	0.9800
C(8)-N(2)	1.1405(17)
C(8)-C(9)	1.4569(18)
C(9)-H(9A)	0.9800
C(9)-H(9B)	0.9800
C(9)-H(9C)	0.9800
C(10)-N(3)	1.1426(17)
C(10)-C(11)	1.4578(18)
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(1A)-C(2A)	1.3990(18)
C(1A)-C(6A)	1.4025(17)
C(2A)-C(3A)	1.3953(19)
C(2A)-H(2A1)	0.9500
C(3A)-C(4A)	1.390(2)
C(3A)-H(3A1)	0.9500
C(4A)-C(5A)	1.388(2)
C(4A)-H(4A1)	0.9500
C(5A)-C(6A)	1.3927(19)
C(5A)-H(5A1)	0.9500
C(6A)-H(6A)	0.9500
C(1B)-C(2B)	1.3953(19)
C(1B)-C(6B)	1.4051(19)
C(2B)-C(3B)	1.398(2)
C(2B)-H(2B1)	0.9500
C(3B)-C(4B)	1.386(3)
C(3B)-H(3B1)	0.9500
C(4B)-C(5B)	1.392(3)
C(4B)-H(4B1)	0.9500

C(5B)-C(6B)	1.391(2)
C(5B)-H(5B1)	0.9500
C(6B)-H(6B)	0.9500
C(1C)-C(2C)	1.4020(18)
C(1C)-C(6C)	1.4022(18)
C(2C)-C(3C)	1.3940(19)
C(2C)-H(2C)	0.9500
C(3C)-C(4C)	1.388(2)
C(3C)-H(3C)	0.9500
C(4C)-C(5C)	1.388(2)
C(4C)-H(4C)	0.9500
C(5C)-C(6C)	1.3934(19)
C(5C)-H(5C1)	0.9500
C(6C)-H(6C)	0.9500
C(1D)-C(6D)	1.3952(18)
C(1D)-C(2D)	1.4033(18)
C(2D)-C(3D)	1.3884(18)
C(2D)-H(2D)	0.9500
C(3D)-C(4D)	1.391(2)
C(3D)-H(3D)	0.9500
C(4D)-C(5D)	1.385(2)
C(4D)-H(4D)	0.9500
C(5D)-C(6D)	1.3954(19)
C(5D)-H(5D)	0.9500
C(6D)-H(6D)	0.9500
C(1E)-C(2E)	1.3881(19)
C(1E)-C(6E)	1.3997(18)
C(2E)-C(3E)	1.398(2)
C(2E)-H(2E)	0.9500
C(3E)-C(4E)	1.382(2)
C(3E)-H(3E)	0.9500
C(4E)-C(5E)	1.387(2)
C(4E)-H(4E)	0.9500
C(5E)-C(6E)	1.3894(18)
C(5E)-H(5E)	0.9500
C(6E)-H(6E)	0.9500

C(1F)-C(6F)	1.3911(17)
C(1F)-C(2F)	1.4032(17)
C(2F)-C(3F)	1.3935(19)
C(2F)-H(2F)	0.9500
C(3F)-C(4F)	1.389(2)
C(3F)-H(3F)	0.9500
C(4F)-C(5F)	1.3843(19)
C(4F)-H(4F)	0.9500
C(5F)-C(6F)	1.3961(18)
C(5F)-H(5F)	0.9500
C(6F)-H(6F)	0.9500
C(1S)-N(1S)	1.150(2)
C(1S)-C(2S)	1.443(2)
C(2S)-H(2S1)	0.9800
C(2S)-H(2S2)	0.9800
C(2S)-H(2S3)	0.9800

