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Table S 1. General Displacement Parameter Expressions - U's

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
NI	0.0268(3)	0.0234(3)	0.0296(3)	0.0041(2)	0.0064(2)	0.0045(2)
N1	0.031(1)	0.020(1)	0.031(1)	0.000(1)	0.004(1)	0.002(1)
C1	0.036(2)	0.024(2)	0.043(2)	0.007(1)	0.004(2)	0.004(1)
C2	0.046(2)	0.029(2)	0.038(2)	0.015(2)	0.004(2)	0.001(2)
C3	0.039(2)	0.034(2)	0.038(2)	0.009(2)	0.009(1)	0.002(2)
N2	0.032(1)	0.026(1)	0.032(1)	0.005(1)	0.009(1)	0.006(1)
C4	0.031(2)	0.036(2)	0.044(2)	0.008(1)	0.011(1)	0.005(2)
C5	0.038(2)	0.032(2)	0.039(2)	0.004(1)	0.014(1)	0.004(1)
N3	0.029(1)	0.025(1)	0.027(1)	0.003(1)	0.008(1)	0.001(1)
C6	0.046(2)	0.029(2)	0.024(2)	0.007(2)	0.004(1)	0.000(1)
C7	0.039(2)	0.034(2)	0.030(2)	0.007(2)	0.001(2)	0.004(1)
C8	0.029(2)	0.040(2)	0.034(2)	0.005(1)	0.003(1)	0.001(2)
N4	0.025(1)	0.027(1)	0.033(1)	0.001(1)	0.007(1)	0.003(1)
C9	0.026(2)	0.034(2)	0.038(2)	0.002(1)	0.006(1)	0.001(1)
C10	0.037(2)	0.025(2)	0.038(2)	0.005(1)	0.010(1)	0.005(1)
C11	0.037(2)	0.030(2)	0.031(2)	0.004(1)	0.007(1)	0.006(1)
C12	0.035(2)	0.023(1)	0.026(1)	0.003(1)	0.012(1)	0.002(1)
C13	0.034(2)	0.026(2)	0.025(1)	0.008(1)	0.004(1)	0.003(1)
C14	0.032(2)	0.025(1)	0.025(1)	0.004(1)	0.008(1)	0.001(1)
C15	0.030(2)	0.030(2)	0.032(2)	0.008(1)	0.006(1)	0.002(1)
C16	0.040(2)	0.030(2)	0.031(2)	0.013(1)	0.005(1)	0.008(1)
C17	0.040(2)	0.024(2)	0.032(2)	0.006(1)	0.012(1)	0.004(1)
C18	0.030(2)	0.030(2)	0.027(1)	0.004(1)	0.005(1)	0.001(1)
CL1	0.0357(4)	0.0355(4)	0.0330(4)	0.0028(4)	0.0113(3)	0.0019(3)
O1	0.046(1)	0.048(1)	0.046(1)	0.006(1)	0.019(1)	0.007(1)

Table S 1. Continued

Name	U(1,1)	U(2,2)	U(3,3)	U(1,2)	U(1,3)	U(2,3)
O2	0.073(2)	0.089(2)	0.034(1)	0.030(2)	0.002(1)	0.016(1)
O3	0.092(2)	0.067(2)	0.109(2)	0.050(1)	0.036(2)	0.012(2)
O4	0.078(2)	0.079(2)	0.057(2)	0.038(2)	0.024(1)	0.005(1)
CL2	0.0390(4)	0.0299(4)	0.0419(4)	0.0009(4)	0.0088(4)	0.0078(3)
O5	0.071(2)	0.114(2)	0.125(3)	0.041(2)	0.013(2)	0.025(2)
O6	0.125(3)	0.093(2)	0.086(2)	0.049(2)	0.036(2)	0.023(2)
O7	0.121(3)	0.050(2)	0.046(2)	0.023(2)	0.009(2)	0.009(1)
O8	0.094(2)	0.038(1)	0.070(2)	0.013(1)	0.005(2)	0.003(1)
C19	0.047(2)	0.060(2)	0.064(2)	0.001(2)	0.000(2)	0.011(2)
C20	0.053(2)	0.037(2)	0.042(2)	0.001(2)	0.014(2)	0.001(2)
N5	0.059(2)	0.073(2)	0.055(2)	0.015(2)	0.003(2)	0.002(2)

The form of the anisotropic displacement parameter is:
$\exp[-2\pi^2[h^2a^2U(1,1) + k^2b^2U(2,2) + l^2c^2U(3,3) + 2hkabU(1,2) + 2hlacU(1,3) + 2klbcU(2,3)]]$
where a,b, and c are reciprocal lattice constants.

Table S 2. Positional Parameters and Their E.S.D.

