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Table 1: Fractional coordinates and equivalent isotropic[a] thermal parameters ($Å^2$) for the non-H atoms of compound **9**.

Atom	x	y	z	U
Ta	0.10032(3)	0.25416(2)	0.16485(3)	0.051(1)
Cl	0.1341(3)	0.2123(2)	-0.0163(2)	0.075(1)
N1	0.2277(6)	0.0911(4)	0.1445(5)	0.050(3)
N2	0.3364(6)	0.0773(4)	0.1793(5)	0.053(3)
N3	0.1409(6)	0.2728(5)	0.3140(5)	0.054(3)
N4	0.2574(6)	0.2216(4)	0.3239(5)	0.053(3)
N5	0.3216(6)	0.2914(4)	0.0988(5)	0.048(2)
N6	0.4148(6)	0.2537(4)	0.1406(5)	0.050(3)
N7	0.0497(7)	0.4048(5)	0.1812(5)	0.058(3)
B	0.3769(9)	0.1709(7)	0.2263(7)	0.053(4)
C1	0.1222(10)	-0.0250(6)	0.0579(8)	0.083(5)
C2	0.2248(9)	-0.0029(6)	0.1025(7)	0.063(4)
C3	0.3312(9)	-0.0737(6)	0.1092(7)	0.069(4)
C4	0.3990(8)	-0.0224(6)	0.1579(7)	0.062(4)
C5	0.5201(10)	-0.0631(7)	0.1840(9)	0.094(5)
C6	-0.0687(9)	0.3898(7)	0.4311(7)	0.081(4)
C7	0.0639(9)	0.3233(6)	0.4082(7)	0.063(4)
C8	0.1296(10)	0.3026(7)	0.4786(7)	0.076(4)
C9	0.2494(9)	0.2391(7)	0.4237(7)	0.064(4)
C10	0.3605(11)	0.1946(9)	0.4604(8)	0.100(6)
C11	0.3174(10)	0.4132(7)	-0.0460(7)	0.081(5)
C12	0.3840(8)	0.3570(6)	0.0207(6)	0.059(3)
C13	0.5174(8)	0.3569(6)	0.0162(7)	0.064(4)
C14	0.5353(8)	0.2919(6)	0.0909(7)	0.061(4)
C15	0.6580(8)	0.2672(7)	0.1202(8)	0.081(4)
C16	-0.0798(9)	0.1823(6)	0.2685(7)	0.074(4)
C17	-0.1200(9)	0.0979(7)	0.3501(9)	0.079(5)
C18	-0.2184(14)	0.0336(10)	0.3269(11)	0.144(9)
C19	-0.1956(13)	0.1465(9)	0.4586(10)	0.142(8)
C20	-0.0047(12)	0.0249(8)	0.3556(9)	0.119(6)
C21	-0.0569(9)	0.3796(6)	0.1565(8)	0.072(4)
C22	0.0769(8)	0.5070(6)	0.2004(6)	0.060(4)
C23	-0.0055(10)	0.5955(6)	0.1890(7)	0.076(4)
C24	0.0208(13)	0.6940(7)	0.2078(8)	0.092(6)
C25	0.1249(12)	0.7067(7)	0.2417(8)	0.087(5)
C26	0.2064(10)	0.6198(7)	0.2531(7)	0.078(4)
C27	0.1847(9)	0.5196(6)	0.2331(6)	0.064(4)
C28	0.465(5)	0.483(3)	0.543(4)	0.20(2)
C29	0.480(4)	0.468(3)	0.630(3)	0.18(2)
C30	0.456(4)	0.393(3)	0.644(3)	0.102(14)

[a]For anisotropic atoms, the U value is U_{eq}, calculated as $U_{eq} = 1/3\ \Sigma_i\Sigma_j\ U_{ij}\ a_i^*\ a_j^*\ A_{ij}$ where A_{ij} is the dot product of the i^{th} and j^{th} direct space unit cell vectors.

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Table 2: Bond Lengths (Å) and Angles (°) for the non-H atoms of compound **9**.

