

ORGANOMETALLICS

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STRUCTURE DETERMINATION SUMMARY

Ja' L866-41

Crystal Data

Empirical Formula	C ₄₆ H ₅₈ Cl F ₆ Fe P ₃ Ru
Color; Habit	red-brown cube
Crystal Size (mm)	0.8 x 0.6 x 0.45
Crystal System	Monoclinic
Space Group	P2 ₁
Unit Cell Dimensions	$\underline{a} = 11.965(2) \text{ \AA}$ $\underline{b} = 14.852(3) \text{ \AA}$ $\underline{c} = 13.999(2) \text{ \AA}$ $\beta = 111.50(2)^\circ$
Volume	2314.6(7) \AA^3
Z	2
Formula Weight	1010.2
Density(calc.)	1.449 Mg/m ³
Absorption Coefficient	0.856 mm ⁻¹
F(000)	1040

9a'

L866-42

Data Collection

Diffractometer Used	Syntex P21
Radiation	MoK α ($\lambda = 0.71073 \text{ \AA}$)
Temperature (K)	293
Monochromator	Highly oriented graphite crystal
2θ Range	3.0 to 40.0 $^\circ$
Scan Type	ω
Scan Speed	Variable; 1.00 to 14.00 $^\circ$ /min. in ω
Scan Range (ω)	1.00 $^\circ$
Background Measurement	Stationary crystal and stationary counter at beginning and end of scan, each for 15.0% of total scan time
Standard Reflections	1 measured every 120 reflections
Index Ranges	$0 \leq h \leq 11, 0 \leq k \leq 14$ $-13 \leq l \leq 12$
Reflections Collected	2433
Independent Reflections	2287 ($R_{\text{int}} = 2.99\%$)
Observed Reflections	2235 ($F > 4.0\sigma(F)$)
Absorption Correction	N/A

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L866-43

Solution and Refinement

System Used	Siemens SHELXTL PLUS (VMS)
Solution	Patterson Methods
Refinement Method	Full-Matrix Least-Squares
Quantity Minimized	$\sum w(F_o - F_c)^2$
Absolute Structure	N/A
Extinction Correction	N/A
Hydrogen Atoms	Riding model, fixed isotropic U
Weighting Scheme	$w^{-1} = \sigma^2(F) + 0.0004F^2$
Number of Parameters Refined	517
Final R Indices (obs. data)	R = 2.72 %, wR = 3.38 %
R Indices (all data)	R = 2.78 %, wR = 3.39 %
Goodness-of-Fit	1.49
Largest and Mean Δ/σ	0.047, 0.004
Data-to-Parameter Ratio	4.3:1
Largest Difference Peak	0.34 eA ⁻³
Largest Difference Hole	-0.50 eA ⁻³

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Table 2. Bond lengths (Å)

