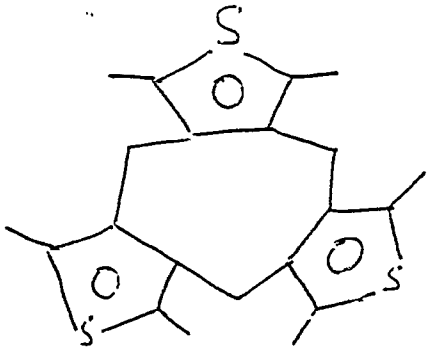
ORGANOMETALLICS
Organometallics, 1998, 17(9), 1732-1740, DOI:10.1021/om970739q

CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM

Compound Name

4

Diagram (conventional chemical structural diagram)



Formula (each residue to be formulated ,eg. $C_2H_3O_2^-$, Na^+, $2H_2O$)

$C_{21}H_{24}S_3$

a(A) with estimated error	b(A) with estimated error	c(A) with estimated error
10.2310(5)	5.2960(2)	34.4670(14)

alpha(deg.) with estimated error	beta(deg.) with estimated error	gamma(deg.) with estimated error
	94.182(1)	

Space Group	Z	R-factor(s)	Temp(K)	Radiation	Powder Data
$P2_1/c$	4	R_1 0.0454 * wF_2 0.1240	20	☒ X ☐ N	Yes ☐ No ☒

Intensity Measurement	Volume(Å^3)	Mol. Weight	Mp(°C)
☐ densit. ☒ diffr. ☐ other (specify)	1862.57(14)		—

Absolute Configuration Determined	Colour	Dm (g cm^{-3})
☐ Yes ☐ No	Colorless	—
	CAS RN —	Dx (g cm^{-3}) 1.329

Polymorph Indicator (eg. low-temp. form) —

Drug (indicate, where appropriate, type of drug, activity, etc.)

—

Disorder (specify nature of disorder with reference to atom labels in coordinate list)

NONE

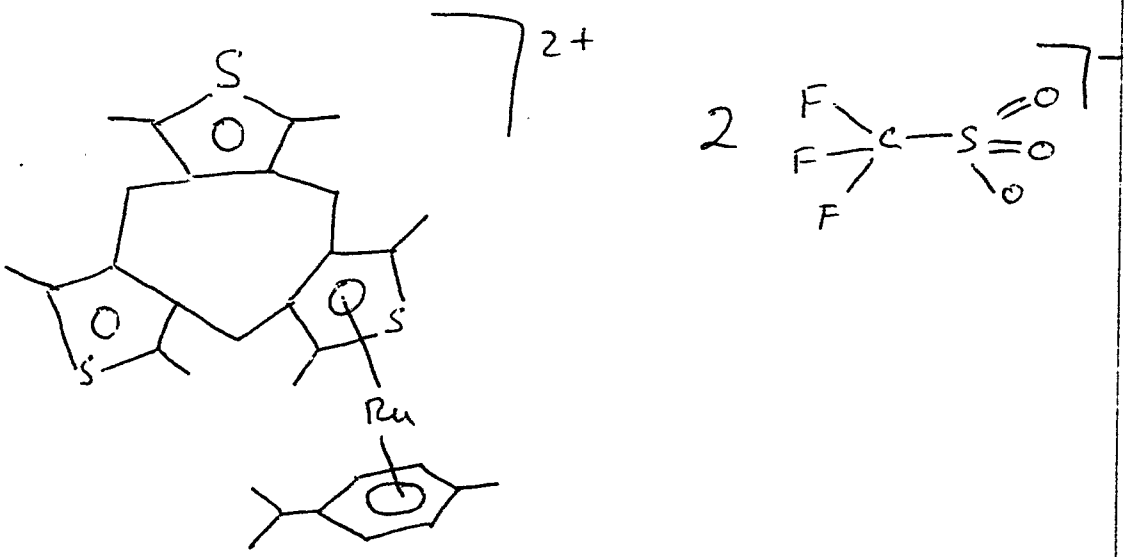
* wR_2 based on F^2, all data
R - F, I > 2σ(I)

CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM

Compound Name

6

Diagram *(conventional chemical structural diagram)*



Formula *(each residue to be formulated ,eg.* $C_2H_3O_2^-\cdot Na^+\cdot 2H_2O$*)*

$[Ru(\eta^6\text{-}MeC_6H_4CHMe_2)(C_{21}H_{24}S_3)][CF_3SO_3]_2$

a(A) *with estimated error*	b(A) *with estimated error*	c(A) *with estimated error*
10·1661 (12)	13·6994 (17)	14·3077 (17)

alpha(deg.)*with estimated error*	beta(deg.) *with estimated error*	gamma(deg.) *with estimated error*
71·267(3)	86·181 (3)	88·430(3)

Space Group	Z	R-factor(s)	Temp(K)	Radiation	Powder Data
PT	2	R 0·0311 * wR 0·0756	160	☒ X ☐ N	Yes ☐ No ☒

Intensity Measurement	Volume(Å^3)	Mol. Weight	Mp(°C)
☐ densit. ☒ diffr. ☐ other(*specify*)	1882·8(4)	906·00	—

Absolute Configuration Determined	Colour PALE YELLOW	Dm (g cm^{-3})
☐ Yes ☐ No	CAS RN —	Dx (g cm^{-3}) 1·598

Polymorph Indicator *(eg. low-temp. form)* —

Drug *(indicate, where appropriate, type of drug, activity, etc.)*

—

Disorder *(specify nature of disorder with reference to atom labels in coordinate list)*

NONE

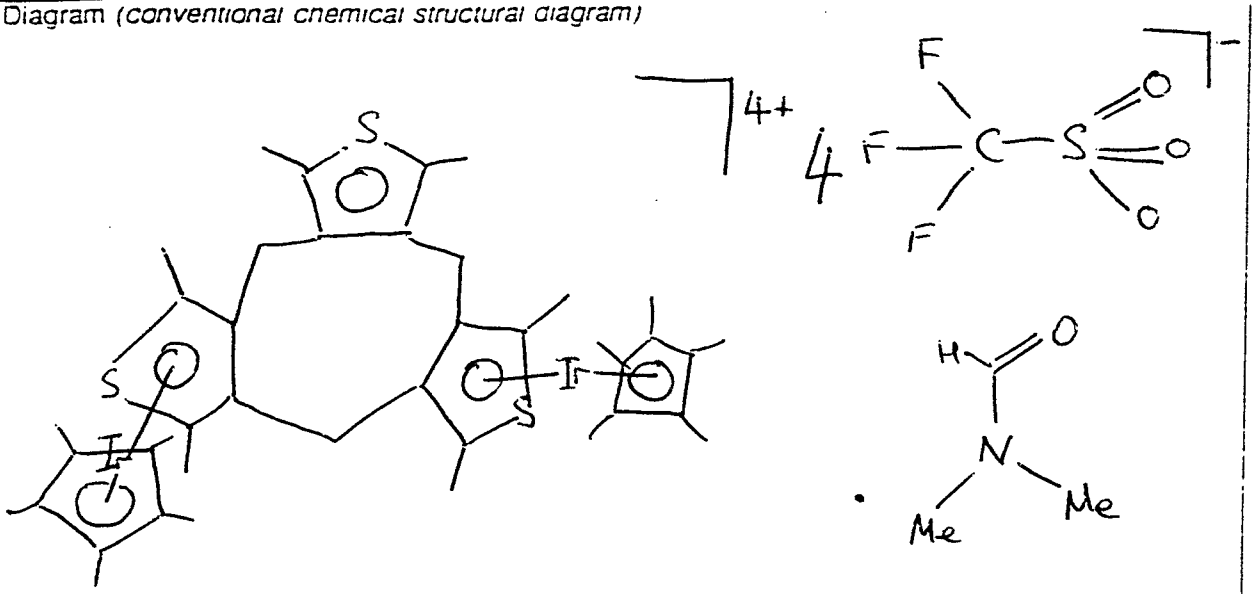
* R for F values with $F^2 > 2(\sigma)(F^2)$

CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM

Compound Name

9

Diagram *(conventional chemical structural diagram)*



Formula *(each residue to be formulated ,eg.* $C_2H_3O_2^-\cdot Na^+\cdot 2H_2O$*)*

$[\{Ir(\eta^5\text{-}C_5Me_5)\}_2(C_{21}H_{24}S_3)][Me_2NCHO]$

a(A) *with estimated error*	b(A) *with estimated error*	c(A) *with estimated error*
20·6686(16)	17·4490(13)	17·0768(13)
alpha(deg.) *with estimated error*	**beta(deg.)** *with estimated error*	**gamma(deg.)** *with estimated error*
90·0	106·158(2)	90·0

Space Group	Z	R-factor(s)	Temp(K)	Radiation	Powder Data
Cc	4	* R 0·0479 wR 0·1290	160	☒ X ☐ N	Yes ☐ No ☒

Intensity Measurement	Volume(Å^3)	Mol. Weight	Mp(°C)
☐ densit. ☒ diffr. ☐ other(*specify*)	5915·4(8)	1696·8	—

Absolute Configuration Determined	Colour PALE YELLOW	Dm (g cm^{-3})
☐ Yes ☐ No	CAS RN —	Dx (g cm^{-3}) 1·905

Polymorph Indicator *(eg. low-temp. form)* —

Drug *(indicate, where appropriate, type of drug, activity, etc.)*

—

Disorder *(specify nature of disorder with reference to atom labels in coordinate list)*

50/50 in DMF MOLECULE FOR ATOMS C1Sa/C1Sab, C2Sa/C2Sab, C3Sa/C3Sab.

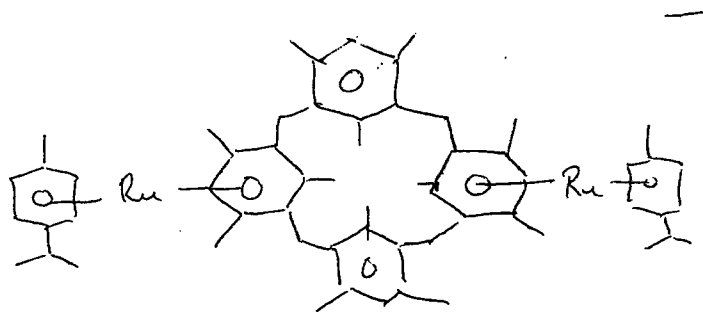
R based on F with $F^2 > 2\sigma(F^2)$

CAMBRIDGE CRYSTALLOGRAPHIC DATA CENTRE: ABSTRACT FORM

Compound Name

11

Diagram (conventional chemical structural diagram)



74*

4 BF_4^-

5 MeCN

Formula (each residue to be formulated .eg. $C_2H_3O_2^- \cdot Na^+ \cdot 2H_2O$)

$C_{60}H_{74}Ru_2^{4+}$ 4× BF_4^- 5× CH_3CN

a(A) with estimated error	b(A) with estimated error	c(A) with estimated error
16.0574(8)	11.6582(6)	19.7603(5)

alpha(deg.) with estimated error	beta(deg.) with estimated error	gamma(deg.) with estimated error
	102.577(1)	

Space Group	Z	R-factor(s)	Temp(K)	Radiation	Powder Data
P2/c	2	* R_1 wR_2	173	☒ X ☐ N	Yes ☐ No ☒

Intensity Measurement	Volume(Å^3)	Mol. Weight	Mp(°C)
☐ densit. ☒ diffr. ☐ other (specify)			

Absolute Configuration Determined	Colour	Dm (g cm^{-3})
☐ Yes ☐ No	CAS RN —	Dx (g cm^{-3})

Polymorph Indicator (eg. low-temp. form) —

Drug (indicate, where appropriate, type of drug, activity, etc.)

—

Disorder (specify nature of disorder with reference to atom labels in coordinate list)

disorder of all acetonitrile atoms

* wR_2 based on F^2, all data
R - F, $I > 2\sigma(I)$

Notes on experimental and computational procedures.

Data collection and data reduction

Measurements were made with graphite-monochromated radiation. Unit cell parameters were refined from the setting angles and recorded spot positions of selected reflections measured on a series of oscillation frames. All machine control calculations were performed with standard Siemens SMART software. Data reduction was carried out with the Siemens SAINT frame integration software, and included corrections for Lp effects. Reflection scaling and averaging of equivalents were part of the structure solution and refinement procedures.

Structure solution and refinement

Programs were all members of the SHELX family (SHELXS-86, SHELXL-93, SHELXTL) written by G. M. Sheldrick, University of Göttingen, Germany. Atoms not revealed in the initial structure solution were subsequently located from difference syntheses. Least-squares refinement was based on F^2 values for all measured reflections except for any flagged for potential systematic errors. Weighted R indices (wR2) are based on F^2, while R1 values are based on F, with F set to zero for negative measured intensities. The observed criteria of $I>2\sigma(I)$ is used only for calculating two of the R indices for comparison with conventional refinements based on F for observed data only (particularly the index R1), and has no effect on the choice of reflections for refinement. Note that R indices based on F^2 are usually substantially greater than those based on F values, especially when all measured data are used. The weighting scheme for refinement is of the form $w^{-1} = \sigma^2(F_o^2) + (aP)^2 + bP$, where P is $(F_o^2+2F_c^2)/3$, F_o^2 being replaced in this expression by zero if it is negative. The extinction correction multiplies F_c by the factor $(1+0.001xF_c^2\lambda^3/\sin 2\theta)^{-1/4}$ as well as by the normal refined overall scale factor; x is the extinction coefficient. For 9 the carbon atoms in the DMF molecule of crystallisation were disordered over two sets of equally occupied postions.

General experimental description: KappaCCD at King's College London

Crystals were mounted on a thin glass fibre using a fast setting epoxy resin and cooled on the diffractometer to the temperature stated using an Oxford Cryostream low temperature attachment. A total of either 90 or 180 oscillation frames each of width either 2° or 1° in ϕ respectively and of 10 - 120 s exposure time (depending on crystal quality) were recorded using a Nonius ^{Kappa}CCD diffractometer, with a detector to crystal distance of 25 - 35 mm. Crystals were indexed from the first ten frames using the DENZO package[1] and positional data were refined along with diffractometer constants to give the final unit cell parameters. Integration and scaling (DENZO, Scalepack[1]) resulted in unique data sets corrected for Lorentz and polarisation effects and for the effects of crystal decay and absorption by a combination of averaging of equivalent reflections and an overall volume and scaling correction. Structures were solved using SHELXS-97[2] and developed *via* alternating least squares cycles and difference Fourier synthesis (SHELXL-97[2]) with the aid of the program RES2INS.[3] In general all non-hydrogen atoms were modelled anisotropically, while hydrogen atoms are assigned an isotropic thermal parameter 1.2 times that of the parent atom (1.5 for terminal atoms) and allowed to ride, except where stated. All calculations were carried out with either a Silicon Graphics Indy 5000 workstation or an IBM compatible PC.

1. Z. Otwinowski and W. Minor, *Methods in Enzymology*, **276**, 1996. C. W. Carter and R. M. Sweet (Eds.), Academic Press.

2. G. M. Sheldrick, 'SHELXL-97', University of Göttingen, 1997.

3. L. J. Barbour, 'RES2INS', University of Missouri - Columbia, 1995.

Acknowledgements

We thank the EPSRC and King's College London for funding of the diffractometer system. Grateful acknowledgement is also given to the Nuffield Foundation for the provision of computing equipment.