1	2	3	1-2	1-2-3
Cl	Ta	N1	2.391(3)	81.4(2)
Cl	Ta	N3		161.53(15)
Cl	Ta	N5		86.4(2)
Cl	Ta	N7		104.2(2)
Cl	Ta	C16		107.4(3)
N1	Ta	N3	2.298(5)	85.3(2)
N1	Ta	N5		77.3(2)
N1	Ta	N7		161.1(3)
N1	Ta	C16		87.2(2)
N1	Ta	C21		160.1(3)
N3	Ta	N5	2.233(8)	78.2(2)
N3	Ta	N7		84.6(3)
N3	Ta	C16		84.5(3)
N3	Ta	C21		111.4(3)
N5	Ta	N7	2.270(6)	84.9(2)
N5	Ta	C16		157.6(3)
N5	Ta	C21		115.6(3)
N7	Ta	C16	1.932(6)	107.8(3)
N7	Ta	C21		37.8(3)
C16	Ta	C21	2.198(8)	83.9(3)
C21	Ta	Cl	2.196(9)	84.3(3)
N2	N1	C2	1.385(10)	105.9(6)
N2	N1	Ta		119.5(4)
C2	N1	Ta	1.345(10)	134.6(6)
B	N2	C4	1.538(12)	129.1(7)
B	N2	N1		120.7(5)
C4	N2	N1	1.344(9)	110.1(7)
N4	N3	C7	1.369(9)	107.0(7)
N4	N3	Ta		121.4(4)
C7	N3	Ta	1.338(10)	131.5(6)
B	N4	C9	1.514(9)	130.2(8)
B	N4	N3		120.3(7)
C9	N4	N3	1.338(12)	108.8(6)
N6	N5	C12	1.349(10)	107.3(6)
N6	N5	Ta		122.2(4)
C12	N5	Ta	1.366(9)	130.3(6)
B	N6	C14	1.544(10)	130.2(7)
B	N6	N5		119.2(6)
C14	N6	N5	1.346(9)	110.4(6)
C21	N7	C22	1.360(13)	127.4(7)
C21	N7	Ta		81.7(4)
C22	N7	Ta	1.423(10)	150.8(6)
N2	B	N4		111.3(6)
N2	B	N6		108.1(7)
N4	B	N6		108.0(6)

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Table 2 continued.

C2	C1		1.48(2)	
C3	C2	N1	1.383(12)	109.0(9)
C3	C2	C1		126.5(8)
N1	C2	C1		124.4(7)
C4	C3	C2	1.360(14)	107.8(7)
C5	C4	N2	1.483(15)	123.8(8)
C5	C4	C3		129.0(7)
N2	C4	C3		107.2(8)
C7	C6		1.467(12)	
C8	C7	N3	1.38(2)	109.1(7)
C8	C7	C6		126.3(8)
N3	C7	C6		124.6(9)
C9	C8	C7	1.358(11)	106.4(8)
C10	C9	N4	1.49(2)	122.3(7)
C10	C9	C8		129.0(9)
N4	C9	C8		108.6(9)
C12	C11		1.475(14)	
C13	C12	N5	1.383(13)	107.1(7)
C13	C12	C11		128.4(7)
N5	C12	C11		124.5(8)
C14	C13	C12	1.361(13)	108.3(7)
C15	C14	N6	1.487(14)	123.6(8)
C15	C14	C13		129.5(7)
N6	C14	C13		106.9(8)
C17	C16	Ta	1.526(13)	141.7(7)
C18	C17	C19	1.52(2)	106.4(9)
C18	C17	C20		107.9(9)
C18	C17	C16		109.9(10)
C19	C17	C20	1.47(2)	106.3(11)
C19	C17	C16		110.4(8)
C20	C17	C16	1.46(2)	115.6(8)
Ta	C21	N7		60.5(4)
C23	C22	C27	1.387(12)	119.0(8)
C23	C22	N7		120.5(9)
C27	C22	N7	1.392(14)	120.5(7)
C24	C23	C22	1.373(14)	120.4(11)
C25	C24	C23	1.36(2)	120.8(10)
C26	C25	C24	1.366(14)	119.1(9)
C27	C26	C25	1.379(13)	121.8(11)
C22	C27	C26		119.0(8)
C29	C28	C30	1.26(7)	
C28a	C28	C29	1.23(6)	135.(5)
C30	C29	C28	1.02(6)	102.(5)

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Supplementary Table 2: Anisotropic thermal parameters[a] for the non-H atoms of compound **9**.