Ru(1)-Cl	2.400 (2)	Ru(1)-P(1)	2.368 (2)
Ru(1)-P(2)	2.390 (2)	Ru(1)-C(32)	2.270 (8)
Ru(1)-C(33)	2.238 (8)	Ru(1)-C(34)	2.272 (8)
Ru(1)-C(35)	2.224 (8)	Ru(1)-C(36)	2.273 (8)
Ru(1)-C(37)	2.321 (8)	Fe(1)-C(1)	2.049 (7)
Fe(1)-C(2)	2.036 (7)	Fe(1)-C(3)	2.039 (6)
Fe(1)-C(4)	2.056 (7)	Fe(1)-C(5)	2.038 (8)
Fe(1)-C(1')	2.046 (8)	Fe(1)-C(2')	2.029 (10)
Fe(1)-C(3')	2.025 (10)	Fe(1)-C(4')	2.027 (12)
Fe(1)-C(5')	2.039 (8)	P(1)-C(1)	1.801 (8)
P(1)-C(20)	1.855 (8)	P(1)-C(26)	1.845 (6)
P(2)-C(6)	1.853 (8)	P(2)-C(8)	1.855 (6)
P(2)-C(14)	1.872 (8)	P(3)-F(1)	1.582 (8)
P(3)-F(2)	1.503 (11)	P(3)-F(3)	1.543 (9)
P(3)-F(4)	1.483 (13)	P(3)-F(5)	1.520 (11)
P(3)-F(6)	1.565 (12)	C(1)-C(2)	1.462 (10)
C(1)-C(5)	1.456 (12)	C(2)-C(3)	1.421 (11)
C(2)-C(6)	1.508 (11)	C(3)-C(4)	1.410 (12)
C(4)-C(5)	1.411 (11)	C(1')-C(2')	1.388 (13)
C(1')-C(5')	1.377 (16)	C(2')-C(3')	1.413 (16)
C(3')-C(4')	1.411 (17)	C(4')-C(5')	1.401 (16)
C(6)-C(7)	1.525 (10)	C(8)-C(9)	1.508 (12)
C(8)-C(13)	1.520 (10)	C(9)-C(10)	1.542 (10)
C(10)-C(11)	1.533 (13)	C(11)-C(12)	1.491 (15)
C(12)-C(13)	1.529 (11)	C(14)-C(15)	1.533 (11)
C(14)-C(19)	1.526 (10)	C(15)-C(16)	1.516 (13)
C(16)-C(17)	1.497 (12)	C(17)-C(18)	1.497 (13)
C(18)-C(19)	1.509 (13)	C(20)-C(21)	1.386 (10)
C(20)-C(25)	1.394 (10)	C(21)-C(22)	1.369 (12)
C(22)-C(23)	1.362 (14)	C(23)-C(24)	1.376 (13)
C(24)-C(25)	1.404 (13)	C(26)-C(27)	1.397 (12)
C(26)-C(31)	1.376 (11)	C(27)-C(28)	1.381 (10)
C(28)-C(29)	1.368 (16)	C(29)-C(30)	1.340 (15)
C(30)-C(31)	1.405 (10)	C(32)-C(33)	1.399 (11)
C(32)-C(37)	1.411 (12)	C(33)-C(34)	1.400 (10)
C(34)-C(35)	1.399 (12)	C(34)-C(38)	1.510 (12)
C(35)-C(36)	1.403 (10)	C(36)-C(37)	1.409 (8)
C(37)-C(39)	1.521 (10)	C(39)-C(40)	1.528 (13)
C(39)-C(41)	1.494 (14)		

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Table 3. Bond angles (°)

