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Table : Bond Distances and Bond Angles of IC3425 complex (5)

W1-Ru1	2.8893(10)
W1-Ru2	2.9097(10)
W1-C1	1.980(9)
W1-C2	1.979(9)
W1-C10	2.037(7)
W1-C18	2.345(8)
W1-C19	2.309(8)
W1-C20	2.369(8)
W1-C21	2.410(8)
W1-C22	2.398(8)
W2-W3	3.0560(7)
W2-Ru1	2.7423(10)
W2-Ru2	2.8734(10)
W2-C3	2.094(8)
W2-C4	1.979(9)
W2-C11	2.128(8)
W2-C28	2.340(8)
W2-C29	2.360(8)
W2-C30	2.396(8)
W2-C31	2.429(8)
W2-C32	2.416(8)
W3-Ru1	2.8873(10)
W3-Ru2	2.7674(10)
W3-C5	1.980(9)
W3-C10	1.992(7)
W3-C11	2.104(8)
W3-C38	2.433(8)
W3-C39	2.339(9)
W3-C40	2.335(8)
W3-C41	2.432(8)
W3-C42	2.463(8)
Ru1-Ru2	2.7391(11)
Ru1-C3	2.145(8)
Ru1-C6	1.894(8)
Ru1-C7	1.874(9)
Ru1-C10	2.125(8)
Ru2-C8	1.907(8)
Ru2-C9	1.902(9)
Ru2-C10	2.141(7)
Ru2-C11	2.120(7)
C1-O1	1.137(11)
C2-O2	1.139(11)
C3-O3	1.174(10)
C4-O4	1.150(11)
C5-O5	1.159(10)
C6-O6	1.147(10)
C7-O7	1.146(11)
C8-O8	1.135(10)
C9-O9	1.142(11)
C11-C12	1.493(11)
C12-C13	1.399(13)
C12-C17	1.403(12)
C13-C14	1.403(12)
C14-C15	1.374(15)
C15-C16	1.349(15)
C16-C17	1.392(12)
C18-C19	1.438(13)
C18-C22	1.397(13)
C18-C23	1.507(13)
C19-C20	1.419(13)
C19-C24	1.509(13)
C20-C21	1.426(12)
C20-C25	1.485(12)
C21-C22	1.428(13)
C21-C26	1.513(13)
C22-C27	1.489(13)
C28-C29	1.433(13)
C28-C32	1.402(12)
C28-C33	1.521(14)
C29-C30	1.412(14)
C29-C34	1.526(13)
C30-C31	1.432(12)
C30-C35	1.482(14)
C31-C32	1.402(13)
C31-C36	1.503(13)
C32-C37	1.502(12)
C38-C39	1.435(13)
C38-C42	1.403(13)
C38-C43	1.481(13)
C39-C40	1.410(13)
C39-C44	1.489(13)
C40-C41	1.418(12)
C40-C45	1.471(13)
C41-C42	1.399(13)
C41-C46	1.477(13)
C42-C47	1.522(13)
C48-Cl1	1.588(8)
C48-Cl1	1.842(7)
C48-Cl2	1.786(11)
Cl1-C48	1.588(8)
Cl1-C48	1.842(7)
Cl1-Cl2	2.526(14)
Cl2-C48	1.786(11)

Ru1-W1-Ru2	56.37(3)
Ru1-W1-C1	132.22(24)
Ru1-W1-C2	90.3(3)
Ru1-W1-C10	47.29(21)
Ru1-W1-C18	148.49(23)
Ru1-W1-C19	138.09(22)
Ru1-W1-C20	103.52(22)
W3-Ru1-C6	103.61(24)
W3-Ru1-C7	159.2(3)
W3-Ru1-C10	43.62(20)
Ru2-Ru1-C3	112.08(22)
Ru2-Ru1-C6	152.67(25)
Ru2-Ru1-C7	100.5(3)
Ru2-Ru1-C10	50.31(20)

Ru1-W1-C21	92.91(21)
Ru1-W1-C22	114.94(23)
Ru2-W1-C1	77.83(25)
Ru2-W1-C2	67.7(3)
Ru2-W1-C10	47.34(20)
Ru2-W1-C18	148.69(22)
Ru2-W1-C19	152.48(21)
Ru2-W1-C20	151.02(20)
Ru2-W1-C21	147.76(21)
Ru2-W1-C22	145.86(21)
C1-W1-C2	83.7(4)
C1-W1-C10	92.7(3)
C1-W1-C18	79.0(3)
C1-W1-C19	79.3(3)
C1-W1-C20	112.2(3)
C1-W1-C21	134.2(3)
C1-W1-C22	110.6(3)
C2-W1-C10	113.8(3)
C2-W1-C18	89.1(3)
C2-W1-C19	124.6(4)
C2-W1-C20	138.4(3)
C2-W1-C21	106.9(3)
C2-W1-C22	80.1(3)
C10-W1-C18	154.7(3)
C10-W1-C19	119.3(3)
C10-W1-C20	103.9(3)
C10-W1-C21	120.4(3)
C10-W1-C22	154.5(3)
C18-W1-C19	36.0(3)
C18-W1-C20	59.0(3)
C18-W1-C21	57.4(3)
C18-W1-C22	34.2(3)
C19-W1-C20	35.3(3)
C19-W1-C21	57.7(3)
C19-W1-C22	58.3(3)
C20-W1-C21	34.7(3)
C20-W1-C22	58.3(3)
C21-W1-C22	34.6(3)
W3-W2-Ru1	59.437(22)
W3-W2-Ru2	55.540(21)
W3-W2-C3	85.56(23)
W3-W2-C4	71.3(3)
W3-W2-C11	43.47(21)
W3-W2-C28	151.39(22)
W3-W2-C29	141.01(23)
W3-W2-C30	140.91(21)
W3-W2-C31	151.57(20)
W3-W2-C32	160.16(20)
Ru1-W2-Ru2	58.33(3)
Ru1-W2-C3	50.51(22)
Ru1-W2-C4	112.2(3)
Ru1-W2-C11	91.73(21)
Ru1-W2-C28	128.52(22)
Ru1-W2-C29	159.55(23)
Ru1-W2-C30	134.53(22)
Ru1-W2-C31	104.93(19)
Ru1-W2-C32	102.41(19)
Ru2-W2-C3	108.81(22)
Ru2-W2-C4	122.8(3)
Ru2-W2-C11	47.32(20)
C3-Ru1-C6	86.5(3)
C3-Ru1-C7	97.5(3)
C3-Ru1-C10	132.7(3)
C6-Ru1-C7	96.5(4)
C6-Ru1-C10	102.4(3)
C7-Ru1-C10	126.7(3)
W1-Ru2-W2	119.83(3)
W1-Ru2-W3	90.113(22)
W1-Ru2-Ru1	61.44(3)
W1-Ru2-C8	107.9(3)
W1-Ru2-C9	99.2(3)
W1-Ru2-C10	44.41(20)
W1-Ru2-C11	138.85(21)
W2-Ru2-W3	65.578(18)
W2-Ru2-Ru1	58.44(3)
W2-Ru2-C8	97.9(3)
W2-Ru2-C9	136.4(3)
W2-Ru2-C10	94.50(20)
W2-Ru2-C11	47.56(21)
W3-Ru2-Ru1	63.247(23)
W3-Ru2-C8	160.4(3)
W3-Ru2-C9	98.0(3)
W3-Ru2-C10	45.72(20)
W3-Ru2-C11	48.83(21)
Ru1-Ru2-C8	118.3(3)
Ru1-Ru2-C9	151.2(3)
Ru1-Ru2-C10	49.79(20)
Ru1-Ru2-C11	91.99(21)
C8-Ru2-C9	86.9(4)
C8-Ru2-C10	151.8(3)
C8-Ru2-C11	112.5(3)
C9-Ru2-C10	101.4(4)
C9-Ru2-C11	90.5(3)
C10-Ru2-C11	94.5(3)
W1-C1-O1	173.5(7)
W1-C2-O2	165.4(8)
W2-C3-Ru1	80.6(3)
W2-C3-O3	145.2(7)
Ru1-C3-O3	134.1(6)
W2-C4-O4	173.5(8)
W3-C5-O5	167.3(7)
Ru1-C6-O6	173.6(7)
Ru1-C7-O7	179.0(8)
Ru2-C8-O8	171.4(9)
Ru2-C9-O9	178.6(8)
W1-C10-W3	172.0(4)
W1-C10-Ru1	87.9(3)
W1-C10-Ru2	88.3(3)
W3-C10-Ru1	89.0(3)
W3-C10-Ru2	84.0(3)
Ru1-C10-Ru2	79.9(3)
W2-C11-W3	92.4(3)
W2-C11-Ru2	85.1(3)
W2-C11-C12	123.7(6)
W3-C11-Ru2	81.9(3)
W3-C11-C12	132.8(6)
Ru2-C11-C12	125.9(6)
C11-C12-C13	123.6(7)
C11-C12-C17	121.0(7)
C13-C12-C17	115.4(7)

Ru2-W2-C28	152.82(22)
Ru2-W2-C29	128.20(25)
Ru2-W2-C30	97.64(22)
Ru2-W2-C31	96.25(21)
Ru2-W2-C32	124.21(21)
C3-W2-C4	84.5(3)
C3-W2-C11	129.0(3)
C3-W2-C28	84.2(3)
C3-W2-C29	119.4(3)
C3-W2-C30	132.8(3)
C3-W2-C31	102.6(3)
C3-W2-C32	75.9(3)
C4-W2-C11	80.5(3)
C4-W2-C28	81.2(3)
C4-W2-C29	81.3(4)
C4-W2-C30	113.2(3)
C4-W2-C31	136.0(3)
C4-W2-C32	113.0(3)
C11-W2-C28	139.7(3)
C11-W2-C29	106.0(3)
C11-W2-C30	97.7(3)
C11-W2-C31	121.7(3)
C11-W2-C32	154.1(3)
C28-W2-C29	35.5(3)
C28-W2-C30	58.1(3)
C28-W2-C31	57.0(3)
C28-W2-C32	34.2(3)
C29-W2-C30	34.5(3)
C29-W2-C31	57.2(3)
C29-W2-C32	57.3(3)
C30-W2-C31	34.5(3)
C30-W2-C32	57.0(3)
C31-W2-C32	33.6(3)
W2-W3-Ru1	54.868(21)
W2-W3-Ru2	58.882(21)
W2-W3-C5	76.5(3)
W2-W3-C10	92.33(21)
W2-W3-C11	44.09(22)
W2-W3-C38	132.97(22)
W2-W3-C39	161.36(22)
W2-W3-C40	163.23(22)
W2-W3-C41	134.62(21)
W2-W3-C42	122.95(21)
Ru1-W3-Ru2	57.900(22)
Ru1-W3-C5	66.73(24)
Ru1-W3-C10	47.37(22)
Ru1-W3-C11	88.29(21)
Ru1-W3-C38	159.80(23)
Ru1-W3-C39	130.65(21)
Ru1-W3-C40	120.76(20)
Ru1-W3-C41	136.09(22)
Ru1-W3-C42	166.04(22)
Ru2-W3-C5	121.97(24)
Ru2-W3-C10	50.29(21)
Ru2-W3-C11	49.32(20)
Ru2-W3-C38	107.60(22)
Ru2-W3-C39	106.93(21)
Ru2-W3-C40	135.27(21)
Ru2-W3-C41	162.90(21)
Ru2-W3-C42	134.85(22)

C12-C13-C14	122.1(9)
C13-C14-C15	119.8(9)
C14-C15-C16	119.6(8)
C15-C16-C17	121.3(9)
C12-C17-C16	121.7(9)
W1-C18-C19	70.7(4)
W1-C18-C22	75.0(5)
W1-C18-C23	127.2(6)
C19-C18-C22	108.0(8)
C19-C18-C23	127.7(9)
C22-C18-C23	123.7(8)
W1-C19-C18	73.4(5)
W1-C19-C20	74.7(5)
W1-C19-C24	127.9(6)
C18-C19-C20	108.7(8)
C18-C19-C24	125.4(8)
C20-C19-C24	124.8(8)
W1-C20-C19	70.0(4)
W1-C20-C21	74.2(5)
W1-C20-C25	129.1(6)
C19-C20-C21	106.5(7)
C19-C20-C25	127.3(8)
C21-C20-C25	125.4(8)
W1-C21-C20	71.1(4)
W1-C21-C22	72.3(5)
W1-C21-C26	132.8(6)
C20-C21-C22	109.0(8)
C20-C21-C26	125.4(8)
C22-C21-C26	124.3(8)
W1-C22-C18	70.8(5)
W1-C22-C21	73.2(4)
W1-C22-C27	128.4(6)
C18-C22-C21	107.8(8)
C18-C22-C27	127.3(9)
C21-C22-C27	124.3(9)
W2-C28-C29	73.0(5)
W2-C28-C32	75.8(5)
W2-C28-C33	126.3(6)
C29-C28-C32	107.9(8)
C29-C28-C33	124.5(8)
C32-C28-C33	126.5(8)
W2-C29-C28	71.5(5)
W2-C29-C30	74.1(5)
W2-C29-C34	125.8(7)
C28-C29-C30	107.8(8)
C28-C29-C34	126.1(9)
C30-C29-C34	125.7(9)
W2-C30-C29	71.3(5)
W2-C30-C31	74.0(5)
W2-C30-C35	131.8(6)
C29-C30-C31	107.4(8)
C29-C30-C35	125.8(8)
C31-C30-C35	125.1(9)
W2-C31-C30	71.5(5)
W2-C31-C32	72.7(5)
W2-C31-C36	131.1(6)
C30-C31-C32	108.2(8)
C30-C31-C36	127.7(8)
C32-C31-C36	123.0(8)
W2-C32-C28	69.9(5)