N(2)-Fe(1)-N(1)	85.75(4)
N(2)-Fe(1)-N(3)	84.99(4)
N(1)-Fe(1)-N(3)	84.08(4)
N(2)-Fe(1)-P(3)	91.30(3)
N(1)-Fe(1)-P(3)	173.34(3)
N(3)-Fe(1)-P(3)	89.71(3)
N(2)-Fe(1)-P(1)	175.88(3)
N(1)-Fe(1)-P(1)	92.20(3)
N(3)-Fe(1)-P(1)	98.37(3)
P(3)-Fe(1)-P(1)	91.104(13)
N(2)-Fe(1)-P(2)	89.97(3)
N(1)-Fe(1)-P(2)	95.94(3)
N(3)-Fe(1)-P(2)	174.95(3)
P(3)-Fe(1)-P(2)	90.028(12)
P(1)-Fe(1)-P(2)	86.678(12)
C(1B)-P(1)-C(1A)	98.02(6)
C(1B)-P(1)-C(2)	107.15(6)
C(1A)-P(1)-C(2)	101.51(6)
C(1B)-P(1)-Fe(1)	114.39(4)

C(1A)-P(1)-Fe(1)	122.64(4)
C(2)-P(1)-Fe(1)	111.25(4)
C(1C)-P(2)-C(1D)	99.67(6)
C(1C)-P(2)-C(3)	103.43(6)
C(1D)-P(2)-C(3)	104.83(6)
C(1C)-P(2)-Fe(1)	119.07(4)
C(1D)-P(2)-Fe(1)	115.19(4)
C(3)-P(2)-Fe(1)	112.77(4)
C(1E)-P(3)-C(1F)	100.01(6)
C(1E)-P(3)-C(4)	106.35(6)
C(1F)-P(3)-C(4)	102.11(6)
C(1E)-P(3)-Fe(1)	115.13(4)
C(1F)-P(3)-Fe(1)	117.78(4)
C(4)-P(3)-Fe(1)	113.66(4)
F(8)-B(2)-F(7)	110.56(14)
F(8)-B(2)-F(6)	108.91(13)
F(7)-B(2)-F(6)	108.91(13)
F(8)-B(2)-F(5)	109.35(13)
F(7)-B(2)-F(5)	110.77(13)
F(6)-B(2)-F(5)	108.29(13)
F(3)-B(1)-F(1)	110.76(15)
F(3)-B(1)-F(2)	109.37(14)
F(1)-B(1)-F(2)	109.08(14)
F(3)-B(1)-F(4)	109.03(13)
F(1)-B(1)-F(4)	108.71(14)
F(2)-B(1)-F(4)	109.87(13)
C(5)-C(1)-C(3)	106.89(10)
C(5)-C(1)-C(2)	107.45(10)
C(3)-C(1)-C(2)	111.08(10)
C(5)-C(1)-C(4)	107.07(10)
C(3)-C(1)-C(4)	112.66(10)
C(2)-C(1)-C(4)	111.36(10)
C(1)-C(2)-P(1)	117.66(8)
C(1)-C(2)-H(2A)	107.9
P(1)-C(2)-H(2A)	107.9
C(1)-C(2)-H(2B)	107.9

P(1)-C(2)-H(2B)	107.9
H(2A)-C(2)-H(2B)	107.2
C(1)-C(3)-P(2)	117.35(8)
C(1)-C(3)-H(3A)	108.0
P(2)-C(3)-H(3A)	108.0
C(1)-C(3)-H(3B)	108.0
P(2)-C(3)-H(3B)	108.0
H(3A)-C(3)-H(3B)	107.2
C(1)-C(4)-P(3)	116.22(8)
C(1)-C(4)-H(4A)	108.2
P(3)-C(4)-H(4A)	108.2
C(1)-C(4)-H(4B)	108.2
P(3)-C(4)-H(4B)	108.2
H(4A)-C(4)-H(4B)	107.4
C(1)-C(5)-H(5A)	109.5
C(1)-C(5)-H(5B)	109.5
H(5A)-C(5)-H(5B)	109.5
C(1)-C(5)-H(5C)	109.5
H(5A)-C(5)-H(5C)	109.5
H(5B)-C(5)-H(5C)	109.5
N(1)-C(6)-C(7)	177.56(15)
C(6)-C(7)-H(7A)	109.5
C(6)-C(7)-H(7B)	109.5
H(7A)-C(7)-H(7B)	109.5
C(6)-C(7)-H(7C)	109.5
H(7A)-C(7)-H(7C)	109.5
H(7B)-C(7)-H(7C)	109.5
N(2)-C(8)-C(9)	177.61(15)
C(8)-C(9)-H(9A)	109.5
C(8)-C(9)-H(9B)	109.5
H(9A)-C(9)-H(9B)	109.5
C(8)-C(9)-H(9C)	109.5
H(9A)-C(9)-H(9C)	109.5
H(9B)-C(9)-H(9C)	109.5
N(3)-C(10)-C(11)	177.99(14)
C(10)-C(11)-H(11A)	109.5

