[Ru(py)4Cl(NO)](PF6)2•1/2H2O

a model system for structural determination and ab initio calculations of photoinduced linkage NO-isomers

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Synopsis: Structure analysis of GS (ground state) and two light-induced (SI, SII) metastable linkage NO isomers of [Ru(py)4Cl(NO)]·(PF6)2·1/2H2O is presented. The experimental results are compared to solid-state calculations based on Density Functional Theory (DFT). The influence of the different occupancies of the metastable isomer SI and ground state on the refinement results was solved by a simulation procedure.

1. Atomic positions for GS
2. Atomic displacement parameters for GS
3. Distances and angles for GS
4. Atomic positions for SI
5. Atomic displacement parameters for SI
6. Distances and angles for SI
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8. Atomic displacement parameters for SII
9. Distances and angles for SII

Atomic positions for GS:

	x	y	z	Ueq/Uiso (Å^2)
Ru1	0.018028(10)	0.232043(12)	0.860632(6)	0.01289(5)
Cl1	0.12910(3)	0.29988(4)	0.81747(2)	0.02121(16)
N1	-0.04137(10)	0.37231(13)	0.85827(6)	0.0144(5)
C1	-0.12680(13)	0.37877(16)	0.84859(9)	0.0201(7)
H1	-0.1597	0.317	0.8401	0.024153
C2	-0.16930(14)	0.46821(17)	0.85020(9)	0.0259(8)
H2	-0.2323	0.4709	0.8429	0.03103
C3	-0.12481(14)	0.55410(17)	0.86190(9)	0.0224(7)
H3	-0.1551	0.6193	0.8639	0.026843
C4	-0.03750(13)	0.54851(16)	0.87084(8)	0.0181(6)
H4	-0.0035	0.6099	0.8785	0.021748
C5	0.00215(13)	0.45693(15)	0.86897(8)	0.0157(6)
H5	0.0652	0.4531	0.8758	0.018809
N2	0.08467(10)	0.27477(13)	0.92693(7)	0.0158(5)
C6	0.04296(13)	0.31996(17)	0.96361(8)	0.0191(6)
H6	-0.0201	0.3292	0.9594	0.02286
C7	0.08427(14)	0.3537(2)	1.00656(9)	0.0276(8)
H7	0.0517	0.3874	1.033	0.033117
C8	0.17125(14)	0.34048(19)	1.01283(9)	0.0278(8)
H8	0.2027	0.3651	1.0436	0.033416
C9	0.21387(14)	0.29286(17)	0.97599(9)	0.0238(7)
H9	0.2768	0.2818	0.9799	0.02859
C10	0.16935(13)	0.26052(17)	0.93374(9)	0.0200(7)
H10	0.2008	0.2254	0.9073	0.023993
N3	0.08356(11)	0.09535(14)	0.86068(8)	0.0232(6)
C11	0.11792(14)	0.05984(19)	0.81923(12)	0.0338(9)
H11	0.1107	0.0975	0.7872	0.040568
C12	0.16373(15)	-0.0293(2)	0.82051(15)	0.0540(13)
H12	0.1894	-0.0548	0.7895	0.064798
C13	0.17361(17)	-0.0821(2)	0.86437(18)	0.0633(15)
H13	0.2066	-0.1457	0.8656	0.07592
C14	0.13721(19)	-0.0458(2)	0.90635(15)	0.0563(12)
H14	0.1431	-0.083	0.9386	0.067554
C15	0.09257(16)	0.04216(18)	0.90367(11)	0.0349(9)
H15	0.0659	0.0678	0.9343	0.041929
N4	-0.04441(10)	0.19400(13)	0.79186(6)	0.0152(5)
C16	-0.03988(13)	0.25101(16)	0.75071(8)	0.0182(6)
H16	-0.0064	0.3142	0.7527	0.021841
C17	-0.08020(13)	0.22451(17)	0.70590(8)	0.0194(6)
H17	-0.0749	0.2676	0.6758	0.023309
C18	-0.12796(13)	0.13828(17)	0.70283(9)	0.0207(7)
H18	-0.1583	0.1186	0.6708	0.024874
C19	-0.13299(13)	0.07989(17)	0.74484(8)	0.0205(7)
H19	-0.167	0.017	0.7437	0.024655
C20	-0.09045(13)	0.10927(16)	0.78852(8)	0.0181(6)
H20	-0.0939	0.0662	0.8188	0.021775
N5	-0.06527(11)	0.18183(13)	0.89426(6)	0.0154(5)
O5	-0.12051(10)	0.15136(12)	0.91630(6)	0.0261(5)
Ru2	0.507111(10)	0.686210(12)	0.880477(6)	0.01118(4)
Cl2	0.62173(3)	0.60915(4)	0.922254(19)	0.01604(14)
N6	0.44807(10)	0.54476(12)	0.87349(6)	0.0125(5)
C21	0.49066(13)	0.46426(15)	0.85756(8)	0.0159(6)
H21	0.5523	0.4714	0.8504	0.019045
C22	0.45248(13)	0.37252(16)	0.85079(8)	0.0190(7)
H22	0.486	0.3145	0.8391	0.022856
C23	0.36652(14)	0.36208(17)	0.86057(9)	0.0225(7)

H23	0.3372	0.2965	0.856	0.026978
C24	0.32244(14)	0.44459(17)	0.87678(9)	0.0225(7)
H24	0.2606	0.4393	0.884	0.027033
C25	0.36478(13)	0.53441(16)	0.88291(8)	0.0169(6)
H25	0.3326	0.5935	0.8947	0.020284
N7	0.57101(10)	0.66105(12)	0.81420(6)	0.0131(5)
C26	0.65511(13)	0.68371(16)	0.81187(8)	0.0160(6)
H26	0.6854	0.7142	0.8417	0.019241
C27	0.69996(13)	0.66598(17)	0.76968(8)	0.0198(7)
H27	0.7615	0.6845	0.7687	0.023795
C28	0.65863(14)	0.62216(17)	0.72860(8)	0.0218(7)
H28	0.6904	0.6068	0.698	0.02611
C29	0.57287(13)	0.59996(17)	0.73051(8)	0.0193(7)
H29	0.5417	0.5694	0.7011	0.023178
C30	0.53069(13)	0.62045(15)	0.77358(8)	0.0146(6)
H30	0.4685	0.6048	0.7747	0.017556
N8	0.57151(10)	0.82317(12)	0.88597(6)	0.0127(5)
C31	0.57110(13)	0.88444(15)	0.84557(8)	0.0164(6)
H31	0.536	0.8659	0.815	0.019658
C32	0.61759(13)	0.97113(16)	0.84564(8)	0.0184(7)
H32	0.6167	1.0146	0.8154	0.022136
C33	0.66584(13)	0.99767(16)	0.88833(9)	0.0194(7)
H33	0.7006	1.06	0.8891	0.023286
C34	0.66487(13)	0.93632(16)	0.92968(8)	0.0174(6)
H34	0.6985	0.9543	0.9609	0.020832
C35	0.61724(12)	0.85019(16)	0.92757(8)	0.0147(6)
H35	0.6165	0.8065	0.9577	0.017604
N9	0.45600(10)	0.70769(12)	0.95099(6)	0.0134(5)
C36	0.42919(12)	0.79852(15)	0.96474(8)	0.0139(6)
H36	0.4305	0.8542	0.9401	0.016658
C37	0.40001(13)	0.81742(17)	1.01155(8)	0.0173(6)
H37	0.3816	0.8859	1.0208	0.020703
C38	0.39648(14)	0.74050(17)	1.04557(8)	0.0204(7)
H38	0.376	0.7525	1.0799	0.024495
C39	0.42179(14)	0.64669(17)	1.03123(8)	0.0216(7)
H39	0.4185	0.5895	1.0549	0.025938
C40	0.45150(13)	0.63257(16)	0.98427(8)	0.0180(6)
H40	0.4704	0.5646	0.9744	0.021552
N10	0.41638(10)	0.74406(12)	0.85337(6)	0.0135(5)
O10	0.35375(9)	0.78226(11)	0.84088(6)	0.0209(5)
P1	-0.12008(4)	-0.14878(4)	0.85673(2)	0.02017(17)
F1	-0.11930(8)	-0.23542(11)	0.81573(5)	0.0295(4)
F2	-0.12025(9)	-0.06141(11)	0.89708(7)	0.0446(6)
F3	-0.19815(8)	-0.20244(9)	0.88262(5)	0.0237(4)
F4	-0.18573(8)	-0.08730(11)	0.82198(6)	0.0395(5)
F5	-0.04156(8)	-0.09640(10)	0.83007(6)	0.0339(5)
F6	-0.05434(8)	-0.21083(10)	0.89146(5)	0.0306(5)
P2	-0.17658(4)	0.35466(5)	1.03919(3)	0.02557(19)
F7	-0.18441(11)	0.27957(17)	0.99382(8)	0.0830(9)
F8	-0.16741(8)	0.43040(10)	1.08532(5)	0.0292(5)
F9	-0.24455(9)	0.29213(11)	1.06872(8)	0.0534(7)
F10	-0.25164(9)	0.42197(14)	1.01631(6)	0.0529(6)
F11	-0.10855(10)	0.41904(13)	1.01066(6)	0.0506(6)
F12	-0.10085(8)	0.28920(11)	1.06336(7)	0.0422(6)
P3	0.38735(3)	1.07446(4)	0.91711(2)	0.01490(16)
F13	0.38769(8)	0.98475(9)	0.87699(5)	0.0204(4)
F14	0.38580(8)	1.16437(10)	0.95652(5)	0.0241(4)
F15	0.32391(8)	1.01134(10)	0.95016(5)	0.0252(4)
F16	0.30590(7)	1.12230(9)	0.88702(5)	0.0207(4)
F17	0.44941(8)	1.13749(9)	0.88342(5)	0.0206(4)

P4	0.33654(3)	0.75664(4)	0.71027(2)	0.01474(15)
F18	0.46731(8)	1.02622(9)	0.94675(5)	0.0230(4)
F19	0.40705(7)	0.69708(9)	0.68076(5)	0.0192(4)
F20	0.26567(7)	0.81646(10)	0.73947(5)	0.0218(4)
F21	0.26247(7)	0.70419(9)	0.67598(5)	0.0208(4)
F22	0.33240(7)	0.66698(9)	0.74990(5)	0.0214(4)
F23	0.41106(7)	0.80835(9)	0.74426(5)	0.0206(4)
F24	0.34099(8)	0.84604(9)	0.67056(5)	0.0215(4)
O3	0.0008(3)	0.1098(4)	1.00704(16)	0.1396(13)
H3a	0.0466(11)	0.097(4)	1.013(2)	0.167576
H3b	-0.013(3)	0.135(4)	1.0302(12)	0.167576

Atomic displacement parameters for GS:

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru1	0.01278(8)	0.01110(8)	0.01493(9)	-0.00002(6)	0.00229(6)	-0.00169(7)
Cl1	0.0190(2)	0.0239(3)	0.0213(3)	-0.0066(2)	0.0069(2)	-0.0054(2)
N1	0.0143(8)	0.0115(9)	0.0174(9)	-0.0020(7)	-0.0004(7)	-0.0010(7)
C1	0.0173(10)	0.0142(11)	0.0283(13)	-0.0015(8)	-0.0070(9)	-0.0014(9)
C2	0.0190(11)	0.0188(12)	0.0388(15)	0.0023(9)	-0.0111(10)	-0.0020(10)
C3	0.0253(12)	0.0120(11)	0.0293(13)	0.0025(9)	-0.0051(10)	0.0001(9)
C4	0.0231(11)	0.0127(11)	0.0185(11)	-0.0046(9)	0.0002(9)	-0.0021(9)
C5	0.0175(10)	0.0139(10)	0.0154(11)	-0.0018(8)	-0.0012(9)	-0.0013(8)
N2	0.0131(8)	0.0161(9)	0.0182(9)	-0.0007(7)	0.0001(7)	-0.0009(8)
C6	0.0156(10)	0.0246(12)	0.0169(11)	0.0014(9)	0.0005(8)	0.0001(9)
C7	0.0197(11)	0.0470(16)	0.0162(12)	0.0024(11)	0.0020(9)	-0.0077(11)
C8	0.0213(12)	0.0428(16)	0.0190(12)	-0.0021(11)	-0.0047(10)	-0.0009(11)
C9	0.0149(10)	0.0283(14)	0.0278(13)	0.0018(9)	-0.0041(9)	0.0034(10)
C10	0.0146(10)	0.0192(11)	0.0263(13)	0.0047(9)	0.0022(9)	-0.0002(9)
N3	0.0151(9)	0.0154(10)	0.0388(13)	0.0016(7)	-0.0024(8)	-0.0081(9)
C11	0.0174(11)	0.0246(14)	0.060(2)	-0.0056(10)	0.0128(12)	-0.0213(13)
C12	0.0135(12)	0.0318(17)	0.118(3)	-0.0074(11)	0.0168(16)	-0.0456(19)
C13	0.0238(15)	0.0182(15)	0.145(4)	0.0049(12)	-0.0326(19)	-0.020(2)
C14	0.0516(19)	0.0171(14)	0.096(3)	0.0078(13)	-0.0478(19)	-0.0107(16)
C15	0.0345(14)	0.0181(13)	0.0502(19)	0.0043(11)	-0.0215(13)	-0.0041(12)
N4	0.0176(8)	0.0119(9)	0.0163(9)	-0.0006(7)	0.0027(7)	-0.0039(7)
C16	0.0203(10)	0.0150(11)	0.0195(11)	-0.0008(8)	0.0039(9)	0.0018(9)
C17	0.0195(11)	0.0202(11)	0.0188(11)	0.0025(9)	0.0041(9)	0.0025(9)
C18	0.0193(11)	0.0248(13)	0.0181(12)	0.0000(9)	0.0007(9)	-0.0068(10)
C19	0.0222(11)	0.0188(12)	0.0208(12)	-0.0043(9)	0.0024(9)	-0.0057(9)
C20	0.0206(11)	0.0145(11)	0.0196(12)	-0.0010(9)	0.0038(9)	-0.0008(9)
N5	0.0175(9)	0.0137(9)	0.0147(9)	0.0017(7)	-0.0008(7)	-0.0037(7)
O5	0.0282(9)	0.0259(9)	0.0248(9)	-0.0088(7)	0.0096(7)	-0.0046(7)
Ru2	0.01278(8)	0.00983(8)	0.01083(8)	0.00111(6)	-0.00074(6)	0.00012(7)
Cl2	0.0168(2)	0.0139(2)	0.0170(3)	0.00191(19)	-0.00439(19)	0.0010(2)
N6	0.0143(8)	0.0110(9)	0.0122(9)	0.0006(7)	-0.0003(7)	0.0003(7)
C21	0.0150(10)	0.0157(11)	0.0170(11)	0.0016(8)	0.0015(8)	-0.0007(8)
C22	0.0195(11)	0.0143(11)	0.0233(12)	0.0015(8)	0.0011(9)	-0.0013(9)
C23	0.0231(12)	0.0148(11)	0.0295(13)	-0.0032(9)	0.0008(10)	-0.0026(10)
C24	0.0175(11)	0.0204(12)	0.0301(14)	-0.0022(9)	0.0055(10)	0.0009(10)
C25	0.0167(10)	0.0151(11)	0.0191(11)	0.0010(8)	0.0027(9)	-0.0011(9)
N7	0.0134(8)	0.0126(9)	0.0133(9)	0.0026(6)	0.0002(7)	0.0011(7)
C26	0.0157(10)	0.0156(10)	0.0166(11)	0.0005(8)	-0.0024(8)	-0.0006(9)
C27	0.0136(10)	0.0272(13)	0.0187(11)	0.0032(9)	0.0010(9)	0.0016(9)
C28	0.0198(11)	0.0302(13)	0.0155(11)	0.0060(10)	0.0034(9)	0.0011(10)
C29	0.0209(11)	0.0227(12)	0.0140(11)	0.0051(9)	-0.0034(9)	-0.0014(9)
C30	0.0142(10)	0.0167(11)	0.0127(10)	0.0013(8)	-0.0022(8)	0.0010(8)
N8	0.0132(8)	0.0109(9)	0.0143(9)	0.0014(7)	0.0027(7)	0.0006(7)
C31	0.0194(10)	0.0150(11)	0.0148(11)	0.0026(8)	0.0016(8)	0.0019(9)
C32	0.0205(11)	0.0131(11)	0.0223(12)	0.0031(8)	0.0071(9)	0.0048(9)
C33	0.0192(11)	0.0128(11)	0.0267(13)	-0.0018(9)	0.0066(9)	-0.0030(9)
C34	0.0170(10)	0.0172(11)	0.0179(11)	0.0014(8)	0.0008(9)	-0.0056(9)
C35	0.0158(10)	0.0140(10)	0.0143(11)	0.0024(8)	0.0024(8)	-0.0001(8)
N9	0.0152(8)	0.0123(9)	0.0126(9)	-0.0007(6)	-0.0010(7)	0.0012(7)
C36	0.0143(10)	0.0123(10)	0.0149(10)	-0.0010(8)	-0.0012(8)	0.0015(8)
C37	0.0169(10)	0.0175(11)	0.0173(11)	-0.0007(9)	0.0005(8)	-0.0046(9)
C38	0.0245(11)	0.0243(12)	0.0124(10)	-0.0027(9)	0.0017(9)	-0.0017(9)
C39	0.0313(12)	0.0181(12)	0.0154(11)	-0.0030(10)	0.0004(9)	0.0043(9)
C40	0.0244(11)	0.0125(11)	0.0168(11)	0.0005(9)	-0.0007(9)	0.0013(9)
N10	0.0174(8)	0.0121(9)	0.0111(8)	-0.0003(7)	0.0009(7)	-0.0008(7)
O10	0.0198(8)	0.0245(9)	0.0180(8)	0.0076(7)	-0.0027(6)	0.0003(7)

