Crystal structure of *bis*-(3-butyl-1-(1,10-phenanthrolin-2-yl) imidazolylidene)iridium(III) *tris*-hexafluorophosphate acetonitrile monosolvate, $[Ir(C_{19}H_{18}N_4)_2(PF_6)_3]\cdot(C_2H_3N)$, $C_{40}H_{39}F_{18}IrN_9P_3$

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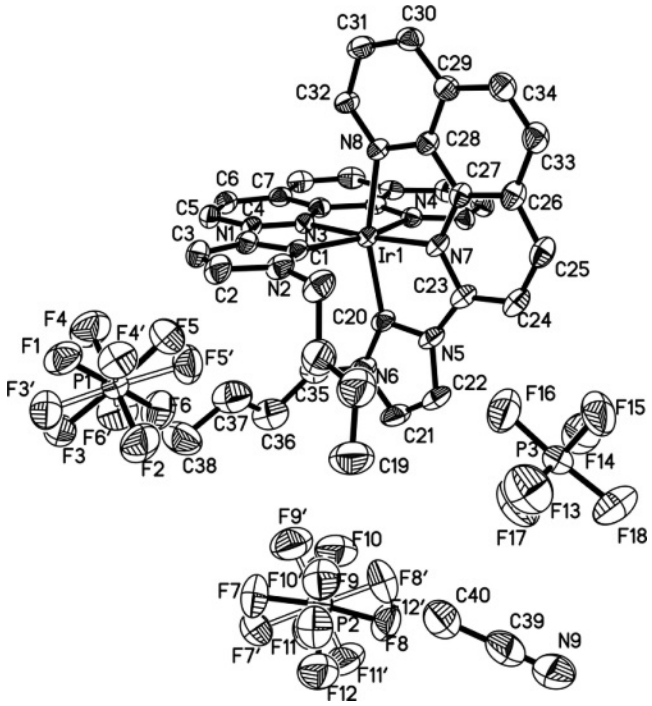

Abstract

$C_{40}H_{39}F_{18}IrN_9P_3$, triclinic, $P\bar{1}$ (no. 2), a = 13.199(1) Å, b = 13.452(1) Å, c = 13.453(1) Å, α = 88.099(2)°, β = 79.526(1)°, γ = 89.597(2)°, V = 2347.4 Å^3, Z = 2, $R_{gt}(F)$ = 0.0500, $wR_{ref}(F^2)$ = 0.1365, T = 298 K.

Table 1. Data collection and handling.

Crystal:	white blocks, size 0.17×0.22×0.45 mm
Wavelength:	Mo K_α radiation (0.71073 Å)
μ:	30.60 cm^{-1}
Diffractometer, scan mode:	Bruker SMART CCD, φ and ω
$2\theta_{max}$:	50.04°
$N(hkl)_{measured}$, $N(hkl)_{unique}$:	12266, 8149
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\ \sigma(I_{obs})$, 6428
$N(param)_{refined}$:	736
Programs:	SHELX [7]

Source of material

A solution of 3-butyl-1-(1,10-phenanthrolin-2-yl)imidazolylidene hexafluorophosphate (90 mg, 0.20 mmol) in 6 mL of acetonitrile was treated with Ag_2O (67 mg, 0.10 mmol) at 50 °C. After 8 h, Ag_2O completely disappeared, and $[IrCl(cod)]_2$ (66 mg, 0.10 mmol) was added. After it was stirred for 6 h at room temperature, the solution was filtered. The filtrate was concentrated to dryness, and the residue was washed with diethyl ether. Yield: 58 mg, 46 %. White air stable single crystals were grown by slow diffusion of Et_2O into concentrated CH_3CN solutions.

