CALIFORNIA INSTITUTE OF TECHNOLOGY

BECKMAN INSTITUTE

X-RAY CRYSTALLOGRAPHY LABORATORY

Date 24 January 2008

Crystal Structure Analysis of:

JHP107

(shown below)

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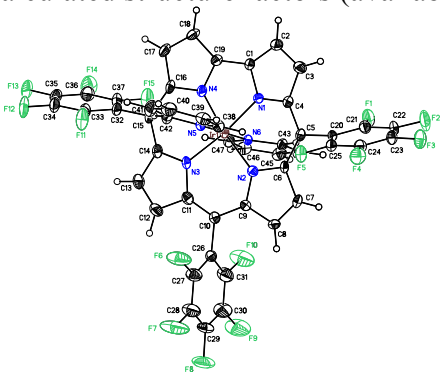


JHP107

Note: The crystallographic data have been deposited in the Cambridge Database (CCDC) and has been placed on hold pending further instructions from me. The deposition number is 657603. Ideally the CCDC would like the publication to contain a footnote of the type: "Crystallographic data have been deposited at the CCDC, 12 Union Road, Cambridge CB2 1EZ, UK and copies can be obtained on request, free of charge, by quoting the publication citation and the deposition number 657603."

Table 1. Crystal data and structure refinement for JHP107 (CCDC 657603).

Empirical formula	$C_{47}H_{18}N_6F_{15}Ir$, $3(CH_4O)$
Formula weight	1240.00
Crystallization Solvent	Methanol
Crystal Habit	Column
Crystal size	0.31 x 0.12 x 0.07 mm^3
Crystal color	Dark red

Data Collection

Type of diffractometer	Bruker KAPPA APEX II
Wavelength	0.71073 Å MoKα
Data Collection Temperature	100(2) K
θ range for 9608 reflections used in lattice determination	2.39 to 32.74°
Unit cell dimensions	a = 48.016(2) Å b = 8.7249(4) Å β= 124.247(2)° c = 27.2703(13) Å
Volume	9443.7(8) $Å^3$
Z	8
Crystal system	Monoclinic
Space group	C2/c
Density (calculated)	1.744 Mg/m^3
F(000)	4864
θ range for data collection	1.81 to 32.95°
Completeness to θ = 32.95°	98.5 %
Index ranges	$-73 \leq h \leq 72$, $-11 \leq k \leq 13$, $-40 \leq l \leq 41$
Data collection scan type	ω scans; 21 settings
Reflections collected	112588
Independent reflections	17484 [R_{int}= 0.0721]
Absorption coefficient	2.938 mm^{-1}
Absorption correction	None
Max. and min. transmission (calc)	0.8208 and 0.4628

Table 1 (cont.)

Structure solution and Refinement

Structure solution program	SHELXS-97 (Sheldrick, 1990)
Primary solution method	Patterson method
Secondary solution method	Difference Fourier map
Hydrogen placement	Geometric positions
Structure refinement program	SHELXL-97 (Sheldrick, 1997)
Refinement method	Full matrix least-squares on F^2
Data / restraints / parameters	17484 / 54 / 695
Treatment of hydrogen atoms	Riding
Goodness-of-fit on F^2	1.520
Final R indices [$I>2\sigma(I)$, 12341 reflections]	R1 = 0.0441, *w*R2 = 0.0563
R indices (all data)	R1 = 0.0761, *w*R2 = 0.0580
Type of weighting scheme used	Sigma
Weighting scheme used	$w=1/\sigma^2(Fo^2)$
Max shift/error	0.007
Average shift/error	0.000
Largest diff. peak and hole	4.237 and -2.827 e.Å^{-3}