P1	0.0155(3)	0.0135(3)	0.0314(3)	0.0000(2)	-0.0007(2)	0.0011(2)
F1	0.0285(7)	0.0344(8)	0.0259(8)	-0.0072(6)	0.0050(6)	-0.0068(6)
F2	0.0312(8)	0.0327(9)	0.0702(12)	-0.0019(7)	0.0057(8)	-0.0285(8)
F3	0.0207(6)	0.0220(7)	0.0288(8)	-0.0013(5)	0.0059(6)	0.0020(6)
F4	0.0179(7)	0.0405(9)	0.0602(11)	0.0060(6)	0.0024(7)	0.0287(8)
F5	0.0167(7)	0.0194(7)	0.0661(11)	-0.0016(5)	0.0078(7)	0.0091(7)
F6	0.0253(7)	0.0337(9)	0.0321(8)	0.0076(6)	-0.0071(6)	0.0035(6)
P2	0.0137(3)	0.0337(4)	0.0292(4)	0.0051(2)	-0.0020(2)	-0.0149(3)
F7	0.0431(10)	0.1173(19)	0.0882(16)	0.0122(11)	-0.0048(10)	-0.0849(14)
F8	0.0278(7)	0.0312(8)	0.0280(8)	-0.0006(6)	-0.0046(6)	-0.0119(6)
F9	0.0279(8)	0.0297(9)	0.1046(15)	-0.0078(7)	0.0249(9)	-0.0157(9)
F10	0.0323(8)	0.0902(14)	0.0348(10)	0.0294(9)	-0.0146(7)	-0.0130(9)
F11	0.0414(9)	0.0582(12)	0.0545(11)	0.0217(8)	0.0282(8)	0.0146(9)
F12	0.0203(7)	0.0245(8)	0.0813(13)	0.0059(6)	-0.0038(8)	0.0031(8)
P3	0.0171(3)	0.0145(3)	0.0130(3)	0.0016(2)	0.0000(2)	0.0007(2)
F13	0.0235(7)	0.0156(7)	0.0220(7)	0.0010(5)	-0.0016(5)	-0.0042(5)
F14	0.0310(7)	0.0254(8)	0.0159(7)	0.0030(6)	0.0004(6)	-0.0055(5)
F15	0.0256(7)	0.0330(8)	0.0169(7)	-0.0054(6)	0.0016(6)	0.0072(6)
F16	0.0212(6)	0.0231(7)	0.0174(7)	0.0078(5)	-0.0024(5)	-0.0002(5)
F17	0.0240(7)	0.0188(7)	0.0193(7)	-0.0031(5)	0.0041(5)	0.0016(5)
P4	0.0135(2)	0.0143(3)	0.0164(3)	0.0017(2)	0.0005(2)	0.0007(2)
F18	0.0209(6)	0.0202(7)	0.0270(8)	0.0011(5)	-0.0084(6)	0.0037(6)
F19	0.0167(6)	0.0164(6)	0.0246(7)	0.0041(5)	0.0038(5)	-0.0019(5)
F20	0.0187(6)	0.0240(7)	0.0230(7)	0.0052(5)	0.0043(5)	-0.0019(6)
F21	0.0176(6)	0.0204(7)	0.0241(7)	0.0002(5)	-0.0041(5)	-0.0013(5)
F22	0.0173(6)	0.0217(7)	0.0250(7)	0.0004(5)	0.0002(5)	0.0093(5)
F23	0.0182(6)	0.0212(7)	0.0221(7)	-0.0013(5)	-0.0019(5)	-0.0026(5)
F24	0.0229(7)	0.0175(7)	0.0242(7)	0.0030(5)	0.0022(5)	0.0060(5)

Distances and angles for GS:

	X-ray	DFT
Ru1-Cl1	2.3206(6)	2.3409
Ru1-N1	2.1044(17)	2.1388
Ru1-N2	2.1041(17)	2.1311
Ru1-N3	2.1069(18)	2.1299
Ru1-N4	2.1142(17)	2.1493
Ru1-N5	1.7550(17)	1.7848
N1-C1	1.358(3)	1.3531
N1-C5	1.352(3)	1.3534
C1-H1	1	1.0876
C1-C2	1.377(3)	1.3904
C2-H2	1	1.0902
C2-C3	1.379(3)	1.3924
C3-H3	1	1.0894
C3-C4	1.384(3)	1.3951
C4-H4	1	1.0894
C4-C5	1.382(3)	1.389
C5-H5	1	1.0874
N2-C6	1.349(3)	1.3531
N2-C10	1.348(3)	1.3524
C6-H6	1	1.0879
C6-C7	1.375(3)	1.3862
C7-H7	1	1.0883
C7-C8	1.380(3)	1.391
C8-H8	1	1.0903
C8-C9	1.375(3)	1.3927
C9-H9	1	1.09
C9-C10	1.376(3)	1.3895
C10-H10	1	1.0864
N3-C11	1.344(4)	1.3531
N3-C15	1.359(3)	1.3543
C11-H11	1	1.0905
C11-C12	1.398(4)	1.3893
C12-H12	1	1.0924
C12-C13	1.377(6)	1.3952
C13-H13	1	1.0892
C13-C14	1.374(6)	1.3905
C14-H14	1	1.0903
C14-C15	1.375(4)	1.3882
C15-H15	1	1.0938
N4-C16	1.348(3)	1.3538
N4-C20	1.350(3)	1.3554
C16-H16	1	1.0891
C16-C17	1.381(3)	1.3898
C17-H17	1	1.0898
C17-C18	1.382(3)	1.3936
C18-H18	1	1.092
C18-C19	1.378(3)	1.3935
C19-H19	1	1.0916
C19-C20	1.381(3)	1.3879
C20-H20	1	1.0858
N5-O5	1.146(2)	1.152
Ru2-Cl2	2.3231(5)	2.3366
Ru2-N6	2.1213(16)	2.1508
Ru2-N7	2.1051(17)	2.1366
Ru2-N8	2.1036(16)	2.1335
Ru2-N9	2.1050(17)	2.1365

Ru2-N10	1.7537(16)	1.7818
N6-C21	1.351(3)	1.3551
N6-C25	1.350(3)	1.3552
C21-H21	1	1.0886
C21-C22	1.381(3)	1.3898
C22-H22	1	1.0897
C22-C23	1.393(3)	1.394
C23-H23	1	1.0913
C23-C24	1.388(3)	1.3932
C24-H24	1	1.0898
C24-C25	1.385(3)	1.389
C25-H25	1	1.0892
N7-C26	1.359(3)	1.3553
N7-C30	1.351(3)	1.3538
C26-H26	1	1.088
C26-C27	1.379(3)	1.3885
C27-H27	1	1.0913
C27-C28	1.386(3)	1.3935
C28-H28	1	1.0886
C28-C29	1.382(3)	1.3943
C29-H29	1	1.089
C29-C30	1.383(3)	1.3869
C30-H30	1	1.0887
N8-C31	1.361(3)	1.3573
N8-C35	1.351(3)	1.3496
C31-H31	1	1.0913
C31-C32	1.376(3)	1.3855
C32-H32	1	1.0901
C32-C33	1.392(3)	1.395
C33-H33	1	1.0912
C33-C34	1.383(3)	1.3908
C34-H34	1	1.0898
C34-C35	1.379(3)	1.3909
C35-H35	1	1.0872
N9-C36	1.349(3)	1.3532
N9-C40	1.352(3)	1.352
C36-H36	1	1.0875
C36-C37	1.378(3)	1.3878
C37-H37	1	1.0876
C37-C38	1.382(3)	1.3904
C38-H38	1	1.0913
C38-C39	1.382(3)	1.3929
C39-H39	1	1.0896
C39-C40	1.374(3)	1.3878
C40-H40	1	1.0882
N10-O10	1.147(2)	1.152
P1-F1	1.6026(15)	1.6472
P1-F2	1.5976(17)	1.6562
P1-F3	1.6057(14)	1.6475
P1-F4	1.5916(15)	1.6411
P1-F5	1.6131(15)	1.6478
P1-F6	1.5961(15)	1.6423
P2-F7	1.582(2)	1.6356
P2-F8	1.6043(15)	1.6635
P2-F9	1.5954(18)	1.657
P2-F10	1.5888(17)	1.632
P2-F11	1.5956(18)	1.6426
P2-F12	1.5949(15)	1.6535
P3-F13	1.6168(13)	1.6588
N3-F14	1.6070(14)	1.6482

P3-F15	1.6043(14)	1.6465
P3-F16	1.6165(13)	1.6613
P3-F17	1.5997(13)	1.6354
P3-F18	1.5951(13)	1.6305
P4-F19	1.6027(13)	1.6381
P4-F20	1.6039(13)	1.6402
P4-F21	1.6139(13)	1.6533
P4-F22	1.6105(14)	1.6518
P4-F23	1.6103(13)	1.65
P4-F24	1.6097(14)	1.6517
O3-H3a	0.75(2)	0.9817
O3-H3b	0.75(4)	0.9811
Cl1-Ru1-N1	88.51(5)	88.2964
Cl1-Ru1-N2	87.51(5)	87.4758
Cl1-Ru1-N3	88.05(5)	88.068
Cl1-Ru1-N4	89.47(5)	88.7326
Cl1-Ru1-N5	178.96(6)	179.1722
N1-Ru1-N2	89.10(7)	88.8753
N1-Ru1-N3	176.56(7)	176.2654
N1-Ru1-N4	90.13(6)	89.7468
N1-Ru1-N5	91.23(7)	91.1786
N2-Ru1-N3	90.72(7)	90.1114
N2-Ru1-N4	176.90(7)	176.0025
N2-Ru1-N5	91.47(7)	91.8741
N3-Ru1-N4	89.87(7)	91.0265
N3-Ru1-N5	92.20(8)	92.4472
N4-Ru1-N5	91.54(7)	91.9058
C1-N1-C5	118.22(18)	119.0312
N1-C1-H1	119.1405	117.3711
N1-C1-C2	121.7(2)	121.9514
H1-C1-C2	119.1391	120.6731
C1-C2-H2	120.0888	118.4608
C1-C2-C3	119.8(2)	119.1245
H2-C2-C3	120.0875	122.4099
C2-C3-H3	120.5798	121.1583
C2-C3-C4	118.8(2)	118.8074
H3-C3-C4	120.5797	120.0334
C3-C4-H4	120.439	121.2926
C3-C4-C5	119.1(2)	119.2931
H4-C4-C5	120.439	119.4
N1-C5-C4	122.25(19)	121.7677
N1-C5-H5	118.873	116.9721
C4-C5-H5	118.8732	121.2556
C6-N2-C10	118.15(18)	118.8886
N2-C6-H6	118.8925	117.7248
N2-C6-C7	122.21(19)	121.9523
H6-C6-C7	118.8939	120.3194
C6-C7-H7	120.3667	118.4198
C6-C7-C8	119.3(2)	119.4027
H7-C7-C8	120.3672	122.1736
C7-C8-H8	120.6006	120.9626
C7-C8-C9	118.8(2)	118.5472
H8-C8-C9	120.6019	120.4891
C8-C9-H9	120.2329	122.0196
C8-C9-C10	119.5(2)	119.4311
H9-C9-C10	120.2339	118.5483
N2-C10-C9	122.0(2)	121.7376
N2-C10-H10	118.9933	117.2925
C9-C10-H10	118.9914	120.969
C11-N3-C15	118.9(2)	119.3911

N3-C11-H11	119.7087	116.5295
N3-C11-C12	120.6(3)	121.6478
H11-C11-C12	119.7083	121.8165
C11-C12-H12	119.9055	119.6135
C11-C12-C13	120.2(3)	119.0708
H12-C12-C13	119.9063	121.3132
C12-C13-H13	120.6521	121.2903
C12-C13-C14	118.7(3)	118.9973
H13-C13-C14	120.6512	119.7112
C13-C14-H14	120.2515	121.4324
C13-C14-C15	119.5(3)	119.3317
H14-C14-C15	120.2513	119.2359
N3-C15-C14	122.1(3)	121.5236
N3-C15-H15	118.947	117.2044
C14-C15-H15	118.9468	121.2712
C16-N4-C20	118.20(18)	118.734
N4-C16-H16	119.0933	116.9581
N4-C16-C17	121.81(19)	121.677
H16-C16-C17	119.0946	121.331
C16-C17-H17	120.1268	118.6464
C16-C17-C18	119.7(2)	119.6308
H17-C17-C18	120.1285	121.7036
C17-C18-H18	120.6757	120.1534
C17-C18-C19	118.6(2)	118.568
H18-C18-C19	120.6744	121.2739
C18-C19-H19	120.4096	122.516
C18-C19-C20	119.2(2)	119.1133
H19-C19-C20	120.4081	118.3693
N4-C20-C19	122.4(2)	122.262
N4-C20-H20	118.7988	117.604
C19-C20-H20	118.7971	120.131
Cl2-Ru2-N6	88.23(4)	88.1759
Cl2-Ru2-N7	87.03(5)	86.7492
Cl2-Ru2-N8	89.82(5)	90.1718
Cl2-Ru2-N9	86.86(5)	86.3765
Cl2-Ru2-N10	175.47(6)	175.092
N6-Ru2-N7	90.19(6)	90.0687
N6-Ru2-N8	176.99(6)	176.7138
N6-Ru2-N9	91.18(6)	91.5419
N6-Ru2-N10	90.98(7)	90.5944
N7-Ru2-N8	87.42(6)	87.0011
N7-Ru2-N9	173.69(6)	172.8856
N7-Ru2-N10	97.43(7)	98.006
N8-Ru2-N9	91.00(6)	91.1882
N8-Ru2-N10	91.15(7)	91.2861
N9-Ru2-N10	88.70(7)	88.9078
C21-N6-C25	118.22(17)	118.6862
N6-C21-H21	118.6638	117.1603
N6-C21-C22	122.67(19)	121.9982
H21-C21-C22	118.6648	120.8389
C21-C22-H22	120.5203	119.036
C21-C22-C23	119.0(2)	119.3563
H22-C22-C23	120.5205	121.5958
C22-C23-H23	120.7057	120.487
C22-C23-C24	118.6(2)	118.5372
H23-C23-C24	120.7062	120.9549
C23-C24-H24	120.28	122.1349
C23-C24-C25	119.4(2)	119.4523
H24-C24-C25	120.2811	118.4097
N6-C25-C24	122.12(19)	121.9578

N6-C25-H25	118.9413	117.3204
C24-C25-H25	118.9414	120.7133
C26-N7-C30	118.45(17)	118.919
N7-C26-H26	118.9962	117.4314
N7-C26-C27	122.01(19)	121.8803
H26-C26-C27	118.9961	120.688
C26-C27-H27	120.4104	118.5034
C26-C27-C28	119.18(19)	119.2237
H27-C27-C28	120.4108	122.2665
C27-C28-H28	120.4531	121.4641
C27-C28-C29	119.1(2)	118.7389
H28-C28-C29	120.4523	119.7747
C28-C29-H29	120.3397	120.6769
C28-C29-C30	119.3(2)	119.3126
H29-C29-C30	120.3408	119.9633
N7-C30-C29	121.93(18)	121.8852
N7-C30-H30	119.0381	116.8796
C29-C30-H30	119.0368	121.2169
C31-N8-C35	118.61(17)	119.0668
N8-C31-H31	119.0758	116.8411
N8-C31-C32	121.85(19)	121.7693
H31-C31-C32	119.0752	121.3864
C31-C32-H32	120.3732	119.959
C31-C32-C33	119.3(2)	119.2646
H32-C32-C33	120.3732	120.7724
C32-C33-H33	120.586	119.7097
C32-C33-C34	118.8(2)	118.8086
H33-C33-C34	120.5846	121.4811
C33-C34-H34	120.2304	122.593
C33-C34-C35	119.5(2)	119.2492
H34-C34-C35	120.2299	118.15
N8-C35-C34	121.89(19)	121.8155
N8-C35-H35	119.0546	117.036
C34-C35-H35	119.0533	121.1471
C36-N9-C40	118.09(18)	118.7989
N9-C36-H36	118.7995	117.5259
N9-C36-C37	122.40(19)	121.8728
H36-C36-C37	118.8008	120.5892
C36-C37-H37	120.415	118.1076
C36-C37-C38	119.2(2)	119.5608
H37-C37-C38	120.415	122.3208
C37-C38-H38	120.6679	121.1459
C37-C38-C39	118.7(2)	118.3311
H38-C38-C39	120.6685	120.5228
C38-C39-H39	120.2078	121.662
C38-C39-C40	119.6(2)	119.5674
H39-C39-C40	120.2074	118.737
N9-C40-C39	122.1(2)	121.836
N9-C40-H40	118.969	116.6071
C39-C40-H40	118.9695	121.5561
F1-P1-F2	179.22(9)	179.672
F1-P1-F3	89.88(7)	90.0169
F1-P1-F4	89.99(8)	89.9371
F1-P1-F5	89.16(8)	89.7682
F1-P1-F6	89.80(7)	90.3165
F2-P1-F3	90.83(8)	90.2556
F2-P1-F4	89.69(8)	89.878
F2-P1-F5	90.13(8)	89.9608
F2-P1-F6	90.53(8)	89.8678

