Inorganic Chemistry
including bioinorganic chemistry
Inorg. Chem., 1998, 37(7), 1555-1562, DOI:10.1021/ic971050g

Terms & Conditions

Electronic Supporting Information files are available without a subscription to ACS Web Editions. The American Chemical Society holds a copyright ownership interest in any copyrightable Supporting Information. Files available from the ACS website may be downloaded for personal use only. Users are not otherwise permitted to reproduce, republish, redistribute, or sell any Supporting Information from the ACS website, either in whole or in part, in either machine-readable form or any other form without permission from the American Chemical Society. For permission to reproduce, republish and redistribute this material, requesters must process their own requests via the RightsLink permission system. Information about how to use the RightsLink permission system can be found at http://pubs.acs.org/page/copyright/permissions.html



ACS Publications
MOST TRUSTED. MOST CITED. MOST READ.

Copyright © 1998 American Chemical Society

Table 1. Crystal data and structure refinement for 1Ru.

Identification code	m9305xco
Empirical formula	$C_{58}HH_{53}P_4RuS$
Formula weight	1008.02
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 11.226(2) Å alpha = 90°
	b = 33.260(7) Å beta = 104.01(3)°
	c = 13.586(3) Å gamma = 90°
Volume, Z	4922(2) Å^3, 4
Density (calculated)	1.360 Mg/m^3
Absorption coefficient	0.529 mm^{-1}
F(000)	2088
Crystal size	0.10 x 0.13 x 0.32 mm
θ range for data collection	2.20 to 26.97°
Limiting indices	$0 \le h \le 14$, $-42 \le k \le 0$, $-17 \le l \le 16$
Reflections collected	11231
Independent reflections	10699 (R_{int} = 0.0516)
Absorption correction	Semi-empirical from psi-scans
Max. and min. transmission	0.4839 and 0.4689
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	10687 / 0 / 581
Goodness-of-fit on F^2	1.135
Final R indices [I>2σ(I)]	R1 = 0.0463, wR2 = 0.1010
R indices (all data)	R1 = 0.1761, wR2 = 0.1291
Largest diff. peak and hole	0.463 and -0.765 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1 Ru, U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Ru(1)	1651(1)	8700(1)	1409(1)	36(1)
H(1RU)	291(35)	8779(11)	1311(28)	53(12)
S(1)	3859(1)	8491(1)	1608(1)	49(1)
P(1)	1902(1)	9392(1)	1646(1)	40(1)
P(2)	998(1)	8857(1)	-305(1)	46(1)
P(3)	1282(1)	8009(1)	1206(1)	45(1)
P(4)	1879(1)	8544(1)	3132(1)	40(1)
C(1)	1423(5)	9640(1)	379(3)	55(1)
C(2)	566(5)	9395(1)	-377(3)	62(1)
C(3)	2167(5)	7776(1)	2392(3)	52(1)
C(4)	1822(4)	7989(1)	3269(3)	49(1)
C(5)	4825(5)	8817(2)	1149(4)	58(1)
C(6)	6087(5)	8775(2)	1467(4)	75(2)
C(7)	6868(6)	9025(2)	1138(5)	88(2)
C(8)	6454(6)	9338(2)	501(4)	80(2)
C(9)	5233(5)	9393(2)	175(4)	63(1)
C(10)	4424(5)	9142(2)	487(4)	58(1)
C(11)	939(5)	9657(1)	2365(4)	48(1)
C(12)	-330(5)	9650(2)	2003(4)	65(2)
C(13)	-1092(6)	9845(2)	2518(6)	87(2)
C(14)	-587(7)	10041(2)	3409(5)	87(2)
C(15)	647(7)	10056(2)	3767(4)	85(2)
C(16)	1418(5)	9864(2)	3245(4)	64(2)
C(21)	3368(4)	9650(1)	2147(3)	44(1)
C(22)	3500(5)	10057(1)	1974(4)	61(1)
C(23)	4609(6)	10247(2)	2326(4)	77(2)
C(24)	5594(6)	10038(2)	2870(4)	75(2)
C(25)	5472(5)	9637(2)	3064(4)	65(2)
C(26)	4372(4)	9446(1)	2705(3)	49(1)
C(31)	-463(5)	8662(1)	-1089(3)	54(1)
C(32)	-1565(5)	8746(2)	-814(4)	79(2)
C(33)	-2687(6)	8626(2)	-1388(5)	100(2)
C(34)	-2723(7)	8417(2)	-2268(5)	96(2)
C(35)	-1680(7)	8319(2)	-2546(4)	77(2)
C(36)	-548(6)	8441(1)	-1962(4)	62(2)
C(41)	1984(5)	8801(1)	-1193(3)	50(1)
C(42)	1914(5)	9047(2)	-2029(4)	62(1)
C(43)	2681(6)	8996(2)	-2659(4)	75(2)
C(44)	3547(6)	8703(2)	-2478(4)	72(2)
C(45)	3629(6)	8444(2)	-1671(4)	75(2)
C(46)	2847(5)	8498(2)	-1033(4)	63(2)
C(51)	-250(5)	7803(1)	1123(3)	50(1)
C(52)	-1269(6)	8041(2)	1014(5)	79(2)
C(53)	-2435(6)	7884(2)	919(5)	99(2)
C(54)	-2581(6)	7478(2)	963(5)	87(2)
C(55)	-1595(7)	7235(2)	1093(4)	82(2)
C(56)	-435(6)	7390(2)	1155(4)	74(2)
C(61)	1751(5)	7704(1)	235(3)	55(1)