C5-W3-C10	102.0(3)
C5-W3-C11	117.0(3)
C5-W3-C38	130.3(3)
C5-W3-C39	122.0(3)
C5-W3-C40	86.9(3)
C5-W3-C41	74.8(3)
C5-W3-C42	99.3(3)
C10-W3-C11	99.6(3)
C10-W3-C38	113.0(3)
C10-W3-C39	85.6(3)
C10-W3-C40	93.8(3)
C10-W3-C41	127.6(3)
C10-W3-C42	142.2(3)
C11-W3-C38	91.3(3)
C11-W3-C39	118.0(3)
C11-W3-C40	148.9(3)
C11-W3-C41	129.1(3)
C11-W3-C42	97.9(3)
C38-W3-C39	34.9(3)
C38-W3-C40	57.6(3)
C38-W3-C41	56.0(3)
C38-W3-C42	33.3(3)
C39-W3-C40	35.1(3)
C39-W3-C41	57.2(3)
C39-W3-C42	56.7(3)
C40-W3-C41	34.5(3)
C40-W3-C42	56.6(3)
C41-W3-C42	33.2(3)
W1-Ru1-W2	125.36(3)
W1-Ru1-W3	88.19(3)
W1-Ru1-Ru2	62.19(3)
W1-Ru1-C3	174.24(22)
W1-Ru1-C6	99.10(25)
W1-Ru1-C7	83.4(3)
W1-Ru1-C10	44.79(20)
W2-Ru1-W3	65.696(24)
W2-Ru1-Ru2	63.23(3)
W2-Ru1-C3	48.89(22)
W2-Ru1-C6	132.28(25)
W2-Ru1-C7	104.2(3)
W2-Ru1-C10	98.74(21)
W3-Ru1-Ru2	58.85(3)
W3-Ru1-C3	89.05(23)

W2-C32-C31	73.7(5)
W2-C32-C37	130.3(6)
C28-C32-C31	108.7(8)
C28-C32-C37	125.8(8)
C31-C32-C37	124.7(8)
W3-C38-C39	69.0(5)
W3-C38-C42	74.5(5)
W3-C38-C43	132.0(7)
C39-C38-C42	107.0(8)
C39-C38-C43	126.2(9)
C42-C38-C43	125.4(9)
W3-C39-C38	76.1(5)
W3-C39-C40	72.3(5)
W3-C39-C44	126.5(6)
C38-C39-C40	107.8(8)
C38-C39-C44	124.4(9)
C40-C39-C44	126.8(9)
W3-C40-C39	72.6(5)
W3-C40-C41	76.5(5)
W3-C40-C45	124.5(6)
C39-C40-C41	107.9(7)
C39-C40-C45	125.5(9)
C41-C40-C45	125.8(9)
W3-C41-C40	69.0(4)
W3-C41-C42	74.6(5)
W3-C41-C46	128.9(6)
C40-C41-C42	107.9(8)
C40-C41-C46	127.6(9)
C42-C41-C46	123.9(9)
W3-C42-C38	72.2(5)
W3-C42-C41	72.2(5)
W3-C42-C47	134.5(7)
C38-C42-C41	109.3(8)
C38-C42-C47	126.9(9)
C41-C42-C47	121.9(9)
Cl1-C48-Cl1	111.4(3)
Cl1-C48-Cl2	96.8(5)
Cl1-C48-Cl2	103.7(5)
C48-Cl1-C48	68.6(3)
C48-Cl1-Cl2	44.6(4)
C48-Cl1-Cl2	86.5(4)
C48-Cl2-Cl1	38.6(3)

Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
W1	0.62431(3)	0.726339(20)	0.067886(15)	2.015(13)
W2	0.35276(3)	0.739848(20)	0.209464(15)	2.059(14)
W3	0.53932(3)	0.854545(19)	0.205124(15)	1.877(13)
Ru1	0.41961(5)	0.77306 (4)	0.10031 (3)	1.95 (3)
Ru2	0.56346(6)	0.69464 (4)	0.18692 (3)	2.02 (3)
C1	0.7646 (8)	0.6964 (6)	0.1183 (4)	3.5 (4)
C2	0.5879 (8)	0.6142 (6)	0.0779 (4)	3.7 (5)
C3	0.2724 (7)	0.8013 (5)	0.1328 (4)	2.6 (4)
C4	0.3274 (7)	0.8364 (6)	0.2552 (4)	3.4 (4)
C5	0.4105 (7)	0.9134 (5)	0.1643 (4)	3.0 (4)
C6	0.3819 (7)	0.8542 (5)	0.0416 (4)	2.4 (4)
C7	0.3656 (7)	0.6893 (5)	0.0488 (4)	2.9 (4)
C8	0.5476 (8)	0.5835 (5)	0.1943 (4)	3.2 (4)
C9	0.7039 (7)	0.6825 (6)	0.2346 (4)	3.4 (4)
C10	0.5850 (6)	0.7980 (4)	0.1347 (3)	1.8 (3)
C11	0.5116 (6)	0.7575 (5)	0.2597 (3)	2.2 (3)
C12	0.5434 (7)	0.7401 (5)	0.3266 (4)	2.6 (4)
C13	0.6046 (8)	0.6744 (6)	0.3496 (4)	3.6 (5)
C14	0.6376 (9)	0.6619 (7)	0.4128 (4)	4.9 (6)
C15	0.6094 (8)	0.7152 (7)	0.4542 (4)	4.6 (6)
C16	0.5474 (8)	0.7779 (6)	0.4336 (4)	4.3 (5)
C17	0.5127 (8)	0.7904 (6)	0.3710 (4)	3.5 (5)
C18	0.7232 (7)	0.6896 (5)	-0.0086 (4)	3.1 (4)
C19	0.7432 (7)	0.7713 (5)	0.0064 (4)	2.9 (4)
C20	0.6461 (7)	0.8142 (5)	-0.0125 (4)	2.8 (4)
C21	0.5667 (7)	0.7583 (5)	-0.0390 (4)	3.0 (4)
C22	0.6147 (8)	0.6818 (5)	-0.0360 (4)	3.1 (4)
C23	0.8051 (9)	0.6240 (6)	-0.0057 (5)	4.5 (5)
C24	0.8534 (8)	0.8078 (6)	0.0264 (5)	4.7 (6)
C25	0.6330 (8)	0.9011 (5)	-0.0153 (4)	3.4 (4)
C26	0.4574 (8)	0.7783 (6)	-0.0766 (4)	3.6 (5)
C27	0.5602 (10)	0.6102 (6)	-0.0655 (5)	5.0 (6)
C28	0.1777 (7)	0.7119 (5)	0.2270 (4)	3.2 (5)
C29	0.2514 (8)	0.6837 (6)	0.2793 (4)	3.7 (5)
C30	0.3115 (7)	0.6212 (5)	0.2596 (4)	3.3 (4)
C31	0.2722 (7)	0.6095 (5)	0.1954 (4)	2.7 (4)
C32	0.1896 (7)	0.6644 (5)	0.1767 (4)	3.0 (4)
C33	0.0881 (8)	0.7715 (7)	0.2299 (5)	4.7 (6)
C34	0.2548 (9)	0.7095 (7)	0.3458 (4)	5.2 (6)
C35	0.3811 (9)	0.5653 (6)	0.3001 (5)	5.1 (6)
C36	0.2951 (9)	0.5414 (5)	0.1560 (5)	4.5 (5)
C37	0.1146 (8)	0.6627 (6)	0.1159 (4)	3.7 (4)
C38	0.6914 (8)	0.8975 (5)	0.2816 (4)	3.3 (4)
C39	0.7129 (7)	0.9097 (5)	0.2206 (4)	3.0 (4)
C40	0.6399 (7)	0.9672 (5)	0.1922 (4)	2.6 (4)
C41	0.5744 (7)	0.9913 (5)	0.2352 (4)	3.1 (4)
C42	0.6052 (8)	0.9474 (5)	0.2889 (4)	3.3 (4)
C43	0.7618 (9)	0.8549 (7)	0.3318 (5)	6.0 (6)
C44	0.8093 (8)	0.8781 (7)	0.1974 (5)	5.4 (6)
C45	0.6437 (10)	1.0048 (6)	0.1326 (5)	5.4 (6)
C46	0.4981 (8)	1.0582 (5)	0.2299 (6)	5.1 (6)
C47	0.5689 (11)	0.9695 (6)	0.3490 (5)	6.0 (7)
O1	0.8490 (5)	0.6791 (4)	0.1421 (3)	4.9 (4)

O2	0.5753 (7)	0.5479 (4)	0.0723 (3)	6.2 (5)
O3	0.1914 (5)	0.8327 (4)	0.1110 (3)	3.5 (3)
O4	0.3034 (6)	0.8895 (4)	0.2823 (3)	5.1 (4)
O5	0.3459 (5)	0.9600 (3)	0.1449 (3)	4.0 (3)
O6	0.3543 (6)	0.9067 (4)	0.0101 (3)	4.4 (4)
O7	0.3311 (6)	0.6381 (4)	0.0176 (3)	5.3 (4)
O8	0.5518 (6)	0.5171 (4)	0.2007 (3)	5.2 (4)
O9	0.7873 (5)	0.6746 (5)	0.2642 (3)	5.4 (4)
C48	-0.00802	0.03259	0.03515	15.8
Cl1	1.1053 (7)	0.9910 (4)	0.0348 (3)	20.3 (6)
Cl2	0.9498 (11)	0.9716 (7)	0.0926 (5)	15.6 (9)
H13	0.628	0.637	0.321	4.5
H14	0.676	0.613	0.427	5.5
H15	0.634	0.707	0.497	5.1
H16	0.530	0.815	0.463	5.0
H17	0.467	0.834	0.358	4.2
H23a	0.771	0.576	-0.018	5.1
H23b	0.856	0.636	-0.033	5.1
H23c	0.845	0.619	0.035	5.1
H24a	0.909	0.768	0.038	5.1
H24b	0.876	0.840	-0.005	5.1
H24c	0.855	0.841	0.062	5.1
H25a	0.698	0.927	0.006	4.3
H25b	0.621	0.921	-0.056	4.3
H25c	0.575	0.919	0.004	4.3
H26a	0.441	0.833	-0.072	4.2
H26b	0.458	0.768	-0.120	4.2
H26c	0.402	0.747	-0.064	4.2
H27a	0.486	0.620	-0.081	5.6
H27b	0.595	0.593	-0.099	5.6
H27c	0.566	0.568	-0.036	5.6
H33a	0.049	0.783	0.190	5.1
H33b	0.039	0.752	0.255	5.1
H33c	0.119	0.820	0.248	5.1
H34a	0.205	0.753	0.346	5.3
H34b	0.231	0.668	0.369	5.3
H34c	0.325	0.726	0.364	5.3
H35a	0.397	0.586	0.343	5.4
H35b	0.348	0.515	0.303	5.4
H35c	0.450	0.558	0.288	5.4
H36a	0.357	0.512	0.177	5.1
H36b	0.235	0.508	0.148	5.1
H36c	0.313	0.560	0.118	5.1
H37a	0.140	0.624	0.089	4.5
H37b	0.043	0.648	0.120	4.5
H37c	0.113	0.713	0.096	4.5
H43a	0.729	0.853	0.369	6.3
H43b	0.770	0.799	0.321	6.3
H43c	0.831	0.876	0.342	6.3
H44a	0.846	0.840	0.224	5.9
H44b	0.787	0.854	0.157	5.9
H44c	0.859	0.920	0.192	5.9
H45a	0.695	0.978	0.110	5.7
H45b	0.574	1.003	0.105	5.7
H45c	0.665	1.059	0.136	5.7
H46a	0.488	1.080	0.189	5.5
H46b	0.429	1.042	0.239	5.5

H46c	0.526	1.100	0.258	5.5
H47a	0.508	1.005	0.341	6.0
H47b	0.546	0.924	0.368	6.0
H47c	0.625	0.995	0.377	6.0