F3-P1-F4	89.96(7)	90.3455
F3-P1-F5	179.04(8)	179.4611
F3-P1-F6	89.96(7)	89.7813
F4-P1-F5	90.10(8)	90.1486
F4-P1-F6	179.77(9)	179.7168
F5-P1-F6	89.98(7)	89.7256
F7-P2-F8	179.28(9)	178.8893
F7-P2-F9	90.77(10)	90.5271
F7-P2-F10	91.99(10)	91.412
F7-P2-F11	90.54(10)	90.6175
F7-P2-F12	89.56(10)	90.0922
F8-P2-F9	89.55(9)	89.1289
F8-P2-F10	88.66(8)	89.6468
F8-P2-F11	89.14(8)	89.7123
F8-P2-F12	89.79(8)	88.8474
F9-P2-F10	89.50(9)	90.467
F9-P2-F11	178.69(10)	178.6146
F9-P2-F12	90.59(8)	89.2443
F10-P2-F11	90.36(9)	90.2849
F10-P2-F12	178.45(10)	178.4709
F11-P2-F12	89.53(8)	89.9735
F13-P3-F14	179.13(7)	178.7373
F13-P3-F15	89.55(7)	89.8176
F13-P3-F16	89.42(7)	89.1264
F13-P3-F17	90.03(7)	89.9751
F13-P3-F18	90.18(7)	90.2553
F14-P3-F15	90.45(7)	90.252
F14-P3-F16	89.71(7)	89.6142
F14-P3-F17	89.95(7)	89.9305
F14-P3-F18	90.69(7)	91.005
F15-P3-F16	89.41(7)	89.091
F15-P3-F17	179.05(7)	178.8531
F15-P3-F18	90.19(7)	90.2792
F16-P3-F17	89.73(7)	89.778
F16-P3-F18	179.44(7)	179.1189
F17-P3-F18	90.67(7)	90.8497
F19-P4-F20	179.62(7)	179.6614
F19-P4-F21	89.79(7)	89.5634
F19-P4-F22	89.98(7)	90.01
F19-P4-F23	89.70(6)	89.9184
F19-P4-F24	89.80(7)	89.7726
F20-P4-F21	89.96(7)	90.1463
F20-P4-F22	90.31(7)	90.164
F20-P4-F23	90.54(7)	90.3712
F20-P4-F24	89.92(7)	90.0516
F21-P4-F22	90.01(7)	89.8567
F21-P4-F23	179.49(7)	179.4243
F21-P4-F24	90.01(7)	89.8036
F22-P4-F23	89.93(7)	90.394
F22-P4-F24	179.77(7)	179.598
F23-P4-F24	90.04(7)	89.9438
H3a-O3-H3b	104(5)	102.4803

Atomic positions for SI:

	Occ	x	y	z	Ueq/Uiso ($Å^2$)
Ru1	1.000	0.021349(9)	0.237396(9)	0.858552(5)	0.01224(4)
Cl1	1.000	0.12948(3)	0.30489(3)	0.815846(17)	0.02070(13)
N1	1.000	-0.04026(9)	0.37614(9)	0.85683(5)	0.0137(4)
C1	1.000	-0.12495(12)	0.38062(12)	0.84761(7)	0.0193(6)
H1	1.000	-0.1565	0.3178	0.8388	0.023105
C2	1.000	-0.16996(13)	0.46900(13)	0.84990(8)	0.0253(6)
H2	1.000	-0.2331	0.4699	0.8433	0.030398
C3	1.000	-0.12624(13)	0.55626(13)	0.86147(8)	0.0228(6)
H3	1.000	-0.1573	0.6212	0.8636	0.027397
C4	1.000	-0.03919(12)	0.55221(12)	0.86999(7)	0.0181(6)
H4	1.000	-0.0062	0.6146	0.8779	0.021767
C5	1.000	0.00225(12)	0.46144(11)	0.86760(6)	0.0149(5)
H5	1.000	0.0654	0.459	0.874	0.017927
N2	1.000	0.08625(10)	0.27980(10)	0.92533(6)	0.0139(4)
C6	1.000	0.04355(12)	0.32440(12)	0.96169(7)	0.0171(5)
H6	1.000	-0.0194	0.3338	0.9568	0.020521
C7	1.000	0.08366(13)	0.35732(15)	1.00524(7)	0.0248(6)
H7	1.000	0.0504	0.3906	1.0315	0.02977
C8	1.000	0.17026(13)	0.34395(15)	1.01239(8)	0.0267(7)
H8	1.000	0.2008	0.3679	1.0437	0.032081
C9	1.000	0.21406(13)	0.29707(13)	0.97570(8)	0.0236(6)
H9	1.000	0.2768	0.2858	0.9801	0.028287
C10	1.000	0.17034(12)	0.26586(12)	0.93283(7)	0.0192(6)
H10	1.000	0.2024	0.2316	0.9063	0.023037
N3	1.000	0.08558(10)	0.10046(10)	0.85921(6)	0.0209(5)
C11	1.000	0.11891(13)	0.06359(14)	0.81776(10)	0.0333(7)
H11	1.000	0.1114	0.1011	0.7856	0.039977
C12	1.000	0.16364(14)	-0.02574(17)	0.81885(13)	0.0566(11)
H12	1.000	0.1882	-0.0521	0.7877	0.067978
C13	1.000	0.17413(16)	-0.07783(17)	0.86290(15)	0.0687(13)
H13	1.000	0.2066	-0.1421	0.8642	0.082398
C14	1.000	0.13965(17)	-0.04058(15)	0.90462(13)	0.0578(11)
H14	1.000	0.1461	-0.0776	0.937	0.069381
C15	1.000	0.09558(14)	0.04858(13)	0.90216(9)	0.0333(7)
H15	1.000	0.0704	0.0753	0.9331	0.040011
N4	1.000	-0.04244(10)	0.19740(10)	0.79076(5)	0.0150(4)
C16	1.000	-0.03981(12)	0.25390(12)	0.74914(7)	0.0183(5)
H16	1.000	-0.0068	0.3177	0.7505	0.021942
C17	1.000	-0.08130(12)	0.22636(13)	0.70485(7)	0.0193(6)
H17	1.000	-0.0771	0.2689	0.6744	0.023123
C18	1.000	-0.12876(12)	0.13959(13)	0.70281(7)	0.0198(6)
H18	1.000	-0.1602	0.1192	0.6711	0.023749
C19	1.000	-0.13200(12)	0.08171(13)	0.74514(7)	0.0201(6)
H19	1.000	-0.1657	0.0184	0.7447	0.024144
C20	1.000	-0.08814(12)	0.11220(12)	0.78816(7)	0.0168(5)
H20	1.000	-0.0903	0.0694	0.8187	0.020112
O5	0.915(16)	-0.06640(8)	0.18357(8)	0.89453(5)	0.0150(4)
N5	0.915(16)	-0.12123(11)	0.15309(11)	0.91645(6)	0.0256(6)
N5'	0.085(16)	-0.06640(8)	0.18357(8)	0.89453(5)	0.0150(4)
O5'	0.085(16)	-0.12123(11)	0.15309(11)	0.91645(6)	0.0256(6)
Ru2	1.000	0.511573(9)	0.685660(9)	0.881559(5)	0.01156(4)
Cl2	1.000	0.62395(3)	0.60898(3)	0.922428(16)	0.01634(12)
N6	1.000	0.45071(9)	0.54607(9)	0.87372(5)	0.0129(4)
C21	1.000	0.49177(12)	0.46466(11)	0.85703(7)	0.0151(5)
H21	1.000	0.5533	0.4706	0.8495	0.018132
C22	1.000	0.45166(12)	0.37375(12)	0.85004(7)	0.0187(6)

H22	1.000	0.4839	0.3147	0.838	0.022411
C23	1.000	0.36649(13)	0.36531(12)	0.85989(8)	0.0225(6)
H23	1.000	0.3361	0.3002	0.8548	0.027025
C24	1.000	0.32386(13)	0.44803(13)	0.87686(7)	0.0216(6)
H24	1.000	0.2622	0.4438	0.8842	0.025899
C25	1.000	0.36790(12)	0.53676(12)	0.88345(7)	0.0169(5)
H25	1.000	0.337	0.5964	0.8959	0.020267
N7	1.000	0.57321(9)	0.66204(9)	0.81479(5)	0.0125(4)
C26	1.000	0.65679(12)	0.68450(12)	0.81209(7)	0.0163(5)
H26	1.000	0.6876	0.7146	0.8419	0.019606
C27	1.000	0.70086(12)	0.66735(13)	0.76966(7)	0.0193(6)
H27	1.000	0.7625	0.6855	0.7686	0.023128
C28	1.000	0.65884(13)	0.62473(13)	0.72846(7)	0.0221(6)
H28	1.000	0.6898	0.61	0.6975	0.026473
C29	1.000	0.57345(13)	0.60297(13)	0.73090(7)	0.0196(6)
H29	1.000	0.5414	0.5731	0.7014	0.023503
C30	1.000	0.53252(12)	0.62271(11)	0.77422(7)	0.0149(5)
H30	1.000	0.4704	0.6072	0.7755	0.0179
N8	1.000	0.57394(9)	0.82333(9)	0.88685(5)	0.0128(4)
C31	1.000	0.57245(12)	0.88439(12)	0.84634(7)	0.0162(5)
H31	1.000	0.5377	0.8647	0.8157	0.019457
C32	1.000	0.61717(12)	0.97239(12)	0.84620(7)	0.0191(6)
H32	1.000	0.6152	1.0158	0.8158	0.022941
C33	1.000	0.66485(12)	1.00040(12)	0.88839(7)	0.0193(6)
H33	1.000	0.6983	1.064	0.8889	0.023198
C34	1.000	0.66566(12)	0.93915(12)	0.92987(7)	0.0175(5)
H34	1.000	0.6995	0.958	0.961	0.021044
C35	1.000	0.61940(11)	0.85189(12)	0.92794(7)	0.0141(5)
H35	1.000	0.6197	0.8083	0.9583	0.016978
N9	1.000	0.45911(9)	0.70788(9)	0.95118(5)	0.0130(4)
C36	1.000	0.43129(11)	0.79892(11)	0.96428(7)	0.0143(5)
H36	1.000	0.4331	0.8545	0.9394	0.017185
C37	1.000	0.40054(11)	0.81840(12)	1.01055(7)	0.0163(5)
H37	1.000	0.3809	0.8871	1.019	0.019503
C38	1.000	0.39700(12)	0.74228(13)	1.04517(7)	0.0206(6)
H38	1.000	0.3756	0.7549	1.0792	0.024738
C39	1.000	0.42379(13)	0.64823(13)	1.03161(7)	0.0219(6)
H39	1.000	0.4207	0.5912	1.0556	0.026304
C40	1.000	0.45475(12)	0.63342(12)	0.98496(7)	0.0178(5)
H40	1.000	0.4747	0.5652	0.9757	0.021384
O10	0.928(17)	0.41549(8)	0.74765(8)	0.85258(5)	0.0147(4)
N10	0.928(17)	0.35278(11)	0.78575(11)	0.84068(6)	0.0215(5)
N10'	0.072(17)	0.41549(8)	0.74765(8)	0.85258(5)	0.0147(4)
O10'	0.072(17)	0.35278(11)	0.78575(11)	0.84068(6)	0.0215(5)
P1	1.000	-0.11953(3)	-0.14565(3)	0.85856(2)	0.01925(15)
F1	1.000	-0.11863(8)	-0.23195(8)	0.81741(4)	0.0303(4)
F2	1.000	-0.11927(8)	-0.05886(9)	0.89930(6)	0.0455(5)
F3	1.000	-0.19764(7)	-0.19935(7)	0.88386(4)	0.0237(4)
F4	1.000	-0.18428(8)	-0.08305(9)	0.82380(5)	0.0407(5)
F5	1.000	-0.04068(7)	-0.09335(8)	0.83262(5)	0.0329(4)
F6	1.000	-0.05442(8)	-0.20862(8)	0.89335(5)	0.0306(4)
P2	1.000	-0.17765(3)	0.35044(4)	1.03998(2)	0.02543(17)
F7	1.000	-0.18754(10)	0.27141(15)	0.99650(7)	0.0889(8)
F8	1.000	-0.16666(8)	0.42907(8)	1.08472(4)	0.0307(4)
F9	1.000	-0.24336(9)	0.28950(9)	1.07183(7)	0.0576(6)
F10	1.000	-0.25362(9)	0.41583(12)	1.01724(5)	0.0549(6)
F11	1.000	-0.11163(9)	0.41259(11)	1.00936(6)	0.0553(6)
F12	1.000	-0.10097(8)	0.28637(8)	1.06428(6)	0.0427(5)
P3	1.000	0.38727(3)	1.07642(3)	0.916941(17)	0.01516(14)
F13	1.000	0.38741(7)	0.98671(7)	0.87672(4)	0.0209(3)

F14	1.000	0.38565(7)	1.16650(7)	0.95630(4)	0.0245(4)
F15	1.000	0.32392(7)	1.01327(8)	0.94990(4)	0.0261(4)
F16	1.000	0.30600(7)	1.12453(7)	0.88667(4)	0.0211(3)
F17	1.000	0.44911(7)	1.13945(7)	0.88337(4)	0.0205(3)
P4	1.000	0.33619(3)	0.75826(3)	0.710162(18)	0.01481(13)
F18	1.000	0.46680(7)	1.02797(7)	0.94663(4)	0.0231(3)
F19	1.000	0.40694(7)	0.69817(7)	0.68141(4)	0.0198(3)
F20	1.000	0.26533(7)	0.81851(7)	0.73877(4)	0.0215(3)
F21	1.000	0.26291(7)	0.70486(7)	0.67591(4)	0.0210(3)
F22	1.000	0.33204(7)	0.66951(7)	0.75037(4)	0.0221(3)
F23	1.000	0.41003(7)	0.81101(7)	0.74430(4)	0.0209(3)
F24	1.000	0.34104(7)	0.84683(7)	0.67006(4)	0.0216(3)
O3	1.000	-0.00163(17)	0.11090(14)	1.00561(9)	0.0829(9)
H1a	1.000	0.0208(17)	0.0536(11)	1.0026(12)	0.099528
H1b	1.000	0.0232(19)	0.1355(19)	1.0317(8)	0.099528

Atomic displacement parameters for SI:

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru1	0.01319(8)	0.00981(5)	0.01392(7)	-0.00055(5)	0.00265(6)	-0.00135(5)
Cl1	0.0211(3)	0.02128(19)	0.0204(2)	-0.00765(17)	0.00826(20)	-0.00446(17)
N1	0.0140(9)	0.0098(6)	0.0171(8)	-0.0017(5)	-0.0014(7)	-0.0005(5)
C1	0.0175(11)	0.0137(7)	0.0259(11)	-0.0021(7)	-0.0072(9)	-0.0021(7)
C2	0.0173(12)	0.0185(8)	0.0390(13)	0.0024(7)	-0.0110(10)	-0.0030(8)
C3	0.0252(12)	0.0137(8)	0.0290(11)	0.0024(7)	-0.0055(9)	-0.0010(7)
C4	0.0237(12)	0.0115(7)	0.0191(10)	-0.0018(7)	0.0000(8)	-0.0006(6)
C5	0.0177(11)	0.0121(7)	0.0149(9)	-0.0019(6)	-0.0012(8)	-0.0013(6)
N2	0.0126(9)	0.0139(6)	0.0152(8)	0.0000(5)	0.0002(6)	0.0008(5)
C6	0.0126(10)	0.0215(8)	0.0173(9)	-0.0004(7)	0.0018(8)	-0.0002(7)
C7	0.0206(12)	0.0373(11)	0.0167(10)	-0.0014(8)	0.0022(9)	-0.0048(8)
C8	0.0199(12)	0.0400(11)	0.0196(11)	-0.0053(9)	-0.0058(9)	-0.0001(9)
C9	0.0143(11)	0.0270(9)	0.0290(12)	0.0020(7)	-0.0040(9)	0.0038(8)
C10	0.0149(11)	0.0169(7)	0.0258(11)	0.0034(7)	0.0015(8)	-0.0015(7)
N3	0.0136(9)	0.0128(6)	0.0362(10)	0.0007(6)	0.0000(8)	-0.0066(6)
C11	0.0155(11)	0.0233(9)	0.0622(17)	-0.0055(8)	0.0134(11)	-0.0218(10)
C12	0.0130(13)	0.0295(12)	0.129(3)	-0.0065(9)	0.0186(15)	-0.0452(15)
C13	0.0206(15)	0.0173(10)	0.165(4)	0.0072(9)	-0.0312(18)	-0.0273(16)
C14	0.0485(18)	0.0134(9)	0.106(3)	0.0060(10)	-0.0532(18)	-0.0075(12)
C15	0.0340(14)	0.0138(8)	0.0501(15)	0.0021(8)	-0.0216(12)	-0.0029(9)
N4	0.0181(9)	0.0128(6)	0.0144(8)	-0.0012(5)	0.0021(6)	-0.0017(5)
C16	0.0220(11)	0.0147(7)	0.0185(9)	-0.0004(7)	0.0044(8)	0.0009(7)
C17	0.0225(11)	0.0189(8)	0.0166(9)	0.0029(7)	0.0038(8)	0.0033(7)
C18	0.0197(11)	0.0225(8)	0.0171(10)	0.0010(7)	-0.0008(8)	-0.0044(7)
C19	0.0222(11)	0.0175(8)	0.0209(10)	-0.0037(7)	0.0028(9)	-0.0048(7)
C20	0.0208(11)	0.0136(7)	0.0162(9)	-0.0015(7)	0.0043(8)	-0.0007(6)
O5	0.0167(8)	0.0137(5)	0.0147(7)	-0.0011(5)	0.0022(5)	-0.0016(5)
N5	0.0295(11)	0.0253(8)	0.0229(9)	-0.0103(7)	0.0105(8)	-0.0064(7)
N5'	0.0167(8)	0.0137(5)	0.0147(7)	-0.0011(5)	0.0022(5)	-0.0016(5)
O5'	0.0295(11)	0.0253(8)	0.0229(9)	-0.0103(7)	0.0105(8)	-0.0064(7)
Ru2	0.01404(8)	0.00973(5)	0.01088(7)	0.00101(5)	0.00000(6)	-0.00001(5)
Cl2	0.0174(2)	0.01382(16)	0.0174(2)	0.00180(15)	-0.00398(19)	0.00121(15)
N6	0.0149(8)	0.0109(6)	0.0127(7)	0.0008(5)	-0.0007(6)	-0.0003(5)
C21	0.0150(10)	0.0149(7)	0.0155(9)	0.0017(6)	0.0010(8)	-0.0006(6)
C22	0.0206(11)	0.0130(7)	0.0224(10)	0.0011(7)	0.0009(8)	-0.0020(7)
C23	0.0233(12)	0.0146(8)	0.0298(11)	-0.0035(7)	0.0031(9)	-0.0028(7)
C24	0.0163(11)	0.0186(8)	0.0302(11)	-0.0020(7)	0.0041(9)	0.0000(7)
C25	0.0174(11)	0.0144(7)	0.0190(10)	0.0017(7)	0.0030(8)	-0.0008(6)
N7	0.0125(8)	0.0137(6)	0.0113(7)	0.0023(5)	0.0002(6)	0.0004(5)
C26	0.0170(10)	0.0167(7)	0.0150(9)	0.0002(7)	-0.0024(8)	-0.0008(7)
C27	0.0124(11)	0.0271(9)	0.0183(10)	0.0013(7)	0.0008(8)	0.0012(7)
C28	0.0199(12)	0.0306(9)	0.0158(10)	0.0061(8)	0.0019(9)	-0.0001(8)
C29	0.0201(11)	0.0246(9)	0.0138(9)	0.0040(7)	-0.0030(8)	-0.0018(7)
C30	0.0144(10)	0.0160(7)	0.0141(9)	0.0016(6)	-0.0015(8)	-0.0004(6)
N8	0.0143(8)	0.0108(6)	0.0136(7)	0.0007(5)	0.0029(6)	-0.0004(5)
C31	0.0180(11)	0.0158(7)	0.0149(9)	0.0031(7)	0.0017(8)	0.0005(6)
C32	0.0206(11)	0.0142(7)	0.0231(10)	0.0027(7)	0.0074(9)	0.0041(7)
C33	0.0192(11)	0.0121(7)	0.0271(11)	-0.0009(7)	0.0054(9)	-0.0029(7)
C34	0.0155(10)	0.0174(8)	0.0196(10)	0.0003(7)	0.0000(8)	-0.0059(7)
C35	0.0145(10)	0.0144(7)	0.0136(9)	0.0024(6)	0.0016(8)	-0.0017(6)
N9	0.0140(8)	0.0120(6)	0.0128(7)	-0.0003(5)	-0.0010(6)	0.0001(5)
C36	0.0133(10)	0.0132(7)	0.0163(9)	-0.0003(6)	-0.0013(8)	0.0002(6)
C37	0.0164(10)	0.0164(7)	0.0160(9)	-0.0006(7)	0.0009(8)	-0.0035(7)
C38	0.0231(11)	0.0258(9)	0.0130(9)	-0.0022(8)	0.0009(8)	-0.0030(7)
C39	0.0335(13)	0.0180(8)	0.0141(9)	-0.0020(8)	-0.0003(9)	0.0035(7)
C40	0.0254(11)	0.0132(7)	0.0146(9)	0.0008(7)	-0.0023(8)	0.0011(6)

O10	0.0177(8)	0.0137(6)	0.0127(6)	0.0012(5)	0.0005(6)	-0.0004(4)
N10	0.0204(11)	0.0241(8)	0.0196(9)	0.0063(7)	-0.0020(7)	-0.0008(6)
N10'	0.0177(8)	0.0137(6)	0.0127(6)	0.0012(5)	0.0005(6)	-0.0004(4)
O10'	0.0204(11)	0.0241(8)	0.0196(9)	0.0063(7)	-0.0020(7)	-0.0008(6)
P1	0.0158(3)	0.01209(19)	0.0297(3)	0.00007(17)	-0.0003(2)	0.00117(18)
F1	0.0302(7)	0.0339(6)	0.0272(7)	-0.0086(5)	0.0060(5)	-0.0080(5)
F2	0.0344(8)	0.0321(6)	0.0704(10)	-0.0011(6)	0.0069(7)	-0.0312(6)
F3	0.0231(7)	0.0209(5)	0.0276(6)	-0.0005(4)	0.0068(5)	0.0027(4)
F4	0.0186(7)	0.0413(7)	0.0624(10)	0.0051(5)	0.0027(6)	0.0319(6)
F5	0.0175(7)	0.0184(5)	0.0634(9)	-0.0008(4)	0.0073(6)	0.0080(5)
F6	0.0256(7)	0.0343(6)	0.0313(7)	0.0089(5)	-0.0059(6)	0.0049(5)
P2	0.0141(3)	0.0324(3)	0.0295(3)	0.0059(2)	-0.0023(2)	-0.0151(2)
F7	0.0477(11)	0.1179(15)	0.0999(15)	0.0177(10)	-0.0113(10)	-0.0932(12)
F8	0.0300(7)	0.0319(6)	0.0293(7)	0.0002(5)	-0.0071(6)	-0.0126(5)
F9	0.0324(9)	0.0289(7)	0.1141(14)	-0.0056(6)	0.0311(9)	-0.0121(7)
F10	0.0333(9)	0.0942(11)	0.0356(9)	0.0345(8)	-0.0168(7)	-0.0173(8)
F11	0.0472(9)	0.0621(9)	0.0596(10)	0.0252(7)	0.0349(8)	0.0187(7)
F12	0.0226(8)	0.0268(6)	0.0780(11)	0.0074(5)	-0.0044(7)	0.0046(6)
P3	0.0175(3)	0.01503(19)	0.0129(2)	0.00066(17)	0.0008(2)	0.00107(16)
F13	0.0235(7)	0.0163(5)	0.0226(6)	0.0001(4)	-0.0023(5)	-0.0034(4)
F14	0.0314(7)	0.0260(5)	0.0160(6)	0.0035(5)	0.0002(5)	-0.0052(4)
F15	0.0257(7)	0.0344(6)	0.0183(6)	-0.0070(5)	0.0014(5)	0.0085(5)
F16	0.0220(7)	0.0234(5)	0.0177(6)	0.0069(4)	-0.0010(5)	0.0003(4)
F17	0.0242(7)	0.0193(5)	0.0183(6)	-0.0037(4)	0.0041(5)	0.0006(4)
P4	0.0139(3)	0.01392(18)	0.0167(2)	0.00177(16)	0.0014(2)	0.00103(16)
F18	0.0210(7)	0.0203(5)	0.0271(6)	0.0000(4)	-0.0083(5)	0.0038(4)
F19	0.0170(6)	0.0166(5)	0.0261(6)	0.0034(4)	0.0048(5)	-0.0022(4)
F20	0.0190(6)	0.0239(5)	0.0219(6)	0.0061(4)	0.0037(5)	-0.0028(4)
F21	0.0174(6)	0.0209(5)	0.0242(6)	0.0000(4)	-0.0036(5)	-0.0023(4)
F22	0.0178(6)	0.0219(5)	0.0266(6)	-0.0001(4)	0.0002(5)	0.0097(4)
F23	0.0179(6)	0.0212(5)	0.0234(6)	-0.0014(4)	-0.0016(5)	-0.0019(4)
F24	0.0224(7)	0.0178(5)	0.0248(6)	0.0025(4)	0.0034(5)	0.0064(4)
O3	0.135(2)	0.0479(11)	0.0610(15)	-0.0509(13)	-0.0464(14)	0.0261(10)

Distances and angles for SI:

	X-ray	DFT
Ru1-Cl1	2.2782(5)	2.3015
Ru1-N1	2.0949(13)	2.1241
Ru1-N2	2.0958(14)	2.1209
Ru1-N3	2.0932(14)	2.1192
Ru1-N4	2.1023(14)	2.1344
Ru1-O5	1.8630(13)	1.9036
N1-C1	1.345(2)	1.3528
N1-H1	2.0259	2.0896
N1-C5	1.348(2)	1.3541
N1-H5	2.0325	2.0857
C1-H1	1	1.0882
C1-C2	1.382(3)	1.3908
C2-H2	1	1.0898
C2-C3	1.384(3)	1.3918
C3-H3	1	1.0892
C3-C4	1.378(3)	1.3953
C4-H4	1	1.0887
C4-C5	1.382(2)	1.3885
C5-H5	1	1.0871
N2-C6	1.347(2)	1.3533
N2-C10	1.341(2)	1.3529
C6-H6	1	1.0886
C6-C7	1.373(3)	1.3872
C7-H7	1	1.0879
C7-C8	1.378(3)	1.3906
C8-H8	1	1.0901
C8-C9	1.376(3)	1.3924
C9-H9	1	1.0892
C9-C10	1.375(3)	1.3892
C10-H10	1	1.0865
N3-C11	1.342(3)	1.3536
N3-H11	2.0303	2.081
N3-C15	1.346(3)	1.3548
N3-H15	2.0306	2.0939
C11-H11	1	1.0905
C11-C12	1.387(3)	1.3898
C12-H12	1	1.0921
C12-C13	1.373(5)	1.3947
C13-H13	1	1.0894
C13-C14	1.358(5)	1.3906
C14-H14	1	1.0903
C14-C15	1.381(3)	1.3882
C15-H15	1	1.0937
N4-C16	1.349(2)	1.3542
N4-H16	2.0317	2.0872
N4-C20	1.348(2)	1.3548
N4-H20	2.0278	2.0927
C16-H16	1	1.0889
C16-C17	1.377(3)	1.3893
C17-H17	1	1.0891
C17-C18	1.381(2)	1.3932
C18-H18	1	1.0921
C18-C19	1.376(3)	1.3928
C19-H19	1	1.0909
C19-C20	1.377(3)	1.3886
C20-H20	1	1.0864

O5-N5	1.140(2)	1.1514
Ru2-Cl2	2.2798(5)	2.295
Ru2-N6	2.1061(13)	2.1363
Ru2-N7	2.0954(15)	2.1252
Ru2-N8	2.0900(13)	2.1227
Ru2-N9	2.0930(15)	2.1246
Ru2-O10	1.8619(12)	1.8962
N6-C21	1.353(2)	1.3557
N6-H21	2.0342	2.0886
N6-C25	1.345(2)	1.3553
N6-H25	2.0251	2.093
C21-H21	1	1.0883
C21-C22	1.380(2)	1.3892
C22-H22	1	1.0891
C22-C23	1.381(3)	1.3939
C23-H23	1	1.0918
C23-C24	1.382(3)	1.3935
C24-H24	1	1.0893
C24-C25	1.383(2)	1.3895
C25-H25	1	1.0899
N7-C26	1.353(2)	1.356
N7-H26	2.0342	2.0918
N7-C30	1.343(2)	1.3544
N7-H30	2.0251	2.0877
C26-H26	1	1.0881
C26-C27	1.376(3)	1.388
C27-H27	1	1.0909
C27-C28	1.383(3)	1.393
C28-H28	1	1.0882
C28-C29	1.378(3)	1.3942
C29-H29	1	1.0889
C29-C30	1.377(3)	1.3867
C30-H30	1	1.0895
N8-C31	1.357(2)	1.3571
N8-H31	2.0393	2.0922
N8-C35	1.340(2)	1.35
N8-H35	2.0221	2.0804
C31-H31	1	1.0919
C31-C32	1.372(2)	1.3859
C32-H32	1	1.0899
C32-C33	1.379(3)	1.3948
C33-H33	1	1.0911
C33-C34	1.380(3)	1.3908
C34-H34	1	1.0897
C34-C35	1.376(2)	1.39
C35-H35	1	1.0867
N9-C36	1.347(2)	1.3532
N9-H36	2.0272	2.0919
N9-C40	1.350(2)	1.3525
N9-H40	2.0316	2.0798
C36-H36	1	1.0878
C36-C37	1.375(3)	1.3885
C37-H37	1	1.0869
C37-C38	1.381(2)	1.3901
C38-H38	1	1.0915
C38-C39	1.382(3)	1.3927
C39-H39	1	1.0888
C39-C40	1.375(3)	1.3874
C40-H40	1	1.0882
O10-N10	1.142(2)	1.1497

P1-F1	1.5970(12)	1.6465
P1-F2	1.5934(14)	1.6597
P1-F3	1.5999(12)	1.6465
P1-F4	1.5871(13)	1.6402
P1-F5	1.6086(13)	1.6471
P1-F6	1.5935(13)	1.6434
P2-F7	1.575(2)	1.6394
P2-F8	1.5982(13)	1.663
P2-F9	1.5938(16)	1.6564
P2-F10	1.5804(15)	1.6317
P2-F11	1.5871(16)	1.6417
P2-F12	1.5941(13)	1.6534
P3-F13	1.6132(11)	1.6613
P3-F14	1.6025(11)	1.6472
P3-F15	1.6018(12)	1.6462
P3-F16	1.6155(11)	1.6609
P3-F17	1.5952(11)	1.6359
P3-F18	1.5892(11)	1.6302
P4-F19	1.5984(11)	1.637
P4-F20	1.5987(11)	1.6397
P4-F21	1.6073(11)	1.6531
P4-F22	1.6066(11)	1.6528
P4-F23	1.6078(11)	1.6526
P4-F24	1.6037(11)	1.6511
O3-H1a	0.850(18)	0.9816
O3-H1b	0.85(2)	0.9814
Cl1-Ru1-N1	89.54(4)	89.353
Cl1-Ru1-N2	88.56(4)	88.9656
Cl1-Ru1-N3	88.91(4)	88.4635
Cl1-Ru1-N4	90.32(4)	89.6152
Cl1-Ru1-O5	178.93(4)	178.978
N1-Ru1-N2	89.15(5)	89.1424
N1-Ru1-N3	178.45(6)	178.2726
N1-Ru1-N4	90.29(5)	89.9357
N1-Ru1-O5	90.11(5)	90.7801
N2-Ru1-N3	90.81(6)	90.417
N2-Ru1-N4	178.76(5)	177.8782
N2-Ru1-O5	90.42(5)	90.5252
N3-Ru1-N4	89.72(6)	90.4486
N3-Ru1-O5	91.43(6)	90.894
N4-Ru1-O5	90.69(5)	91.3983
Ru1-N1-C1	119.78(10)	119.5033
Ru1-N1-H1	94.2536	92.0228
Ru1-N1-C5	121.51(12)	121.5375
Ru1-N1-H5	96.1332	93.8971
C1-N1-H1	25.6211	27.5573
C1-N1-C5	118.60(14)	118.858
C1-N1-H5	144.0391	146.5431
H1-N1-C5	144.207	146.4079
H1-N1-H5	169.604	174.0785
C5-N1-H5	25.445	27.6851
N1-C1-H1	118.8303	117.3341
N1-C1-C2	122.34(16)	122.0736
H1-C1-C2	118.8289	120.5914
C1-C2-H2	120.5544	118.6555
C1-C2-C3	118.89(19)	119.1199
H2-C2-C3	120.5544	122.2242
C2-C3-H3	120.5493	121.2462
C2-C3-C4	118.90(17)	118.751
H3-C3-C4	120.5483	120.0026