Special Refinement Details

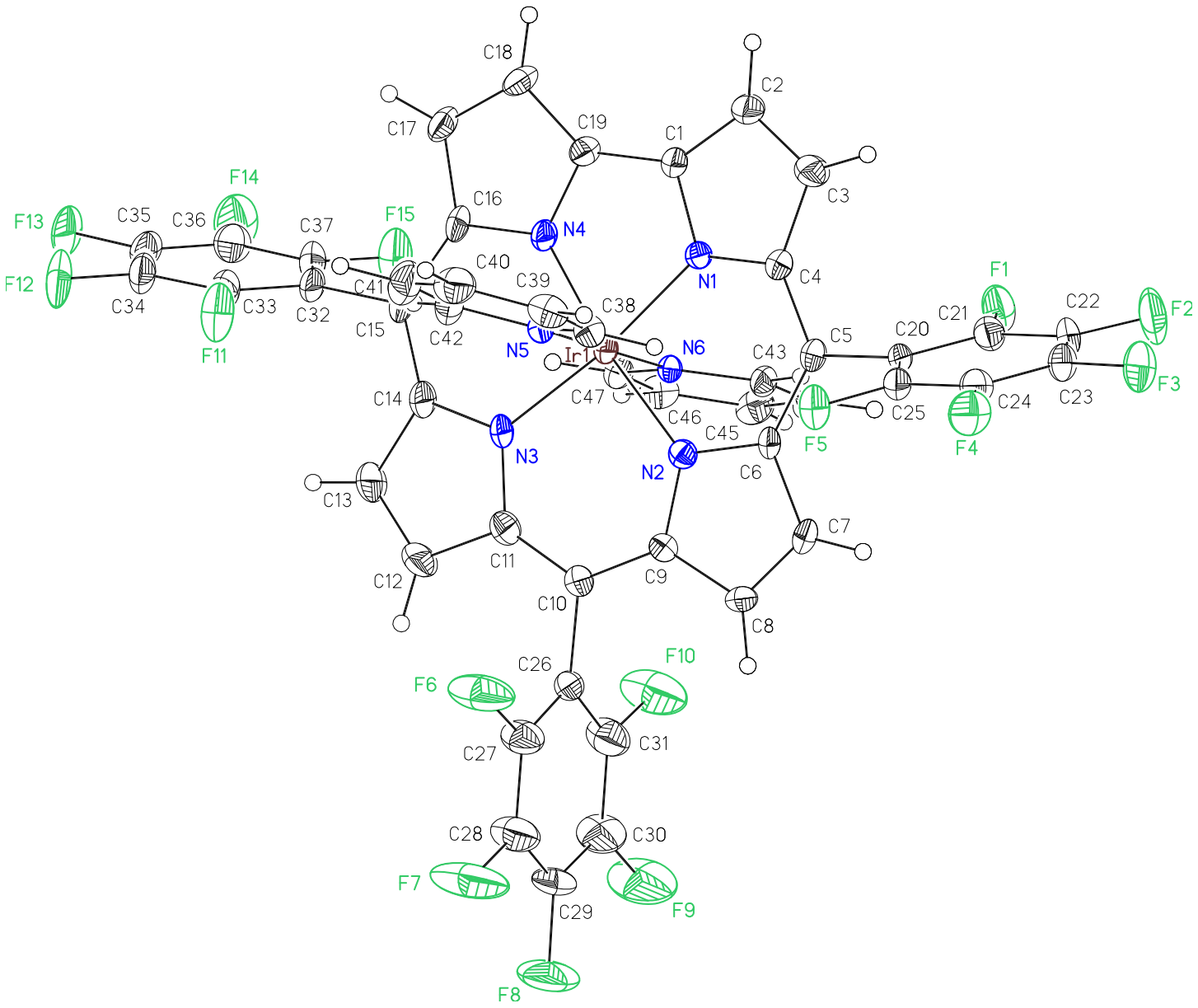
Crystals were mounted on a glass fiber using Paratone oil then placed on the diffractometer under a nitrogen stream at 100K.

The crystals contain methanol as a solvent of crystallization, three in the asymmetric unit. One of those three is disordered between two positions. The disorder was model with restraint on the C-O bond distances and on the anisotropic displacement parameters (ADP). In the solvent only C-O distances were restrained to have similar distances, the ADP's restrained to mimic isotropic behavior and for the disordered site the population was restrained so the occupancies summed to one.

See tables at the end for planarity of the corrole and comparison to JHP104.

Refinement of F^2 against ALL reflections. The weighted R-factor (*w*R) and goodness 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 threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) 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.

All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.


C18
C2
C17
C19
C1
C3
F14
F13
C35
C36
C16
N4
F15
C37
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C39
N1
C4
F1
F12
C34
C33
C32
C41
C38
C21
C22
F2
C15
C42
N5
Ir1
N6
C43
C5
C20
F11
C14
C47
C46
C25
C24
C23
F3
C45
F5
F4
N3
N2
C6
C13
C7
C11
C9
C12
C10
C8
C26
F10
F6
C27
C31
C28
C30
F7
C29
F9
F8

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for JHP107 (CCDC 657603). U(eq) is defined a the trace of the orthogonalized U^{ij} tensor.