^{1}H NMR (DMSO-d$_6$, 400 Hz): 9.47 (*d*, J = 8.8 Hz, phen, 2*H*), 9.05 (*d*, J = 9.2 Hz, phen, 2*H*), 8.90 (*d*, J = 7.6 Hz, phen, 2*H*), 8.86 (*d*, J = 2.4 Hz, NCHCHN, 2*H*), 8.58 (*d*, J = 8.4 Hz, phen, 2*H*), 8.46 (*d*, J = 9.2 Hz, phen, 2*H*), 8.17 (*d*, J = 5.6 Hz, phen, 2*H*), 7.80-7.76 (*m*, phen, 2*H*), 7.73 (*d*, J = 2.8 Hz, NCHCHN, 2*H*), 3.13-3.07 (*m*, CH2, 2*H*), 2.88-2.82 (*m*, CH2, 2*H*), 0.72-0.69 (*m*, CH2, 2*H*), 0.41-0.22 (*m*, CH2 + CH3, 12*H*).

Discussion

N-Heterocyclic carbene (NHC) compounds have become a class of important ligands in organometallic chemistry and homogeneous catalysis due to their unique electronic and structural properties [1-2]. Transition metal complexes of *N*-heterocyclic carbenes are an important class of catalysts in organometallic chemistry [3] and organic synthesis [4]. We here report the crystal structure of the title compound. In the title crystal structure, the Ir ion is hexacoordinate and surrounded by two 3-butyl-1-(1,10-phenanthrolin-2-yl)imidazolylidene ligands with one acetonitrile of crystallization. The high R value of title compound may be caused by disorder of the F atoms in the PF_6 group.The geometry around the iridium is distorted octahedral with two NHC units *trans* to two phenanthroline nitrogen atoms, similar to reported iridium(III) complex [5]. The two phenanthroline rings are perpendicular to each other with a bite angle of 86.67°. The compound crystallized in the triclinic space group $P\bar{1}$, whereas the previously reported analogous Ru(II) complex $[Ru(C_{19}H_{18}N_4)_2(PF_6)_2]$ crystallized in the monoclinic space group *C*2/*c* [6].

Table 2. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	x	y	z	U_{iso}
H(2)	2*i*	0.4359	0.1148	0.0580	0.086
H(3)	2*i*	0.5163	–0.0260	0.1303	0.078
H(5)	2*i*	0.6579	–0.1157	0.2237	0.070
H(6)	2*i*	0.7894	–0.1614	0.3053	0.069
H(11)	2*i*	1.1036	0.2055	0.3900	0.073
H(12)	2*i*	1.0578	0.3616	0.3434	0.073
H(13)	2*i*	0.9165	0.3853	0.2666	0.058
H(14)	2*i*	0.9580	–0.1088	0.3737	0.072
H(15)	2*i*	1.0639	0.0141	0.3958	0.074
H(16A)	2*i*	0.4959	0.2997	0.0031	0.099
H(16B)	2*i*	0.5783	0.3461	0.0595	0.099
H(17A)	2*i*	0.3790	0.2809	0.1636	0.126
H(17B)	2*i*	0.4603	0.3317	0.2170	0.126
H(18A)	2*i*	0.3616	0.4298	0.0732	0.160
H(18B)	2*i*	0.4408	0.4805	0.1299	0.160

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Table 2. continued.

Atom	Site	x	y	z	U_{iso}
H(19A)	2*i*	0.2444	0.4077	0.2219	0.213
H(19B)	2*i*	0.2799	0.5189	0.2187	0.213
H(19C)	2*i*	0.3256	0.4397	0.2865	0.213
H(21)	2*i*	0.4882	0.3697	0.4899	0.093
H(22)	2*i*	0.5460	0.5061	0.3767	0.087
H(24)	2*i*	0.6694	0.5982	0.2188	0.078
H(25)	2*i*	0.7746	0.6469	0.0689	0.079
H(30)	2*i*	1.0104	0.2752	–0.2060	0.070
H(31)	2*i*	0.9752	0.1213	–0.1400	0.078
H(32)	2*i*	0.8827	0.0965	0.0216	0.060
H(33)	2*i*	0.9042	0.5922	–0.0939	0.082
H(34)	2*i*	0.9796	0.4661	–0.1863	0.080

Table 2. continued.