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
W1	2.620(19)	2.841(18)	2.323(17)	0.153(16)	0.789(14)	-0.099(15)
W2	2.187(18)	3.513(19)	2.189(17)	-0.035(16)	0.556(14)	0.022(15)
W3	2.246(18)	2.640(17)	2.193(16)	0.144(15)	0.234(14)	-0.237(15)
Ru1	2.28 (4)	3.09 (4)	2.00 (3)	0.08 (3)	0.22 (3)	0.11 (3)
Ru2	2.56 (4)	2.80 (4)	2.33 (4)	0.42 (3)	0.48 (3)	0.29 (3)
C1	4.3 (6)	5.9 (7)	3.3 (5)	2.2 (5)	1.6 (5)	0.5 (5)
C2	5.4 (7)	5.0 (6)	4.1 (6)	-0.5 (5)	1.5 (5)	-0.2 (5)
C3	3.0 (5)	3.7 (5)	3.2 (5)	0.1 (4)	1.0 (4)	0.2 (4)
C4	3.2 (6)	6.1 (7)	3.6 (5)	0.6 (5)	0.6 (4)	-1.1 (5)
C5	3.9 (6)	3.0 (5)	4.5 (6)	0.4 (4)	0.4 (5)	-1.1 (4)
C6	2.9 (5)	3.1 (5)	3.0 (5)	-0.2 (4)	0.1 (4)	0.1 (4)
C7	4.0 (6)	4.5 (5)	2.6 (5)	0.7 (5)	0.9 (4)	-0.4 (4)
C8	4.9 (6)	3.2 (5)	4.5 (6)	-0.1 (5)	1.9 (5)	0.6 (4)
C9	3.6 (6)	6.2 (6)	3.5 (5)	1.5 (5)	1.3 (4)	0.7 (5)
C10	1.8 (4)	1.8 (4)	3.4 (5)	-0.2 (3)	0.5 (4)	0.0 (3)
C11	2.6 (5)	3.2 (5)	2.5 (4)	0.2 (4)	0.6 (4)	-0.7 (4)
C12	2.5 (5)	4.8 (6)	2.4 (4)	-0.3 (4)	0.1 (4)	0.2 (4)
C13	4.3 (6)	5.9 (6)	3.3 (5)	0.3 (5)	0.4 (5)	0.5 (5)
C14	5.6 (7)	9.3 (9)	3.2 (6)	0.7 (7)	-0.4 (5)	2.9 (6)
C15	4.5 (7)	10.6 (9)	2.0 (5)	-0.1 (6)	-0.4 (4)	0.6 (6)
C16	5.5 (7)	8.6 (8)	2.2 (5)	-0.1 (6)	1.0 (5)	-0.6 (5)
C17	5.2 (7)	5.9 (6)	2.5 (5)	-0.5 (5)	1.3 (5)	-0.1 (4)
C18	4.4 (6)	4.2 (5)	3.7 (5)	0.5 (5)	2.1 (5)	-0.4 (4)
C19	2.8 (5)	6.3 (6)	2.2 (4)	-0.3 (5)	1.0 (4)	0.3 (4)
C20	5.1 (6)	3.7 (5)	2.0 (4)	-0.1 (5)	1.3 (4)	0.3 (4)
C21	3.7 (6)	5.4 (6)	2.4 (5)	-0.4 (5)	0.9 (4)	0.0 (4)
C22	5.0 (6)	4.5 (5)	2.6 (5)	-0.3 (5)	1.8 (4)	-1.0 (4)
C23	6.2 (8)	6.4 (7)	5.3 (7)	2.0 (6)	2.5 (6)	-0.6 (6)
C24	4.5 (7)	7.9 (8)	5.5 (7)	-1.1 (6)	1.5 (5)	0.4 (6)
C25	5.4 (7)	4.5 (6)	3.3 (5)	-0.7 (5)	0.9 (5)	0.1 (4)
C26	5.9 (7)	5.8 (6)	1.8 (5)	-0.2 (5)	-0.2 (4)	-0.1 (4)
C27	8.9 (9)	5.1 (7)	4.9 (7)	-0.3 (6)	1.1 (6)	-2.3 (5)
C28	2.5 (5)	5.5 (6)	4.4 (6)	-0.6 (5)	1.0 (4)	0.1 (5)
C29	3.8 (6)	7.2 (7)	3.6 (5)	-1.5 (5)	1.8 (5)	0.1 (5)
C30	3.1 (6)	5.7 (6)	4.0 (5)	-1.6 (5)	0.9 (4)	1.4 (5)
C31	3.6 (6)	3.6 (5)	3.3 (5)	-0.7 (4)	0.8 (4)	0.2 (4)
C32	3.0 (5)	5.1 (6)	3.5 (5)	-1.3 (5)	1.6 (4)	0.2 (4)
C33	3.3 (6)	9.1 (9)	5.7 (7)	-0.9 (6)	1.9 (5)	-0.3 (6)
C34	5.9 (8)	11.0 (10)	3.5 (6)	-1.7 (7)	2.6 (5)	-1.0 (6)
C35	6.3 (8)	8.1 (8)	4.7 (7)	-0.1 (7)	0.6 (6)	3.2 (6)
C36	7.0 (8)	3.6 (6)	6.8 (7)	-0.5 (6)	2.2 (6)	0.2 (5)
C37	3.4 (6)	5.8 (7)	4.6 (6)	-1.8 (5)	-0.2 (5)	-0.1 (5)
C38	4.4 (6)	4.1 (5)	3.4 (5)	-1.1 (5)	-1.6 (4)	-0.2 (4)
C39	2.7 (5)	3.7 (5)	5.0 (6)	-0.5 (4)	0.3 (4)	-1.6 (4)
C40	3.8 (6)	3.4 (5)	2.7 (5)	-1.1 (4)	0.4 (4)	-0.8 (4)
C41	3.3 (6)	2.6 (5)	5.8 (6)	-0.5 (4)	1.0 (5)	-1.0 (4)
C42	4.6 (6)	3.8 (5)	4.4 (6)	-1.0 (5)	1.1 (5)	-1.7 (5)
C43	7.0 (9)	8.0 (8)	5.9 (7)	-0.3 (7)	-3.9 (6)	0.3 (7)
C44	3.2 (6)	8.1 (8)	9.7 (9)	-1.4 (6)	2.0 (6)	-3.8 (7)
C45	8.7 (10)	6.5 (8)	5.3 (7)	-3.5 (7)	0.7 (6)	0.4 (6)
C46	4.3 (7)	3.1 (6)	11.9 (10)	0.3 (5)	0.6 (7)	-2.4 (6)
C47	12.8 (12)	6.5 (8)	4.3 (7)	-3.3 (8)	3.6 (7)	-2.7 (6)

01	3.7	(4)	9.6	(6)	5.4	(4)	2.4	(4)	0.4	(3)	1.1	(4)
02	14.3	(8)	3.5	(4)	6.7	(5)	-1.7	(5)	4.2	(5)	-0.8	(4)
03	3.0	(4)	5.8	(4)	4.5	(4)	1.0	(3)	0.4	(3)	0.1	(3)
04	5.7	(5)	7.0	(5)	7.0	(5)	1.4	(4)	2.2	(4)	-2.8	(4)
05	4.8	(4)	3.4	(4)	6.4	(5)	1.4	(3)	-1.0	(4)	-0.5	(3)
06	7.8	(6)	4.2	(4)	4.5	(4)	0.8	(4)	0.2	(4)	1.3	(3)
07	7.1	(6)	6.5	(5)	6.5	(5)	-1.8	(4)	0.9	(4)	-2.7	(4)
08	9.2	(6)	3.2	(4)	7.6	(5)	0.5	(4)	2.3	(5)	1.9	(4)
09	3.8	(5)	11.3	(6)	5.0	(4)	1.7	(4)	-0.4	(3)	1.7	(4)
C48	20.0											
Cl1	37.4	(12)	24.1	(7)	14.3	(5)	10.8	(8)	0.6	(6)	1.5	(5)
Cl2	24.2	(15)	20.8	(12)	16.1	(10)	-11.9	(11)	8.1	(10)	-4.7	(9)
H13	5.7											
H14	7.0											
H15	6.4											
H16	6.4											
H17	5.4											
H23a	6.5											
H23b	6.5											
H23c	6.5											
H24a	6.4											
H24b	6.4											
H24c	6.4											
H25a	5.5											
H25b	5.5											
H25c	5.5											
H26a	5.3											
H26b	5.3											
H26c	5.3											
H27a	7.1											
H27b	7.1											
H27c	7.1											
H33a	6.4											
H33b	6.4											
H33c	6.4											
H34a	6.7											
H34b	6.7											
H34c	6.7											
H35a	6.9											
H35b	6.9											
H35c	6.9											
H36a	6.5											
H36b	6.5											
H36c	6.5											
H37a	5.7											
H37b	5.7											
H37c	5.7											
H43a	8.0											
H43b	8.0											
H43c	8.0											
H44a	7.4											
H44b	7.4											
H44c	7.4											
H45a	7.2											
H45b	7.2											
H45c	7.2											
H46a	7.0											

H46b	7.0
H46c	7.0
H47a	7.6
H47b	7.6
H47c	7.6

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)

Table : Bond Distances and Bond Angles of IC3313 complex (6)

W1a-Ru1a	2.8534(20)
W1a-Ru2a	2.9211(19)
W1a-C1a	2.487(20)
W1a-C2a	1.974(22)
W1a-C3a	2.108(24)
W1a-C16a	2.50(3)
W1a-C17a	2.279(21)
W1a-C18a	2.278(21)
W1a-C19a	2.38(3)
W1a-C20a	2.465(23)
W1a-O1a	2.103(14)
W2a-W3a	3.0075(14)
W2a-Ru1a	2.8825(18)
W2a-Ru2a	2.8242(19)
W2a-C1a	1.997(20)
W2a-C4a	1.995(23)
W2a-C10a	1.966(20)
W2a-C26a	2.377(19)
W2a-C27a	2.383(24)
W2a-C28a	2.402(22)
W2a-C29a	2.397(21)
W2a-C30a	2.378(21)
W3a-Ru1a	2.8296(19)
W3a-Ru2a	2.8113(20)
W3a-C5a	1.945(24)
W3a-C10a	2.125(18)
W3a-C11a	2.215(20)
W3a-C36a	2.502(22)
W3a-C37a	2.479(23)
W3a-C38a	2.328(22)
W3a-C39a	2.372(21)
W3a-C40a	2.404(24)
Ru1a-Ru2a	2.7821(23)
Ru1a-C1a	2.179(19)
Ru1a-C4a	2.329(22)
Ru1a-C6a	1.793(21)
Ru1a-C7a	1.920(23)
Ru2a-C1a	2.293(18)
Ru2a-C8a	1.898(22)
Ru2a-C9a	1.899(23)
Ru2a-C10a	2.263(18)
Ru2a-C11a	2.312(20)
C1a-O1a	1.277(23)
C2a-O2a	1.16(3)
C3a-O3a	1.08(3)
C4a-O4a	1.24(3)
C5a-O5a	1.22(3)
C6a-O6a	1.207(25)
C7a-O7a	1.18(3)
C8a-O8a	1.12(3)
C9a-O9a	1.18(3)
C10a-C11a	1.35(3)
C11a-C12a	1.56(3)
C12a-C13a	1.48(3)
C12a-C14a	1.56(4)
C12a-C15a	1.54(3)
C16a-C17a	1.50(3)

W1b-C1b	2.495(19)
W1b-C2b	1.908(21)
W1b-C3b	1.84(3)
W1b-C16b	2.370(20)
W1b-C17b	2.265(24)
W1b-C18b	2.283(21)
W1b-C19b	2.328(21)
W1b-C20b	2.356(20)
W1b-O1b	2.141(13)
W2b-W3b	2.9993(14)
W2b-Ru1b	2.8752(18)
W2b-Ru2b	2.8230(19)
W2b-C1b	1.997(19)
W2b-C4b	2.006(19)
W2b-C10b	2.016(20)
W2b-C26b	2.350(20)
W2b-C27b	2.383(18)
W2b-C28b	2.326(19)
W2b-C29b	2.332(19)
W2b-C30b	2.291(21)
W3b-Ru1b	2.8355(19)
W3b-Ru2b	2.8186(20)
W3b-C5b	1.878(22)
W3b-C10b	2.252(18)
W3b-C11b	2.210(19)
W3b-C36b	2.369(22)
W3b-C37b	2.431(20)
W3b-C38b	2.362(23)
W3b-C39b	2.263(22)
W3b-C40b	2.357(20)
Ru1b-Ru2b	2.7779(23)
Ru1b-C1b	2.240(18)
Ru1b-C4b	2.305(18)
Ru1b-C6b	1.857(18)
Ru1b-C7b	1.875(22)
Ru2b-C1b	2.265(17)
Ru2b-C8b	1.845(20)
Ru2b-C9b	1.901(22)
Ru2b-C10b	2.198(18)
Ru2b-C11b	2.266(20)
C1b-O1b	1.248(22)
C2b-O2b	1.18(3)
C3b-O3b	1.28(4)
C4b-O4b	1.186(24)
C5b-O5b	1.20(3)
C6b-O6b	1.139(24)
C7b-O7b	1.11(3)
C8b-O8b	1.19(3)
C9b-O9b	1.14(3)
C10b-C11b	1.30(3)
C11b-C12b	1.53(3)
C12b-C13b	1.58(3)
C12b-C14b	1.50(3)
C12b-C15b	1.46(4)
C16b-C17b	1.35(3)
C16b-C20b	1.36(3)
C16b-C21b	1.49(4)

C16a-C20a	1.46(4)
C16a-C21a	1.35(4)
C17a-C18a	1.32(3)
C17a-C22a	1.52(4)
C18a-C19a	1.49(3)
C18a-C23a	1.46(3)
C19a-C20a	1.44(4)
C19a-C24a	1.60(4)
C20a-C25a	1.45(4)
C26a-C27a	1.35(3)
C26a-C30a	1.41(3)
C26a-C31a	1.60(4)
C27a-C28a	1.55(4)
C27a-C32a	1.44(4)
C28a-C29a	1.52(3)
C28a-C33a	1.41(3)
C29a-C30a	1.39(3)
C29a-C34a	1.51(3)
C30a-C35a	1.48(3)
C36a-C37a	1.44(3)
C36a-C40a	1.50(3)
C36a-C41a	1.38(3)
C37a-C38a	1.55(3)
C37a-C42a	1.46(4)
C38a-C39a	1.34(3)
C38a-C43a	1.60(4)
C39a-C40a	1.49(3)
C39a-C44a	1.48(3)
C40a-C45a	1.48(4)
W1b-Ru1b	2.8449(20)
W1b-Ru2b	2.9202(19)

C17b-C18b	1.42(4)
C17b-C22b	1.57(4)
C18b-C19b	1.38(3)
C18b-C23b	1.51(3)
C19b-C20b	1.29(3)
C19b-C24b	1.56(4)
C20b-C25b	1.58(3)
C26b-C27b	1.40(3)
C26b-C30b	1.45(3)
C26b-C31b	1.44(3)
C27b-C28b	1.30(3)
C27b-C32b	1.57(3)
C28b-C29b	1.33(3)
C28b-C33b	1.56(3)
C29b-C30b	1.41(3)
C29b-C34b	1.47(3)
C30b-C35b	1.57(3)
C36b-C37b	1.41(3)
C36b-C40b	1.32(3)
C36b-C41b	1.62(3)
C37b-C38b	1.35(3)
C37b-C42b	1.48(3)
C38b-C39b	1.36(3)
C38b-C43b	1.51(4)
C39b-C40b	1.44(3)
C39b-C44b	1.54(4)
C40b-C45b	1.54(4)
C1-Cl1	1.74(3)
C1-Cl2	1.68(4)
C2-Cl3	1.64(4)
C2-Cl4	1.59(4)

Ru1a-W1a-Ru2a	57.59(5)
Ru1a-W1a-C1a	47.6(4)
Ru1a-W1a-C2a	65.6(6)
Ru1a-W1a-C3a	72.9(6)
Ru1a-W1a-C16a	149.6(6)
Ru1a-W1a-C17a	142.4(6)
Ru1a-W1a-C18a	144.3(5)
Ru1a-W1a-C19a	152.0(7)
Ru1a-W1a-C20a	155.6(6)
Ru1a-W1a-O1a	73.3(3)
Ru2a-W1a-C1a	49.4(4)
Ru2a-W1a-C2a	123.1(6)
Ru2a-W1a-C3a	81.7(6)
Ru2a-W1a-C16a	113.9(6)
Ru2a-W1a-C17a	149.9(6)
Ru2a-W1a-C18a	151.0(5)
Ru2a-W1a-C19a	113.8(7)
Ru2a-W1a-C20a	98.1(6)
Ru2a-W1a-O1a	74.8(3)
C1a-W1a-C2a	93.3(7)
C1a-W1a-C3a	115.5(8)
C1a-W1a-C16a	103.3(7)
C1a-W1a-C17a	120.5(7)
C1a-W1a-C18a	154.1(7)
C1a-W1a-C19a	150.4(8)
C1a-W1a-C20a	117.0(7)