	x	y	z		U_{eq}
Ir(1)	5966(1)	2657(1)	37(1)	17(1)	1
F(1)	5516(1)	3864(2)	1516(1)	36(1)	1
F(2)	5321(1)	2868(2)	2209(1)	50(1)	1
F(3)	5304(1)	-171(2)	2394(1)	45(1)	1
F(4)	5495(1)	-2227(2)	1892(1)	36(1)	1
F(5)	5695(1)	-1256(2)	1201(1)	29(1)	1
F(6)	7064(1)	-1186(2)	1111(1)	60(1)	1
F(7)	7708(1)	-1870(2)	1935(1)	79(1)	1
F(8)	8128(1)	299(2)	2706(1)	67(1)	1
F(9)	7893(1)	3140(2)	2662(1)	79(1)	1
F(10)	7246(1)	3836(2)	1831(1)	66(1)	1
F(11)	6131(1)	1475(2)	-1786(1)	44(1)	1
F(12)	6229(1)	2374(2)	-2618(1)	48(1)	1
F(13)	6261(1)	5398(2)	-2813(1)	44(1)	1
F(14)	6212(1)	7524(2)	-2139(1)	50(1)	1
F(15)	6118(1)	6640(2)	-1299(1)	44(1)	1
N(1)	5548(1)	2875(2)	-7(1)	18(1)	1
N(2)	6212(1)	1834(2)	853(1)	17(1)	1
N(3)	6356(1)	2535(3)	-27(1)	21(1)	1
N(4)	5672(1)	3499(2)	-758(1)	19(1)	1
N(5)	5804(1)	504(2)	-333(1)	19(1)	1
N(6)	6125(1)	4806(2)	395(1)	17(1)	1
C(1)	5268(1)	3338(3)	-542(1)	20(1)	1
C(2)	4995(1)	3231(3)	-476(2)	26(1)	1
C(3)	5117(1)	2679(3)	84(1)	27(1)	1
C(4)	5474(1)	2447(3)	381(1)	19(1)	1
C(5)	5725(1)	1839(3)	948(1)	19(1)	1
C(6)	6070(1)	1600(3)	1170(1)	16(1)	1
C(7)	6342(1)	1145(3)	1757(1)	19(1)	1
C(8)	6631(1)	1139(3)	1778(1)	19(1)	1
C(9)	6552(1)	1570(3)	1205(1)	16(1)	1
C(10)	6765(1)	1702(3)	1000(1)	21(1)	1
C(11)	6678(1)	2154(3)	440(2)	25(1)	1
C(12)	6893(1)	2367(4)	223(2)	38(1)	1
C(13)	6694(1)	2873(3)	-344(2)	35(1)	1
C(14)	6351(1)	2996(3)	-511(2)	26(1)	1
C(15)	6066(1)	3559(3)	-1046(1)	24(1)	1
C(16)	5735(1)	3776(3)	-1179(1)	21(1)	1
C(17)	5416(1)	4175(3)	-1707(1)	25(1)	1
C(18)	5178(1)	4109(3)	-1579(1)	24(1)	1
C(19)	5340(1)	3684(3)	-977(1)	19(1)	1
C(20)	5612(1)	1341(3)	1330(1)	19(1)	1
C(21)	5509(1)	2351(3)	1595(1)	24(1)	1
C(22)	5406(1)	1847(3)	1947(2)	30(1)	1
C(23)	5399(1)	318(4)	2045(2)	30(1)	1
C(24)	5497(1)	-717(3)	1791(2)	25(1)	1
C(25)	5602(1)	-200(3)	1442(1)	23(1)	1

C(26)	7129(1)	1337(3)	1446(1)	21(1)	1
C(27)	7262(1)	-81(3)	1490(2)	33(1)	1
C(28)	7595(1)	-444(4)	1909(2)	42(1)	1
C(29)	7804(1)	637(4)	2292(2)	40(1)	1
C(30)	7686(1)	2067(4)	2269(2)	43(1)	1
C(31)	7352(1)	2408(4)	1847(2)	37(1)	1
C(32)	6117(1)	4024(3)	-1516(2)	24(1)	1
C(33)	6151(1)	2980(3)	-1861(2)	30(1)	1
C(34)	6201(1)	3435(4)	-2291(2)	32(1)	1
C(35)	6219(1)	4956(4)	-2390(2)	32(1)	1
C(36)	6187(1)	6030(4)	-2054(2)	32(1)	1
C(37)	6140(1)	5553(3)	-1626(2)	30(1)	1
C(38)	5692(1)	-525(3)	-113(2)	24(1)	1
C(39)	5561(1)	-1926(3)	-378(2)	29(1)	1
C(40)	5536(1)	-2285(3)	-893(2)	33(1)	1
C(41)	5648(1)	-1245(3)	-1120(2)	35(1)	1
C(42)	5780(1)	122(3)	-832(2)	29(1)	1
C(43)	6110(1)	5276(3)	851(1)	20(1)	1
C(44)	6235(1)	6665(3)	1127(1)	26(1)	1
C(45)	6378(1)	7628(3)	929(1)	27(1)	1
C(46)	6387(1)	7189(3)	451(2)	26(1)	1
C(47)	6258(1)	5777(3)	192(1)	22(1)	1
C(51)	7183(5)	6190(20)	349(12)	179(11)	0.314(3)
O(51)	7428(5)	5226(18)	363(9)	202(8)	0.314(3)
C(52)	7911(1)	9259(6)	1017(3)	122(2)	1
O(52)	7660(1)	10415(4)	759(2)	123(2)	1
C(53)	6840(2)	8859(7)	9592(4)	84(2)	0.686(3)
O(53)	7116(1)	9625(4)	9631(2)	83(2)	0.686(3)
C(54)	6988(2)	865(6)	8397(3)	131(2)	1
O(54)	7050(1)	1778(4)	8876(2)	133(2)	1

Table 3. Selected bond lengths [Å] and angles [°] for JHP107 (CCDC 657603).