Atom	Site	x	y	z	U_{iso}
H(35A)	2*i*	0.6049	0.1782	0.4987	0.103
H(35B)	2*i*	0.6089	0.1326	0.3926	0.103
H(36A)	2*i*	0.4596	0.0896	0.5200	0.153
H(36B)	2*i*	0.4204	0.1984	0.5039	0.153
H(37A)	2*i*	0.4643	0.0627	0.3493	0.15
H(37B)	2*i*	0.4201	0.1697	0.3368	0.15
H(38A)	2*i*	0.306	0.0173	0.4574	0.199
H(38B)	2*i*	0.2894	0.0477	0.348	0.199
H(38C)	2*i*	0.262	0.1228	0.4356	0.199
H(40A)	2*i*	0.1993	0.6129	0.4475	0.188
H(40B)	2*i*	0.1938	0.6501	0.337	0.188
H(40C)	2*i*	0.0923	0.637	0.4173	0.188

Table 3. Atomic coordinates and displacement parameters (in Å^2).

Atom	Site	Occ.	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ir(1)	2*i*		0.74848(2)	0.24097(2)	0.19084(2)	0.0444(2)	0.0380(2)	0.0384(2)	0.0022(1)	–0.0095(1)	–0.0078(1)
F(1)	2*i*		0.2540(6)	0.0375(6)	0.0379(8)	0.106(6)	0.115(6)	0.179(9)	0.039(5)	–0.026(6)	–0.047(6)
F(2)	2*i*		0.1025(6)	0.2179(5)	0.0781(7)	0.115(6)	0.083(5)	0.168(8)	0.031(4)	–0.031(5)	–0.022(5)
F(3)	2*i*	0.68	0.090(1)	0.061(1)	0.123(1)	0.12(1)	0.106(9)	0.09(1)	–0.037(7)	0.03(1)	–0.024(9)
F(4)	2*i*	0.68	0.1404(9)	0.088(1)	–0.0364(9)	0.104(9)	0.12(1)	0.074(8)	0.012(8)	–0.021(6)	–0.034(8)
F(5)	2*i*	0.68	0.271(1)	0.185(1)	–0.004(2)	0.11(1)	0.11(1)	0.11(1)	–0.028(8)	0.02(1)	0.000(9)
F(6)	2*i*	0.68	0.217(1)	0.154(2)	0.161(1)	0.12(1)	0.13(2)	0.10(1)	–0.01(1)	–0.044(8)	–0.04(1)
F(7)	2*i*	0.49	0.133(3)	0.285(2)	0.563(2)	0.16(3)	0.08(1)	0.13(3)	–0.03(2)	–0.05(2)	–0.00(2)
F(8)	2*i*	0.49	0.205(2)	0.494(2)	0.605(2)	0.13(2)	0.09(1)	0.12(2)	–0.01(1)	–0.04(2)	–0.03(1)
F(9)	2*i*	0.49	0.175(2)	0.414(2)	0.469(1)	0.16(2)	0.13(2)	0.08(1)	–0.02(2)	–0.03(1)	–0.00(1)
F(10)	2*i*	0.49	0.285(2)	0.360(3)	0.565(3)	0.11(2)	0.16(3)	0.15(3)	0.03(2)	–0.00(2)	–0.01(2)
F(11)	2*i*	0.49	0.166(2)	0.347(2)	0.691(1)	0.15(2)	0.12(2)	0.10(1)	–0.02(2)	–0.01(1)	0.02(1)
F(12)	2*i*	0.49	0.063(2)	0.440(2)	0.609(2)	0.12(2)	0.15(2)	0.16(3)	0.02(1)	–0.02(2)	–0.02(2)