C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(2A)-C(1A)-C(6A)	118.86(12)
C(2A)-C(1A)-P(1)	120.20(10)
C(6A)-C(1A)-P(1)	120.92(10)
C(3A)-C(2A)-C(1A)	120.45(13)
C(3A)-C(2A)-H(2A1)	119.8
C(1A)-C(2A)-H(2A1)	119.8
C(4A)-C(3A)-C(2A)	120.13(14)
C(4A)-C(3A)-H(3A1)	119.9
C(2A)-C(3A)-H(3A1)	119.9
C(5A)-C(4A)-C(3A)	119.87(13)
C(5A)-C(4A)-H(4A1)	120.1
C(3A)-C(4A)-H(4A1)	120.1
C(4A)-C(5A)-C(6A)	120.30(13)
C(4A)-C(5A)-H(5A1)	119.8
C(6A)-C(5A)-H(5A1)	119.8
C(5A)-C(6A)-C(1A)	120.37(13)
C(5A)-C(6A)-H(6A)	119.8
C(1A)-C(6A)-H(6A)	119.8
C(2B)-C(1B)-C(6B)	118.65(12)
C(2B)-C(1B)-P(1)	124.30(10)
C(6B)-C(1B)-P(1)	117.02(10)
C(1B)-C(2B)-C(3B)	120.43(14)
C(1B)-C(2B)-H(2B1)	119.8
C(3B)-C(2B)-H(2B1)	119.8
C(4B)-C(3B)-C(2B)	120.25(15)
C(4B)-C(3B)-H(3B1)	119.9
C(2B)-C(3B)-H(3B1)	119.9
C(3B)-C(4B)-C(5B)	119.94(14)
C(3B)-C(4B)-H(4B1)	120.0
C(5B)-C(4B)-H(4B1)	120.0
C(6B)-C(5B)-C(4B)	119.93(15)

C(6B)-C(5B)-H(5B1)	120.0
C(4B)-C(5B)-H(5B1)	120.0
C(5B)-C(6B)-C(1B)	120.67(15)
C(5B)-C(6B)-H(6B)	119.7
C(1B)-C(6B)-H(6B)	119.7
C(2C)-C(1C)-C(6C)	118.84(12)
C(2C)-C(1C)-P(2)	122.22(10)
C(6C)-C(1C)-P(2)	118.64(10)
C(3C)-C(2C)-C(1C)	120.34(13)
C(3C)-C(2C)-H(2C)	119.8
C(1C)-C(2C)-H(2C)	119.8
C(4C)-C(3C)-C(2C)	120.16(14)
C(4C)-C(3C)-H(3C)	119.9
C(2C)-C(3C)-H(3C)	119.9
C(5C)-C(4C)-C(3C)	120.13(13)
C(5C)-C(4C)-H(4C)	119.9
C(3C)-C(4C)-H(4C)	119.9
C(4C)-C(5C)-C(6C)	120.08(13)
C(4C)-C(5C)-H(5C1)	120.0
C(6C)-C(5C)-H(5C1)	120.0
C(5C)-C(6C)-C(1C)	120.45(13)
C(5C)-C(6C)-H(6C)	119.8
C(1C)-C(6C)-H(6C)	119.8
C(6D)-C(1D)-C(2D)	118.49(12)
C(6D)-C(1D)-P(2)	122.62(10)
C(2D)-C(1D)-P(2)	118.89(9)
C(3D)-C(2D)-C(1D)	120.78(12)
C(3D)-C(2D)-H(2D)	119.6
C(1D)-C(2D)-H(2D)	119.6
C(2D)-C(3D)-C(4D)	120.26(13)
C(2D)-C(3D)-H(3D)	119.9
C(4D)-C(3D)-H(3D)	119.9
C(5D)-C(4D)-C(3D)	119.40(13)
C(5D)-C(4D)-H(4D)	120.3
C(3D)-C(4D)-H(4D)	120.3
C(4D)-C(5D)-C(6D)	120.64(13)

