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Table 2. Anisotropic Displacement Parameters

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Ta(1)	0.0326(2)	0.0280(2)	0.0426(3)	-0.0028(2)	0.0047(2)	0.0030(3)
Ta(2)	0.0481(3)	0.0445(3)	0.0342(3)	-0.0047(2)	-0.0036(3)	0.0043(3)
Cl(11)	0.052(2)	0.035(2)	0.075(3)	-0.009(1)	-0.005(2)	0.000(2)
Cl(21)	0.063(2)	0.055(2)	0.050(2)	-0.002(1)	0.005(2)	0.011(2)
Cl(31)	0.041(2)	0.046(2)	0.078(2)	0.004(1)	0.012(1)	0.004(2)
Cl(41)	0.110(3)	0.051(2)	0.038(2)	-0.016(2)	-0.007(2)	0.003(2)
Cl(42)	0.071(2)	0.119(3)	0.126(4)	-0.044(2)	-0.041(2)	0.061(3)
Cl(43)	0.100(2)	0.058(2)	0.082(3)	0.012(2)	0.037(2)	0.005(2)
Cl(44)	0.107(3)	0.101(3)	0.050(2)	-0.013(2)	0.006(2)	0.008(2)
Cl(45)	0.058(2)	0.127(3)	0.087(3)	-0.023(2)	-0.012(2)	-0.005(3)
Cl(46)	0.135(3)	0.055(2)	0.096(3)	0.021(2)	0.025(3)	0.016(3)
N(11)	0.030(5)	0.038(5)	0.037(6)	0.001(4)	0.005(4)	-0.003(5)
N(12)	0.043(5)	0.030(5)	0.019(5)	-0.002(4)	0.007(4)	-0.002(5)
N(21)	0.035(5)	0.040(5)	0.040(6)	0.006(4)	-0.004(4)	-0.004(5)
N(22)	0.048(5)	0.022(5)	0.029(6)	-0.002(4)	0.007(4)	0.004(4)
N(31)	0.025(4)	0.033(5)	0.038(6)	0.000(4)	0.005(4)	0.014(4)
N(32)	0.039(5)	0.023(5)	0.042(6)	-0.005(4)	0.007(4)	0.002(5)
C(11)	0.032(6)	0.027(6)	0.052(8)	0.000(5)	-0.006(6)	-0.003(6)
C(12)	0.053(7)	0.030(6)	0.041(8)	0.000(5)	0.000(6)	-0.009(6)
C(13)	0.037(6)	0.038(7)	0.043(9)	0.007(5)	-0.007(5)	0.001(6)
C(14)	0.044(6)	0.047(7)	0.070(10)	-0.012(5)	-0.013(7)	-0.004(8)
C(15)	0.065(8)	0.063(8)	0.049(9)	0.003(6)	0.016(7)	-0.001(7)
C(21)	0.067(8)	0.029(7)	0.044(9)	0.008(6)	0.020(7)	-0.003(7)
C(22)	0.070(8)	0.048(8)	0.034(8)	0.016(6)	-0.005(6)	-0.002(7)

Table 2. Anisotropic Displacement Parameters (continued)

atom	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
C(23)	0.058(7)	0.030(7)	0.054(9)	0.006(5)	-0.009(7)	0.000(6)
C(24)	0.097(10)	0.056(8)	0.042(9)	0.009(7)	0.018(8)	0.003(8)
C(25)	0.054(7)	0.077(9)	0.12(1)	-0.027(7)	-0.031(9)	0.002(9)
C(31)	0.026(5)	0.061(7)	0.061(9)	0.002(6)	0.017(5)	0.006(8)
C(32)	0.039(6)	0.036(6)	0.074(10)	0.006(5)	0.011(6)	0.012(7)
C(33)	0.032(5)	0.026(6)	0.050(8)	0.007(5)	0.008(5)	0.003(6)
C(34)	0.048(7)	0.058(8)	0.13(1)	0.022(6)	0.037(8)	0.038(10)
C(35)	0.049(7)	0.042(7)	0.066(10)	0.015(5)	0.004(7)	0.009(8)
B(1)	0.040(7)	0.025(6)	0.037(9)	-0.012(5)	-0.003(6)	-0.003(6)