F(3')	2*i*	0.32	0.083(2)	0.064(2)	0.054(4)	0.10(2)	0.10(2)	0.13(4)	–0.01(1)	–0.02(3)	–0.02(2)
F(4')	2*i*	0.32	0.166(2)	0.176(3)	–0.052(2)	0.10(2)	0.10(3)	0.08(2)	0.02(2)	–0.03(1)	–0.00(1)
F(5')	2*i*	0.32	0.266(3)	0.210(3)	0.053(3)	0.09(2)	0.09(2)	0.13(3)	–0.02(1)	–0.04(2)	–0.02(2)
F(6')	2*i*	0.32	0.185(3)	0.095(3)	0.162(3)	0.13(3)	0.12(3)	0.10(2)	0.02(2)	–0.02(2)	0.00(2)
F(7')	2*i*	0.51	0.090(2)	0.303(3)	0.604(2)	0.11(2)	0.11(2)	0.12(2)	–0.03(1)	0.02(1)	0.01(1)
F(8')	2*i*	0.51	0.255(2)	0.472(2)	0.548(3)	0.12(2)	0.13(2)	0.17(3)	–0.05(2)	–0.03(2)	0.01(2)
F(9')	2*i*	0.51	0.225(2)	0.324(2)	0.482(2)	0.14(2)	0.17(2)	0.14(2)	0.02(2)	–0.00(1)	–0.06(2)
F(10')	2*i*	0.51	0.257(2)	0.334(2)	0.627(2)	0.13(3)	0.12(2)	0.12(2)	0.02(2)	–0.06(2)	0.01(2)
F(11')	2*i*	0.51	0.133(2)	0.439(2)	0.674(2)	0.15(2)	0.15(2)	0.13(2)	0.02(2)	–0.01(2)	–0.06(2)
F(12')	2*i*	0.51	0.100(2)	0.435(2)	0.510(2)	0.12(2)	0.11(1)	0.12(2)	0.00(1)	–0.07(2)	0.02(1)
F(13)	2*i*		0.3595(7)	0.7390(9)	0.2057(9)	0.123(7)	0.19(1)	0.19(1)	0.002(7)	–0.063(7)	0.022(8)
F(14)	2*i*		0.5601(7)	0.7270(7)	0.2964(8)	0.109(6)	0.135(7)	0.189(9)	0.015(5)	–0.055(6)	–0.033(7)
F(15)	2*i*		0.5218(9)	0.7880(7)	0.1551(6)	0.22(1)	0.161(8)	0.089(6)	–0.104(8)	0.034(6)	–0.031(6)
F(16)	2*i*		0.4852(7)	0.6357(6)	0.1937(8)	0.149(8)	0.101(6)	0.187(9)	–0.013(5)	–0.035(7)	–0.042(6)
F(17)	2*i*		0.4039(8)	0.6816(9)	0.3431(8)	0.165(9)	0.20(1)	0.137(8)	–0.062(8)	–0.013(7)	0.039(7)
F(18)	2*i*		0.4441(8)	0.8392(6)	0.2995(7)	0.188(9)	0.111(6)	0.128(7)	0.048(6)	–0.021(6)	–0.037(5)
N(1)	2*i*		0.6221(5)	0.0780(6)	0.1605(5)	0.051(4)	0.061(5)	0.044(4)	–0.004(4)	–0.012(3)	–0.015(3)
N(2)	2*i*		0.5514(6)	0.2016(6)	0.0954(6)	0.057(5)	0.077(6)	0.057(5)	0.009(4)	–0.023(4)	–0.024(4)
N(3)	2*i*		0.7594(5)	0.0983(5)	0.2313(5)	0.045(4)	0.039(4)	0.039(4)	–0.003(3)	–0.006(3)	–0.007(3)
N(4)	2*i*		0.8798(5)	0.2455(5)	0.2622(5)	0.041(4)	0.053(4)	0.040(4)	–0.002(3)	–0.008(3)	–0.009(3)