Ir(1)-N(4)	1.947(2)	N(4)-Ir(1)-N(1)	79.55(10)
Ir(1)-N(1)	1.953(2)	N(4)-Ir(1)-N(2)	172.23(10)
Ir(1)-N(2)	1.976(2)	N(1)-Ir(1)-N(2)	92.69(10)
Ir(1)-N(3)	1.979(2)	N(4)-Ir(1)-N(3)	92.92(10)
Ir(1)-N(6)	2.052(2)	N(1)-Ir(1)-N(3)	172.47(10)
Ir(1)-N(5)	2.066(2)	N(2)-Ir(1)-N(3)	94.84(10)
		N(4)-Ir(1)-N(6)	91.55(9)
		N(1)-Ir(1)-N(6)	91.87(9)
		N(2)-Ir(1)-N(6)	88.27(9)
		N(3)-Ir(1)-N(6)	88.60(9)
		N(4)-Ir(1)-N(5)	87.80(9)
		N(1)-Ir(1)-N(5)	88.04(9)
		N(2)-Ir(1)-N(5)	92.38(9)
		N(3)-Ir(1)-N(5)	91.41(9)
		N(6)-Ir(1)-N(5)	179.34(12)

Table 4. Bond lengths [Å] and angles [°] for JHP107 (CCDC 657603).

Ir(1)-N(4)	1.947(2)	C(15)-C(32)	1.494(4)
Ir(1)-N(1)	1.953(2)	C(16)-C(17)	1.434(4)
Ir(1)-N(2)	1.976(2)	C(17)-C(18)	1.370(4)
Ir(1)-N(3)	1.979(2)	C(18)-C(19)	1.416(4)
Ir(1)-N(6)	2.052(2)	C(20)-C(25)	1.386(4)
Ir(1)-N(5)	2.066(2)	C(20)-C(21)	1.396(4)
F(1)-C(21)	1.340(3)	C(21)-C(22)	1.376(4)
F(2)-C(22)	1.342(3)	C(22)-C(23)	1.366(4)
F(3)-C(23)	1.335(3)	C(23)-C(24)	1.372(4)
F(4)-C(24)	1.346(3)	C(24)-C(25)	1.382(4)
F(5)-C(25)	1.344(3)	C(26)-C(27)	1.365(4)
F(6)-C(27)	1.340(3)	C(26)-C(31)	1.377(4)
F(7)-C(28)	1.344(3)	C(27)-C(28)	1.381(5)
F(8)-C(29)	1.343(4)	C(28)-C(29)	1.345(5)
F(9)-C(30)	1.348(3)	C(29)-C(30)	1.358(4)
F(10)-C(31)	1.338(3)	C(30)-C(31)	1.381(5)
F(11)-C(33)	1.341(3)	C(32)-C(33)	1.383(4)
F(12)-C(34)	1.344(3)	C(32)-C(37)	1.384(4)
F(13)-C(35)	1.337(4)	C(33)-C(34)	1.383(4)
F(14)-C(36)	1.342(3)	C(34)-C(35)	1.365(4)
F(15)-C(37)	1.347(3)	C(35)-C(36)	1.378(4)
N(1)-C(4)	1.348(3)	C(36)-C(37)	1.369(4)
N(1)-C(1)	1.375(4)	C(38)-C(39)	1.378(4)
N(2)-C(9)	1.368(3)	C(39)-C(40)	1.374(5)
N(2)-C(6)	1.387(4)	C(40)-C(41)	1.368(4)
N(3)-C(14)	1.367(4)	C(41)-C(42)	1.371(4)
N(3)-C(11)	1.378(4)	C(43)-C(44)	1.373(4)
N(4)-C(19)	1.361(3)	C(44)-C(45)	1.373(4)
N(4)-C(16)	1.362(4)	C(45)-C(46)	1.383(4)
N(5)-C(42)	1.343(4)	C(46)-C(47)	1.381(4)
N(5)-C(38)	1.350(4)	C(51)-O(51)	1.425(5)
N(6)-C(43)	1.347(4)	C(52)-O(52)	1.418(4)
N(6)-C(47)	1.353(3)	C(53)-O(53)	1.432(4)
C(1)-C(2)	1.426(4)	C(54)-O(54)	1.410(4)
C(1)-C(19)	1.442(4)		
C(2)-C(3)	1.378(4)	N(4)-Ir(1)-N(1)	79.55(10)
C(3)-C(4)	1.437(4)	N(4)-Ir(1)-N(2)	172.23(10)
C(4)-C(5)	1.424(4)	N(1)-Ir(1)-N(2)	92.69(10)
C(5)-C(6)	1.422(4)	N(4)-Ir(1)-N(3)	92.92(10)
C(5)-C(20)	1.482(4)	N(1)-Ir(1)-N(3)	172.47(10)
C(6)-C(7)	1.440(4)	N(2)-Ir(1)-N(3)	94.84(10)
C(7)-C(8)	1.359(4)	N(4)-Ir(1)-N(6)	91.55(9)
C(8)-C(9)	1.433(4)	N(1)-Ir(1)-N(6)	91.87(9)
C(9)-C(10)	1.421(4)	N(2)-Ir(1)-N(6)	88.27(9)
C(10)-C(11)	1.395(4)	N(3)-Ir(1)-N(6)	88.60(9)
C(10)-C(26)	1.497(4)	N(4)-Ir(1)-N(5)	87.80(9)
C(11)-C(12)	1.462(4)	N(1)-Ir(1)-N(5)	88.04(9)
C(12)-C(13)	1.354(5)	N(2)-Ir(1)-N(5)	92.38(9)
C(13)-C(14)	1.445(4)	N(3)-Ir(1)-N(5)	91.41(9)
C(14)-C(15)	1.413(4)	N(6)-Ir(1)-N(5)	179.34(12)
C(15)-C(16)	1.427(4)	C(4)-N(1)-C(1)	112.4(2)