The general temperature factor expression:

$$\exp(-2\pi^2(a^{*2}U_{11}h^2 + b^{*2}U_{22}k^2 + c^{*2}U_{33}l^2 + 2a^*b^*U_{12}hk + 2a^*c^*U_{13}hl + 2b^*c^*U_{23}kl))$$

Table 3. Bond Lengths($\text{\AA}$)

atom	atom	distance	atom	atom	distance
Ta(1)	Cl(11)	2.281(3)	Ta(1)	Cl(21)	2.273(3)
Ta(1)	Cl(31)	2.278(2)	Ta(1)	N(11)	2.171(8)
Ta(1)	N(21)	2.153(8)	Ta(1)	N(31)	2.149(7)
Ta(2)	Cl(41)	2.361(3)	Ta(2)	Cl(42)	2.331(3)
Ta(2)	Cl(43)	2.330(3)	Ta(2)	Cl(44)	2.301(4)
Ta(2)	Cl(45)	2.305(3)	Ta(2)	Cl(46)	2.349(4)
N(11)	N(12)	1.390(9)	N(11)	C(13)	1.38(1)
N(12)	C(11)	1.34(1)	N(12)	B(1)	1.52(1)
N(21)	N(22)	1.397(10)	N(21)	C(23)	1.39(1)
N(22)	C(21)	1.34(1)	N(22)	B(1)	1.54(1)
N(31)	N(32)	1.401(9)	N(31)	C(33)	1.39(1)
N(32)	C(31)	1.34(1)	N(32)	B(1)	1.54(1)
C(11)	C(12)	1.37(1)	C(11)	C(14)	1.48(1)
C(12)	C(13)	1.35(1)	C(12)	H(4)	1.01
C(13)	C(15)	1.49(1)	C(14)	H(1)	0.95
C(14)	H(2)	0.96	C(14)	H(3)	0.98
C(15)	H(5)	0.97	C(15)	H(6)	0.95
C(15)	H(7)	0.98	C(21)	C(22)	1.38(1)
C(21)	C(24)	1.44(1)	C(22)	C(23)	1.37(1)
C(22)	H(18)	0.99	C(23)	C(25)	1.48(1)
C(24)	H(15)	0.98	C(24)	H(16)	0.98
C(24)	H(17)	0.97	C(25)	H(19)	1.00
C(25)	H(20)	0.95	C(25)	H(21)	0.98
C(31)	C(32)	1.39(1)	C(31)	C(34)	1.46(1)

Table 3. Bond Lengths($\text{\AA}$) (continued)

atom	atom	distance	atom	atom	distance
C(32)	C(33)	1.34(1)	C(32)	H(11)	0.98
C(33)	C(35)	1.48(1)	C(34)	H(8)	0.94
C(34)	H(9)	0.94	C(34)	H(10)	1.03
C(35)	H(12)	0.95	C(35)	H(13)	1.00
C(35)	H(14)	0.95	B(1)	H(22)	1.01

Table 4. Bond Angles(°)