N(5)	2*i*		0.6434(6)	0.4051(6)	0.2912(6)	0.065(5)	0.055(5)	0.052(5)	0.012(4)	–0.010(4)	–0.024(4)
N(6)	2*i*		0.5873(6)	0.2808(6)	0.3909(6)	0.074(5)	0.074(6)	0.051(5)	0.003(4)	–0.005(4)	–0.026(4)
N(7)	2*i*		0.7513(5)	0.3844(5)	0.1471(5)	0.054(4)	0.040(4)	0.043(4)	0.010(3)	–0.017(3)	–0.014(3)
N(8)	2*i*		0.8468(5)	0.2361(5)	0.0461(5)	0.049(4)	0.041(4)	0.038(4)	0.004(3)	–0.010(3)	–0.007(3)
N(9)	2*i*		0.182(1)	0.837(1)	0.471(1)	0.14(1)	0.15(1)	0.14(1)	–0.01(1)	0.04(1)	–0.00(1)
P(1)	2*i*		0.1778(2)	0.1285(2)	0.0592(2)	0.059(2)	0.063(2)	0.061(2)	–0.003(1)	–0.004(1)	–0.011(1)
P(2)	2*i*		0.1743(2)	0.3875(2)	0.5757(2)	0.083(2)	0.065(2)	0.064(2)	–0.007(2)	–0.027(2)	0.001(1)
P(3)	2*i*		0.4602(2)	0.7366(2)	0.2477(3)	0.068(2)	0.083(2)	0.081(2)	–0.007(2)	0.004(2)	–0.005(2)
C(1)	2*i*		0.6289(6)	0.1797(6)	0.1395(6)	0.048(5)	0.052(5)	0.040(5)	0.001(4)	–0.010(4)	–0.015(4)
C(2)	2*i*		0.4948(8)	0.1170(9)	0.0869(8)	0.067(7)	0.085(8)	0.072(7)	–0.002(6)	–0.031(5)	–0.029(6)
C(3)	2*i*		0.5379(8)	0.0399(8)	0.1263(7)	0.065(6)	0.075(7)	0.061(6)	–0.011(5)	–0.020(5)	–0.026(5)
C(4)	2*i*		0.6947(6)	0.0319(6)	0.2098(6)	0.055(5)	0.048(5)	0.037(4)	–0.006(4)	–0.004(4)	–0.011(4)
C(5)	2*i*		0.7042(8)	–0.0685(7)	0.2375(7)	0.069(6)	0.047(5)	0.054(6)	–0.011(5)	0.000(5)	–0.006(4)
C(6)	2*i*		0.7832(8)	–0.0951(7)	0.2854(7)	0.075(7)	0.042(5)	0.050(5)	0.000(5)	0.001(5)	0.002(4)
C(7)	2*i*		0.8561(7)	–0.0258(6)	0.3059(6)	0.060(5)	0.049(5)	0.038(5)	0.005(4)	0.001(4)	–0.001(4)
C(8)	2*i*		0.8405(6)	0.0732(6)	0.2769(6)	0.048(5)	0.047(5)	0.036(4)	0.003(4)	–0.004(4)	0.001(4)
C(9)	2*i*		0.9042(6)	0.1522(6)	0.2931(6)	0.046(5)	0.046(5)	0.034(4)	–0.001(4)	–0.004(3)	–0.005(4)
C(10)	2*i*		0.9882(6)	0.1317(7)	0.3394(6)	0.043(5)	0.068(6)	0.042(5)	0.006(4)	–0.003(4)	–0.002(4)
C(11)	2*i*		1.0468(7)	0.2147(8)	0.3586(7)	0.053(6)	0.076(7)	0.054(6)	–0.001(5)	–0.012(4)	–0.004(5)

Table 3. continued.

Atom	Site	Occ.	*x*	*y*	*z*	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(12)	2*i*		1.0197(7)	0.3070(8)	0.3309(7)	0.056(6)	0.077(7)	0.052(6)	–0.017(5)	–0.013(4)	–0.007(5)
C(13)	2*i*		0.9349(6)	0.3209(7)	0.2836(6)	0.048(5)	0.053(5)	0.044(5)	–0.013(4)	–0.008(4)	–0.005(4)
C(14)	2*i*		0.9442(7)	–0.0442(7)	0.3528(7)	0.067(6)	0.059(6)	0.050(5)	0.015(5)	–0.005(5)	0.008(5)
C(15)	2*i*		1.0065(8)	0.0292(8)	0.3670(7)	0.061(6)	0.077(7)	0.046(5)	0.014(5)	–0.009(4)	0.005(5)
C(16)	2*i*		0.5208(9)	0.3003(9)	0.0666(9)	0.086(8)	0.089(8)	0.084(8)	0.017(6)	–0.041(6)	–0.030(7)
C(17)	2*i*		0.433(1)	0.331(1)	0.155(1)	0.088(9)	0.10(1)	0.13(1)	0.006(8)	–0.034(8)	–0.015(9)
C(18)	2*i*		0.388(1)	0.430(1)	0.136(1)	0.12(1)	0.14(1)	0.15(2)	0.00(1)	–0.03(1)	–0.04(1)
C(19)	2*i*		0.302(1)	0.451(1)	0.224(1)	0.10(1)	0.18(2)	0.15(2)	0.02(1)	–0.01(1)	–0.06(1)
C(20)	2*i*		0.6530(7)	0.3021(7)	0.3066(6)	0.054(5)	0.059(6)	0.041(5)	0.002(4)	–0.011(4)	–0.021(4)
C(21)	2*i*		0.5365(9)	0.3666(9)	0.4304(9)	0.078(7)	0.086(8)	0.063(7)	0.010(6)	0.004(6)	–0.034(6)
C(22)	2*i*		0.5686(8)	0.4406(9)	0.3697(8)	0.085(8)	0.065(7)	0.066(7)	0.017(6)	–0.005(6)	–0.031(6)
C(23)	2*i*		0.6995(7)	0.4511(7)	0.2062(7)	0.064(6)	0.049(5)	0.049(5)	0.014(4)	–0.014(4)	–0.015(4)
C(24)	2*i*		0.7064(8)	0.5511(7)	0.1778(8)	0.081(7)	0.047(6)	0.071(7)	0.017(5)	–0.025(6)	–0.017(5)
C(25)	2*i*		0.7687(8)	0.5798(7)	0.0882(8)	0.090(7)	0.041(5)	0.069(7)	0.008(5)	–0.025(6)	–0.003(5)
C(26)	2*i*		0.8242(8)	0.5077(7)	0.0250(7)	0.076(6)	0.046(5)	0.057(6)	0.005(5)	–0.024(5)	0.000(4)
C(27)	2*i*		0.8133(6)	0.4097(6)	0.0591(6)	0.057(5)	0.041(5)	0.042(5)	0.001(4)	–0.016(4)	–0.002(4)
C(28)	2*i*		0.8637(6)	0.3299(6)	0.0040(6)	0.054(5)	0.039(5)	0.045(5)	0.005(4)	–0.013(4)	–0.001(4)
C(29)	2*i*		0.9249(7)	0.3495(7)	–0.0902(7)	0.062(6)	0.052(5)	0.045(5)	–0.001(4)	–0.007(4)	0.004(4)
C(30)	2*i*		0.9683(7)	0.2665(7)	–0.1430(7)	0.065(6)	0.059(6)	0.046(5)	0.003(5)	0.000(4)	0.002(4)
C(31)	2*i*		0.9492(8)	0.1760(8)	–0.1030(7)	0.070(6)	0.060(6)	0.059(6)	0.010(5)	0.003(5)	–0.011(5)
C(32)	2*i*		0.8909(7)	0.1608(7)	–0.0064(6)	0.058(5)	0.046(5)	0.045(5)	0.008(4)	–0.004(4)	–0.003(4)
C(33)	2*i*		0.8919(8)	0.5270(7)	–0.0698(8)	0.091(8)	0.050(6)	0.064(6)	–0.003(5)	–0.015(6)	0.012(5)
C(34)	2*i*		0.9378(8)	0.4515(7)	–0.1242(8)	0.083(7)	0.059(6)	0.056(6)	–0.005(5)	–0.006(5)	0.011(5)
C(35)	2*i*		0.5726(9)	0.1799(9)	0.4394(9)	0.087(8)	0.088(9)	0.074(8)	–0.006(7)	0.010(6)	–0.015(7)
C(36)	2*i*		0.462(1)	0.145(1)	0.471(1)	0.13(1)	0.13(1)	0.12(1)	0.01(1)	0.00(1)	–0.03(1)
C(37)	2*i*		0.419(1)	0.113(1)	0.384(1)	0.12(1)	0.15(2)	0.11(1)	0.02(1)	–0.02(1)	–0.02(1)
C(38)	2*i*		0.309(1)	0.071(1)	0.409(1)	0.08(1)	0.18(2)	0.13(1)	–0.00(1)	–0.014(9)	–0.01(1)
C(39)	2*i*		0.172(1)	0.761(2)	0.437(2)	0.11(1)	0.15(2)	0.12(1)	–0.03(1)	0.03(1)	–0.00(1)
C(40)	2*i*		0.164(1)	0.656(1)	0.407(1)	0.11(1)	0.13(1)	0.13(1)	–0.02(1)	–0.006(9)	0.00(1)

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