C(4)-N(1)-Ir(1)	130.07(19)	C(17)-C(18)-C(19)	108.2(3)
C(1)-N(1)-Ir(1)	116.8(2)	N(4)-C(19)-C(18)	106.4(3)
C(9)-N(2)-C(6)	110.5(2)	N(4)-C(19)-C(1)	112.3(3)
C(9)-N(2)-Ir(1)	124.9(2)	C(18)-C(19)-C(1)	141.2(3)
C(6)-N(2)-Ir(1)	124.27(19)	C(25)-C(20)-C(21)	115.5(3)
C(14)-N(3)-C(11)	111.4(2)	C(25)-C(20)-C(5)	120.8(3)
C(14)-N(3)-Ir(1)	124.5(2)	C(21)-C(20)-C(5)	123.7(2)
C(11)-N(3)-Ir(1)	123.62(19)	F(1)-C(21)-C(22)	118.5(3)
C(19)-N(4)-C(16)	111.8(3)	F(1)-C(21)-C(20)	119.4(3)
C(19)-N(4)-Ir(1)	118.0(2)	C(22)-C(21)-C(20)	122.1(3)
C(16)-N(4)-Ir(1)	129.7(2)	F(2)-C(22)-C(23)	119.6(3)
C(42)-N(5)-C(38)	117.3(3)	F(2)-C(22)-C(21)	119.8(3)
C(42)-N(5)-Ir(1)	120.9(2)	C(23)-C(22)-C(21)	120.6(3)
C(38)-N(5)-Ir(1)	121.6(2)	F(3)-C(23)-C(22)	120.6(3)
C(43)-N(6)-C(47)	117.9(2)	F(3)-C(23)-C(24)	120.1(3)
C(43)-N(6)-Ir(1)	121.29(19)	C(22)-C(23)-C(24)	119.3(3)
C(47)-N(6)-Ir(1)	120.8(2)	F(4)-C(24)-C(23)	119.9(3)
N(1)-C(1)-C(2)	105.5(3)	F(4)-C(24)-C(25)	120.4(3)
N(1)-C(1)-C(19)	113.0(3)	C(23)-C(24)-C(25)	119.7(3)
C(2)-C(1)-C(19)	141.4(3)	F(5)-C(25)-C(24)	117.6(2)
C(3)-C(2)-C(1)	108.2(3)	F(5)-C(25)-C(20)	119.7(3)
C(2)-C(3)-C(4)	107.8(3)	C(24)-C(25)-C(20)	122.8(3)
N(1)-C(4)-C(5)	121.2(3)	C(27)-C(26)-C(31)	115.5(3)
N(1)-C(4)-C(3)	106.0(3)	C(27)-C(26)-C(10)	122.6(3)
C(5)-C(4)-C(3)	132.7(3)	C(31)-C(26)-C(10)	122.0(3)
C(6)-C(5)-C(4)	126.1(3)	F(6)-C(27)-C(26)	119.3(3)
C(6)-C(5)-C(20)	117.1(3)	F(6)-C(27)-C(28)	117.6(3)
C(4)-C(5)-C(20)	116.7(3)	C(26)-C(27)-C(28)	123.1(3)
N(2)-C(6)-C(5)	125.4(3)	F(7)-C(28)-C(29)	120.4(3)
N(2)-C(6)-C(7)	106.0(2)	F(7)-C(28)-C(27)	120.1(3)
C(5)-C(6)-C(7)	128.6(3)	C(29)-C(28)-C(27)	119.5(3)
C(8)-C(7)-C(6)	108.4(3)	F(8)-C(29)-C(28)	120.3(3)
C(7)-C(8)-C(9)	108.3(3)	F(8)-C(29)-C(30)	119.8(3)
N(2)-C(9)-C(10)	123.3(3)	C(28)-C(29)-C(30)	119.8(3)
N(2)-C(9)-C(8)	106.8(2)	F(9)-C(30)-C(29)	119.9(3)
C(10)-C(9)-C(8)	129.9(3)	F(9)-C(30)-C(31)	120.3(3)
C(11)-C(10)-C(9)	127.9(3)	C(29)-C(30)-C(31)	119.8(3)
C(11)-C(10)-C(26)	116.4(3)	F(10)-C(31)-C(26)	119.7(3)
C(9)-C(10)-C(26)	115.7(3)	F(10)-C(31)-C(30)	118.0(3)
N(3)-C(11)-C(10)	124.8(3)	C(26)-C(31)-C(30)	122.3(3)
N(3)-C(11)-C(12)	105.9(3)	C(33)-C(32)-C(37)	115.7(3)
C(10)-C(11)-C(12)	129.3(3)	C(33)-C(32)-C(15)	123.0(3)
C(13)-C(12)-C(11)	107.5(3)	C(37)-C(32)-C(15)	121.3(3)
C(12)-C(13)-C(14)	109.1(3)	F(11)-C(33)-C(34)	118.2(3)
N(3)-C(14)-C(15)	125.3(3)	F(11)-C(33)-C(32)	119.7(3)
N(3)-C(14)-C(13)	106.0(3)	C(34)-C(33)-C(32)	122.1(3)
C(15)-C(14)-C(13)	128.6(3)	F(12)-C(34)-C(35)	120.0(3)
C(14)-C(15)-C(16)	127.1(3)	F(12)-C(34)-C(33)	119.7(3)
C(14)-C(15)-C(32)	116.5(3)	C(35)-C(34)-C(33)	120.3(3)
C(16)-C(15)-C(32)	116.4(3)	F(13)-C(35)-C(34)	120.3(3)
N(4)-C(16)-C(15)	120.3(3)	F(13)-C(35)-C(36)	120.4(3)
N(4)-C(16)-C(17)	105.7(3)	C(34)-C(35)-C(36)	119.3(3)
C(15)-C(16)-C(17)	133.9(3)	F(14)-C(36)-C(37)	121.2(3)
C(18)-C(17)-C(16)	107.9(3)	F(14)-C(36)-C(35)	119.4(3)