atom	atom	atom	angle	atom	atom	atom	angle
Cl(11)	Ta(1)	Cl(21)	96.1(1)	Cl(11)	Ta(1)	Cl(31)	95.77(10)
Cl(11)	Ta(1)	N(11)	171.9(2)	Cl(11)	Ta(1)	N(21)	89.4(2)
Cl(11)	Ta(1)	N(31)	91.4(2)	Cl(21)	Ta(1)	Cl(31)	96.1(1)
Cl(21)	Ta(1)	N(11)	89.8(2)	Cl(21)	Ta(1)	N(21)	171.5(2)
Cl(21)	Ta(1)	N(31)	90.1(2)	Cl(31)	Ta(1)	N(11)	89.1(2)
Cl(31)	Ta(1)	N(21)	89.8(2)	Cl(31)	Ta(1)	N(31)	170.0(2)
N(11)	Ta(1)	N(21)	84.2(3)	N(11)	Ta(1)	N(31)	83.0(3)
N(21)	Ta(1)	N(31)	83.2(3)	Cl(41)	Ta(2)	Cl(42)	89.8(1)
Cl(41)	Ta(2)	Cl(43)	87.6(1)	Cl(41)	Ta(2)	Cl(44)	178.2(1)
Cl(41)	Ta(2)	Cl(45)	88.2(1)	Cl(41)	Ta(2)	Cl(46)	89.9(1)
Cl(42)	Ta(2)	Cl(43)	91.3(1)	Cl(42)	Ta(2)	Cl(44)	90.3(1)
Cl(42)	Ta(2)	Cl(45)	175.8(1)	Cl(42)	Ta(2)	Cl(46)	88.0(1)
Cl(43)	Ta(2)	Cl(44)	90.6(1)	Cl(43)	Ta(2)	Cl(45)	92.2(1)
Cl(43)	Ta(2)	Cl(46)	177.4(1)	Cl(44)	Ta(2)	Cl(45)	91.9(1)
Cl(44)	Ta(2)	Cl(46)	92.0(1)	Cl(45)	Ta(2)	Cl(46)	88.4(1)
Ta(1)	N(11)	N(12)	119.9(6)	Ta(1)	N(11)	C(13)	133.6(7)
N(12)	N(11)	C(13)	105.8(8)	N(11)	N(12)	C(11)	109.1(8)
N(11)	N(12)	B(1)	120.4(8)	C(11)	N(12)	B(1)	130.5(9)
Ta(1)	N(21)	N(22)	121.2(6)	Ta(1)	N(21)	C(23)	134.6(7)
N(22)	N(21)	C(23)	104.0(8)	N(21)	N(22)	C(21)	110.0(9)
N(21)	N(22)	B(1)	118.9(8)	C(21)	N(22)	B(1)	131.0(9)
Ta(1)	N(31)	N(32)	120.4(5)	Ta(1)	N(31)	C(33)	133.8(6)
N(32)	N(31)	C(33)	105.8(7)	N(31)	N(32)	C(31)	108.0(8)
N(31)	N(32)	B(1)	119.8(7)	C(31)	N(32)	B(1)	132.1(9)

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(12)	C(11)	C(12)	108.0(9)	N(12)	C(11)	C(14)	122(1)
C(12)	C(11)	C(14)	129(1)	C(11)	C(12)	C(13)	108(1)
C(11)	C(12)	H(4)	125.3	C(13)	C(12)	H(4)	126.3
N(11)	C(13)	C(12)	108.7(10)	N(11)	C(13)	C(15)	124.9(10)
C(12)	C(13)	C(15)	126(1)	C(11)	C(14)	H(1)	112.1
C(11)	C(14)	H(2)	111.3	C(11)	C(14)	H(3)	111.1
H(1)	C(14)	H(2)	108.5	H(1)	C(14)	H(3)	106.8
H(2)	C(14)	H(3)	106.7	C(13)	C(15)	H(5)	111.9
C(13)	C(15)	H(6)	112.9	C(13)	C(15)	H(7)	111.2
H(5)	C(15)	H(6)	107.8	H(5)	C(15)	H(7)	105.2
H(6)	C(15)	H(7)	107.4	N(22)	C(21)	C(22)	109(1)
N(22)	C(21)	C(24)	122(1)	C(22)	C(21)	C(24)	128(1)
C(21)	C(22)	C(23)	106(1)	C(21)	C(22)	H(18)	124.7
C(23)	C(22)	H(18)	129.0	N(21)	C(23)	C(22)	110.5(10)
N(21)	C(23)	C(25)	123(1)	C(22)	C(23)	C(25)	126(1)
C(21)	C(24)	H(15)	113.8	C(21)	C(24)	H(16)	113.5
C(21)	C(24)	H(17)	112.8	H(15)	C(24)	H(16)	105.0
H(15)	C(24)	H(17)	105.3	H(16)	C(24)	H(17)	105.6
C(23)	C(25)	H(19)	112.2	C(23)	C(25)	H(20)	114.6
C(23)	C(25)	H(21)	112.9	H(19)	C(25)	H(20)	105.6
H(19)	C(25)	H(21)	103.7	H(20)	C(25)	H(21)	107.1
N(32)	C(31)	C(32)	109.2(9)	N(32)	C(31)	C(34)	121(1)
C(32)	C(31)	C(34)	129.2(10)	C(31)	C(32)	C(33)	107.1(9)
C(31)	C(32)	H(11)	124.5	C(33)	C(32)	H(11)	128.3