C(4D)-C(5D)-H(5D)	119.7
C(6D)-C(5D)-H(5D)	119.7
C(1D)-C(6D)-C(5D)	120.41(13)
C(1D)-C(6D)-H(6D)	119.8
C(5D)-C(6D)-H(6D)	119.8
C(2E)-C(1E)-C(6E)	118.48(12)
C(2E)-C(1E)-P(3)	124.74(10)
C(6E)-C(1E)-P(3)	116.77(9)
C(1E)-C(2E)-C(3E)	120.30(14)
C(1E)-C(2E)-H(2E)	119.9
C(3E)-C(2E)-H(2E)	119.9
C(4E)-C(3E)-C(2E)	120.89(14)
C(4E)-C(3E)-H(3E)	119.6
C(2E)-C(3E)-H(3E)	119.6
C(3E)-C(4E)-C(5E)	119.15(13)
C(3E)-C(4E)-H(4E)	120.4
C(5E)-C(4E)-H(4E)	120.4
C(4E)-C(5E)-C(6E)	120.30(13)
C(4E)-C(5E)-H(5E)	119.8
C(6E)-C(5E)-H(5E)	119.8
C(5E)-C(6E)-C(1E)	120.87(13)
C(5E)-C(6E)-H(6E)	119.6
C(1E)-C(6E)-H(6E)	119.6
C(6F)-C(1F)-C(2F)	118.02(12)
C(6F)-C(1F)-P(3)	121.65(9)
C(2F)-C(1F)-P(3)	120.30(10)
C(3F)-C(2F)-C(1F)	120.43(13)
C(3F)-C(2F)-H(2F)	119.8
C(1F)-C(2F)-H(2F)	119.8
C(4F)-C(3F)-C(2F)	120.78(13)
C(4F)-C(3F)-H(3F)	119.6
C(2F)-C(3F)-H(3F)	119.6
C(5F)-C(4F)-C(3F)	119.27(12)
C(5F)-C(4F)-H(4F)	120.4
C(3F)-C(4F)-H(4F)	120.4
C(4F)-C(5F)-C(6F)	120.04(12)