Cl-Ru(1)-P(1)	85.1(1)	Cl-Ru(1)-P(2)	85.9(1)
P(1)-Ru(1)-P(2)	92.6(1)	Cl-Ru(1)-C(32)	98.6(2)
P(1)-Ru(1)-C(32)	103.3(2)	P(2)-Ru(1)-C(32)	163.8(2)
Cl-Ru(1)-C(33)	131.3(2)	P(1)-Ru(1)-C(33)	89.7(3)
P(2)-Ru(1)-C(33)	142.8(2)	C(32)-Ru(1)-C(33)	36.1(3)
Cl-Ru(1)-C(34)	163.0(2)	P(1)-Ru(1)-C(34)	103.6(2)
P(2)-Ru(1)-C(34)	107.9(2)	C(32)-Ru(1)-C(34)	65.4(3)
C(33)-Ru(1)-C(34)	36.2(3)	Cl-Ru(1)-C(35)	137.7(2)
P(1)-Ru(1)-C(35)	137.1(2)	P(2)-Ru(1)-C(35)	89.9(2)
C(32)-Ru(1)-C(35)	76.2(3)	C(33)-Ru(1)-C(35)	64.4(3)
C(34)-Ru(1)-C(35)	36.2(3)	Cl-Ru(1)-C(36)	103.3(2)
P(1)-Ru(1)-C(36)	165.5(2)	P(2)-Ru(1)-C(36)	99.8(2)
C(32)-Ru(1)-C(36)	64.0(3)	C(33)-Ru(1)-C(36)	75.8(3)
C(34)-Ru(1)-C(36)	65.3(3)	C(35)-Ru(1)-C(36)	36.3(3)
Cl-Ru(1)-C(37)	86.1(2)	P(1)-Ru(1)-C(37)	135.6(2)
P(2)-Ru(1)-C(37)	130.1(2)	C(32)-Ru(1)-C(37)	35.8(3)
C(33)-Ru(1)-C(37)	64.8(3)	C(34)-Ru(1)-C(37)	77.4(3)
C(35)-Ru(1)-C(37)	65.1(2)	C(36)-Ru(1)-C(37)	35.7(2)
C(1)-Fe(1)-C(2)	41.9(3)	C(1)-Fe(1)-C(3)	68.9(3)
C(2)-Fe(1)-C(3)	40.8(3)	C(1)-Fe(1)-C(4)	69.2(3)
C(2)-Fe(1)-C(4)	69.2(3)	C(3)-Fe(1)-C(4)	40.3(3)
C(1)-Fe(1)-C(5)	41.7(3)	C(2)-Fe(1)-C(5)	70.0(3)
C(3)-Fe(1)-C(5)	68.1(3)	C(4)-Fe(1)-C(5)	40.3(3)
C(1)-Fe(1)-C(1')	110.7(3)	C(2)-Fe(1)-C(1')	124.5(4)
C(3)-Fe(1)-C(1')	158.9(4)	C(4)-Fe(1)-C(1')	160.7(4)
C(5)-Fe(1)-C(1')	126.6(3)	C(1)-Fe(1)-C(2')	124.1(4)
C(2)-Fe(1)-C(2')	106.7(3)	C(3)-Fe(1)-C(2')	121.7(3)
C(4)-Fe(1)-C(2')	156.6(3)	C(5)-Fe(1)-C(2')	161.9(4)
C(1')-Fe(1)-C(2')	39.8(4)	C(1)-Fe(1)-C(3')	158.8(4)
C(2)-Fe(1)-C(3')	120.1(4)	C(3)-Fe(1)-C(3')	104.7(3)
C(4)-Fe(1)-C(3')	119.9(4)	C(5)-Fe(1)-C(3')	156.4(4)
C(1')-Fe(1)-C(3')	67.6(4)	C(2')-Fe(1)-C(3')	40.8(5)
C(1)-Fe(1)-C(4')	159.9(4)	C(2)-Fe(1)-C(4')	156.4(4)
C(3)-Fe(1)-C(4')	120.8(4)	C(4)-Fe(1)-C(4')	106.0(4)
C(5)-Fe(1)-C(4')	122.1(4)	C(1')-Fe(1)-C(4')	67.1(4)
C(2')-Fe(1)-C(4')	68.0(5)	C(3')-Fe(1)-C(4')	40.8(5)
C(1)-Fe(1)-C(5')	125.1(4)	C(2)-Fe(1)-C(5')	160.9(4)
C(3)-Fe(1)-C(5')	158.0(4)	C(4)-Fe(1)-C(5')	123.8(4)
C(5)-Fe(1)-C(5')	109.8(4)	C(1')-Fe(1)-C(5')	39.4(5)
C(2')-Fe(1)-C(5')	67.2(4)	C(3')-Fe(1)-C(5')	68.0(4)
C(4')-Fe(1)-C(5')	40.3(4)	Ru(1)-P(1)-C(1)	116.5(2)
Ru(1)-P(1)-C(20)	114.8(3)	C(1)-P(1)-C(20)	103.1(3)
Ru(1)-P(1)-C(26)	114.9(3)	C(1)-P(1)-C(26)	107.1(3)
C(20)-P(1)-C(26)	98.4(3)	Ru(1)-P(2)-C(6)	110.0(2)
Ru(1)-P(2)-C(8)	115.8(2)	C(6)-P(2)-C(8)	110.4(3)
Ru(1)-P(2)-C(14)	115.9(2)	C(6)-P(2)-C(14)	102.4(3)
C(8)-P(2)-C(14)	101.3(3)	F(1)-P(3)-F(2)	92.0(6)
F(1)-P(3)-F(3)	175.7(6)	F(2)-P(3)-F(3)	87.4(7)
F(1)-P(3)-F(4)	89.2(7)	F(2)-P(3)-F(4)	94.7(10)
F(3)-P(3)-F(4)	95.1(6)	F(1)-P(3)-F(5)	83.8(6)
F(2)-P(3)-F(5)	88.9(8)	F(3)-P(3)-F(5)	91.8(6)
F(4)-P(3)-F(5)	172.3(7)	F(1)-P(3)-F(6)	89.5(6)
F(2)-P(3)-F(6)	175.4(10)	F(3)-P(3)-F(6)	90.8(6)
F(4)-P(3)-F(6)	89.7(10)	F(5)-P(3)-F(6)	86.9(8)
Fe(1)-C(1)-P(1)	133.8(3)	Fe(1)-C(1)-C(2)	68.6(4)
P(1)-C(1)-C(2)	128.3(6)	Fe(1)-C(1)-C(5)	68.7(4)