Table 1. Crystal data and structure refinement for tri(2,5-dimethylthiophenylene).

Identification code	thio
Empirical formula	C21 H24 S3
Formula weight	372.58
Temperature	293(2) K
Wavelength	0.71070 A
Data collection	KappaCCD, phi rotation, 2^{o} frames, 30 s, DX = 25mm
Crystal system, space group	Monoclinic, P21/c
Unit cell dimensions	a = 10.2310(5) A alpha = 90.0 deg. b = 5.2960(2) A beta = 94.1820(10) deg. c = 34.4670(14) A gamma = 90.0 deg.
Volume	1862.57(14) A^3
Z, Calculated density	4, 1.329 Mg/m^3
Absorption coefficient	0.398 mm^-1
F(000)	792
Crystal size	0.40 x 0.10 x 0.10 mm
Theta range for data collection	4.03 to 25.00 deg.
Index ranges	0<=h<=12, 0<=k<=6, -40<=l<=40
Reflections collected / unique	25828 / 3224 [R(int) = 0.0530]
Completeness to 2theta = 25.00	87.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3224 / 0 / 218
Goodness-of-fit on F^2	1.026
Final R indices [I>2sigma(I)]	R1 = 0.0454, wR2 = 0.1205
R indices (all data)	R1 = 0.0507, wR2 = 0.1240
Extinction coefficient	0.033(5)
Largest diff. peak and hole	0.233 and -0.242 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for tri(2,5-dimethylthiophenylene). U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
S(1A)	8901(1)	1438(1)	2241(1)	52(1)
C(1A)	9920(2)	2694(5)	1916(1)	43(1)
C(2A)	9282(2)	4447(4)	1684(1)	38(1)
C(3A)	7946(2)	4800(4)	1777(1)	39(1)
C(4A)	7606(2)	3291(5)	2070(1)	46(1)
C(5A)	7006(2)	6594(5)	1561(1)	42(1)
C(6A)	11331(3)	1889(6)	1937(1)	56(1)
C(7A)	6318(3)	3101(7)	2246(1)	66(1)
S(1B)	3702(1)	3729(1)	1044(1)	51(1)
C(1B)	4638(2)	5663(5)	1355(1)	44(1)
C(2B)	5939(2)	5230(4)	1321(1)	38(1)
C(3B)	6186(2)	3300(4)	1044(1)	38(1)
C(4B)	5061(2)	2287(5)	872(1)	44(1)
C(5B)	7551(2)	2499(4)	948(1)	38(1)
C(6B)	3990(3)	7490(6)	1608(1)	59(1)
C(7B)	4872(3)	199(6)	581(1)	58(1)
S(1C)	9103(1)	7632(1)	264(1)	48(1)
C(1C)	8087(2)	5255(5)	392(1)	41(1)
C(2C)	8319(2)	4599(4)	774(1)	36(1)
C(3C)	9349(2)	6077(4)	965(1)	37(1)
C(4C)	9861(2)	7802(4)	722(1)	40(1)
C(5C)	9922(2)	5970(5)	1384(1)	47(1)
C(6C)	7125(3)	4146(6)	91(1)	57(1)
C(7C)	10937(3)	9672(6)	811(1)	55(1)

Table 3. Bond lengths [A] and angles [deg] for tri(2,5-dimethylthiophenylene).

S(1A)-C(4A)	1.719(3)
S(1A)-C(1A)	1.719(3)
C(1A)-C(2A)	1.360(3)
C(1A)-C(6A)	1.503(3)
C(2A)-C(3A)	1.439(3)
C(2A)-C(5C)	1.500(3)
C(3A)-C(4A)	1.353(3)
C(3A)-C(5A)	1.509(3)
C(4A)-C(7A)	1.494(4)
C(5A)-C(2B)	1.505(3)
S(1B)-C(1B)	1.722(2)
S(1B)-C(4B)	1.727(3)
C(1B)-C(2B)	1.364(3)
C(1B)-C(6B)	1.491(4)
C(2B)-C(3B)	1.434(3)
C(3B)-C(4B)	1.365(3)
C(3B)-C(5B)	1.520(3)
C(4B)-C(7B)	1.497(4)
C(5B)-C(2C)	1.511(3)
S(1C)-C(4C)	1.710(2)
S(1C)-C(1C)	1.712(2)
C(1C)-C(2C)	1.363(3)
C(1C)-C(6C)	1.496(3)
C(2C)-C(3C)	1.435(3)
C(3C)-C(4C)	1.370(3)
C(3C)-C(5C)	1.518(3)
C(4C)-C(7C)	1.495(3)
C(4A)-S(1A)-C(1A)	92.52(12)
C(2A)-C(1A)-C(6A)	129.8(2)
C(2A)-C(1A)-S(1A)	111.07(18)
C(6A)-C(1A)-S(1A)	118.98(19)
C(1A)-C(2A)-C(3A)	112.4(2)
C(1A)-C(2A)-C(5C)	123.9(2)
C(3A)-C(2A)-C(5C)	123.6(2)
C(4A)-C(3A)-C(2A)	112.9(2)
C(4A)-C(3A)-C(5A)	123.5(2)
C(2A)-C(3A)-C(5A)	123.6(2)
C(3A)-C(4A)-C(7A)	128.7(2)
C(3A)-C(4A)-S(1A)	111.10(18)
C(7A)-C(4A)-S(1A)	120.2(2)
C(2B)-C(5A)-C(3A)	112.30(19)
C(1B)-S(1B)-C(4B)	92.91(11)
C(2B)-C(1B)-C(6B)	129.5(2)
C(2B)-C(1B)-S(1B)	110.47(18)
C(6B)-C(1B)-S(1B)	119.99(18)
C(1B)-C(2B)-C(3B)	113.3(2)
C(1B)-C(2B)-C(5A)	123.2(2)
C(3B)-C(2B)-C(5A)	123.45(19)
C(4B)-C(3B)-C(2B)	112.6(2)
C(4B)-C(3B)-C(5B)	123.7(2)
C(2B)-C(3B)-C(5B)	123.64(19)
C(3B)-C(4B)-C(7B)	130.1(2)
C(3B)-C(4B)-S(1B)	110.65(18)
C(7B)-C(4B)-S(1B)	119.23(18)
C(2C)-C(5B)-C(3B)	113.20(19)
C(4C)-S(1C)-C(1C)	92.48(11)
C(2C)-C(1C)-C(6C)	128.9(2)
C(2C)-C(1C)-S(1C)	111.72(17)
C(6C)-C(1C)-S(1C)	119.40(18)
C(1C)-C(2C)-C(3C)	112.1(2)
C(1C)-C(2C)-C(5B)	120.8(2)
C(3C)-C(2C)-C(5B)	127.13(19)
C(4C)-C(3C)-C(2C)	112.47(19)
C(4C)-C(3C)-C(5C)	117.9(2)
C(2C)-C(3C)-C(5C)	129.6(2)
C(3C)-C(4C)-C(7C)	128.7(2)
C(3C)-C(4C)-S(1C)	111.25(17)
C(7C)-C(4C)-S(1C)	120.08(18)
C(2A)-C(5C)-C(3C)	121.17(19)

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for tri(2,5-dimethylthiophenylene). The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
S(1A)	56(1)	60(1)	41(1)	11(1)	-3(1)	-2(1)
C(1A)	42(1)	50(1)	37(1)	-3(1)	-4(1)	1(1)
C(2A)	37(1)	44(1)	33(1)	-3(1)	-3(1)	-5(1)
C(3A)	38(1)	44(1)	33(1)	-4(1)	-3(1)	-3(1)
C(4A)	45(1)	58(2)	34(1)	0(1)	-1(1)	-3(1)
C(5A)	39(1)	41(1)	44(1)	-4(1)	0(1)	0(1)
C(6A)	48(1)	67(2)	53(2)	-1(1)	-7(1)	8(1)
C(7A)	52(2)	95(2)	50(2)	10(2)	11(1)	-5(2)
S(1B)	35(1)	66(1)	51(1)	1(1)	-1(1)	-9(1)
C(1B)	39(1)	52(1)	40(1)	2(1)	0(1)	0(1)
C(2B)	34(1)	42(1)	36(1)	4(1)	-2(1)	-1(1)
C(3B)	36(1)	41(1)	36(1)	3(1)	1(1)	-5(1)
C(4B)	41(1)	50(1)	41(1)	0(1)	2(1)	-12(1)
C(5B)	38(1)	38(1)	37(1)	0(1)	2(1)	-5(1)
C(6B)	47(2)	68(2)	61(2)	-4(1)	6(1)	11(1)
C(7B)	57(2)	64(2)	50(2)	-8(1)	-2(1)	-21(1)
S(1C)	51(1)	55(1)	38(1)	7(1)	6(1)	-8(1)
C(1C)	40(1)	47(1)	37(1)	-1(1)	4(1)	-3(1)
C(2C)	33(1)	39(1)	36(1)	-1(1)	4(1)	-1(1)
C(3C)	31(1)	42(1)	37(1)	1(1)	2(1)	-1(1)
C(4C)	36(1)	44(1)	41(1)	1(1)	4(1)	-3(1)
C(5C)	38(1)	61(2)	40(1)	5(1)	-3(1)	-12(1)
C(6C)	61(2)	67(2)	40(1)	1(1)	-7(1)	-14(1)
C(7C)	49(1)	60(2)	57(2)	7(1)	4(1)	-17(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for tri(2,5-dimethylthiophenylene).

	x	y	z	U(eq)
H(5A2)	6614	7683	1746	50
H(5A1)	7488	7652	1391	50
H(6A3)	11782	2589	2167	68
H(6A2)	11733	2484	1711	68
H(6A1)	11382	80	1948	68
H(7A3)	5671	2439	2057	79
H(7A2)	6052	4747	2327	79
H(7A1)	6401	1997	2467	79
H(5B2)	8031	1907	1183	45
H(5B1)	7477	1098	766	45
H(6B3)	4059	9163	1504	71
H(6B2)	4412	7433	1866	71
H(6B1)	3082	7050	1617	71
H(7B3)	5604	-937	609	69
H(7B2)	4810	896	323	69
H(7B1)	4081	-702	624	69
H(5C2)	10814	5358	1378	56
H(5C1)	9979	7695	1478	56
H(6C3)	6255	4670	142	68
H(6C2)	7179	2338	101	68
H(6C1)	7324	4721	-162	68
H(7C3)	11738	8792	883	66
H(7C2)	10715	10738	1022	66
H(7C1)	11048	10687	585	66

Table 6. Torsion angles [deg] for tri(2,5-dimethylthiophenylene).

C(4A)-S(1A)-C(1A)-C(2A)	-0.48(19)
C(4A)-S(1A)-C(1A)-C(6A)	176.1(2)
C(6A)-C(1A)-C(2A)-C(3A)	-175.2(2)
S(1A)-C(1A)-C(2A)-C(3A)	0.8(3)
C(6A)-C(1A)-C(2A)-C(5C)	0.9(4)
S(1A)-C(1A)-C(2A)-C(5C)	176.97(18)
C(1A)-C(2A)-C(3A)-C(4A)	-0.9(3)
C(5C)-C(2A)-C(3A)-C(4A)	-177.0(2)
C(1A)-C(2A)-C(3A)-C(5A)	-178.8(2)
C(5C)-C(2A)-C(3A)-C(5A)	5.1(3)
C(2A)-C(3A)-C(4A)-C(7A)	-179.7(3)
C(5A)-C(3A)-C(4A)-C(7A)	-1.8(4)
C(2A)-C(3A)-C(4A)-S(1A)	0.5(3)
C(5A)-C(3A)-C(4A)-S(1A)	178.39(17)
C(1A)-S(1A)-C(4A)-C(3A)	0.0(2)
C(1A)-S(1A)-C(4A)-C(7A)	-179.8(2)
C(4A)-C(3A)-C(5A)-C(2B)	-67.2(3)
C(2A)-C(3A)-C(5A)-C(2B)	110.5(2)
C(4B)-S(1B)-C(1B)-C(2B)	0.9(2)
C(4B)-S(1B)-C(1B)-C(6B)	-179.5(2)
C(6B)-C(1B)-C(2B)-C(3B)	179.9(3)
S(1B)-C(1B)-C(2B)-C(3B)	-0.5(3)
C(6B)-C(1B)-C(2B)-C(5A)	1.6(4)
S(1B)-C(1B)-C(2B)-C(5A)	-178.84(18)
C(3A)-C(5A)-C(2B)-C(1B)	125.3(2)
C(3A)-C(5A)-C(2B)-C(3B)	-52.9(3)
C(1B)-C(2B)-C(3B)-C(4B)	-0.4(3)
C(5A)-C(2B)-C(3B)-C(4B)	178.0(2)
C(1B)-C(2B)-C(3B)-C(5B)	178.8(2)
C(5A)-C(2B)-C(3B)-C(5B)	-2.8(3)
C(2B)-C(3B)-C(4B)-C(7B)	-177.7(2)
C(5B)-C(3B)-C(4B)-C(7B)	3.1(4)
C(2B)-C(3B)-C(4B)-S(1B)	1.0(3)
C(5B)-C(3B)-C(4B)-S(1B)	-178.15(17)
C(1B)-S(1B)-C(4B)-C(3B)	-1.1(2)
C(1B)-S(1B)-C(4B)-C(7B)	177.8(2)
C(4B)-C(3B)-C(5B)-C(2C)	116.8(2)
C(2B)-C(3B)-C(5B)-C(2C)	-62.3(3)
C(4C)-S(1C)-C(1C)-C(2C)	-0.17(19)
C(4C)-S(1C)-C(1C)-C(6C)	-178.7(2)
C(6C)-C(1C)-C(2C)-C(3C)	178.5(2)
S(1C)-C(1C)-C(2C)-C(3C)	0.2(3)
C(6C)-C(1C)-C(2C)-C(5B)	-0.4(4)
S(1C)-C(1C)-C(2C)-C(5B)	-178.76(17)
C(3B)-C(5B)-C(2C)-C(1C)	-78.3(3)
C(3B)-C(5B)-C(2C)-C(3C)	103.0(3)
C(1C)-C(2C)-C(3C)-C(4C)	0.0(3)
C(5B)-C(2C)-C(3C)-C(4C)	178.8(2)
C(1C)-C(2C)-C(3C)-C(5C)	-179.7(2)
C(5B)-C(2C)-C(3C)-C(5C)	-0.8(4)
C(2C)-C(3C)-C(4C)-C(7C)	180.0(2)
C(5C)-C(3C)-C(4C)-C(7C)	-0.3(4)
C(2C)-C(3C)-C(4C)-S(1C)	-0.1(3)
C(5C)-C(3C)-C(4C)-S(1C)	179.59(18)
C(1C)-S(1C)-C(4C)-C(3C)	0.15(19)
C(1C)-S(1C)-C(4C)-C(7C)	-179.9(2)
C(1A)-C(2A)-C(5C)-C(3C)	127.3(3)
C(3A)-C(2A)-C(5C)-C(3C)	-57.0(3)
C(4C)-C(3C)-C(5C)-C(2A)	170.0(2)
C(2C)-C(3C)-C(5C)-C(2A)	-10.4(4)

Symmetry transformations used to generate equivalent atoms:

Table 1. Crystal data, structure solution and refinement for 6.