C(4F)-C(5F)-H(5F)	120.0
C(6F)-C(5F)-H(5F)	120.0
C(1F)-C(6F)-C(5F)	121.45(12)
C(1F)-C(6F)-H(6F)	119.3
C(5F)-C(6F)-H(6F)	119.3
N(1S)-C(1S)-C(2S)	178.80(18)
C(1S)-C(2S)-H(2S1)	109.5
C(1S)-C(2S)-H(2S2)	109.5
H(2S1)-C(2S)-H(2S2)	109.5
C(1S)-C(2S)-H(2S3)	109.5
H(2S1)-C(2S)-H(2S3)	109.5
H(2S2)-C(2S)-H(2S3)	109.5
C(6)-N(1)-Fe(1)	171.99(10)
C(8)-N(2)-Fe(1)	178.05(11)
C(10)-N(3)-Fe(1)	171.75(11)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for g473. 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)	9(1)	8(1)	10(1)	1(1)	0(1)	0(1)
P(1)	9(1)	8(1)	12(1)	1(1)	0(1)	0(1)
P(2)	10(1)	9(1)	11(1)	1(1)	-1(1)	0(1)
P(3)	9(1)	10(1)	11(1)	1(1)	0(1)	1(1)
B(2)	25(1)	20(1)	24(1)	9(1)	5(1)	1(1)
B(1)	28(1)	18(1)	25(1)	2(1)	2(1)	1(1)
C(1)	13(1)	10(1)	13(1)	2(1)	0(1)	1(1)
C(2)	13(1)	9(1)	15(1)	2(1)	0(1)	0(1)
C(3)	15(1)	11(1)	12(1)	2(1)	-2(1)	-1(1)
C(4)	13(1)	13(1)	14(1)	3(1)	0(1)	3(1)
C(5)	21(1)	12(1)	17(1)	5(1)	-1(1)	2(1)
C(6)	14(1)	14(1)	18(1)	1(1)	1(1)	-1(1)
C(7)	24(1)	21(1)	43(1)	-3(1)	-1(1)	11(1)
C(8)	16(1)	14(1)	16(1)	-1(1)	2(1)	0(1)
C(9)	24(1)	20(1)	29(1)	-1(1)	8(1)	-11(1)
C(10)	15(1)	15(1)	17(1)	-1(1)	0(1)	2(1)
C(11)	30(1)	33(1)	13(1)	1(1)	-3(1)	4(1)
C(1A)	10(1)	13(1)	17(1)	-2(1)	0(1)	-1(1)
C(2A)	15(1)	16(1)	24(1)	0(1)	-5(1)	0(1)
C(3A)	21(1)	25(1)	30(1)	-1(1)	-12(1)	2(1)
C(4A)	21(1)	27(1)	36(1)	-11(1)	-14(1)	0(1)
C(5A)	19(1)	16(1)	36(1)	-7(1)	-5(1)	-2(1)
C(6A)	15(1)	14(1)	23(1)	-1(1)	-1(1)	-1(1)
C(1B)	11(1)	12(1)	20(1)	-3(1)	4(1)	-3(1)
C(2B)	14(1)	30(1)	17(1)	-3(1)	2(1)	-2(1)
C(3B)	20(1)	48(1)	19(1)	-8(1)	6(1)	-5(1)
C(4B)	22(1)	33(1)	39(1)	-17(1)	16(1)	-5(1)
C(5B)	21(1)	15(1)	54(1)	-3(1)	16(1)	1(1)
C(6B)	17(1)	12(1)	35(1)	3(1)	9(1)	-1(1)
C(1C)	11(1)	15(1)	15(1)	-3(1)	-1(1)	-1(1)
C(2C)	17(1)	18(1)	18(1)	-3(1)	1(1)	-3(1)