Ru1b-W1b-C1b	49.1(4)
Ru1b-W1b-C2b	64.7(6)
Ru1b-W1b-C3b	75.0(10)
Ru1b-W1b-C16b	151.3(5)
Ru1b-W1b-C17b	144.1(6)
Ru1b-W1b-C18b	142.7(5)
Ru1b-W1b-C19b	153.1(6)
Ru1b-W1b-C20b	157.9(5)
Ru1b-W1b-O1b	74.0(3)
Ru2b-W1b-C1b	48.7(4)
Ru2b-W1b-C2b	122.3(6)
Ru2b-W1b-C3b	83.2(9)
Ru2b-W1b-C16b	115.2(5)
Ru2b-W1b-C17b	148.9(6)
Ru2b-W1b-C18b	149.5(6)
Ru2b-W1b-C19b	115.3(5)
Ru2b-W1b-C20b	100.3(5)
Ru2b-W1b-O1b	73.5(3)
C1b-W1b-C2b	94.3(7)
C1b-W1b-C3b	118.5(10)
C1b-W1b-C16b	103.9(7)
C1b-W1b-C17b	120.8(8)
C1b-W1b-C18b	157.0(7)
C1b-W1b-C19b	149.2(7)
C1b-W1b-C20b	117.9(7)
C1b-W1b-O1b	30.0(5)

C1a-W1a-O1a	30.9(5)
C2a-W1a-C3a	80.0(10)
C2a-W1a-C16a	116.0(9)
C2a-W1a-C17a	82.2(9)
C2a-W1a-C18a	81.5(8)
C2a-W1a-C19a	115.0(9)
C2a-W1a-C20a	138.8(8)
C2a-W1a-O1a	92.0(7)
C3a-W1a-C16a	137.3(9)
C3a-W1a-C17a	121.8(8)
C3a-W1a-C18a	88.7(8)
C3a-W1a-C19a	79.6(10)
C3a-W1a-C20a	107.6(9)
C3a-W1a-O1a	145.5(7)
C16a-W1a-C17a	36.3(8)
C16a-W1a-C18a	57.9(8)
C16a-W1a-C19a	57.7(10)
C16a-W1a-C20a	34.1(9)
C16a-W1a-O1a	76.3(7)
C17a-W1a-C18a	33.8(8)
C17a-W1a-C19a	59.3(9)
C17a-W1a-C20a	59.0(8)
C17a-W1a-O1a	89.7(6)
C18a-W1a-C19a	37.2(9)
C18a-W1a-C20a	58.8(8)
C18a-W1a-O1a	123.5(6)
C19a-W1a-C20a	34.5(10)
C19a-W1a-O1a	133.0(8)
C20a-W1a-O1a	100.4(7)
W3a-W2a-Ru1a	57.38(4)
W3a-W2a-Ru2a	57.54(4)
W3a-W2a-C1a	96.1(5)
W3a-W2a-C4a	62.3(6)
W3a-W2a-C10a	44.8(5)
W3a-W2a-C26a	122.8(5)
W3a-W2a-C27a	130.1(6)
W3a-W2a-C28a	158.1(5)
W3a-W2a-C29a	165.0(5)
W3a-W2a-C30a	136.4(5)
Ru1a-W2a-Ru2a	58.34(5)
Ru1a-W2a-C1a	49.0(5)
Ru1a-W2a-C4a	53.3(6)
Ru1a-W2a-C10a	93.5(5)
Ru1a-W2a-C26a	162.0(5)
Ru1a-W2a-C27a	130.7(6)
Ru1a-W2a-C28a	113.3(6)
Ru1a-W2a-C29a	128.3(5)
Ru1a-W2a-C30a	159.2(5)
Ru2a-W2a-C1a	53.5(5)
Ru2a-W2a-C4a	105.1(6)
Ru2a-W2a-C10a	52.7(5)
Ru2a-W2a-C26a	138.9(5)
Ru2a-W2a-C27a	169.6(6)
Ru2a-W2a-C28a	138.0(6)
Ru2a-W2a-C29a	111.6(5)
Ru2a-W2a-C30a	112.2(6)
C1a-W2a-C4a	96.3(8)
C1a-W2a-C10a	106.2(7)
C1a-W2a-C26a	139.9(8)
C1a-W2a-C27a	126.0(8)
C2b-W1b-C3b	80.5(12)
C2b-W1b-C16b	116.0(9)
C2b-W1b-C17b	84.6(9)
C2b-W1b-C18b	82.0(8)
C2b-W1b-C19b	114.8(8)
C2b-W1b-C20b	137.3(8)
C2b-W1b-O1b	93.5(8)
C3b-W1b-C16b	133.5(11)
C3b-W1b-C17b	119.5(12)
C3b-W1b-C18b	83.4(11)
C3b-W1b-C19b	78.4(11)
C3b-W1b-C20b	104.6(11)
C3b-W1b-O1b	147.9(10)
C16b-W1b-C17b	33.8(8)
C16b-W1b-C18b	58.7(7)
C16b-W1b-C19b	55.1(8)
C16b-W1b-C20b	33.5(8)
C16b-W1b-O1b	77.4(6)
C17b-W1b-C18b	36.4(9)
C17b-W1b-C19b	56.2(9)
C17b-W1b-C20b	55.7(8)
C17b-W1b-O1b	90.8(8)
C18b-W1b-C19b	34.8(8)
C18b-W1b-C20b	57.2(7)
C18b-W1b-O1b	127.2(7)
C19b-W1b-C20b	32.0(8)
C19b-W1b-O1b	131.4(7)
C20b-W1b-O1b	101.1(6)
W3b-W2b-Ru1b	57.68(4)
W3b-W2b-Ru2b	57.81(4)
W3b-W2b-C1b	97.2(5)
W3b-W2b-C4b	62.7(5)
W3b-W2b-C10b	48.7(5)
W3b-W2b-C26b	120.6(5)
W3b-W2b-C27b	132.2(5)
W3b-W2b-C28b	157.6(5)
W3b-W2b-C29b	168.9(5)
W3b-W2b-C30b	137.0(6)
Ru1b-W2b-Ru2b	58.35(5)
Ru1b-W2b-C1b	50.9(5)
Ru1b-W2b-C4b	52.8(5)
Ru1b-W2b-C10b	95.1(5)
Ru1b-W2b-C26b	161.1(5)
Ru1b-W2b-C27b	130.2(4)
Ru1b-W2b-C28b	116.5(5)
Ru1b-W2b-C29b	126.6(5)
Ru1b-W2b-C30b	158.7(6)
Ru2b-W2b-C1b	52.7(5)
Ru2b-W2b-C4b	104.9(5)
Ru2b-W2b-C10b	50.8(5)
Ru2b-W2b-C26b	139.1(5)
Ru2b-W2b-C27b	168.4(4)
Ru2b-W2b-C28b	140.9(5)
Ru2b-W2b-C29b	114.2(5)
Ru2b-W2b-C30b	112.5(5)
C1b-W2b-C4b	97.8(7)
C1b-W2b-C10b	102.7(7)
C1b-W2b-C26b	140.5(8)
C1b-W2b-C27b	123.9(7)
C1b-W2b-C28b	92.4(7)

C1a-W2a-C28a	88.9(8)
C1a-W2a-C29a	82.9(7)
C1a-W2a-C30a	110.2(8)
C4a-W2a-C10a	104.7(8)
C4a-W2a-C26a	109.4(8)
C4a-W2a-C27a	85.4(8)
C4a-W2a-C28a	95.9(8)
C4a-W2a-C29a	132.6(8)
C4a-W2a-C30a	142.3(8)
C10a-W2a-C26a	96.6(7)
C10a-W2a-C27a	125.6(8)
C10a-W2a-C28a	152.7(8)
C10a-W2a-C29a	121.1(7)
C10a-W2a-C30a	93.5(7)
C26a-W2a-C27a	33.0(7)
C26a-W2a-C28a	59.1(8)
C26a-W2a-C29a	57.1(8)
C26a-W2a-C30a	34.5(8)
C27a-W2a-C28a	37.8(9)
C27a-W2a-C29a	59.4(8)
C27a-W2a-C30a	57.5(8)
C28a-W2a-C29a	36.8(7)
C28a-W2a-C30a	59.5(7)
C29a-W2a-C30a	33.9(7)
W2a-W3a-Ru1a	59.09(4)
W2a-W3a-Ru2a	57.95(4)
W2a-W3a-C5a	126.7(7)
W2a-W3a-C10a	40.7(5)
W2a-W3a-C11a	75.5(5)
W2a-W3a-C36a	113.9(5)
W2a-W3a-C37a	96.3(5)
W2a-W3a-C38a	112.8(6)
W2a-W3a-C39a	145.6(6)
W2a-W3a-C40a	149.5(6)
Ru1a-W3a-Ru2a	59.10(5)
Ru1a-W3a-C5a	82.1(7)
Ru1a-W3a-C10a	91.7(5)
Ru1a-W3a-C11a	111.1(5)
Ru1a-W3a-C36a	97.0(5)
Ru1a-W3a-C37a	113.2(5)
Ru1a-W3a-C38a	150.6(6)
Ru1a-W3a-C39a	149.4(6)
Ru1a-W3a-C40a	113.2(6)
Ru2a-W3a-C5a	71.5(7)
Ru2a-W3a-C10a	52.3(5)
Ru2a-W3a-C11a	53.2(5)
Ru2a-W3a-C36a	155.9(5)
Ru2a-W3a-C37a	154.0(5)
Ru2a-W3a-C38a	144.5(5)
Ru2a-W3a-C39a	140.9(6)
Ru2a-W3a-C40a	147.7(6)
C5a-W3a-C10a	116.3(9)
C5a-W3a-C11a	88.1(9)
C5a-W3a-C36a	105.0(9)
C5a-W3a-C37a	134.1(9)
C5a-W3a-C38a	118.2(9)
C5a-W3a-C39a	85.4(9)
C5a-W3a-C40a	76.4(9)
C10a-W3a-C11a	36.3(8)
C10a-W3a-C36a	138.6(7)
C1b-W2b-C29b	81.4(7)
C1b-W2b-C30b	107.8(8)
C4b-W2b-C10b	109.9(7)
C4b-W2b-C26b	108.7(7)
C4b-W2b-C27b	86.4(7)
C4b-W2b-C28b	96.1(7)
C4b-W2b-C29b	128.4(7)
C4b-W2b-C30b	142.4(8)
C10b-W2b-C26b	95.3(7)
C10b-W2b-C27b	128.4(7)
C10b-W2b-C28b	147.5(7)
C10b-W2b-C29b	120.7(7)
C10b-W2b-C30b	91.2(7)
C26b-W2b-C27b	34.4(7)
C26b-W2b-C28b	56.9(7)
C26b-W2b-C29b	59.2(7)
C26b-W2b-C30b	36.3(8)
C27b-W2b-C28b	31.9(7)
C27b-W2b-C29b	55.0(6)
C27b-W2b-C30b	56.5(7)
C28b-W2b-C29b	33.1(7)
C28b-W2b-C30b	56.6(7)
C29b-W2b-C30b	35.6(7)
W2b-W3b-Ru1b	58.96(4)
W2b-W3b-Ru2b	57.95(4)
W2b-W3b-C5b	129.9(6)
W2b-W3b-C10b	42.2(5)
W2b-W3b-C11b	75.0(5)
W2b-W3b-C36b	115.0(5)
W2b-W3b-C37b	96.4(5)
W2b-W3b-C38b	109.6(5)
W2b-W3b-C39b	143.4(7)
W2b-W3b-C40b	147.4(5)
Ru1b-W3b-Ru2b	58.85(5)
Ru1b-W3b-C5b	85.0(6)
Ru1b-W3b-C10b	91.1(5)
Ru1b-W3b-C11b	109.6(5)
Ru1b-W3b-C36b	100.1(5)
Ru1b-W3b-C37b	116.1(5)
Ru1b-W3b-C38b	148.6(5)
Ru1b-W3b-C39b	150.2(6)
Ru1b-W3b-C40b	114.2(5)
Ru2b-W3b-C5b	74.3(6)
Ru2b-W3b-C10b	49.9(5)
Ru2b-W3b-C11b	51.9(5)
Ru2b-W3b-C36b	158.8(5)
Ru2b-W3b-C37b	153.5(5)
Ru2b-W3b-C38b	143.9(5)
Ru2b-W3b-C39b	142.6(6)
Ru2b-W3b-C40b	150.3(5)
C5b-W3b-C10b	114.8(8)
C5b-W3b-C11b	87.8(8)
C5b-W3b-C36b	103.8(8)
C5b-W3b-C37b	132.2(8)
C5b-W3b-C38b	118.2(8)
C5b-W3b-C39b	84.6(9)
C5b-W3b-C40b	76.3(8)
C10b-W3b-C11b	33.8(7)
C10b-W3b-C36b	140.7(7)
C10b-W3b-C37b	107.5(7)