Identification code	jws3
Chemical formula	$C_{33}H_{38}F_6O_6RuS_5$
Formula weight	906.00
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	triclinic, $P\bar{1}$
Unit cell dimensions	a = 10.1661(12) Å α = 71.267(3)°
	b = 13.6994(17) Å β = 86.181(3)°
	c = 14.3077(17) Å γ = 88.430(3)°
Volume	1882.8(4) Å^3
Z	2
Density (calculated)	1.598 g/cm^3
Absorption coefficient μ	0.766 mm^{-1}
F(000)	924
Reflections for cell refinement	12168 (θ range 1.79 to 28.30°)
Crystal colour	pale yellow
Crystal size	0.47 x 0.31 x 0.11 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.51 to 28.35°
Index ranges	$-12 \le h \le 12$, $-17 \le k \le 17$, $-18 \le l \le 14$
Intensity decay of standards	0%
Reflections collected	14630
Independent reflections	8279 (R_{int} = 0.0190)
Reflections with I>2σ(I)	7446
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.875 and 0.608
Structure solution	Patterson synthesis
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0283, 1.7414
Data / restraints / parameters	8279 / 0 / 470
Goodness-of-fit on F^2	1.056
Final R indices [I>2σ(I)]	R1 = 0.0311, wR2 = 0.0724
R indices (all data)	R1 = 0.0367, wR2 = 0.0756
Extinction coefficient	0.0007(2)
Largest and mean shift/esd	0.003 and 0.000
Largest diff. peak and hole	0.756 and -0.648 eÅ^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for 6. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	2215.67(16)	2744.07(12)	4081.80(12)	18.29(6)
S(1A)	4229.8(5)	1854.1(4)	4180.0(4)	23.68(12)
S(1B)	3153.8(7)	796.0(5)	133.0(5)	38.23(15)
S(1C)	1686.0(7)	5590.7(5)	-521.0(5)	35.92(15)
C(1A)	4270(2)	3170.8(16)	3525.9(16)	22.3(4)
C(2A)	3497(2)	3425.7(16)	2688.1(16)	22.1(4)
C(3A)	2811(2)	2546.2(16)	2629.3(16)	22.0(4)
C(4A)	3089(2)	1631.4(16)	3414.4(16)	23.2(4)
C(5A)	1897(2)	2500.4(17)	1847.9(16)	23.4(4)
C(6A)	5180(2)	3860.0(19)	3794.8(19)	29.7(5)
C(7A)	2641(3)	555.3(17)	3563.3(19)	32.3(5)
C(11A)	94(2)	3253.6(18)	3920.8(17)	25.3(5)
C(12A)	157(2)	2216.0(17)	4535.9(17)	24.3(4)
C(13A)	910(2)	1930.7(17)	5374.3(16)	23.9(4)
C(14A)	1593(2)	2683.4(17)	5643.2(16)	23.7(4)
C(15A)	1539(2)	3714.5(17)	5025.6(18)	25.8(5)
C(16A)	821(2)	3994.3(17)	4168.6(18)	26.5(5)
C(17A)	-680(2)	3571(2)	3022(2)	36.7(6)
C(18A)	2370(2)	2344(2)	6563.5(18)	32.8(5)
C(19A)	3350(3)	3149(3)	6599(2)	50.5(8)
C(20A)	1392(3)	2079(3)	7468(2)	45.3(7)
C(1B)	2110(3)	1153.1(19)	975.0(18)	31.2(5)
C(2B)	2575(2)	2013.0(17)	1127.3(16)	24.9(4)
C(3B)	3771(2)	2397.8(18)	538.3(17)	26.6(5)
C(4B)	4209(3)	1808.4(19)	-28.7(18)	34.0(5)
C(5B)	4417(2)	3392.6(18)	491.9(18)	27.8(5)
C(6B)	887(3)	537(2)	1389(2)	43.4(7)
C(7B)	5411(3)	1941(2)	-724(2)	47.3(7)
C(1C)	2800(2)	4631.3(18)	-564.9(18)	30.3(5)
C(2C)	3429(2)	4273.7(17)	294.4(17)	26.0(5)
C(3C)	2980(2)	4771.0(17)	1001.4(17)	25.8(5)
C(4C)	2035(2)	5510.0(18)	663.3(18)	30.4(5)
C(6C)	2907(3)	4236(2)	-1430.2(18)	37.4(6)
C(7C)	1328(3)	6219(2)	1148(2)	41.9(6)
C(5C)	3563(2)	4530.3(17)	1990.8(17)	28.4(5)
S(1D)	7582.9(6)	3507.7(5)	6154.8(5)	34.66(15)
O(1D)	7583(3)	3851.0(18)	5095.6(18)	62.4(7)
O(2D)	6550(2)	3900.3(18)	6667(2)	66.8(7)
O(3D)	8866.2(19)	3523.3(15)	6503.0(16)	45.4(5)
C(1D)	7203(3)	2149(2)	6495(3)	46.3(7)
F(1D)	8122(2)	1637.0(13)	6139.5(18)	72.9(7)
F(2D)	6045(2)	1992.5(16)	6184(2)	91.9(9)
F(3D)	7144(3)	1700.9(17)	7446.8(18)	99.1(9)
S(1E)	2585.7(6)	9124.9(5)	6552.6(5)	29.40(13)
O(1E)	2968.2(19)	8157.1(15)	6422.3(17)	49.5(5)
O(2E)	1184.8(18)	9320.3(16)	6574.8(16)	43.1(5)
O(3E)	3370(2)	9990.4(15)	5972.1(14)	45.1(5)
C(1E)	3016(3)	8961(2)	7806(2)	44.1(7)
F(1E)	2721(2)	9783.2(16)	8068.4(14)	66.1(6)
F(2E)	4305(2)	8776(2)	7878.8(17)	83.7(7)
F(3E)	2376(3)	8177.7(17)	8459.1(15)	84.2(7)

Table 3. Bond lengths (Å) and angles (°) for 6.

Ru(1)-C(4A)	2.184(2)	Ru(1)-C(13A)	2.203(2)
Ru(1)-C(1A)	2.210(2)	Ru(1)-C(12A)	2.219(2)
Ru(1)-C(16A)	2.222(2)	Ru(1)-C(3A)	2.223(2)
Ru(1)-C(15A)	2.246(2)	Ru(1)-C(2A)	2.252(2)
Ru(1)-C(11A)	2.252(2)	Ru(1)-C(14A)	2.257(2)
Ru(1)-S(1A)	2.3432(6)	S(1A)-C(4A)	1.744(2)
S(1A)-C(1A)	1.745(2)	S(1B)-C(4B)	1.724(3)
S(1B)-C(1B)	1.731(3)	S(1C)-C(4C)	1.723(3)
S(1C)-C(1C)	1.725(3)	C(1A)-C(2A)	1.421(3)
C(1A)-C(6A)	1.492(3)	C(2A)-C(3A)	1.437(3)
C(2A)-C(5C)	1.522(3)	C(3A)-C(4A)	1.425(3)
C(3A)-C(5A)	1.518(3)	C(4A)-C(7A)	1.499(3)
C(5A)-C(2B)	1.519(3)	C(11A)-C(12A)	1.414(3)
C(11A)-C(16A)	1.417(3)	C(11A)-C(17A)	1.489(3)
C(12A)-C(13A)	1.408(3)	C(13A)-C(14A)	1.422(3)
C(14A)-C(15A)	1.407(3)	C(14A)-C(18A)	1.516(3)
C(15A)-C(16A)	1.409(3)	C(18A)-C(19A)	1.521(4)
C(18A)-C(20A)	1.531(4)	C(1B)-C(2B)	1.367(3)
C(1B)-C(6B)	1.499(4)	C(2B)-C(3B)	1.442(3)
C(3B)-C(4B)	1.364(3)	C(3B)-C(5B)	1.509(3)
C(4B)-C(7B)	1.500(4)	C(5B)-C(2C)	1.516(3)
C(1C)-C(2C)	1.364(3)	C(1C)-C(6C)	1.499(3)
C(2C)-C(3C)	1.435(3)	C(3C)-C(4C)	1.370(3)
C(3C)-C(5C)	1.505(3)	C(4C)-C(7C)	1.506(4)
S(1D)-O(3D)	1.430(2)	S(1D)-O(2D)	1.432(2)
S(1D)-O(1D)	1.435(2)	S(1D)-C(1D)	1.812(3)
C(1D)-F(3D)	1.300(4)	C(1D)-F(1D)	1.325(3)
C(1D)-F(2D)	1.332(4)	S(1E)-O(3E)	1.436(2)
S(1E)-O(1E)	1.4369(19)	S(1E)-O(2E)	1.4420(19)
S(1E)-C(1E)	1.817(3)	C(1E)-F(1E)	1.318(3)
C(1E)-F(3E)	1.326(4)	C(1E)-F(2E)	1.333(4)

C(4A)-Ru(1)-C(13A)	109.26(8)	C(4A)-Ru(1)-C(1A)	69.63(8)
C(13A)-Ru(1)-C(1A)	145.66(8)	C(4A)-Ru(1)-C(12A)	104.71(8)
C(13A)-Ru(1)-C(12A)	37.13(8)	C(1A)-Ru(1)-C(12A)	174.01(8)
C(4A)-Ru(1)-C(16A)	154.34(9)	C(13A)-Ru(1)-C(16A)	78.56(8)
C(1A)-Ru(1)-C(16A)	117.99(8)	C(12A)-Ru(1)-C(16A)	66.22(8)
C(4A)-Ru(1)-C(3A)	37.71(8)	C(13A)-Ru(1)-C(3A)	135.80(8)
C(1A)-Ru(1)-C(3A)	64.56(8)	C(12A)-Ru(1)-C(3A)	109.84(8)
C(16A)-Ru(1)-C(3A)	120.31(8)	C(4A)-Ru(1)-C(15A)	168.72(8)
C(13A)-Ru(1)-C(15A)	66.12(8)	C(1A)-Ru(1)-C(15A)	107.95(8)
C(12A)-Ru(1)-C(15A)	77.99(8)	C(16A)-Ru(1)-C(15A)	36.76(8)
C(3A)-Ru(1)-C(15A)	152.05(8)	C(4A)-Ru(1)-C(2A)	64.79(8)
C(13A)-Ru(1)-C(2A)	173.22(8)	C(1A)-Ru(1)-C(2A)	37.12(8)
C(12A)-Ru(1)-C(2A)	139.22(8)	C(16A)-Ru(1)-C(2A)	105.42(8)
C(3A)-Ru(1)-C(2A)	37.44(7)	C(15A)-Ru(1)-C(2A)	120.35(8)
C(4A)-Ru(1)-C(11A)	122.31(8)	C(13A)-Ru(1)-C(11A)	66.85(8)
C(1A)-Ru(1)-C(11A)	144.40(8)	C(12A)-Ru(1)-C(11A)	36.85(8)
C(16A)-Ru(1)-C(11A)	36.92(8)	C(3A)-Ru(1)-C(11A)	103.21(8)
C(15A)-Ru(1)-C(11A)	66.35(8)	C(2A)-Ru(1)-C(11A)	112.95(8)
C(4A)-Ru(1)-C(14A)	134.25(8)	C(13A)-Ru(1)-C(14A)	37.16(8)
C(1A)-Ru(1)-C(14A)	118.48(8)	C(12A)-Ru(1)-C(14A)	66.73(8)
C(16A)-Ru(1)-C(14A)	66.31(8)	C(3A)-Ru(1)-C(14A)	171.36(8)
C(15A)-Ru(1)-C(14A)	36.42(8)	C(2A)-Ru(1)-C(14A)	149.43(8)
C(11A)-Ru(1)-C(14A)	78.87(8)	C(4A)-Ru(1)-S(1A)	45.14(6)
C(13A)-Ru(1)-S(1A)	108.66(6)	C(1A)-Ru(1)-S(1A)	44.96(6)
C(12A)-Ru(1)-S(1A)	132.31(6)	C(16A)-Ru(1)-S(1A)	157.13(6)
C(3A)-Ru(1)-S(1A)	70.19(6)	C(15A)-Ru(1)-S(1A)	125.19(6)