C(3C)	21(1)	28(1)	19(1)	-6(1)	6(1)	-5(1)
C(4C)	15(1)	28(1)	28(1)	-13(1)	4(1)	0(1)
C(5C)	17(1)	19(1)	30(1)	-8(1)	-2(1)	3(1)
C(6C)	15(1)	17(1)	20(1)	-3(1)	-3(1)	1(1)
C(1D)	12(1)	14(1)	13(1)	0(1)	-2(1)	-2(1)
C(2D)	16(1)	14(1)	18(1)	-1(1)	-1(1)	-1(1)
C(3D)	20(1)	16(1)	20(1)	-2(1)	-1(1)	-6(1)
C(4D)	15(1)	26(1)	23(1)	-1(1)	-3(1)	-7(1)
C(5D)	14(1)	24(1)	36(1)	4(1)	-8(1)	0(1)
C(6D)	16(1)	16(1)	29(1)	4(1)	-6(1)	-1(1)
C(1E)	11(1)	14(1)	15(1)	-1(1)	2(1)	-1(1)
C(2E)	16(1)	42(1)	25(1)	13(1)	-2(1)	-4(1)
C(3E)	13(1)	60(1)	35(1)	14(1)	-5(1)	-9(1)
C(4E)	17(1)	32(1)	31(1)	0(1)	6(1)	-9(1)
C(5E)	21(1)	19(1)	22(1)	1(1)	8(1)	-2(1)
C(6E)	15(1)	17(1)	17(1)	1(1)	2(1)	1(1)
C(1F)	14(1)	10(1)	13(1)	1(1)	1(1)	0(1)
C(2F)	14(1)	19(1)	25(1)	-6(1)	1(1)	2(1)
C(3F)	20(1)	20(1)	28(1)	-9(1)	6(1)	3(1)
C(4F)	25(1)	16(1)	16(1)	-4(1)	2(1)	-1(1)
C(5F)	18(1)	18(1)	17(1)	-2(1)	-2(1)	0(1)
C(6F)	14(1)	15(1)	15(1)	-2(1)	1(1)	2(1)
C(1S)	28(1)	16(1)	24(1)	-1(1)	-1(1)	0(1)
C(2S)	28(1)	29(1)	56(1)	1(1)	10(1)	5(1)
F(4)	37(1)	32(1)	25(1)	5(1)	-2(1)	2(1)
F(2)	41(1)	29(1)	36(1)	-9(1)	-2(1)	7(1)
F(6)	50(1)	23(1)	43(1)	-1(1)	19(1)	-6(1)
F(7)	34(1)	29(1)	50(1)	3(1)	21(1)	4(1)
F(5)	33(1)	23(1)	31(1)	14(1)	2(1)	-3(1)
F(8)	36(1)	62(1)	35(1)	24(1)	-5(1)	-4(1)
F(3)	61(1)	78(1)	32(1)	2(1)	-5(1)	47(1)
F(1)	79(1)	39(1)	72(1)	-2(1)	23(1)	-34(1)
N(1)	12(1)	11(1)	12(1)	2(1)	1(1)	-2(1)
N(2)	13(1)	12(1)	12(1)	0(1)	1(1)	1(1)
N(3)	13(1)	11(1)	14(1)	0(1)	0(1)	1(1)
N(1S)	26(1)	30(1)	34(1)	-11(1)	0(1)	-2(1)

O(1W)	164(9)	137(8)	68(5)	-26(6)	-4(6)	-69(7)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for g473.

	x	y	z	U(eq)
H(2A)	4088	9080	4188	15
H(2B)	4596	8964	3474	15
H(3A)	3673	8070	2671	15
H(3B)	2471	8067	2672	15
H(4A)	1624	8452	3775	16
H(4B)	2172	9056	4222	16
H(5A)	3339	9378	2693	25
H(5B)	2945	9761	3363	25
H(5C)	2176	9322	2886	25
H(7A)	6226	5214	3839	44
H(7B)	5538	4757	4337	44
H(7C)	6397	5276	4639	44
H(9A)	684	5489	4757	36
H(9B)	1401	5166	5343	36
H(9C)	1478	4868	4587	36
H(11A)	5042	6855	6778	38
H(11B)	4316	6167	6738	38
H(11C)	3865	6942	6920	38
H(2A1)	6002	7363	5250	22
H(3A1)	7159	7849	6033	31
H(4A1)	7548	9080	6006	34
H(5A1)	6815	9819	5176	29
H(6A)	5654	9341	4393	20
H(2B1)	5296	8310	2717	24
H(3B1)	6484	7886	1952	35
H(4B1)	7554	6934	2251	38
H(5B1)	7530	6462	3349	36
H(6B)	6386	6909	4128	25
H(2C)	3796	7336	1925	21
H(3C)	4531	6605	1106	27

H(4C)	4920	5404	1351	29
H(5C1)	4622	4936	2425	26
H(6C)	3907	5665	3253	21
H(2D)	2190	5689	3281	19
H(3D)	573	5219	3125	23
H(4D)	-795	5991	2909	25
H(5D)	-524	7232	2831	30
H(6D)	1098	7708	2970	24
H(2E)	375	7980	4169	33
H(3E)	-1135	7463	4522	43
H(4E)	-1169	6738	5483	32
H(5E)	321	6543	6109	25
H(6E)	1829	7058	5765	19
H(2F)	1341	8846	5562	23
H(3F)	1707	9611	6471	27
H(4F)	3366	9754	6869	23
H(5F)	4657	9090	6375	21
H(6F)	4291	8297	5488	18
H(2S1)	2843	6075	9050	57
H(2S2)	2480	6012	8276	57
H(2S3)	2719	6787	8598	57

Table 6. Torsion angles [°] for g473.