Table 4. Bond Angles(°) (continued)

atom	atom	atom	angle	atom	atom	atom	angle
N(31)	C(33)	C(32)	109.8(9)	N(31)	C(33)	C(35)	122.9(8)
C(32)	C(33)	C(35)	127.3(9)	C(31)	C(34)	H(8)	112.6
C(31)	C(34)	H(9)	114.3	C(31)	C(34)	H(10)	110.4
H(8)	C(34)	H(9)	111.2	H(8)	C(34)	H(10)	103.7
H(9)	C(34)	H(10)	103.8	C(33)	C(35)	H(12)	113.9
C(33)	C(35)	H(13)	109.9	C(33)	C(35)	H(14)	112.9
H(12)	C(35)	H(13)	105.2	H(12)	C(35)	H(14)	109.4
H(13)	C(35)	H(14)	104.9	N(12)	B(1)	N(22)	107.7(8)
N(12)	B(1)	N(32)	109.4(9)	N(12)	B(1)	H(22)	111.1
N(22)	B(1)	N(32)	108.0(8)	N(22)	B(1)	H(22)	110.2
N(32)	B(1)	H(22)	110.4				

Table 5. Torsion Angles(°)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
Ta(1)	N(11)	N(12)	C(11)	171.2(6)	Ta(1)	N(11)	N(12)	B(1)	-6(1)
Ta(1)	N(11)	C(13)	C(12)	-169.6(7)	Ta(1)	N(11)	C(13)	C(15)	9(1)
Ta(1)	N(21)	N(22)	C(21)	-178.4(6)	Ta(1)	N(21)	N(22)	B(1)	0(1)
Ta(1)	N(21)	C(23)	C(22)	177.7(7)	Ta(1)	N(21)	C(23)	C(25)	-3(1)
Ta(1)	N(31)	N(32)	C(31)	-177.6(7)	Ta(1)	N(31)	N(32)	B(1)	0(1)
Ta(1)	N(31)	C(33)	C(32)	178.7(8)	Ta(1)	N(31)	C(33)	C(35)	0(1)
Cl(11)	Ta(1)	N(11)	N(12)	0(1)	Cl(11)	Ta(1)	N(11)	C(13)	169(1)
Cl(11)	Ta(1)	N(21)	N(22)	-134.4(6)	Cl(11)	Ta(1)	N(21)	C(23)	49.3(9)
Cl(11)	Ta(1)	N(31)	N(32)	132.1(7)	Cl(11)	Ta(1)	N(31)	C(33)	-46.7(9)
Cl(21)	Ta(1)	N(11)	N(12)	136.4(6)	Cl(21)	Ta(1)	N(11)	C(13)	-53.8(9)
Cl(21)	Ta(1)	N(21)	N(22)	-4(1)	Cl(21)	Ta(1)	N(21)	C(23)	179.6(10)
Cl(21)	Ta(1)	N(31)	N(32)	-131.8(7)	Cl(21)	Ta(1)	N(31)	C(33)	49.4(9)
Cl(31)	Ta(1)	N(11)	N(12)	-127.5(6)	Cl(31)	Ta(1)	N(11)	C(13)	42.3(9)
Cl(31)	Ta(1)	N(21)	N(22)	129.8(6)	Cl(31)	Ta(1)	N(21)	C(23)	-46.5(9)
Cl(31)	Ta(1)	N(31)	N(32)	-3(1)	Cl(31)	Ta(1)	N(31)	C(33)	177.7(9)
N(11)	Ta(1)	N(21)	N(22)	40.7(6)	N(11)	Ta(1)	N(21)	C(23)	-135.6(9)
N(11)	Ta(1)	N(31)	N(32)	-42.0(7)	N(11)	Ta(1)	N(31)	C(33)	139.1(10)
N(11)	N(12)	C(11)	C(12)	0(1)	N(11)	N(12)	C(11)	C(14)	-178.6(8)
N(11)	N(12)	B(1)	N(22)	63(1)	N(11)	N(12)	B(1)	N(32)	-53(1)
N(11)	C(13)	C(12)	C(11)	0(1)	N(12)	N(11)	Ta(1)	N(21)	-37.6(6)
N(12)	N(11)	Ta(1)	N(31)	46.3(6)	N(12)	N(11)	C(13)	C(12)	1(1)
N(12)	N(11)	C(13)	C(15)	179.8(9)	N(12)	C(11)	C(12)	C(13)	0(1)
N(12)	B(1)	N(22)	N(21)	-59(1)	N(12)	B(1)	N(22)	C(21)	118(1)
N(12)	B(1)	N(32)	N(31)	58(1)	N(12)	B(1)	N(32)	C(31)	-125(1)