C(62)	917(5)	7621(2)	-679(4)	65(2)
C(63)	1264(7)	7403(2)	-1436(4)	90(2)
C(64)	2433(8)	7265(2)	-1278(5)	97(2)
C(65)	3270(7)	7343(2)	-395(5)	87(2)
C(66)	2934(6)	7562(2)	368(4)	68(2)
C(71)	721(4)	8677(1)	3835(3)	46(1)
C(72)	-427(5)	8802(2)	3331(4)	66(2)
C(73)	-1327(6)	8872(2)	3839(5)	86(2)
C(74)	-1092(6)	8820(2)	4858(5)	81(2)
C(75)	41(6)	8697(2)	5378(4)	81(2)
C(76)	938(5)	8624(2)	4867(4)	68(2)
C(81)	3294(4)	8684(1)	4054(3)	42(1)
C(82)	4341(5)	8449(2)	4206(4)	57(1)
C(83)	5424(5)	8572(2)	4851(4)	74(2)
C(84)	5488(5)	8927(2)	5359(4)	75(2)
C(85)	4470(6)	9167(2)	5220(4)	65(2)
C(86)	3377(5)	9047(2)	4569(3)	52(1)

Table 3. Bond lengths [Å] and angles [°] for 1Ru

Ru(1)-H(1RU)	1.52(4)	Ru(1)-P(2)	2.3246(13)
Ru(1)-P(1)	2.3317(13)	Ru(1)-P(3)	2.3396(13)
Ru(1)-P(4)	2.3513(12)	Ru(1)-S(1)	2.5257(14)
S(1)-C(5)	1.754(5)	P(1)-C(21)	1.834(5)
P(1)-C(11)	1.846(5)	P(1)-C(1)	1.866(4)
P(2)-C(41)	1.833(5)	P(2)-C(31)	1.844(5)
P(2)-C(2)	1.852(5)	P(3)-C(51)	1.829(5)
P(3)-C(61)	1.839(5)	P(3)-C(3)	1.848(4)
P(4)-C(81)	1.829(4)	P(4)-C(71)	1.844(5)
P(4)-C(4)	1.857(4)	C(1)-C(2)	1.472(6)
C(3)-C(4)	1.516(6)	C(5)-C(6)	1.385(7)
C(5)-C(10)	1.408(6)	C(6)-C(7)	1.358(7)
C(7)-C(8)	1.362(7)	C(8)-C(9)	1.347(7)
C(9)-C(10)	1.373(6)	C(11)-C(16)	1.372(6)
C(11)-C(12)	1.390(7)	C(12)-C(13)	1.389(7)
C(13)-C(14)	1.370(8)	C(14)-C(15)	1.353(8)
C(15)-C(16)	1.400(7)	C(21)-C(26)	1.374(6)
C(21)-C(22)	1.390(6)	C(22)-C(23)	1.375(7)
C(23)-C(24)	1.363(8)	C(24)-C(25)	1.373(7)
C(25)-C(26)	1.369(6)	C(31)-C(36)	1.378(6)
C(31)-C(32)	1.404(7)	C(32)-C(33)	1.371(8)
C(33)-C(34)	1.375(9)	C(34)-C(35)	1.354(8)
C(35)-C(36)	1.385(7)	C(41)-C(46)	1.378(7)
C(41)-C(42)	1.388(6)	C(42)-C(43)	1.364(7)
C(43)-C(44)	1.357(8)	C(44)-C(45)	1.380(7)
C(45)-C(46)	1.386(7)	C(51)-C(52)	1.369(7)
C(51)-C(56)	1.390(6)	C(52)-C(53)	1.386(7)
C(53)-C(54)	1.365(8)	C(54)-C(55)	1.346(8)
C(55)-C(56)	1.385(7)	C(61)-C(66)	1.379(7)
C(61)-C(62)	1.391(6)	C(62)-C(63)	1.390(7)
C(63)-C(64)	1.357(9)	C(64)-C(65)	1.357(8)
C(65)-C(66)	1.392(7)	C(71)-C(72)	1.369(6)
C(71)-C(76)	1.375(6)	C(72)-C(73)	1.374(7)
C(73)-C(74)	1.356(8)	C(74)-C(75)	1.360(8)
C(75)-C(76)	1.377(7)	C(81)-C(82)	1.385(6)
C(81)-C(86)	1.386(6)	C(82)-C(83)	1.377(7)
C(83)-C(84)	1.361(8)	C(84)-C(85)	1.370(7)
C(85)-C(86)	1.387(7)		