Atom	U11	U22	U33	U12	U13	U23
Ta	0.0483(2)	0.0463(2)	0.0654(2)	-0.01178(12)	-0.0290(2)	0.00860(13)
Cl	0.096(2)	0.0710(13)	0.0759(15)	-0.0195(12)	-0.0513(14)	0.0073(11)
N1	0.051(4)	0.051(3)	0.055(4)	-0.018(3)	-0.024(3)	-0.002(3)
N2	0.046(4)	0.044(3)	0.066(4)	-0.007(3)	-0.019(3)	0.006(3)
N3	0.042(3)	0.056(4)	0.064(4)	-0.008(3)	-0.019(3)	0.004(3)
N4	0.050(4)	0.051(3)	0.063(4)	-0.010(3)	-0.028(3)	0.008(3)
N5	0.046(3)	0.045(3)	0.056(4)	-0.014(3)	-0.022(3)	0.006(3)
N6	0.038(3)	0.051(3)	0.066(4)	-0.011(3)	-0.023(3)	0.000(3)
N7	0.069(4)	0.050(3)	0.073(4)	-0.008(3)	-0.047(4)	0.011(3)
B	0.043(5)	0.055(5)	0.070(6)	-0.009(4)	-0.030(5)	0.009(4)
C1	0.094(7)	0.061(5)	0.112(8)	-0.022(5)	-0.055(6)	-0.008(5)
C2	0.065(5)	0.052(4)	0.072(6)	-0.014(4)	-0.023(5)	0.004(4)
C3	0.071(6)	0.044(4)	0.093(7)	-0.006(4)	-0.033(5)	0.002(4)
C4	0.050(5)	0.050(4)	0.080(6)	-0.001(4)	-0.020(4)	0.008(4)
C5	0.081(7)	0.060(5)	0.147(10)	0.006(5)	-0.053(7)	-0.001(6)
C6	0.070(6)	0.086(6)	0.076(6)	-0.010(5)	-0.015(5)	0.004(5)
C7	0.067(5)	0.055(5)	0.067(6)	-0.012(4)	-0.023(5)	0.003(4)
C8	0.080(7)	0.099(7)	0.049(5)	-0.021(6)	-0.021(5)	0.000(5)
C9	0.066(6)	0.068(5)	0.070(6)	-0.018(4)	-0.036(5)	0.015(4)
C10	0.108(8)	0.128(9)	0.081(7)	-0.016(7)	-0.057(7)	0.020(6)
C11	0.105(7)	0.075(6)	0.073(6)	-0.036(5)	-0.038(6)	0.026(5)
C12	0.067(5)	0.052(4)	0.050(5)	-0.021(4)	-0.010(4)	0.003(4)
C13	0.058(5)	0.056(5)	0.072(6)	-0.022(4)	-0.015(4)	0.005(4)
C14	0.048(5)	0.053(4)	0.078(6)	-0.017(4)	-0.017(4)	-0.008(4)
C15	0.051(5)	0.074(6)	0.119(8)	-0.020(4)	-0.029(5)	0.003(5)
C16	0.076(6)	0.067(5)	0.084(6)	-0.031(5)	-0.029(5)	0.018(5)
C17	0.057(5)	0.079(6)	0.098(8)	-0.024(5)	-0.021(6)	0.025(6)
C18	0.162(12)	0.144(11)	0.172(13)	-0.104(10)	-0.090(11)	0.084(10)
C19	0.115(10)	0.122(10)	0.142(12)	-0.009(8)	-0.000(9)	0.067(9)
C20	0.120(10)	0.102(8)	0.111(9)	-0.011(7)	-0.017(7)	0.060(7)
C21	0.060(5)	0.064(5)	0.103(7)	-0.009(4)	-0.044(5)	0.024(5)
C22	0.065(5)	0.051(4)	0.065(5)	-0.009(4)	-0.025(4)	0.008(4)
C23	0.092(7)	0.060(5)	0.082(6)	-0.003(5)	-0.040(5)	0.012(4)
C24	0.142(10)	0.050(5)	0.080(7)	-0.009(6)	-0.039(7)	0.014(5)
C25	0.122(9)	0.054(5)	0.076(7)	-0.024(6)	-0.025(6)	0.001(5)
C26	0.076(6)	0.080(6)	0.074(6)	-0.027(5)	-0.020(5)	-0.001(5)
C27	0.072(6)	0.056(5)	0.067(5)	-0.018(4)	-0.027(5)	0.008(4)