C3-C4-H4	120.213	121.2604
C3-C4-C5	119.57(16)	119.3327
H4-C4-C5	120.2139	119.3953
N1-C5-C4	121.68(17)	121.8489
N1-C5-H5	119.163	116.9569
C4-C5-H5	119.1615	121.188
Ru1-N2-C6	119.81(12)	119.5633
Ru1-N2-H6	94.2877	92.2453
Ru1-N2-C10	121.90(12)	121.679
Ru1-N2-H10	96.2658	94.1436
C6-N2-H6	25.5423	27.3641
C6-N2-C10	118.28(15)	118.7087
C6-N2-H10	143.9278	146.289
H6-N2-C10	143.8153	146.0647
H6-N2-H10	169.4105	173.5139
C10-N2-H10	25.6534	27.6013
N2-C6-H6	118.9572	117.7886
N2-C6-C7	122.09(18)	122.0648
H6-C6-C7	118.9568	120.1444
C6-C7-H7	120.3562	118.5639
C6-C7-C8	119.29(19)	119.3515
H7-C7-C8	120.358	122.0789
C7-C8-H8	120.5449	120.9636
C7-C8-C9	118.91(19)	118.5521
H8-C8-C9	120.5449	120.4842
C8-C9-H9	120.4427	121.9872
C8-C9-C10	119.11(19)	119.4335
H9-C9-C10	120.4433	118.5792
N2-C10-C9	122.31(18)	121.8474
N2-C10-H10	118.8467	117.1641
C9-C10-H10	118.8473	120.9884
Ru1-N3-C11	121.44(13)	121.2279
Ru1-N3-H11	96.0541	93.2459
Ru1-N3-C15	119.79(13)	119.5993
Ru1-N3-H15	94.3279	91.9383
C11-N3-H11	25.3956	28.0111
C11-N3-C15	118.75(16)	119.1363
C11-N3-H15	144.2311	146.8264
H11-N3-C15	144.1484	147.1444
H11-N3-H15	169.6138	174.7792
C15-N3-H15	25.478	27.6968
N3-C11-H11	119.4586	116.3282
N3-C11-C12	121.1(2)	121.7894
H11-C11-C12	119.4565	121.879
C11-C12-H12	120.0988	119.6357
C11-C12-C13	119.8(3)	119.0464
H12-C12-C13	120.0987	121.3167
C12-C13-H13	120.5789	121.2251
C12-C13-C14	118.8(2)	119.0241
H13-C13-C14	120.5792	119.7497
C13-C14-H14	120.1099	121.3237
C13-C14-C15	119.8(3)	119.2452
H14-C14-C15	120.1087	119.4304
N3-C15-C14	121.7(2)	121.7341
N3-C15-H15	119.1347	117.1515
C14-C15-H15	119.1351	121.1124
Ru1-N4-C16	122.58(11)	122.3325
Ru1-N4-H16	97.0889	94.6364
Ru1-N4-C20	119.50(11)	119.0807
Ru1-N4-H20	93.8592	91.705

C16-N4-H16	25.4944	27.7095
C16-N4-C20	117.92(15)	118.5848
C16-N4-H20	143.5584	145.9597
H16-N4-C20	143.4126	146.2807
H16-N4-H20	169.051	173.51
C20-N4-H20	25.6385	27.3916
N4-C16-H16	119.0156	116.9607
N4-C16-C17	121.97(15)	121.7332
H16-C16-C17	119.0147	121.2769
C16-C17-H17	120.2158	118.5686
C16-C17-C18	119.57(17)	119.6776
H17-C17-C18	120.216	121.7374
C17-C18-H18	120.5949	120.1951
C17-C18-C19	118.81(17)	118.5277
H18-C18-C19	120.5944	121.2721
C18-C19-H19	120.4737	122.4087
C18-C19-C20	119.05(16)	119.0833
H19-C19-C20	120.4736	118.5049
N4-C20-C19	122.66(16)	122.3726
N4-C20-H20	118.6692	117.5965
C19-C20-H20	118.6688	120.0266
Ru1-O5-N5	178.12(12)	179.0422
Cl2-Ru2-N6	89.24(4)	89.2108
Cl2-Ru2-N7	87.87(4)	87.8854
Cl2-Ru2-N8	90.80(4)	90.7965
Cl2-Ru2-N9	88.00(4)	87.5402
Cl2-Ru2-O10	175.73(4)	175.6313
N6-Ru2-N7	90.38(5)	90
N6-Ru2-N8	177.93(6)	177.2904
N6-Ru2-N9	91.10(5)	91.3973
N6-Ru2-O10	89.88(5)	90.0559
N7-Ru2-N8	87.55(5)	87.2897
N7-Ru2-N9	175.59(6)	175.197
N7-Ru2-O10	96.31(5)	96.4218
N8-Ru2-N9	90.97(5)	91.3102
N8-Ru2-O10	90.24(5)	90.1394
N9-Ru2-O10	87.85(5)	88.1722
Ru2-N6-C21	121.77(12)	121.7724
Ru2-N6-H21	96.2923	94.1796
Ru2-N6-C25	120.16(10)	119.6554
Ru2-N6-H25	94.5208	92.2017
C21-N6-H21	25.499	27.6604
C21-N6-C25	118.02(14)	118.4851
C21-N6-H25	143.6801	146.0153
H21-N6-C25	143.5148	146.1389
H21-N6-H25	169.1791	173.5138
C25-N6-H25	25.6643	27.5603
N6-C21-H21	118.8721	117.007
N6-C21-C22	122.26(17)	122.1431
H21-C21-C22	118.8722	120.8481
C21-C22-H22	120.4151	119.0205
C21-C22-C23	119.17(16)	119.3796
H22-C22-C23	120.4155	121.5869
C22-C23-H23	120.463	120.4658
C22-C23-C24	119.07(16)	118.4597
H23-C23-C24	120.4622	121.0556
C23-C24-H24	120.5525	122.0891
C23-C24-C25	118.89(18)	119.4675
H24-C24-C25	120.5525	118.4378
N6-C25-C24	122.59(16)	122.0595

N6-C25-H25	118.7071	117.3171
C24-C25-H25	118.7073	120.6108
Ru2-N7-C26	119.99(11)	119.9891
Ru2-N7-H26	94.5049	92.4896
Ru2-N7-C30	121.81(12)	121.1663
Ru2-N7-H30	96.2229	93.5551
C26-N7-H26	25.4962	27.5339
C26-N7-C30	118.19(15)	118.8053
C26-N7-H30	143.7905	146.454
H26-N7-C30	143.6829	146.3342
H26-N7-H30	169.2512	173.6868
C30-N7-H30	25.6114	27.7264
N7-C26-H26	118.8806	117.2897
N7-C26-C27	122.24(16)	121.955
H26-C26-C27	118.8814	120.7541
C26-C27-H27	120.4405	118.584
C26-C27-C28	119.12(18)	119.185
H27-C27-C28	120.4385	122.2269
C27-C28-H28	120.6315	121.401
C27-C28-C29	118.74(18)	118.7756
H28-C28-C29	120.6312	119.7999
C28-C29-H29	120.2413	120.5732
C28-C29-C30	119.52(17)	119.2905
H29-C29-C30	120.242	120.0957
N7-C30-C29	122.17(17)	121.9277
N7-C30-H30	118.9127	116.9383
C29-C30-H30	118.914	121.1186
Ru2-N8-C31	119.10(11)	118.7827
Ru2-N8-H31	93.7851	91.164
Ru2-N8-C35	122.58(11)	122.245
Ru2-N8-H35	96.9931	94.5917
C31-N8-H31	25.392	27.7222
C31-N8-C35	118.22(14)	118.8278
C31-N8-H35	143.8801	146.5909
H31-N8-C35	143.6069	146.5418
H31-N8-H35	169.2013	174.1704
C35-N8-H35	25.6686	27.781
N8-C31-H31	119.0194	116.9578
N8-C31-C32	121.96(16)	121.9068
H31-C31-C32	119.0187	121.1321
C31-C32-H32	120.3039	119.9614
C31-C32-C33	119.39(17)	119.2399
H32-C32-C33	120.3032	120.7914
C32-C33-H33	120.589	119.7842
C32-C33-C34	118.82(16)	118.7656
H33-C33-C34	120.5908	121.4495
C33-C34-H34	120.3574	122.6061
C33-C34-C35	119.28(17)	119.2232
H34-C34-C35	120.3594	118.1664
N8-C35-C34	122.30(16)	122.0035
N8-C35-H35	118.8499	116.8384
C34-C35-H35	118.8501	121.158
Ru2-N9-C36	120.41(11)	119.8577
Ru2-N9-H36	94.819	92.4293
Ru2-N9-C40	121.69(11)	121.5867
Ru2-N9-H40	96.1922	93.7225
C36-N9-H36	25.6302	27.4585
C36-N9-C40	117.86(15)	118.512
C36-N9-H40	143.3815	146.4169
H36-N9-C40	143.4815	145.9684

H36-N9-H40	168.9835	173.7833
C40-N9-H40	25.5236	27.9263
N9-C36-H36	118.7312	117.5407
N9-C36-C37	122.54(15)	122.0362
H36-C36-C37	118.7311	120.4124
C36-C37-H37	120.289	118.2239
C36-C37-C38	119.42(16)	119.5979
H37-C37-C38	120.2891	122.1635
C37-C38-H38	120.8359	121.2796
C37-C38-C39	118.33(17)	118.1847
H38-C38-C39	120.8356	120.5352
C38-C39-H39	120.1727	121.5691
C38-C39-C40	119.65(16)	119.6339
H39-C39-C40	120.1732	118.7633
N9-C40-C39	122.18(15)	122.0026
N9-C40-H40	118.9116	116.4746
C39-C40-H40	118.9104	121.5198
Ru2-O10-N10	171.43(13)	173.225
F1-P1-F2	179.20(7)	179.6412
F1-P1-F3	89.86(6)	90.1161
F1-P1-F4	90.20(7)	90.0594
F1-P1-F5	89.22(7)	89.791
F1-P1-F6	89.68(6)	90.366
F2-P1-F3	90.94(7)	90.2381
F2-P1-F4	89.86(7)	89.8799
F2-P1-F5	89.98(7)	89.8554
F2-P1-F6	90.26(7)	89.6945
F3-P1-F4	90.07(6)	90.339
F3-P1-F5	179.04(6)	179.4128
F3-P1-F6	89.99(6)	89.6992
F4-P1-F5	90.20(7)	90.2408
F4-P1-F6	179.87(8)	179.573
F5-P1-F6	89.74(6)	89.7216
F7-P2-F8	178.91(9)	178.9865
F7-P2-F9	90.37(9)	90.4921
F7-P2-F10	92.31(9)	91.243
F7-P2-F11	90.91(9)	90.6112
F7-P2-F12	89.27(8)	90.0256
F8-P2-F9	89.27(8)	89.1639
F8-P2-F10	88.71(7)	89.7132
F8-P2-F11	89.45(7)	89.7186
F8-P2-F12	89.71(7)	89.0165
F9-P2-F10	89.58(8)	90.4946
F9-P2-F11	178.69(9)	178.6014
F9-P2-F12	90.16(7)	89.2093
F10-P2-F11	90.64(8)	90.3409
F10-P2-F12	178.40(8)	178.6998
F11-P2-F12	89.58(8)	89.9305
F13-P3-F14	178.91(6)	178.7003
F13-P3-F15	89.66(6)	89.7306
F13-P3-F16	89.28(6)	89.1862
F13-P3-F17	89.94(6)	89.8603
F13-P3-F18	90.27(6)	90.2463
F14-P3-F15	90.38(6)	90.4342
F14-P3-F16	89.63(6)	89.5276
F14-P3-F17	90.01(6)	89.9497
F14-P3-F18	90.82(6)	91.0419
F15-P3-F16	89.39(6)	89.0477
F15-P3-F17	179.02(6)	178.8089
F15-P3-F18	90.22(6)	90.3036

F16-P3-F17	89.71(6)	89.828
F16-P3-F18	179.40(6)	179.1402
F17-P3-F18	90.68(6)	90.8168
F19-P4-F20	179.83(6)	179.8052
F19-P4-F21	89.88(6)	89.6627
F19-P4-F22	90.02(6)	89.9784
F19-P4-F23	89.68(6)	89.9874
F19-P4-F24	89.71(6)	89.7751
F20-P4-F21	90.04(6)	90.1574
F20-P4-F22	90.13(6)	90.0935
F20-P4-F23	90.40(6)	90.1921
F20-P4-F24	90.14(6)	90.1525
F21-P4-F22	90.17(6)	90.053
F21-P4-F23	179.54(6)	179.5621
F21-P4-F24	90.11(6)	89.7876
F22-P4-F23	89.70(6)	90.2101
F22-P4-F24	179.61(6)	179.7072
F23-P4-F24	90.02(6)	89.9478
H3a-O3-H3b	105(3)	102.6607

Atomic positions for SII:

	Occ	x	y	z	Ueq/Uiso (Å^2)
Ru1	1	0.020971(16)	0.23149(2)	0.861134(10)	0.01764(9)
Cl1	1	0.13068(5)	0.29890(6)	0.81782(3)	0.0237(3)
N1	1	-0.03828(15)	0.37138(19)	0.85936(9)	0.0159(10)
C1	1	-0.12278(19)	0.3778(3)	0.84911(12)	0.0251(13)
H1	1	-0.1553	0.316	0.84	0.030154
C2	1	-0.1653(2)	0.4670(3)	0.85084(13)	0.0294(14)
H2	1	-0.2282	0.4697	0.8441	0.035313
C3	1	-0.1206(2)	0.5525(2)	0.86187(12)	0.0232(13)
H3	1	-0.1509	0.6178	0.8632	0.027806
C4	1	-0.0343(2)	0.5481(2)	0.87104(12)	0.0216(13)
H4	1	-0.0009	0.6098	0.8789	0.025929
C5	1	0.0055(2)	0.4567(2)	0.86917(11)	0.0187(12)
H5	1	0.0685	0.4532	0.8752	0.02249
N2	1	0.08644(15)	0.27387(18)	0.92678(9)	0.0186(9)
C6	1	0.04503(19)	0.3193(2)	0.96383(12)	0.0215(12)
H6	1	-0.0179	0.3285	0.9598	0.025787
C7	1	0.0860(2)	0.3531(2)	1.00663(12)	0.0283(14)
H7	1	0.0533	0.3875	1.0328	0.033971
C8	1	0.1724(2)	0.3394(2)	1.01319(13)	0.0284(14)
H8	1	0.2032	0.3638	1.0441	0.034108
C9	1	0.2155(2)	0.2917(2)	0.97671(13)	0.0264(13)
H9	1	0.2781	0.2798	0.9808	0.031706
C10	1	0.17085(19)	0.2601(2)	0.93410(12)	0.0224(12)
H10	1	0.2027	0.2257	0.9076	0.026869
N3	1	0.08808(16)	0.0957(2)	0.85912(12)	0.0269(11)
C11	1	0.1193(2)	0.0618(3)	0.81609(17)	0.0396(17)
H11	1	0.1095	0.1003	0.7845	0.047479
C12	1	0.1645(2)	-0.0254(3)	0.8157(2)	0.074(3)
H12	1	0.1876	-0.0491	0.7837	0.088858
C13	1	0.1787(3)	-0.0805(4)	0.8577(3)	0.109(4)
H13	1	0.2111	-0.1444	0.8569	0.131133