H(1RU)-Ru(1)-P(2)	78.9(14)	H(1RU)-Ru(1)-P(1)	85.8(14)
P(2)-Ru(1)-P(1)	85.18(4)	H(1RU)-Ru(1)-P(3)	90.8(14)
P(2)-Ru(1)-P(3)	95.60(4)	P(1)-Ru(1)-P(3)	176.31(5)
H(1RU)-Ru(1)-P(4)	89.5(14)	P(2)-Ru(1)-P(4)	168.25(5)
P(1)-Ru(1)-P(4)	95.81(4)	P(3)-Ru(1)-P(4)	82.70(4)
H(1RU)-Ru(1)-S(1)	173.7(14)	P(2)-Ru(1)-S(1)	103.44(5)
P(1)-Ru(1)-S(1)	100.11(4)	P(3)-Ru(1)-S(1)	83.24(4)
P(4)-Ru(1)-S(1)	87.95(5)	C(5)-S(1)-Ru(1)	117.8(2)
C(21)-P(1)-C(11)	99.7(2)	C(21)-P(1)-C(1)	99.7(2)
C(11)-P(1)-C(1)	101.7(2)	C(21)-P(1)-Ru(1)	125.4(2)
C(11)-P(1)-Ru(1)	118.4(2)	C(1)-P(1)-Ru(1)	108.1(2)
C(41)-P(2)-C(31)	100.3(2)	C(41)-P(2)-C(2)	104.8(2)
C(31)-P(2)-C(2)	97.2(2)	C(41)-P(2)-Ru(1)	122.9(2)
C(31)-P(2)-Ru(1)	121.4(2)	C(2)-P(2)-Ru(1)	106.5(2)
C(51)-P(3)-C(61)	100.2(2)	C(51)-P(3)-C(3)	101.2(2)
C(61)-P(3)-C(3)	101.9(2)	C(51)-P(3)-Ru(1)	120.9(2)