Atom	x	y	z	B(Å^2)
H1	0.5593	0.3971	0.4697	3*
H2	0.6831	0.4767	0.5092	3*
H3	0.5935	0.5089	0.7011	3*
H4	0.7037	0.4422	0.7611	3*
H5	0.4428	0.3840	0.7059	3*
H6	0.5494	0.3585	0.8368	3*
H7	0.4218	0.1133	0.6306	3*
H8	0.3823	0.1978	0.7385	3*
H9	0.5057	0.0715	0.8591	3*
H10	0.5586	0.1883	0.9187	3*
H11	0.7493	0.0658	0.9863	3*
H12	0.7648	0.1880	0.9962	3*
H13	0.9113	0.0587	0.8611	3*
H14	0.9616	0.1253	1.0157	3*
H15	1.0392	0.2146	0.8528	3*
H16	0.9333	0.2775	0.8970	3*
H17	0.9430	0.2430	0.5085	3*
H18	1.0258	0.3037	0.6570	3*
H19	0.8732	0.4127	0.6734	3*
H20	0.8865	0.4092	0.5102	3*
H21	0.7561	0.2257	0.3611	3*
H22	0.7235	0.3341	0.3107	3*
H23	0.5708	0.0974	0.3877	2*
H24	0.2323	0.1088	0.0923	3*
H25	0.3141	0.2687	0.0341	3*

Table S 2. Continued.

Atom	x	y	z	B(Å^2)
H26	0.5194	0.3481	0.1589	3*
H27	0.2576	-0.0035	0.3109	3*
H28	0.3961	-0.0192	0.3941	3*
H29	0.0030	0.3241	0.3060	6*
H30	0.0844	0.3907	0.2223	6*
H31	0.0558	0.2693	0.1789	6*
H32	0.4876	0.2652	0.5474	3*
H33	0.8842	0.1295	0.6402	2*

Table S 3. Bond Distances in Angstroms

Atom 1	Atom 2	Distance	Atom 1	Atom 2	Distance
NI	N1	1.956(2)	C9	C10	1.501(4)
NI	N2	1.909(2)	C11	C12	1.504(3)
NI	N3	1.969(2)	C12	C13	1.389(3)
NI	N4	1.939(2)	C12	C17	1.392(3)
N1	C1	1.500(3)	C13	C14	1.386(3)
N1	C10	1.500(3)	C14	C15	1.406(3)
N1	C11	1.520(3)	C14	C18	1.516(3)
C1	C2	1.515(4)	C15	C16	1.375(3)
C2	C3	1.517(4)	C16	C17	1.391(4)
C3	N2	1.496(3)	CL1	O1	1.426(2)
N2	C4	1.479(3)	CL1	O2	1.417(2)
C4	C5	1.490(4)	CL1	O3	1.411(2)
C5	N3	1.501(3)	CL1	O4	1.421(2)
N3	C6	1.493(3)	CL2	O5	1.410(3)
N3	C18	1.508(3)	CL2	O6	1.396(2)
C6	C7	1.513(4)	CL2	O7	1.419(2)
C7	C8	1.498(4)	CL2	O8	1.406(2)
C8	N4	1.489(3)	C19	C20	1.444(5)
N4	C9	1.491(3)	C20	N5	1.144(4)

Numbers in parentheses are estimated standard deviations in the least significant digits.

Table S 4. Bond Angles in Degrees

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
N1	NI	N2	90.61(8)	NI	N3	C6	115.0(1)
N1	NI	N3	177.26(7)	NI	N3	C18	104.4(1)
N1	NI	N4	88.04(8)	C5	N3	C6	107.4(2)
N2	NI	N3	87.48(8)	C5	N3	C18	111.4(2)
N2	NI	N4	174.76(7)	C6	N3	C18	111.6(2)
N3	NI	N4	94.03(8)	N3	C6	C7	115.5(2)
NI	N1	C1	112.9(1)	C6	C7	C8	112.9(2)
NI	N1	C10	103.0(1)	C7	C8	N4	111.2(2)
NI	N1	C11	114.8(1)	NI	N4	C8	112.2(1)
C1	N1	C10	108.5(2)	NI	N4	C9	109.8(1)
C1	N1	C11	109.5(2)	C8	N4	C9	112.5(2)
C10	N1	C11	107.7(2)	N4	C9	C10	108.1(2)
N1	C1	C2	111.4(2)	N1	C10	C9	109.0(2)
C1	C2	C3	113.6(2)	N1	C11	C12	115.9(2)
C2	C3	N2	110.4(2)	C11	C12	C13	121.1(2)
NI	N2	C3	110.0(1)	C11	C12	C17	120.7(2)
NI	N2	C4	110.4(1)	C13	C12	C17	118.1(2)
C3	N2	C4	112.7(2)	C12	C13	C14	122.5(2)
N2	C4	C5	107.3(2)	C13	C14	C15	118.4(2)
C4	C5	N3	109.7(2)	C13	C14	C18	119.3(2)
NI	N3	C5	106.9(1)	C15	C14	C18	122.0(2)
C14	C15	C16	119.7(2)	O3	CL1	O4	111.2(2)
C15	C16	C17	121.1(2)	O5	CL2	O6	108.0(2)
C12	C17	C16	120.2(2)	O5	CL2	O7	110.0(2)
N3	C18	C14	119.6(2)	O5	CL2	O8	106.0(2)
O1	CL1	O2	109.6(1)	O6	CL2	O7	111.0(2)

Table S 4. Continued

Atom 1	Atom 2	Atom 3	Angle	Atom 1	Atom 2	Atom 3	Angle
O1	CL1	O3	107.9(1)	O6	CL2	O8	111.9(2)
O1	CL1	O4	109.7(1)	O7	CL2	O8	109.7(1)
O2	CL1	O3	109.3(2)	C19	C20	N5	177.5(3)
O2	CL1	O4	109.2(1)				

Numbers in parentheses are estimated standard deviations in the least significant digits.