C14	1	0.1470(3)	-0.0453(3)	0.9009(2)	0.105(3)
H14	1	0.1566	-0.0834	0.9326	0.125742
C15	1	0.1017(2)	0.0427(3)	0.90104(17)	0.0556(19)
H15	1	0.0786	0.0673	0.933	0.066741
N4	1	-0.04266(14)	0.19359(20)	0.79325(9)	0.0186(9)
C16	1	-0.03901(18)	0.2512(2)	0.75208(12)	0.0188(12)
H16	1	-0.0052	0.3141	0.7539	0.022563
C17	1	-0.08028(18)	0.2261(2)	0.70774(12)	0.0200(12)
H17	1	-0.076	0.2701	0.6779	0.023946
C18	1	-0.12734(19)	0.1404(3)	0.70476(13)	0.0260(13)
H18	1	-0.1578	0.1211	0.6728	0.031207
C19	1	-0.13200(18)	0.0807(2)	0.74676(13)	0.0232(13)
H19	1	-0.166	0.0178	0.7458	0.027797
C20	1	-0.08901(18)	0.1098(2)	0.78954(13)	0.0202(12)
H20	1	-0.0922	0.0664	0.8197	0.024186
N5'	0.650(13)	-0.0651(4)	0.1817(8)	0.8968(2)	0.014(2)
O5'	0.650(13)	-0.1191(3)	0.1517(4)	0.91700(18)	0.041(2)
N5	0.350(13)	-0.0416(7)	0.1337(11)	0.8969(3)	0.037(4)
O5	0.350(13)	-0.0869(9)	0.1923(14)	0.9034(5)	0.049(5)
Ru2	1	0.506550(16)	0.68920(2)	0.881866(10)	0.01713(9)
Cl2	1	0.61820(5)	0.61190(6)	0.92361(3)	0.0236(3)
N6	1	0.44732(16)	0.54836(19)	0.87426(9)	0.0171(10)
C21	1	0.4896(2)	0.4683(2)	0.85846(12)	0.0199(12)
H21	1	0.5511	0.4756	0.8512	0.02391
C22	1	0.4515(2)	0.3763(3)	0.85181(12)	0.0249(13)
H22	1	0.4846	0.3184	0.8394	0.029873
C23	1	0.3673(2)	0.3660(3)	0.86264(13)	0.0303(14)
H23	1	0.3388	0.2997	0.8594	0.036404
C24	1	0.3227(2)	0.4470(3)	0.87786(13)	0.0345(15)
H24	1	0.2609	0.4416	0.8845	0.041355
C25	1	0.3647(2)	0.5361(2)	0.88387(12)	0.0244(13)
H25	1	0.3323	0.5947	0.896	0.029248
N7	1	0.57089(15)	0.66349(18)	0.81586(9)	0.0169(10)
C26	1	0.65434(19)	0.6841(2)	0.81368(12)	0.0207(12)
H26	1	0.685	0.7119	0.8439	0.024897
C27	1	0.6988(2)	0.6681(2)	0.77128(12)	0.0237(13)
H27	1	0.7604	0.6862	0.7705	0.028478
C28	1	0.6577(2)	0.6267(2)	0.72955(13)	0.0264(13)
H28	1	0.6891	0.6124	0.6987	0.031687
C29	1	0.57222(20)	0.6058(2)	0.73208(13)	0.0236(13)
H29	1	0.5405	0.5762	0.7027	0.028311
C30	1	0.5308(2)	0.6259(2)	0.77506(12)	0.0194(12)
H30	1	0.4684	0.6119	0.776	0.023306
N8	1	0.57121(14)	0.82582(18)	0.88675(9)	0.0143(9)
C31	1	0.57190(19)	0.8854(2)	0.84628(12)	0.0192(12)
H31	1	0.5378	0.8663	0.8156	0.023006
C32	1	0.61873(19)	0.9722(2)	0.84652(13)	0.0210(13)
H32	1	0.6179	1.0157	0.8163	0.02524
C33	1	0.66668(19)	0.9988(2)	0.88841(13)	0.0232(13)
H33	1	0.7017	1.0609	0.8889	0.027794
C34	1	0.66521(19)	0.9378(2)	0.92968(12)	0.0182(12)
H34	1	0.6989	0.9554	0.9608	0.021796
C35	1	0.61733(18)	0.8534(2)	0.92757(12)	0.0158(12)
H35	1	0.6165	0.8099	0.9578	0.019007
N9	1	0.45661(14)	0.70914(19)	0.95301(9)	0.0165(10)
C36	1	0.43167(18)	0.7997(3)	0.96751(13)	0.0243(13)
H36	1	0.4356	0.8565	0.9437	0.029202
C37	1	0.40089(18)	0.8174(3)	1.01392(13)	0.0269(13)
H37	1	0.3836	0.886	1.0237	0.032337
C38	1	0.39419(19)	0.7395(3)	1.04677(13)	0.0289(13)

H38	1	0.3721	0.7505	1.0808	0.034636
C39	1	0.4183(2)	0.6465(3)	1.03202(13)	0.0269(14)
H39	1	0.413	0.5886	1.055	0.032256
C40	1	0.44986(19)	0.6331(3)	0.98545(12)	0.0229(13)
H40	1	0.4683	0.5651	0.9753	0.027529
N10'	0.398(9)	0.4152(6)	0.7336(7)	0.8517(4)	0.025(2)
O10'	0.398(9)	0.3508(5)	0.7827(4)	0.8409(2)	0.025(3)
N10	0.602(9)	0.3985(4)	0.7621(5)	0.8691(3)	0.044(2)
O10	0.602(9)	0.4122(4)	0.7651(4)	0.8358(2)	0.049(2)
P1	1	-0.11980(6)	-0.14964(7)	0.85768(4)	0.0276(4)
F1	1	-0.11786(10)	-0.23475(14)	0.81585(7)	0.0359(7)
F2	1	-0.12133(11)	-0.06486(15)	0.89895(9)	0.0558(9)
F3	1	-0.19854(10)	-0.20488(13)	0.88227(6)	0.0295(7)
F4	1	-0.18467(11)	-0.08715(15)	0.82302(8)	0.0468(9)
F5	1	-0.04078(11)	-0.09637(13)	0.83261(8)	0.0434(8)
F6	1	-0.05519(10)	-0.21269(13)	0.89217(7)	0.0345(7)
P2	1	-0.17534(6)	0.35410(8)	1.03862(4)	0.0330(4)
F7	1	-0.18127(13)	0.2849(2)	0.99130(10)	0.1053(13)
F8	1	-0.16837(11)	0.42409(14)	1.08669(7)	0.0382(8)
F9	1	-0.24570(11)	0.29024(15)	1.06521(9)	0.0674(10)
F10	1	-0.24793(12)	0.42418(17)	1.01605(8)	0.0558(10)
F11	1	-0.10410(12)	0.41966(16)	1.01347(8)	0.0538(9)
F12	1	-0.10254(11)	0.28490(15)	1.06225(9)	0.0601(10)
P3	1	0.38862(5)	1.07507(7)	0.91658(3)	0.0213(3)
F13	1	0.38877(10)	0.98492(13)	0.87703(6)	0.0267(7)
F14	1	0.38771(11)	1.16517(13)	0.95583(6)	0.0283(7)
F15	1	0.32459(11)	1.01320(14)	0.94981(6)	0.0341(7)
F16	1	0.30783(10)	1.12306(13)	0.88617(6)	0.0269(7)
F17	1	0.45148(10)	1.13689(13)	0.88310(6)	0.0261(7)
P4	1	0.33508(5)	0.76064(7)	0.70798(3)	0.0229(3)
F18	1	0.46761(10)	1.02656(13)	0.94636(7)	0.0296(7)
F19	1	0.40526(10)	0.70034(12)	0.67882(6)	0.0281(7)
F20	1	0.26428(10)	0.82014(13)	0.73695(7)	0.0333(7)
F21	1	0.26151(10)	0.70651(13)	0.67447(6)	0.0279(7)
F22	1	0.33214(10)	0.67243(13)	0.74815(7)	0.0286(7)
F23	1	0.40916(10)	0.81418(13)	0.74087(7)	0.0327(7)
F24	1	0.33827(11)	0.84829(13)	0.66758(7)	0.0334(7)
O3	1	0.0039(3)	0.1073(4)	1.00598(13)	0.1111(12)
H3a	1	0.0491(10)	0.091(3)	1.0107(16)	0.133269
H3b	1	-0.009(3)	0.129(3)	1.0303(9)	0.133269

Ru1	0.01798(15)	0.01520(16)	0.01990(17)	-0.00078(13)	0.00295(12)	-0.00115(14)
Cl1	0.0223(4)	0.0252(5)	0.0241(5)	-0.0058(4)	0.0071(4)	-0.0034(4)
N1	0.0127(15)	0.0171(17)	0.0178(17)	-0.0005(13)	0.0018(13)	-0.0059(13)
C1	0.019(2)	0.023(2)	0.034(2)	-0.0028(17)	-0.0007(17)	-0.0099(18)
C2	0.021(2)	0.023(2)	0.044(3)	0.0051(18)	-0.0122(19)	-0.0050(19)
C3	0.029(2)	0.014(2)	0.026(2)	0.0006(17)	-0.0046(18)	-0.0025(17)
C4	0.027(2)	0.016(2)	0.022(2)	-0.0027(17)	0.0017(17)	0.0015(17)
C5	0.0183(19)	0.022(2)	0.016(2)	-0.0031(17)	-0.0049(17)	-0.0006(16)
N2	0.0167(15)	0.0158(16)	0.0233(17)	-0.0006(13)	0.0019(13)	0.0032(13)
C6	0.0159(18)	0.025(2)	0.024(2)	0.0028(17)	0.0058(17)	-0.0019(18)
C7	0.030(2)	0.041(3)	0.015(2)	-0.0051(19)	0.0059(18)	-0.0056(18)
C8	0.019(2)	0.042(3)	0.025(2)	-0.0084(18)	0.0032(18)	-0.0110(19)
C9	0.0162(18)	0.029(2)	0.034(2)	0.0052(17)	-0.0010(18)	0.0048(18)
C10	0.0194(19)	0.016(2)	0.032(2)	0.0024(16)	0.0012(17)	0.0007(17)
N3	0.0225(17)	0.0112(18)	0.046(2)	-0.0006(14)	-0.0141(17)	-0.0088(16)
C11	0.019(2)	0.020(2)	0.080(4)	-0.0027(18)	0.013(2)	-0.022(2)
C12	0.022(3)	0.031(3)	0.170(7)	-0.010(2)	0.016(3)	-0.044(3)
C13	0.029(3)	0.020(4)	0.273(10)	0.004(2)	-0.062(5)	-0.051(5)

C14	0.116(5)	0.011(3)	0.178(7)	-0.004(3)	-0.123(5)	0.000(3)
C15	0.076(3)	0.017(3)	0.069(4)	-0.002(2)	-0.051(3)	-0.006(2)
N4	0.0183(15)	0.0140(16)	0.0235(18)	0.0030(13)	-0.0016(13)	0.0029(14)
C16	0.0254(19)	0.014(2)	0.018(2)	0.0009(15)	0.0031(16)	0.0036(16)
C17	0.0206(18)	0.020(2)	0.019(2)	0.0060(17)	0.0040(16)	0.0069(17)
C18	0.024(2)	0.030(2)	0.024(2)	0.0006(18)	-0.0004(18)	-0.0102(19)
C19	0.021(2)	0.017(2)	0.032(2)	-0.0034(16)	-0.0010(18)	-0.0025(18)
C20	0.0134(18)	0.019(2)	0.028(2)	0.0014(16)	-0.0011(17)	0.0007(17)
Ru2	0.01932(15)	0.01649(17)	0.01552(16)	-0.00019(13)	-0.00035(12)	0.00052(13)
Cl2	0.0275(5)	0.0185(5)	0.0244(6)	0.0013(4)	-0.0068(4)	0.0020(4)
N6	0.0168(16)	0.0198(18)	0.0150(17)	-0.0006(14)	0.0036(13)	-0.0030(13)
C21	0.0162(19)	0.021(2)	0.023(2)	-0.0020(17)	0.0018(17)	-0.0028(17)
C22	0.030(2)	0.022(2)	0.023(2)	-0.0007(18)	0.0022(18)	-0.0062(17)
C23	0.032(2)	0.022(2)	0.038(3)	-0.0060(19)	0.009(2)	0.0000(19)
C24	0.021(2)	0.035(3)	0.049(3)	-0.0099(19)	0.016(2)	-0.008(2)
C25	0.033(2)	0.017(2)	0.024(2)	-0.0046(18)	0.0111(18)	-0.0071(17)
N7	0.0185(15)	0.0149(17)	0.0170(17)	0.0005(12)	-0.0034(13)	-0.0020(12)
C26	0.0183(19)	0.018(2)	0.026(2)	0.0020(16)	-0.0026(16)	-0.0033(17)
C27	0.0144(18)	0.036(2)	0.022(2)	0.0043(17)	0.0052(17)	0.0039(18)
C28	0.025(2)	0.039(3)	0.016(2)	0.0122(18)	0.0066(17)	-0.0002(18)
C29	0.018(2)	0.034(2)	0.019(2)	0.0047(17)	0.0013(17)	-0.0052(17)
C30	0.0183(19)	0.018(2)	0.022(2)	0.0058(16)	-0.0007(18)	0.0023(17)
N8	0.0142(14)	0.0160(17)	0.0129(16)	-0.0011(12)	0.0030(12)	0.0009(13)
C31	0.026(2)	0.021(2)	0.011(2)	0.0083(17)	0.0019(16)	-0.0023(17)
C32	0.025(2)	0.012(2)	0.027(2)	0.0084(17)	0.0131(18)	0.0085(17)
C33	0.024(2)	0.018(2)	0.028(2)	-0.0026(16)	0.0062(18)	-0.0051(19)
C34	0.023(2)	0.013(2)	0.019(2)	-0.0013(16)	0.0038(16)	-0.0074(16)
C35	0.0172(18)	0.014(2)	0.016(2)	0.0058(16)	0.0055(16)	0.0027(16)
N9	0.0166(14)	0.0119(18)	0.0204(17)	-0.0005(12)	-0.0074(12)	0.0011(13)
C36	0.0179(18)	0.020(2)	0.035(2)	-0.0051(17)	0.0037(17)	-0.0005(18)
C37	0.0201(19)	0.028(2)	0.033(2)	-0.0009(18)	0.0085(17)	-0.011(2)
C38	0.026(2)	0.040(3)	0.021(2)	-0.0048(19)	0.0027(17)	-0.007(2)
C39	0.039(2)	0.021(2)	0.021(2)	0.0040(19)	-0.0057(19)	0.0006(18)
C40	0.032(2)	0.020(2)	0.017(2)	0.0055(17)	0.0001(18)	0.0019(18)
P1	0.0205(5)	0.0221(6)	0.0401(7)	0.0006(5)	-0.0007(5)	0.0023(5)
F1	0.0314(11)	0.0437(14)	0.0332(13)	-0.0099(10)	0.0068(9)	-0.0079(11)
F2	0.0320(13)	0.0407(15)	0.095(2)	0.0008(11)	0.0075(13)	-0.0425(13)
F3	0.0246(10)	0.0305(14)	0.0337(12)	0.0002(9)	0.0053(9)	0.0036(10)
F4	0.0207(11)	0.0460(15)	0.0741(18)	0.0067(10)	0.0054(11)	0.0302(12)
F5	0.0216(11)	0.0231(13)	0.0859(18)	-0.0004(9)	0.0077(11)	0.0137(11)
F6	0.0269(11)	0.0383(15)	0.0378(13)	0.0092(10)	-0.0057(9)	0.0025(10)
P2	0.0193(5)	0.0365(7)	0.0430(7)	0.0057(5)	-0.0042(5)	-0.0172(6)
F7	0.0405(14)	0.143(3)	0.131(3)	0.0181(16)	-0.0113(15)	-0.120(2)
F8	0.0343(12)	0.0482(15)	0.0317(14)	-0.0011(11)	-0.0057(10)	-0.0143(11)
F9	0.0237(12)	0.0343(16)	0.145(2)	-0.0077(11)	0.0189(13)	-0.0065(14)
F10	0.0315(12)	0.092(2)	0.0428(16)	0.0293(12)	-0.0122(11)	-0.0043(13)
F11	0.0415(14)	0.0680(18)	0.0536(17)	0.0192(12)	0.0256(12)	0.0088(13)
F12	0.0243(11)	0.0300(15)	0.125(2)	0.0065(10)	-0.0097(12)	0.0162(13)
P3	0.0218(5)	0.0235(6)	0.0187(6)	0.0027(4)	0.0018(4)	0.0013(5)
F13	0.0317(12)	0.0198(12)	0.0279(13)	0.0017(9)	-0.0055(10)	-0.0047(9)
F14	0.0351(11)	0.0320(13)	0.0176(12)	0.0047(9)	-0.0020(9)	-0.0066(9)
F15	0.0295(11)	0.0490(14)	0.0238(13)	-0.0082(10)	0.0018(10)	0.0127(10)
F16	0.0288(11)	0.0313(13)	0.0204(12)	0.0108(9)	-0.0011(9)	0.0022(9)
F17	0.0294(11)	0.0272(12)	0.0221(12)	-0.0044(9)	0.0050(9)	-0.0004(9)
P4	0.0201(5)	0.0216(6)	0.0272(6)	0.0046(4)	0.0025(4)	-0.0004(5)
F18	0.0280(11)	0.0263(13)	0.0337(13)	0.0019(9)	-0.0108(10)	0.0054(10)
F19	0.0270(10)	0.0209(12)	0.0369(13)	0.0084(9)	0.0073(9)	-0.0030(9)
F20	0.0295(11)	0.0361(14)	0.0349(13)	0.0076(10)	0.0104(9)	-0.0080(10)
F21	0.0222(10)	0.0311(13)	0.0300(12)	0.0037(9)	-0.0047(9)	-0.0046(9)
F22	0.0238(10)	0.0279(13)	0.0339(13)	-0.0021(9)	-0.0008(9)	0.0079(10)

F23	0.0254(11)	0.0317(13)	0.0410(13)	-0.0022(10)	-0.0002(10)	-0.0065(10)
F24	0.0345(12)	0.0281(13)	0.0382(14)	0.0059(10)	0.0086(10)	0.0102(10)

Atomic displacement parameters for SII:

	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ru1	0.01798(15)	0.01520(16)	0.01990(17)	-0.00078(13)	0.00295(12)	-0.00115(14)
Cl1	0.0223(4)	0.0252(5)	0.0241(5)	-0.0058(4)	0.0071(4)	-0.0034(4)
N1	0.0127(15)	0.0171(17)	0.0178(17)	-0.0005(13)	0.0018(13)	-0.0059(13)
C1	0.019(2)	0.023(2)	0.034(2)	-0.0028(17)	-0.0007(17)	-0.0099(18)
C2	0.021(2)	0.023(2)	0.044(3)	0.0051(18)	-0.0122(19)	-0.0050(19)
C3	0.029(2)	0.014(2)	0.026(2)	0.0006(17)	-0.0046(18)	-0.0025(17)
C4	0.027(2)	0.016(2)	0.022(2)	-0.0027(17)	0.0017(17)	0.0015(17)
C5	0.0183(19)	0.022(2)	0.016(2)	-0.0031(17)	-0.0049(17)	-0.0006(16)
N2	0.0167(15)	0.0158(16)	0.0233(17)	-0.0006(13)	0.0019(13)	0.0032(13)
C6	0.0159(18)	0.025(2)	0.024(2)	0.0028(17)	0.0058(17)	-0.0019(18)
C7	0.030(2)	0.041(3)	0.015(2)	-0.0051(19)	0.0059(18)	-0.0056(18)
C8	0.019(2)	0.042(3)	0.025(2)	-0.0084(18)	0.0032(18)	-0.0110(19)
C9	0.0162(18)	0.029(2)	0.034(2)	0.0052(17)	-0.0010(18)	0.0048(18)
C10	0.0194(19)	0.016(2)	0.032(2)	0.0024(16)	0.0012(17)	0.0007(17)
N3	0.0225(17)	0.0112(18)	0.046(2)	-0.0006(14)	-0.0141(17)	-0.0088(16)
C11	0.019(2)	0.020(2)	0.080(4)	-0.0027(18)	0.013(2)	-0.022(2)
C12	0.022(3)	0.031(3)	0.170(7)	-0.010(2)	0.016(3)	-0.044(3)
C13	0.029(3)	0.020(4)	0.273(10)	0.004(2)	-0.062(5)	-0.051(5)
C14	0.116(5)	0.011(3)	0.178(7)	-0.004(3)	-0.123(5)	0.000(3)
C15	0.076(3)	0.017(3)	0.069(4)	-0.002(2)	-0.051(3)	-0.006(2)
N4	0.0183(15)	0.0140(16)	0.0235(18)	0.0030(13)	-0.0016(13)	0.0029(14)
C16	0.0254(19)	0.014(2)	0.018(2)	0.0009(15)	0.0031(16)	0.0036(16)
C17	0.0206(18)	0.020(2)	0.019(2)	0.0060(17)	0.0040(16)	0.0069(17)
C18	0.024(2)	0.030(2)	0.024(2)	0.0006(18)	-0.0004(18)	-0.0102(19)
C19	0.021(2)	0.017(2)	0.032(2)	-0.0034(16)	-0.0010(18)	-0.0025(18)
C20	0.0134(18)	0.019(2)	0.028(2)	0.0014(16)	-0.0011(17)	0.0007(17)
Ru2	0.01932(15)	0.01649(17)	0.01552(16)	-0.00019(13)	-0.00035(12)	0.00052(13)
Cl2	0.0275(5)	0.0185(5)	0.0244(6)	0.0013(4)	-0.0068(4)	0.0020(4)
N6	0.0168(16)	0.0198(18)	0.0150(17)	-0.0006(14)	0.0036(13)	-0.0030(13)
C21	0.0162(19)	0.021(2)	0.023(2)	-0.0020(17)	0.0018(17)	-0.0028(17)
C22	0.030(2)	0.022(2)	0.023(2)	-0.0007(18)	0.0022(18)	-0.0062(17)
C23	0.032(2)	0.022(2)	0.038(3)	-0.0060(19)	0.009(2)	0.0000(19)
C24	0.021(2)	0.035(3)	0.049(3)	-0.0099(19)	0.016(2)	-0.008(2)
C25	0.033(2)	0.017(2)	0.024(2)	-0.0046(18)	0.0111(18)	-0.0071(17)
N7	0.0185(15)	0.0149(17)	0.0170(17)	0.0005(12)	-0.0034(13)	-0.0020(12)
C26	0.0183(19)	0.018(2)	0.026(2)	0.0020(16)	-0.0026(16)	-0.0033(17)
C27	0.0144(18)	0.036(2)	0.022(2)	0.0043(17)	0.0052(17)	0.0039(18)
C28	0.025(2)	0.039(3)	0.016(2)	0.0122(18)	0.0066(17)	-0.0002(18)
C29	0.018(2)	0.034(2)	0.019(2)	0.0047(17)	0.0013(17)	-0.0052(17)
C30	0.0183(19)	0.018(2)	0.022(2)	0.0058(16)	-0.0007(18)	0.0023(17)
N8	0.0142(14)	0.0160(17)	0.0129(16)	-0.0011(12)	0.0030(12)	0.0009(13)
C31	0.026(2)	0.021(2)	0.011(2)	0.0083(17)	0.0019(16)	-0.0023(17)
C32	0.025(2)	0.012(2)	0.027(2)	0.0084(17)	0.0131(18)	0.0085(17)
C33	0.024(2)	0.018(2)	0.028(2)	-0.0026(16)	0.0062(18)	-0.0051(19)
C34	0.023(2)	0.013(2)	0.019(2)	-0.0013(16)	0.0038(16)	-0.0074(16)
C35	0.0172(18)	0.014(2)	0.016(2)	0.0058(16)	0.0055(16)	0.0027(16)
N9	0.0166(14)	0.0119(18)	0.0204(17)	-0.0005(12)	-0.0074(12)	0.0011(13)
C36	0.0179(18)	0.020(2)	0.035(2)	-0.0051(17)	0.0037(17)	-0.0005(18)
C37	0.0201(19)	0.028(2)	0.033(2)	-0.0009(18)	0.0085(17)	-0.011(2)
C38	0.026(2)	0.040(3)	0.021(2)	-0.0048(19)	0.0027(17)	-0.007(2)
C39	0.039(2)	0.021(2)	0.021(2)	0.0040(19)	-0.0057(19)	0.0006(18)
C40	0.032(2)	0.020(2)	0.017(2)	0.0055(17)	0.0001(18)	0.0019(18)
P1	0.0205(5)	0.0221(6)	0.0401(7)	0.0006(5)	-0.0007(5)	0.0023(5)
F1	0.0314(11)	0.0437(14)	0.0332(13)	-0.0099(10)	0.0068(9)	-0.0079(11)
F2	0.0320(13)	0.0407(15)	0.095(2)	0.0008(11)	0.0075(13)	-0.0425(13)

F3	0.0246(10)	0.0305(14)	0.0337(12)	0.0002(9)	0.0053(9)	0.0036(10)
F4	0.0207(11)	0.0460(15)	0.0741(18)	0.0067(10)	0.0054(11)	0.0302(12)
F5	0.0216(11)	0.0231(13)	0.0859(18)	-0.0004(9)	0.0077(11)	0.0137(11)
F6	0.0269(11)	0.0383(15)	0.0378(13)	0.0092(10)	-0.0057(9)	0.0025(10)
P2	0.0193(5)	0.0365(7)	0.0430(7)	0.0057(5)	-0.0042(5)	-0.0172(6)
F7	0.0405(14)	0.143(3)	0.131(3)	0.0181(16)	-0.0113(15)	-0.120(2)
F8	0.0343(12)	0.0482(15)	0.0317(14)	-0.0011(11)	-0.0057(10)	-0.0143(11)
F9	0.0237(12)	0.0343(16)	0.145(2)	-0.0077(11)	0.0189(13)	-0.0065(14)
F10	0.0315(12)	0.092(2)	0.0428(16)	0.0293(12)	-0.0122(11)	-0.0043(13)
F11	0.0415(14)	0.0680(18)	0.0536(17)	0.0192(12)	0.0256(12)	0.0088(13)
F12	0.0243(11)	0.0300(15)	0.125(2)	0.0065(10)	-0.0097(12)	0.0162(13)
P3	0.0218(5)	0.0235(6)	0.0187(6)	0.0027(4)	0.0018(4)	0.0013(5)
F13	0.0317(12)	0.0198(12)	0.0279(13)	0.0017(9)	-0.0055(10)	-0.0047(9)
F14	0.0351(11)	0.0320(13)	0.0176(12)	0.0047(9)	-0.0020(9)	-0.0066(9)
F15	0.0295(11)	0.0490(14)	0.0238(13)	-0.0082(10)	0.0018(10)	0.0127(10)
F16	0.0288(11)	0.0313(13)	0.0204(12)	0.0108(9)	-0.0011(9)	0.0022(9)
F17	0.0294(11)	0.0272(12)	0.0221(12)	-0.0044(9)	0.0050(9)	-0.0004(9)
P4	0.0201(5)	0.0216(6)	0.0272(6)	0.0046(4)	0.0025(4)	-0.0004(5)
F18	0.0280(11)	0.0263(13)	0.0337(13)	0.0019(9)	-0.0108(10)	0.0054(10)
F19	0.0270(10)	0.0209(12)	0.0369(13)	0.0084(9)	0.0073(9)	-0.0030(9)
F20	0.0295(11)	0.0361(14)	0.0349(13)	0.0076(10)	0.0104(9)	-0.0080(10)
F21	0.0222(10)	0.0311(13)	0.0300(12)	0.0037(9)	-0.0047(9)	-0.0046(9)
F22	0.0238(10)	0.0279(13)	0.0339(13)	-0.0021(9)	-0.0008(9)	0.0079(10)
F23	0.0254(11)	0.0317(13)	0.0410(13)	-0.0022(10)	-0.0002(10)	-0.0065(10)
F24	0.0345(12)	0.0281(13)	0.0382(14)	0.0059(10)	0.0086(10)	0.0102(10)

Distances and angles for SII:

	X-ray	DFT
Ru1-Cl1	2.3045(8)	2.3217
Ru1-N1	2.099(2)	2.1354
Ru1-N2	2.086(2)	2.1154
Ru1-N3	2.111(3)	2.1714
Ru1-N4	2.108(2)	2.1424
Ru1-N5'	1.816(7)	-
Ru1-N5	1.921(13)	1.9774
Ru1-O5	2.144(14)	2.2184
N1-C1	1.351(4)	1.3535
N1-H1	2.0352	2.0918
N1-C5	1.359(4)	1.3541
N1-H5	2.04	2.0873
C1-H1	1	1.0869
C1-C2	1.376(5)	1.3908
C2-H2	1	1.0906
C2-C3	1.374(5)	1.3919
C3-H3	1	1.0889
C3-C4	1.374(4)	1.3957
C4-H4	1	1.0893
C4-C5	1.381(5)	1.3881
C5-H5	1	1.0879
N2-C6	1.355(4)	1.3524
N2-H6	2.0339	2.0925
N2-C10	1.349(4)	1.3546
N2-H10	2.0265	2.0892
C6-H6	1	1.0891
C6-C7	1.373(4)	1.3874
C7-H7	1	1.0873
C7-C8	1.378(5)	1.3902
C8-H8	1	1.0904
C8-C9	1.372(5)	1.3931
C9-H9	1	1.0899
C9-C10	1.386(5)	1.388
C10-H10	1	1.0865
N3-C11	1.352(5)	1.3521
N3-H11	2.0442	2.0835
N3-C15	1.342(5)	1.3518
N3-H15	2.0298	2.0894
C11-H11	1	1.0889
C11-C12	1.371(6)	1.3875
C12-H12	1	1.0911
C12-C13	1.359(9)	1.3947
C13-H13	1	1.0916
C13-C14	1.364(10)	1.3909
C14-H14	1	1.0895
C14-C15	1.382(6)	1.3914
C15-H15	1	1.0911
N4-C16	1.352(4)	1.3575
N4-H16	2.0337	2.0909
N4-C20	1.344(4)	1.3547
N4-H20	2.0201	2.091
C16-H16	1	1.0894
C16-C17	1.376(4)	1.3884
C17-H17	1	1.0905
C17-C18	1.371(5)	1.3954
C18-H18	1	1.0913

C18-C19	1.388(5)	1.3921
C19-H19	1	1.0918
C19-C20	1.367(5)	1.3877
C20-H20	1	1.0859
N5'-O5'	1.102(9)	-
N5'-N5	0.744(17)	-
N5'-O5	0.418(16)	-
O5'-N5	1.375(12)	-
O5'-O5	0.838(17)	-
N5-O5	1.08(2)	1.1875
Ru2-Cl2	2.2967(8)	2.3141
Ru2-N6	2.117(3)	2.1421
Ru2-N7	2.103(3)	2.1389
Ru2-N8	2.102(2)	2.1231
Ru2-N9	2.110(2)	2.163
Ru2-N10'	1.729(9)	-
Ru2-N10	1.982(6)	1.9659
Ru2-O10	2.153(6)	2.2097
N6-C21	1.342(4)	1.357
N6-H21	2.0216	2.0916
N6-C25	1.346(4)	1.3575
N6-H25	2.0224	2.0948
C21-H21	1	1.0891
C21-C22	1.384(5)	1.391
C22-H22	1	1.0896
C22-C23	1.376(5)	1.3932
C23-H23	1	1.0919
C23-C24	1.367(5)	1.3946
C24-H24	1	1.0899
C24-C25	1.375(5)	1.3889
C25-H25	1	1.0899
N7-C26	1.346(4)	1.3545
N7-H26	2.0283	2.0923
N7-C30	1.342(4)	1.3549
N7-H30	2.0239	2.0887
C26-H26	1	1.0875
C26-C27	1.376(5)	1.3888
C27-H27	1	1.0913
C27-C28	1.388(5)	1.394
C28-H28	1	1.0891
C28-C29	1.379(4)	1.3948
C29-H29	1	1.0896
C29-C30	1.374(5)	1.3863
C30-H30	1	1.0886
N8-C31	1.350(4)	1.3575
N8-H31	2.0361	2.0925
N8-C35	1.343(4)	1.3513
N8-H35	2.0216	2.0844
C31-H31	1	1.0916
C31-C32	1.380(4)	1.3854
C32-H32	1	1.0906
C32-C33	1.378(5)	1.3954
C33-H33	1	1.0911
C33-C34	1.379(5)	1.391
C34-H34	1	1.0896
C34-C35	1.363(4)	1.3908
C35-H35	1	1.0875
N9-C36	1.341(4)	1.3502
N9-H36	2.0224	2.0936
N9-C40	1.350(4)	1.3517

N9-H40	2.0334	2.0841
C36-H36	1	1.0875
C36-C37	1.374(5)	1.3883
C37-H37	1	1.0874
C37-C38	1.376(5)	1.3887
C38-H38	1	1.0907
C38-C39	1.369(5)	1.3932
C39-H39	1	1.0893
C39-C40	1.374(5)	1.3865
C40-H40	1	1.0885
N10'-O10'	1.236(12)	-
N10'-N10	0.664(13)	-
N10'-O10	0.603(12)	-
O10'-N10	1.082(9)	-
O10'-O10	1.010(10)	-
N10-O10	0.928(9)	1.1892
P1-F1	1.604(2)	1.6526
P1-F2	1.590(2)	1.6489
P1-F3	1.6084(19)	1.65
P1-F4	1.594(2)	1.6433
P1-F5	1.606(2)	1.6464
P1-F6	1.5933(19)	1.6401
P2-F7	1.574(3)	1.636
P2-F8	1.597(2)	1.6681
P2-F9	1.592(2)	1.6466
P2-F10	1.584(2)	1.6338
P2-F11	1.597(2)	1.6421
P2-F12	1.589(2)	1.6568
P3-F13	1.6113(19)	1.6551
P3-F14	1.6061(19)	1.6496
P3-F15	1.604(2)	1.6447
P3-F16	1.6190(18)	1.6617
P3-F17	1.5956(19)	1.6357
P3-F18	1.5921(19)	1.6338
P4-F19	1.5990(19)	1.6381
P4-F20	1.598(2)	1.6416
P4-F21	1.6126(18)	1.6542
P4-F22	1.605(2)	1.6516
P4-F23	1.6060(19)	1.643
P4-F24	1.604(2)	1.6546
O3-H3a	0.75(2)	0.9819
O3-H3b	0.75(3)	0.9824
Cl1-Ru1-N1	88.69(7)	87.9271
Cl1-Ru1-N2	87.88(7)	88.417
Cl1-Ru1-N3	86.65(8)	82.5695
Cl1-Ru1-N4	89.98(7)	89.9433
Cl1-Ru1-N5'	178.1(3)	-
Cl1-Ru1-N5	158.4(4)	157.2164
Cl1-Ru1-O5	171.1(5)	170.3403
N1-Ru1-N2	88.81(9)	88.4647
N1-Ru1-N3	175.32(10)	170.4412
N1-Ru1-N4	90.05(10)	88.4059
N1-Ru1-N5'	90.1(3)	-
N1-Ru1-N5	112.9(4)	114.7995
N1-Ru1-O5	82.6(5)	82.5656
N2-Ru1-N3	91.50(11)	92.2827
N2-Ru1-N4	177.60(10)	176.5177
N2-Ru1-N5'	90.6(2)	-
N2-Ru1-N5	90.6(3)	90.5178
N2-Ru1-O5	89.8(4)	89.6189

N3-Ru1-N4	89.46(11)	90.551
N3-Ru1-N5'	94.5(3)	-
N3-Ru1-N5	71.8(4)	74.7317
N3-Ru1-O5	102.0(5)	106.9634
N4-Ru1-N5'	91.5(2)	92.1815
N4-Ru1-N5	91.7(3)	-
N4-Ru1-O5	92.2(4)	91.4907
N5'-Ru1-N5	22.7(5)	-
N5'-Ru1-O5	7.5(6)	-
N5-Ru1-O5	30.2(6)	32.234
Ru1-N1-C1	119.7(2)	118.9319
Ru1-N1-H1	94.3156	91.5598
Ru1-N1-C5	122.02(19)	121.7725
Ru1-N1-H5	96.6776	94.174
C1-N1-H1	25.4078	27.4231
C1-N1-C5	118.3(3)	119.1829
C1-N1-H5	143.6604	146.8405
H1-N1-C5	143.6579	146.6059
H1-N1-H5	168.7462	174.2624
C5-N1-H5	25.397	27.6581
N1-C1-H1	119.1669	117.5797
N1-C1-C2	121.7(3)	121.7777
H1-C1-C2	119.1671	120.6305
C1-C2-H2	120.2811	118.2292
C1-C2-C3	119.4(3)	119.1894
H2-C2-C3	120.2811	122.5682
C2-C3-H3	120.0816	121.2241
C2-C3-C4	119.8(3)	118.8473
H3-C3-C4	120.083	119.9286
C3-C4-H4	120.6976	121.3452
C3-C4-C5	118.6(3)	119.2822
H4-C4-C5	120.696	119.3495
N1-C5-C4	122.1(3)	121.7041
N1-C5-H5	118.9625	117.046
C4-C5-H5	118.9632	121.2461
Ru1-N2-C6	120.45(19)	119.3715
Ru1-N2-H6	94.9304	91.9513
Ru1-N2-C10	122.5(2)	121.6505
Ru1-N2-H10	96.8621	94.204
C6-N2-H6	25.5569	27.4718
C6-N2-C10	117.0(3)	118.8851
C6-N2-H10	142.686	146.4021
H6-N2-C10	142.5362	146.356
H6-N2-H10	168.1633	173.8252
C10-N2-H10	25.6945	27.5289
N2-C6-H6	118.6645	117.5791
N2-C6-C7	122.7(3)	121.9513
H6-C6-C7	118.6645	120.4593
C6-C7-H7	120.2678	118.2689
C6-C7-C8	119.5(3)	119.3313
H7-C7-C8	120.2682	122.3842
C7-C8-H8	120.5008	120.875
C7-C8-C9	119.0(3)	118.6777
H8-C8-C9	120.5023	120.4458
C8-C9-H9	120.5568	121.9408
C8-C9-C10	118.9(3)	119.3693
H9-C9-C10	120.5561	118.6871
N2-C10-C9	123.0(3)	121.7493
N2-C10-H10	118.5221	117.2816
C9-C10-H10	118.5212	120.968

Ru1-N3-C11	120.8(2)	119.9908
Ru1-N3-H11	95.7748	92.1824
Ru1-N3-C15	120.1(3)	120.9969
Ru1-N3-H15	94.7302	93.3329
C11-N3-H11	25.0688	27.813
C11-N3-C15	119.0(3)	119.0122
C11-N3-H15	144.4283	146.6612
H11-N3-C15	144.0791	146.8161
H11-N3-H15	169.495	174.2629
C15-N3-H15	25.4177	27.6802
N3-C11-H11	119.9888	116.7836
N3-C11-C12	120.0(4)	121.8445
H11-C11-C12	119.9885	121.3697
C11-C12-H12	119.0356	119.4071
C11-C12-C13	121.9(5)	119.2531
H12-C12-C13	119.0367	121.3396
C12-C13-H13	121.2604	120.7898
C12-C13-C14	117.5(5)	118.839
H13-C13-C14	121.2616	120.3712
C13-C14-H14	119.8242	121.6187
C13-C14-C15	120.4(5)	119.0803
H14-C14-C15	119.8236	119.2989
N3-C15-C14	121.2(4)	121.9363
N3-C15-H15	119.3971	117.1846
C14-C15-H15	119.3984	120.8764
Ru1-N4-C16	122.3(2)	121.1155
Ru1-N4-H16	96.7873	93.4858
Ru1-N4-C20	120.4(2)	120.6584
Ru1-N4-H20	94.5044	93.2663
C16-N4-H16	25.4978	27.6642
C16-N4-C20	117.4(3)	118.2106
C16-N4-H20	143.2108	145.6181
H16-N4-C20	142.8551	145.8558
H16-N4-H20	168.7079	173.0756
C20-N4-H20	25.853	27.4301
N4-C16-H16	118.8988	116.9864
N4-C16-C17	122.2(3)	121.965
H16-C16-C17	118.9005	121.0262
C16-C17-H17	120.2383	118.7001
C16-C17-C18	119.5(3)	119.589
H17-C17-C18	120.2399	121.7025
C17-C18-H18	120.5218	120.1715
C17-C18-C19	119.0(3)	118.4556
H18-C18-C19	120.5215	121.3641
C18-C19-H19	120.766	122.5969
C18-C19-C20	118.5(3)	119.1501
H19-C19-C20	120.7645	118.2513
N4-C20-C19	123.5(3)	122.6111
N4-C20-H20	118.2539	117.4902
C19-C20-H20	118.2546	119.8927
Ru1-N5'-O5'	177.6(6)	-
Ru1-N5'-N5	86.6(10)	-
Ru1-N5'-O5	138(3)	-
O5'-N5'-N5	94.3(13)	-
O5'-N5'-O5	42(3)	-
N5-N5'-O5	135(3)	-
N5'-O5'-N5	32.6(8)	-
N5'-O5'-O5	19.4(13)	-
N5-O5'-O5	51.9(13)	-
Ru1-N5-N5'	70.7(11)	-

Ru1-N5-O5'	123.7(9)	-
Ru1-N5-O5	86.3(12)	85.122
N5'-N5-O5'	53.1(9)	-
N5'-N5-O5	15.7(11)	-
O5'-N5-O5	37.6(10)	-
Ru1-O5-N5'	35(2)	-
Ru1-O5-O5'	153.5(17)	-
Ru1-O5-N5	63.4(9)	62.644
N5'-O5-O5'	119(4)	-
N5'-O5-N5	29(2)	-
O5'-O5-N5	90.5(18)	-
Cl2-Ru2-N6	88.19(7)	89.5244
Cl2-Ru2-N7	87.26(7)	86.8816
Cl2-Ru2-N8	90.30(7)	90.5459
Cl2-Ru2-N9	85.45(7)	81.6495
Cl2-Ru2-N10'	172.6(3)	-
Cl2-Ru2-N10	160.8(2)	155.7676
Cl2-Ru2-O10	173.18(16)	171.8007
N6-Ru2-N7	89.79(9)	89.1724
N6-Ru2-N8	176.55(10)	175.5701
N6-Ru2-N9	91.31(10)	91.3053
N6-Ru2-N10'	84.7(3)	-
N6-Ru2-N10	93.1(2)	89.9709
N6-Ru2-O10	94.40(17)	90.9221
N7-Ru2-N8	87.04(9)	86.4087
N7-Ru2-N9	172.59(9)	168.5163
N7-Ru2-N10'	94.7(4)	-
N7-Ru2-N10	111.9(2)	117.3358
N7-Ru2-O10	86.45(17)	84.9387
N8-Ru2-N9	91.66(10)	93.0874
N8-Ru2-N10'	96.9(3)	-
N8-Ru2-N10	89.4(2)	91.7798
N8-Ru2-O10	86.76(17)	88.3794
N9-Ru2-N10'	92.7(4)	-
N9-Ru2-N10	75.3(2)	74.1414
N9-Ru2-O10	100.77(17)	106.5231
N10'-Ru2-N10	19.1(4)	-
N10'-Ru2-O10	12.8(4)	-
N10-Ru2-O10	25.5(3)	32.4278
Ru2-N6-C21	121.7(2)	121.045
Ru2-N6-H21	95.9929	93.4588
Ru2-N6-C25	121.1(2)	120.8098
Ru2-N6-H25	95.3062	93.3333
C21-N6-H21	25.7319	27.6123
C21-N6-C25	117.2(3)	118.1211
C21-N6-H25	142.973	145.6216
H21-N6-C25	142.9225	145.7275
H21-N6-H25	168.7008	173.0704
C25-N6-H25	25.7838	27.5361
N6-C21-H21	118.631	117.1115
N6-C21-C22	122.7(3)	122.3068
H21-C21-C22	118.6316	120.5787
C21-C22-H22	120.7101	119.1427
C21-C22-C23	118.6(3)	119.4272
H22-C22-C23	120.7104	121.4219
C22-C23-H23	120.2241	120.7147
C22-C23-C24	119.6(3)	118.3552
H23-C23-C24	120.224	120.912
C23-C24-H24	120.6604	122.1087
C23-C24-C25	118.7(3)	119.5097

H24-C24-C25	120.6617	118.3572
N6-C25-C24	123.2(3)	122.2772
N6-C25-H25	118.3924	117.3065
C24-C25-H25	118.3935	120.3933
Ru2-N7-C26	120.4(2)	120.5396
Ru2-N7-H26	94.7861	93.0846
Ru2-N7-C30	121.5(2)	120.3292
Ru2-N7-H30	95.8564	92.6972
C26-N7-H26	25.5669	27.4551
C26-N7-C30	118.2(3)	119.1298
C26-N7-H30	143.7885	146.7303
H26-N7-C30	143.7195	146.5827
H26-N7-H30	169.3459	173.9953
C30-N7-H30	25.6487	27.652
N7-C26-H26	118.9178	117.4985
N7-C26-C27	122.2(3)	121.727
H26-C26-C27	118.9183	120.7729
C26-C27-H27	120.2019	118.4559
C26-C27-C28	119.6(3)	119.2721
H27-C27-C28	120.2015	122.2564
C27-C28-H28	121.0775	121.4485
C27-C28-C29	117.8(3)	118.7577
H28-C28-C29	121.0768	119.7809
C28-C29-H29	120.0732	120.6972
C28-C29-C30	119.9(3)	119.3222
H29-C29-C30	120.0725	119.9406
N7-C30-C29	122.3(3)	121.7667
N7-C30-H30	118.8299	117.0615
C29-C30-H30	118.8292	121.1532
Ru2-N8-C31	119.2(2)	118.6958
Ru2-N8-H31	93.8982	91.0886
Ru2-N8-C35	122.5(2)	122.191
Ru2-N8-H35	96.8286	94.6372
C31-N8-H31	25.3391	27.7068
C31-N8-C35	118.2(3)	118.9153
C31-N8-H35	143.9326	146.5985
H31-N8-C35	143.5101	146.6215
H31-N8-H35	169.2659	174.2694
C35-N8-H35	25.7643	27.6917
N8-C31-H31	119.3754	116.9689
N8-C31-C32	121.2(3)	121.9171
H31-C31-C32	119.3763	121.1111
C31-C32-H32	120.0138	120.0244
C31-C32-C33	120.0(3)	119.2143
H32-C32-C33	120.0124	120.7495
C32-C33-H33	120.8118	119.7371
C32-C33-C34	118.4(3)	118.8044
H33-C33-C34	120.8134	121.455
C33-C34-H34	120.3775	122.4591
C33-C34-C35	119.2(3)	119.271
H34-C34-C35	120.3766	118.2584
N8-C35-C34	123.0(3)	121.8564
N8-C35-H35	118.5109	117.0381
C34-C35-H35	118.5129	121.1048
Ru2-N9-C36	120.1(2)	119.8624
Ru2-N9-H36	94.4058	92.5887
Ru2-N9-C40	121.9(2)	121.0084
Ru2-N9-H40	96.4775	93.2712
C36-N9-H36	25.6902	27.305
C36-N9-C40	118.0(3)	119.0457

C36-N9-H40	143.4316	146.7998
H36-N9-C40	143.6641	146.3502
H36-N9-H40	169.1162	174.0833
C40-N9-H40	25.454	27.7587
N9-C36-H36	118.7513	117.9752
N9-C36-C37	122.5(3)	121.8281
H36-C36-C37	118.7496	120.1965
C36-C37-H37	120.4146	118.2217
C36-C37-C38	119.2(3)	119.4516
H37-C37-C38	120.4159	122.3226
C37-C38-H38	120.6321	121.1577
C37-C38-C39	118.7(3)	118.4528
H38-C38-C39	120.6319	120.3893
C38-C39-H39	120.1134	121.5721
C38-C39-C40	119.8(3)	119.5504
H39-C39-C40	120.1128	118.8484
N9-C40-C39	121.8(3)	121.6694
N9-C40-H40	119.0848	116.9031
C39-C40-H40	119.0862	121.4174
Ru2-N10'-O10'	162.8(9)	-
Ru2-N10'-N10	102.5(12)	-
Ru2-N10'-O10	128.0(13)	-
O10'-N10'-N10	60.9(9)	-
O10'-N10'-O10	54.2(10)	-
N10-N10'-O10	94.0(15)	-
N10'-O10'-N10	32.4(7)	-
N10'-O10'-O10	29.0(6)	-
N10-O10'-O10	52.5(6)	-
Ru2-N10-N10'	58.4(10)	-
Ru2-N10-O10'	144.7(6)	-
Ru2-N10-O10	87.6(6)	85.1394
N10'-N10-O10'	86.6(11)	-
N10'-N10-O10	40.4(10)	-
O10'-N10-O10	59.7(7)	-
Ru2-O10-N10'	39.3(10)	-
Ru2-O10-O10'	132.6(5)	-
Ru2-O10-N10	66.9(5)	-
N10'-O10-O10'	96.8(12)	-
N10'-O10-N10	45.6(11)	-
O10'-O10-N10	67.8(6)	-
F1-P1-F2	179.65(12)	179.4902
F1-P1-F3	89.63(10)	89.7325
F1-P1-F4	89.80(11)	89.4696
F1-P1-F5	89.37(11)	89.6486
F1-P1-F6	89.90(10)	90.2674
F2-P1-F3	90.72(11)	90.1253
F2-P1-F4	90.13(11)	90.0417
F2-P1-F5	90.28(11)	90.4971
F2-P1-F6	90.17(11)	90.2214
F3-P1-F4	89.78(10)	90.1944
F3-P1-F5	178.94(11)	179.2603
F3-P1-F6	90.05(10)	89.864
F4-P1-F5	90.56(11)	90.2052
F4-P1-F6	179.66(12)	179.7295
F5-P1-F6	89.61(10)	89.7335
F7-P2-F8	179.45(12)	178.9688
F7-P2-F9	91.27(13)	90.7998
F7-P2-F10	91.34(13)	91.4222
F7-P2-F11	90.34(13)	90.5891
F7-P2-F12	89.75(13)	90.289

F8-P2-F9	89.03(12)	89.1943
F8-P2-F10	89.13(11)	89.6089
F8-P2-F11	89.35(11)	89.3987
F8-P2-F12	89.79(12)	88.6799
F9-P2-F10	89.32(11)	90.7722
F9-P2-F11	178.34(14)	178.2778
F9-P2-F12	90.51(11)	89.3331
F10-P2-F11	91.04(12)	90.2111
F10-P2-F12	178.91(14)	178.284
F11-P2-F12	89.10(11)	89.6418
F13-P3-F14	179.53(10)	178.8223
F13-P3-F15	89.60(10)	90.1513
F13-P3-F16	89.34(9)	89.2396
F13-P3-F17	90.25(10)	90.0164
F13-P3-F18	90.11(10)	90.2886
F14-P3-F15	90.27(10)	90.0247
F14-P3-F16	90.21(10)	89.5979
F14-P3-F17	89.87(10)	89.7891
F14-P3-F18	90.34(10)	90.8754
F15-P3-F16	89.35(9)	89.3612
F15-P3-F17	179.38(10)	179.0761
F15-P3-F18	90.22(10)	90.1735
F16-P3-F17	90.04(9)	89.7325
F16-P3-F18	179.31(11)	179.3368
F17-P3-F18	90.38(10)	90.7342
F19-P4-F20	179.46(10)	179.5502
F19-P4-F21	89.62(9)	89.4808
F19-P4-F22	89.56(10)	89.9169
F19-P4-F23	89.74(9)	89.941
F19-P4-F24	90.09(10)	90.096
F20-P4-F21	89.87(9)	90.1296
F20-P4-F22	90.25(10)	89.8564
F20-P4-F23	90.77(10)	90.4519
F20-P4-F24	90.09(10)	90.1254
F21-P4-F22	90.14(10)	89.7098
F21-P4-F23	179.33(11)	178.9692
F21-P4-F24	89.71(10)	89.5055
F22-P4-F23	90.06(10)	91.1426
F22-P4-F24	179.63(11)	179.2152
F23-P4-F24	90.09(10)	89.6423
H3a-O3-H3b	105(4)	103.4949