[a] Uij are the mean-square amplitudes of vibration in $Å^2$ from the general temperature factor expression

$$\exp[-2\pi^2(h^2a^{*2}U11 + k^2b^{*2}U22 + l^2c^{*2}U33 + 2hka^*b^*U12 + 2hla^*c^*U13 + 2klb^*c^*U23)]$$

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Suppelementary Table 3: Fractional coordinates and isotropic thermal parameters ($Å^2$) for the H atoms of compound **9**.

Atom	x	y	z	U
H	0.45307	0.146	0.24646	0.08
H1a	0.14047	-0.0971	0.03223	0.08
H1b	0.12779	0.01985	-0.00003	0.08
H1c	0.03105	-0.01172	0.11291	0.08
H3	0.35237	-0.14636	0.08509	0.08
H5a	0.54874	-0.13592	0.16137	0.08
H5b	0.49456	-0.05528	0.25997	0.08
H5c	0.59499	-0.02364	0.14838	0.08
H6a	-0.1044	0.41632	0.50416	0.08
H6b	-0.1334	0.34941	0.42002	0.08
H6c	-0.05492	0.44751	0.38463	0.08
H8	0.09678	0.32878	0.55162	0.08
H10a	0.33745	0.21545	0.53393	0.08
H10b	0.44574	0.2191	0.41678	0.08
H10c	0.37084	0.11939	0.45266	0.08
H11a	0.38146	0.45381	-0.09564	0.08
H11b	0.23691	0.45912	-0.00103	0.08
H11c	0.2905	0.36336	-0.08461	0.08
H13	0.58567	0.39588	-0.03145	0.08
H15a	0.73303	0.30216	0.07494	0.08
H15b	0.68629	0.19273	0.11252	0.08
H15c	0.63287	0.29071	0.19336	0.08
H16a	-0.11397	0.15928	0.21683	0.08
H16b	-0.1397	0.2429	0.30903	0.08
H18a	-0.17305	-0.00148	0.25745	0.08
H18b	-0.2976	0.08053	0.32852	0.08
H18c	-0.2476	-0.01756	0.37994	0.08
H19a	-0.27419	0.19311	0.45836	0.08
H19b	-0.13545	0.18571	0.47736	0.08
H19c	-0.22656	0.09413	0.50992	0.08
H20a	0.04727	-0.01019	0.28685	0.08
H20b	-0.03747	-0.02626	0.4079	0.08
H20c	0.05364	0.06532	0.37534	0.08
H21a	-0.14903	0.38734	0.2103	0.08
H21b	-0.0608(9)	0.3968(6)	0.0886(8)	0.08
H23	-0.08018	0.58707	0.16667	0.08
H24	-0.03427	0.7551	0.19724	0.08
H25	0.14021	0.77569	0.25777	0.08
H26	0.28071	0.62907	0.27554	0.08
H27	0.24206	0.45887	0.24156	0.08

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Supplementary Table 4: Bond Lengths (Å) and Angles (°) of the H atoms of compound **9**.