C(2A)-Ru(1)-S(1A)	69.81(6)	C(11A)-Ru(1)-S(1A)	165.90(6)
C(14A)-Ru(1)-S(1A)	105.85(6)	C(4A)-S(1A)-C(1A)	91.95(10)
C(4A)-S(1A)-Ru(1)	62.61(7)	C(1A)-S(1A)-Ru(1)	63.47(7)
C(4B)-S(1B)-C(1B)	93.11(12)	C(4C)-S(1C)-C(1C)	93.13(12)
C(2A)-C(1A)-C(6A)	127.3(2)	C(2A)-C(1A)-S(1A)	111.97(16)
C(6A)-C(1A)-S(1A)	120.22(17)	C(2A)-C(1A)-Ru(1)	73.04(12)
C(6A)-C(1A)-Ru(1)	129.20(16)	S(1A)-C(1A)-Ru(1)	71.57(7)
C(1A)-C(2A)-C(3A)	111.92(19)	C(1A)-C(2A)-C(5C)	117.30(18)
C(3A)-C(2A)-C(5C)	130.7(2)	C(1A)-C(2A)-Ru(1)	69.84(12)
C(3A)-C(2A)-Ru(1)	70.22(12)	C(5C)-C(2A)-Ru(1)	129.56(15)
C(4A)-C(3A)-C(2A)	112.35(19)	C(4A)-C(3A)-C(5A)	119.70(19)
C(2A)-C(3A)-C(5A)	127.95(19)	C(4A)-C(3A)-Ru(1)	69.66(12)
C(2A)-C(3A)-Ru(1)	72.34(12)	C(5A)-C(3A)-Ru(1)	126.47(15)
C(3A)-C(4A)-C(7A)	128.0(2)	C(3A)-C(4A)-S(1A)	111.61(16)
C(7A)-C(4A)-S(1A)	120.05(17)	C(3A)-C(4A)-Ru(1)	72.63(12)
C(7A)-C(4A)-Ru(1)	127.90(16)	S(1A)-C(4A)-Ru(1)	72.25(8)
C(3A)-C(5A)-C(2B)	111.41(18)	C(12A)-C(11A)-C(16A)	118.0(2)
C(12A)-C(11A)-C(17A)	121.8(2)	C(16A)-C(11A)-C(17A)	120.2(2)
C(12A)-C(11A)-Ru(1)	70.33(12)	C(16A)-C(11A)-Ru(1)	70.40(12)
C(17A)-C(11A)-Ru(1)	129.49(17)	C(13A)-C(12A)-C(11A)	120.9(2)
C(13A)-C(12A)-Ru(1)	70.80(12)	C(11A)-C(12A)-Ru(1)	72.82(12)
C(12A)-C(13A)-C(14A)	120.9(2)	C(12A)-C(13A)-Ru(1)	72.07(12)
C(14A)-C(13A)-Ru(1)	73.48(13)	C(15A)-C(14A)-C(13A)	118.1(2)
C(15A)-C(14A)-C(18A)	122.7(2)	C(13A)-C(14A)-C(18A)	119.1(2)
C(15A)-C(14A)-Ru(1)	71.35(12)	C(13A)-C(14A)-Ru(1)	69.36(12)
C(18A)-C(14A)-Ru(1)	129.56(15)	C(14A)-C(15A)-C(16A)	120.9(2)
C(14A)-C(15A)-Ru(1)	72.23(12)	C(16A)-C(15A)-Ru(1)	70.72(12)
C(15A)-C(16A)-C(11A)	121.1(2)	C(15A)-C(16A)-Ru(1)	72.51(12)
C(11A)-C(16A)-Ru(1)	72.67(13)	C(14A)-C(18A)-C(19A)	113.0(2)
C(14A)-C(18A)-C(20A)	108.3(2)	C(19A)-C(18A)-C(20A)	110.9(2)
C(2B)-C(1B)-C(6B)	130.8(2)	C(2B)-C(1B)-S(1B)	110.32(19)
C(6B)-C(1B)-S(1B)	118.84(18)	C(1B)-C(2B)-C(3B)	112.9(2)
C(1B)-C(2B)-C(5A)	123.0(2)	C(3B)-C(2B)-C(5A)	124.1(2)
C(4B)-C(3B)-C(2B)	113.0(2)	C(4B)-C(3B)-C(5B)	123.2(2)
C(2B)-C(3B)-C(5B)	123.6(2)	C(3B)-C(4B)-C(7B)	129.3(3)
C(3B)-C(4B)-S(1B)	110.59(19)	C(7B)-C(4B)-S(1B)	120.1(2)
C(3B)-C(5B)-C(2C)	111.32(19)	C(2C)-C(1C)-C(6C)	128.1(2)
C(2C)-C(1C)-S(1C)	110.75(18)	C(6C)-C(1C)-S(1C)	120.97(19)
C(1C)-C(2C)-C(3C)	112.6(2)	C(1C)-C(2C)-C(5B)	122.8(2)
C(3C)-C(2C)-C(5B)	124.5(2)	C(4C)-C(3C)-C(2C)	113.4(2)
C(4C)-C(3C)-C(5C)	124.3(2)	C(2C)-C(3C)-C(5C)	122.2(2)
C(3C)-C(4C)-C(7C)	130.7(2)	C(3C)-C(4C)-S(1C)	110.12(18)
C(7C)-C(4C)-S(1C)	119.17(19)	C(3C)-C(5C)-C(2A)	118.32(18)
O(3D)-S(1D)-O(2D)	114.68(14)	O(3D)-S(1D)-O(1D)	112.79(14)
O(2D)-S(1D)-O(1D)	116.49(16)	O(3D)-S(1D)-C(1D)	104.14(14)
O(2D)-S(1D)-C(1D)	103.32(13)	O(1D)-S(1D)-C(1D)	103.32(15)
F(3D)-C(1D)-F(1D)	105.2(3)	F(3D)-C(1D)-F(2D)	106.6(3)
F(1D)-C(1D)-F(2D)	108.5(3)	F(3D)-C(1D)-S(1D)	112.2(2)
F(1D)-C(1D)-S(1D)	111.88(19)	F(2D)-C(1D)-S(1D)	112.0(2)
O(3E)-S(1E)-O(1E)	114.99(13)	O(3E)-S(1E)-O(2E)	114.66(13)
O(1E)-S(1E)-O(2E)	114.86(12)	O(3E)-S(1E)-C(1E)	102.95(13)
O(1E)-S(1E)-C(1E)	103.15(14)	O(2E)-S(1E)-C(1E)	103.95(13)
F(1E)-C(1E)-F(3E)	106.7(3)	F(1E)-C(1E)-F(2E)	108.6(3)
F(3E)-C(1E)-F(2E)	108.2(3)	F(1E)-C(1E)-S(1E)	112.09(19)
F(3E)-C(1E)-S(1E)	111.6(2)	F(2E)-C(1E)-S(1E)	109.6(2)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for 6.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Ru(1)	18.47(9)	17.27(9)	20.18(9)	-7.15(6)	-2.45(6)	-0.63(6)
S(1A)	22.3(3)	22.4(3)	25.3(3)	-6.4(2)	-1.9(2)	3.2(2)
S(1B)	55.3(4)	32.8(3)	31.3(3)	-17.7(3)	0.5(3)	2.9(3)
S(1C)	42.5(4)	32.1(3)	30.9(3)	-5.8(3)	-10.5(3)	5.9(3)
C(1A)	19.9(10)	21.4(10)	24.6(11)	-6.2(9)	0.9(8)	-0.8(8)
C(2A)	22.5(10)	21.9(10)	22.0(11)	-7.6(8)	1.1(8)	-1.6(8)
C(3A)	25.8(11)	22.7(10)	18.7(10)	-8.8(8)	2.7(8)	-2.7(8)
C(4A)	25.7(11)	21.4(10)	23.7(11)	-9.4(9)	0.8(9)	-0.4(8)
C(5A)	25.3(11)	24.8(11)	21.9(11)	-9.7(9)	-1.8(9)	-3.9(8)
C(6A)	23.7(11)	32.2(12)	34.2(13)	-10.8(10)	-6.0(10)	-4.3(9)
C(7A)	47.1(15)	20.1(11)	30.1(12)	-8.9(9)	1.6(11)	-5.4(10)
C(11A)	16.9(10)	31.2(12)	26.2(11)	-6.9(9)	-1.9(8)	1.4(8)
C(12A)	19.6(10)	28.0(11)	25.7(11)	-9.2(9)	1.7(8)	-5.8(8)
C(13A)	23.5(11)	23.6(10)	23.5(11)	-6.7(9)	2.1(9)	0.6(8)
C(14A)	21.6(10)	30.1(11)	21.8(11)	-12.0(9)	-1.0(8)	4.1(8)
C(15A)	23.4(11)	25.8(11)	34.1(13)	-18.4(10)	0.0(9)	2.1(8)
C(16A)	23.1(11)	21.6(10)	33.4(13)	-7.3(9)	-0.3(9)	3.0(8)
C(17A)	27.4(13)	44.2(15)	34.8(14)	-6.1(12)	-9.0(10)	3.1(11)
C(18A)	33.4(13)	43.7(14)	27.2(12)	-19.0(11)	-8.9(10)	11.2(11)
C(19A)	42.3(16)	79(2)	41.2(16)	-31.7(16)	-14.2(13)	-2.5(15)
C(20A)	45.0(16)	61.2(19)	26.2(13)	-9.1(13)	-5.8(12)	6.0(14)
C(1B)	38.9(13)	30.2(12)	27.3(12)	-13.0(10)	-2.1(10)	-2.2(10)
C(2B)	30.5(12)	25.4(11)	19.1(10)	-7.2(9)	-3.2(9)	-0.2(9)
C(3B)	29.2(12)	26.5(11)	21.9(11)	-4.6(9)	-2.9(9)	2.5(9)
C(4B)	41.4(14)	31.1(12)	26.5(12)	-6.6(10)	0.8(10)	8.0(10)
C(5B)	25.4(11)	28.7(11)	26.8(12)	-5.9(9)	1.4(9)	-1.0(9)
C(6B)	49.7(17)	40.8(15)	47.8(17)	-25.0(13)	0.0(13)	-14.6(12)
C(7B)	53.2(18)	45.7(16)	38.9(16)	-11.6(13)	12.0(13)	11.3(13)
C(1C)	34.9(13)	29.1(12)	23.6(12)	-3.8(9)	0.7(10)	-3.9(10)
C(2C)	27.3(11)	22.1(10)	24.7(11)	-2.3(9)	1.2(9)	-5.1(9)
C(3C)	30.2(12)	20.8(10)	23.9(11)	-3.1(9)	-2.0(9)	-5.7(9)
C(4C)	34.8(13)	23.6(11)	31.0(13)	-5.8(10)	-3.4(10)	-2.0(9)
C(6C)	44.1(15)	41.9(15)	23.8(12)	-7.1(11)	-1.8(11)	-1.4(12)
C(7C)	48.3(16)	31.3(13)	47.4(17)	-14.7(12)	-5.0(13)	7.4(12)
C(5C)	33.8(12)	21.9(11)	28.4(12)	-5.6(9)	-5.8(10)	-4.5(9)
S(1D)	37.1(3)	23.6(3)	48.9(4)	-17.9(3)	-11.7(3)	2.8(2)
O(1D)	83.7(17)	49.4(13)	53.3(14)	-9.1(11)	-32.1(12)	-11.8(12)
O(2D)	48.7(13)	49.3(13)	120(2)	-53.9(15)	-4.0(13)	12.4(10)
O(3D)	42.7(11)	41.4(11)	57.3(13)	-20.6(10)	-18.0(10)	2.7(8)
C(1D)	42.5(16)	28.8(13)	67(2)	-20.1(14)	24.9(14)	-4.4(11)
F(1D)	68.8(12)	32.0(9)	119.6(18)	-37.7(10)	55.8(12)	-12.4(8)
F(2D)	57.5(13)	51.7(12)	177(3)	-50.6(15)	-5.2(15)	-19.1(10)
F(3D)	142(2)	52.4(13)	75.8(16)	4.2(11)	58.2(16)	5.5(13)
S(1E)	27.1(3)	28.7(3)	34.2(3)	-12.8(2)	-0.6(2)	-1.3(2)
O(1E)	38.7(11)	40.6(11)	76.8(16)	-32.6(11)	12.2(10)	-1.3(8)
O(2E)	28.8(9)	53.2(12)	55.6(13)	-28.4(10)	-7.3(9)	5.2(8)
O(3E)	54.4(12)	41.3(11)	35.6(10)	-6.0(9)	0.2(9)	-15.1(9)
C(1E)	49.1(17)	41.8(15)	35.5(15)	-3.8(12)	-8.5(13)	9.1(13)
F(1E)	98.5(16)	65.2(13)	46.3(11)	-32.3(10)	-18.4(10)	7.6(11)
F(2E)	60.4(13)	122(2)	67.9(14)	-24.8(14)	-36.6(11)	31.3(13)
F(3E)	126(2)	60.3(13)	43.5(11)	11.2(10)	11.6(12)	-0.4(13)

Table 5. Hydrogen atom coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 6.

	x	y	z	U
H(5A)	1603	3207	1481	28
H(5B)	1106	2094	2173	28
H(6A)	4768	4540	3682	45
H(6B)	6006	3931	3386	45
H(6C)	5365	3562	4494	45
H(7A)	2808	117	4236	48
H(7B)	3127	283	3085	48
H(7C)	1695	562	3466	48
H(12A)	-316	1704	4382	29
H(13A)	963	1226	5766	29
H(15A)	1994	4229	5188	31
H(16A)	824	4691	3750	32
H(17A)	-1566	3787	3191	55
H(17B)	-745	2988	2772	55
H(17C)	-238	4146	2513	55
H(18A)	2872	1704	6572	39
H(19A)	2872	3763	6650	76
H(19B)	3931	3338	5994	76
H(19C)	3879	2866	7174	76
H(20A)	1876	1845	8072	68
H(20B)	805	1531	7451	68
H(20C)	869	2693	7462	68
H(5C)	5130	3560	-40	33
H(5D)	4817	3306	1126	33
H(6D)	1104	-200	1581	65
H(6E)	234	700	886	65
H(6F)	524	708	1969	65
H(7D)	5398	2630	-1217	71
H(7E)	5416	1419	-1059	71
H(7F)	6203	1862	-352	71
H(6G)	2587	4765	-2013	56
H(6H)	2373	3613	-1280	56
H(6I)	3830	4072	-1564	56
H(7G)	1726	6157	1770	63
H(7H)	396	6029	1284	63
H(7I)	1403	6932	707	63
H(5E)	3119	4977	2340	34
H(5F)	4503	4732	1870	34

Table 1. Crystal data, structure solution and refinement for 9.

Identification code	jws1
Chemical formula	$C_{48}H_{61}F_{12}Ir_2NO_{13}S_7$
Formula weight	1696.80
Temperature	160(2) K
Radiation and wavelength	MoKα, 0.71073 Å
Crystal system, space group	monoclinic, Cc
Unit cell dimensions	a = 20.6686(16) Å α = 90°
	b = 17.4490(13) Å β = 106.158(2)°
	c = 17.0768(13) Å γ = 90°
Volume	5915.4(8) Å^3
Z	4
Density (calculated)	1.905 g/cm^3
Absorption coefficient μ	4.840 mm^{-1}
F(000)	3336
Reflections for cell refinement	15417 (θ range 2.05 to 28.43°)
Crystal colour	pale yellow
Crystal size	0.80 × 0.30 × 0.09 mm
Data collection method	Siemens SMART CCD diffractometer,
	ω rotation with narrow frames
θ range for data collection	1.55 to 25.00°
Index ranges	$-15 \le h \le 27$, $-20 \le k \le 22$, $-22 \le l \le 22$
Intensity decay of standards	0%
Reflections collected	15221
Independent reflections	7144 (R_{int} = 0.0398)
Reflections with I>2σ(I)	6797
Absorption correction	semi-empirical from ψ-scans
Max. and min. transmission	0.379 and 0.241
Structure solution	direct methods
Refinement method	full-matrix least-squares on F^2
Weighting parameters a, b	0.0877, 38.0859
Data / restraints / parameters	7144 / 461 / 801
Goodness-of-fit on F^2	1.049
Final R indices [I>2σ(I)]	R1 = 0.0479, wR2 = 0.1265
R indices (all data)	R1 = 0.0506, wR2 = 0.1290
Absolute structure parameter	0.416(13)
Largest and mean shift/esd	0.009 and 0.001
Largest diff. peak and hole	2.861 and -2.524 eÅ^{-3}

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

	x	y	z	U(eq)
Ir(1A)	7317.1(2)	8438.9(2)	1794.0(2)	27.97(15)
Ir(1B)	10441.4(2)	8564.3(3)	1400.1(2)	30.99(16)
S(1A)	7035(2)	8046(2)	408(2)	36.9(9)
S(1C)	8952(3)	5021.7(14)	1546(3)	36.0(9)
S(1B)	10790(2)	8099.2(19)	2753(2)	33.6(8)
C(1A)	7410(8)	7344(6)	1165(9)	29(3)
C(2A)	8071(7)	7589(6)	1610(8)	24(3)
C(3A)	8240(10)	8327(9)	1342(14)	48(4)
C(4A)	7738(10)	8658(8)	753(12)	40(4)
C(5A)	8892(11)	8747(8)	1767(17)	78(6)
C(6A)	7080(10)	6630(10)	1191(12)	43(4)
C(7A)	7719(13)	9404(9)	303(14)	67(6)
C(11A)	6998(9)	9466(9)	2317(9)	42(3)
C(12A)	6457(9)	8985(9)	2068(10)	41(3)
C(13A)	6592(10)	8271(9)	2517(10)	37(3)
C(14A)	7310(13)	8364(10)	3059(11)	53(5)
C(15A)	7509(9)	9091(9)	2905(10)	50(4)
C(16A)	7071(12)	10318(9)	1995(14)	69(6)
C(17A)	5776(10)	9212(8)	1429(10)	44(4)
C(18A)	6149(9)	7595(10)	2483(10)	51(4)
C(19A)	7615(10)	7813(11)	3667(10)	55(5)
C(20A)	8191(11)	9465(10)	3376(14)	70(7)
C(1B)	10056(10)	8679(8)	2512(12)	39(4)
C(2B)	9550(8)	8355(7)	1878(11)	33(3)
C(3B)	9738(8)	7665(7)	1570(9)	31(3)
C(4B)	10414(8)	7452(8)	2011(8)	30(3)
C(5B)	9279(7)	7155(7)	926(8)	26(3)
C(6B)	10039(12)	9400(9)	2995(13)	59(5)
C(7B)	10789(10)	6718(9)	1889(11)	37(4)
C(11B)	10147(10)	9328(10)	331(10)	56(4)
C(12B)	10395(13)	8647(13)	118(12)	66(5)
C(13B)	11066(11)	8524(10)	602(10)	50(5)
C(14B)	11277(9)	9182(10)	1133(9)	47(4)
C(15B)	10681(9)	9705(8)	973(10)	41(3)
C(16B)	9489(15)	9652(14)	-44(18)	102(10)
C(17B)	10055(13)	8062(16)	-564(12)	90(8)
C(18B)	11600(12)	7869(12)	585(11)	67(5)
C(19B)	11918(11)	9388(14)	1670(12)	71(6)
C(20B)	10612(14)	10410(10)	1297(15)	94(9)
C(1C)	9207(8)	5723(7)	979(9)	29(3)
C(2C)	9096(9)	6427(6)	1251(9)	22(3)
C(3C)	8769(8)	6394(6)	1895(10)	23(3)
C(4C)	8658(8)	5677(7)	2127(9)	26(3)
C(5C)	8497(8)	7093(6)	2267(9)	28(3)
C(6C)	9470(10)	5501(8)	302(10)	46(4)
C(7C)	8397(10)	5398(8)	2816(10)	46(4)
S(1D)	5053(3)	7190(2)	-370(3)	54.0(12)
O(1D)	5128(13)	7236(10)	469(10)	111(8)
O(2D)	4504(11)	6829(9)	-869(15)	112(8)
O(3D)	5659(9)	6929(7)	-519(11)	78(5)
C(1D)	4972(14)	8145(10)	-714(12)	67(7)