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P(1)-C(1)-C(5)	124.7(5)	C(2)-C(1)-C(5)	106.5(6)
Fe(1)-C(2)-C(1)	69.5(4)	Fe(1)-C(2)-C(3)	69.7(4)
C(1)-C(2)-C(3)	106.7(7)	Fe(1)-C(2)-C(6)	124.0(5)
C(1)-C(2)-C(6)	127.8(7)	C(3)-C(2)-C(6)	125.5(6)
Fe(1)-C(3)-C(2)	69.5(4)	Fe(1)-C(3)-C(4)	70.5(4)
C(2)-C(3)-C(4)	110.2(7)	Fe(1)-C(4)-C(3)	69.2(4)
Fe(1)-C(4)-C(5)	69.1(4)	C(3)-C(4)-C(5)	108.0(7)
Fe(1)-C(5)-C(1)	69.5(4)	Fe(1)-C(5)-C(4)	70.5(4)
C(1)-C(5)-C(4)	108.7(7)	Fe(1)-C(1')-C(2')	69.4(5)
Fe(1)-C(1')-C(5')	70.0(5)	C(2')-C(1')-C(5')	109.0(9)
Fe(1)-C(2')-C(1')	70.7(6)	Fe(1)-C(2')-C(3')	69.5(6)
C(1')-C(2')-C(3')	108.0(9)	Fe(1)-C(3')-C(2')	69.7(6)
Fe(1)-C(3')-C(4')	69.7(7)	C(2')-C(3')-C(4')	106.9(9)
Fe(1)-C(4')-C(3')	69.5(6)	Fe(1)-C(4')-C(5')	70.3(6)
C(3')-C(4')-C(5')	107.8(10)	Fe(1)-C(5')-C(1')	70.6(5)
Fe(1)-C(5')-C(4')	69.4(5)	C(1')-C(5')-C(4')	108.3(9)
P(2)-C(6)-C(2)	112.4(5)	P(2)-C(6)-C(7)	117.2(5)
C(2)-C(6)-C(7)	111.4(7)	P(2)-C(8)-C(9)	112.5(5)
P(2)-C(8)-C(13)	117.7(5)	C(9)-C(8)-C(13)	110.3(6)
C(8)-C(9)-C(10)	111.4(6)	C(9)-C(10)-C(11)	109.1(8)
C(10)-C(11)-C(12)	112.3(7)	C(11)-C(12)-C(13)	110.9(7)
C(8)-C(13)-C(12)	111.5(7)	P(2)-C(14)-C(15)	113.9(5)
P(2)-C(14)-C(19)	113.1(5)	C(15)-C(14)-C(19)	110.4(7)
C(14)-C(15)-C(16)	110.9(7)	C(15)-C(16)-C(17)	111.0(6)
C(16)-C(17)-C(18)	111.6(8)	C(17)-C(18)-C(19)	111.9(7)
C(14)-C(19)-C(18)	112.0(6)	P(1)-C(20)-C(21)	119.5(5)
P(1)-C(20)-C(25)	121.8(6)	C(21)-C(20)-C(25)	118.7(7)
C(20)-C(21)-C(22)	120.8(7)	C(21)-C(22)-C(23)	121.2(8)
C(22)-C(23)-C(24)	119.5(9)	C(23)-C(24)-C(25)	120.4(8)
C(20)-C(25)-C(24)	119.3(7)	P(1)-C(26)-C(27)	118.5(5)
P(1)-C(26)-C(31)	123.2(6)	C(27)-C(26)-C(31)	118.3(6)
C(26)-C(27)-C(28)	121.0(8)	C(27)-C(28)-C(29)	118.7(10)
C(28)-C(29)-C(30)	122.2(7)	C(29)-C(30)-C(31)	119.5(8)
C(26)-C(31)-C(30)	120.2(8)	Ru(1)-C(32)-C(33)	70.7(5)
Ru(1)-C(32)-C(37)	74.1(4)	C(33)-C(32)-C(37)	120.8(6)
Ru(1)-C(33)-C(32)	73.2(5)	Ru(1)-C(33)-C(34)	73.2(4)
C(32)-C(33)-C(34)	122.4(8)	Ru(1)-C(34)-C(33)	70.6(4)
Ru(1)-C(34)-C(35)	70.0(4)	C(33)-C(34)-C(35)	116.4(7)
Ru(1)-C(34)-C(38)	135.6(7)	C(33)-C(34)-C(38)	121.9(8)
C(35)-C(34)-C(38)	121.4(7)	Ru(1)-C(35)-C(34)	73.7(5)
Ru(1)-C(35)-C(36)	73.7(4)	C(34)-C(35)-C(36)	122.2(6)
Ru(1)-C(36)-C(35)	70.0(5)	Ru(1)-C(36)-C(37)	74.0(5)
C(35)-C(36)-C(37)	120.9(7)	Ru(1)-C(37)-C(32)	70.1(5)
Ru(1)-C(37)-C(36)	70.3(4)	C(32)-C(37)-C(36)	117.2(6)
Ru(1)-C(37)-C(39)	133.5(5)	C(32)-C(37)-C(39)	118.8(6)
C(36)-C(37)-C(39)	124.0(7)	C(37)-C(39)-C(40)	106.8(7)
C(37)-C(39)-C(41)	115.9(6)	C(40)-C(39)-C(41)	110.9(8)