C(37)-C(36)-C(35)	119.4(3)	C(40)-C(41)-C(42)	119.4(3)
F(15)-C(37)-C(36)	117.5(3)	N(5)-C(42)-C(41)	122.9(3)
F(15)-C(37)-C(32)	119.3(3)	N(6)-C(43)-C(44)	122.8(3)
C(36)-C(37)-C(32)	123.3(3)	C(43)-C(44)-C(45)	119.0(3)
N(5)-C(38)-C(39)	122.2(3)	C(44)-C(45)-C(46)	119.2(3)
C(40)-C(39)-C(38)	119.4(3)	C(47)-C(46)-C(45)	119.2(3)
C(41)-C(40)-C(39)	118.7(3)	N(6)-C(47)-C(46)	121.9(3)

Table 5. Anisotropic displacement parameters ($Å^2 x 10^4$) for JHP107 (CCDC 657603). 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}
Ir(1)	170(1)	230(1)	136(1)	13(1)	103(1)	8(1)
F(1)	488(14)	323(10)	423(14)	21(8)	345(12)	83(8)
F(2)	695(16)	565(12)	531(15)	27(10)	528(14)	154(10)
F(3)	524(15)	679(13)	383(14)	115(10)	396(14)	18(10)
F(4)	411(12)	362(10)	380(12)	95(9)	266(11)	-37(9)
F(5)	405(12)	266(9)	325(12)	-23(8)	277(11)	-17(8)
F(6)	274(13)	413(12)	699(19)	-202(11)	25(13)	32(9)
F(7)	323(14)	533(13)	950(20)	-92(13)	21(15)	173(10)
F(8)	167(13)	908(16)	600(20)	-107(13)	19(13)	68(11)
F(9)	318(14)	775(15)	830(20)	-448(14)	53(15)	-113(11)
F(10)	357(14)	452(12)	840(20)	-272(12)	138(15)	1(10)
F(11)	701(16)	372(11)	456(15)	-71(9)	462(14)	-80(10)
F(12)	677(15)	607(12)	393(13)	-136(11)	444(13)	-73(11)
F(13)	524(15)	686(13)	313(13)	85(10)	359(13)	-10(10)
F(14)	695(15)	452(11)	523(15)	125(11)	451(14)	32(11)
F(15)	680(16)	386(10)	460(15)	-35(10)	447(14)	-17(10)
N(1)	145(13)	257(13)	150(13)	20(10)	94(12)	1(9)
N(2)	181(14)	153(11)	176(14)	-2(9)	101(12)	7(9)
N(3)	217(13)	287(13)	190(13)	-5(11)	158(12)	7(11)
N(4)	195(14)	243(12)	159(14)	11(10)	122(12)	-11(10)
N(5)	177(14)	258(13)	160(14)	16(10)	106(13)	44(10)
N(6)	155(14)	258(12)	133(13)	37(10)	99(12)	27(10)
C(1)	192(17)	252(15)	160(16)	-3(12)	109(15)	3(12)
C(2)	167(17)	393(17)	202(18)	-19(14)	89(16)	-22(13)
C(3)	190(16)	356(17)	261(17)	34(15)	134(15)	1(14)
C(4)	207(15)	223(14)	163(14)	12(13)	112(13)	12(13)
C(5)	230(17)	200(14)	167(16)	11(11)	136(15)	-12(11)
C(6)	220(17)	155(13)	165(16)	-3(11)	143(14)	1(11)
C(7)	283(19)	176(14)	150(16)	-16(11)	139(16)	-8(12)
C(8)	152(16)	200(14)	165(17)	11(11)	57(14)	17(11)
C(9)	160(16)	145(13)	185(16)	1(11)	101(14)	-12(11)
C(10)	197(17)	264(15)	202(18)	8(12)	125(15)	11(12)
C(11)	210(17)	314(16)	266(18)	-1(13)	166(16)	-16(13)
C(12)	240(18)	640(20)	330(20)	114(19)	209(17)	117(18)