F(1D)	4445(13)	8473(9)	-637(12)	123(8)
F(2D)	5473(10)	8579(6)	-348(8)	85(5)
F(3D)	4946(8)	8174(7)	-1519(7)	81(4)
S(1E)	1717(3)	10526(3)	3666(3)	61.4(13)
O(1E)	1589(12)	9687(11)	3434(16)	131(9)
O(2E)	2000(9)	10962(9)	3140(9)	80(4)
O(3E)	1239(9)	10880(10)	3968(10)	87(5)
C(1E)	2418(15)	10360(10)	4530(12)	65(7)
F(1E)	2684(9)	10992(7)	4907(9)	111(6)
F(2E)	2263(13)	9911(11)	5068(11)	139(8)
F(3E)	2927(9)	10016(8)	4351(8)	83(4)
S(1F)	6111(3)	10744(3)	-497(3)	65.8(14)
O(1F)	5803(11)	11256(14)	-132(14)	140(10)
O(2F)	6699(10)	10935(9)	-735(9)	89(6)
O(3F)	6223(9)	10066(13)	-1(10)	122(9)
C(1F)	5498(17)	10403(14)	-1385(15)	79(7)
F(1F)	5267(9)	11013(8)	-1889(10)	103(5)
F(2F)	4987(9)	10091(8)	-1217(9)	85(4)
F(3F)	5744(10)	9904(7)	-1817(8)	91(5)
S(1G)	2736(3)	7087(3)	3521(3)	63.9(15)
O(1G)	2756(17)	7118(17)	2712(14)	192(16)
O(2G)	3287(9)	6715(10)	4051(19)	139(11)
O(3G)	2082(9)	6938(10)	3628(9)	81(5)
C(1G)	2889(15)	7990(15)	3788(16)	96(10)
F(1G)	2497(20)	8526(9)	3296(14)	198(17)
F(2G)	3489(13)	8275(11)	3746(12)	130(8)
F(3G)	2894(9)	8159(8)	4572(8)	95(5)
N(1S)	8843(15)	11825(7)	1519(15)	69(5)
O1Sa	8858(13)	10564(10)	1852(18)	45(6)
C1Sa	9032(28)	11177(24)	2046(30)	75(9)
C2Sa	8442(25)	11754(21)	772(26)	72(10)
C3Sa	9076(25)	12553(16)	1925(27)	70(9)
O1SAb	8914(28)	10538(23)	1324(34)	127(16)
C1SAb	8792(30)	11207(23)	1056(33)	84(10)
C2SAb	8784(29)	12700(20)	1102(31)	89(12)
C3SAb	9336(32)	11864(31)	2249(33)	100(13)

Table 3. Bond lengths (Å) and angles (°) for 9.

Ir(1A)-C(15A)	2.152(15)	Ir(1A)-C(14A)	2.168(19)
Ir(1A)-C(12A)	2.180(17)	Ir(1A)-C(11A)	2.185(14)
Ir(1A)-C(13A)	2.212(18)	Ir(1A)-C(4A)	2.219(19)
Ir(1A)-C(1A)	2.226(11)	Ir(1A)-C(2A)	2.236(12)
Ir(1A)-C(3A)	2.26(2)	Ir(1A)-S(1A)	2.376(4)
Ir(1B)-C(13B)	2.124(19)	Ir(1B)-C(12B)	2.170(20)
Ir(1B)-C(14B)	2.188(15)	Ir(1B)-C(11B)	2.204(14)
Ir(1B)-C(4B)	2.211(14)	Ir(1B)-C(3B)	2.213(14)
Ir(1B)-C(15B)	2.223(12)	Ir(1B)-C(2B)	2.243(15)
Ir(1B)-C(1B)	2.263(19)	Ir(1B)-S(1B)	2.365(4)
S(1A)-C(4A)	1.767(19)	S(1A)-C(1A)	1.794(15)
S(1C)-C(1C)	1.731(15)	S(1C)-C(4C)	1.731(14)
S(1B)-C(4B)	1.714(14)	S(1B)-C(1B)	1.773(19)
C(1A)-C(6A)	1.43(2)	C(1A)-C(2A)	1.43(2)
C(2A)-C(3A)	1.44(2)	C(2A)-C(5C)	1.495(20)
C(3A)-C(4A)	1.36(3)	C(3A)-C(5A)	1.53(3)
C(4A)-C(7A)	1.51(2)	C(5A)-C(2B)	1.49(3)
C(11A)-C(12A)	1.37(2)	C(11A)-C(15A)	1.40(2)
C(11A)-C(16A)	1.61(2)	C(12A)-C(13A)	1.45(2)
C(12A)-C(17A)	1.57(2)	C(13A)-C(18A)	1.48(3)
C(13A)-C(14A)	1.52(3)	C(14A)-C(15A)	1.38(3)
C(14A)-C(19A)	1.43(3)	C(15A)-C(20A)	1.56(3)
C(1B)-C(2B)	1.40(3)	C(1B)-C(6B)	1.51(2)
C(2B)-C(3B)	1.411(20)	C(3B)-C(4B)	1.44(2)
C(3B)-C(5B)	1.522(20)	C(4B)-C(7B)	1.54(2)
C(5B)-C(2C)	1.477(18)	C(11B)-C(12B)	1.38(3)
C(11B)-C(16B)	1.45(3)	C(11B)-C(15B)	1.48(2)
C(12B)-C(13B)	1.42(3)	C(12B)-C(17B)	1.56(3)
C(13B)-C(14B)	1.45(2)	C(13B)-C(18B)	1.59(3)
C(14B)-C(19B)	1.43(2)	C(14B)-C(15B)	1.50(3)
C(15B)-C(20B)	1.37(3)	C(1C)-C(2C)	1.357(18)
C(1C)-C(6C)	1.46(2)	C(2C)-C(3C)	1.443(16)
C(3C)-C(4C)	1.350(18)	C(3C)-C(5C)	1.553(18)
C(4C)-C(7C)	1.51(2)	S(1D)-O(2D)	1.368(20)
S(1D)-O(1D)	1.399(17)	S(1D)-O(3D)	1.421(18)
S(1D)-C(1D)	1.760(19)	C(1D)-F(1D)	1.27(3)
C(1D)-F(2D)	1.29(3)	C(1D)-F(3D)	1.36(2)
S(1E)-O(3E)	1.381(17)	S(1E)-O(2E)	1.420(15)
S(1E)-O(1E)	1.522(17)	S(1E)-C(1E)	1.78(3)
C(1E)-F(2E)	1.31(2)	C(1E)-F(1E)	1.32(2)
C(1E)-F(3E)	1.32(3)	S(1F)-O(1F)	1.347(19)
S(1F)-O(2F)	1.423(18)	S(1F)-O(3F)	1.436(17)
S(1F)-C(1F)	1.79(3)	C(1F)-F(2F)	1.29(3)
C(1F)-F(3F)	1.33(3)	C(1F)-F(1F)	1.37(3)
S(1G)-O(1G)	1.395(20)	S(1G)-O(2G)	1.40(2)
S(1G)-O(3G)	1.437(17)	S(1G)-C(1G)	1.65(3)
C(1G)-F(2G)	1.36(4)	C(1G)-F(1G)	1.36(3)
C(1G)-F(3G)	1.37(3)	N(1S)-C2Sa	1.32(4)
N(1S)-C1SAb	1.32(5)	N(1S)-C3SAb	1.38(5)
N(1S)-C1Sa	1.43(5)	N(1S)-C3Sa	1.46(3)
N(1S)-C2SAb	1.68(4)	O1Sa-C1Sa	1.15(5)
O1SAb-C1SAb	1.25(4)		

C(15A)-Ir(1A)-C(14A)	37.3(7)	C(15A)-Ir(1A)-C(12A)	62.7(6)
C(14A)-Ir(1A)-C(12A)	65.2(8)	C(15A)-Ir(1A)-C(11A)	37.7(6)
C(14A)-Ir(1A)-C(11A)	63.6(6)	C(12A)-Ir(1A)-C(11A)	36.6(6)
C(15A)-Ir(1A)-C(13A)	64.2(7)	C(14A)-Ir(1A)-C(13A)	40.7(8)
C(12A)-Ir(1A)-C(13A)	38.5(6)	C(11A)-Ir(1A)-C(13A)	63.4(6)

C(15A)-Ir(1A)-C(4A)	126.7(7)	C(14A)-Ir(1A)-C(4A)	157.1(8)
C(12A)-Ir(1A)-C(4A)	128.4(6)	C(11A)-Ir(1A)-C(4A)	114.6(5)
C(13A)-Ir(1A)-C(4A)	161.5(7)	C(15A)-Ir(1A)-C(1A)	149.2(6)
C(14A)-Ir(1A)-C(1A)	117.0(6)	C(12A)-Ir(1A)-C(1A)	131.6(6)
C(11A)-Ir(1A)-C(1A)	167.9(6)	C(13A)-Ir(1A)-C(1A)	108.6(6)
C(4A)-Ir(1A)-C(1A)	69.9(5)	C(15A)-Ir(1A)-C(2A)	120.7(6)
C(14A)-Ir(1A)-C(2A)	107.3(6)	C(12A)-Ir(1A)-C(2A)	164.2(5)
C(11A)-Ir(1A)-C(2A)	154.6(6)	C(13A)-Ir(1A)-C(2A)	126.7(5)
C(4A)-Ir(1A)-C(2A)	63.7(5)	C(1A)-Ir(1A)-C(2A)	37.4(5)
C(15A)-Ir(1A)-C(3A)	112.4(7)	C(14A)-Ir(1A)-C(3A)	125.2(9)
C(12A)-Ir(1A)-C(3A)	158.3(6)	C(11A)-Ir(1A)-C(3A)	126.2(6)
C(13A)-Ir(1A)-C(3A)	161.5(6)	C(4A)-Ir(1A)-C(3A)	35.3(7)
C(1A)-Ir(1A)-C(3A)	64.3(6)	C(2A)-Ir(1A)-C(3A)	37.4(5)
C(15A)-Ir(1A)-S(1A)	164.7(5)	C(14A)-Ir(1A)-S(1A)	155.1(6)
C(12A)-Ir(1A)-S(1A)	110.5(5)	C(11A)-Ir(1A)-S(1A)	128.7(4)
C(13A)-Ir(1A)-S(1A)	120.1(5)	C(4A)-Ir(1A)-S(1A)	45.1(5)
C(1A)-Ir(1A)-S(1A)	45.7(4)	C(2A)-Ir(1A)-S(1A)	69.9(4)
C(3A)-Ir(1A)-S(1A)	68.3(5)	C(13B)-Ir(1B)-C(12B)	38.6(9)
C(13B)-Ir(1B)-C(14B)	39.3(6)	C(12B)-Ir(1B)-C(14B)	64.7(7)
C(13B)-Ir(1B)-C(11B)	64.3(8)	C(12B)-Ir(1B)-C(11B)	36.8(8)
C(14B)-Ir(1B)-C(11B)	65.3(7)	C(13B)-Ir(1B)-C(4B)	112.0(6)
C(12B)-Ir(1B)-C(4B)	122.3(7)	C(14B)-Ir(1B)-C(4B)	131.0(7)
C(11B)-Ir(1B)-C(4B)	152.1(6)	C(13B)-Ir(1B)-C(3B)	126.9(6)
C(12B)-Ir(1B)-C(3B)	109.5(6)	C(14B)-Ir(1B)-C(3B)	164.1(6)
C(11B)-Ir(1B)-C(3B)	119.8(6)	C(4B)-Ir(1B)-C(3B)	38.0(5)
C(13B)-Ir(1B)-C(15B)	65.6(7)	C(12B)-Ir(1B)-C(15B)	63.9(7)
C(14B)-Ir(1B)-C(15B)	39.6(7)	C(11B)-Ir(1B)-C(15B)	38.9(6)
C(4B)-Ir(1B)-C(15B)	168.0(6)	C(3B)-Ir(1B)-C(15B)	153.2(6)
C(13B)-Ir(1B)-C(2B)	159.4(6)	C(12B)-Ir(1B)-C(2B)	124.6(8)
C(14B)-Ir(1B)-C(2B)	158.7(6)	C(11B)-Ir(1B)-C(2B)	109.5(7)
C(4B)-Ir(1B)-C(2B)	63.5(5)	C(3B)-Ir(1B)-C(2B)	36.9(5)
C(15B)-Ir(1B)-C(2B)	123.1(6)	C(13B)-Ir(1B)-C(1B)	163.8(7)
C(12B)-Ir(1B)-C(1B)	156.0(9)	C(14B)-Ir(1B)-C(1B)	127.9(6)
C(11B)-Ir(1B)-C(1B)	124.1(7)	C(4B)-Ir(1B)-C(1B)	67.7(5)
C(3B)-Ir(1B)-C(1B)	63.6(5)	C(15B)-Ir(1B)-C(1B)	111.1(6)
C(2B)-Ir(1B)-C(1B)	36.1(7)	C(13B)-Ir(1B)-S(1B)	122.8(6)
C(12B)-Ir(1B)-S(1B)	157.7(8)	C(14B)-Ir(1B)-S(1B)	109.2(4)
C(11B)-Ir(1B)-S(1B)	162.8(6)	C(4B)-Ir(1B)-S(1B)	43.8(4)
C(3B)-Ir(1B)-S(1B)	70.2(4)	C(15B)-Ir(1B)-S(1B)	126.4(4)
C(2B)-Ir(1B)-S(1B)	69.2(5)	C(1B)-Ir(1B)-S(1B)	45.0(5)
C(4A)-S(1A)-C(1A)	91.2(8)	C(4A)-S(1A)-Ir(1A)	62.8(6)
C(1A)-S(1A)-Ir(1A)	62.7(4)	C(1C)-S(1C)-C(4C)	93.7(5)
C(4B)-S(1B)-C(1B)	91.2(8)	C(4B)-S(1B)-Ir(1B)	63.3(5)
C(1B)-S(1B)-Ir(1B)	64.5(6)	C(6A)-C(1A)-C(2A)	129.7(14)
C(6A)-C(1A)-S(1A)	120.3(13)	C(2A)-C(1A)-S(1A)	109.6(9)
C(6A)-C(1A)-Ir(1A)	128.9(12)	C(2A)-C(1A)-Ir(1A)	71.7(6)
S(1A)-C(1A)-Ir(1A)	71.5(4)	C(1A)-C(2A)-C(3A)	112.2(14)
C(1A)-C(2A)-C(5C)	120.1(11)	C(3A)-C(2A)-C(5C)	127.7(14)
C(1A)-C(2A)-Ir(1A)	70.9(7)	C(3A)-C(2A)-Ir(1A)	72.0(9)
C(5C)-C(2A)-Ir(1A)	124.4(9)	C(4A)-C(3A)-C(2A)	114.4(16)
C(4A)-C(3A)-C(5A)	122.6(16)	C(2A)-C(3A)-C(5A)	122.5(18)
C(4A)-C(3A)-Ir(1A)	70.8(11)	C(2A)-C(3A)-Ir(1A)	70.5(9)
C(5A)-C(3A)-Ir(1A)	120.9(14)	C(3A)-C(4A)-C(7A)	130.7(19)
C(3A)-C(4A)-S(1A)	112.2(12)	C(7A)-C(4A)-S(1A)	116.7(15)
C(3A)-C(4A)-Ir(1A)	73.9(12)	C(7A)-C(4A)-Ir(1A)	126.6(12)
S(1A)-C(4A)-Ir(1A)	72.2(6)	C(2B)-C(5A)-C(3A)	119.6(13)
C(12A)-C(11A)-C(15A)	108.9(15)	C(12A)-C(11A)-C(16A)	127.4(16)
C(15A)-C(11A)-C(16A)	123.7(16)	C(12A)-C(11A)-Ir(1A)	71.5(9)
C(15A)-C(11A)-Ir(1A)	69.9(9)	C(16A)-C(11A)-Ir(1A)	123.4(11)
C(11A)-C(12A)-C(13A)	110.0(16)	C(11A)-C(12A)-C(17A)	123.9(15)
C(13A)-C(12A)-C(17A)	126.0(15)	C(11A)-C(12A)-Ir(1A)	72.0(10)
C(13A)-C(12A)-Ir(1A)	71.9(9)	C(17A)-C(12A)-Ir(1A)	126.0(11)