9a

Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

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	x	y	z	U(eq)
Ru(1)	1045(1)	131	7622(1)	25(1)
Fe(1)	3006(1)	1687(1)	5361(1)	35(1)
Cl	40(2)	1378(1)	6566(1)	38(1)
P(1)	1848(2)	-143(1)	6335(1)	27(1)
P(2)	2594(2)	1185(1)	8491(1)	27(1)
P(3)	6271(3)	-5518(2)	7482(2)	80(2)
F(1)	7635(7)	-5317(7)	8144(8)	162(5)
F(2)	6451(12)	-6514(7)	7659(11)	221(9)
F(3)	4923(8)	-5717(8)	6914(7)	175(5)
F(4)	6570(12)	-5515(13)	6543(8)	254(10)
F(5)	6111(10)	-5438(9)	8507(7)	189(6)
F(6)	6026(11)	-4482(8)	7358(12)	219(8)
C(1)	2994(6)	621(5)	6287(5)	28(3)
C(2)	3429(6)	1441(5)	6885(5)	29(3)
C(3)	4467(6)	1718(5)	6697(5)	36(3)
C(4)	4688(6)	1125(6)	5999(6)	40(3)
C(5)	3792(6)	453(5)	5732(5)	37(3)
C(1')	1309(8)	1949(7)	4342(6)	55(4)
C(2')	1765(9)	2687(7)	4974(6)	59(4)
C(3')	2823(9)	2969(7)	4834(7)	69(5)
C(4')	2997(9)	2379(9)	4110(8)	74(5)
C(5')	2056(10)	1752(7)	3821(6)	70(4)
C(6)	2879(6)	1935(5)	7547(5)	30(3)
C(7)	3530(6)	2818(6)	7948(6)	44(2)
C(8)	4024(6)	692(5)	9376(5)	34(3)
C(9)	4519(6)	-14(6)	8865(6)	48(3)
C(10)	5560(7)	-539(6)	9657(6)	55(4)
C(11)	6538(7)	127(9)	10275(6)	70(4)
C(12)	6065(7)	837(7)	10779(7)	64(4)
C(13)	5012(7)	1337(6)	9990(6)	51(3)
C(14)	2239(7)	2004(5)	9355(5)	36(3)
C(15)	2261(7)	1592(6)	10366(5)	41(3)
C(16)	2037(8)	2305(6)	11050(6)	57(4)
C(17)	869(8)	2778(7)	10512(6)	63(4)
C(18)	825(8)	3194(6)	9525(7)	57(4)
C(19)	1064(7)	2512(5)	8824(5)	40(3)
C(20)	2560(6)	-1264(5)	6408(5)	32(3)
C(21)	1853(7)	-2000(5)	5954(6)	42(3)
C(22)	2347(9)	-2841(6)	6024(7)	60(4)
C(23)	3545(10)	-2978(6)	6533(8)	65(5)
C(24)	4277(8)	-2257(7)	6965(7)	58(4)
C(25)	3796(7)	-1386(5)	6889(6)	38(3)
C(26)	722(6)	-229(5)	5019(5)	35(3)
C(27)	1114(7)	-443(7)	4222(6)	53(4)
C(28)	312(9)	-515(8)	3222(6)	69(5)
C(29)	-886(10)	-403(7)	3028(6)	70(4)
C(30)	-1302(7)	-207(6)	3771(7)	55(4)
C(31)	-491(7)	-119(5)	4789(5)	40(3)
C(32)	-531(7)	-835(5)	7214(6)	41(3)
C(33)	542(8)	-1324(5)	7582(6)	46(4)
C(34)	1428(7)	-1165(5)	8549(6)	36(3)
C(35)	1204(6)	-466(5)	9124(5)	33(3)
C(36)	127(6)	24(6)	8780(5)	33(3)
C(37)	-769(6)	-152(5)	7814(5)	34(3)