C(13)	320(20)	550(20)	300(20)	86(16)	257(19)	50(16)
C(14)	269(19)	370(18)	225(18)	19(13)	194(17)	-3(13)
C(15)	300(20)	293(16)	179(17)	-13(13)	174(17)	-16(13)
C(16)	275(19)	255(15)	157(17)	-21(12)	157(16)	-46(12)
C(17)	280(20)	327(17)	139(17)	4(13)	115(16)	-29(13)
C(18)	208(18)	318(16)	132(17)	21(12)	54(15)	-35(12)
C(19)	186(17)	208(14)	168(17)	-1(11)	87(15)	-15(11)
C(20)	148(16)	288(16)	151(16)	11(12)	104(14)	11(12)
C(21)	260(17)	262(16)	246(16)	27(14)	164(15)	39(13)
C(22)	300(20)	444(19)	260(20)	-14(14)	216(18)	77(14)
C(23)	290(20)	500(20)	240(20)	76(15)	215(18)	24(15)
C(24)	235(19)	313(17)	250(20)	61(13)	167(17)	-8(13)
C(25)	204(18)	321(17)	191(18)	-29(13)	123(16)	-1(13)

C(26)	162(17)	307(16)	191(18)	12(13)	111(15)	-13(12)
C(27)	210(20)	345(18)	360(20)	-69(15)	106(19)	-32(14)
C(28)	270(20)	390(20)	460(30)	-37(17)	120(20)	73(16)
C(29)	124(19)	600(20)	340(20)	-35(18)	58(19)	34(16)
C(30)	219(19)	480(20)	440(30)	-191(17)	96(19)	-136(16)
C(31)	266(19)	377(19)	440(20)	-70(18)	173(18)	-1(16)
C(32)	236(19)	384(18)	169(18)	6(13)	148(16)	-6(13)
C(33)	330(20)	390(19)	253(19)	-25(14)	209(18)	-59(14)
C(34)	320(20)	490(20)	230(20)	-60(16)	205(18)	-34(15)
C(35)	270(20)	550(20)	200(20)	58(16)	166(18)	-15(16)
C(36)	320(20)	393(19)	300(20)	83(15)	208(19)	12(15)
C(37)	360(20)	373(18)	250(20)	-11(14)	225(19)	37(15)
C(38)	231(19)	258(16)	233(19)	5(13)	140(16)	22(12)
C(39)	227(18)	268(17)	340(20)	1(14)	138(18)	15(13)
C(40)	299(19)	279(17)	320(20)	-65(16)	115(17)	12(15)
C(41)	470(20)	318(18)	280(20)	-36(15)	220(20)	33(15)
C(42)	390(20)	294(17)	240(20)	6(14)	213(19)	51(14)
C(43)	243(18)	232(15)	162(17)	45(12)	129(16)	58(12)
C(44)	330(20)	254(15)	170(17)	-19(13)	131(16)	32(13)
C(45)	298(17)	195(15)	237(17)	-36(14)	103(15)	-8(14)
C(46)	238(17)	230(16)	275(18)	31(13)	121(16)	-21(13)
C(47)	231(18)	266(16)	182(17)	36(12)	129(16)	16(12)
C(51)	1790(120)	1790(120)	1800(120)	-110(40)	1020(70)	30(40)
O(51)	2030(90)	1980(90)	2020(90)	0(40)	1130(60)	-20(40)
C(52)	990(30)	1390(30)	1380(40)	-20(30)	730(30)	260(30)
O(52)	1170(30)	1270(20)	1180(30)	50(20)	630(20)	240(20)
C(53)	990(40)	840(30)	820(40)	-120(30)	580(30)	-190(30)
O(53)	950(30)	880(30)	720(30)	-40(20)	500(30)	130(20)
C(54)	1430(40)	1350(40)	1220(40)	-90(30)	800(30)	-10(30)
O(54)	1610(30)	1240(20)	1190(30)	-120(20)	810(30)	180(20)

Table 6. Hydrogen bonds for JHP107 (CCDC 657603) [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(51)-H(51)...O(54)#1	0.84	2.25	2.791(19)	122.4
O(52)-H(52)...O(54)#2	0.84	1.89	2.714(6)	168.1
O(53)-H(53)...O(52)#3	0.84	2.04	2.777(7)	146.7
O(54)-H(54)...O(51)#1	0.84	2.25	2.791(19)	122.7

Symmetry transformations used to generate equivalent atoms:
#1 -x+3/2,-y+1/2,-z+1
#2 -x+3/2,-y+3/2,-z+1
#3 x,y,z+1

JHP107

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Least-squares plane number 3 (XO = orthogonal, x = Crystal coordinates)

0.2104 XO + 0.9429 YO + 0.2583 ZO = 3.0255
1.373 x + 8.226 y + 7.044 z = 3.0255

	Deviation	Weight					
+	0.0052	1.0000	IR1	+	-0.0500	1.0000	C17
	1.9780	1.0000	F1		-0.1007	1.0000	H17
	1.6204	1.0000	F2	+	-0.0475	1.0000	C18
	-0.7523	1.0000	F3		-0.1017	1.0000	H18
	-2.7707	1.0000	F4	+	0.0499	1.0000	C19
	-2.4312	1.0000	F5		-0.2149	1.0000	C20
	-2.2490	1.0000	F6		0.7883	1.0000	C21
	-2.1434	1.0000	F7		0.6078	1.0000	C22
	0.2423	1.0000	F8		-0.5826	1.0000	C23
	2.5160	1.0000	F9		-1.5993	1.0000	C24
	2.4150	1.0000	F10		-1.4052	1.0000	C25
	-2.2291	1.0000	F11		0.0710	1.0000	C26
	-2.0620	1.0000	F12		-1.0460	1.0000	C27
	0.2926	1.0000	F13		-1.0036	1.0000	C28
	2.5103	1.0000	F14		0.1842	1.0000	C29
	2.3613	1.0000	F15		1.3277	1.0000	C30
+	0.0966	1.0000	N1		1.2650	1.0000	C31
+	-0.0631	1.0000	N2		0.0568	1.0000	C32
+	-0.0864	1.0000	N3		-1.0406	1.0000	C33
+	0.0976	1.0000	N4		-0.9627	1.0000	C34
	-2.0490	1.0000	N5		0.2215	1.0000	C35
	2.0469	1.0000	N6		1.3376	1.0000	C36
+	0.0620	1.0000	C1		1.2396	1.0000	C37
+	-0.0170	1.0000	C2		-2.7559	1.0000	C38
	-0.0363	1.0000	H2		-2.3027	1.0000	H38
+	-0.0602	1.0000	C3		-4.1129	1.0000	C39
	-0.1232	1.0000	H3		-4.5872	1.0000	H39
+	0.0070	1.0000	C4		-4.7741	1.0000	C40
+	-0.0589	1.0000	C5		-5.7057	1.0000	H40
+	-0.0526	1.0000	C6		-4.0635	1.0000	C41
+	0.0238	1.0000	C7		-4.4984	1.0000	H41
	0.0369	1.0000	H7		-2.7179	1.0000	C42
+	0.0740	1.0000	C8		-2.2377	1.0000	H42
	0.1381	1.0000	H8		2.7524	1.0000	C43
+	0.0138	1.0000	C9		2.2935	1.0000	H43
+	0.0078	1.0000	C10		4.1066	1.0000	C44
+	-0.0278	1.0000	C11		4.5707	1.0000	H44
+	0.0249	1.0000	C12		4.7799	1.0000	C45
	0.0602	1.0000	H12		5.7131	1.0000	H45
+	0.0142	1.0000	C13		4.0824	1.0000	C46
	0.0435	1.0000	H13		4.5342	1.0000	H46
+	-0.0489	1.0000	C14		2.7211	1.0000	C47
+	-0.0020	1.0000	C15		2.2442	1.0000	H47
+	0.0377	1.0000	C16				

Mean deviation from plane = 0.0429 Angstroms

JHP107 over JHP104

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MODEL FITTING FOR jhp104 in P-1

ORTHOGONAL COORDINATES FROM jhp107.ort

ATOM MODEL DEVIATION

IR	IR1	0.008	C8	C8	0.042
N1	N1	0.076	C9	C9	0.063
N2	N2	0.041	C10	C10	0.039
N3	N3	0.059	C11	C11	0.038
N4	N4	0.032	C12	C12	0.022
C1	C1	0.038	C13	C13	0.015
C2	C2	0.017	C14	C14	0.037
C3	C3	0.031	C15	C15	0.017
C4	C4	0.013	C16	C16	0.010
C5	C5	0.047	C17	C17	0.023
C6	C6	0.023	C18	C18	0.013
C7	C7	0.035	C19	C19	0.012

WEIGHTED R.M.S. DEVIATION = 0.0360 ANGSTROMS