C(12A)-C(13A)-C(18A)	129.5(17)	C(12A)-C(13A)-C(14A)	104.0(15)
C(18A)-C(13A)-C(14A)	126.5(15)	C(12A)-C(13A)-Ir(1A)	69.5(9)
C(18A)-C(13A)-Ir(1A)	126.1(11)	C(14A)-C(13A)-Ir(1A)	68.1(11)
C(15A)-C(14A)-C(19A)	131(2)	C(15A)-C(14A)-C(13A)	105.9(15)
C(19A)-C(14A)-C(13A)	121.9(19)	C(15A)-C(14A)-Ir(1A)	70.8(11)
C(19A)-C(14A)-Ir(1A)	130.0(13)	C(13A)-C(14A)-Ir(1A)	71.2(9)
C(14A)-C(15A)-C(11A)	111.2(17)	C(14A)-C(15A)-C(20A)	124.1(17)
C(11A)-C(15A)-C(20A)	124.5(17)	C(14A)-C(15A)-Ir(1A)	72.0(9)
C(11A)-C(15A)-Ir(1A)	72.4(9)	C(20A)-C(15A)-Ir(1A)	126.4(14)
C(2B)-C(1B)-C(6B)	129.3(17)	C(2B)-C(1B)-S(1B)	110.9(12)
C(6B)-C(1B)-S(1B)	119.8(15)	C(2B)-C(1B)-Ir(1B)	71.1(10)
C(6B)-C(1B)-Ir(1B)	126.8(12)	S(1B)-C(1B)-Ir(1B)	70.5(7)
C(1B)-C(2B)-C(3B)	114.2(15)	C(1B)-C(2B)-C(5A)	111.9(15)
C(3B)-C(2B)-C(5A)	133.0(16)	C(1B)-C(2B)-Ir(1B)	72.7(10)
C(3B)-C(2B)-Ir(1B)	70.4(9)	C(5A)-C(2B)-Ir(1B)	133.9(12)
C(2B)-C(3B)-C(4B)	110.6(14)	C(2B)-C(3B)-C(5B)	125.9(14)
C(4B)-C(3B)-C(5B)	123.1(12)	C(2B)-C(3B)-Ir(1B)	72.7(8)
C(4B)-C(3B)-Ir(1B)	71.0(9)	C(5B)-C(3B)-Ir(1B)	128.3(10)
C(3B)-C(4B)-C(7B)	126.5(13)	C(3B)-C(4B)-S(1B)	113.0(10)
C(7B)-C(4B)-S(1B)	120.4(11)	C(3B)-C(4B)-Ir(1B)	71.1(7)
C(7B)-C(4B)-Ir(1B)	125.9(11)	S(1B)-C(4B)-Ir(1B)	72.9(5)
C(2C)-C(5B)-C(3B)	113.8(12)	C(12B)-C(11B)-C(16B)	126(2)
C(12B)-C(11B)-C(15B)	108.8(17)	C(16B)-C(11B)-C(15B)	125(2)
C(12B)-C(11B)-Ir(1B)	70.2(10)	C(16B)-C(11B)-Ir(1B)	127.7(16)
C(15B)-C(11B)-Ir(1B)	71.2(8)	C(11B)-C(12B)-C(13B)	110.5(18)
C(11B)-C(12B)-C(17B)	129(2)	C(13B)-C(12B)-C(17B)	120(2)
C(11B)-C(12B)-Ir(1B)	72.9(12)	C(13B)-C(12B)-Ir(1B)	68.9(11)
C(17B)-C(12B)-Ir(1B)	126.3(12)	C(12B)-C(13B)-C(14B)	108.6(19)
C(12B)-C(13B)-C(18B)	131.8(17)	C(14B)-C(13B)-C(18B)	119.3(18)
C(12B)-C(13B)-Ir(1B)	72.5(12)	C(14B)-C(13B)-Ir(1B)	72.7(10)
C(18B)-C(13B)-Ir(1B)	125.6(11)	C(19B)-C(14B)-C(13B)	131(2)
C(19B)-C(14B)-C(15B)	122.2(17)	C(13B)-C(14B)-C(15B)	106.2(15)
C(19B)-C(14B)-Ir(1B)	129.3(12)	C(13B)-C(14B)-Ir(1B)	68.0(9)
C(15B)-C(14B)-Ir(1B)	71.4(8)	C(20B)-C(15B)-C(11B)	124.0(18)
C(20B)-C(15B)-C(14B)	130.2(17)	C(11B)-C(15B)-C(14B)	105.8(14)
C(20B)-C(15B)-Ir(1B)	127.8(14)	C(11B)-C(15B)-Ir(1B)	69.9(7)
C(14B)-C(15B)-Ir(1B)	68.9(7)	C(2C)-C(1C)-C(6C)	130.4(14)
C(2C)-C(1C)-S(1C)	110.0(12)	C(6C)-C(1C)-S(1C)	119.6(10)
C(1C)-C(2C)-C(3C)	112.6(12)	C(1C)-C(2C)-C(5B)	124.4(14)
C(3C)-C(2C)-C(5B)	123.0(12)	C(4C)-C(3C)-C(2C)	114.5(13)
C(4C)-C(3C)-C(5C)	119.8(14)	C(2C)-C(3C)-C(5C)	125.5(12)
C(3C)-C(4C)-C(7C)	131.0(14)	C(3C)-C(4C)-S(1C)	109.2(12)
C(7C)-C(4C)-S(1C)	119.5(10)	C(2A)-C(5C)-C(3C)	110.6(12)
O(2D)-S(1D)-O(1D)	120.0(14)	O(2D)-S(1D)-O(3D)	111.1(10)
O(1D)-S(1D)-O(3D)	110.5(13)	O(2D)-S(1D)-C(1D)	104.0(13)
O(1D)-S(1D)-C(1D)	105.1(10)	O(3D)-S(1D)-C(1D)	104.5(12)
F(1D)-C(1D)-F(2D)	106.3(18)	F(1D)-C(1D)-F(3D)	107.1(18)
F(2D)-C(1D)-F(3D)	105(2)	F(1D)-C(1D)-S(1D)	113(2)
F(2D)-C(1D)-S(1D)	113.8(16)	F(3D)-C(1D)-S(1D)	110.2(12)
O(3E)-S(1E)-O(2E)	117.4(11)	O(3E)-S(1E)-O(1E)	115.9(12)
O(2E)-S(1E)-O(1E)	115.0(11)	O(3E)-S(1E)-C(1E)	105.3(10)
O(2E)-S(1E)-C(1E)	103.2(11)	O(1E)-S(1E)-C(1E)	95.8(13)
F(2E)-C(1E)-F(1E)	108(2)	F(2E)-C(1E)-F(3E)	104.9(18)
F(1E)-C(1E)-F(3E)	104(2)	F(2E)-C(1E)-S(1E)	112(2)
F(1E)-C(1E)-S(1E)	113.6(14)	F(3E)-C(1E)-S(1E)	113.5(14)
O(1F)-S(1F)-O(2F)	121.8(11)	O(1F)-S(1F)-O(3F)	107.0(16)
O(2F)-S(1F)-O(3F)	110.6(11)	O(1F)-S(1F)-C(1F)	107.4(14)
O(2F)-S(1F)-C(1F)	107.3(11)	O(3F)-S(1F)-C(1F)	100.8(12)
F(2F)-C(1F)-F(3F)	108.1(18)	F(2F)-C(1F)-F(1F)	108(3)
F(3F)-C(1F)-F(1F)	106(2)	F(2F)-C(1F)-S(1F)	112.6(16)
F(3F)-C(1F)-S(1F)	113(2)	F(1F)-C(1F)-S(1F)	108.4(15)
O(1G)-S(1G)-O(2G)	114(2)	O(1G)-S(1G)-O(3G)	115.0(14)

O(2G)-S(1G)-O(3G)	117.3(13)	O(1G)-S(1G)-C(1G)	100.4(14)
O(2G)-S(1G)-C(1G)	101.9(13)	O(3G)-S(1G)-C(1G)	104.6(14)
F(2G)-C(1G)-F(1G)	96(2)	F(2G)-C(1G)-F(3G)	102(2)
F(1G)-C(1G)-F(3G)	107(3)	F(2G)-C(1G)-S(1G)	116(3)
F(1G)-C(1G)-S(1G)	117(2)	F(3G)-C(1G)-S(1G)	115.3(16)
C1SAb-N(1S)-C3SAb	120(4)	C2Sa-N(1S)-C1Sa	121(3)
C2Sa-N(1S)-C3Sa	125(3)	C1Sa-N(1S)-C3Sa	113(3)
C1SAb-N(1S)-C2SAb	120(4)	C3SAb-N(1S)-C2SAb	107(3)
O1Sa-C1Sa-N(1S)	123(4)	O1SAb-C1SAb-N(1S)	124(5)

Table 4. Anisotropic displacement parameters ($Å^2$ x 10^3) for 9.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2(h^2a^{*2}U_{11} + \ldots + 2hka^*b^*U_{12})$.

	U(11)	U(22)	U(33)	U(23)	U(13)	U(12)
Ir(1A)	24.1(3)	33.1(2)	25.4(3)	-8.26(19)	4.5(2)	10.1(2)
Ir(1B)	24.1(3)	38.3(2)	28.4(3)	14.7(2)	3.5(2)	-9.3(2)
S(1A)	42(3)	43.3(18)	24.4(19)	-3.5(14)	7.4(18)	8.0(17)
S(1C)	54(2)	16.1(11)	37.3(17)	-0.3(14)	10.7(15)	4.9(16)
S(1B)	38(2)	41.0(17)	23.1(18)	3.9(13)	10.7(17)	-4.6(16)
C(1A)	40(8)	17(5)	35(7)	-14(5)	20(7)	1(5)
C(2A)	17(6)	18(5)	42(7)	-10(4)	18(6)	1(4)
C(3A)	24(8)	28(6)	92(11)	-14(7)	15(8)	1(6)
C(4A)	28(9)	30(6)	67(11)	0(7)	21(8)	10(7)
C(5A)	40(8)	28(6)	163(15)	-9(8)	21(10)	-11(7)
C(6A)	27(9)	60(9)	45(10)	-7(8)	16(8)	-14(8)
C(7A)	81(17)	41(8)	93(15)	28(9)	45(13)	0(9)
C(11A)	37(8)	57(7)	33(7)	-13(6)	13(6)	7(7)
C(12A)	37(8)	52(7)	38(8)	-17(6)	15(7)	6(6)
C(13A)	37(5)	46(4)	33(5)	-4(4)	18(4)	9(4)
C(14A)	65(11)	69(8)	17(7)	-14(6)	-3(8)	28(8)
C(15A)	41(9)	59(8)	39(8)	-28(6)	-6(7)	18(7)
C(16A)	59(13)	44(8)	84(14)	-27(8)	-15(11)	30(8)
C(17A)	48(11)	48(7)	29(8)	-3(6)	-3(7)	30(7)
C(18A)	36(10)	82(10)	41(9)	9(8)	20(8)	25(8)
C(19A)	42(10)	99(12)	19(7)	-9(7)	1(7)	30(10)
C(20A)	51(12)	60(10)	74(14)	-33(9)	-24(11)	33(9)
C(1B)	35(9)	31(6)	52(9)	5(6)	13(8)	-4(7)
C(2B)	21(7)	16(5)	68(9)	3(5)	25(7)	-8(5)
C(3B)	24(7)	31(5)	37(7)	11(5)	11(6)	-2(5)
C(4B)	21(7)	51(7)	17(6)	0(5)	3(6)	11(6)
C(5B)	22(7)	25(5)	29(7)	5(5)	3(6)	6(5)
C(6B)	62(13)	41(8)	78(13)	-15(8)	28(11)	-19(8)
C(7B)	28(9)	44(7)	34(8)	-1(7)	-1(7)	-1(7)
C(11B)	50(9)	69(8)	35(8)	37(7)	-12(7)	-20(8)
C(12B)	53(11)	115(11)	23(8)	22(8)	1(8)	-54(9)
C(13B)	45(10)	90(11)	14(7)	5(6)	9(7)	-25(8)
C(14B)	32(8)	82(9)	25(7)	3(6)	7(6)	-38(7)
C(15B)	42(5)	37(4)	43(5)	22(4)	9(4)	-19(4)
C(16B)	84(17)	96(15)	96(17)	81(14)	-21(14)	-25(12)
C(17B)	67(15)	167(20)	32(10)	8(11)	7(10)	-73(15)
C(18B)	78(14)	99(13)	32(9)	-8(8)	28(9)	-44(11)
C(19B)	33(10)	137(17)	41(10)	22(10)	6(9)	-17(11)
C(20B)	99(19)	52(9)	102(16)	59(10)	-19(14)	-42(10)
C(1C)	29(8)	29(6)	28(7)	2(5)	7(6)	7(5)
C(2C)	19(7)	28(5)	23(6)	-3(4)	11(5)	0(5)
C(3C)	15(7)	19(5)	34(7)	-2(5)	8(5)	1(5)
C(4C)	30(8)	19(5)	33(7)	-3(5)	12(6)	-1(5)
C(5C)	23(7)	15(5)	50(8)	-7(5)	18(7)	-3(5)
C(6C)	56(11)	44(7)	40(9)	-3(6)	19(8)	32(8)
C(7C)	51(11)	48(7)	37(9)	7(6)	10(8)	-17(7)
S(1D)	64(4)	48(2)	49(3)	-5.9(18)	14(3)	1(2)
O(1D)	180(24)	89(11)	56(10)	10(7)	16(12)	-4(12)
O(2D)	95(16)	62(9)	191(22)	-61(12)	61(15)	-37(10)
O(3D)	60(11)	59(8)	102(12)	-6(7)	2(9)	18(7)
C(1D)	103(21)	53(10)	32(9)	-6(8)	0(11)	19(11)