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Table 1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	x	y	z	U(eq)
C(38)	2498(8)	-1781(7)	9000(8)	71(5)
C(39)	-1989(6)	308(6)	7416(6)	50(3)
C(40)	-2896(7)	-368(7)	7527(8)	69(4)
C(41)	-2067(8)	1184(7)	7914(8)	77(5)

* Equivalent isotropic U defined as one third of the trace of the orthogonalized U_{ij} tensor.

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Table 4. Anisotropic displacement coefficients ($\text{\AA}^2 \times 10^3$)

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru(1)	26(1)	24(1)	26(1)	-1(1)	11(1)	-1(1)
Fe(1)	43(1)	37(1)	28(1)	3(1)	16(1)	8(1)
Cl	39(1)	32(1)	37(1)	2(1)	8(1)	2(1)
P(1)	28(1)	26(1)	25(1)	1(1)	9(1)	-2(1)
P(2)	31(1)	27(1)	25(1)	0(1)	12(1)	-1(1)
P(3)	113(2)	80(3)	67(2)	-49(2)	57(2)	-28(2)
F(1)	102(6)	185(10)	192(9)	-32(6)	45(6)	-29(8)
F(2)	238(12)	93(8)	300(16)	-30(8)	59(11)	-24(8)
F(3)	131(7)	217(11)	146(7)	-101(7)	15(6)	4(8)
F(4)	292(13)	398(22)	141(8)	-110(15)	161(9)	-21(11)
F(5)	211(9)	261(13)	127(6)	-42(9)	101(7)	-68(8)
F(6)	189(11)	103(8)	301(16)	-19(6)	12(11)	22(9)
C(1)	27(4)	32(4)	22(4)	11(3)	8(3)	8(3)
C(2)	34(4)	30(5)	25(4)	-1(4)	13(4)	4(4)
C(3)	41(5)	38(5)	28(4)	-5(4)	13(4)	4(4)
C(4)	36(4)	49(5)	41(4)	-2(4)	19(4)	9(4)
C(5)	42(4)	37(5)	34(4)	8(4)	18(4)	5(3)
C(1')	60(6)	56(6)	40(5)	8(5)	9(5)	16(5)
C(2')	84(7)	51(6)	43(5)	35(6)	24(5)	15(5)
C(3')	86(7)	53(6)	51(6)	-10(6)	7(5)	27(5)
C(4')	78(7)	105(9)	50(6)	16(7)	36(5)	43(7)
C(5')	105(8)	62(7)	30(5)	19(7)	8(5)	6(5)
C(6)	32(4)	23(4)	34(4)	-3(3)	13(3)	-1(3)
C(8)	27(4)	34(4)	39(4)	-1(4)	10(3)	-6(4)
C(9)	46(4)	49(6)	46(4)	11(4)	12(4)	2(5)
C(10)	49(5)	63(6)	43(5)	24(5)	6(4)	-3(5)
C(11)	40(5)	99(7)	55(5)	13(7)	1(4)	-4(7)
C(12)	41(5)	73(7)	58(6)	0(5)	-5(4)	0(5)
C(13)	45(5)	51(6)	50(5)	-2(4)	11(4)	-6(4)
C(14)	42(5)	29(4)	37(4)	3(4)	14(4)	-1(4)
C(15)	50(5)	45(5)	25(4)	5(4)	12(3)	-8(4)
C(16)	76(6)	60(6)	40(5)	-2(5)	26(5)	-12(5)
C(17)	78(7)	67(6)	58(6)	16(6)	40(5)	-12(5)
C(18)	60(5)	46(5)	71(6)	18(5)	31(5)	-4(5)
C(19)	51(5)	36(5)	34(4)	9(4)	17(4)	0(4)
C(20)	34(5)	38(5)	24(4)	4(4)	10(3)	-3(4)
C(21)	45(5)	28(5)	53(5)	-2(4)	18(4)	-4(4)
C(22)	65(7)	37(6)	71(6)	-3(5)	19(5)	-21(5)
C(23)	85(8)	33(6)	84(7)	8(6)	39(6)	-3(5)
C(24)	51(5)	65(7)	57(6)	24(6)	16(5)	5(5)
C(25)	43(5)	35(5)	40(5)	3(4)	18(4)	-6(4)
C(26)	34(5)	35(4)	31(4)	-2(3)	4(3)	2(3)
C(27)	50(5)	77(7)	27(5)	-13(5)	8(4)	-13(4)
C(28)	74(7)	91(8)	35(5)	-10(6)	12(5)	-20(5)
C(29)	83(8)	85(7)	16(5)	-2(6)	-14(5)	-2(5)
C(30)	39(5)	51(6)	50(6)	-3(4)	-13(5)	-6(4)
C(31)	48(5)	27(5)	37(4)	1(3)	5(4)	-1(3)
C(32)	39(5)	45(6)	44(5)	-14(4)	22(4)	-4(4)
C(33)	69(6)	26(5)	60(6)	-18(5)	45(5)	-5(4)
C(34)	44(5)	23(4)	54(5)	3(4)	31(4)	14(4)
C(35)	34(5)	36(5)	31(4)	-5(4)	14(4)	9(4)
C(36)	37(4)	30(4)	38(4)	-8(4)	22(3)	-6(4)
C(37)	29(4)	37(5)	44(5)	-7(3)	22(4)	1(4)
C(38)	74(6)	56(6)	96(8)	18(5)	47(6)	25(6)
C(39)	37(5)	59(7)	55(5)	1(4)	17(4)	17(5)