Table 5. Torsion Angles(°) (continued)

atom	atom	atom	atom	angle	atom	atom	atom	atom	angle
N(21)	Ta(1)	N(11)	C(13)	132.2(9)	N(21)	Ta(1)	N(31)	N(32)	42.9(7)
N(21)	Ta(1)	N(31)	C(33)	-135.9(9)	N(21)	N(22)	C(21)	C(22)	0(1)
N(21)	N(22)	C(21)	C(24)	-179.7(9)	N(21)	N(22)	B(1)	N(32)	58(1)
N(21)	C(23)	C(22)	C(21)	0(1)	N(22)	N(21)	Ta(1)	N(31)	-43.0(6)
N(22)	N(21)	C(23)	C(22)	0(1)	N(22)	N(21)	C(23)	C(25)	-179.8(9)
N(22)	C(21)	C(22)	C(23)	0(1)	N(22)	B(1)	N(12)	C(11)	-113(1)
N(22)	B(1)	N(32)	N(31)	-58(1)	N(22)	B(1)	N(32)	C(31)	117(1)
N(31)	Ta(1)	N(11)	C(13)	-143.9(9)	N(31)	Ta(1)	N(21)	C(23)	140.7(9)
N(31)	N(32)	C(31)	C(32)	-2(1)	N(31)	N(32)	C(31)	C(34)	176(1)
N(31)	C(33)	C(32)	C(31)	-1(1)	N(32)	N(31)	C(33)	C(32)	0(1)
N(32)	N(31)	C(33)	C(35)	-178(1)	N(32)	C(31)	C(32)	C(33)	2(1)
N(32)	B(1)	N(12)	C(11)	129.2(10)	N(32)	B(1)	N(22)	C(21)	-123(1)
C(11)	N(12)	N(11)	C(13)	-1(1)	C(11)	C(12)	C(13)	C(15)	-179.5(9)
C(12)	C(11)	N(12)	B(1)	177.9(9)	C(13)	N(11)	N(12)	B(1)	-178.7(8)
C(13)	C(12)	C(11)	C(14)	179.3(10)	C(14)	C(11)	N(12)	B(1)	-1(1)
C(21)	N(22)	N(21)	C(23)	-1(1)	C(21)	C(22)	C(23)	C(25)	-179(1)
C(22)	C(21)	N(22)	B(1)	-177.5(10)	C(23)	N(21)	N(22)	B(1)	177.6(8)
C(23)	C(22)	C(21)	C(24)	-179(1)	C(24)	C(21)	N(22)	B(1)	1(1)
C(31)	N(32)	N(31)	C(33)	1(1)	C(31)	C(32)	C(33)	C(35)	177(1)
C(32)	C(31)	N(32)	B(1)	-178(1)	C(33)	N(31)	N(32)	B(1)	178.3(9)
C(33)	C(32)	C(31)	C(34)	-176(1)	C(34)	C(31)	N(32)	B(1)	0(1)

Table 6. Least Squares Planes

Plane number 1

Atoms defining plane	Distance
N(11)	-0.006(7)
N(12)	0.004(7)
C(11)	-0.003(9)
C(12)	-0.003(10)
C(13)	0.007(9)

Plane number 2

Atoms defining plane	Distance
N(21)	0.005(7)
N(22)	-0.005(8)
C(21)	0.005(10)
C(22)	0.00(1)
C(23)	-0.01(1)

Plane number 3

Atoms defining plane	Distance
N(31)	-0.004(8)
N(32)	0.007(9)
C(31)	-0.01(1)
C(32)	0.01(1)
C(33)	0.00(1)

Plane number 4

Atoms defining plane	Distance
Cl(11)	0.0000
Cl(21)	0.0000
Cl(31)	0.0000
Additional Atoms	Distance
Ta(1)	1.170

Summary

plane	mean deviation	χ^2
1	0.0047	1.6
2	0.0041	1.2
3	0.0073	2.6
4	0.0000	0.0

Dihedral angles between planes (°)

plane	1	2	3
2	66.31		
3	53.70	119.85	
4	84.62	88.45	90.05