C10a-W3a-C37a	106.6(7)
C10a-W3a-C38a	97.0(7)
C10a-W3a-C39a	118.9(8)
C10a-W3a-C40a	154.0(8)
C11a-W3a-C36a	150.6(7)
C11a-W3a-C37a	121.2(8)
C11a-W3a-C38a	91.8(8)
C11a-W3a-C39a	96.2(8)
C11a-W3a-C40a	130.0(8)
C36a-W3a-C37a	33.6(8)
C36a-W3a-C38a	58.7(8)
C36a-W3a-C39a	59.7(7)
C36a-W3a-C40a	35.5(8)
C37a-W3a-C38a	37.3(7)
C37a-W3a-C39a	59.1(8)
C37a-W3a-C40a	57.8(8)
C38a-W3a-C39a	33.2(8)
C38a-W3a-C40a	57.7(8)
C39a-W3a-C40a	36.3(8)
W1a-Ru1a-W2a	99.18(6)
W1a-Ru1a-W3a	120.61(6)
W1a-Ru1a-Ru2a	62.43(5)
W1a-Ru1a-C1a	57.4(5)
W1a-Ru1a-C4a	139.7(5)
W1a-Ru1a-C6a	107.0(7)
W1a-Ru1a-C7a	106.6(7)
W2a-Ru1a-W3a	63.53(4)
W2a-Ru1a-Ru2a	59.78(5)
W2a-Ru1a-C1a	43.8(5)
W2a-Ru1a-C4a	43.4(6)
W2a-Ru1a-C6a	105.2(7)
W2a-Ru1a-C7a	143.5(7)
W3a-Ru1a-Ru2a	60.12(5)
W3a-Ru1a-C1a	97.3(5)
W3a-Ru1a-C4a	63.0(5)
W3a-Ru1a-C6a	132.0(7)
W3a-Ru1a-C7a	81.0(6)
Ru2a-Ru1a-C1a	53.4(5)
Ru2a-Ru1a-C4a	97.7(5)
Ru2a-Ru1a-C6a	157.0(7)
Ru2a-Ru1a-C7a	110.7(6)
C1a-Ru1a-C4a	82.5(8)
C1a-Ru1a-C6a	103.6(9)
C1a-Ru1a-C7a	160.4(8)
C4a-Ru1a-C6a	77.4(8)
C4a-Ru1a-C7a	113.4(9)
C6a-Ru1a-C7a	91.6(9)
W1a-Ru2a-W2a	98.95(6)
W1a-Ru2a-W3a	118.89(6)
W1a-Ru2a-Ru1a	59.98(5)
W1a-Ru2a-C1a	55.4(5)
W1a-Ru2a-C8a	87.1(6)
W1a-Ru2a-C9a	82.2(6)
W1a-Ru2a-C10a	142.2(5)
W1a-Ru2a-C11a	168.8(5)
W2a-Ru2a-W3a	64.51(5)
W2a-Ru2a-Ru1a	61.88(5)
W2a-Ru2a-C1a	44.4(5)
W2a-Ru2a-C8a	95.4(7)
W2a-Ru2a-C9a	173.0(7)
C10b-W3b-C38b	96.9(7)
C10b-W3b-C39b	118.5(8)
C10b-W3b-C40b	153.7(7)
C11b-W3b-C36b	149.1(7)
C11b-W3b-C37b	119.5(7)
C11b-W3b-C38b	93.1(7)
C11b-W3b-C39b	97.8(8)
C11b-W3b-C40b	131.5(7)
C36b-W3b-C37b	34.2(7)
C36b-W3b-C38b	56.0(7)
C36b-W3b-C39b	56.0(8)
C36b-W3b-C40b	32.3(7)
C37b-W3b-C38b	32.7(7)
C37b-W3b-C39b	55.3(8)
C37b-W3b-C40b	56.0(7)
C38b-W3b-C39b	34.1(9)
C38b-W3b-C40b	57.9(7)
C39b-W3b-C40b	36.1(8)
W1b-Ru1b-W2b	99.51(6)
W1b-Ru1b-W3b	120.90(6)
W1b-Ru1b-Ru2b	62.56(5)
W1b-Ru1b-C1b	57.3(5)
W1b-Ru1b-C4b	140.2(5)
W1b-Ru1b-C6b	106.6(6)
W1b-Ru1b-C7b	109.4(7)
W2b-Ru1b-W3b	63.36(4)
W2b-Ru1b-Ru2b	59.89(5)
W2b-Ru1b-C1b	43.8(5)
W2b-Ru1b-C4b	43.9(5)
W2b-Ru1b-C6b	105.2(6)
W2b-Ru1b-C7b	142.7(7)
W3b-Ru1b-Ru2b	60.27(5)
W3b-Ru1b-C1b	96.5(4)
W3b-Ru1b-C4b	63.4(5)
W3b-Ru1b-C6b	132.1(6)
W3b-Ru1b-C7b	81.4(7)
Ru2b-Ru1b-C1b	52.3(4)
Ru2b-Ru1b-C4b	98.4(5)
Ru2b-Ru1b-C6b	156.8(7)
Ru2b-Ru1b-C7b	113.8(7)
C1b-Ru1b-C4b	83.2(7)
C1b-Ru1b-C6b	104.5(8)
C1b-Ru1b-C7b	163.1(8)
C4b-Ru1b-C6b	76.9(7)
C4b-Ru1b-C7b	110.3(8)
C6b-Ru1b-C7b	88.9(9)
W1b-Ru2b-W2b	98.95(6)
W1b-Ru2b-W3b	118.86(6)
W1b-Ru2b-Ru1b	59.84(5)
W1b-Ru2b-C1b	55.8(5)
W1b-Ru2b-C8b	88.0(6)
W1b-Ru2b-C9b	83.5(6)
W1b-Ru2b-C10b	144.2(5)
W1b-Ru2b-C11b	168.8(5)
W2b-Ru2b-W3b	64.23(4)
W2b-Ru2b-Ru1b	61.77(5)
W2b-Ru2b-C1b	44.6(5)
W2b-Ru2b-C8b	93.9(6)
W2b-Ru2b-C9b	172.0(7)
W2b-Ru2b-C10b	45.2(5)

W2a-Ru2a-C10a	43.8(5)
W2a-Ru2a-C11a	78.0(5)
W3a-Ru2a-Ru1a	60.78(5)
W3a-Ru2a-C1a	95.1(5)
W3a-Ru2a-C8a	148.2(6)
W3a-Ru2a-C9a	108.8(7)
W3a-Ru2a-C10a	48.0(4)
W3a-Ru2a-C11a	50.1(5)
Ru1a-Ru2a-C1a	49.7(5)
Ru1a-Ru2a-C8a	133.2(7)
Ru1a-Ru2a-C9a	113.5(7)
Ru1a-Ru2a-C10a	90.1(5)
Ru1a-Ru2a-C11a	109.7(5)
C1a-Ru2a-C8a	84.8(8)
C1a-Ru2a-C9a	137.5(8)
C1a-Ru2a-C10a	88.1(7)
C1a-Ru2a-C11a	122.5(7)
C8a-Ru2a-C9a	91.6(10)
C8a-Ru2a-C10a	100.3(8)
C8a-Ru2a-C11a	103.8(8)
C9a-Ru2a-C10a	133.9(8)
C9a-Ru2a-C11a	99.5(8)
C10a-Ru2a-C11a	34.4(7)
W1a-C1a-W2a	153.7(9)
W1a-C1a-Ru1a	75.1(6)
W1a-C1a-Ru2a	75.2(5)
W1a-C1a-O1a	57.7(10)
W2a-C1a-Ru1a	87.2(7)
W2a-C1a-Ru2a	82.0(7)
W2a-C1a-O1a	148.0(14)
Ru1a-C1a-Ru2a	76.9(6)
Ru1a-C1a-O1a	119.5(13)
Ru2a-C1a-O1a	119.0(13)
W1a-C2a-O2a	164.0(19)
W1a-C3a-O3a	167.0(21)
W2a-C4a-Ru1a	83.2(8)
W2a-C4a-O4a	150.4(17)
Ru1a-C4a-O4a	121.9(15)
W3a-C5a-O5a	169.2(20)
Ru1a-C6a-O6a	179.4(21)
Ru1a-C7a-O7a	172.4(19)
Ru2a-C8a-O8a	172.1(21)
Ru2a-C9a-O9a	173.9(20)
W2a-C10a-W3a	94.6(7)
W2a-C10a-Ru2a	83.5(6)
W2a-C10a-C11a	157.3(15)
W3a-C10a-Ru2a	79.6(6)
W3a-C10a-C11a	75.5(12)
Ru2a-C10a-C11a	74.8(12)
W3a-C11a-Ru2a	76.8(6)
W3a-C11a-C10a	68.2(11)
W3a-C11a-C12a	147.0(15)
Ru2a-C11a-C10a	70.8(11)
Ru2a-C11a-C12a	120.7(14)
C10a-C11a-C12a	141.5(19)
C11a-C12a-C13a	109.9(16)
C11a-C12a-C14a	110.0(18)
C11a-C12a-C15a	109.2(17)
C13a-C12a-C14a	108.8(19)
C13a-C12a-C15a	108.5(19)
W2b-Ru2b-C11b	78.1(5)
W3b-Ru2b-Ru1b	60.88(5)
W3b-Ru2b-C1b	96.4(5)
W3b-Ru2b-C8b	146.6(6)
W3b-Ru2b-C9b	107.9(7)
W3b-Ru2b-C10b	51.6(5)
W3b-Ru2b-C11b	50.1(5)
Ru1b-Ru2b-C1b	51.5(5)
Ru1b-Ru2b-C8b	132.6(6)
Ru1b-Ru2b-C9b	113.9(7)
Ru1b-Ru2b-C10b	93.8(5)
Ru1b-Ru2b-C11b	109.8(5)
C1b-Ru2b-C8b	82.1(7)
C1b-Ru2b-C9b	139.2(8)
C1b-Ru2b-C10b	89.2(7)
C1b-Ru2b-C11b	122.6(7)
C8b-Ru2b-C9b	93.8(9)
C8b-Ru2b-C10b	95.0(8)
C8b-Ru2b-C11b	102.9(8)
C9b-Ru2b-C10b	131.6(8)
C9b-Ru2b-C11b	98.0(8)
C10b-Ru2b-C11b	33.7(7)
W1b-C1b-W2b	152.6(9)
W1b-C1b-Ru1b	73.6(5)
W1b-C1b-Ru2b	75.5(6)
W1b-C1b-O1b	59.1(9)
W2b-C1b-Ru1b	85.3(7)
W2b-C1b-Ru2b	82.7(6)
W2b-C1b-O1b	148.3(15)
Ru1b-C1b-Ru2b	76.1(6)
Ru1b-C1b-O1b	119.3(13)
Ru2b-C1b-O1b	120.6(13)
W1b-C2b-O2b	163.9(18)
W1b-C3b-O3b	176.6(25)
W2b-C4b-Ru1b	83.3(7)
W2b-C4b-O4b	147.2(15)
Ru1b-C4b-O4b	125.7(14)
W3b-C5b-O5b	175.9(18)
Ru1b-C6b-O6b	178.3(20)
Ru1b-C7b-O7b	166.6(21)
Ru2b-C8b-O8b	175.4(17)
Ru2b-C9b-O9b	174.9(20)
W2b-C10b-W3b	89.1(7)
W2b-C10b-Ru2b	84.0(7)
W2b-C10b-C11b	154.2(15)
W3b-C10b-Ru2b	78.6(6)
W3b-C10b-C11b	71.3(12)
Ru2b-C10b-C11b	76.0(12)
W3b-C11b-Ru2b	78.1(6)
W3b-C11b-C10b	74.9(12)
W3b-C11b-C12b	147.7(15)
Ru2b-C11b-C10b	70.3(12)
Ru2b-C11b-C12b	122.0(14)
C10b-C11b-C12b	133.3(18)
C11b-C12b-C13b	110.1(17)
C11b-C12b-C14b	111.4(18)
C11b-C12b-C15b	112.7(19)
C13b-C12b-C14b	108.8(20)
C13b-C12b-C15b	106.2(19)
C14b-C12b-C15b	107.4(20)

C14a-C12a-C15a	110.4(18)
W1a-C16a-C17a	63.7(12)
W1a-C16a-C20a	71.5(14)
W1a-C16a-C21a	124.8(19)
C17a-C16a-C20a	104.4(21)
C17a-C16a-C21a	124.7(25)
C20a-C16a-C21a	130.8(24)
W1a-C17a-C16a	80.0(13)
W1a-C17a-C18a	73.1(13)
W1a-C17a-C22a	127.8(16)
C16a-C17a-C18a	110.3(20)
C16a-C17a-C22a	119.1(21)
C18a-C17a-C22a	128.4(21)
W1a-C18a-C17a	73.2(13)
W1a-C18a-C19a	75.0(13)
W1a-C18a-C23a	128.1(16)
C17a-C18a-C19a	110.0(20)
C17a-C18a-C23a	124.9(21)
C19a-C18a-C23a	124.0(22)
W1a-C19a-C18a	67.8(13)
W1a-C19a-C20a	76.1(14)
W1a-C19a-C24a	120.4(20)
C18a-C19a-C20a	105.9(22)
C18a-C19a-C24a	119.2(24)
C20a-C19a-C24a	134(3)
W1a-C20a-C16a	74.4(14)
W1a-C20a-C19a	69.4(14)
W1a-C20a-C25a	136.0(19)
C16a-C20a-C19a	109.0(21)
C16a-C20a-C25a	123(3)
C19a-C20a-C25a	125(3)
W2a-C26a-C27a	73.7(13)
W2a-C26a-C30a	72.8(12)
W2a-C26a-C31a	125.0(16)
C27a-C26a-C30a	111.9(20)
C27a-C26a-C31a	123.2(22)
C30a-C26a-C31a	124.8(20)
W2a-C27a-C26a	73.3(13)
W2a-C27a-C28a	71.8(12)
W2a-C27a-C32a	128.2(18)
C26a-C27a-C28a	108.5(21)
C26a-C27a-C32a	129(3)
C28a-C27a-C32a	121.8(23)
W2a-C28a-C27a	70.4(12)
W2a-C28a-C29a	71.4(12)
W2a-C28a-C33a	124.0(15)
C27a-C28a-C29a	101.2(18)
C27a-C28a-C33a	125.9(21)
C29a-C28a-C33a	132.8(22)
W2a-C29a-C28a	71.8(11)
W2a-C29a-C30a	72.3(12)
W2a-C29a-C34a	128.5(14)
C28a-C29a-C30a	109.4(19)
C28a-C29a-C34a	118.3(18)
C30a-C29a-C34a	131.7(20)
W2a-C30a-C26a	72.7(12)
W2a-C30a-C29a	73.8(12)
W2a-C30a-C35a	121.7(15)
C26a-C30a-C29a	109.0(19)
C26a-C30a-C35a	124.8(19)
W1b-C16b-C17b	68.8(13)
W1b-C16b-C20b	72.7(12)
W1b-C16b-C21b	126.4(15)
C17b-C16b-C20b	105.5(20)
C17b-C16b-C21b	130.2(23)
C20b-C16b-C21b	124.2(21)
W1b-C17b-C16b	77.4(14)
W1b-C17b-C18b	72.5(13)
W1b-C17b-C22b	125.8(17)
C16b-C17b-C18b	110.9(21)
C16b-C17b-C22b	124.7(23)
C18b-C17b-C22b	123.5(21)
W1b-C18b-C17b	71.1(13)
W1b-C18b-C19b	74.4(13)
W1b-C18b-C23b	124.3(16)
C17b-C18b-C19b	101.2(19)
C17b-C18b-C23b	130.3(22)
C19b-C18b-C23b	128.0(22)
W1b-C19b-C18b	70.8(12)
W1b-C19b-C20b	75.2(13)
W1b-C19b-C24b	127.4(17)
C18b-C19b-C20b	112.5(21)
C18b-C19b-C24b	127.5(22)
C20b-C19b-C24b	119.7(21)
W1b-C20b-C16b	73.8(11)
W1b-C20b-C19b	72.7(13)
W1b-C20b-C25b	132.5(15)
C16b-C20b-C19b	109.8(19)
C16b-C20b-C25b	122.1(21)
C19b-C20b-C25b	126.2(21)
W2b-C26b-C27b	74.1(11)
W2b-C26b-C30b	69.6(11)
W2b-C26b-C31b	127.3(16)
C27b-C26b-C30b	102.1(17)
C27b-C26b-C31b	131.2(20)
C30b-C26b-C31b	125.8(19)
W2b-C27b-C26b	71.5(11)
W2b-C27b-C28b	71.6(11)
W2b-C27b-C32b	127.9(14)
C26b-C27b-C28b	111.4(17)
C26b-C27b-C32b	122.1(18)
C28b-C27b-C32b	126.2(18)
W2b-C28b-C27b	76.4(12)
W2b-C28b-C29b	73.7(12)
W2b-C28b-C33b	121.7(14)
C27b-C28b-C29b	112.3(18)
C27b-C28b-C33b	124.4(20)
C29b-C28b-C33b	123.0(20)
W2b-C29b-C28b	73.2(11)
W2b-C29b-C30b	70.6(12)
W2b-C29b-C34b	129.4(14)
C28b-C29b-C30b	105.9(18)
C28b-C29b-C34b	132.7(20)
C30b-C29b-C34b	120.3(19)
W2b-C30b-C26b	74.1(12)
W2b-C30b-C29b	73.8(11)
W2b-C30b-C35b	126.7(15)
C26b-C30b-C29b	108.0(18)
C26b-C30b-C35b	125.2(19)
C29b-C30b-C35b	125.8(20)

C29a-C30a-C35a	126.1(21)
W3a-C36a-C37a	72.4(12)
W3a-C36a-C40a	68.7(12)
W3a-C36a-C41a	132.0(16)
C37a-C36a-C40a	106.9(19)
C37a-C36a-C41a	127.8(22)
C40a-C36a-C41a	124.5(21)
W3a-C37a-C36a	74.0(13)
W3a-C37a-C38a	66.0(11)
W3a-C37a-C42a	131.9(15)
C36a-C37a-C38a	105.3(19)
C36a-C37a-C42a	129.3(21)
C38a-C37a-C42a	124.5(21)
W3a-C38a-C37a	76.7(12)
W3a-C38a-C39a	75.2(14)
W3a-C38a-C43a	128.9(15)
C37a-C38a-C39a	111.8(20)
C37a-C38a-C43a	116.4(20)
C39a-C38a-C43a	129.7(21)
W3a-C39a-C38a	71.6(13)
W3a-C39a-C40a	73.0(13)
W3a-C39a-C44a	127.2(16)
C38a-C39a-C40a	107.3(20)
C38a-C39a-C44a	130.8(23)
C40a-C39a-C44a	121.3(22)
W3a-C40a-C36a	75.8(12)
W3a-C40a-C39a	70.7(12)
W3a-C40a-C45a	129.0(18)
C36a-C40a-C39a	108.6(20)
C36a-C40a-C45a	121.2(21)
C39a-C40a-C45a	129.2(22)
W1a-O1a-C1a	91.4(11)
Ru1b-W1b-Ru2b	57.60(5)
W3b-C36b-C37b	75.3(12)
W3b-C36b-C40b	73.4(13)
W3b-C36b-C41b	130.0(14)
C37b-C36b-C40b	111.1(20)
C37b-C36b-C41b	121.8(19)
C40b-C36b-C41b	125.5(19)
W3b-C37b-C36b	70.5(12)
W3b-C37b-C38b	70.8(13)
W3b-C37b-C42b	132.5(15)
C36b-C37b-C38b	107.1(19)
C36b-C37b-C42b	129.4(20)
C38b-C37b-C42b	122.5(20)
W3b-C38b-C37b	76.5(13)
W3b-C38b-C39b	69.0(13)
W3b-C38b-C43b	131.2(17)
C37b-C38b-C39b	107.5(20)
C37b-C38b-C43b	122.2(22)
C39b-C38b-C43b	128.8(22)
W3b-C39b-C38b	77.0(14)
W3b-C39b-C40b	75.5(12)
W3b-C39b-C44b	127.9(17)
C38b-C39b-C40b	109.7(21)
C38b-C39b-C44b	126.4(23)
C40b-C39b-C44b	121.6(22)
W3b-C40b-C36b	74.3(12)
W3b-C40b-C39b	68.4(11)
W3b-C40b-C45b	127.4(17)
C36b-C40b-C39b	104.4(20)
C36b-C40b-C45b	130.0(21)
C39b-C40b-C45b	125.0(21)
W1b-O1b-C1b	90.9(11)
Cl1-C1-Cl2	112.2(20)
Cl3-C2-Cl4	119(3)

Table . Atomic Parameters x,y,z and Beq.
E.S.Ds. refer to the last digit printed.

	x	y	z	Beq
W1a	0.97517(6)	0.40760(5)	0.14935 (3)	3.06(4)
W2a	1.01549(5)	0.16480(4)	0.120003(24)	2.08(3)
W3a	1.18248(5)	0.22103(5)	0.11106 (3)	2.78(4)
Ru1a	1.08066(10)	0.28542(9)	0.17018 (5)	2.42(7)
Ru2a	1.05240(10)	0.31180(9)	0.08806 (5)	2.47(7)
C1a	0.9703 (11)	0.2657 (11)	0.1378 (5)	2.7 (8)
C2a	0.9947 (15)	0.3964 (12)	0.2082 (7)	4.5 (12)
C3a	1.0891 (15)	0.4558 (13)	0.1532 (7)	4.8 (13)
C4a	1.0879 (12)	0.1512 (13)	0.1673 (6)	3.7 (10)
C5a	1.2170 (14)	0.3278 (14)	0.1065 (7)	4.9 (12)
C6a	1.0582 (14)	0.2577 (12)	0.2214 (6)	3.6 (10)
C7a	1.1776 (13)	0.3332 (13)	0.1868 (6)	4.0 (11)
C8a	0.9588 (14)	0.3213 (12)	0.0568 (7)	4.0 (11)
C9a	1.0895 (13)	0.4092 (13)	0.0697 (6)	4.0 (11)
C10a	1.0855 (11)	0.1881 (11)	0.0740 (6)	2.4 (8)
C11a	1.1315 (12)	0.2317 (13)	0.0493 (6)	3.2 (10)
C12a	1.1466 (12)	0.2493 (13)	0.0036 (6)	3.2 (10)
C13a	1.0712 (14)	0.2663 (15)	-0.0171 (6)	4.8 (13)
C14a	1.2020 (17)	0.3205 (16)	-0.0007 (8)	6.6 (15)
C15a	1.1841 (15)	0.1779 (14)	-0.0167 (7)	5.3 (13)
C16a	0.8398 (16)	0.4516 (14)	0.1296 (8)	5.9 (14)
C17a	0.8665 (13)	0.4722 (13)	0.1719 (7)	3.9 (11)
C18a	0.9248 (13)	0.5229 (12)	0.1703 (6)	3.5 (10)
C19a	0.9490 (18)	0.5358 (15)	0.1273 (9)	7.1 (16)
C20a	0.8969 (16)	0.4893 (14)	0.1031 (7)	5.8 (14)
C21a	0.7790 (16)	0.4043 (18)	0.1210 (9)	7.4 (18)
C22a	0.8140 (17)	0.4520 (15)	0.2077 (8)	6.7 (16)
C23a	0.9507 (17)	0.5707 (14)	0.2042 (8)	6.3 (15)
C24a	1.0199 (24)	0.5938 (15)	0.1178 (10)	10.3 (24)
C25a	0.8870 (23)	0.4958 (20)	0.0594 (9)	10.6 (24)
C26a	0.9734 (14)	0.0417 (11)	0.0965 (6)	3.8 (11)
C27a	0.9666 (15)	0.0401 (14)	0.1375 (7)	5.3 (13)
C28a	0.9043 (12)	0.1009 (15)	0.1504 (7)	4.5 (12)
C29a	0.8794 (13)	0.1328 (12)	0.1094 (6)	3.6 (10)
C30a	0.9230 (13)	0.0972 (13)	0.0789 (7)	4.0 (11)
C31a	1.0268 (20)	-0.0176 (16)	0.0716 (10)	8.7 (20)
C32a	0.9989 (19)	-0.0143 (17)	0.1660 (10)	8.6 (19)
C33a	0.8780 (13)	0.1146 (13)	0.1902 (6)	3.9 (11)
C34a	0.8093 (13)	0.1860 (12)	0.1078 (7)	4.0 (11)
C35a	0.9161 (13)	0.1121 (13)	0.0349 (6)	4.1 (11)
C36a	1.2774 (12)	0.1598 (14)	0.1595 (7)	4.1 (12)
C37a	1.2467 (12)	0.0998 (14)	0.1337 (7)	4.4 (12)
C38a	1.2687 (13)	0.1243 (13)	0.0900 (7)	4.2 (12)
C39a	1.3121 (12)	0.1891 (14)	0.0896 (7)	4.5 (12)
C40a	1.3181 (14)	0.2168 (15)	0.1324 (7)	5.4 (13)
C41a	1.2819 (14)	0.1603 (15)	0.2014 (7)	5.1 (13)
C42a	1.2146 (14)	0.0244 (15)	0.1447 (8)	5.7 (14)
C43a	1.2567 (17)	0.0608 (16)	0.0554 (8)	6.5 (16)
C44a	1.3578 (14)	0.2257 (18)	0.0566 (8)	6.4 (17)
C45a	1.3676 (15)	0.2796 (17)	0.1494 (8)	6.4 (16)
O1a	0.9092 (7)	0.3048 (8)	0.1475 (4)	2.8 (6)
O2a	0.9925 (11)	0.4028 (9)	0.2433 (4)	5.3 (9)
O3a	1.1401 (11)	0.4924 (10)	0.1566 (6)	8.2 (12)
O4a	1.1122 (9)	0.1124 (8)	0.1963 (4)	4.2 (8)
O5a	1.2497 (11)	0.3894 (10)	0.1008 (5)	7.1 (11)
O6a	1.0438 (11)	0.2392 (9)	0.2560 (4)	6.3 (10)

O7a	1.2336 (11)	0.3621 (11)	0.2015 (5)	7.7 (11)
O8a	0.9007 (10)	0.3194 (11)	0.0406 (5)	6.5 (10)
O9a	1.1116 (14)	0.4673 (11)	0.0547 (6)	10.0 (15)
W1b	0.48756(6)	0.59941(5)	0.14832 (3)	2.85(4)
W2b	0.50980(5)	0.84470(4)	0.119848(24)	2.03(3)
W3b	0.67968(5)	0.80069(5)	0.10909 (3)	2.84(4)
Ru1b	0.58437(10)	0.72792(10)	0.16866 (5)	2.41(7)
Ru2b	0.55550(10)	0.70108(9)	0.08677 (5)	2.41(7)
C1b	0.4698 (11)	0.7403 (11)	0.1354 (5)	2.3 (8)
C2b	0.5082 (15)	0.6123 (12)	0.2049 (6)	4.4 (12)
C3b	0.5885 (20)	0.5604 (17)	0.1505 (9)	8.1 (20)
C4b	0.5821 (11)	0.8610 (11)	0.1674 (6)	2.4 (8)
C5b	0.7258 (12)	0.7028 (13)	0.1028 (6)	3.7 (11)
C6b	0.5604 (13)	0.7538 (11)	0.2220 (6)	2.9 (9)
C7b	0.6831 (13)	0.6925 (13)	0.1863 (6)	4.0 (11)
C8b	0.4636 (12)	0.6893 (11)	0.0573 (5)	2.7 (9)
C9b	0.6007 (13)	0.6081 (13)	0.0668 (6)	3.7 (10)
C10b	0.5736 (11)	0.8224 (10)	0.0695 (6)	2.6 (8)
C11b	0.6259 (12)	0.7851 (12)	0.0485 (6)	2.9 (9)
C12b	0.6384 (12)	0.7730 (13)	0.0029 (6)	3.8 (11)
C13b	0.5582 (15)	0.7484 (15)	-0.0180 (6)	4.9 (13)
C14b	0.6992 (17)	0.7119 (16)	-0.0052 (7)	6.7 (17)
C15b	0.6642 (16)	0.8430 (17)	-0.0178 (7)	6.5 (16)
C16b	0.3635 (12)	0.5451 (12)	0.1314 (6)	3.5 (10)
C17b	0.3852 (15)	0.5256 (15)	0.1695 (7)	5.3 (14)
C18b	0.4535 (14)	0.4781 (12)	0.1691 (6)	3.9 (11)
C19b	0.4676 (14)	0.4722 (13)	0.1279 (6)	4.2 (11)
C20b	0.4182 (14)	0.5122 (12)	0.1066 (6)	4.0 (11)
C21b	0.2926 (17)	0.5879 (16)	0.1167 (9)	7.5 (17)
C22b	0.3340 (16)	0.5402 (16)	0.2086 (8)	6.3 (15)
C23b	0.4936 (18)	0.4350 (15)	0.2031 (8)	7.2 (17)
C24b	0.5278 (22)	0.4179 (15)	0.1061 (9)	9.1 (21)
C25b	0.4064 (17)	0.5073 (15)	0.0592 (7)	6.0 (14)
C26b	0.4636 (13)	0.9655 (12)	0.0976 (6)	3.5 (10)
C27b	0.4481 (11)	0.9626 (11)	0.1394 (5)	2.4 (8)
C28b	0.4010 (11)	0.9062 (12)	0.1483 (6)	2.6 (9)
C29b	0.3749 (11)	0.8698 (11)	0.1155 (6)	2.7 (9)
C30b	0.4139 (14)	0.9043 (13)	0.0821 (6)	3.9 (11)
C31b	0.5055 (15)	1.0213 (13)	0.0735 (7)	5.0 (13)
C32b	0.4800 (15)	1.0257 (13)	0.1697 (8)	5.5 (13)
C33b	0.3719 (17)	0.8871 (17)	0.1920 (8)	6.8 (16)
C34b	0.3091 (13)	0.8159 (13)	0.1087 (8)	5.2 (14)
C35b	0.3948 (14)	0.8898 (15)	0.0361 (7)	4.7 (13)
C36b	0.7695 (12)	0.8674 (13)	0.1516 (7)	3.7 (11)
C37b	0.7345 (12)	0.9256 (12)	0.1276 (6)	3.2 (10)
C38b	0.7529 (13)	0.9099 (14)	0.0885 (7)	4.2 (12)
C39b	0.7985 (13)	0.8454 (15)	0.0883 (7)	5.0 (13)
C40b	0.8117 (12)	0.8200 (13)	0.1292 (7)	3.8 (10)
C41b	0.7727 (13)	0.8736 (14)	0.2007 (7)	4.4 (12)
C42b	0.6975 (16)	0.9995 (15)	0.1402 (8)	5.9 (14)
C43b	0.7392 (18)	0.9673 (18)	0.0547 (9)	7.8 (18)
C44b	0.8495 (15)	0.8159 (19)	0.0526 (9)	7.5 (17)
C45b	0.8720 (15)	0.7579 (20)	0.1420 (9)	7.8 (20)
O1b	0.4127 (7)	0.6988 (7)	0.1452 (4)	2.7 (6)
O2b	0.5115 (14)	0.6036 (9)	0.2405 (5)	7.7 (11)
O3b	0.6569 (10)	0.5299 (10)	0.1532 (6)	7.6 (11)
O4b	0.6022 (8)	0.9022 (8)	0.1942 (4)	3.9 (7)
O5b	0.7594 (9)	0.6428 (10)	0.0980 (5)	6.5 (10)
O6b	0.5476 (11)	0.7691 (9)	0.2550 (5)	6.1 (10)
O7b	0.7342 (10)	0.6586 (12)	0.1978 (5)	7.9 (12)

O8b	0.4025 (10)	0.6859 (9)	0.0399 (4)	5.0 (8)
O9b	0.6222 (10)	0.5508 (10)	0.0542 (5)	6.5 (10)
C1	0.1151 (20)	0.8030 (20)	0.1885 (10)	9.2 (10)
C2	0.6092 (24)	0.2043 (23)	0.1901 (12)	12.4 (13)
Cl1	0.1010 (6)	0.7891 (7)	0.1366 (3)	10.9 (7)
Cl2	0.1713 (9)	0.7337 (12)	0.2093 (4)	22.4 (15)
Cl3	0.6031 (5)	0.2148 (5)	0.1406 (3)	8.9 (6)
Cl4	0.6734 (7)	0.2526 (9)	0.2146 (4)	16.5 (10)
H13aa	1.078	0.280	−0.046	5.0
H13ab	1.035	0.225	−0.016	5.0
H13ac	1.045	0.312	−0.005	5.0
H14aa	1.213	0.333	−0.028	5.8
H14ab	1.181	0.365	0.013	5.8
H14ac	1.253	0.309	0.013	5.8
H15aa	1.195	0.187	−0.045	5.5
H15ab	1.233	0.166	−0.003	5.5
H15ac	1.150	0.134	−0.014	5.5
H21aa	0.752	0.388	0.146	7.5
H21ab	0.741	0.427	0.104	7.5
H21ac	0.797	0.357	0.109	7.5
H22aa	0.836	0.466	0.233	6.4
H22ab	0.763	0.475	0.205	6.4
H22ac	0.805	0.395	0.209	6.4
H23aa	0.995	0.604	0.198	5.5
H23ab	0.908	0.604	0.214	5.5
H23ac	0.967	0.540	0.228	5.5
H24aa	1.034	0.602	0.090	8.0
H24ab	1.017	0.645	0.131	8.0
H24ac	1.072	0.573	0.131	8.0
H25aa	0.859	0.466	0.046	8.7
H25ab	0.881	0.552	0.052	8.7
H25ac	0.947	0.491	0.048	8.7
H31aa	1.029	−0.007	0.044	7.1
H31ab	1.084	−0.012	0.081	7.1
H31ac	1.014	−0.069	0.077	7.1
H32aa	0.983	−0.001	0.195	7.6
H32ab	0.982	−0.066	0.162	7.6
H32ac	1.056	−0.014	0.167	7.6
H33aa	0.839	0.155	0.190	4.2
H33ab	0.858	0.072	0.204	4.2
H33ac	0.922	0.135	0.206	4.2
H34aa	0.800	0.202	0.080	4.8
H34ab	0.761	0.163	0.118	4.8
H34ac	0.818	0.232	0.124	4.8
H35aa	0.951	0.083	0.019	4.2
H35ab	0.863	0.102	0.025	4.2
H35ac	0.926	0.166	0.029	4.2
H41aa	1.250	0.117	0.212	4.7
H41ab	1.334	0.151	0.210	4.7
H41ac	1.262	0.205	0.213	4.7
H42aa	1.199	−0.006	0.121	5.7
H42ab	1.252	−0.008	0.159	5.7
H42ac	1.168	0.027	0.162	5.7
H43aa	1.272	0.080	0.028	6.3
H43ab	1.287	0.014	0.059	6.3
H43ac	1.202	0.044	0.052	6.3
H44aa	1.384	0.275	0.066	5.7
H44ab	1.399	0.196	0.046	5.7
H44ac	1.324	0.243	0.035	5.7
H45aa	1.356	0.286	0.178	6.7

H45ab	1.422	0.268	0.147	6.7
H45ac	1.359	0.329	0.137	6.7
H13ba	0.564	0.743	−0.046	4.5
H13bb	0.540	0.703	−0.005	4.5
H13bc	0.520	0.789	−0.012	4.5
H14ba	0.708	0.704	−0.034	6.2
H14bb	0.748	0.723	0.007	6.2
H14bc	0.680	0.663	0.005	6.2
H15ba	0.673	0.835	−0.045	6.0
H15bb	0.625	0.882	−0.013	6.0
H15bc	0.713	0.860	−0.004	6.0
H21ba	0.259	0.610	0.138	7.0
H21bb	0.308	0.636	0.100	7.0
H21bc	0.258	0.561	0.098	7.0
H22ba	0.358	0.523	0.233	6.0
H22bb	0.324	0.595	0.212	6.0
H22bc	0.283	0.516	0.207	6.0
H23ba	0.538	0.406	0.193	6.9
H23bb	0.509	0.467	0.225	6.9
H23bc	0.457	0.396	0.215	6.9
H24ba	0.526	0.428	0.076	7.0
H24bb	0.582	0.426	0.113	7.0
H24bc	0.516	0.365	0.109	7.0
H25ba	0.363	0.545	0.051	7.2
H25bb	0.450	0.523	0.043	7.2
H25bc	0.387	0.459	0.049	7.2
H31ba	0.498	1.072	0.080	5.1
H31bb	0.562	1.010	0.072	5.1
H31bc	0.487	1.015	0.044	5.1
H32ba	0.462	1.012	0.197	5.8
H32bb	0.536	1.025	0.169	5.8
H32bc	0.461	1.074	0.162	5.8
H33ba	0.337	0.843	0.192	5.8
H33bb	0.413	0.878	0.210	5.8
H33bc	0.340	0.930	0.203	5.8
H34ba	0.307	0.799	0.082	4.8
H34bb	0.316	0.771	0.127	4.8
H34bc	0.261	0.840	0.117	4.8
H35ba	0.430	0.920	0.019	5.2
H35bb	0.403	0.836	0.029	5.2
H35bc	0.342	0.904	0.030	5.2
H41ba	0.736	0.915	0.210	4.2
H41bb	0.755	0.828	0.214	4.2
H41bc	0.823	0.888	0.211	4.2
H42ba	0.680	1.028	0.117	6.6
H42bb	0.656	0.993	0.159	6.6
H42bc	0.737	1.033	0.153	6.6
H43ba	0.755	0.947	0.029	7.2
H43bb	0.684	0.981	0.052	7.2
H43bc	0.767	1.016	0.059	7.2
H44ba	0.875	0.765	0.059	6.9
H44bb	0.815	0.801	0.028	6.9
H44bc	0.887	0.848	0.042	6.9
H45ba	0.871	0.744	0.171	6.6
H45bb	0.857	0.705	0.129	6.6
H45bc	0.924	0.766	0.134	6.6
H1	0.118	0.850	0.195	8.2
H1'	0.052	0.788	0.199	8.2
H2	0.647	0.140	0.193	12.0
H2'	0.571	0.183	0.206	12.0

Beq is the Mean of the Principal Axes of the Thermal Ellipsoid

Table of u(i,j) or U values *100.
E.S.Ds. refer to the last digit printed

	u11(U)	u22	u33	u12	u13	u23
W1a	6.32(7)	2.63(4)	2.67(5)	0.64(5)	0.54(5)	-0.22(4)
W2a	3.09(5)	2.44(4)	2.36(4)	-0.01(4)	-0.07(4)	-0.17(4)
W3a	2.49(4)	5.43(5)	2.66(5)	0.37(5)	0.08(4)	-0.10(5)
Ru1a	3.69(10)	3.44(10)	2.04(9)	-0.42(9)	-0.05(8)	-0.25(8)
Ru2a	3.93(10)	3.06(9)	2.38(9)	0.24(9)	0.54(8)	0.06(8)
C1a	3.3 (12)	4.4 (12)	2.5 (11)	-1.5 (11)	0.1 (9)	0.8 (10)
C2a	8.4 (19)	3.6 (13)	5.1 (15)	1.4 (15)	-0.4 (15)	-0.1 (11)
C3a	8.1 (19)	3.9 (14)	6.2 (17)	-0.8 (14)	0.3 (15)	-0.8 (13)
C4a	4.3 (14)	4.8 (14)	4.9 (14)	-1.3 (12)	1.8 (12)	0.0 (12)
C5a	5.5 (16)	7.7 (18)	5.4 (16)	-0.8 (15)	0.7 (14)	-0.2 (15)
C6a	6.4 (16)	3.8 (13)	3.6 (13)	-0.2 (13)	0.6 (12)	-1.4 (11)
C7a	5.6 (15)	6.4 (16)	3.4 (13)	-0.3 (15)	0.4 (12)	0.0 (12)
C8a	6.4 (16)	4.3 (13)	4.3 (14)	0.9 (13)	-0.7 (13)	-0.8 (12)
C9a	5.6 (15)	6.1 (16)	3.5 (13)	0.0 (14)	2.8 (12)	0.1 (12)
C10a	2.9 (11)	3.0 (11)	3.2 (11)	1.9 (10)	-1.6 (9)	-1.6 (9)
C11a	3.4 (13)	5.4 (14)	3.5 (13)	1.1 (12)	0.8 (10)	-0.5 (12)
C12a	4.5 (13)	4.6 (13)	3.2 (12)	0.1 (12)	1.0 (11)	0.9 (11)
C13a	5.8 (17)	9.7 (20)	2.6 (13)	0.8 (16)	1.5 (12)	1.3 (14)
C14a	9.3 (22)	9.9 (22)	5.9 (18)	0.4 (20)	2.2 (17)	1.5 (17)
C15a	7.4 (18)	7.9 (19)	4.7 (15)	1.0 (18)	1.7 (15)	0.8 (15)
C16a	9.0 (21)	6.3 (17)	7.0 (19)	2.0 (17)	-2.1 (17)	-2.0 (15)
C17a	5.7 (16)	4.8 (14)	4.2 (14)	0.8 (13)	1.1 (12)	-0.7 (12)
C18a	5.3 (15)	4.6 (14)	3.3 (13)	0.7 (13)	-0.2 (11)	-1.0 (11)
C19a	10.5 (24)	6.2 (18)	10.2 (24)	1.8 (19)	2.6 (20)	1.0 (18)
C20a	9.9 (22)	7.0 (18)	5.2 (17)	4.4 (17)	-0.6 (16)	0.0 (15)
C21a	6.5 (19)	12.6 (26)	8.9 (23)	3.0 (20)	-0.3 (18)	-0.2 (22)
C22a	10.1 (23)	7.5 (19)	7.7 (20)	3.7 (20)	0.2 (19)	-0.2 (17)
C23a	9.8 (22)	4.7 (16)	9.6 (23)	1.8 (17)	0.3 (19)	-2.1 (16)
C24a	22.1 (42)	5.4 (18)	11.8 (28)	0.0 (26)	5.5 (30)	1.1 (21)
C25a	20.2 (40)	13.1 (31)	6.8 (23)	7.5 (31)	-0.6 (26)	0.4 (23)
C26a	7.3 (17)	3.6 (12)	3.7 (13)	-0.9 (13)	1.0 (12)	-1.5 (10)
C27a	8.3 (19)	6.2 (17)	5.5 (17)	-2.0 (16)	-0.2 (15)	-0.7 (14)
C28a	3.7 (14)	7.8 (18)	5.7 (16)	-2.0 (14)	-0.8 (13)	-0.1 (15)
C29a	5.0 (14)	5.5 (14)	3.2 (13)	-1.4 (12)	-0.1 (11)	-0.7 (12)
C30a	4.6 (14)	5.7 (15)	4.8 (15)	-0.9 (14)	0.5 (12)	-1.5 (13)
C31a	15.0 (31)	6.3 (19)	12.0 (28)	-0.9 (23)	3.2 (25)	-2.3 (20)
C32a	12.3 (28)	8.4 (22)	12.1 (27)	-3.7 (23)	-3.3 (24)	2.5 (21)
C33a	5.2 (15)	6.4 (16)	3.5 (13)	-2.4 (14)	0.7 (12)	-0.6 (12)
C34a	4.7 (15)	4.7 (13)	5.7 (15)	-0.3 (13)	-1.3 (13)	0.1 (13)
C35a	6.3 (16)	5.8 (16)	3.5 (13)	-2.6 (14)	-2.1 (12)	-0.6 (12)
C36a	3.1 (13)	7.4 (17)	5.2 (15)	0.0 (13)	0.1 (12)	0.3 (14)
C37a	3.6 (14)	6.9 (17)	6.1 (16)	2.7 (13)	0.7 (12)	-0.6 (14)
C38a	3.8 (14)	6.8 (17)	5.5 (16)	1.2 (13)	-0.1 (12)	0.2 (14)
C39a	2.8 (13)	8.1 (17)	6.4 (16)	0.6 (14)	0.3 (13)	1.2 (15)
C40a	4.4 (15)	8.7 (20)	7.4 (19)	-0.9 (16)	-0.8 (14)	-1.1 (16)
C41a	5.9 (17)	9.7 (21)	3.7 (15)	2.4 (17)	-1.2 (13)	0.2 (15)
C42a	5.6 (17)	7.5 (19)	8.6 (21)	4.1 (15)	-0.8 (16)	0.2 (17)
C43a	8.9 (22)	7.4 (20)	8.6 (22)	1.9 (19)	1.0 (19)	-1.4 (18)
C44a	4.1 (16)	14.3 (28)	6.0 (18)	0.3 (19)	-0.3 (14)	0.1 (19)
C45a	5.4 (18)	11.5 (25)	7.5 (20)	-1.3 (18)	-1.4 (16)	0.3 (20)
O1a	2.4 (7)	4.6 (8)	3.7 (8)	2.5 (7)	0.5 (7)	-1.0 (7)
O2a	11.8 (14)	6.2 (10)	2.2 (8)	2.0 (12)	0.1 (10)	-0.7 (8)
O3a	10.0 (16)	7.2 (13)	13.9 (19)	-4.4 (13)	2.1 (15)	0.2 (14)
O4a	7.8 (12)	5.4 (10)	2.7 (8)	0.9 (10)	-1.5 (8)	1.4 (8)
O5a	10.1 (15)	8.5 (13)	8.3 (14)	-5.0 (13)	-0.1 (12)	0.2 (12)

O6a	14.6 (18)	6.1 (11)	3.2 (9)	2.4 (13)	3.9 (11)	2.3 (9)
O7a	8.5 (14)	12.2 (17)	8.4 (14)	-6.2 (14)	-3.9 (12)	-0.6 (13)
O8a	6.6 (12)	12.1 (17)	5.9 (12)	1.5 (13)	-2.6 (10)	0.1 (12)
O9a	19.7 (25)	5.9 (13)	12.2 (18)	-0.9 (16)	2.1 (19)	4.2 (14)
W1b	5.69(6)	2.49(4)	2.66(5)	-0.35(5)	0.13(5)	0.33(4)
W2b	2.87(4)	2.50(4)	2.36(4)	0.04(4)	-0.15(4)	0.25(4)
W3b	2.83(5)	5.20(5)	2.78(5)	-0.39(5)	0.45(4)	0.11(5)
Ru1b	3.67(10)	3.31(9)	2.17(9)	0.53(9)	-0.18(8)	0.08(8)
Ru2b	3.78(10)	3.38(9)	2.00(9)	0.18(9)	0.07(8)	-0.23(8)
C1b	2.9 (11)	3.8 (11)	1.9 (10)	0.1 (10)	0.8 (9)	0.1 (9)
C2b	8.7 (19)	4.0 (13)	4.1 (14)	-1.7 (15)	-0.5 (14)	0.4 (11)
C3b	15.3 (31)	7.1 (21)	8.4 (23)	2.3 (22)	-0.4 (24)	0.3 (19)
C4b	3.2 (12)	2.7 (11)	3.2 (12)	0.2 (10)	0.7 (10)	0.5 (9)
C5b	2.9 (13)	7.1 (16)	3.9 (13)	-1.0 (12)	1.4 (11)	0.4 (12)
C6b	6.3 (15)	2.2 (11)	2.6 (11)	0.6 (11)	1.2 (11)	-0.3 (9)
C7b	5.0 (15)	6.2 (15)	4.2 (14)	0.0 (14)	-0.3 (12)	1.1 (13)
C8b	3.9 (13)	4.3 (12)	1.9 (11)	-0.7 (11)	0.7 (9)	0.0 (10)
C9b	4.6 (15)	5.4 (15)	4.1 (14)	-0.7 (13)	0.9 (12)	-0.3 (12)
C10b	3.7 (12)	2.5 (11)	3.6 (12)	-0.5 (10)	-1.6 (10)	1.4 (9)
C11b	4.0 (13)	4.8 (14)	2.0 (11)	0.9 (11)	0.1 (10)	0.1 (10)
C12b	4.0 (14)	7.0 (17)	3.4 (13)	0.9 (13)	0.2 (11)	-0.2 (13)
C13b	6.9 (18)	9.2 (19)	2.4 (12)	-0.2 (17)	1.2 (12)	1.3 (14)
C14b	9.2 (22)	12.4 (27)	3.8 (16)	0.8 (21)	2.0 (15)	-1.4 (17)
C15b	8.8 (22)	11.2 (24)	4.7 (16)	-3.1 (21)	0.7 (16)	0.5 (17)
C16b	4.3 (14)	3.8 (13)	5.1 (15)	-1.2 (11)	-1.7 (11)	0.6 (11)
C17b	7.5 (19)	7.5 (19)	5.0 (16)	-2.3 (17)	-0.2 (15)	0.2 (15)
C18b	6.3 (16)	4.5 (14)	4.1 (14)	-0.6 (13)	-1.2 (12)	0.5 (12)
C19b	6.9 (17)	5.3 (14)	3.7 (13)	-1.4 (14)	0.2 (12)	-1.5 (12)
C20b	8.3 (18)	3.8 (13)	3.0 (12)	-1.1 (13)	-0.3 (13)	-1.8 (11)
C21b	7.8 (21)	8.6 (21)	11.9 (26)	-3.3 (19)	0.9 (20)	-0.8 (22)
C22b	9.3 (22)	7.9 (20)	6.7 (19)	-2.2 (19)	2.3 (17)	-0.8 (17)
C23b	12.2 (27)	6.4 (18)	8.7 (22)	0.8 (21)	-1.3 (21)	0.3 (17)
C24b	19.2 (37)	6.1 (18)	9.3 (24)	1.1 (24)	3.0 (26)	-3.7 (18)
C25b	10.9 (23)	6.9 (19)	4.9 (16)	-4.2 (18)	-0.2 (16)	-1.8 (15)
C26b	5.3 (15)	4.3 (13)	3.7 (13)	0.4 (12)	-0.9 (11)	0.1 (11)
C27b	3.6 (12)	3.0 (11)	2.5 (11)	1.0 (10)	-1.0 (10)	-1.1 (9)
C28b	2.7 (11)	4.0 (12)	3.3 (12)	0.6 (10)	-0.5 (10)	0.8 (11)
C29b	3.4 (12)	3.2 (11)	3.7 (13)	0.9 (10)	-0.4 (10)	-0.9 (10)
C30b	6.5 (16)	4.6 (14)	3.6 (13)	0.3 (13)	-0.5 (12)	0.8 (12)
C31b	7.1 (18)	4.6 (14)	7.4 (18)	-0.7 (15)	-0.3 (16)	2.0 (13)
C32b	8.3 (20)	5.0 (15)	7.7 (19)	0.9 (16)	0.4 (17)	-1.8 (14)
C33b	9.2 (23)	10.3 (24)	6.3 (19)	4.5 (21)	1.5 (17)	0.0 (18)
C34b	3.9 (15)	5.5 (15)	10.5 (22)	0.7 (14)	-0.3 (15)	-0.9 (16)
C35b	5.9 (17)	8.2 (19)	3.8 (14)	1.4 (15)	-1.1 (13)	1.8 (14)
C36b	2.8 (12)	6.0 (15)	5.3 (15)	0.6 (12)	0.1 (12)	0.1 (13)
C37b	2.9 (12)	4.8 (14)	4.6 (14)	-0.7 (11)	-0.9 (11)	0.1 (11)
C38b	4.2 (14)	6.8 (16)	5.1 (15)	-0.8 (14)	-0.6 (12)	-0.8 (14)
C39b	4.2 (15)	10.1 (21)	4.8 (15)	-2.3 (16)	-0.8 (12)	0.1 (16)
C40b	2.3 (12)	6.3 (15)	5.8 (15)	0.5 (12)	-0.9 (11)	0.9 (13)
C41b	5.1 (15)	7.5 (18)	4.2 (15)	-0.3 (14)	-1.9 (12)	-0.5 (14)
C42b	8.2 (20)	6.1 (17)	8.0 (20)	-1.1 (17)	-1.1 (17)	1.4 (16)
C43b	10.4 (25)	10.6 (26)	8.6 (23)	-3.2 (23)	-0.1 (20)	2.2 (21)
C44b	4.1 (16)	13.5 (28)	11.0 (25)	-2.4 (19)	3.4 (17)	-2.7 (23)
C45b	5.0 (18)	14.6 (30)	10.2 (25)	1.1 (21)	-0.7 (18)	0.5 (24)
O1b	3.3 (8)	3.7 (8)	3.1 (8)	-0.9 (7)	0.2 (7)	-0.6 (7)
O2b	19.3 (21)	6.0 (11)	3.9 (10)	-5.0 (15)	2.1 (13)	1.0 (9)
O3b	7.8 (13)	6.6 (12)	14.6 (19)	2.8 (12)	-4.0 (14)	-1.7 (13)
O4b	5.5 (10)	4.5 (9)	4.8 (10)	-0.6 (9)	1.0 (8)	1.4 (8)
O5b	5.1 (11)	9.8 (14)	9.8 (15)	2.2 (12)	-0.3 (11)	0.3 (13)
O6b	12.8 (16)	6.1 (11)	4.3 (10)	2.7 (12)	0.2 (11)	-0.5 (9)

O7b	7.5 (13)	15.5 (20)	7.2 (13)	8.0 (14)	1.0 (11)	3.6 (14)
O8b	8.4 (13)	6.5 (11)	3.9 (10)	-1.6 (10)	-0.7 (9)	1.6 (9)
O9b	9.5 (14)	7.7 (13)	7.5 (13)	3.5 (12)	3.3 (11)	-3.8 (11)
C1	11.7 (12)					
C2	15.7 (17)					
Cl1	12.3 (8)	18.1 (11)	11.1 (8)	-1.8 (8)	0.1 (7)	-2.8 (8)
Cl2	19.5 (14)	49.9 (30)	15.7 (12)	8.3 (19)	3.1 (11)	11.2 (17)
Cl3	8.8 (6)	11.1 (7)	14.0 (8)	0.9 (6)	1.6 (6)	0.5 (7)
Cl4	16.0 (11)	31.4 (18)	15.3 (11)	-5.1 (14)	-3.5 (9)	-6.5 (12)
H13aa	6.3					
H13ab	6.3					
H13ac	6.3					
H14aa	7.4					
H14ab	7.4					
H14ac	7.4					
H15aa	7.0					
H15ab	7.0					
H15ac	7.0					
H21aa	9.6					
H21ab	9.6					
H21ac	9.6					
H22aa	8.1					
H22ab	8.1					
H22ac	8.1					
H23aa	7.0					
H23ab	7.0					
H23ac	7.0					
H24aa	10.1					
H24ab	10.1					
H24ac	10.1					
H25aa	11.0					
H25ab	11.0					
H25ac	11.0					
H31aa	9.0					
H31ab	9.0					
H31ac	9.0					
H32aa	9.6					
H32ab	9.6					
H32ac	9.6					
H33aa	5.3					
H33ab	5.3					
H33ac	5.3					
H34aa	6.1					
H34ab	6.1					
H34ac	6.1					
H35aa	5.4					
H35ab	5.4					
H35ac	5.4					
H41aa	5.9					
H41ab	5.9					
H41ac	5.9					
H42aa	7.2					
H42ab	7.2					
H42ac	7.2					
H43aa	8.0					
H43ab	8.0					
H43ac	8.0					
H44aa	7.2					
H44ab	7.2					
H44ac	7.2					

H45aa	8.5
H45ab	8.5
H45ac	8.5
H13ba	5.7
H13bb	5.7
H13bc	5.7
H14ba	7.9
H14bb	7.9
H14bc	7.9
H15ba	7.6
H15bb	7.6
H15bc	7.6
H21ba	8.8
H21bb	8.8
H21bc	8.8
H22ba	7.6
H22bb	7.6
H22bc	7.6
H23ba	8.7
H23bb	8.7
H23bc	8.7
H24ba	8.9
H24bb	8.9
H24bc	8.9
H25ba	9.2
H25bb	9.2
H25bc	9.2
H31ba	6.5
H31bb	6.5
H31bc	6.5
H32ba	7.4
H32bb	7.4
H32bc	7.4
H33ba	7.3
H33bb	7.3
H33bc	7.3
H34ba	6.1
H34bb	6.1
H34bc	6.1
H35ba	6.6
H35bb	6.6
H35bc	6.6
H41ba	5.4
H41bb	5.4
H41bc	5.4
H42ba	8.4
H42bb	8.4
H42bc	8.4
H43ba	9.2
H43bb	9.2
H43bc	9.2
H44ba	8.7
H44bb	8.7
H44bc	8.7
H45ba	8.4
H45bb	8.4
H45bc	8.4
H1	10.4
H1'	10.4
H2	15.1
H2'	15.1

Anisotropic Temperature Factors are of the form
Temp=-2*Pi*Pi*(h*h*u11*astar*astar+---+2*h*k*u12*astar*bstar+---)