C(61)-P(3)-Ru(1)	123.6(2)	C(3)-P(3)-Ru(1)	105.6(2)
C(81)-P(4)-C(71)	100.8(2)	C(81)-P(4)-C(4)	103.3(2)
C(71)-P(4)-C(4)	98.1(2)	C(81)-P(4)-Ru(1)	119.5(2)
C(71)-P(4)-Ru(1)	122.8(2)	C(4)-P(4)-Ru(1)	108.81(14)
C(2)-C(1)-P(1)	113.1(3)	C(1)-C(2)-P(2)	112.3(3)
C(4)-C(3)-P(3)	107.7(3)	C(3)-C(4)-P(4)	111.3(3)
C(6)-C(5)-C(10)	114.9(5)	C(6)-C(5)-S(1)	120.1(4)
C(10)-C(5)-S(1)	125.0(4)	C(7)-C(6)-C(5)	121.9(6)
C(6)-C(7)-C(8)	121.9(6)	C(9)-C(8)-C(7)	118.4(6)
C(8)-C(9)-C(10)	120.8(5)	C(9)-C(10)-C(5)	122.0(5)
C(16)-C(11)-C(12)	117.9(5)	C(16)-C(11)-P(1)	123.0(4)
C(12)-C(11)-P(1)	119.1(4)	C(11)-C(12)-C(13)	121.1(6)
C(14)-C(13)-C(12)	119.6(6)	C(15)-C(14)-C(13)	120.3(6)
C(14)-C(15)-C(16)	120.3(6)	C(11)-C(16)-C(15)	120.7(5)
C(26)-C(21)-C(22)	117.8(4)	C(26)-C(21)-P(1)	121.1(3)
C(22)-C(21)-P(1)	121.0(4)	C(23)-C(22)-C(21)	120.9(5)
C(24)-C(23)-C(22)	120.1(5)	C(23)-C(24)-C(25)	119.6(5)
C(26)-C(25)-C(24)	120.3(5)	C(25)-C(26)-C(21)	121.1(5)
C(36)-C(31)-C(32)	117.0(5)	C(36)-C(31)-P(2)	123.4(4)
C(32)-C(31)-P(2)	119.6(4)	C(33)-C(32)-C(31)	122.5(6)
C(32)-C(33)-C(34)	118.1(7)	C(35)-C(34)-C(33)	121.2(6)
C(34)-C(35)-C(36)	120.4(6)	C(31)-C(36)-C(35)	120.7(6)
C(46)-C(41)-C(42)	117.4(5)	C(46)-C(41)-P(2)	118.9(4)
C(42)-C(41)-P(2)	123.7(4)	C(43)-C(42)-C(41)	121.4(5)
C(44)-C(43)-C(42)	120.6(5)	C(43)-C(44)-C(45)	120.1(5)
C(44)-C(45)-C(46)	119.0(6)	C(41)-C(46)-C(45)	121.5(5)
C(52)-C(51)-C(56)	116.5(5)	C(52)-C(51)-P(3)	122.6(4)
C(56)-C(51)-P(3)	120.9(4)	C(51)-C(52)-C(53)	122.6(5)
C(54)-C(53)-C(52)	119.3(6)	C(55)-C(54)-C(53)	119.7(6)
C(54)-C(55)-C(56)	121.1(6)	C(55)-C(56)-C(51)	120.7(6)
C(66)-C(61)-C(62)	117.9(5)	C(66)-C(61)-P(3)	122.0(4)
C(62)-C(61)-P(3)	120.1(4)	C(63)-C(62)-C(61)	121.1(6)
C(64)-C(63)-C(62)	119.5(6)	C(65)-C(64)-C(63)	120.8(6)
C(64)-C(65)-C(66)	120.2(7)	C(61)-C(66)-C(65)	120.5(6)
C(72)-C(71)-C(76)	117.5(5)	C(72)-C(71)-P(4)	120.7(3)
C(76)-C(71)-P(4)	121.6(4)	C(71)-C(72)-C(73)	121.2(5)
C(74)-C(73)-C(72)	120.4(6)	C(73)-C(74)-C(75)	119.6(5)
C(74)-C(75)-C(76)	119.9(5)	C(71)-C(76)-C(75)	121.4(5)
C(82)-C(81)-C(86)	117.7(4)	C(82)-C(81)-P(4)	121.6(4)
C(86)-C(81)-P(4)	120.6(4)	C(83)-C(82)-C(81)	121.0(5)
C(84)-C(83)-C(82)	120.6(5)	C(83)-C(84)-C(85)	119.8(5)
C(84)-C(85)-C(86)	119.9(5)	C(81)-C(86)-C(85)	121.0(5)