F(1D)	162(20)	127(12)	100(13)	16(9)	70(14)	99(13)
F(2D)	118(13)	66(7)	46(7)	-13(5)	-17(8)	0(7)
F(3D)	114(13)	77(7)	40(6)	-4(5)	2(7)	9(7)
S(1E)	58(3)	85(3)	48(3)	-12(2)	26(3)	-6(3)
O(1E)	127(19)	105(12)	195(24)	-92(14)	100(18)	-37(13)
O(2E)	80(12)	109(11)	58(8)	24(7)	31(8)	14(9)
O(3E)	71(11)	109(11)	88(12)	-35(9)	35(9)	6(9)
C(1E)	114(21)	52(9)	38(10)	1(8)	37(12)	8(11)
F(1E)	124(14)	76(8)	96(11)	-20(7)	-33(10)	22(8)
F(2E)	197(22)	156(14)	95(12)	53(10)	94(14)	19(14)
F(3E)	94(11)	103(9)	55(7)	24(6)	27(7)	33(8)
S(1F)	52(3)	96(3)	53(3)	-14(3)	19(3)	-4(3)
O(1F)	93(15)	200(20)	151(19)	-131(17)	77(15)	-82(15)
O(2F)	127(16)	97(10)	60(9)	5(7)	55(10)	-47(10)
O(3F)	61(10)	216(20)	73(10)	102(13)	-8(8)	-42(12)
C(1F)	102(21)	89(14)	60(14)	-18(11)	44(15)	-27(15)
F(1F)	114(14)	76(8)	101(11)	26(7)	-2(10)	-1(8)
F(2F)	100(12)	94(8)	59(8)	-12(6)	18(8)	-19(8)
F(3F)	160(16)	74(7)	56(7)	-22(6)	57(9)	-3(8)
S(1G)	76(4)	57(2)	69(4)	-16(2)	38(3)	-14(3)
O(1G)	263(36)	252(27)	110(18)	-107(18)	132(22)	-187(27)
O(2G)	41(11)	63(9)	291(35)	13(14)	10(16)	-2(8)
O(3G)	60(11)	142(13)	39(7)	-11(8)	9(7)	-34(10)
C(1G)	82(19)	115(19)	71(17)	64(15)	-13(14)	-1(16)
F(1G)	328(47)	106(13)	102(17)	46(10)	-38(20)	26(16)
F(2G)	164(21)	123(12)	106(14)	-12(11)	44(14)	-79(14)
F(3G)	118(14)	97(9)	62(9)	-18(7)	11(9)	-8(9)
N(1S)	85(13)	37(6)	70(11)	7(8)	-4(9)	-3(9)
O1Sa	57(10)	6(6)	64(10)	0(6)	4(8)	12(6)
C1Sa	79(12)	65(11)	76(12)	-2(9)	14(9)	-2(9)
C2Sa	72(18)	53(14)	76(17)	-15(13)	-4(14)	-9(14)
C3Sa	92(18)	23(11)	81(16)	-10(11)	4(14)	-2(12)
O1SAb	138(23)	97(19)	137(23)	2(16)	26(18)	42(16)
C1SAb	87(12)	77(12)	84(12)	1(9)	16(9)	-2(9)
C2SAb	97(20)	43(14)	109(20)	-12(14)	8(15)	33(14)
C3SAb	104(20)	99(18)	91(19)	6(15)	20(16)	-2(14)

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

	x	y	z	U
H(5B)	8903	9225	1459	94
H(5A)	8862	8900	2314	94
H(6C)	6592	6707	1019	64
H(6B)	7216	6429	1749	64
H(6A)	7207	6265	823	64
H(7C)	7903	9814	694	101
H(7B)	7252	9526	7	101
H(7A)	7989	9358	-84	101
H(16C)	7077	10688	2429	104
H(16B)	6689	10427	1521	104
H(16A)	7492	10357	1839	104
H(17C)	5842	9681	1145	67
H(17B)	5430	9300	1711	67
H(17A)	5632	8796	1032	67
H(18C)	5806	7584	1954	76
H(18B)	5929	7630	2921	76
H(18A)	6419	7126	2550	76
H(19C)	7573	7984	4198	82
H(19B)	8093	7758	3694	82
H(19A)	7388	7317	3528	82
H(20C)	8471	9085	3740	105
H(20B)	8105	9898	3698	105
H(20A)	8426	9647	2985	105
H(5C)	8861	7442	664	32
H(5D)	9506	7039	501	32
H(6D)	10499	9591	3224	88
H(6E)	9838	9287	3439	88
H(6F)	9769	9790	2637	88
H(7D)	10597	6276	2100	56
H(7E)	11267	6766	2183	56
H(7F)	10741	6645	1307	56
H(16D)	9505	9951	-524	152
H(16E)	9359	9987	348	152
H(16F)	9159	9239	-209	152
H(17D)	10191	7540	-375	135
H(17E)	10195	8170	-1056	135
H(17F)	9564	8108	-689	135
H(18D)	11874	7763	1142	100
H(18E)	11893	8040	256	100
H(18F)	11362	7402	347	100
H(19D)	11852	9681	2131	107
H(19E)	12166	9701	1374	107
H(19F)	12176	8922	1872	107
H(20D)	10924	10449	1845	141
H(20E)	10149	10472	1328	141
H(20F)	10715	10812	949	141
H(5E)	8226	6912	2626	34
H(5F)	8879	7396	2603	34
H(6H)	9956	5597	449	68
H(6I)	9246	5802	-182	68
H(6J)	9384	4955	185	68
H(7K)	7962	5641	2781	69

H(7L)	8719	5530	3338	69
H(7M)	8340	4840	2778	69
H1Sa	9315	11258	2582	90
H2S1a	8368	12258	510	86
H2S2a	8009	11538	793	86
H2S3a	8651	11412	457	86
H3S1a	9392	12453	2460	83
H3S2a	8689	12842	1995	83
H3S3a	9302	12851	1592	83
H1SAb	8652	11276	482	101
H2S4b	8808	13087	1524	106
H2S5b	8354	12747	680	106
H2S6b	9155	12776	857	106
H3S4b	9281	12336	2535	120
H3S5b	9780	11864	2147	120
H3S6b	9300	11420	2586	120

Table 1. Crystal data and structure refinement for GB12D.

Identification code	gb12d (11)
Empirical formula	C70 H91 B4 F16 N5 Ru2
Formula weight	1551.86
Temperature	173(2) K
Wavelength	0.71070 A
Crystal system, space group	Monoclinic, P2/c
Unit cell dimensions	a = 16.0574(8) A alpha = 90 deg. b = 11.6582(6) A beta = 102.577(1) deg. c = 19.7603(5) A gamma = 90 deg.
Volume	3610.4(3) A^3
Z, Calculated density	2, 1.428 Mg/m^3
Absorption coefficient	0.504 mm^-1
F(000)	1596
Crystal size	0.20 x 0.10 x 0.03 mm
Theta range for data collection	3.62 to 25.00 deg.
Index ranges	0<=h<=19, 0<=k<=13, -22<=l<=20
Reflections collected / unique	31329 / 6004 [R(int) = 0.0790]
Completeness to 2theta = 25.00	89.4%
Max. and min. transmission	0.9851 and 0.9060
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6004 / 0 / 446
Goodness-of-fit on F^2	1.070
Final R indices [I>2sigma(I)]	R1 = 0.0484, wR2 = 0.1201
R indices (all data)	R1 = 0.0636, wR2 = 0.1319
Extinction coefficient	0.0024(6)
Largest diff. peak and hole	0.706 and -0.691 e.A^-3

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for GB12D.
U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
Ru(1)	2860(1)	8615(1)	3478(1)	25(1)
C(1A)	1593(2)	9440(3)	3056(2)	24(1)
C(2A)	1546(2)	8847(3)	3693(2)	27(1)
C(3A)	1779(2)	7673(4)	3772(2)	29(1)
C(4A)	2033(2)	7094(4)	3216(2)	30(1)
C(5A)	2078(2)	7654(4)	2585(2)	28(1)
C(6A)	1847(2)	8832(3)	2497(2)	26(1)
C(7A)	1910(2)	9464(4)	1835(2)	28(1)
C(8A)	1409(3)	10701(4)	2992(2)	31(1)
C(9A)	1791(3)	6997(4)	4421(2)	37(1)
C(10A)	2408(3)	6950(4)	2061(2)	37(1)
C(11A)	3865(3)	9959(4)	3401(2)	39(1)
C(12A)	3653(3)	10032(4)	4050(2)	39(1)
C(13A)	3720(3)	9065(5)	4480(2)	40(1)
C(14A)	3994(3)	7999(4)	4286(3)	42(1)
C(15A)	4172(3)	7909(4)	3617(3)	45(1)
C(16A)	4096(3)	8879(5)	3175(2)	43(1)
C(17A)	3845(3)	11002(5)	2947(3)	55(1)
C(18A)	4103(4)	6998(5)	4783(3)	61(2)
C(19A)	4889(4)	7233(6)	5366(3)	74(2)
C(20A)	4149(5)	5851(5)	4454(4)	88(2)
C(1B)	325(3)	9506(4)	1254(2)	26(1)
C(2B)	1111(2)	10076(4)	1432(2)	27(1)
C(3B)	1187(3)	11207(4)	1209(2)	30(1)
C(4B)	462(3)	11730(4)	819(2)	33(1)
C(5B)	-339(3)	11214(4)	662(2)	30(1)
C(6B)	-405(2)	10088(4)	899(2)	26(1)
C(7B)	1278(2)	9489(4)	4283(2)	29(1)
C(8B)	274(3)	8245(4)	1406(2)	33(1)
C(9B)	2014(3)	11873(4)	1352(2)	37(1)
C(10B)	-1084(3)	11864(4)	244(2)	38(1)
B(1A)	6235(3)	9382(5)	4023(3)	42(1)
F(1A)	7069(2)	9502(3)	4390(2)	58(1)
F(2A)	5942(3)	10447(4)	3764(2)	91(1)
F(3A)	5733(2)	9033(3)	4455(2)	69(1)
F(4A)	6186(2)	8648(3)	3476(2)	74(1)
B(1B)	2335(8)	3716(7)	3371(5)	88(3)
F(1B)	2743(3)	2805(4)	3745(3)	102(1)
F(2B)	2841(7)	4347(6)	3055(4)	199(4)
F(3B)	2090(4)	4463(4)	3805(3)	124(2)
F(4B)	1712(6)	3323(5)	2880(4)	200(4)
N(1S)	0	6122(11)	2500	130(4)
N(2S)	2988(7)	3589(8)	5395(5)	141(3)
N(3S)	5000	6280(3)	2500	122(11)
N(4S)	258(17)	5100(3)	187(16)	190(10)
N(5S)	4630(4)	4380(5)	6590(3)	200(2)
C(1S)	38(10)	5276(14)	2052(8)	86(4)
C(2S)	124(12)	4194(17)	1691(10)	102(5)
C(3S)	3133(8)	4756(12)	5761(7)	63(3)
C(4S)	3295(12)	5584(17)	6017(10)	102(5)
C(5S)	5000	5240(4)	2500	119(13)
C(6S)	5000	3920(3)	2500	126(12)
C(7S)	2550(12)	4363(16)	5527(9)	94(5)
C(8S)	2095(17)	5120(2)	5678(14)	68(7)

C(9S)	278(17)	4690(2)	1290(16)	66(7)
C(10S)	270(2)	4920(3)	810(2)	100(10)
C(11S)	4250(3)	5350(4)	6710(2)	121(13)
C(12S)	3930(3)	6310(3)	7010(2)	103(11)
C(13S)	4640(3)	3840(3)	7280(2)	79(8)
C(14S)	5390(3)	4740(6)	7660(3)	115(13)
C(15S)	4520(3)	6110(4)	7510(2)	106(11)

Table 3. Bond lengths [A] and angles [deg] for GB12D.

Ru(1)-C(4A)	2.209(4)
Ru(1)-C(13A)	2.216(4)
Ru(1)-C(16A)	2.215(4)
Ru(1)-C(15A)	2.222(4)
Ru(1)-C(12A)	2.236(4)
Ru(1)-C(5A)	2.231(4)
Ru(1)-C(3A)	2.236(4)
Ru(1)-C(1A)	2.240(4)
Ru(1)-C(6A)	2.257(4)
Ru(1)-C(2A)	2.258(4)
Ru(1)-C(14A)	2.261(4)
Ru(1)-C(11A)	2.277(4)
C(1A)-C(6A)	1.444(5)
C(1A)-C(2A)	1.451(6)
C(1A)-C(8A)	1.500(6)
C(2A)-C(3A)	1.418(6)
C(2A)-C(7B)	1.525(6)
C(3A)-C(4A)	1.422(6)
C(3A)-C(9A)	1.502(6)
C(4A)-C(5A)	1.422(6)
C(5A)-C(6A)	1.424(6)
C(5A)-C(10A)	1.507(6)
C(6A)-C(7A)	1.523(5)
C(7A)-C(2B)	1.532(5)
C(11A)-C(12A)	1.398(7)
C(11A)-C(16A)	1.413(7)
C(11A)-C(17A)	1.506(7)
C(12A)-C(13A)	1.402(7)
C(13A)-C(14A)	1.401(7)
C(14A)-C(15A)	1.415(7)
C(14A)-C(18A)	1.512(7)
C(15A)-C(16A)	1.418(7)
C(18A)-C(20A)	1.496(9)
C(18A)-C(19A)	1.537(7)
C(1B)-C(2B)	1.401(6)
C(1B)-C(6B)	1.403(6)
C(1B)-C(8B)	1.506(6)
C(2B)-C(3B)	1.405(6)
C(3B)-C(4B)	1.389(6)
C(3B)-C(9B)	1.512(6)
C(4B)-C(5B)	1.392(6)
C(5B)-C(6B)	1.406(6)
C(5B)-C(10B)	1.502(6)
C(6B)-C(7B)#1	1.537(5)
C(7B)-C(6B)#1	1.537(5)
B(1A)-F(3A)	1.358(6)
B(1A)-F(4A)	1.368(6)
B(1A)-F(1A)	1.383(6)
B(1A)-F(2A)	1.386(7)
B(1B)-F(4B)	1.316(11)
B(1B)-F(3B)	1.339(10)
B(1B)-F(2B)	1.346(12)
B(1B)-F(1B)	1.377(10)
C(4A)-Ru(1)-C(13A)	128.71(17)
C(4A)-Ru(1)-C(16A)	125.23(17)
C(13A)-Ru(1)-C(16A)	77.80(18)
C(4A)-Ru(1)-C(15A)	103.74(17)
C(13A)-Ru(1)-C(15A)	65.68(19)
C(16A)-Ru(1)-C(15A)	37.29(19)
C(4A)-Ru(1)-C(12A)	163.50(17)