1	2	3	1-2	1-2-3
H	B	N2	0.960(10)	108.6(7)
H	B	N4		108.9(8)
H	B	N6		112.0(7)
H1a	C1	H1b	0.960(8)	109.5(10)
H1a	C1	H1c		109.5(9)
H1a	C1	C2		109.8(9)
H1b	C1	H1c	0.960(10)	109.5(9)
H1b	C1	C2		109.4(8)
H1c	C1	C2	0.960(8)	109.2(9)
H3	C3	C4	0.960(8)	126.1(9)
H3	C3	C2		126.2(11)
H5a	C5	H5b	0.960(8)	109.5(10)
H5a	C5	H5c		109.5(8)
H5a	C5	C4		110.1(11)
H5b	C5	H5c	0.960(12)	109.5(12)
H5b	C5	C4		108.9(7)
H5c	C5	C4	0.960(9)	109.4(9)
H6a	C6	H6b	0.960(9)	109.5(8)
H6a	C6	H6c		109.5(9)
H6a	C6	C7		109.0(10)
H6b	C6	H6c	0.960(11)	109.5(11)
H6b	C6	C7		109.8(8)
H6c	C6	C7	0.960(9)	109.6(7)
H8	C8	C9	0.960(9)	127.2(11)
H8	C8	C7		126.4(9)
H10a	C10	H10b	0.960(11)	109.5(13)
H10a	C10	H10c		109.5(11)
H10a	C10	C9		110.8(8)
H10b	C10	H10c	0.960(10)	109.5(9)
H10b	C10	C9		109.1(10)
H10c	C10	C9	0.960(11)	108.5(11)
H11a	C11	H11b	0.960(9)	109.5(9)
H11a	C11	H11c		109.5(9)
H11a	C11	C12		109.5(10)
H11b	C11	H11c	0.960(8)	109.5(11)
H11b	C11	C12		109.5(8)
H11c	C11	C12	0.960(11)	109.5(8)
H13	C13	C14	0.960(8)	125.9(9)
H13	C13	C12		125.8(9)
H15a	C15	H15b	0.960(8)	109.5(7)
H15a	C15	H15c		109.5(10)
H15a	C15	C14		110.3(9)
H15b	C15	H15c	0.960(8)	109.5(10)
H15b	C15	C14		109.4(9)
H15c	C15	C14	0.960(11)	108.7(7)

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Supplementary Table 4 continued.

H16a	C16	H16b	0.960(11)	109.5(10)
H16a	C16	C17		100.7(8)
H16a	C16	Ta		100.9(6)
H16b	C16	C17	0.960(7)	101.0(7)
H16b	C16	Ta		101.1(6)
H18a	C18	H18b	0.960(13)	109.(2)
H18a	C18	H18c		109.5(12)
H18a	C18	C17		109.8(11)
H18b	C18	H18c	0.960(14)	109.5(12)
H18b	C18	C17		108.2(11)
H18c	C18	C17	0.960(13)	110.4(14)
H19a	C19	H19b	0.960(13)	109.5(12)
H19a	C19	H19c		109.5(11)
H19a	C19	C17		108.4(13)
H19b	C19	H19c	0.960(15)	109.5(15)
H19b	C19	C17		108.9(10)
H19c	C19	C17	0.960(12)	111.1(10)
H20a	C20	H20b	0.960(10)	109.5(10)
H20a	C20	H20c		109.5(10)
H20a	C20	C17		109.7(12)
H20b	C20	H20c	0.960(11)	109.5(13)
H20b	C20	C17		111.1(10)
H20c	C20	C17	0.960(14)	107.6(9)
H21a	C21	H21b	0.960(7)	109.5(11)
H21a	C21	Ta		120.1(7)
H21a	C21	N7		119.9(10)
H21b	C21	Ta	0.96(2)	119.9(7)
H21b	C21	N7		119.8(9)
H23	C23	C24	0.960(12)	120.4(10)
H23	C23	C22		119.2(9)
H24	C24	C25	0.960(11)	119.1(10)
H24	C24	C23		120.1(13)
H25	C25	C26	0.960(10)	120.5(13)
H25	C25	C24		120.4(10)
H26	C26	C27	0.960(11)	119.4(9)
H26	C26	C25		118.9(10)
H27	C27	C22	0.960(8)	119.7(8)
H27	C27	C26		121.4(10)