Table 4. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1 Ru

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Ru(1)	46(1)	30(1)	31(1)	1(1)	7(1)	1(1)
S(1)	54(1)	43(1)	53(1)	5(1)	18(1)	6(1)
P(1)	49(1)	32(1)	40(1)	0(1)	11(1)	-1(1)
P(2)	67(1)	37(1)	33(1)	2(1)	10(1)	4(1)
P(3)	64(1)	32(1)	36(1)	0(1)	6(1)	-1(1)
P(4)	48(1)	38(1)	33(1)	1(1)	7(1)	1(1)
C(1)	68(4)	39(3)	54(3)	6(2)	7(3)	4(2)
C(2)	92(4)	45(3)	45(3)	5(2)	10(3)	8(3)
C(3)	75(4)	34(3)	42(3)	0(2)	3(3)	2(2)
C(4)	62(3)	41(3)	38(3)	5(2)	1(2)	-2(2)
C(5)	66(4)	57(3)	53(3)	-11(2)	20(3)	8(3)
C(6)	56(4)	92(5)	77(4)	12(3)	14(3)	20(3)
C(7)	55(4)	111(6)	103(5)	26(4)	31(4)	7(4)
C(8)	61(4)	100(5)	83(4)	20(4)	26(3)	-4(4)
C(9)	70(4)	64(4)	59(3)	10(3)	25(3)	-2(3)
C(10)	61(4)	53(3)	58(3)	-3(3)	12(3)	10(3)
C(11)	63(4)	33(3)	53(3)	1(2)	24(3)	3(2)
C(12)	69(4)	53(3)	79(4)	-4(3)	30(3)	2(3)
C(13)	87(5)	78(4)	111(5)	17(4)	53(4)	19(4)
C(14)	109(6)	85(5)	83(5)	14(4)	57(5)	35(4)
C(15)	122(6)	77(4)	63(4)	-9(3)	35(4)	17(4)
C(16)	77(4)	66(4)	54(3)	-3(3)	24(3)	13(3)
C(21)	55(3)	39(3)	40(3)	-6(2)	18(2)	-8(2)
C(22)	78(4)	44(3)	58(3)	-2(2)	11(3)	-11(3)
C(23)	101(5)	56(4)	72(4)	-7(3)	18(4)	-36(4)
C(24)	71(4)	82(5)	76(4)	-30(4)	26(3)	-26(4)
C(25)	58(4)	67(4)	71(4)	-21(3)	19(3)	-1(3)
C(26)	56(3)	52(3)	42(3)	-10(2)	20(2)	-8(3)
C(31)	69(4)	48(3)	39(3)	10(2)	3(2)	1(3)
C(32)	67(4)	97(5)	67(4)	-18(3)	5(3)	1(4)
C(33)	65(4)	120(6)	103(6)	-8(5)	-2(4)	5(4)
C(34)	95(6)	93(5)	77(5)	4(4)	-25(4)	-7(4)
C(35)	98(5)	71(4)	57(4)	-9(3)	9(4)	-23(4)
C(36)	87(4)	52(3)	48(3)	-2(2)	19(3)	-13(3)
C(41)	70(4)	45(3)	35(2)	-4(2)	13(2)	-13(2)
C(42)	86(4)	55(3)	47(3)	4(2)	21(3)	-8(3)
C(43)	102(5)	79(4)	48(3)	3(3)	26(3)	-22(4)
C(44)	93(5)	75(4)	61(4)	-20(3)	41(3)	-31(4)
C(45)	93(5)	69(4)	71(4)	-13(3)	34(4)	-4(3)
C(46)	90(4)	58(3)	47(3)	0(3)	29(3)	0(3)
C(51)	71(4)	35(3)	41(3)	-4(2)	9(2)	-8(2)
C(52)	76(4)	49(3)	109(5)	-13(3)	16(4)	-16(3)
C(53)	69(5)	79(5)	146(7)	-19(4)	23(4)	-18(4)
C(54)	83(5)	101(6)	81(4)	-23(4)	26(4)	-42(4)
C(55)	108(6)	66(4)	65(4)	13(3)	6(4)	-40(4)
C(56)	91(5)	52(3)	67(4)	13(3)	-6(3)	-11(3)
C(61)	89(4)	31(3)	43(3)	2(2)	13(3)	-3(3)
C(62)	87(4)	61(3)	47(3)	-3(3)	17(3)	-6(3)

C(63)	140(7)	79(5)	52(4)	-22(3)	22(4)	-16(4)
C(64)	159(8)	71(5)	72(5)	-22(4)	49(5)	1(5)
C(65)	119(6)	63(4)	85(5)	-7(3)	39(4)	22(4)
C(66)	89(5)	51(3)	65(4)	-1(3)	17(3)	11(3)
C(71)	54(3)	46(3)	38(2)	5(2)	12(2)	-5(2)
C(72)	60(4)	88(4)	51(3)	19(3)	19(3)	18(3)
C(73)	69(4)	116(5)	77(4)	18(4)	27(4)	28(4)
C(74)	74(5)	102(5)	82(4)	-8(4)	49(4)	-9(4)
C(75)	72(4)	129(6)	48(3)	3(4)	27(3)	-14(4)
C(76)	62(4)	96(5)	48(3)	8(3)	17(3)	-2(3)
C(81)	44(3)	47(3)	32(2)	0(2)	6(2)	-4(2)
C(82)	53(3)	67(4)	46(3)	4(2)	1(3)	10(3)
C(83)	52(4)	97(5)	67(4)	8(3)	0(3)	11(3)
C(84)	58(4)	108(5)	53(3)	-3(3)	3(3)	-17(4)
C(85)	82(4)	71(4)	46(3)	-16(3)	21(3)	-22(3)
C(86)	56(3)	62(3)	40(3)	-2(2)	12(2)	-2(3)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1Ru

	x	y	z	U(eq)
H(1A)	1036(5)	9896(1)	455(3)	66
H(1B)	2148(5)	9696(1)	132(3)	66
H(2A)	549(5)	9496(1)	-1051(3)	74
H(2B)	-254(5)	9422(1)	-270(3)	74
H(3A)	1972(5)	7492(1)	2400(3)	63
H(3B)	3040(5)	7803(1)	2444(3)	63
H(4A)	2382(4)	7908(1)	3900(3)	59
H(4B)	1000(4)	7909(1)	3299(3)	59
H(6A)	6410(5)	8570(2)	1919(4)	90
H(7A)	7709(6)	8980(2)	1354(5)	105
H(8A)	7002(6)	9509(2)	296(4)	96
H(9A)	4935(5)	9603(2)	-266(4)	75
H(10A)	3586(5)	9188(2)	254(4)	69
H(12A)	-676(5)	9512(2)	1406(4)	78
H(13A)	-1938(6)	9842(2)	2260(6)	104
H(14A)	-1094(7)	10163(2)	3769(5)	104
H(15A)	983(7)	10196(2)	4363(4)	102
H(16A)	2265(5)	9877(2)	3497(4)	77
H(22A)	2829(5)	10204(1)	1614(4)	73
H(23A)	4687(6)	10519(2)	2193(4)	92
H(24A)	6345(6)	10166(2)	3108(4)	90
H(25A)	6140(5)	9494(2)	3441(4)	78
H(26A)	4302(4)	9175(1)	2840(3)	59
H(32A)	-1532(5)	8888(2)	-218(4)	95
H(33A)	-3404(6)	8684(2)	-1189(5)	120
H(34A)	-3478(7)	8341(2)	-2680(5)	115
H(35A)	-1723(7)	8170(2)	-3131(4)	92
H(36A)	162(6)	8374(1)	-2162(4)	75
H(42A)	1331(5)	9252(2)	-2163(4)	74
H(43A)	2610(6)	9164(2)	-3218(4)	91
H(44A)	4085(6)	8677(2)	-2897(4)	87
H(45A)	4201(6)	8236(2)	-1556(4)	90
H(46A)	2906(5)	8325(2)	-484(4)	76
H(52A)	-1175(6)	8318(2)	1003(5)	95
H(53A)	-3111(6)	8054(2)	826(5)	118
H(54A)	-3358(6)	7369(2)	903(5)	105
H(55A)	-1695(7)	6959(2)	1142(4)	99
H(56A)	229(6)	7217(2)	1219(4)	89
H(62A)	114(5)	7714(2)	-787(4)	78
H(63A)	699(7)	7351(2)	-2046(4)	108
H(64A)	2664(8)	7116(2)	-1781(5)	116
H(65A)	4070(7)	7249(2)	-300(5)	104
H(66A)	3512(6)	7614(2)	971(4)	82
H(72A)	-601(5)	8839(2)	2633(4)	79
H(73A)	-2101(6)	8956(2)	3482(5)	103
H(74A)	-1703(6)	8869(2)	5199(5)	97
H(75A)	209(6)	8663(2)	6077(4)	97
H(76A)	1708(5)	8537(2)	5227(4)	82
H(82A)	4313(5)	8205(2)	3868(4)	69

H(83A)	6118(5)	8410(2)	4941(4)	89
H(84A)	6220(5)	9006(2)	5800(4)	89
H(85A)	4513(6)	9411(2)	5561(4)	79
H(86A)	2690(5)	9211(2)	4476(3)	63