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C(40)	36(5)	74(7)	98(7)	0(5)	27(5)	22(6)
C(41)	37(5)	75(8)	118(9)	14(5)	26(5)	-10(7)

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The anisotropic displacement factor exponent takes the form:

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

Table 5. H-Atom coordinates ($\times 10^4$) and isotropic displacement coefficients ($\text{Å}^2 \times 10^3$)

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	x	y	z	U
H(3A)	4943	2239	6993	80
H(4A)	5328	1175	5743	80
H(5A)	3717	-32	5259	80
H(1'A)	606	1614	4296	80
H(2'A)	1416	2957	5422	80
H(3'A)	3314	3475	5159	80
H(4'A)	3646	2404	3863	80
H(5'A)	1962	1264	3348	80
H(6A)	2096	2112	7084	80
H(7A)	3626	3147	7393	80
H(7B)	4305	2691	8459	80
H(7C)	3071	3172	8247	80
H(8A)	3808	372	9879	80
H(9A)	4796	267	8375	80
H(9B)	3890	-427	8501	80
H(10A)	5889	-960	9310	80
H(10B)	5274	-869	10112	80
H(11A)	6872	409	9823	80
H(11B)	7172	-195	10789	80
H(12A)	5808	566	11285	80
H(12B)	6695	1258	11121	80
H(13A)	4691	1763	10338	80
H(13B)	5294	1666	9532	80
H(14A)	2865	2449	9540	80
H(15A)	1655	1134	10221	80
H(15B)	3027	1314	10716	80
H(16A)	2683	2733	11245	80
H(16B)	2020	2027	11663	80
H(17A)	217	2359	10376	80
H(17B)	768	3241	10953	80
H(18A)	1412	3666	9670	80
H(18B)	48	3458	9182	80
H(19A)	1099	2815	8230	80
H(19B)	413	2089	8596	80
H(21A)	1007	-1920	5588	80
H(22A)	1842	-3343	5706	80
H(23A)	3878	-3573	6592	80
H(24A)	5122	-2348	7328	80
H(25A)	4311	-878	7158	80
H(27A)	1954	-540	4371	80
H(28A)	591	-640	2674	80
H(29A)	-1446	-471	2336	80
H(30A)	-2147	-127	3610	80
H(31A)	-784	22	5324	80
H(32A)	-1053	-902	6509	80
H(33A)	730	-1716	7116	80
H(35A)	1844	-269	9734	80
H(36A)	55	549	9154	80
H(38A)	2289	-2273	9346	80
H(38B)	3155	-1451	9479	80
H(38C)	2730	-2010	8458	80
H(39A)	-2195	423	6697	80
H(40A)	-3681	-100	7285	80
H(40B)	-2675	-533	8235	80
H(40C)	-2903	-895	7127	80
H(41A)	-1490	1597	7838	80
H(41B)	-1902	1085	8631	80
H(41C)	-2860	1430	7595	80