C(5)-C(1)-C(2)-P(1)	-163.59(9)
C(3)-C(1)-C(2)-P(1)	-47.01(12)
C(4)-C(1)-C(2)-P(1)	79.45(11)
C(1B)-P(1)-C(2)-C(1)	99.06(10)
C(1A)-P(1)-C(2)-C(1)	-158.71(9)
Fe(1)-P(1)-C(2)-C(1)	-26.65(10)
C(5)-C(1)-C(3)-P(2)	-169.06(9)
C(2)-C(1)-C(3)-P(2)	74.01(12)
C(4)-C(1)-C(3)-P(2)	-51.72(13)
C(1C)-P(2)-C(3)-C(1)	-148.78(9)
C(1D)-P(2)-C(3)-C(1)	107.22(10)
Fe(1)-P(2)-C(3)-C(1)	-18.84(10)
C(5)-C(1)-C(4)-P(3)	-167.13(9)
C(3)-C(1)-C(4)-P(3)	75.64(12)
C(2)-C(1)-C(4)-P(3)	-49.93(12)
C(1E)-P(3)-C(4)-C(1)	-148.26(9)
C(1F)-P(3)-C(4)-C(1)	107.37(10)
Fe(1)-P(3)-C(4)-C(1)	-20.54(10)
C(1B)-P(1)-C(1A)-C(2A)	-86.94(11)
C(2)-P(1)-C(1A)-C(2A)	163.63(11)
Fe(1)-P(1)-C(1A)-C(2A)	38.90(12)
C(1B)-P(1)-C(1A)-C(6A)	91.59(11)
C(2)-P(1)-C(1A)-C(6A)	-17.84(12)
Fe(1)-P(1)-C(1A)-C(6A)	-142.58(9)
C(6A)-C(1A)-C(2A)-C(3A)	1.4(2)
P(1)-C(1A)-C(2A)-C(3A)	179.91(11)
C(1A)-C(2A)-C(3A)-C(4A)	-0.2(2)
C(2A)-C(3A)-C(4A)-C(5A)	-1.0(2)
C(3A)-C(4A)-C(5A)-C(6A)	1.1(2)
C(4A)-C(5A)-C(6A)-C(1A)	0.0(2)
C(2A)-C(1A)-C(6A)-C(5A)	-1.3(2)
P(1)-C(1A)-C(6A)-C(5A)	-179.81(11)
C(1A)-P(1)-C(1B)-C(2B)	-113.63(12)
C(2)-P(1)-C(1B)-C(2B)	-8.89(13)