C(13A)-Ru(1)-C(12A)	36.70(18)
C(16A)-Ru(1)-C(12A)	65.73(18)
C(15A)-Ru(1)-C(12A)	77.94(18)
C(4A)-Ru(1)-C(5A)	37.37(15)
C(13A)-Ru(1)-C(5A)	163.55(18)
C(16A)-Ru(1)-C(5A)	103.84(16)
C(15A)-Ru(1)-C(5A)	105.49(16)
C(12A)-Ru(1)-C(5A)	158.58(17)
C(4A)-Ru(1)-C(3A)	37.32(15)
C(13A)-Ru(1)-C(3A)	104.59(16)
C(16A)-Ru(1)-C(3A)	158.52(18)
C(15A)-Ru(1)-C(3A)	123.69(18)
C(12A)-Ru(1)-C(3A)	128.36(17)
C(5A)-Ru(1)-C(3A)	67.88(15)
C(4A)-Ru(1)-C(1A)	78.81(14)
C(13A)-Ru(1)-C(1A)	124.67(17)
C(16A)-Ru(1)-C(1A)	129.35(17)
C(15A)-Ru(1)-C(1A)	164.71(18)
C(12A)-Ru(1)-C(1A)	104.00(16)
C(5A)-Ru(1)-C(1A)	67.19(14)
C(3A)-Ru(1)-C(1A)	67.27(14)
C(4A)-Ru(1)-C(6A)	66.68(15)
C(13A)-Ru(1)-C(6A)	158.89(18)
C(16A)-Ru(1)-C(6A)	105.85(16)
C(15A)-Ru(1)-C(6A)	129.40(17)
C(12A)-Ru(1)-C(6A)	125.16(16)
C(5A)-Ru(1)-C(6A)	36.98(14)
C(3A)-Ru(1)-C(6A)	79.78(14)
C(1A)-Ru(1)-C(6A)	37.44(14)
C(4A)-Ru(1)-C(2A)	66.47(15)
C(13A)-Ru(1)-C(2A)	103.25(16)
C(16A)-Ru(1)-C(2A)	164.38(18)
C(15A)-Ru(1)-C(2A)	157.03(18)
C(12A)-Ru(1)-C(2A)	105.62(16)
C(5A)-Ru(1)-C(2A)	79.66(15)
C(3A)-Ru(1)-C(2A)	36.80(15)
C(1A)-Ru(1)-C(2A)	37.65(14)
C(6A)-Ru(1)-C(2A)	67.62(14)
C(4A)-Ru(1)-C(14A)	105.15(16)
C(13A)-Ru(1)-C(14A)	36.44(19)
C(16A)-Ru(1)-C(14A)	66.69(18)
C(15A)-Ru(1)-C(14A)	36.78(19)
C(12A)-Ru(1)-C(14A)	66.15(18)
C(5A)-Ru(1)-C(14A)	128.79(17)
C(3A)-Ru(1)-C(14A)	102.23(16)
C(1A)-Ru(1)-C(14A)	157.69(17)
C(6A)-Ru(1)-C(14A)	163.92(17)
C(2A)-Ru(1)-C(14A)	123.17(17)
C(4A)-Ru(1)-C(11A)	159.31(17)
C(13A)-Ru(1)-C(11A)	65.45(17)
C(16A)-Ru(1)-C(11A)	36.62(18)
C(15A)-Ru(1)-C(11A)	66.25(18)
C(12A)-Ru(1)-C(11A)	36.08(17)
C(5A)-Ru(1)-C(11A)	125.29(16)
C(3A)-Ru(1)-C(11A)	163.09(17)
C(1A)-Ru(1)-C(11A)	106.19(15)
C(6A)-Ru(1)-C(11A)	104.73(15)
C(2A)-Ru(1)-C(11A)	129.40(16)
C(14A)-Ru(1)-C(11A)	78.04(17)
C(6A)-C(1A)-C(2A)	120.4(4)
C(6A)-C(1A)-C(8A)	119.9(3)
C(2A)-C(1A)-C(8A)	119.6(3)
C(6A)-C(1A)-Ru(1)	71.9(2)
C(2A)-C(1A)-Ru(1)	71.8(2)
C(8A)-C(1A)-Ru(1)	126.8(3)

C(3A)-C(2A)-C(1A)	119.5(4)
C(3A)-C(2A)-C(7B)	120.1(4)
C(1A)-C(2A)-C(7B)	120.3(4)
C(3A)-C(2A)-Ru(1)	70.8(2)
C(1A)-C(2A)-Ru(1)	70.5(2)
C(7B)-C(2A)-Ru(1)	129.4(3)
C(2A)-C(3A)-C(4A)	119.0(4)
C(2A)-C(3A)-C(9A)	123.6(4)
C(4A)-C(3A)-C(9A)	117.3(4)
C(2A)-C(3A)-Ru(1)	72.4(2)
C(4A)-C(3A)-Ru(1)	70.3(2)
C(9A)-C(3A)-Ru(1)	127.9(3)
C(5A)-C(4A)-C(3A)	122.5(4)
C(5A)-C(4A)-Ru(1)	72.2(2)
C(3A)-C(4A)-Ru(1)	72.4(2)
C(4A)-C(5A)-C(6A)	119.2(4)
C(4A)-C(5A)-C(10A)	116.5(4)
C(6A)-C(5A)-C(10A)	124.3(4)
C(4A)-C(5A)-Ru(1)	70.5(2)
C(6A)-C(5A)-Ru(1)	72.5(2)
C(10A)-C(5A)-Ru(1)	126.6(3)
C(5A)-C(6A)-C(1A)	119.3(3)
C(5A)-C(6A)-C(7A)	120.5(3)
C(1A)-C(6A)-C(7A)	120.2(3)
C(5A)-C(6A)-Ru(1)	70.5(2)
C(1A)-C(6A)-Ru(1)	70.6(2)
C(7A)-C(6A)-Ru(1)	128.4(3)
C(6A)-C(7A)-C(2B)	117.8(3)
C(12A)-C(11A)-C(16A)	118.5(4)
C(12A)-C(11A)-C(17A)	121.3(5)
C(16A)-C(11A)-C(17A)	120.2(5)
C(12A)-C(11A)-Ru(1)	70.4(3)
C(16A)-C(11A)-Ru(1)	69.3(3)
C(17A)-C(11A)-Ru(1)	132.2(3)
C(11A)-C(12A)-C(13A)	120.4(4)
C(11A)-C(12A)-Ru(1)	73.6(3)
C(13A)-C(12A)-Ru(1)	70.9(3)
C(12A)-C(13A)-C(14A)	122.3(5)
C(12A)-C(13A)-Ru(1)	72.4(3)
C(14A)-C(13A)-Ru(1)	73.5(3)
C(13A)-C(14A)-C(15A)	117.5(5)
C(13A)-C(14A)-C(18A)	120.4(5)
C(15A)-C(14A)-C(18A)	122.2(5)
C(13A)-C(14A)-Ru(1)	70.0(3)
C(15A)-C(14A)-Ru(1)	70.1(2)
C(18A)-C(14A)-Ru(1)	131.7(3)
C(14A)-C(15A)-C(16A)	120.6(5)
C(14A)-C(15A)-Ru(1)	73.1(3)
C(16A)-C(15A)-Ru(1)	71.1(2)
C(11A)-C(16A)-C(15A)	120.6(4)
C(11A)-C(16A)-Ru(1)	74.1(3)
C(15A)-C(16A)-Ru(1)	71.6(3)
C(20A)-C(18A)-C(14A)	114.7(6)
C(20A)-C(18A)-C(19A)	112.1(5)
C(14A)-C(18A)-C(19A)	108.0(5)
C(2B)-C(1B)-C(6B)	120.3(4)
C(2B)-C(1B)-C(8B)	119.9(4)
C(6B)-C(1B)-C(8B)	119.8(4)
C(1B)-C(2B)-C(3B)	120.1(4)
C(1B)-C(2B)-C(7A)	121.1(4)
C(3B)-C(2B)-C(7A)	118.7(4)
C(4B)-C(3B)-C(2B)	117.8(4)
C(4B)-C(3B)-C(9B)	118.3(4)
C(2B)-C(3B)-C(9B)	123.8(4)
C(3B)-C(4B)-C(5B)	123.8(4)

C(4B)-C(5B)-C(6B)	117.5(4)
C(4B)-C(5B)-C(10B)	119.4(4)
C(6B)-C(5B)-C(10B)	123.1(4)
C(1B)-C(6B)-C(5B)	120.2(4)
C(1B)-C(6B)-C(7B)#1	121.1(4)
C(5B)-C(6B)-C(7B)#1	118.5(4)
C(2A)-C(7B)-C(6B)#1	116.1(3)
F(3A)-B(1A)-F(4A)	111.7(5)
F(3A)-B(1A)-F(1A)	109.9(4)
F(4A)-B(1A)-F(1A)	111.1(4)
F(3A)-B(1A)-F(2A)	107.5(5)
F(4A)-B(1A)-F(2A)	108.2(5)
F(1A)-B(1A)-F(2A)	108.4(5)
F(4B)-B(1B)-F(3B)	114.6(10)
F(4B)-B(1B)-F(2B)	106.7(9)
F(3B)-B(1B)-F(2B)	103.5(7)
F(4B)-B(1B)-F(1B)	108.9(6)
F(3B)-B(1B)-F(1B)	109.2(7)
F(2B)-B(1B)-F(1B)	114.0(10)

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

Table 4. Anisotropic displacement parameters (A^2 x 10^3) for GB12D. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Ru(1)	20(1)	32(1)	23(1)	-1(1)	3(1)	0(1)
C(1A)	17(2)	32(2)	24(2)	1(2)	4(1)	-1(2)
C(2A)	19(2)	37(2)	25(2)	1(2)	3(2)	1(2)
C(3A)	22(2)	38(2)	26(2)	2(2)	2(2)	0(2)
C(4A)	24(2)	32(2)	31(2)	-1(2)	1(2)	-1(2)
C(5A)	21(2)	34(2)	26(2)	-4(2)	1(2)	-1(2)
C(6A)	18(2)	35(2)	23(2)	0(2)	2(1)	-2(2)
C(7A)	23(2)	38(2)	25(2)	1(2)	8(2)	3(2)
C(8A)	29(2)	35(2)	29(2)	0(2)	7(2)	-1(2)
C(9A)	34(2)	45(3)	33(3)	8(2)	10(2)	3(2)
C(10A)	39(3)	39(3)	33(3)	-7(2)	8(2)	3(2)
C(11A)	23(2)	50(3)	39(3)	7(2)	-2(2)	-9(2)
C(12A)	26(2)	46(3)	40(3)	-10(2)	-1(2)	-7(2)
C(13A)	34(2)	58(3)	25(2)	-4(2)	1(2)	-10(2)
C(14A)	23(2)	52(3)	44(3)	7(2)	-8(2)	-4(2)
C(15A)	18(2)	49(3)	64(3)	-13(2)	2(2)	8(2)
C(16A)	19(2)	79(4)	30(3)	-7(2)	6(2)	-4(2)
C(17A)	42(3)	71(4)	48(3)	11(3)	0(2)	-16(3)
C(18A)	42(3)	59(4)	71(4)	23(3)	-10(3)	-2(3)
C(19A)	57(4)	85(5)	67(4)	25(3)	-16(3)	-4(3)
C(20A)	77(5)	46(4)	119(6)	9(4)	-28(4)	4(3)
C(1B)	28(2)	35(2)	17(2)	0(2)	7(2)	-2(2)
C(2B)	26(2)	38(2)	20(2)	-1(2)	7(2)	0(2)
C(3B)	28(2)	39(2)	24(2)	-1(2)	9(2)	-2(2)
C(4B)	37(2)	35(2)	30(2)	4(2)	12(2)	-2(2)
C(5B)	32(2)	34(2)	24(2)	4(2)	7(2)	3(2)
C(6B)	26(2)	37(2)	17(2)	-1(2)	7(2)	-1(2)
C(7B)	23(2)	41(2)	23(2)	-3(2)	4(2)	-2(2)
C(8B)	23(2)	40(2)	34(2)	2(2)	4(2)	-1(2)
C(9B)	32(2)	41(3)	37(3)	5(2)	9(2)	-7(2)
C(10B)	34(2)	44(3)	36(3)	10(2)	6(2)	5(2)
B(1A)	30(3)	62(4)	35(3)	-5(2)	8(2)	-3(3)
F(1A)	27(1)	101(3)	45(2)	-7(2)	5(1)	-2(2)
F(2A)	80(3)	83(3)	99(3)	22(2)	-5(2)	12(2)
F(3A)	48(2)	122(3)	43(2)	-22(2)	20(1)	-37(2)
F(4A)	58(2)	113(3)	50(2)	-34(2)	12(2)	4(2)
B(1B)	142(9)	46(4)	72(6)	0(4)	16(6)	-12(5)
F(1B)	127(4)	66(3)	105(3)	-5(2)	8(3)	16(3)
F(2B)	325(11)	129(5)	184(7)	13(5)	147(8)	-30(6)
F(3B)	212(6)	71(3)	88(3)	-3(2)	34(3)	38(3)
F(4B)	286(9)	76(3)	166(6)	-25(4)	-105(6)	9(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for GB12D.

	x	y	z	U(eq)
H(4A)	2177	6304	3267	36
H(7A2)	2091	8904	1519	34
H(7A1)	2370	10041	1957	34
H(8A3)	803	10819	2782	37
H(8A2)	1757	11053	2698	37
H(8A1)	1545	11055	3452	37
H(9A3)	2045	6242	4383	44
H(9A2)	1206	6900	4483	44
H(9A1)	2128	7408	4821	44
H(10C)	2673	6247	2281	44
H(10B)	2833	7395	1883	44
H(10A)	1934	6749	1676	44
H(13A)	3540(3)	9080(4)	4940(3)	48
H(15A)	4344	7193	3463	53
H(16A)	4202	8802	2722	51
H(17C)	3426	11551	3048	66
H(17B)	3684	10772	2459	66
H(17A)	4411	11359	3039	66
H(18A)	3594	6988	4998	73
H(19C)	4926	6650	5729	89
H(19B)	4836	7994	5564	89
H(19A)	5405	7207	5178	89
H(20C)	3626	5720	4100	106
H(20B)	4207	5251	4809	106
H(20A)	4642	5830	4237	106
H(4B)	515	12484	650	40
H(7B2)	1717	10075	4462	35
H(7B1)	1272	8939	4663	35
H(8B3)	823	7881	1403	39
H(8B2)	-174	7889	1052	39
H(8B1)	140	8144	1863	39
H(9B3)	1934	12596	1092	44
H(9B2)	2459	11419	1207	44
H(9B1)	2187	12038	1849	44
H(10F)	-882	12585	80	46
H(10E)	-1493	12031	533	46
H(10D)	-1362	11400	-155	46