Fe(1)-P(1)-C(1B)-C(2B)	114.92(11)
C(1A)-P(1)-C(1B)-C(6B)	64.19(11)
C(2)-P(1)-C(1B)-C(6B)	168.93(10)
Fe(1)-P(1)-C(1B)-C(6B)	-67.26(11)
C(6B)-C(1B)-C(2B)-C(3B)	2.8(2)
P(1)-C(1B)-C(2B)-C(3B)	-179.44(11)
C(1B)-C(2B)-C(3B)-C(4B)	0.6(2)
C(2B)-C(3B)-C(4B)-C(5B)	-2.8(2)
C(3B)-C(4B)-C(5B)-C(6B)	1.7(2)
C(4B)-C(5B)-C(6B)-C(1B)	1.8(2)
C(2B)-C(1B)-C(6B)-C(5B)	-3.9(2)
P(1)-C(1B)-C(6B)-C(5B)	178.10(11)
C(1D)-P(2)-C(1C)-C(2C)	94.33(11)
C(3)-P(2)-C(1C)-C(2C)	-13.59(12)
Fe(1)-P(2)-C(1C)-C(2C)	-139.59(9)
C(1D)-P(2)-C(1C)-C(6C)	-79.33(11)
C(3)-P(2)-C(1C)-C(6C)	172.75(10)
Fe(1)-P(2)-C(1C)-C(6C)	46.74(11)
C(6C)-C(1C)-C(2C)-C(3C)	-0.21(19)
P(2)-C(1C)-C(2C)-C(3C)	-173.86(10)
C(1C)-C(2C)-C(3C)-C(4C)	0.8(2)
C(2C)-C(3C)-C(4C)-C(5C)	-0.9(2)
C(3C)-C(4C)-C(5C)-C(6C)	0.5(2)
C(4C)-C(5C)-C(6C)-C(1C)	0.1(2)
C(2C)-C(1C)-C(6C)-C(5C)	-0.23(19)
P(2)-C(1C)-C(6C)-C(5C)	173.66(10)
C(1C)-P(2)-C(1D)-C(6D)	-124.82(12)
C(3)-P(2)-C(1D)-C(6D)	-18.03(13)
Fe(1)-P(2)-C(1D)-C(6D)	106.51(11)
C(1C)-P(2)-C(1D)-C(2D)	56.22(11)
C(3)-P(2)-C(1D)-C(2D)	163.01(10)
Fe(1)-P(2)-C(1D)-C(2D)	-72.45(11)
C(6D)-C(1D)-C(2D)-C(3D)	-1.2(2)
P(2)-C(1D)-C(2D)-C(3D)	177.82(10)
C(1D)-C(2D)-C(3D)-C(4D)	0.0(2)
C(2D)-C(3D)-C(4D)-C(5D)	0.7(2)

C(3D)-C(4D)-C(5D)-C(6D)	-0.2(2)
C(2D)-C(1D)-C(6D)-C(5D)	1.7(2)
P(2)-C(1D)-C(6D)-C(5D)	-177.29(12)
C(4D)-C(5D)-C(6D)-C(1D)	-1.0(2)
C(1F)-P(3)-C(1E)-C(2E)	117.47(13)
C(4)-P(3)-C(1E)-C(2E)	11.58(14)
Fe(1)-P(3)-C(1E)-C(2E)	-115.26(13)
C(1F)-P(3)-C(1E)-C(6E)	-63.62(11)
C(4)-P(3)-C(1E)-C(6E)	-169.51(10)
Fe(1)-P(3)-C(1E)-C(6E)	63.65(11)
C(6E)-C(1E)-C(2E)-C(3E)	-1.1(2)
P(3)-C(1E)-C(2E)-C(3E)	177.83(14)
C(1E)-C(2E)-C(3E)-C(4E)	0.2(3)
C(2E)-C(3E)-C(4E)-C(5E)	0.6(3)
C(3E)-C(4E)-C(5E)-C(6E)	-0.5(2)
C(4E)-C(5E)-C(6E)-C(1E)	-0.4(2)
C(2E)-C(1E)-C(6E)-C(5E)	1.2(2)
P(3)-C(1E)-C(6E)-C(5E)	-177.79(10)
C(1E)-P(3)-C(1F)-C(6F)	144.88(11)
C(4)-P(3)-C(1F)-C(6F)	-105.84(11)
Fe(1)-P(3)-C(1F)-C(6F)	19.39(12)
C(1E)-P(3)-C(1F)-C(2F)	-37.40(12)
C(4)-P(3)-C(1F)-C(2F)	71.88(12)
Fe(1)-P(3)-C(1F)-C(2F)	-162.88(9)
C(6F)-C(1F)-C(2F)-C(3F)	0.2(2)
P(3)-C(1F)-C(2F)-C(3F)	-177.59(11)
C(1F)-C(2F)-C(3F)-C(4F)	1.0(2)
C(2F)-C(3F)-C(4F)-C(5F)	-1.2(2)
C(3F)-C(4F)-C(5F)-C(6F)	0.2(2)
C(2F)-C(1F)-C(6F)-C(5F)	-1.24(19)
P(3)-C(1F)-C(6F)-C(5F)	176.54(10)
C(4F)-C(5F)-C(6F)-C(1F)	1.0(2)

Symmetry transformations used to generate equivalent atoms: