Supplementary Material (ESI) for Dalton Transactions

'Pincer' pyridine dicarbene complexes of nickel and their derivatives: unexpected ring opening of a coordinated imidazol-2-ylidene.

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Electronic Supplementary information. List of bond lengths, angles etc. for crystal structures.

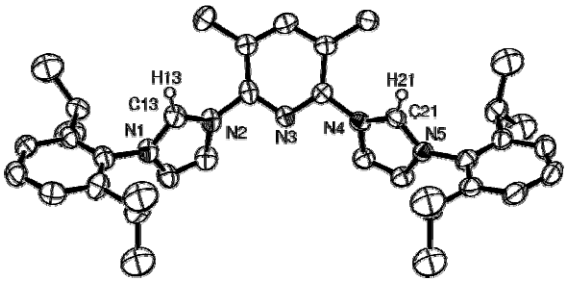


Table 1. Crystal data and structure refinement for $\mathbf{1^{Me}(I)^-_2}$

Identification code	$\mathbf{1^{Me}(I)^-_2}$	
Empirical formula	C38.67 H48.67 Cl5 I2 N5	
Formula weight	1014.54	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R-3	
Unit cell dimensions	a = 52.325(4) Å	α= 90°.
	b = 52.325(4) Å	β= 90°.
	c = 9.4345(5) Å	γ = 120°.
Volume	22370(3) $Å^3$	
Z	18	
Density (calculated)	1.356 Mg/m^3	
Absorption coefficient	1.563 mm^{-1}	
F(000)	9120	
Crystal size	0.36 x 0.16 x 0.16 mm^3	
Theta range for data collection	2.46 to 27.63°.	
Index ranges	-60<=h<=67, -67<=k<=66, -12<=l<=12	
Reflections collected	40406	
Independent reflections	11431 [R(int) = 0.0842]	
Completeness to theta = 27.63°	98.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7881 and 0.6031	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11431 / 0 / 437	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0665, wR2 = 0.1500	
R indices (all data)	R1 = 0.1396, wR2 = 0.1754	
Largest diff. peak and hole	1.194 and -0.847 e.$Å^{-3}$	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{1^{Me}(I)^-_2}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6304(2)	318(2)	7891(6)	40(2)
C(2)	6051(2)	63(2)	7443(7)	45(2)
C(3)	6069(2)	-192(2)	7299(7)	46(2)
C(4)	6330(2)	-191(2)	7638(7)	46(2)
C(5)	6575(2)	70(2)	8071(7)	40(2)
C(6)	6570(2)	332(1)	8209(6)	38(2)
C(7)	5761(2)	57(2)	7135(8)	56(2)
C(8)	5648(2)	-49(2)	5645(9)	76(1)
C(9)	5532(2)	-118(2)	8214(9)	76(1)
C(10)	6843(2)	615(2)	8677(7)	43(2)
C(11)	6890(2)	622(2)	10253(9)	76(1)
C(12)	7130(2)	653(2)	7993(9)	76(1)
C(13)	6350(2)	788(2)	7071(6)	40(2)
C(14)	6224(2)	678(2)	9312(7)	45(2)
C(15)	6243(2)	936(2)	9071(7)	45(2)
C(16)	6357(2)	1262(1)	6917(6)	38(2)
C(17)	6590(1)	1427(1)	5979(6)	37(2)
C(18)	6580(1)	1657(2)	5343(7)	40(2)
C(19)	6365(1)	1730(1)	5604(6)	36(2)
C(20)	6148(1)	1544(1)	6579(6)	35(2)
C(21)	5737(1)	1631(1)	6068(7)	36(2)
C(22)	5796(2)	1563(2)	8329(7)	41(2)
C(23)	5562(2)	1602(2)	8220(6)	41(2)
C(24)	5298(2)	1690(2)	6198(6)	39(2)
C(25)	5043(2)	1446(2)	5704(7)	42(2)
C(26)	4832(2)	1496(2)	5087(7)	51(2)
C(27)	4877(2)	1781(2)	5000(7)	51(2)
C(28)	5131(2)	2016(2)	5476(7)	49(2)
C(29)	5356(2)	1982(2)	6102(7)	43(2)
C(30)	4991(2)	1135(2)	5826(7)	48(2)
C(31)	4769(2)	975(2)	6993(9)	76(1)

C(32)	4887(2)	961(2)	4448(9)	76(1)
C(33)	5638(2)	2244(2)	6566(8)	49(2)
C(34)	5811(2)	2423(2)	5299(9)	76(1)
C(35)	5590(2)	2427(2)	7643(9)	76(1)
C(36)	6836(2)	1365(2)	5673(8)	48(2)
C(37)	6373(2)	1993(2)	4933(7)	44(2)
C(38)	1093(2)	2673(2)	9093(11)	80(3)
C(39)	1844(3)	3842(3)	3252(13)	62(3)
N(1)	6288(1)	584(1)	8075(5)	40(1)
N(2)	6326(1)	1007(1)	7655(5)	38(1)
N(3)	6142(1)	1318(1)	7243(5)	33(1)
N(4)	5906(1)	1585(1)	6968(5)	35(1)
N(5)	5527(1)	1645(1)	6805(5)	36(1)
I(1)	6290(1)	678(1)	3237(1)	47(1)
I(2)	996(1)	1643(1)	1160(1)	51(1)
Cl(1)	1045(1)	2337(1)	9787(3)	90(1)
Cl(2)	1085(1)	2660(1)	7226(3)	95(1)
Cl(3)	1424(1)	2973(1)	9643(4)	111(1)
Cl(4)	2197(1)	3910(1)	3099(5)	113(2)
Cl(5)	1822(1)	4157(1)	3403(6)	124(2)
Cl(6)	1613(1)	3611(1)	1915(4)	93(1)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{1^{Me}(I)^-_2}$.

C(1)-C(6)	1.387(9)	C(14)-N(1)	1.371(8)
C(1)-C(2)	1.397(10)	C(14)-H(14)	0.9500
C(1)-N(1)	1.448(8)	C(15)-N(2)	1.396(8)
C(2)-C(3)	1.389(10)	C(15)-H(15)	0.9500
C(2)-C(7)	1.526(10)	C(16)-N(3)	1.335(8)
C(3)-C(4)	1.400(10)	C(16)-C(17)	1.399(9)
C(3)-H(3)	0.9500	C(16)-N(2)	1.439(8)
C(4)-C(5)	1.389(10)	C(17)-C(18)	1.368(9)
C(4)-H(4)	0.9500	C(17)-C(36)	1.507(9)
C(5)-C(6)	1.392(9)	C(18)-C(19)	1.381(9)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.520(9)	C(19)-C(20)	1.406(9)
C(7)-C(9)	1.487(11)	C(19)-C(37)	1.496(9)
C(7)-C(8)	1.518(11)	C(20)-N(3)	1.321(8)
C(7)-H(7)	1.0000	C(20)-N(4)	1.433(8)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.331(8)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.335(8)
C(8)-H(8C)	0.9800	C(21)-H(21)	0.9500
C(9)-H(9A)	0.9800	C(22)-C(23)	1.343(9)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.388(8)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(11)	1.505(10)	C(23)-N(5)	1.382(8)
C(10)-C(12)	1.551(11)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.389(9)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.403(10)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.449(8)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.385(9)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.511(10)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.390(11)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(2)	1.333(8)	C(27)-C(28)	1.359(11)
C(13)-N(1)	1.341(8)	C(27)-H(27)	0.9500
C(13)-H(13)	0.9500	C(28)-C(29)	1.403(10)
C(14)-C(15)	1.324(9)	C(28)-H(28)	0.9500

C(29)-C(33)	1.492(10)	C(2)-C(1)-N(1)	118.0(6)
C(30)-C(31)	1.513(11)	C(3)-C(2)-C(1)	117.2(6)
C(30)-C(32)	1.525(11)	C(3)-C(2)-C(7)	120.3(7)
C(30)-H(30)	1.0000	C(1)-C(2)-C(7)	122.5(7)
C(31)-H(31A)	0.9800	C(2)-C(3)-C(4)	120.8(7)
C(31)-H(31B)	0.9800	C(2)-C(3)-H(3)	119.6
C(31)-H(31C)	0.9800	C(4)-C(3)-H(3)	119.6
C(32)-H(32A)	0.9800	C(5)-C(4)-C(3)	119.3(7)
C(32)-H(32B)	0.9800	C(5)-C(4)-H(4)	120.4
C(32)-H(32C)	0.9800	C(3)-C(4)-H(4)	120.4
C(33)-C(35)	1.502(11)	C(4)-C(5)-C(6)	122.3(7)
C(33)-C(34)	1.511(11)	C(4)-C(5)-H(5)	118.9
C(33)-H(33)	1.0000	C(6)-C(5)-H(5)	118.9
C(34)-H(34A)	0.9800	C(1)-C(6)-C(5)	116.1(6)
C(34)-H(34B)	0.9800	C(1)-C(6)-C(10)	123.1(6)
C(34)-H(34C)	0.9800	C(5)-C(6)-C(10)	120.9(6)
C(35)-H(35A)	0.9800	C(9)-C(7)-C(8)	111.3(7)
C(35)-H(35B)	0.9800	C(9)-C(7)-C(2)	111.6(7)
C(35)-H(35C)	0.9800	C(8)-C(7)-C(2)	112.8(7)
C(36)-H(36A)	0.9800	C(9)-C(7)-H(7)	107.0
C(36)-H(36B)	0.9800	C(8)-C(7)-H(7)	107.0
C(36)-H(36C)	0.9800	C(2)-C(7)-H(7)	107.0
C(37)-H(37A)	0.9800	C(7)-C(8)-H(8A)	109.5
C(37)-H(37B)	0.9800	C(7)-C(8)-H(8B)	109.5
C(37)-H(37C)	0.9800	H(8A)-C(8)-H(8B)	109.5
C(38)-Cl(3)	1.737(9)	C(7)-C(8)-H(8C)	109.5
C(38)-Cl(2)	1.762(11)	H(8A)-C(8)-H(8C)	109.5
C(38)-Cl(1)	1.774(10)	H(8B)-C(8)-H(8C)	109.5
C(38)-H(38)	1.0000	C(7)-C(9)-H(9A)	109.5
C(39)-Cl(4)	1.705(12)	C(7)-C(9)-H(9B)	109.5
C(39)-Cl(5)	1.714(13)	H(9A)-C(9)-H(9B)	109.5
C(39)-Cl(6)	1.747(12)	C(7)-C(9)-H(9C)	109.5
C(39)-H(39)	1.0000	H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.5
C(6)-C(1)-C(2)	124.4(6)	C(11)-C(10)-C(6)	112.0(6)
C(6)-C(1)-N(1)	117.5(6)	C(11)-C(10)-C(12)	105.8(6)

C(6)-C(10)-C(12)	112.6(6)	C(20)-C(19)-C(37)	124.0(6)
C(11)-C(10)-H(10)	108.8	N(3)-C(20)-C(19)	125.4(6)
C(6)-C(10)-H(10)	108.8	N(3)-C(20)-N(4)	112.6(5)
C(12)-C(10)-H(10)	108.8	C(19)-C(20)-N(4)	122.0(6)
C(10)-C(11)-H(11A)	109.5	N(5)-C(21)-N(4)	108.6(5)
C(10)-C(11)-H(11B)	109.5	N(5)-C(21)-H(21)	125.7
H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-H(21)	125.7
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	106.8(6)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	126.6
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	126.6
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	107.7(6)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	126.1
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.1
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	124.4(6)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	118.3(6)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	117.2(6)
N(2)-C(13)-N(1)	107.7(5)	C(26)-C(25)-C(24)	117.2(7)
N(2)-C(13)-H(13)	126.1	C(26)-C(25)-C(30)	120.3(7)
N(1)-C(13)-H(13)	126.1	C(24)-C(25)-C(30)	122.5(6)
C(15)-C(14)-N(1)	108.2(6)	C(25)-C(26)-C(27)	120.4(7)
C(15)-C(14)-H(14)	125.9	C(25)-C(26)-H(26)	119.8
N(1)-C(14)-H(14)	125.9	C(27)-C(26)-H(26)	119.8
C(14)-C(15)-N(2)	106.9(6)	C(28)-C(27)-C(26)	121.0(7)
C(14)-C(15)-H(15)	126.5	C(28)-C(27)-H(27)	119.5
N(2)-C(15)-H(15)	126.5	C(26)-C(27)-H(27)	119.5
N(3)-C(16)-C(17)	125.4(6)	C(27)-C(28)-C(29)	121.8(7)
N(3)-C(16)-N(2)	112.0(6)	C(27)-C(28)-H(28)	119.1
C(17)-C(16)-N(2)	122.6(6)	C(29)-C(28)-H(28)	119.1
C(18)-C(17)-C(16)	114.6(6)	C(28)-C(29)-C(24)	115.3(7)
C(18)-C(17)-C(36)	121.3(6)	C(28)-C(29)-C(33)	120.9(7)
C(16)-C(17)-C(36)	124.1(6)	C(24)-C(29)-C(33)	123.7(6)
C(17)-C(18)-C(19)	124.0(6)	C(25)-C(30)-C(31)	109.2(7)
C(17)-C(18)-H(18)	118.0	C(25)-C(30)-C(32)	113.5(6)
C(19)-C(18)-H(18)	118.0	C(31)-C(30)-C(32)	110.0(7)
C(18)-C(19)-C(20)	114.4(6)	C(25)-C(30)-H(30)	108.0
C(18)-C(19)-C(37)	121.6(6)	C(31)-C(30)-H(30)	108.0

C(32)-C(30)-H(30)	108.0	H(36B)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31A)	109.5	C(19)-C(37)-H(37A)	109.5
C(30)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37B)	109.5
H(31A)-C(31)-H(31B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(30)-C(31)-H(31C)	109.5	C(19)-C(37)-H(37C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32A)	109.5	Cl(3)-C(38)-Cl(2)	109.1(6)
C(30)-C(32)-H(32B)	109.5	Cl(3)-C(38)-Cl(1)	111.6(5)
H(32A)-C(32)-H(32B)	109.5	Cl(2)-C(38)-Cl(1)	109.9(5)
C(30)-C(32)-H(32C)	109.5	Cl(3)-C(38)-H(38)	108.7
H(32A)-C(32)-H(32C)	109.5	Cl(2)-C(38)-H(38)	108.7
H(32B)-C(32)-H(32C)	109.5	Cl(1)-C(38)-H(38)	108.7
C(29)-C(33)-C(35)	112.4(6)	Cl(4)-C(39)-Cl(5)	113.1(8)
C(29)-C(33)-C(34)	110.4(6)	Cl(4)-C(39)-Cl(6)	112.6(7)
C(35)-C(33)-C(34)	112.2(7)	Cl(5)-C(39)-Cl(6)	111.8(7)
C(29)-C(33)-H(33)	107.2	Cl(4)-C(39)-H(39)	106.2
C(35)-C(33)-H(33)	107.2	Cl(5)-C(39)-H(39)	106.2
C(34)-C(33)-H(33)	107.2	Cl(6)-C(39)-H(39)	106.2
C(33)-C(34)-H(34A)	109.5	C(13)-N(1)-C(14)	108.7(6)
C(33)-C(34)-H(34B)	109.5	C(13)-N(1)-C(1)	125.1(5)
H(34A)-C(34)-H(34B)	109.5	C(14)-N(1)-C(1)	126.1(5)
C(33)-C(34)-H(34C)	109.5	C(13)-N(2)-C(15)	108.5(5)
H(34A)-C(34)-H(34C)	109.5	C(13)-N(2)-C(16)	125.5(5)
H(34B)-C(34)-H(34C)	109.5	C(15)-N(2)-C(16)	125.9(5)
C(33)-C(35)-H(35A)	109.5	C(20)-N(3)-C(16)	116.2(5)
C(33)-C(35)-H(35B)	109.5	C(21)-N(4)-C(22)	108.5(5)
H(35A)-C(35)-H(35B)	109.5	C(21)-N(4)-C(20)	125.6(5)
C(33)-C(35)-H(35C)	109.5	C(22)-N(4)-C(20)	125.8(5)
H(35A)-C(35)-H(35C)	109.5	C(21)-N(5)-C(23)	108.4(5)
H(35B)-C(35)-H(35C)	109.5	C(21)-N(5)-C(24)	125.0(5)
C(17)-C(36)-H(36A)	109.5	C(23)-N(5)-C(24)	126.6(5)
C(17)-C(36)-H(36B)	109.5		
H(36A)-C(36)-H(36B)	109.5		
C(17)-C(36)-H(36C)	109.5		
H(36A)-C(36)-H(36C)	109.5		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $\mathbf{1^{Me}(I)^-_2}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	61(5)	42(4)	26(3)	1(3)	0(3)	31(4)
C(2)	44(4)	53(5)	44(4)	-10(3)	-8(3)	29(4)
C(3)	43(4)	43(4)	41(4)	-3(3)	-2(3)	14(4)
C(4)	62(5)	45(4)	39(4)	-2(3)	3(3)	32(4)
C(5)	41(4)	43(4)	36(3)	-3(3)	0(3)	21(3)
C(6)	47(4)	35(4)	32(3)	0(3)	-2(3)	21(3)
C(7)	46(5)	64(5)	60(5)	-15(4)	-12(4)	28(4)
C(8)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(9)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(10)	45(4)	41(4)	37(4)	-1(3)	-1(3)	17(3)
C(11)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(12)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(13)	48(4)	51(4)	26(3)	-1(3)	-6(3)	28(4)
C(14)	57(5)	50(5)	33(4)	2(3)	-7(3)	31(4)
C(15)	58(5)	54(5)	30(3)	-9(3)	-6(3)	32(4)
C(16)	50(4)	37(4)	32(3)	-6(3)	-10(3)	27(4)
C(17)	35(4)	39(4)	32(3)	-3(3)	-4(3)	16(3)
C(18)	32(4)	42(4)	37(4)	-7(3)	-3(3)	12(3)
C(19)	35(4)	40(4)	27(3)	-3(3)	-2(3)	14(3)
C(20)	34(4)	37(4)	33(3)	-5(3)	-2(3)	17(3)
C(21)	41(4)	36(4)	31(3)	6(3)	4(3)	20(3)
C(22)	43(4)	48(4)	30(3)	0(3)	-2(3)	22(4)
C(23)	41(4)	51(4)	27(3)	-3(3)	0(3)	21(4)
C(24)	35(4)	54(5)	31(3)	0(3)	2(3)	24(4)
C(25)	37(4)	53(5)	35(3)	9(3)	8(3)	22(4)
C(26)	38(4)	71(6)	47(4)	7(4)	6(3)	29(4)
C(27)	45(5)	89(6)	36(4)	9(4)	5(3)	46(5)
C(28)	62(5)	67(5)	38(4)	8(4)	9(4)	46(5)
C(29)	48(4)	59(5)	32(3)	5(3)	7(3)	34(4)
C(30)	33(4)	48(4)	50(4)	7(3)	-3(3)	12(3)
C(31)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)

C(32)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(33)	49(5)	52(5)	51(4)	-6(4)	2(4)	28(4)
C(34)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(35)	68(2)	83(2)	65(2)	-8(2)	1(2)	30(2)
C(36)	37(4)	55(5)	56(4)	-6(4)	-3(3)	25(4)
C(37)	38(4)	48(4)	44(4)	9(3)	1(3)	19(4)
C(38)	64(6)	62(6)	116(8)	-16(5)	-27(6)	34(5)
C(39)	46(7)	77(9)	61(7)	-16(6)	-1(6)	31(7)
N(1)	55(4)	47(3)	28(3)	-4(2)	-5(2)	32(3)
N(2)	47(3)	42(3)	29(3)	-6(2)	-9(2)	26(3)
N(3)	38(3)	31(3)	29(3)	-4(2)	-4(2)	18(3)
N(4)	38(3)	37(3)	29(3)	3(2)	0(2)	18(3)
N(5)	32(3)	45(3)	33(3)	5(2)	2(2)	21(3)
I(1)	58(1)	50(1)	33(1)	-2(1)	-2(1)	26(1)
I(2)	48(1)	86(1)	32(1)	-3(1)	-2(1)	43(1)
Cl(1)	79(2)	79(2)	122(2)	9(2)	1(2)	46(2)
Cl(2)	94(2)	87(2)	99(2)	-12(2)	-16(2)	42(2)
Cl(3)	93(2)	82(2)	136(3)	-13(2)	-51(2)	28(2)
Cl(4)	68(3)	153(4)	115(3)	-35(3)	7(2)	53(3)
Cl(5)	166(5)	89(3)	140(4)	-13(3)	-28(4)	80(4)
Cl(6)	67(2)	99(3)	89(3)	-23(2)	7(2)	24(2)

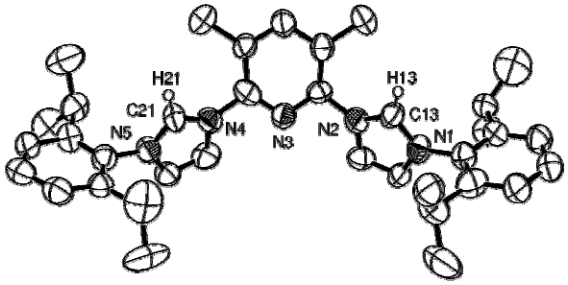


Table 1. Crystal data and structure refinement for $\mathbf{1^{Me}(Br)^-_2}$.

Identification code	$\mathbf{1^{Me}(Br)^-_2}$	
Empirical formula	C37 H47 Br2 N5	
Formula weight	721.62	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R-3	
Unit cell dimensions	a = 52.1838(13) Å	α= 90°.
	b = 52.1838(13) Å	β= 90°.
	c = 9.4150(3) Å	γ = 120°.
Volume	22203.5(11) Å^3	
Z	18	
Density (calculated)	0.971 Mg/m^3	
Absorption coefficient	1.666 mm^{-1}	
F(000)	6732	
Crystal size	0.24 x 0.22 x 0.20 mm^3	
Theta range for data collection	2.92 to 25.02°.	
Index ranges	-62<=h<=62, -61<=k<=62, -11<=l<=11	
Reflections collected	60773	
Independent reflections	8591 [R(int) = 0.0739]	
Completeness to theta = 25.02°	98.5 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7217 and 0.6805	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	8591 / 12 / 407	
Goodness-of-fit on F^2	1.059	
Final R indices [I>2sigma(I)]	R1 = 0.0995, wR2 = 0.2847	
R indices (all data)	R1 = 0.1366, wR2 = 0.3094	
Largest diff. peak and hole	3.818 and -1.838 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for $\mathbf{1^{Me}(Br)^-_2}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3621(2)	679(2)	8788(10)	64(2)
C(2)	3651(2)	431(2)	8513(10)	63(2)
C(3)	3396(2)	156(2)	8667(11)	70(3)
C(4)	3131(2)	142(2)	9101(11)	72(3)
C(5)	3112(3)	390(2)	9399(12)	84(3)
C(6)	3365(2)	670(3)	9216(11)	79(3)
C(7)	3941(2)	451(2)	8025(11)	66(3)
C(8)	3996(4)	211(4)	8592(18)	144(6)
C(9)	3964(3)	436(3)	6472(12)	92(3)
C(10)	3344(2)	951(2)	9506(11)	77(3)
C(11)	3108(4)	956(3)	8546(15)	124(5)
C(12)	3281(3)	973(3)	11062(13)	91(3)
C(13)	4097(2)	1109(2)	9642(10)	62(2)
C(14)	3984(2)	1125(2)	7371(10)	63(2)
C(15)	4245(2)	1370(2)	7634(10)	65(2)
C(16)	4580(2)	1575(2)	9762(9)	57(2)
C(17)	4736(2)	1504(2)	10672(10)	59(2)
C(18)	4984(2)	1740(2)	11329(11)	66(2)
C(19)	5056(2)	2030(2)	11045(9)	57(2)
C(20)	4875(2)	2067(2)	10070(10)	65(2)
C(21)	4975(2)	2577(2)	10554(9)	55(2)
C(22)	4911(2)	2441(2)	8301(10)	73(3)
C(23)	4958(2)	2723(2)	8400(10)	61(2)
C(24)	5047(2)	3081(2)	10428(10)	62(2)
C(25)	4802(2)	3096(2)	10888(9)	59(2)
C(26)	4862(3)	3358(2)	11498(11)	76(3)
C(27)	5143(2)	3595(2)	11635(10)	71(3)
C(28)	5379(2)	3571(2)	11156(11)	72(3)
C(29)	5341(2)	3312(2)	10524(10)	63(2)
C(30)	4492(2)	2838(2)	10712(11)	74(3)
C(31)	4302(3)	2773(3)	12145(14)	113(5)

C(32)	4331(3)	2874(4)	9517(14)	126(5)
C(33)	5606(2)	3284(2)	10124(11)	77(3)
C(34)	5773(3)	3276(4)	11432(15)	120(5)
C(35)	5793(4)	3524(3)	8994(16)	128(5)
C(36)	4675(2)	1188(2)	10986(11)	76(3)
C(37)	5331(2)	2286(2)	11763(11)	74(3)
N(1)	3894(2)	968(2)	8632(8)	63(2)
N(2)	4319(2)	1356(2)	9036(8)	63(2)
N(3)	4643(2)	1848(2)	9406(8)	59(2)
N(4)	4929(2)	2357(2)	9675(8)	60(2)
N(5)	4995(2)	2797(2)	9807(8)	62(2)
Br(1)	4010(1)	1071(1)	3477(1)	41(1)
Br(2)	6037(1)	4336(1)	12222(1)	64(1)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{1^{Me}(Br)^-_2}$.

C(1)-C(6)	1.375(13)	C(14)-N(1)	1.385(11)
C(1)-C(2)	1.405(13)	C(14)-H(14)	0.9500
C(1)-N(1)	1.474(11)	C(15)-N(2)	1.388(11)
C(2)-C(3)	1.391(13)	C(15)-H(15)	0.9500
C(2)-C(7)	1.536(13)	C(16)-N(3)	1.335(11)
C(3)-C(4)	1.412(13)	C(16)-C(17)	1.351(12)
C(3)-H(3)	0.9500	C(16)-N(2)	1.440(11)
C(4)-C(5)	1.376(15)	C(17)-C(18)	1.408(12)
C(4)-H(4)	0.9500	C(17)-C(36)	1.545(12)
C(5)-C(6)	1.407(15)	C(18)-C(19)	1.390(13)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.547(15)	C(19)-C(20)	1.400(13)
C(7)-C(9)	1.473(14)	C(19)-C(37)	1.543(12)
C(7)-C(8)	1.513(18)	C(20)-N(3)	1.332(12)
C(7)-H(7)	1.0000	C(20)-N(4)	1.443(11)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.306(11)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.337(10)
C(8)-H(8C)	0.9800	C(21)-H(21)	0.9500
C(9)-H(9A)	0.9800	C(22)-C(23)	1.365(13)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.385(11)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(12)	1.518(14)	C(23)-N(5)	1.367(11)
C(10)-C(11)	1.540(16)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.388(12)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.401(13)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.486(11)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.369(13)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.510(13)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.371(14)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(1)	1.339(12)	C(27)-C(28)	1.377(14)
C(13)-N(2)	1.356(11)	C(27)-H(27)	0.9500
C(13)-H(13)	0.9500	C(28)-C(29)	1.396(13)
C(14)-C(15)	1.347(12)	C(28)-H(28)	0.9500

C(29)-C(33)	1.507(14)	C(5)-C(4)-H(4)	118.6
C(30)-C(32)	1.473(14)	C(3)-C(4)-H(4)	118.6
C(30)-C(31)	1.608(14)	C(4)-C(5)-C(6)	118.7(11)
C(30)-H(30)	1.0000	C(4)-C(5)-H(5)	120.7
C(31)-H(31A)	0.9800	C(6)-C(5)-H(5)	120.7
C(31)-H(31B)	0.9800	C(1)-C(6)-C(5)	117.6(11)
C(31)-H(31C)	0.9800	C(1)-C(6)-C(10)	123.2(10)
C(32)-H(32A)	0.9800	C(5)-C(6)-C(10)	119.2(10)
C(32)-H(32B)	0.9800	C(9)-C(7)-C(8)	104.6(10)
C(32)-H(32C)	0.9800	C(9)-C(7)-C(2)	113.4(8)
C(33)-C(34)	1.521(16)	C(8)-C(7)-C(2)	115.1(10)
C(33)-C(35)	1.559(17)	C(9)-C(7)-H(7)	107.8
C(33)-H(33)	1.0000	C(8)-C(7)-H(7)	107.8
C(34)-H(34A)	0.9800	C(2)-C(7)-H(7)	107.8
C(34)-H(34B)	0.9800	C(7)-C(8)-H(8A)	109.5
C(34)-H(34C)	0.9800	C(7)-C(8)-H(8B)	109.5
C(35)-H(35A)	0.9800	H(8A)-C(8)-H(8B)	109.5
C(35)-H(35B)	0.9800	C(7)-C(8)-H(8C)	109.5
C(35)-H(35C)	0.9800	H(8A)-C(8)-H(8C)	109.5
C(36)-H(36A)	0.9800	H(8B)-C(8)-H(8C)	109.5
C(36)-H(36B)	0.9800	C(7)-C(9)-H(9A)	109.5
C(36)-H(36C)	0.9800	C(7)-C(9)-H(9B)	109.5
C(37)-H(37A)	0.9800	H(9A)-C(9)-H(9B)	109.5
C(37)-H(37B)	0.9800	C(7)-C(9)-H(9C)	109.5
C(37)-H(37C)	0.9800	H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.5
C(6)-C(1)-C(2)	125.2(9)	C(12)-C(10)-C(11)	111.1(10)
C(6)-C(1)-N(1)	119.2(9)	C(12)-C(10)-C(6)	111.2(9)
C(2)-C(1)-N(1)	115.6(8)	C(11)-C(10)-C(6)	110.4(9)
C(3)-C(2)-C(1)	116.3(9)	C(12)-C(10)-H(10)	108.0
C(3)-C(2)-C(7)	120.2(8)	C(11)-C(10)-H(10)	108.0
C(1)-C(2)-C(7)	123.5(8)	C(6)-C(10)-H(10)	108.0
C(2)-C(3)-C(4)	119.4(9)	C(10)-C(11)-H(11A)	109.5
C(2)-C(3)-H(3)	120.3	C(10)-C(11)-H(11B)	109.5
C(4)-C(3)-H(3)	120.3	H(11A)-C(11)-H(11B)	109.5
C(5)-C(4)-C(3)	122.7(10)	C(10)-C(11)-H(11C)	109.5

H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	127.0
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	127.0
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	107.2(8)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	126.4
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.4
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	125.1(9)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	117.4(8)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	117.5(8)
N(1)-C(13)-N(2)	106.8(8)	C(26)-C(25)-C(24)	115.4(9)
N(1)-C(13)-H(13)	126.6	C(26)-C(25)-C(30)	123.0(9)
N(2)-C(13)-H(13)	126.6	C(24)-C(25)-C(30)	121.7(8)
C(15)-C(14)-N(1)	106.7(8)	C(25)-C(26)-C(27)	123.4(10)
C(15)-C(14)-H(14)	126.7	C(25)-C(26)-H(26)	118.3
N(1)-C(14)-H(14)	126.7	C(27)-C(26)-H(26)	118.3
C(14)-C(15)-N(2)	107.5(8)	C(26)-C(27)-C(28)	119.0(10)
C(14)-C(15)-H(15)	126.2	C(26)-C(27)-H(27)	120.5
N(2)-C(15)-H(15)	126.2	C(28)-C(27)-H(27)	120.5
N(3)-C(16)-C(17)	126.2(8)	C(27)-C(28)-C(29)	122.0(10)
N(3)-C(16)-N(2)	111.0(7)	C(27)-C(28)-H(28)	119.0
C(17)-C(16)-N(2)	122.8(8)	C(29)-C(28)-H(28)	119.0
C(16)-C(17)-C(18)	117.1(8)	C(28)-C(29)-C(24)	115.1(9)
C(16)-C(17)-C(36)	125.6(9)	C(28)-C(29)-C(33)	120.5(9)
C(18)-C(17)-C(36)	117.1(9)	C(24)-C(29)-C(33)	124.1(9)
C(19)-C(18)-C(17)	119.8(9)	C(32)-C(30)-C(25)	113.3(10)
C(19)-C(18)-H(18)	120.1	C(32)-C(30)-C(31)	109.7(10)
C(17)-C(18)-H(18)	120.1	C(25)-C(30)-C(31)	111.7(9)
C(18)-C(19)-C(20)	116.2(8)	C(32)-C(30)-H(30)	107.3
C(18)-C(19)-C(37)	119.3(9)	C(25)-C(30)-H(30)	107.3
C(20)-C(19)-C(37)	124.5(8)	C(31)-C(30)-H(30)	107.3
N(3)-C(20)-C(19)	125.3(8)	C(30)-C(31)-H(31A)	109.5
N(3)-C(20)-N(4)	113.3(8)	C(30)-C(31)-H(31B)	109.5
C(19)-C(20)-N(4)	121.5(9)	H(31A)-C(31)-H(31B)	109.5
N(5)-C(21)-N(4)	108.9(7)	C(30)-C(31)-H(31C)	109.5
N(5)-C(21)-H(21)	125.6	H(31A)-C(31)-H(31C)	109.5
N(4)-C(21)-H(21)	125.6	H(31B)-C(31)-H(31C)	109.5
C(23)-C(22)-N(4)	105.9(8)	C(30)-C(32)-H(32A)	109.5

C(30)-C(32)-H(32B)	109.5	C(13)-N(1)-C(1)	125.8(8)
H(32A)-C(32)-H(32B)	109.5	C(14)-N(1)-C(1)	124.0(8)
C(30)-C(32)-H(32C)	109.5	C(13)-N(2)-C(15)	108.8(8)
H(32A)-C(32)-H(32C)	109.5	C(13)-N(2)-C(16)	125.1(8)
H(32B)-C(32)-H(32C)	109.5	C(15)-N(2)-C(16)	126.0(7)
C(29)-C(33)-C(34)	111.4(9)	C(20)-N(3)-C(16)	115.4(8)
C(29)-C(33)-C(35)	109.1(10)	C(21)-N(4)-C(22)	108.5(7)
C(34)-C(33)-C(35)	116.0(10)	C(21)-N(4)-C(20)	126.8(8)
C(29)-C(33)-H(33)	106.6	C(22)-N(4)-C(20)	124.5(8)
C(34)-C(33)-H(33)	106.6	C(21)-N(5)-C(23)	109.5(8)
C(35)-C(33)-H(33)	106.6	C(21)-N(5)-C(24)	124.0(7)
C(33)-C(34)-H(34A)	109.5	C(23)-N(5)-C(24)	126.5(8)
C(33)-C(34)-H(34B)	109.5		
H(34A)-C(34)-H(34B)	109.5		
C(33)-C(34)-H(34C)	109.5		
H(34A)-C(34)-H(34C)	109.5		
H(34B)-C(34)-H(34C)	109.5		
C(33)-C(35)-H(35A)	109.5		
C(33)-C(35)-H(35B)	109.5		
H(35A)-C(35)-H(35B)	109.5		
C(33)-C(35)-H(35C)	109.5		
H(35A)-C(35)-H(35C)	109.5		
H(35B)-C(35)-H(35C)	109.5		
C(17)-C(36)-H(36A)	109.5		
C(17)-C(36)-H(36B)	109.5		
H(36A)-C(36)-H(36B)	109.5		
C(17)-C(36)-H(36C)	109.5		
H(36A)-C(36)-H(36C)	109.5		
H(36B)-C(36)-H(36C)	109.5		
C(19)-C(37)-H(37A)	109.5		
C(19)-C(37)-H(37B)	109.5		
H(37A)-C(37)-H(37B)	109.5		
C(19)-C(37)-H(37C)	109.5		
H(37A)-C(37)-H(37C)	109.5		
H(37B)-C(37)-H(37C)	109.5		
C(13)-N(1)-C(14)	110.1(8)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $\mathbf{1^{Me}(Br)^-_2}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	61(6)	57(6)	69(6)	3(5)	4(5)	25(5)
C(2)	66(6)	59(6)	65(6)	6(5)	-2(5)	32(5)
C(3)	62(6)	64(6)	80(7)	6(5)	8(5)	29(5)
C(4)	71(7)	60(6)	78(7)	5(5)	3(5)	28(5)
C(5)	83(8)	68(7)	84(8)	15(6)	-8(6)	26(6)
C(6)	62(6)	98(8)	75(7)	4(6)	7(5)	40(6)
C(7)	60(6)	62(6)	81(7)	5(5)	-5(5)	34(5)
C(8)	144(6)	144(6)	145(6)	0(1)	0(1)	72(3)
C(9)	94(8)	112(9)	81(8)	3(7)	5(6)	58(8)
C(10)	88(7)	79(7)	76(7)	4(6)	13(6)	50(6)
C(11)	190(16)	114(11)	111(11)	3(8)	-24(10)	109(12)
C(12)	90(8)	80(7)	111(10)	-25(7)	-15(7)	50(7)
C(13)	58(5)	58(6)	59(6)	-6(5)	-9(5)	21(5)
C(14)	59(6)	56(5)	59(6)	0(4)	-13(4)	18(5)
C(15)	65(6)	75(6)	58(6)	12(5)	2(5)	37(5)
C(16)	66(6)	62(6)	45(5)	-2(4)	-9(4)	33(5)
C(17)	53(5)	53(5)	64(6)	3(4)	8(4)	21(4)
C(18)	60(6)	55(6)	80(7)	1(5)	1(5)	27(5)
C(19)	63(5)	56(5)	47(5)	-6(4)	-6(4)	26(4)
C(20)	72(6)	67(6)	64(6)	16(5)	12(5)	41(5)
C(21)	83(6)	45(5)	31(4)	-1(4)	9(4)	28(4)
C(22)	94(8)	90(8)	41(5)	-13(5)	-9(5)	50(6)
C(23)	78(6)	67(6)	46(5)	-3(4)	-4(4)	42(5)
C(24)	67(6)	58(5)	57(6)	-2(4)	-2(5)	29(5)
C(25)	68(6)	62(6)	53(5)	-2(4)	-7(4)	37(5)
C(26)	84(8)	80(7)	77(7)	1(6)	-2(6)	51(7)
C(27)	84(8)	77(7)	67(7)	9(5)	-1(5)	50(6)
C(28)	82(7)	52(6)	74(7)	2(5)	-15(5)	27(5)
C(29)	65(6)	62(6)	61(6)	2(5)	11(5)	31(5)
C(30)	66(6)	92(7)	67(7)	1(5)	3(5)	41(6)
C(31)	81(8)	125(11)	124(11)	2(9)	41(8)	44(8)

C(32)	74(8)	196(16)	104(10)	23(10)	-20(7)	64(10)
C(33)	63(6)	75(7)	74(7)	9(5)	6(5)	21(5)
C(34)	106(10)	154(13)	107(10)	-18(9)	-32(8)	71(10)
C(35)	128(5)	128(5)	128(5)	0(1)	0(1)	64(3)
C(36)	84(7)	56(6)	87(7)	11(5)	7(6)	35(5)
C(37)	64(6)	79(7)	69(7)	-15(5)	-5(5)	28(5)
N(1)	59(5)	58(4)	58(5)	1(4)	7(4)	19(4)
N(2)	67(5)	56(4)	57(5)	9(4)	-2(4)	25(4)
N(3)	55(4)	55(5)	63(5)	-3(4)	-1(4)	25(4)
N(4)	62(5)	58(4)	61(5)	10(4)	3(4)	31(4)
N(5)	73(5)	57(4)	56(5)	0(4)	0(4)	34(4)
Br(1)	44(1)	49(1)	30(1)	-3(1)	0(1)	23(1)
Br(2)	62(1)	51(1)	26(1)	1(1)	-2(1)	-12(1)

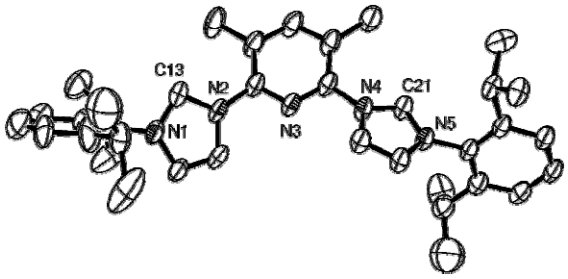


Table 1. Crystal data and structure refinement for **2**^{Me}.

Identification code	**2**^{Me}	
Empirical formula	C37 H45 N5	
Formula weight	559.78	
Temperature	120(2) K	
Wavelength	0.7848 Å	
Crystal system	Monoclinic	
Space group	P21/c	
Unit cell dimensions	a = 15.058(3) Å	α= 90°.
	b = 24.920(6) Å	β= 91.360(3)°.
	c = 10.967(3) Å	γ = 90°.
Volume	4114.2(17) Å^3	
Z	4	
Density (calculated)	0.904 Mg/m^3	
Absorption coefficient	0.054 mm^{-1}	
F(000)	1208	
Crystal size	0.10 x 0.10 x 0.10 mm^3	
Theta range for data collection	4.63 to 26.34°.	
Index ranges	-16<=h<=16, -27<=k<=27, -12<=l<=12	
Reflections collected	22457	
Independent reflections	5879 [R(int) = 0.0579]	
Completeness to theta = 26.34°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9947 and 0.9947	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5879 / 15 / 448	
Goodness-of-fit on F^2	0.976	
Final R indices [I>2sigma(I)]	R1 = 0.0700, wR2 = 0.1937	
R indices (all data)	R1 = 0.1048, wR2 = 0.2125	
Largest diff. peak and hole	0.427 and -0.313 e.Å^{-3}	

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **2**^{Me}. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1A)	1915(11)	9021(4)	4761(12)	49(1)
C(2A)	2331(10)	8907(5)	3673(12)	101(8)
C(3A)	2160(10)	8425(5)	3073(11)	69(2)
C(4A)	1571(9)	8058(4)	3560(14)	94(8)
C(5A)	1154(8)	8172(4)	4647(14)	75(5)
C(6A)	1326(9)	8653(4)	5248(11)	52(1)
C(7A)	3050(10)	9290(6)	3236(15)	59(2)
C(8A)	2640(30)	9670(9)	2280(20)	135(12)
C(9A)	3885(14)	9005(10)	2770(20)	121(8)
C(10A)	893(15)	8770(7)	6479(15)	79(7)
C(11A)	654(14)	8261(6)	7200(20)	86(6)
C(12A)	-28(18)	9076(11)	6230(30)	101(3)
C(1B)	2081(3)	9091(1)	4434(3)	49(1)
C(2B)	2591(3)	9078(1)	3394(3)	48(2)
C(3B)	2509(3)	8651(2)	2582(3)	69(2)
C(4B)	1916(3)	8238(1)	2810(4)	78(2)
C(5B)	1407(3)	8250(1)	3850(5)	68(2)
C(6B)	1489(3)	8677(1)	4662(4)	52(1)
C(7B)	3231(4)	9546(2)	3100(5)	59(2)
C(8B)	2780(7)	9925(3)	2157(7)	78(2)
C(9B)	4135(5)	9342(3)	2699(6)	78(2)
C(10B)	927(6)	8691(3)	5804(7)	68(2)
C(11B)	698(5)	8134(3)	6303(8)	88(2)
C(12B)	77(6)	9000(3)	5568(9)	101(3)
C(13)	2736(2)	9556(1)	6225(3)	48(1)
C(14)	1697(2)	10018(1)	5067(3)	49(1)
C(15)	2015(2)	10360(1)	5906(3)	47(1)
C(16)	3158(2)	10318(1)	7571(3)	43(1)
C(17)	3418(2)	10037(1)	8616(3)	53(1)
C(18)	3903(3)	10340(1)	9469(3)	57(1)
C(19)	4117(2)	10878(1)	9331(3)	50(1)

C(20)	3801(2)	11106(1)	8229(2)	41(1)
C(21)	4061(2)	12076(1)	8672(2)	41(1)
C(22)	4007(2)	11801(1)	6658(2)	43(1)
C(23)	4129(2)	12333(1)	6658(2)	42(1)
C(24)	4300(2)	13042(1)	8254(2)	38(1)
C(25)	3552(2)	13375(1)	8372(3)	44(1)
C(26)	3713(2)	13904(1)	8733(3)	49(1)
C(27)	4563(2)	14089(1)	8941(3)	47(1)
C(28)	5282(2)	13755(1)	8806(2)	44(1)
C(29)	5171(2)	13220(1)	8462(2)	40(1)
C(30)	2619(2)	13170(1)	8142(3)	55(1)
C(31)	2090(4)	13513(2)	7278(5)	122(2)
C(32)	2127(3)	13101(2)	9327(4)	92(1)
C(33)	5964(2)	12849(1)	8343(3)	48(1)
C(34)	6683(2)	13098(1)	7556(3)	53(1)
C(35)	6342(2)	12692(1)	9594(3)	68(1)
C(36)	3193(3)	9458(1)	8855(3)	76(1)
C(37)	4641(3)	11170(1)	10299(3)	64(1)
N(1)	2136(2)	9535(1)	5275(2)	46(1)
N(2)	2644(2)	10077(1)	6612(2)	42(1)
N(3)	3337(2)	10833(1)	7386(2)	40(1)
N(4)	3970(2)	11649(1)	7886(2)	40(1)
N(5)	4159(2)	12489(1)	7873(2)	39(1)

Table 3. Bond lengths [Å] and angles [°] for **2**^{Me}.

C(1A)-C(2A)	1.3900	C(2B)-C(7B)	1.552(5)
C(1A)-C(6A)	1.3900	C(3B)-C(4B)	1.3900
C(1A)-N(1)	1.435(6)	C(3B)-H(3B)	0.9500
C(2A)-C(3A)	1.3900	C(4B)-C(5B)	1.3900
C(2A)-C(7A)	1.529(9)	C(4B)-H(4B)	0.9500
C(3A)-C(4A)	1.3900	C(5B)-C(6B)	1.3900
C(3A)-H(3A)	0.9500	C(5B)-H(5B)	0.9500
C(4A)-C(5A)	1.3900	C(6B)-C(10B)	1.529(7)
C(4A)-H(4A)	0.9500	C(7B)-C(9B)	1.527(8)
C(5A)-C(6A)	1.3900	C(7B)-C(8B)	1.547(9)
C(5A)-H(5A)	0.9500	C(7B)-H(7B)	1.0000
C(6A)-C(10A)	1.541(10)	C(8B)-H(8B1)	0.9800
C(7A)-C(8A)	1.538(10)	C(8B)-H(8B2)	0.9800
C(7A)-C(9A)	1.539(10)	C(8B)-H(8B3)	0.9800
C(7A)-H(7A)	1.0000	C(9B)-H(9B1)	0.9800
C(8A)-H(8A1)	0.9800	C(9B)-H(9B2)	0.9800
C(8A)-H(8A2)	0.9800	C(9B)-H(9B3)	0.9800
C(8A)-H(8A3)	0.9800	C(10B)-C(12B)	1.510(12)
C(9A)-H(9A1)	0.9800	C(10B)-C(11B)	1.535(8)
C(9A)-H(9A2)	0.9800	C(10B)-H(10B)	1.0000
C(9A)-H(9A3)	0.9800	C(11B)-H(11D)	0.9800
C(10A)-C(11A)	1.542(10)	C(11B)-H(11E)	0.9800
C(10A)-C(12A)	1.60(4)	C(11B)-H(11F)	0.9800
C(10A)-H(10A)	1.0000	C(12B)-H(12D)	0.9800
C(11A)-H(11A)	0.9800	C(12B)-H(12E)	0.9800
C(11A)-H(11B)	0.9800	C(12B)-H(12F)	0.9800
C(11A)-H(11C)	0.9800	C(13)-N(1)	1.364(4)
C(12A)-H(12A)	0.9800	C(13)-N(2)	1.374(3)
C(12A)-H(12B)	0.9800	C(14)-C(15)	1.336(4)
C(12A)-H(12C)	0.9800	C(14)-N(1)	1.391(3)
C(1B)-C(2B)	1.3900	C(14)-H(14)	0.9500
C(1B)-C(6B)	1.3900	C(15)-N(2)	1.398(4)
C(1B)-N(1)	1.441(3)	C(15)-H(15)	0.9500
C(2B)-C(3B)	1.3900	C(16)-N(3)	1.329(3)

C(16)-C(17)	1.391(4)	C(32)-H(32B)	0.9800
C(16)-N(2)	1.424(4)	C(32)-H(32C)	0.9800
C(17)-C(18)	1.396(4)	C(33)-C(35)	1.524(4)
C(17)-C(36)	1.507(4)	C(33)-C(34)	1.532(4)
C(18)-C(19)	1.387(4)	C(33)-H(33)	1.0000
C(18)-H(18)	0.9500	C(34)-H(34A)	0.9800
C(19)-C(20)	1.409(4)	C(34)-H(34B)	0.9800
C(19)-C(37)	1.497(4)	C(34)-H(34C)	0.9800
C(20)-N(3)	1.332(3)	C(35)-H(35A)	0.9800
C(20)-N(4)	1.428(3)	C(35)-H(35B)	0.9800
C(21)-N(5)	1.363(3)	C(35)-H(35C)	0.9800
C(21)-N(4)	1.375(3)	C(36)-H(36A)	0.9800
C(22)-C(23)	1.336(4)	C(36)-H(36B)	0.9800
C(22)-N(4)	1.402(3)	C(36)-H(36C)	0.9800
C(22)-H(22)	0.9500	C(37)-H(37A)	0.9800
C(23)-N(5)	1.389(3)	C(37)-H(37B)	0.9800
C(23)-H(23)	0.9500	C(37)-H(37C)	0.9800
C(24)-C(29)	1.399(4)		
C(24)-C(25)	1.407(4)	C(2A)-C(1A)-C(6A)	120.0
C(24)-N(5)	1.452(3)	C(2A)-C(1A)-N(1)	114.5(8)
C(25)-C(26)	1.398(4)	C(6A)-C(1A)-N(1)	125.5(8)
C(25)-C(30)	1.511(4)	C(1A)-C(2A)-C(3A)	120.0
C(26)-C(27)	1.373(4)	C(1A)-C(2A)-C(7A)	118.6(10)
C(26)-H(26)	0.9500	C(3A)-C(2A)-C(7A)	121.0(10)
C(27)-C(28)	1.378(4)	C(4A)-C(3A)-C(2A)	120.0
C(27)-H(27)	0.9500	C(4A)-C(3A)-H(3A)	120.0
C(28)-C(29)	1.394(4)	C(2A)-C(3A)-H(3A)	120.0
C(28)-H(28)	0.9500	C(5A)-C(4A)-C(3A)	120.0
C(29)-C(33)	1.519(4)	C(5A)-C(4A)-H(4A)	120.0
C(30)-C(31)	1.492(6)	C(3A)-C(4A)-H(4A)	120.0
C(30)-C(32)	1.521(5)	C(4A)-C(5A)-C(6A)	120.0
C(30)-H(30)	1.0000	C(4A)-C(5A)-H(5A)	120.0
C(31)-H(31A)	0.9800	C(6A)-C(5A)-H(5A)	120.0
C(31)-H(31B)	0.9800	C(5A)-C(6A)-C(1A)	120.0
C(31)-H(31C)	0.9800	C(5A)-C(6A)-C(10A)	120.0(10)
C(32)-H(32A)	0.9800	C(1A)-C(6A)-C(10A)	119.9(10)

C(2A)-C(7A)-C(8A)	108.7(16)	C(7B)-C(8B)-H(8B1)	109.5
C(2A)-C(7A)-C(9A)	113.9(15)	C(7B)-C(8B)-H(8B2)	109.5
C(8A)-C(7A)-C(9A)	112(2)	H(8B1)-C(8B)-H(8B2)	109.5
C(2A)-C(7A)-H(7A)	107.2	C(7B)-C(8B)-H(8B3)	109.5
C(8A)-C(7A)-H(7A)	107.2	H(8B1)-C(8B)-H(8B3)	109.5
C(9A)-C(7A)-H(7A)	107.2	H(8B2)-C(8B)-H(8B3)	109.5
C(6A)-C(10A)-C(11A)	113.8(14)	C(7B)-C(9B)-H(9B1)	109.5
C(6A)-C(10A)-C(12A)	109.0(16)	C(7B)-C(9B)-H(9B2)	109.5
C(11A)-C(10A)-C(12A)	105.4(17)	H(9B1)-C(9B)-H(9B2)	109.5
C(6A)-C(10A)-H(10A)	109.5	C(7B)-C(9B)-H(9B3)	109.5
C(11A)-C(10A)-H(10A)	109.5	H(9B1)-C(9B)-H(9B3)	109.5
C(12A)-C(10A)-H(10A)	109.5	H(9B2)-C(9B)-H(9B3)	109.5
C(2B)-C(1B)-C(6B)	120.0	C(12B)-C(10B)-C(6B)	110.8(6)
C(2B)-C(1B)-N(1)	121.2(2)	C(12B)-C(10B)-C(11B)	108.9(6)
C(6B)-C(1B)-N(1)	118.8(2)	C(6B)-C(10B)-C(11B)	113.8(5)
C(3B)-C(2B)-C(1B)	120.0	C(12B)-C(10B)-H(10B)	107.7
C(3B)-C(2B)-C(7B)	119.2(3)	C(6B)-C(10B)-H(10B)	107.7
C(1B)-C(2B)-C(7B)	120.8(3)	C(11B)-C(10B)-H(10B)	107.7
C(4B)-C(3B)-C(2B)	120.0	C(10B)-C(11B)-H(11D)	109.5
C(4B)-C(3B)-H(3B)	120.0	C(10B)-C(11B)-H(11E)	109.5
C(2B)-C(3B)-H(3B)	120.0	H(11D)-C(11B)-H(11E)	109.5
C(3B)-C(4B)-C(5B)	120.0	C(10B)-C(11B)-H(11F)	109.5
C(3B)-C(4B)-H(4B)	120.0	H(11D)-C(11B)-H(11F)	109.5
C(5B)-C(4B)-H(4B)	120.0	H(11E)-C(11B)-H(11F)	109.5
C(4B)-C(5B)-C(6B)	120.0	C(10B)-C(12B)-H(12D)	109.5
C(4B)-C(5B)-H(5B)	120.0	C(10B)-C(12B)-H(12E)	109.5
C(6B)-C(5B)-H(5B)	120.0	H(12D)-C(12B)-H(12E)	109.5
C(5B)-C(6B)-C(1B)	120.0	C(10B)-C(12B)-H(12F)	109.5
C(5B)-C(6B)-C(10B)	120.0(3)	H(12D)-C(12B)-H(12F)	109.5
C(1B)-C(6B)-C(10B)	120.0(3)	H(12E)-C(12B)-H(12F)	109.5
C(9B)-C(7B)-C(8B)	113.0(6)	N(1)-C(13)-N(2)	101.7(2)
C(9B)-C(7B)-C(2B)	111.9(4)	C(15)-C(14)-N(1)	106.2(3)
C(8B)-C(7B)-C(2B)	109.5(5)	C(15)-C(14)-H(14)	126.9
C(9B)-C(7B)-H(7B)	107.4	N(1)-C(14)-H(14)	126.9
C(8B)-C(7B)-H(7B)	107.4	C(14)-C(15)-N(2)	106.7(2)
C(2B)-C(7B)-H(7B)	107.4	C(14)-C(15)-H(15)	126.7

N(2)-C(15)-H(15)	126.7	C(27)-C(28)-H(28)	119.4
N(3)-C(16)-C(17)	123.9(3)	C(29)-C(28)-H(28)	119.4
N(3)-C(16)-N(2)	113.7(2)	C(28)-C(29)-C(24)	117.0(3)
C(17)-C(16)-N(2)	122.3(2)	C(28)-C(29)-C(33)	121.1(3)
C(16)-C(17)-C(18)	114.4(3)	C(24)-C(29)-C(33)	121.9(2)
C(16)-C(17)-C(36)	124.4(3)	C(31)-C(30)-C(25)	113.1(3)
C(18)-C(17)-C(36)	121.2(3)	C(31)-C(30)-C(32)	110.1(4)
C(19)-C(18)-C(17)	124.7(3)	C(25)-C(30)-C(32)	111.5(3)
C(19)-C(18)-H(18)	117.7	C(31)-C(30)-H(30)	107.3
C(17)-C(18)-H(18)	117.7	C(25)-C(30)-H(30)	107.3
C(18)-C(19)-C(20)	114.2(3)	C(32)-C(30)-H(30)	107.3
C(18)-C(19)-C(37)	120.8(3)	C(30)-C(31)-H(31A)	109.5
C(20)-C(19)-C(37)	125.1(3)	C(30)-C(31)-H(31B)	109.5
N(3)-C(20)-C(19)	123.4(2)	H(31A)-C(31)-H(31B)	109.5
N(3)-C(20)-N(4)	113.2(2)	C(30)-C(31)-H(31C)	109.5
C(19)-C(20)-N(4)	123.3(3)	H(31A)-C(31)-H(31C)	109.5
N(5)-C(21)-N(4)	101.1(2)	H(31B)-C(31)-H(31C)	109.5
C(23)-C(22)-N(4)	106.1(2)	C(30)-C(32)-H(32A)	109.5
C(23)-C(22)-H(22)	126.9	C(30)-C(32)-H(32B)	109.5
N(4)-C(22)-H(22)	126.9	H(32A)-C(32)-H(32B)	109.5
C(22)-C(23)-N(5)	106.3(2)	C(30)-C(32)-H(32C)	109.5
C(22)-C(23)-H(23)	126.9	H(32A)-C(32)-H(32C)	109.5
N(5)-C(23)-H(23)	126.9	H(32B)-C(32)-H(32C)	109.5
C(29)-C(24)-C(25)	123.2(2)	C(29)-C(33)-C(35)	110.9(2)
C(29)-C(24)-N(5)	118.5(2)	C(29)-C(33)-C(34)	111.7(2)
C(25)-C(24)-N(5)	118.3(3)	C(35)-C(33)-C(34)	110.9(3)
C(26)-C(25)-C(24)	116.7(3)	C(29)-C(33)-H(33)	107.7
C(26)-C(25)-C(30)	121.4(3)	C(35)-C(33)-H(33)	107.7
C(24)-C(25)-C(30)	121.9(2)	C(34)-C(33)-H(33)	107.7
C(27)-C(26)-C(25)	121.2(3)	C(33)-C(34)-H(34A)	109.5
C(27)-C(26)-H(26)	119.4	C(33)-C(34)-H(34B)	109.5
C(25)-C(26)-H(26)	119.4	H(34A)-C(34)-H(34B)	109.5
C(26)-C(27)-C(28)	120.7(3)	C(33)-C(34)-H(34C)	109.5
C(26)-C(27)-H(27)	119.7	H(34A)-C(34)-H(34C)	109.5
C(28)-C(27)-H(27)	119.7	H(34B)-C(34)-H(34C)	109.5
C(27)-C(28)-C(29)	121.2(3)	C(33)-C(35)-H(35A)	109.5

C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(17)-C(36)-H(36A)	109.5
C(17)-C(36)-H(36B)	109.5
H(36A)-C(36)-H(36B)	109.5
C(17)-C(36)-H(36C)	109.5
H(36A)-C(36)-H(36C)	109.5
H(36B)-C(36)-H(36C)	109.5
C(19)-C(37)-H(37A)	109.5
C(19)-C(37)-H(37B)	109.5
H(37A)-C(37)-H(37B)	109.5
C(19)-C(37)-H(37C)	109.5
H(37A)-C(37)-H(37C)	109.5
H(37B)-C(37)-H(37C)	109.5
C(13)-N(1)-C(14)	113.2(2)
C(13)-N(1)-C(1A)	118.6(7)
C(14)-N(1)-C(1A)	127.2(8)
C(13)-N(1)-C(1B)	123.1(3)
C(14)-N(1)-C(1B)	122.7(3)
C(13)-N(2)-C(15)	112.2(3)
C(13)-N(2)-C(16)	124.7(2)
C(15)-N(2)-C(16)	123.1(2)
C(16)-N(3)-C(20)	119.5(2)
C(21)-N(4)-C(22)	112.8(2)
C(21)-N(4)-C(20)	125.7(2)
C(22)-N(4)-C(20)	121.4(2)
C(21)-N(5)-C(23)	113.7(2)
C(21)-N(5)-C(24)	123.3(2)
C(23)-N(5)-C(24)	123.0(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **2**^{Me}. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1A)	50(3)	31(2)	65(4)	-11(2)	-5(3)	5(2)
C(2A)	124(19)	56(12)	123(18)	2(12)	-24(14)	-56(11)
C(3A)	78(4)	49(3)	80(4)	-33(3)	9(3)	0(3)
C(4A)	85(14)	56(13)	140(20)	-24(13)	-22(13)	19(11)
C(5A)	75(11)	50(9)	100(13)	2(9)	12(9)	0(7)
C(6A)	50(3)	32(2)	73(4)	4(3)	6(3)	-1(2)
C(7A)	79(4)	49(4)	48(3)	-14(3)	19(2)	-11(3)
C(8A)	210(30)	56(16)	150(20)	5(17)	70(20)	30(20)
C(9A)	140(20)	122(19)	106(15)	-13(16)	18(14)	-5(16)
C(10A)	63(11)	43(9)	130(19)	6(12)	-23(14)	10(8)
C(11A)	89(12)	51(9)	118(15)	16(11)	10(13)	-8(8)
C(12A)	67(4)	67(4)	172(10)	43(6)	52(6)	15(3)
C(1B)	50(3)	31(2)	65(4)	-11(2)	-5(3)	5(2)
C(2B)	55(4)	32(3)	56(3)	-20(3)	-3(3)	-2(3)
C(3B)	78(4)	49(3)	80(4)	-33(3)	9(3)	0(3)
C(4B)	89(5)	37(3)	107(5)	-31(3)	-25(4)	7(3)
C(5B)	63(4)	21(3)	117(6)	-5(4)	-20(4)	0(3)
C(6B)	50(3)	32(2)	73(4)	4(3)	6(3)	-1(2)
C(7B)	79(4)	49(4)	48(3)	-14(3)	19(2)	-11(3)
C(8B)	128(6)	49(5)	57(4)	-8(3)	8(4)	2(4)
C(9B)	89(5)	95(5)	51(3)	-17(4)	18(3)	-4(4)
C(10B)	63(4)	39(3)	102(6)	14(4)	-3(5)	-17(3)
C(11B)	77(4)	62(4)	125(7)	35(4)	-4(5)	2(3)
C(12B)	67(4)	67(4)	172(10)	43(6)	52(6)	15(3)
C(13)	57(2)	29(2)	56(2)	-4(1)	7(2)	-2(1)
C(14)	56(2)	27(2)	63(2)	0(2)	2(2)	4(1)
C(15)	62(2)	24(2)	56(2)	3(1)	7(2)	7(1)
C(16)	62(2)	26(2)	42(2)	-3(1)	12(2)	2(1)
C(17)	91(3)	29(2)	40(2)	4(1)	9(2)	1(2)
C(18)	106(3)	31(2)	35(2)	4(1)	7(2)	3(2)
C(19)	81(2)	33(2)	38(2)	-4(1)	12(2)	1(2)

C(20)	66(2)	26(2)	32(2)	0(1)	16(1)	1(1)
C(21)	56(2)	30(2)	38(2)	-1(1)	10(1)	-2(1)
C(22)	65(2)	36(2)	28(2)	-2(1)	9(1)	-3(1)
C(23)	63(2)	33(2)	32(2)	-2(1)	11(1)	-5(1)
C(24)	58(2)	25(1)	32(2)	1(1)	7(1)	-2(1)
C(25)	60(2)	34(2)	39(2)	0(1)	7(1)	1(1)
C(26)	65(2)	33(2)	50(2)	1(1)	6(2)	9(2)
C(27)	73(2)	24(2)	44(2)	1(1)	4(2)	0(2)
C(28)	61(2)	29(2)	43(2)	0(1)	5(1)	-4(1)
C(29)	55(2)	26(2)	37(2)	4(1)	6(1)	-3(1)
C(30)	55(2)	45(2)	65(2)	-2(2)	1(2)	5(2)
C(31)	120(2)	123(2)	123(2)	5(1)	0(1)	-2(1)
C(32)	80(3)	110(3)	88(3)	-22(2)	28(2)	-23(3)
C(33)	56(2)	28(2)	59(2)	2(1)	6(2)	-3(1)
C(34)	60(2)	38(2)	62(2)	-6(2)	14(2)	-2(2)
C(35)	68(2)	68(2)	70(2)	21(2)	7(2)	16(2)
C(36)	145(4)	33(2)	50(2)	6(2)	6(2)	-13(2)
C(37)	104(3)	42(2)	46(2)	-1(2)	-5(2)	0(2)
N(1)	50(2)	27(1)	60(2)	-6(1)	3(1)	1(1)
N(2)	59(2)	22(1)	45(1)	1(1)	10(1)	1(1)
N(3)	57(2)	25(1)	38(1)	0(1)	10(1)	0(1)
N(4)	59(2)	27(1)	33(1)	-2(1)	10(1)	-4(1)
N(5)	56(2)	27(1)	33(1)	-1(1)	8(1)	-3(1)

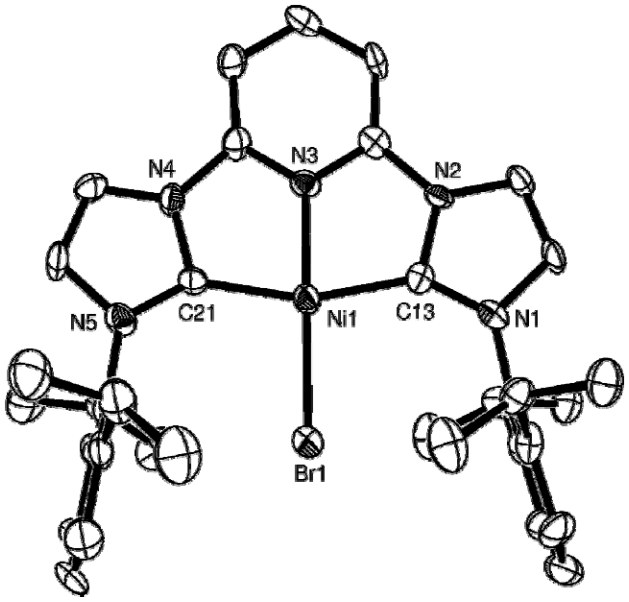


Table 1. Crystal data and structure refinement for **3(Br)**$^-$.

Identification code	**3(Br)**$^-$	
Empirical formula	C36 H43 Br2 Cl2 N5 Ni	
Formula weight	835.18	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.7728(5) Å	α= 87.286(2)°.
	b = 13.6700(5) Å	β= 75.428(2)°.
	c = 25.2292(10) Å	γ = 71.776(2)°.
Volume	4047.2(3) Å^3	
Z	4	
Density (calculated)	1.371 Mg/m^3	
Absorption coefficient	2.616 mm^{-1}	
F(000)	1704	
Crystal size	0.08 x 0.08 x 0.02 mm^3	
Theta range for data collection	2.91 to 27.73°.	
Index ranges	-16<=h<=16, -17<=k<=16, -32<=l<=32	
Reflections collected	69924	
Independent reflections	18589 [R(int) = 0.1227]	
Completeness to theta = 27.73°	97.7 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9495 and 0.8180
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	18589 / 12 / 846
Goodness-of-fit on F^2	1.008
Final R indices [I>2sigma(I)]	R1 = 0.0900, wR2 = 0.1668
R indices (all data)	R1 = 0.1837, wR2 = 0.1947
Largest diff. peak and hole	0.869 and -0.665 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3(Br)$^-$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7395(6)	5068(5)	1384(3)	22(2)
C(2)	7797(6)	5928(5)	1273(3)	25(2)
C(3)	7615(6)	6593(6)	1694(3)	32(2)
C(4)	7036(7)	6435(6)	2228(3)	36(2)
C(5)	6666(6)	5582(6)	2327(3)	34(2)
C(6)	6846(6)	4870(5)	1905(3)	29(2)
C(7)	8410(7)	6093(6)	696(3)	32(2)
C(8)	9673(7)	5931(6)	660(3)	45(2)
C(9)	7829(7)	7145(6)	492(3)	39(2)
C(10)	6472(6)	3919(6)	2027(3)	30(2)
C(11)	5180(7)	4173(6)	2223(3)	38(2)
C(12)	7079(7)	3254(6)	2429(3)	45(2)
C(13)	8359(6)	3563(5)	700(3)	21(2)
C(14)	6655(6)	4629(5)	646(3)	27(2)
C(15)	6971(6)	3950(5)	230(3)	25(2)
C(16)	8751(6)	2434(5)	-40(3)	21(2)
C(17)	8667(6)	2056(5)	-513(3)	26(2)
C(18)	9543(6)	1194(6)	-769(3)	31(2)
C(19)	10467(6)	733(6)	-549(3)	28(2)
C(20)	10473(6)	1182(5)	-78(3)	25(2)
C(21)	11128(6)	1468(5)	681(3)	21(2)

C(22)	12288(6)	48(6)	148(3)	29(2)
C(23)	12750(6)	111(5)	552(3)	30(2)
C(24)	12348(6)	1353(6)	1337(3)	28(2)
C(25)	13120(6)	1905(6)	1220(3)	30(2)
C(26)	13444(7)	2211(6)	1661(3)	37(2)
C(27)	12981(7)	1958(6)	2186(3)	43(2)
C(28)	12207(7)	1413(6)	2289(3)	39(2)
C(29)	11874(6)	1090(6)	1868(3)	34(2)
C(30)	13589(7)	2216(6)	643(3)	34(2)
C(31)	14835(8)	1619(7)	424(4)	56(3)
C(32)	13384(9)	3378(6)	607(4)	55(3)
C(33)	11005(7)	510(6)	1982(3)	40(2)
C(34)	11559(7)	-639(6)	2059(4)	48(2)
C(35)	10004(7)	969(7)	2475(4)	54(3)
C(36)	4292(7)	1598(5)	3954(3)	29(2)
C(37)	5089(7)	1460(6)	4261(3)	38(2)
C(38)	4648(9)	1892(7)	4799(4)	50(2)
C(39)	3524(10)	2431(7)	4994(4)	57(3)
C(40)	2777(8)	2544(7)	4667(3)	47(2)
C(41)	3147(7)	2139(6)	4131(3)	37(2)
C(42)	6328(7)	868(7)	4049(4)	47(2)
C(43)	6647(10)	-88(7)	4374(4)	76(4)
C(44)	7088(9)	1556(9)	4054(6)	102(5)
C(45)	2340(7)	2334(7)	3760(3)	44(2)
C(46)	1180(8)	2227(8)	4066(4)	66(3)
C(47)	2171(8)	3398(7)	3533(4)	60(3)
C(48)	4653(6)	422(6)	3125(3)	30(2)
C(49)	5287(6)	1798(6)	3001(3)	31(2)
C(50)	5577(6)	1331(6)	2510(3)	33(2)
C(51)	5162(6)	-193(5)	2204(3)	25(2)
C(52)	5553(6)	-221(6)	1646(3)	30(2)
C(53)	5380(6)	-981(6)	1363(3)	33(2)
C(54)	4859(7)	-1678(6)	1620(3)	33(2)
C(55)	4505(6)	-1587(5)	2184(3)	27(2)
C(56)	3673(6)	-1936(6)	3096(3)	28(2)
C(57)	3557(6)	-2983(5)	2445(3)	26(2)

C(58)	3053(6)	-3249(6)	2934(3)	31(2)
C(59)	2693(7)	-2709(6)	3908(3)	32(2)
C(60)	3333(7)	-3484(6)	4182(3)	33(2)
C(61)	2846(8)	-3576(7)	4740(3)	52(2)
C(62)	1811(8)	-2938(7)	4995(3)	51(2)
C(63)	1194(8)	-2176(7)	4718(3)	52(2)
C(64)	1619(7)	-2039(6)	4158(3)	38(2)
C(65)	4516(7)	-4174(6)	3901(3)	42(2)
C(66)	4653(9)	-5313(8)	3992(4)	74(3)
C(67)	5415(8)	-3861(8)	4078(5)	76(3)
C(68)	933(7)	-1213(7)	3858(3)	48(2)
C(69)	204(9)	-1607(8)	3603(4)	80(4)
C(70)	227(8)	-228(7)	4209(4)	65(3)
C(71)	1676(8)	5502(7)	1727(4)	59(3)
C(72)	9150(11)	4457(12)	2926(5)	121(6)
N(1)	7493(5)	4398(4)	929(2)	25(1)
N(2)	8024(5)	3309(4)	268(2)	21(1)
N(3)	9656(5)	2016(4)	168(2)	23(1)
N(4)	11311(5)	860(4)	228(2)	24(1)
N(5)	12037(5)	997(4)	879(2)	27(1)
N(6)	4728(5)	1228(5)	3374(2)	31(2)
N(7)	5190(5)	503(4)	2585(2)	26(1)
N(8)	4651(5)	-860(5)	2465(2)	25(1)
N(9)	3940(5)	-2192(4)	2543(2)	26(1)
N(10)	3140(5)	-2600(4)	3326(2)	27(1)
Ni(1)	9771(1)	2624(1)	792(1)	24(1)
Ni(2)	4113(1)	-758(1)	3229(1)	26(1)
Br(1)	10009(1)	3452(1)	1495(1)	33(1)
Br(2)	3520(1)	-643(1)	4153(1)	40(1)
Br(3)	7261(1)	1509(1)	1143(1)	41(1)
Br(4)	3901(1)	6617(1)	972(1)	38(1)
Cl(1)	748(3)	6754(2)	1884(1)	85(1)
Cl(2)	2079(2)	4898(2)	2297(1)	72(1)
Cl(3)	8830(5)	5659(4)	3240(2)	173(2)
Cl(4)	8652(4)	3642(3)	3409(2)	132(2)

Table 3. Bond lengths [Å] and angles [°] for **3(Br)**$^-$.

C(1)-C(6)	1.383(9)	C(14)-N(1)	1.381(8)
C(1)-C(2)	1.412(10)	C(14)-H(14)	0.9500
C(1)-N(1)	1.459(8)	C(15)-N(2)	1.380(8)
C(2)-C(3)	1.359(9)	C(15)-H(15)	0.9500
C(2)-C(7)	1.512(9)	C(16)-N(3)	1.342(8)
C(3)-C(4)	1.406(10)	C(16)-C(17)	1.364(9)
C(3)-H(3)	0.9500	C(16)-N(2)	1.389(8)
C(4)-C(5)	1.380(10)	C(17)-C(18)	1.392(10)
C(4)-H(4)	0.9500	C(17)-H(17)	0.9500
C(5)-C(6)	1.404(10)	C(18)-C(19)	1.388(10)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.513(10)	C(19)-C(20)	1.367(9)
C(7)-C(9)	1.530(10)	C(19)-H(19)	0.9500
C(7)-C(8)	1.537(10)	C(20)-N(3)	1.330(8)
C(7)-H(7)	1.0000	C(20)-N(4)	1.423(9)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.344(8)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.372(8)
C(8)-H(8C)	0.9800	C(21)-Ni(1)	1.914(7)
C(9)-H(9A)	0.9800	C(22)-C(23)	1.319(10)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.362(9)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(12)	1.525(10)	C(23)-N(5)	1.416(8)
C(10)-C(11)	1.529(10)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.389(10)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.403(10)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.462(9)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.402(10)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.525(10)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.383(11)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(1)	1.346(8)	C(27)-C(28)	1.383(11)
C(13)-N(2)	1.364(8)	C(27)-H(27)	0.9500
C(13)-Ni(1)	1.920(7)	C(28)-C(29)	1.378(10)
C(14)-C(15)	1.331(9)	C(28)-H(28)	0.9500

C(29)-C(33)	1.519(11)	C(43)-H(43C)	0.9800
C(30)-C(31)	1.513(11)	C(44)-H(44A)	0.9800
C(30)-C(32)	1.529(11)	C(44)-H(44B)	0.9800
C(30)-H(30)	1.0000	C(44)-H(44C)	0.9800
C(31)-H(31A)	0.9800	C(45)-C(47)	1.509(12)
C(31)-H(31B)	0.9800	C(45)-C(46)	1.536(12)
C(31)-H(31C)	0.9800	C(45)-H(45)	1.0000
C(32)-H(32A)	0.9800	C(46)-H(46A)	0.9800
C(32)-H(32B)	0.9800	C(46)-H(46B)	0.9800
C(32)-H(32C)	0.9800	C(46)-H(46C)	0.9800
C(33)-C(35)	1.533(11)	C(47)-H(47A)	0.9800
C(33)-C(34)	1.534(11)	C(47)-H(47B)	0.9800
C(33)-H(33)	1.0000	C(47)-H(47C)	0.9800
C(34)-H(34A)	0.9800	C(48)-N(6)	1.334(9)
C(34)-H(34B)	0.9800	C(48)-N(7)	1.379(9)
C(34)-H(34C)	0.9800	C(48)-Ni(2)	1.927(8)
C(35)-H(35A)	0.9800	C(49)-C(50)	1.332(9)
C(35)-H(35B)	0.9800	C(49)-N(6)	1.394(9)
C(35)-H(35C)	0.9800	C(49)-H(49)	0.9500
C(36)-C(41)	1.382(10)	C(50)-N(7)	1.358(9)
C(36)-C(37)	1.389(10)	C(50)-H(50)	0.9500
C(36)-N(6)	1.480(8)	C(51)-N(8)	1.337(9)
C(37)-C(38)	1.410(11)	C(51)-C(52)	1.369(9)
C(37)-C(42)	1.503(11)	C(51)-N(7)	1.398(8)
C(38)-C(39)	1.366(13)	C(52)-C(53)	1.390(10)
C(38)-H(38)	0.9500	C(52)-H(52)	0.9500
C(39)-C(40)	1.381(12)	C(53)-C(54)	1.376(10)
C(39)-H(39)	0.9500	C(53)-H(53)	0.9500
C(40)-C(41)	1.394(10)	C(54)-C(55)	1.379(10)
C(40)-H(40)	0.9500	C(54)-H(54)	0.9500
C(41)-C(45)	1.517(11)	C(55)-N(8)	1.332(9)
C(42)-C(43)	1.510(12)	C(55)-N(9)	1.414(9)
C(42)-C(44)	1.550(12)	C(56)-N(10)	1.328(9)
C(42)-H(42)	1.0000	C(56)-N(9)	1.385(8)
C(43)-H(43A)	0.9800	C(56)-Ni(2)	1.932(8)
C(43)-H(43B)	0.9800	C(57)-C(58)	1.333(10)

C(57)-N(9)	1.374(9)	C(71)-H(71A)	0.9900
C(57)-H(57)	0.9500	C(71)-H(71B)	0.9900
C(58)-N(10)	1.406(9)	C(72)-Cl(3)	1.742(15)
C(58)-H(58)	0.9500	C(72)-Cl(4)	1.748(15)
C(59)-C(60)	1.393(10)	C(72)-H(72A)	0.9900
C(59)-C(64)	1.397(11)	C(72)-H(72B)	0.9900
C(59)-N(10)	1.455(9)	N(3)-Ni(1)	1.872(5)
C(60)-C(61)	1.405(10)	N(8)-Ni(2)	1.873(5)
C(60)-C(65)	1.519(11)	Ni(1)-Br(1)	2.2813(11)
C(61)-C(62)	1.352(12)	Ni(2)-Br(2)	2.2591(11)
C(61)-H(61)	0.9500		
C(62)-C(63)	1.375(12)	C(6)-C(1)-C(2)	122.6(6)
C(62)-H(62)	0.9500	C(6)-C(1)-N(1)	118.3(6)
C(63)-C(64)	1.405(11)	C(2)-C(1)-N(1)	119.0(6)
C(63)-H(63)	0.9500	C(3)-C(2)-C(1)	118.4(7)
C(64)-C(68)	1.500(11)	C(3)-C(2)-C(7)	121.4(7)
C(65)-C(67)	1.512(12)	C(1)-C(2)-C(7)	120.2(6)
C(65)-C(66)	1.524(12)	C(2)-C(3)-C(4)	120.9(7)
C(65)-H(65)	1.0000	C(2)-C(3)-H(3)	119.5
C(66)-H(66A)	0.9800	C(4)-C(3)-H(3)	119.5
C(66)-H(66B)	0.9800	C(5)-C(4)-C(3)	119.5(7)
C(66)-H(66C)	0.9800	C(5)-C(4)-H(4)	120.2
C(67)-H(67A)	0.9800	C(3)-C(4)-H(4)	120.2
C(67)-H(67B)	0.9800	C(4)-C(5)-C(6)	121.4(7)
C(67)-H(67C)	0.9800	C(4)-C(5)-H(5)	119.3
C(68)-C(69)	1.490(12)	C(6)-C(5)-H(5)	119.3
C(68)-C(70)	1.538(11)	C(1)-C(6)-C(5)	117.1(7)
C(68)-H(68)	1.0000	C(1)-C(6)-C(10)	122.4(6)
C(69)-H(69A)	0.9800	C(5)-C(6)-C(10)	120.5(7)
C(69)-H(69B)	0.9800	C(2)-C(7)-C(9)	111.8(6)
C(69)-H(69C)	0.9800	C(2)-C(7)-C(8)	110.5(6)
C(70)-H(70A)	0.9800	C(9)-C(7)-C(8)	112.1(6)
C(70)-H(70B)	0.9800	C(2)-C(7)-H(7)	107.4
C(70)-H(70C)	0.9800	C(9)-C(7)-H(7)	107.4
C(71)-Cl(2)	1.735(10)	C(8)-C(7)-H(7)	107.4
C(71)-Cl(1)	1.746(9)	C(7)-C(8)-H(8A)	109.5

C(7)-C(8)-H(8B)	109.5	C(14)-C(15)-H(15)	128.0
H(8A)-C(8)-H(8B)	109.5	N(2)-C(15)-H(15)	128.0
C(7)-C(8)-H(8C)	109.5	N(3)-C(16)-C(17)	121.8(6)
H(8A)-C(8)-H(8C)	109.5	N(3)-C(16)-N(2)	110.0(6)
H(8B)-C(8)-H(8C)	109.5	C(17)-C(16)-N(2)	128.0(6)
C(7)-C(9)-H(9A)	109.5	C(16)-C(17)-C(18)	117.6(6)
C(7)-C(9)-H(9B)	109.5	C(16)-C(17)-H(17)	121.2
H(9A)-C(9)-H(9B)	109.5	C(18)-C(17)-H(17)	121.2
C(7)-C(9)-H(9C)	109.5	C(19)-C(18)-C(17)	121.3(7)
H(9A)-C(9)-H(9C)	109.5	C(19)-C(18)-H(18)	119.4
H(9B)-C(9)-H(9C)	109.5	C(17)-C(18)-H(18)	119.4
C(6)-C(10)-C(12)	110.4(6)	C(20)-C(19)-C(18)	116.3(7)
C(6)-C(10)-C(11)	112.8(6)	C(20)-C(19)-H(19)	121.9
C(12)-C(10)-C(11)	111.9(6)	C(18)-C(19)-H(19)	121.9
C(6)-C(10)-H(10)	107.1	N(3)-C(20)-C(19)	123.5(7)
C(12)-C(10)-H(10)	107.1	N(3)-C(20)-N(4)	109.2(6)
C(11)-C(10)-H(10)	107.1	C(19)-C(20)-N(4)	127.3(6)
C(10)-C(11)-H(11A)	109.5	N(5)-C(21)-N(4)	102.6(6)
C(10)-C(11)-H(11B)	109.5	N(5)-C(21)-Ni(1)	143.7(5)
H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-Ni(1)	113.7(5)
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	106.1(6)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	126.9
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	126.9
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	107.3(6)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	126.3
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.3
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	123.9(7)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	118.0(6)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	118.0(7)
N(1)-C(13)-N(2)	103.0(6)	C(24)-C(25)-C(26)	117.6(7)
N(1)-C(13)-Ni(1)	143.0(5)	C(24)-C(25)-C(30)	122.9(6)
N(2)-C(13)-Ni(1)	113.9(5)	C(26)-C(25)-C(30)	119.5(7)
C(15)-C(14)-N(1)	109.1(6)	C(27)-C(26)-C(25)	119.0(8)
C(15)-C(14)-H(14)	125.4	C(27)-C(26)-H(26)	120.5
N(1)-C(14)-H(14)	125.4	C(25)-C(26)-H(26)	120.5
C(14)-C(15)-N(2)	104.1(6)	C(28)-C(27)-C(26)	122.0(7)

C(28)-C(27)-H(27)	119.0	H(34A)-C(34)-H(34C)	109.5
C(26)-C(27)-H(27)	119.0	H(34B)-C(34)-H(34C)	109.5
C(29)-C(28)-C(27)	120.8(8)	C(33)-C(35)-H(35A)	109.5
C(29)-C(28)-H(28)	119.6	C(33)-C(35)-H(35B)	109.5
C(27)-C(28)-H(28)	119.6	H(35A)-C(35)-H(35B)	109.5
C(28)-C(29)-C(24)	116.6(8)	C(33)-C(35)-H(35C)	109.5
C(28)-C(29)-C(33)	120.9(7)	H(35A)-C(35)-H(35C)	109.5
C(24)-C(29)-C(33)	122.5(7)	H(35B)-C(35)-H(35C)	109.5
C(31)-C(30)-C(25)	111.5(6)	C(41)-C(36)-C(37)	125.3(7)
C(31)-C(30)-C(32)	111.4(7)	C(41)-C(36)-N(6)	117.4(6)
C(25)-C(30)-C(32)	112.3(6)	C(37)-C(36)-N(6)	117.0(7)
C(31)-C(30)-H(30)	107.1	C(36)-C(37)-C(38)	115.2(7)
C(25)-C(30)-H(30)	107.1	C(36)-C(37)-C(42)	123.3(7)
C(32)-C(30)-H(30)	107.1	C(38)-C(37)-C(42)	121.6(7)
C(30)-C(31)-H(31A)	109.5	C(39)-C(38)-C(37)	122.0(8)
C(30)-C(31)-H(31B)	109.5	C(39)-C(38)-H(38)	119.0
H(31A)-C(31)-H(31B)	109.5	C(37)-C(38)-H(38)	119.0
C(30)-C(31)-H(31C)	109.5	C(38)-C(39)-C(40)	119.9(8)
H(31A)-C(31)-H(31C)	109.5	C(38)-C(39)-H(39)	120.0
H(31B)-C(31)-H(31C)	109.5	C(40)-C(39)-H(39)	120.0
C(30)-C(32)-H(32A)	109.5	C(39)-C(40)-C(41)	121.5(8)
C(30)-C(32)-H(32B)	109.5	C(39)-C(40)-H(40)	119.2
H(32A)-C(32)-H(32B)	109.5	C(41)-C(40)-H(40)	119.2
C(30)-C(32)-H(32C)	109.5	C(36)-C(41)-C(40)	116.1(7)
H(32A)-C(32)-H(32C)	109.5	C(36)-C(41)-C(45)	122.6(7)
H(32B)-C(32)-H(32C)	109.5	C(40)-C(41)-C(45)	121.2(7)
C(29)-C(33)-C(35)	112.7(7)	C(37)-C(42)-C(43)	110.3(8)
C(29)-C(33)-C(34)	111.5(7)	C(37)-C(42)-C(44)	111.1(8)
C(35)-C(33)-C(34)	110.0(7)	C(43)-C(42)-C(44)	111.7(8)
C(29)-C(33)-H(33)	107.4	C(37)-C(42)-H(42)	107.9
C(35)-C(33)-H(33)	107.4	C(43)-C(42)-H(42)	107.9
C(34)-C(33)-H(33)	107.4	C(44)-C(42)-H(42)	107.9
C(33)-C(34)-H(34A)	109.5	C(42)-C(43)-H(43A)	109.5
C(33)-C(34)-H(34B)	109.5	C(42)-C(43)-H(43B)	109.5
H(34A)-C(34)-H(34B)	109.5	H(43A)-C(43)-H(43B)	109.5
C(33)-C(34)-H(34C)	109.5	C(42)-C(43)-H(43C)	109.5

H(43A)-C(43)-H(43C)	109.5	N(8)-C(51)-N(7)	109.7(6)
H(43B)-C(43)-H(43C)	109.5	C(52)-C(51)-N(7)	128.0(7)
C(42)-C(44)-H(44A)	109.5	C(51)-C(52)-C(53)	116.1(7)
C(42)-C(44)-H(44B)	109.5	C(51)-C(52)-H(52)	121.9
H(44A)-C(44)-H(44B)	109.5	C(53)-C(52)-H(52)	121.9
C(42)-C(44)-H(44C)	109.5	C(54)-C(53)-C(52)	122.9(7)
H(44A)-C(44)-H(44C)	109.5	C(54)-C(53)-H(53)	118.6
H(44B)-C(44)-H(44C)	109.5	C(52)-C(53)-H(53)	118.6
C(47)-C(45)-C(41)	110.1(7)	C(53)-C(54)-C(55)	116.4(7)
C(47)-C(45)-C(46)	109.4(7)	C(53)-C(54)-H(54)	121.8
C(41)-C(45)-C(46)	111.5(7)	C(55)-C(54)-H(54)	121.8
C(47)-C(45)-H(45)	108.6	N(8)-C(55)-C(54)	121.9(7)
C(41)-C(45)-H(45)	108.6	N(8)-C(55)-N(9)	110.4(6)
C(46)-C(45)-H(45)	108.6	C(54)-C(55)-N(9)	127.7(7)
C(45)-C(46)-H(46A)	109.5	N(10)-C(56)-N(9)	102.8(6)
C(45)-C(46)-H(46B)	109.5	N(10)-C(56)-Ni(2)	144.9(5)
H(46A)-C(46)-H(46B)	109.5	N(9)-C(56)-Ni(2)	112.2(5)
C(45)-C(46)-H(46C)	109.5	C(58)-C(57)-N(9)	105.9(6)
H(46A)-C(46)-H(46C)	109.5	C(58)-C(57)-H(57)	127.0
H(46B)-C(46)-H(46C)	109.5	N(9)-C(57)-H(57)	127.0
C(45)-C(47)-H(47A)	109.5	C(57)-C(58)-N(10)	107.0(6)
C(45)-C(47)-H(47B)	109.5	C(57)-C(58)-H(58)	126.5
H(47A)-C(47)-H(47B)	109.5	N(10)-C(58)-H(58)	126.5
C(45)-C(47)-H(47C)	109.5	C(60)-C(59)-C(64)	123.6(7)
H(47A)-C(47)-H(47C)	109.5	C(60)-C(59)-N(10)	119.0(7)
H(47B)-C(47)-H(47C)	109.5	C(64)-C(59)-N(10)	117.4(7)
N(6)-C(48)-N(7)	103.3(6)	C(59)-C(60)-C(61)	116.6(7)
N(6)-C(48)-Ni(2)	144.7(6)	C(59)-C(60)-C(65)	122.1(7)
N(7)-C(48)-Ni(2)	111.9(5)	C(61)-C(60)-C(65)	121.2(7)
C(50)-C(49)-N(6)	107.4(7)	C(62)-C(61)-C(60)	121.3(8)
C(50)-C(49)-H(49)	126.3	C(62)-C(61)-H(61)	119.3
N(6)-C(49)-H(49)	126.3	C(60)-C(61)-H(61)	119.3
C(49)-C(50)-N(7)	106.2(7)	C(61)-C(62)-C(63)	121.1(8)
C(49)-C(50)-H(50)	126.9	C(61)-C(62)-H(62)	119.4
N(7)-C(50)-H(50)	126.9	C(63)-C(62)-H(62)	119.4
N(8)-C(51)-C(52)	122.2(7)	C(62)-C(63)-C(64)	121.0(8)

C(62)-C(63)-H(63)	119.5	C(68)-C(70)-H(70B)	109.5
C(64)-C(63)-H(63)	119.5	H(70A)-C(70)-H(70B)	109.5
C(59)-C(64)-C(63)	116.3(8)	C(68)-C(70)-H(70C)	109.5
C(59)-C(64)-C(68)	123.1(7)	H(70A)-C(70)-H(70C)	109.5
C(63)-C(64)-C(68)	120.5(8)	H(70B)-C(70)-H(70C)	109.5
C(67)-C(65)-C(60)	110.6(7)	Cl(2)-C(71)-Cl(1)	112.2(5)
C(67)-C(65)-C(66)	111.4(8)	Cl(2)-C(71)-H(71A)	109.2
C(60)-C(65)-C(66)	112.4(7)	Cl(1)-C(71)-H(71A)	109.2
C(67)-C(65)-H(65)	107.4	Cl(2)-C(71)-H(71B)	109.2
C(60)-C(65)-H(65)	107.4	Cl(1)-C(71)-H(71B)	109.2
C(66)-C(65)-H(65)	107.4	H(71A)-C(71)-H(71B)	107.9
C(65)-C(66)-H(66A)	109.5	Cl(3)-C(72)-Cl(4)	108.9(7)
C(65)-C(66)-H(66B)	109.5	Cl(3)-C(72)-H(72A)	109.9
H(66A)-C(66)-H(66B)	109.5	Cl(4)-C(72)-H(72A)	109.9
C(65)-C(66)-H(66C)	109.5	Cl(3)-C(72)-H(72B)	109.9
H(66A)-C(66)-H(66C)	109.5	Cl(4)-C(72)-H(72B)	109.9
H(66B)-C(66)-H(66C)	109.5	H(72A)-C(72)-H(72B)	108.3
C(65)-C(67)-H(67A)	109.5	C(13)-N(1)-C(14)	110.6(6)
C(65)-C(67)-H(67B)	109.5	C(13)-N(1)-C(1)	129.0(6)
H(67A)-C(67)-H(67B)	109.5	C(14)-N(1)-C(1)	120.3(6)
C(65)-C(67)-H(67C)	109.5	C(13)-N(2)-C(15)	113.2(5)
H(67A)-C(67)-H(67C)	109.5	C(13)-N(2)-C(16)	115.9(6)
H(67B)-C(67)-H(67C)	109.5	C(15)-N(2)-C(16)	130.8(6)
C(69)-C(68)-C(64)	111.5(8)	C(20)-N(3)-C(16)	119.5(6)
C(69)-C(68)-C(70)	111.0(8)	C(20)-N(3)-Ni(1)	120.6(5)
C(64)-C(68)-C(70)	113.7(7)	C(16)-N(3)-Ni(1)	119.9(5)
C(69)-C(68)-H(68)	106.7	C(22)-N(4)-C(21)	113.2(6)
C(64)-C(68)-H(68)	106.7	C(22)-N(4)-C(20)	131.2(6)
C(70)-C(68)-H(68)	106.7	C(21)-N(4)-C(20)	115.6(5)
C(68)-C(69)-H(69A)	109.5	C(21)-N(5)-C(23)	110.7(6)
C(68)-C(69)-H(69B)	109.5	C(21)-N(5)-C(24)	127.1(6)
H(69A)-C(69)-H(69B)	109.5	C(23)-N(5)-C(24)	122.0(6)
C(68)-C(69)-H(69C)	109.5	C(48)-N(6)-C(49)	111.0(6)
H(69A)-C(69)-H(69C)	109.5	C(48)-N(6)-C(36)	130.7(6)
H(69B)-C(69)-H(69C)	109.5	C(49)-N(6)-C(36)	118.3(6)
C(68)-C(70)-H(70A)	109.5	C(50)-N(7)-C(48)	112.1(6)

C(50)-N(7)-C(51)	130.6(6)
C(48)-N(7)-C(51)	117.0(6)
C(55)-N(8)-C(51)	120.5(6)
C(55)-N(8)-Ni(2)	119.7(5)
C(51)-N(8)-Ni(2)	119.8(5)
C(57)-N(9)-C(56)	112.4(6)
C(57)-N(9)-C(55)	131.5(6)
C(56)-N(9)-C(55)	116.1(6)
C(56)-N(10)-C(58)	112.0(6)
C(56)-N(10)-C(59)	127.2(6)
C(58)-N(10)-C(59)	120.8(6)
N(3)-Ni(1)-C(21)	80.8(3)
N(3)-Ni(1)-C(13)	80.3(3)
C(21)-Ni(1)-C(13)	161.1(3)
N(3)-Ni(1)-Br(1)	174.43(18)
C(21)-Ni(1)-Br(1)	99.1(2)
C(13)-Ni(1)-Br(1)	99.8(2)
N(8)-Ni(2)-C(48)	81.3(3)
N(8)-Ni(2)-C(56)	81.6(3)
C(48)-Ni(2)-C(56)	162.7(3)
N(8)-Ni(2)-Br(2)	178.24(18)
C(48)-Ni(2)-Br(2)	97.9(2)
C(56)-Ni(2)-Br(2)	99.2(2)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3(Br)$^-$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	19(4)	20(4)	28(4)	1(3)	-10(3)	-3(3)
C(2)	14(4)	33(4)	22(4)	5(3)	-3(3)	-1(3)
C(3)	35(5)	32(5)	33(4)	-2(4)	-9(4)	-14(4)
C(4)	38(5)	45(5)	30(4)	-1(4)	-14(4)	-15(4)
C(5)	33(5)	38(5)	21(4)	-6(4)	3(3)	-6(4)
C(6)	21(4)	26(4)	33(4)	7(3)	-3(3)	-2(3)
C(7)	36(5)	38(5)	30(4)	5(4)	-6(4)	-25(4)
C(8)	35(5)	48(5)	47(5)	15(4)	-5(4)	-10(4)
C(9)	36(5)	30(5)	47(5)	2(4)	-9(4)	-5(4)
C(10)	29(4)	31(5)	24(4)	-1(3)	-1(3)	-7(4)
C(11)	36(5)	29(5)	43(5)	8(4)	-8(4)	-5(4)
C(12)	33(5)	47(5)	57(6)	19(4)	-13(4)	-16(4)
C(13)	18(4)	20(4)	24(4)	3(3)	0(3)	-9(3)
C(14)	20(4)	33(5)	25(4)	5(3)	-13(3)	2(3)
C(15)	19(4)	35(4)	21(4)	4(3)	-10(3)	-6(3)
C(16)	22(4)	28(4)	16(3)	9(3)	-2(3)	-15(3)
C(17)	13(4)	34(4)	26(4)	7(3)	-8(3)	-2(3)
C(18)	27(4)	48(5)	28(4)	3(4)	-12(4)	-20(4)
C(19)	20(4)	31(4)	28(4)	-1(3)	-1(3)	-4(3)
C(20)	22(4)	28(4)	19(4)	2(3)	-1(3)	-4(3)
C(21)	24(4)	26(4)	13(3)	2(3)	-5(3)	-6(3)
C(22)	33(5)	29(4)	20(4)	-7(3)	-4(3)	-5(4)
C(23)	24(4)	22(4)	36(4)	3(3)	-7(4)	6(3)
C(24)	22(4)	33(5)	21(4)	-5(3)	-6(3)	5(4)
C(25)	26(4)	34(5)	26(4)	2(3)	-11(3)	-1(4)
C(26)	44(5)	36(5)	39(5)	4(4)	-22(4)	-15(4)
C(27)	40(5)	55(6)	34(5)	-2(4)	-29(4)	1(4)
C(28)	37(5)	44(5)	31(5)	5(4)	-5(4)	-10(4)
C(29)	24(4)	38(5)	29(4)	-4(4)	-10(4)	10(4)
C(30)	34(5)	40(5)	33(4)	0(4)	-17(4)	-13(4)
C(31)	48(6)	62(6)	40(5)	-4(5)	10(5)	-7(5)

C(32)	72(7)	48(6)	43(5)	6(4)	-3(5)	-25(5)
C(33)	33(5)	49(6)	29(4)	5(4)	-5(4)	-5(4)
C(34)	35(5)	52(6)	56(6)	1(5)	-8(5)	-12(4)
C(35)	37(5)	62(6)	60(6)	9(5)	-4(5)	-18(5)
C(36)	36(5)	28(4)	18(4)	-4(3)	-4(3)	-6(4)
C(37)	43(5)	39(5)	34(5)	2(4)	-21(4)	-10(4)
C(38)	64(7)	45(6)	46(6)	-7(4)	-33(5)	-10(5)
C(39)	95(9)	43(6)	31(5)	1(4)	-27(6)	-10(6)
C(40)	43(6)	61(6)	29(5)	-2(4)	-6(4)	-5(5)
C(41)	35(5)	56(6)	23(4)	5(4)	-11(4)	-15(4)
C(42)	38(5)	62(6)	53(6)	5(5)	-31(5)	-18(5)
C(43)	100(9)	65(7)	41(6)	-13(5)	-33(6)	20(6)
C(44)	40(7)	92(9)	187(15)	-23(9)	-48(8)	-18(6)
C(45)	22(5)	61(6)	41(5)	-9(4)	-1(4)	-4(4)
C(46)	48(6)	85(8)	63(7)	6(6)	-6(5)	-23(6)
C(47)	55(7)	66(7)	63(7)	16(5)	-29(5)	-14(5)
C(48)	22(4)	37(5)	29(4)	-3(4)	-13(3)	-1(4)
C(49)	34(5)	40(5)	21(4)	-1(4)	-6(3)	-15(4)
C(50)	32(5)	38(5)	27(4)	1(4)	-3(4)	-9(4)
C(51)	28(4)	26(4)	15(4)	5(3)	-1(3)	-4(3)
C(52)	27(4)	36(5)	28(4)	6(4)	-3(3)	-13(4)
C(53)	34(5)	34(5)	19(4)	2(3)	-8(4)	5(4)
C(54)	39(5)	39(5)	22(4)	4(4)	-6(4)	-13(4)
C(55)	25(4)	26(4)	31(4)	8(3)	-14(4)	-4(3)
C(56)	24(4)	36(5)	24(4)	6(3)	-12(3)	-4(4)
C(57)	30(4)	22(4)	29(4)	-4(3)	-8(4)	-9(3)
C(58)	36(5)	32(5)	31(4)	-1(4)	-5(4)	-20(4)
C(59)	31(5)	48(5)	22(4)	5(4)	-2(4)	-24(4)
C(60)	36(5)	42(5)	24(4)	6(4)	-6(4)	-17(4)
C(61)	63(7)	64(6)	26(5)	17(4)	-15(5)	-17(5)
C(62)	58(7)	65(7)	24(4)	13(4)	1(5)	-22(5)
C(63)	43(6)	69(7)	36(5)	-3(5)	-2(4)	-13(5)
C(64)	42(5)	48(5)	31(5)	4(4)	-12(4)	-24(4)
C(65)	44(6)	48(6)	27(4)	11(4)	-15(4)	-3(4)
C(66)	72(8)	72(8)	55(7)	-1(6)	6(6)	-7(6)
C(67)	34(6)	90(8)	93(9)	-12(7)	-15(6)	-4(6)

C(68)	36(5)	64(6)	38(5)	1(5)	-5(4)	-9(5)
C(69)	77(8)	83(8)	82(8)	-17(6)	-43(7)	-6(7)
C(70)	53(7)	60(7)	76(7)	-10(6)	-24(6)	0(5)
C(71)	59(7)	58(6)	55(6)	-3(5)	-10(5)	-14(5)
C(72)	71(9)	176(15)	66(8)	6(9)	-13(7)	27(9)
N(1)	25(3)	30(4)	24(3)	3(3)	-13(3)	-9(3)
N(2)	19(3)	29(3)	20(3)	-3(3)	-8(3)	-10(3)
N(3)	23(3)	30(4)	16(3)	-1(3)	-5(3)	-9(3)
N(4)	20(3)	23(3)	23(3)	0(3)	-4(3)	0(3)
N(5)	29(4)	32(4)	19(3)	6(3)	-9(3)	-7(3)
N(6)	34(4)	39(4)	21(3)	5(3)	-4(3)	-14(3)
N(7)	29(4)	33(4)	18(3)	-1(3)	-1(3)	-15(3)
N(8)	16(3)	40(4)	19(3)	2(3)	-4(3)	-9(3)
N(9)	28(4)	25(4)	18(3)	0(3)	-4(3)	3(3)
N(10)	29(4)	35(4)	19(3)	0(3)	-6(3)	-14(3)
Ni(1)	21(1)	27(1)	20(1)	1(1)	-7(1)	-3(1)
Ni(2)	26(1)	36(1)	18(1)	2(1)	-7(1)	-11(1)
Br(1)	30(1)	36(1)	31(1)	-4(1)	-13(1)	-3(1)
Br(2)	50(1)	53(1)	20(1)	2(1)	-7(1)	-24(1)
Br(3)	48(1)	35(1)	30(1)	-3(1)	9(1)	-15(1)
Br(4)	28(1)	53(1)	30(1)	-10(1)	-14(1)	-1(1)
Cl(1)	71(2)	74(2)	90(2)	18(2)	-14(2)	-2(2)
Cl(2)	76(2)	62(2)	89(2)	13(2)	-42(2)	-21(2)
Cl(3)	189(5)	168(4)	156(4)	13(3)	-35(4)	-53(4)
Cl(4)	145(4)	167(4)	108(3)	30(3)	-72(3)	-53(3)

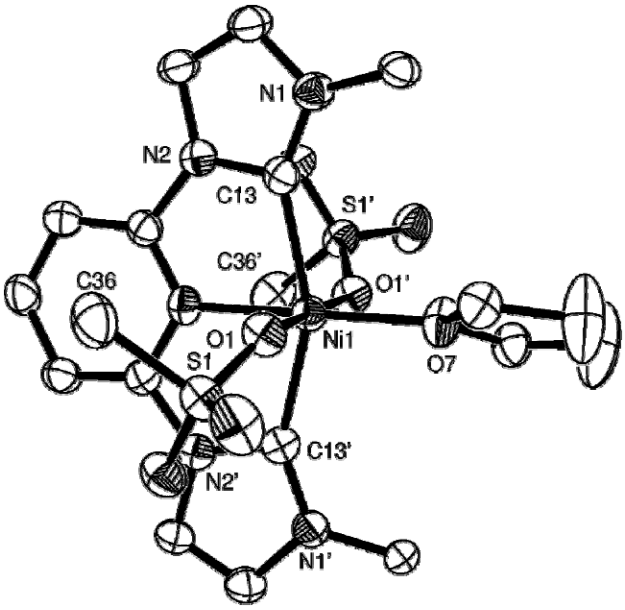


Table 1. Crystal data and structure refinement for **5**.

Identification code	**5**	
Empirical formula	C49 H65 F6 N5 Ni O9 S2	
Formula weight	1104.89	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 22.7194(19) Å	α= 90°.
	b = 25.510(3) Å	β= 125.520(4)°.
	c = 14.1716(13) Å	γ = 90°.
Volume	6685.2(11) $Å^3$	
Z	4	
Density (calculated)	1.098 Mg/m^3	
Absorption coefficient	0.415 mm^{-1}	
F(000)	2320	
Crystal size	0.30 x 0.20 x 0.20 mm^3	
Theta range for data collection	3.13 to 27.52°.	
Index ranges	-27<=h<=29, -33<=k<=32, -18<=l<=18	
Reflections collected	28442	
Independent reflections	7590 [R(int) = 0.0715]	
Completeness to theta = 27.50°	98.8 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9216 and 0.8856
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7590 / 0 / 331
Goodness-of-fit on F^2	1.056
Final R indices [I>2sigma(I)]	R1 = 0.0869, wR2 = 0.1959
R indices (all data)	R1 = 0.1390, wR2 = 0.2181
Largest diff. peak and hole	1.280 and -0.330 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **5**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	3893(2)	1851(2)	-705(3)	35(1)
C(2)	3172(2)	1972(2)	-1141(4)	44(1)
C(3)	2952(3)	2491(2)	-1523(4)	52(1)
C(4)	3418(3)	2852(2)	-1454(4)	55(1)
C(5)	4127(3)	2718(2)	-995(4)	48(1)
C(6)	4380(2)	2208(2)	-611(4)	40(1)
C(7)	2646(3)	1582(2)	-1208(4)	54(1)
C(8)	2331(3)	1791(2)	-571(5)	69(2)
C(9)	2067(3)	1432(3)	-2463(5)	80(2)
C(10)	5150(2)	2050(2)	-133(4)	46(1)
C(11)	5693(3)	2500(2)	343(5)	59(1)
C(12)	5174(3)	1752(3)	-1028(6)	78(2)
C(13)	4441(2)	1113(2)	727(3)	31(1)
C(14)	3892(2)	903(2)	-1181(3)	39(1)
C(15)	4091(2)	449(2)	-597(3)	37(1)
C(16)	4717(2)	235(2)	1517(3)	30(1)
C(17)	4701(2)	-303(2)	1455(4)	38(1)

C(18)	5000	-568(2)	2500	43(2)
C(36)	3036(3)	554(2)	1753(4)	52(1)
C(38)	4361(2)	2424(2)	1986(4)	40(1)
C(39)	4626(3)	2979(2)	2185(7)	87(2)
C(42)	2931(4)	9021(3)	186(6)	100(2)
C(43)	2251(4)	8773(4)	-677(7)	115(3)
C(44)	2331(6)	8231(4)	-277(7)	155(4)
C(45)	3038(4)	8187(3)	914(6)	87(2)
N(1)	4109(2)	1307(1)	-359(3)	35(1)
N(2)	4420(2)	583(1)	559(3)	31(1)
N(3)	5000	498(2)	2500	31(1)
O(1)	3950(1)	1296(1)	2237(2)	36(1)
O(2)	3103(2)	1445(1)	2711(3)	53(1)
O(3)	4078(2)	814(1)	3829(2)	42(1)
O(7)	5000	2100(2)	2500	41(1)
O(8)	3306(3)	8713(2)	1207(4)	87(1)
F(1)	2659(2)	334(1)	2094(3)	72(1)
F(2)	3442(2)	181(1)	1756(3)	78(1)
F(3)	2577(2)	721(2)	689(3)	93(1)
S(1)	3602(1)	1089(1)	2750(1)	36(1)
Ni(1)	5000	1289(1)	2500	30(1)

Table 3. Bond lengths [Å] and angles [°] for **5**.

C(1)-C(6)	1.380(6)	C(14)-N(1)	1.413(5)
C(1)-C(2)	1.407(6)	C(14)-H(14)	0.9500
C(1)-N(1)	1.458(5)	C(15)-N(2)	1.392(5)
C(2)-C(3)	1.409(6)	C(15)-H(15)	0.9500
C(2)-C(7)	1.515(7)	C(16)-N(3)	1.329(4)
C(3)-C(4)	1.363(7)	C(16)-C(17)	1.373(6)
C(3)-H(3)	0.9500	C(16)-N(2)	1.423(5)
C(4)-C(5)	1.384(7)	C(17)-C(18)	1.393(5)
C(4)-H(4)	0.9500	C(17)-H(17)	0.9500
C(5)-C(6)	1.397(6)	C(18)-C(17)#1	1.393(5)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.519(6)	C(36)-F(3)	1.310(5)
C(7)-C(9)	1.525(7)	C(36)-F(2)	1.322(6)
C(7)-C(8)	1.538(7)	C(36)-F(1)	1.327(5)
C(7)-H(7)	1.0000	C(36)-S(1)	1.844(5)
C(8)-H(8A)	0.9800	C(38)-O(7)	1.446(4)
C(8)-H(8B)	0.9800	C(38)-C(39)	1.499(7)
C(8)-H(8C)	0.9800	C(38)-H(38A)	0.9900
C(9)-H(9A)	0.9800	C(38)-H(38B)	0.9900
C(9)-H(9B)	0.9800	C(39)-C(39)#1	1.388(10)
C(9)-H(9C)	0.9800	C(39)-H(39A)	0.9900
C(10)-C(12)	1.506(7)	C(39)-H(39B)	0.9900
C(10)-C(11)	1.525(7)	C(42)-O(8)	1.416(8)
C(10)-H(10)	1.0000	C(42)-C(43)	1.444(9)
C(11)-H(11A)	0.9800	C(42)-H(42A)	0.9900
C(11)-H(11B)	0.9800	C(42)-H(42B)	0.9900
C(11)-H(11C)	0.9800	C(43)-C(44)	1.467(11)
C(12)-H(12A)	0.9800	C(43)-H(43A)	0.9900
C(12)-H(12B)	0.9800	C(43)-H(43B)	0.9900
C(12)-H(12C)	0.9800	C(44)-C(45)	1.514(10)
C(13)-N(1)	1.355(5)	C(44)-H(44A)	0.9900
C(13)-N(2)	1.368(5)	C(44)-H(44B)	0.9900
C(13)-Ni(1)	2.103(4)	C(45)-O(8)	1.432(7)
C(14)-C(15)	1.341(6)	C(45)-H(45A)	0.9900

C(45)-H(45B)	0.9900	C(7)-C(8)-H(8A)	109.5
N(3)-C(16)#1	1.329(4)	C(7)-C(8)-H(8B)	109.5
N(3)-Ni(1)	2.017(4)	H(8A)-C(8)-H(8B)	109.5
O(1)-S(1)	1.450(3)	C(7)-C(8)-H(8C)	109.5
O(1)-Ni(1)	2.190(3)	H(8A)-C(8)-H(8C)	109.5
O(2)-S(1)	1.429(3)	H(8B)-C(8)-H(8C)	109.5
O(3)-S(1)	1.442(3)	C(7)-C(9)-H(9A)	109.5
O(7)-C(38)#1	1.446(4)	C(7)-C(9)-H(9B)	109.5
O(7)-Ni(1)	2.069(4)	H(9A)-C(9)-H(9B)	109.5
Ni(1)-C(13)#1	2.103(4)	C(7)-C(9)-H(9C)	109.5
Ni(1)-O(1)#1	2.190(3)	H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.5
C(6)-C(1)-C(2)	124.1(4)	C(12)-C(10)-C(6)	110.8(4)
C(6)-C(1)-N(1)	120.1(4)	C(12)-C(10)-C(11)	109.7(4)
C(2)-C(1)-N(1)	115.8(4)	C(6)-C(10)-C(11)	114.9(4)
C(1)-C(2)-C(3)	116.0(4)	C(12)-C(10)-H(10)	107.0
C(1)-C(2)-C(7)	123.9(4)	C(6)-C(10)-H(10)	107.0
C(3)-C(2)-C(7)	120.2(4)	C(11)-C(10)-H(10)	107.0
C(4)-C(3)-C(2)	121.3(4)	C(10)-C(11)-H(11A)	109.5
C(4)-C(3)-H(3)	119.3	C(10)-C(11)-H(11B)	109.5
C(2)-C(3)-H(3)	119.3	H(11A)-C(11)-H(11B)	109.5
C(3)-C(4)-C(5)	120.7(4)	C(10)-C(11)-H(11C)	109.5
C(3)-C(4)-H(4)	119.7	H(11A)-C(11)-H(11C)	109.5
C(5)-C(4)-H(4)	119.7	H(11B)-C(11)-H(11C)	109.5
C(4)-C(5)-C(6)	121.1(5)	C(10)-C(12)-H(12A)	109.5
C(4)-C(5)-H(5)	119.5	C(10)-C(12)-H(12B)	109.5
C(6)-C(5)-H(5)	119.5	H(12A)-C(12)-H(12B)	109.5
C(1)-C(6)-C(5)	116.8(4)	C(10)-C(12)-H(12C)	109.5
C(1)-C(6)-C(10)	121.3(4)	H(12A)-C(12)-H(12C)	109.5
C(5)-C(6)-C(10)	121.9(4)	H(12B)-C(12)-H(12C)	109.5
C(2)-C(7)-C(9)	110.6(4)	N(1)-C(13)-N(2)	103.0(3)
C(2)-C(7)-C(8)	110.8(4)	N(1)-C(13)-Ni(1)	146.1(3)
C(9)-C(7)-C(8)	113.0(4)	N(2)-C(13)-Ni(1)	110.8(3)
C(2)-C(7)-H(7)	107.4	C(15)-C(14)-N(1)	107.0(3)
C(9)-C(7)-H(7)	107.4	C(15)-C(14)-H(14)	126.5
C(8)-C(7)-H(7)	107.4	N(1)-C(14)-H(14)	126.5

C(14)-C(15)-N(2)	105.7(4)	C(42)-C(43)-C(44)	104.7(7)
C(14)-C(15)-H(15)	127.1	C(42)-C(43)-H(43A)	110.8
N(2)-C(15)-H(15)	127.1	C(44)-C(43)-H(43A)	110.8
N(3)-C(16)-C(17)	123.5(4)	C(42)-C(43)-H(43B)	110.8
N(3)-C(16)-N(2)	110.8(3)	C(44)-C(43)-H(43B)	110.8
C(17)-C(16)-N(2)	125.7(4)	H(43A)-C(43)-H(43B)	108.9
C(16)-C(17)-C(18)	116.0(4)	C(43)-C(44)-C(45)	108.3(7)
C(16)-C(17)-H(17)	122.0	C(43)-C(44)-H(44A)	110.0
C(18)-C(17)-H(17)	122.0	C(45)-C(44)-H(44A)	110.0
C(17)#1-C(18)-C(17)	121.9(6)	C(43)-C(44)-H(44B)	110.0
C(17)#1-C(18)-H(18)	119.0	C(45)-C(44)-H(44B)	110.0
C(17)-C(18)-H(18)	119.0	H(44A)-C(44)-H(44B)	108.4
F(3)-C(36)-F(2)	109.0(5)	O(8)-C(45)-C(44)	104.6(6)
F(3)-C(36)-F(1)	107.8(4)	O(8)-C(45)-H(45A)	110.8
F(2)-C(36)-F(1)	106.9(4)	C(44)-C(45)-H(45A)	110.8
F(3)-C(36)-S(1)	112.0(4)	O(8)-C(45)-H(45B)	110.8
F(2)-C(36)-S(1)	110.8(3)	C(44)-C(45)-H(45B)	110.8
F(1)-C(36)-S(1)	110.1(4)	H(45A)-C(45)-H(45B)	108.9
O(7)-C(38)-C(39)	105.6(4)	C(13)-N(1)-C(14)	111.5(3)
O(7)-C(38)-H(38A)	110.6	C(13)-N(1)-C(1)	126.0(3)
C(39)-C(38)-H(38A)	110.6	C(14)-N(1)-C(1)	122.0(3)
O(7)-C(38)-H(38B)	110.6	C(13)-N(2)-C(15)	112.9(3)
C(39)-C(38)-H(38B)	110.6	C(13)-N(2)-C(16)	120.1(3)
H(38A)-C(38)-H(38B)	108.8	C(15)-N(2)-C(16)	127.0(3)
C(39)#1-C(39)-C(38)	109.2(3)	C(16)-N(3)-C(16)#1	119.1(5)
C(39)#1-C(39)-H(39A)	109.8	C(16)-N(3)-Ni(1)	120.4(2)
C(38)-C(39)-H(39A)	109.8	C(16)#1-N(3)-Ni(1)	120.4(2)
C(39)#1-C(39)-H(39B)	109.8	S(1)-O(1)-Ni(1)	140.30(17)
C(38)-C(39)-H(39B)	109.8	C(38)#1-O(7)-C(38)	110.4(4)
H(39A)-C(39)-H(39B)	108.3	C(38)#1-O(7)-Ni(1)	124.8(2)
O(8)-C(42)-C(43)	109.7(7)	C(38)-O(7)-Ni(1)	124.8(2)
O(8)-C(42)-H(42A)	109.7	C(42)-O(8)-C(45)	108.7(5)
C(43)-C(42)-H(42A)	109.7	O(2)-S(1)-O(3)	116.11(19)
O(8)-C(42)-H(42B)	109.7	O(2)-S(1)-O(1)	113.63(18)
C(43)-C(42)-H(42B)	109.7	O(3)-S(1)-O(1)	114.66(17)
H(42A)-C(42)-H(42B)	108.2	O(2)-S(1)-C(36)	104.9(2)

O(3)-S(1)-C(36)	102.2(2)	O(7)-Ni(1)-O(1)	89.52(8)
O(1)-S(1)-C(36)	103.1(2)	C(13)-Ni(1)-O(1)	87.49(12)
N(3)-Ni(1)-O(7)	180.0	C(13)#1-Ni(1)-O(1)	92.71(12)
N(3)-Ni(1)-C(13)	77.63(11)	N(3)-Ni(1)-O(1)#1	90.48(8)
O(7)-Ni(1)-C(13)	102.37(11)	O(7)-Ni(1)-O(1)#1	89.52(8)
N(3)-Ni(1)-C(13)#1	77.63(11)	C(13)-Ni(1)-O(1)#1	92.71(12)
O(7)-Ni(1)-C(13)#1	102.37(11)	C(13)#1-Ni(1)-O(1)#1	87.49(12)
C(13)-Ni(1)-C(13)#1	155.3(2)	O(1)-Ni(1)-O(1)#1	179.03(15)
N(3)-Ni(1)-O(1)	90.48(8)		

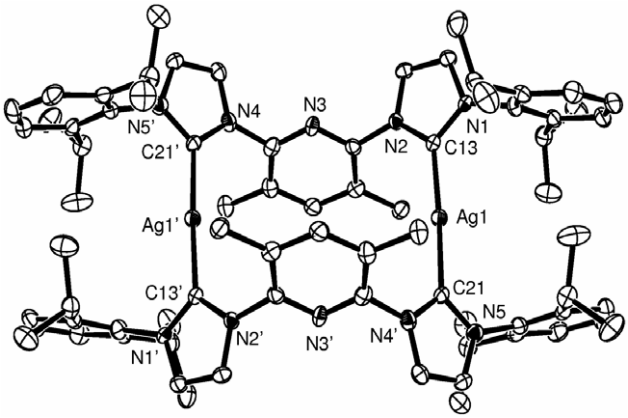
Symmetry transformations used to generate equivalent atoms:

#1 -x+1,y,-z+1/2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **5**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	42(2)	33(2)	27(2)	5(2)	18(2)	9(2)
C(2)	42(3)	50(3)	37(2)	10(2)	21(2)	13(2)
C(3)	50(3)	55(3)	52(3)	18(2)	30(2)	21(2)
C(4)	74(4)	46(3)	55(3)	18(2)	43(3)	21(3)
C(5)	61(3)	43(3)	45(3)	6(2)	33(2)	4(2)
C(6)	48(3)	37(3)	35(2)	3(2)	23(2)	6(2)
C(7)	41(3)	53(3)	65(3)	11(2)	29(3)	9(2)
C(8)	48(3)	77(4)	87(4)	20(3)	43(3)	15(3)
C(9)	50(3)	85(4)	70(4)	5(3)	16(3)	-2(3)
C(10)	41(2)	46(3)	49(3)	3(2)	26(2)	0(2)
C(11)	60(3)	63(4)	60(3)	-9(3)	37(3)	-15(3)
C(12)	68(4)	84(4)	95(5)	-31(4)	54(4)	-5(3)
C(13)	27(2)	33(2)	32(2)	1(2)	17(2)	-2(2)
C(14)	38(2)	44(3)	27(2)	-2(2)	14(2)	0(2)
C(15)	39(2)	39(3)	26(2)	-4(2)	16(2)	-1(2)
C(16)	30(2)	32(2)	32(2)	1(2)	19(2)	-1(2)
C(17)	46(2)	38(3)	35(2)	-2(2)	26(2)	-2(2)
C(18)	65(4)	28(3)	51(4)	0	42(4)	0
C(36)	42(3)	52(3)	55(3)	6(2)	24(2)	-7(2)
C(38)	33(2)	39(3)	43(2)	1(2)	20(2)	6(2)
C(39)	49(3)	37(3)	144(6)	7(3)	39(4)	-2(2)
C(42)	106(6)	92(5)	66(4)	-7(4)	30(4)	-11(4)
C(43)	94(6)	116(7)	91(6)	-9(5)	28(5)	-18(5)
C(44)	155(9)	125(8)	80(6)	-14(5)	8(6)	-56(7)
C(45)	99(5)	97(5)	73(4)	-24(4)	55(4)	-26(4)
N(1)	35(2)	36(2)	31(2)	0(2)	18(2)	4(2)
N(2)	29(2)	34(2)	30(2)	-1(1)	17(2)	-1(1)
N(3)	31(2)	26(3)	38(3)	0	22(2)	0
O(1)	30(1)	42(2)	39(2)	3(1)	21(1)	2(1)
O(2)	54(2)	49(2)	72(2)	12(2)	45(2)	14(2)
O(3)	40(2)	45(2)	38(2)	9(1)	21(1)	3(1)

O(7)	30(2)	32(2)	50(3)	0	16(2)	0
O(8)	102(3)	90(3)	55(2)	-19(2)	38(2)	-21(3)
F(1)	54(2)	74(2)	88(2)	1(2)	40(2)	-21(2)
F(2)	77(2)	64(2)	103(3)	-39(2)	59(2)	-24(2)
F(3)	79(2)	97(3)	48(2)	7(2)	4(2)	-40(2)
S(1)	32(1)	38(1)	38(1)	4(1)	21(1)	3(1)
Ni(1)	29(1)	31(1)	28(1)	0	15(1)	0



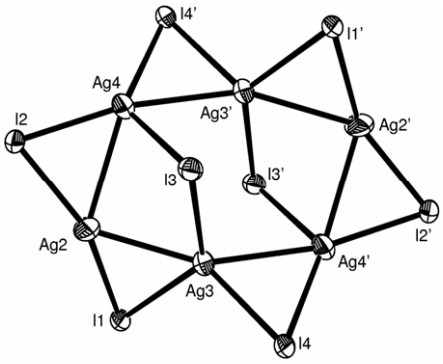


Table 1. Crystal data and structure refinement for $\mathbf{6^{Me}(Ag_6I_8)^{2-}}$.

Identification code	$\mathbf{6^{Me}(Ag_6I_8)^{2-}}$	
Empirical formula	C82 H110 Ag8 I8 N10 O2	
Formula weight	3145.96	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P21/n	
Unit cell dimensions	a = 13.6353(4) Å	α= 90°.
	b = 22.1211(6) Å	β= 98.0900(10)°.
	c = 17.0640(5) Å	γ = 90°.
Volume	5095.8(3) Å^3	
Z	2	
Density (calculated)	2.050 Mg/m^3	
Absorption coefficient	3.972 mm^{-1}	
F(000)	2976	
Crystal size	0.08 x 0.08 x 0.01 mm^3	
Theta range for data collection	3.01 to 27.63°.	
Index ranges	-17<=h<=17, -28<=k<=28, -22<=l<=22	
Reflections collected	78859	
Independent reflections	11729 [R(int) = 0.0516]	
Completeness to theta = 27.63°	98.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9614 and 0.7417	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	11729 / 6 / 508	

Goodness-of-fit on F^2	1.166
Final R indices [I>2sigma(I)]	R1 = 0.0560, wR2 = 0.1026
R indices (all data)	R1 = 0.0753, wR2 = 0.1121
Largest diff. peak and hole	2.834 and -3.554 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for $\mathbf{6^{Me}(Ag_6I_8)^{2-}}$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6926(5)	7547(3)	4828(4)	23(2)
C(2)	7505(5)	7548(3)	5572(4)	24(2)
C(3)	7671(6)	6992(4)	5945(4)	28(2)
C(4)	7272(6)	6466(4)	5601(5)	31(2)
C(5)	6665(6)	6486(3)	4881(5)	27(2)
C(6)	6485(5)	7031(3)	4475(4)	22(1)
C(7)	7924(6)	8136(3)	5956(4)	27(2)
C(8)	8074(7)	8104(4)	6865(5)	41(2)
C(9)	8899(7)	8316(4)	5684(5)	36(2)
C(10)	5765(6)	7055(3)	3698(4)	27(2)
C(11)	4701(6)	7018(4)	3882(5)	39(2)
C(12)	5973(7)	6563(4)	3122(5)	37(2)
C(13)	6060(5)	8509(3)	4373(4)	20(1)
C(14)	7458(5)	8268(3)	3851(4)	22(1)
C(15)	7102(5)	8790(3)	3515(4)	22(1)
C(16)	5672(5)	9459(3)	3619(4)	20(1)
C(17)	4661(5)	9421(3)	3304(4)	22(1)
C(18)	4213(6)	9972(3)	3099(4)	26(2)
C(19)	4708(6)	10516(3)	3198(4)	24(2)
C(20)	5698(6)	10480(3)	3526(4)	22(1)
C(21)	3843(5)	8549(3)	5816(4)	19(1)
C(22)	7139(6)	11116(3)	3305(4)	26(2)

C(23)	2488(6)	8353(3)	6409(4)	24(2)
C(24)	2955(5)	7572(3)	5471(4)	23(1)
C(25)	3434(5)	7077(3)	5854(4)	22(1)
C(26)	3232(6)	6513(3)	5503(5)	27(2)
C(27)	2588(6)	6456(3)	4812(5)	30(2)
C(28)	2146(6)	6961(4)	4437(5)	30(2)
C(29)	2333(5)	7536(3)	4745(4)	23(2)
C(30)	4172(6)	7137(4)	6606(4)	27(2)
C(31)	5218(6)	7038(5)	6419(5)	46(2)
C(32)	3937(7)	6707(4)	7258(5)	40(2)
C(33)	1869(6)	8095(4)	4333(4)	28(2)
C(34)	1777(7)	8040(4)	3439(5)	41(2)
C(35)	858(7)	8230(4)	4597(6)	39(2)
C(36)	4094(6)	8841(3)	3143(4)	26(2)
C(37)	4207(6)	11096(3)	2917(5)	29(2)
C(38)	2322(12)	9984(6)	4433(7)	86(5)
C(39)	1405(13)	9915(6)	3839(9)	96(5)
C(40)	902(13)	9996(8)	2425(10)	108(6)
C(41)	1237(14)	10244(9)	1679(11)	117(6)
N(1)	6810(4)	8108(3)	4380(3)	20(1)
N(2)	6250(4)	8927(2)	3830(3)	18(1)
N(3)	6184(5)	9969(3)	3732(3)	21(1)
N(4)	6305(5)	11010(3)	3665(3)	22(1)
N(5)	3091(5)	8155(3)	5864(3)	22(1)
Ag(1)	4947(1)	8505(1)	5091(1)	20(1)
Ag(2)	5400(1)	1558(1)	9688(1)	73(1)
Ag(3)	6020(1)	525(1)	10724(1)	40(1)
Ag(4)	4024(1)	723(1)	8661(1)	44(1)
I(1)	5880(1)	1717(1)	11246(1)	28(1)
I(2)	4272(1)	1925(1)	8355(1)	29(1)
I(3)	5880(1)	141(1)	9101(1)	33(1)
I(4)	7654(1)	-50(1)	11644(1)	31(1)
O(1)	1685(7)	10084(4)	3066(5)	75(2)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{6^{Me}(Ag_6I_8)^{2-}}$.

C(1)-C(6)	1.387(10)	C(14)-N(1)	1.395(8)
C(1)-C(2)	1.397(10)	C(14)-H(14)	0.9500
C(1)-N(1)	1.456(8)	C(15)-N(2)	1.381(9)
C(2)-C(3)	1.388(10)	C(15)-H(15)	0.9500
C(2)-C(7)	1.531(10)	C(16)-N(3)	1.326(9)
C(3)-C(4)	1.379(12)	C(16)-C(17)	1.411(10)
C(3)-H(3)	0.9500	C(16)-N(2)	1.435(9)
C(4)-C(5)	1.383(11)	C(17)-C(18)	1.386(10)
C(4)-H(4)	0.9500	C(17)-C(36)	1.503(10)
C(5)-C(6)	1.395(10)	C(18)-C(19)	1.380(10)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.535(10)	C(19)-C(20)	1.390(10)
C(7)-C(9)	1.522(11)	C(19)-C(37)	1.499(10)
C(7)-C(8)	1.537(11)	C(20)-N(3)	1.330(9)
C(7)-H(7)	1.0000	C(20)-N(4)	1.436(9)
C(8)-H(8A)	0.9800	C(21)-N(4)#1	1.351(9)
C(8)-H(8B)	0.9800	C(21)-N(5)	1.357(9)
C(8)-H(8C)	0.9800	C(21)-Ag(1)	2.082(7)
C(9)-H(9A)	0.9800	C(22)-C(23)#1	1.343(10)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.387(9)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(12)	1.520(10)	C(23)-C(22)#1	1.343(10)
C(10)-C(11)	1.529(11)	C(23)-N(5)	1.396(9)
C(10)-H(10)	1.0000	C(23)-H(23)	0.9500
C(11)-H(11A)	0.9800	C(24)-C(25)	1.389(10)
C(11)-H(11B)	0.9800	C(24)-C(29)	1.402(10)
C(11)-H(11C)	0.9800	C(24)-N(5)	1.454(9)
C(12)-H(12A)	0.9800	C(25)-C(26)	1.395(10)
C(12)-H(12B)	0.9800	C(25)-C(30)	1.521(10)
C(12)-H(12C)	0.9800	C(26)-C(27)	1.374(11)
C(13)-N(1)	1.352(9)	C(26)-H(26)	0.9500
C(13)-N(2)	1.359(8)	C(27)-C(28)	1.382(11)
C(13)-Ag(1)	2.079(7)	C(27)-H(27)	0.9500
C(14)-C(15)	1.347(10)	C(28)-C(29)	1.387(10)

C(28)-H(28)	0.9500	C(40)-H(40B)	0.9900
C(29)-C(33)	1.515(11)	C(41)-H(41A)	0.9800
C(30)-C(31)	1.521(11)	C(41)-H(41B)	0.9800
C(30)-C(32)	1.530(10)	C(41)-H(41C)	0.9800
C(30)-H(30)	1.0000	N(4)-C(21)#1	1.351(9)
C(31)-H(31A)	0.9800	Ag(2)-I(1)	2.6704(9)
C(31)-H(31B)	0.9800	Ag(2)-I(2)	2.6861(9)
C(31)-H(31C)	0.9800	Ag(2)-Ag(3)	2.9392(11)
C(32)-H(32A)	0.9800	Ag(2)-Ag(4)	3.0114(11)
C(32)-H(32B)	0.9800	Ag(3)-I(1)	2.7970(8)
C(32)-H(32C)	0.9800	Ag(3)-I(4)	2.8392(9)
C(33)-C(34)	1.519(10)	Ag(3)-I(3)	2.8776(9)
C(33)-C(35)	1.540(11)	Ag(3)-Ag(4)#2	2.9576(9)
C(33)-H(33)	1.0000	Ag(3)-I(3)#2	3.0311(9)
C(34)-H(34A)	0.9800	Ag(4)-I(4)#2	2.7193(9)
C(34)-H(34B)	0.9800	Ag(4)-I(2)	2.7399(8)
C(34)-H(34C)	0.9800	Ag(4)-I(3)	2.8437(10)
C(35)-H(35A)	0.9800	Ag(4)-Ag(3)#2	2.9576(9)
C(35)-H(35B)	0.9800	I(3)-Ag(3)#2	3.0311(9)
C(35)-H(35C)	0.9800	I(4)-Ag(4)#2	2.7193(9)
C(36)-H(36A)	0.9800		
C(36)-H(36B)	0.9800	C(6)-C(1)-C(2)	123.5(6)
C(36)-H(36C)	0.9800	C(6)-C(1)-N(1)	117.7(6)
C(37)-H(37A)	0.9800	C(2)-C(1)-N(1)	118.8(6)
C(37)-H(37B)	0.9800	C(3)-C(2)-C(1)	116.7(7)
C(37)-H(37C)	0.9800	C(3)-C(2)-C(7)	122.0(7)
C(38)-C(39)	1.502(19)	C(1)-C(2)-C(7)	121.3(6)
C(38)-H(38A)	0.9800	C(4)-C(3)-C(2)	121.5(7)
C(38)-H(38B)	0.9800	C(4)-C(3)-H(3)	119.2
C(38)-H(38C)	0.9800	C(2)-C(3)-H(3)	119.2
C(39)-O(1)	1.473(17)	C(3)-C(4)-C(5)	120.2(7)
C(39)-H(39A)	0.9900	C(3)-C(4)-H(4)	119.9
C(39)-H(39B)	0.9900	C(5)-C(4)-H(4)	119.9
C(40)-O(1)	1.430(16)	C(4)-C(5)-C(6)	120.6(7)
C(40)-C(41)	1.51(2)	C(4)-C(5)-H(5)	119.7
C(40)-H(40A)	0.9900	C(6)-C(5)-H(5)	119.7

C(1)-C(6)-C(5)	117.3(7)	C(10)-C(12)-H(12C)	109.5
C(1)-C(6)-C(10)	122.2(6)	H(12A)-C(12)-H(12C)	109.5
C(5)-C(6)-C(10)	120.3(7)	H(12B)-C(12)-H(12C)	109.5
C(9)-C(7)-C(2)	112.4(6)	N(1)-C(13)-N(2)	103.6(6)
C(9)-C(7)-C(8)	108.8(7)	N(1)-C(13)-Ag(1)	127.3(5)
C(2)-C(7)-C(8)	112.5(7)	N(2)-C(13)-Ag(1)	129.0(5)
C(9)-C(7)-H(7)	107.7	C(15)-C(14)-N(1)	105.6(6)
C(2)-C(7)-H(7)	107.7	C(15)-C(14)-H(14)	127.2
C(8)-C(7)-H(7)	107.7	N(1)-C(14)-H(14)	127.2
C(7)-C(8)-H(8A)	109.5	C(14)-C(15)-N(2)	107.1(6)
C(7)-C(8)-H(8B)	109.5	C(14)-C(15)-H(15)	126.4
H(8A)-C(8)-H(8B)	109.5	N(2)-C(15)-H(15)	126.4
C(7)-C(8)-H(8C)	109.5	N(3)-C(16)-C(17)	125.0(6)
H(8A)-C(8)-H(8C)	109.5	N(3)-C(16)-N(2)	113.8(6)
H(8B)-C(8)-H(8C)	109.5	C(17)-C(16)-N(2)	121.2(6)
C(7)-C(9)-H(9A)	109.5	C(18)-C(17)-C(16)	114.5(7)
C(7)-C(9)-H(9B)	109.5	C(18)-C(17)-C(36)	120.5(7)
H(9A)-C(9)-H(9B)	109.5	C(16)-C(17)-C(36)	124.9(7)
C(7)-C(9)-H(9C)	109.5	C(19)-C(18)-C(17)	123.1(7)
H(9A)-C(9)-H(9C)	109.5	C(19)-C(18)-H(18)	118.5
H(9B)-C(9)-H(9C)	109.5	C(17)-C(18)-H(18)	118.5
C(12)-C(10)-C(11)	111.3(7)	C(18)-C(19)-C(20)	115.5(7)
C(12)-C(10)-C(6)	112.3(6)	C(18)-C(19)-C(37)	121.0(7)
C(11)-C(10)-C(6)	109.3(6)	C(20)-C(19)-C(37)	123.5(7)
C(12)-C(10)-H(10)	107.9	N(3)-C(20)-C(19)	125.1(7)
C(11)-C(10)-H(10)	107.9	N(3)-C(20)-N(4)	113.4(6)
C(6)-C(10)-H(10)	107.9	C(19)-C(20)-N(4)	121.5(7)
C(10)-C(11)-H(11A)	109.5	N(4)#1-C(21)-N(5)	103.9(6)
C(10)-C(11)-H(11B)	109.5	N(4)#1-C(21)-Ag(1)	127.7(5)
H(11A)-C(11)-H(11B)	109.5	N(5)-C(21)-Ag(1)	128.4(5)
C(10)-C(11)-H(11C)	109.5	C(23)#1-C(22)-N(4)	106.2(6)
H(11A)-C(11)-H(11C)	109.5	C(23)#1-C(22)-H(22)	126.9
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	126.9
C(10)-C(12)-H(12A)	109.5	C(22)#1-C(23)-N(5)	106.7(6)
C(10)-C(12)-H(12B)	109.5	C(22)#1-C(23)-H(23)	126.6
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.6

C(25)-C(24)-C(29)	123.8(7)	C(29)-C(33)-C(34)	111.8(7)
C(25)-C(24)-N(5)	117.5(6)	C(29)-C(33)-C(35)	110.8(6)
C(29)-C(24)-N(5)	118.7(6)	C(34)-C(33)-C(35)	111.0(7)
C(24)-C(25)-C(26)	116.9(7)	C(29)-C(33)-H(33)	107.7
C(24)-C(25)-C(30)	122.7(6)	C(34)-C(33)-H(33)	107.7
C(26)-C(25)-C(30)	120.5(7)	C(35)-C(33)-H(33)	107.7
C(27)-C(26)-C(25)	121.0(7)	C(33)-C(34)-H(34A)	109.5
C(27)-C(26)-H(26)	119.5	C(33)-C(34)-H(34B)	109.5
C(25)-C(26)-H(26)	119.5	H(34A)-C(34)-H(34B)	109.5
C(26)-C(27)-C(28)	120.5(7)	C(33)-C(34)-H(34C)	109.5
C(26)-C(27)-H(27)	119.8	H(34A)-C(34)-H(34C)	109.5
C(28)-C(27)-H(27)	119.8	H(34B)-C(34)-H(34C)	109.5
C(27)-C(28)-C(29)	121.4(7)	C(33)-C(35)-H(35A)	109.5
C(27)-C(28)-H(28)	119.3	C(33)-C(35)-H(35B)	109.5
C(29)-C(28)-H(28)	119.3	H(35A)-C(35)-H(35B)	109.5
C(28)-C(29)-C(24)	116.3(7)	C(33)-C(35)-H(35C)	109.5
C(28)-C(29)-C(33)	122.0(7)	H(35A)-C(35)-H(35C)	109.5
C(24)-C(29)-C(33)	121.7(6)	H(35B)-C(35)-H(35C)	109.5
C(25)-C(30)-C(31)	109.8(6)	C(17)-C(36)-H(36A)	109.5
C(25)-C(30)-C(32)	112.2(6)	C(17)-C(36)-H(36B)	109.5
C(31)-C(30)-C(32)	111.2(7)	H(36A)-C(36)-H(36B)	109.5
C(25)-C(30)-H(30)	107.8	C(17)-C(36)-H(36C)	109.5
C(31)-C(30)-H(30)	107.8	H(36A)-C(36)-H(36C)	109.5
C(32)-C(30)-H(30)	107.8	H(36B)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31A)	109.5	C(19)-C(37)-H(37A)	109.5
C(30)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37B)	109.5
H(31A)-C(31)-H(31B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(30)-C(31)-H(31C)	109.5	C(19)-C(37)-H(37C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32A)	109.5	C(39)-C(38)-H(38A)	109.5
C(30)-C(32)-H(32B)	109.5	C(39)-C(38)-H(38B)	109.5
H(32A)-C(32)-H(32B)	109.5	H(38A)-C(38)-H(38B)	109.5
C(30)-C(32)-H(32C)	109.5	C(39)-C(38)-H(38C)	109.5
H(32A)-C(32)-H(32C)	109.5	H(38A)-C(38)-H(38C)	109.5
H(32B)-C(32)-H(32C)	109.5	H(38B)-C(38)-H(38C)	109.5

O(1)-C(39)-C(38)	106.4(13)	I(2)-Ag(2)-Ag(4)	57.14(2)
O(1)-C(39)-H(39A)	110.4	Ag(3)-Ag(2)-Ag(4)	88.66(3)
C(38)-C(39)-H(39A)	110.4	I(1)-Ag(3)-I(4)	109.23(3)
O(1)-C(39)-H(39B)	110.4	I(1)-Ag(3)-I(3)	125.89(3)
C(38)-C(39)-H(39B)	110.4	I(4)-Ag(3)-I(3)	109.90(3)
H(39A)-C(39)-H(39B)	108.6	I(1)-Ag(3)-Ag(2)	55.42(2)
O(1)-C(40)-C(41)	108.2(14)	I(4)-Ag(3)-Ag(2)	144.85(4)
O(1)-C(40)-H(40A)	110.1	I(3)-Ag(3)-Ag(2)	71.08(3)
C(41)-C(40)-H(40A)	110.1	I(1)-Ag(3)-Ag(4)#2	139.60(3)
O(1)-C(40)-H(40B)	110.1	I(4)-Ag(3)-Ag(4)#2	55.91(2)
C(41)-C(40)-H(40B)	110.1	I(3)-Ag(3)-Ag(4)#2	93.64(3)
H(40A)-C(40)-H(40B)	108.4	Ag(2)-Ag(3)-Ag(4)#2	156.98(3)
C(40)-C(41)-H(41A)	109.5	I(1)-Ag(3)-I(3)#2	109.25(3)
C(40)-C(41)-H(41B)	109.5	I(4)-Ag(3)-I(3)#2	110.06(3)
H(41A)-C(41)-H(41B)	109.5	I(3)-Ag(3)-I(3)#2	90.51(2)
C(40)-C(41)-H(41C)	109.5	Ag(2)-Ag(3)-I(3)#2	105.04(3)
H(41A)-C(41)-H(41C)	109.5	Ag(4)#2-Ag(3)-I(3)#2	56.68(2)
H(41B)-C(41)-H(41C)	109.5	I(4)#2-Ag(4)-I(2)	128.17(3)
C(13)-N(1)-C(14)	112.1(6)	I(4)#2-Ag(4)-I(3)	119.73(3)
C(13)-N(1)-C(1)	126.1(6)	I(2)-Ag(4)-I(3)	111.16(3)
C(14)-N(1)-C(1)	121.7(6)	I(4)#2-Ag(4)-Ag(3)#2	59.84(2)
C(13)-N(2)-C(15)	111.6(6)	I(2)-Ag(4)-Ag(3)#2	169.43(3)
C(13)-N(2)-C(16)	125.4(6)	I(3)-Ag(4)-Ag(3)#2	62.96(2)
C(15)-N(2)-C(16)	123.0(6)	I(4)#2-Ag(4)-Ag(2)	152.36(4)
C(16)-N(3)-C(20)	116.8(6)	I(2)-Ag(4)-Ag(2)	55.44(2)
C(21)#1-N(4)-C(22)	112.0(6)	I(3)-Ag(4)-Ag(2)	70.49(3)
C(21)#1-N(4)-C(20)	124.2(6)	Ag(3)#2-Ag(4)-Ag(2)	114.11(3)
C(22)-N(4)-C(20)	123.7(6)	Ag(2)-I(1)-Ag(3)	64.99(3)
C(21)-N(5)-C(23)	111.1(6)	Ag(2)-I(2)-Ag(4)	67.41(3)
C(21)-N(5)-C(24)	126.2(6)	Ag(4)-I(3)-Ag(3)	93.24(3)
C(23)-N(5)-C(24)	122.5(6)	Ag(4)-I(3)-Ag(3)#2	60.35(2)
C(13)-Ag(1)-C(21)	177.0(3)	Ag(3)-I(3)-Ag(3)#2	89.49(2)
I(1)-Ag(2)-I(2)	146.54(5)	Ag(4)#2-I(4)-Ag(3)	64.25(2)
I(1)-Ag(2)-Ag(3)	59.59(2)	C(40)-O(1)-C(39)	113.0(12)
I(2)-Ag(2)-Ag(3)	145.76(4)		
I(1)-Ag(2)-Ag(4)	134.86(4)		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+2,-z+1 #2 -x+1,-y,-z+2

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $\mathbf{6^{Me}(Ag_6I_8)^{2-}}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(4)	20(3)	23(3)	6(3)	1(3)	4(3)
C(2)	23(4)	22(4)	28(4)	-1(3)	9(3)	5(3)
C(3)	31(4)	31(4)	22(3)	9(3)	2(3)	5(3)
C(4)	29(4)	27(4)	39(4)	15(3)	7(3)	10(3)
C(5)	31(4)	21(4)	32(4)	4(3)	11(3)	7(3)
C(6)	25(4)	19(3)	23(3)	2(3)	8(3)	5(3)
C(7)	26(4)	24(4)	29(4)	2(3)	-1(3)	6(3)
C(8)	51(6)	41(5)	28(4)	-2(4)	-8(4)	13(4)
C(9)	39(5)	27(4)	41(5)	-5(4)	2(4)	-6(4)
C(10)	31(4)	21(4)	27(4)	-2(3)	4(3)	-2(3)
C(11)	28(4)	55(6)	32(4)	-7(4)	3(3)	2(4)
C(12)	40(5)	39(5)	34(4)	-8(4)	8(4)	7(4)
C(13)	20(3)	16(3)	24(3)	2(3)	5(3)	-2(3)
C(14)	24(4)	22(3)	21(3)	2(3)	8(3)	2(3)
C(15)	24(4)	25(4)	19(3)	2(3)	10(3)	-1(3)
C(16)	24(4)	20(3)	19(3)	2(3)	7(3)	3(3)
C(17)	24(4)	25(4)	18(3)	-3(3)	2(3)	-4(3)
C(18)	23(4)	25(4)	28(4)	3(3)	4(3)	2(3)
C(19)	33(4)	21(3)	18(3)	-1(3)	3(3)	1(3)
C(20)	29(4)	22(3)	16(3)	0(3)	5(3)	-5(3)
C(21)	22(4)	17(3)	20(3)	3(3)	7(3)	-1(3)
C(22)	30(4)	20(3)	28(4)	-7(3)	8(3)	1(3)
C(23)	24(4)	23(4)	27(4)	1(3)	11(3)	-3(3)
C(24)	21(4)	19(3)	29(4)	-4(3)	7(3)	-1(3)

C(25)	24(4)	20(3)	22(3)	-1(3)	8(3)	-5(3)
C(26)	29(4)	19(3)	34(4)	-1(3)	5(3)	1(3)
C(27)	41(5)	20(4)	29(4)	-8(3)	7(3)	1(3)
C(28)	25(4)	33(4)	32(4)	-4(3)	2(3)	-9(3)
C(29)	19(3)	26(4)	26(4)	-4(3)	8(3)	-4(3)
C(30)	31(4)	27(4)	22(3)	0(3)	1(3)	-4(3)
C(31)	27(5)	79(7)	32(4)	8(5)	7(4)	-2(5)
C(32)	48(5)	44(5)	27(4)	8(4)	7(4)	-14(4)
C(33)	32(4)	27(4)	23(4)	-2(3)	-2(3)	-4(3)
C(34)	49(6)	44(5)	27(4)	5(4)	-3(4)	1(4)
C(35)	36(5)	34(5)	47(5)	-2(4)	9(4)	5(4)
C(36)	27(4)	24(4)	27(4)	-1(3)	6(3)	-5(3)
C(37)	34(4)	21(4)	30(4)	1(3)	0(3)	2(3)
C(38)	119(13)	73(9)	55(7)	8(7)	-23(8)	3(9)
C(39)	130(14)	47(7)	101(12)	19(7)	-11(10)	-10(8)
C(40)	89(12)	100(12)	119(14)	16(11)	-36(10)	-22(10)
C(41)	115(9)	139(10)	99(9)	8(8)	19(7)	34(8)
N(1)	21(3)	16(3)	26(3)	5(2)	9(2)	-1(2)
N(2)	21(3)	16(3)	19(3)	3(2)	5(2)	2(2)
N(3)	28(3)	15(3)	19(3)	2(2)	3(2)	-3(2)
N(4)	29(3)	17(3)	19(3)	-1(2)	4(2)	2(2)
N(5)	25(3)	21(3)	21(3)	0(2)	5(2)	-1(2)
Ag(1)	24(1)	18(1)	20(1)	0(1)	6(1)	0(1)
Ag(2)	112(1)	60(1)	37(1)	18(1)	-31(1)	-36(1)
Ag(3)	48(1)	24(1)	45(1)	-2(1)	-6(1)	2(1)
Ag(4)	58(1)	31(1)	41(1)	3(1)	0(1)	-13(1)
I(1)	32(1)	24(1)	27(1)	-2(1)	2(1)	0(1)
I(2)	33(1)	24(1)	29(1)	3(1)	1(1)	2(1)
I(3)	36(1)	34(1)	29(1)	-2(1)	4(1)	-6(1)
I(4)	38(1)	22(1)	32(1)	-3(1)	0(1)	2(1)
O(1)	63(5)	90(7)	73(6)	6(5)	12(5)	8(5)

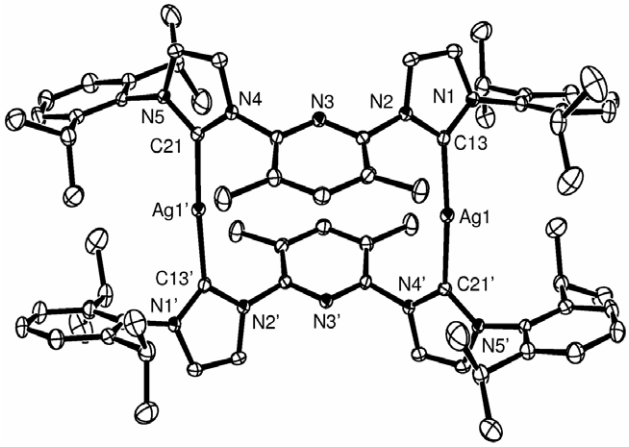


Table 1. Crystal data and structure refinement for $\mathbf{6^{Me}(OTf)^-_2}$.

Identification code	$\mathbf{6^{Me}(OTf)^-_2}$	
Empirical formula	C84 H106 Ag2 F6 N10 O8 S2	
Formula weight	1777.65	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.7012(3) Å	α= 89.4130(10)°.
	b = 13.0999(3) Å	β= 74.8100(10)°.
	c = 13.2765(3) Å	γ = 80.2370(10)°.
Volume	2099.59(8) $Å^3$	
Z	1	
Density (calculated)	1.406 Mg/m^3	
Absorption coefficient	0.590 mm^{-1}	
F(000)	924	
Crystal size	0.24 x 0.24 x 0.20 mm^3	
Theta range for data collection	3.31 to 27.54°.	
Index ranges	-16<=h<=16, -17<=k<=17, -16<=l<=17	
Reflections collected	42521	
Independent reflections	9617 [R(int) = 0.0435]	
Completeness to theta = 27.54°	99.3 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.8912 and 0.8714	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9617 / 0 / 516	

Goodness-of-fit on F^2	1.055
Final R indices [I>2sigma(I)]	R1 = 0.0381, wR2 = 0.0889
R indices (all data)	R1 = 0.0476, wR2 = 0.0932
Largest diff. peak and hole	1.357 and -0.634 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **6^{Me}(OTf)$^-_2$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7082(2)	2892(2)	2754(2)	18(1)
C(2)	7129(2)	3951(2)	2669(2)	22(1)
C(3)	6978(2)	4414(2)	1755(2)	27(1)
C(4)	6781(2)	3847(2)	974(2)	27(1)
C(5)	6747(2)	2796(2)	1073(2)	25(1)
C(6)	6906(2)	2289(2)	1968(2)	20(1)
C(7)	7316(2)	4603(2)	3529(2)	27(1)
C(8)	6423(4)	5561(3)	3823(3)	54(1)
C(9)	8481(3)	4884(3)	3196(3)	43(1)
C(10)	6833(2)	1142(2)	2064(2)	24(1)
C(11)	5625(3)	988(2)	2260(3)	37(1)
C(12)	7546(3)	504(2)	1083(2)	34(1)
C(13)	8024(2)	2160(2)	4112(2)	15(1)
C(14)	6147(2)	2376(2)	4520(2)	21(1)
C(15)	6444(2)	2060(2)	5391(2)	20(1)
C(16)	8213(2)	1611(2)	5877(2)	14(1)
C(17)	8918(2)	2212(2)	6135(2)	18(1)
C(18)	9438(2)	1813(2)	6891(2)	20(1)
C(19)	9225(2)	901(2)	7391(2)	18(1)
C(20)	8454(2)	418(2)	7088(2)	15(1)
C(21)	8656(2)	-1429(2)	7575(2)	15(1)
C(22)	7010(2)	-384(2)	8307(2)	19(1)
C(23)	6944(2)	-1336(2)	8687(2)	18(1)
C(24)	8165(2)	-3064(2)	8403(2)	16(1)

C(25)	7803(2)	-3732(2)	7802(2)	20(1)
C(26)	7981(2)	-4783(2)	8000(2)	25(1)
C(27)	8483(2)	-5146(2)	8771(2)	26(1)
C(28)	8807(2)	-4462(2)	9368(2)	25(1)
C(29)	8657(2)	-3402(2)	9204(2)	18(1)
C(30)	7239(2)	-3335(2)	6959(2)	24(1)
C(31)	8075(3)	-3485(3)	5895(2)	46(1)
C(32)	6237(3)	-3838(3)	6963(3)	50(1)
C(33)	9023(2)	-2656(2)	9861(2)	22(1)
C(34)	10254(2)	-2621(2)	9425(2)	32(1)
C(35)	8789(2)	-2927(2)	11012(2)	30(1)
C(36)	9054(2)	3261(2)	5694(2)	26(1)
C(37)	9764(3)	494(2)	8235(2)	29(1)
C(75)	4217(3)	6702(2)	1670(2)	37(1)
C(77)	3256(3)	868(2)	4638(3)	37(1)
C(78)	2237(3)	831(3)	5523(3)	52(1)
C(79)	2431(4)	1434(3)	6414(3)	56(1)
C(80)	3670(4)	1480(3)	6021(3)	60(1)
N(1)	7117(2)	2431(2)	3749(2)	16(1)
N(2)	7594(2)	1941(2)	5130(2)	15(1)
N(3)	7964(2)	743(2)	6344(2)	15(1)
N(4)	8066(2)	-458(2)	7635(2)	15(1)
N(5)	7954(2)	-1963(1)	8226(2)	15(1)
O(1)	4679(2)	8385(2)	2258(2)	35(1)
O(2)	4802(2)	8141(2)	437(2)	43(1)
O(3)	6177(2)	7141(2)	1190(3)	72(1)
O(7)	3848(2)	1592(2)	4907(2)	55(1)
F(1)	4521(2)	5924(2)	960(2)	54(1)
F(2)	4256(3)	6295(2)	2579(2)	79(1)
F(3)	3162(2)	7086(2)	1729(2)	58(1)
S(1)	5079(1)	7701(1)	1349(1)	26(1)
Ag(1)	9690(1)	1885(1)	3272(1)	16(1)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{6^{Me}(OTf)^-_2}$.

C(1)-C(6)	1.399(3)	C(14)-N(1)	1.393(3)
C(1)-C(2)	1.401(3)	C(14)-H(14)	0.9500
C(1)-N(1)	1.455(3)	C(15)-N(2)	1.392(3)
C(2)-C(3)	1.395(3)	C(15)-H(15)	0.9500
C(2)-C(7)	1.523(4)	C(16)-N(3)	1.335(3)
C(3)-C(4)	1.380(4)	C(16)-C(17)	1.395(3)
C(3)-H(3)	0.9500	C(16)-N(2)	1.439(3)
C(4)-C(5)	1.388(4)	C(17)-C(18)	1.391(3)
C(4)-H(4)	0.9500	C(17)-C(36)	1.507(3)
C(5)-C(6)	1.399(3)	C(18)-C(19)	1.393(3)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.524(4)	C(19)-C(20)	1.395(3)
C(7)-C(8)	1.519(4)	C(19)-C(37)	1.508(3)
C(7)-C(9)	1.536(4)	C(20)-N(3)	1.329(3)
C(7)-H(7)	1.0000	C(20)-N(4)	1.439(3)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.352(3)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.355(3)
C(8)-H(8C)	0.9800	C(21)-Ag(1)#1	2.094(2)
C(9)-H(9A)	0.9800	C(22)-C(23)	1.347(3)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.392(3)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(11)	1.535(4)	C(23)-N(5)	1.391(3)
C(10)-C(12)	1.537(4)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.398(3)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.402(3)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.449(3)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.392(3)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.522(3)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.383(4)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(1)	1.354(3)	C(27)-C(28)	1.382(4)
C(13)-N(2)	1.366(3)	C(27)-H(27)	0.9500
C(13)-Ag(1)	2.089(2)	C(28)-C(29)	1.392(3)
C(14)-C(15)	1.348(3)	C(28)-H(28)	0.9500

C(29)-C(33)	1.523(3)	C(79)-C(80)	1.534(6)
C(30)-C(31)	1.521(4)	C(79)-H(79A)	0.9900
C(30)-C(32)	1.527(4)	C(79)-H(79B)	0.9900
C(30)-H(30)	1.0000	C(80)-O(7)	1.446(5)
C(31)-H(31A)	0.9800	C(80)-H(80A)	0.9900
C(31)-H(31B)	0.9800	C(80)-H(80B)	0.9900
C(31)-H(31C)	0.9800	O(1)-S(1)	1.437(2)
C(32)-H(32A)	0.9800	O(2)-S(1)	1.435(2)
C(32)-H(32B)	0.9800	O(3)-S(1)	1.425(2)
C(32)-H(32C)	0.9800	Ag(1)-C(21)#1	2.094(2)
C(33)-C(34)	1.526(4)		
C(33)-C(35)	1.528(4)	C(6)-C(1)-C(2)	123.3(2)
C(33)-H(33)	1.0000	C(6)-C(1)-N(1)	119.1(2)
C(34)-H(34A)	0.9800	C(2)-C(1)-N(1)	117.4(2)
C(34)-H(34B)	0.9800	C(3)-C(2)-C(1)	117.3(2)
C(34)-H(34C)	0.9800	C(3)-C(2)-C(7)	119.7(2)
C(35)-H(35A)	0.9800	C(1)-C(2)-C(7)	123.0(2)
C(35)-H(35B)	0.9800	C(4)-C(3)-C(2)	120.9(2)
C(35)-H(35C)	0.9800	C(4)-C(3)-H(3)	119.5
C(36)-H(36A)	0.9800	C(2)-C(3)-H(3)	119.5
C(36)-H(36B)	0.9800	C(3)-C(4)-C(5)	120.6(2)
C(36)-H(36C)	0.9800	C(3)-C(4)-H(4)	119.7
C(37)-H(37A)	0.9800	C(5)-C(4)-H(4)	119.7
C(37)-H(37B)	0.9800	C(4)-C(5)-C(6)	120.9(2)
C(37)-H(37C)	0.9800	C(4)-C(5)-H(5)	119.6
C(75)-F(2)	1.324(3)	C(6)-C(5)-H(5)	119.6
C(75)-F(3)	1.331(4)	C(5)-C(6)-C(1)	117.0(2)
C(75)-F(1)	1.331(4)	C(5)-C(6)-C(10)	119.5(2)
C(75)-S(1)	1.823(3)	C(1)-C(6)-C(10)	123.5(2)
C(77)-O(7)	1.409(4)	C(8)-C(7)-C(2)	111.2(2)
C(77)-C(78)	1.509(5)	C(8)-C(7)-C(9)	111.8(3)
C(77)-H(77A)	0.9900	C(2)-C(7)-C(9)	110.1(2)
C(77)-H(77B)	0.9900	C(8)-C(7)-H(7)	107.8
C(78)-C(79)	1.524(5)	C(2)-C(7)-H(7)	107.8
C(78)-H(78A)	0.9900	C(9)-C(7)-H(7)	107.8
C(78)-H(78B)	0.9900	C(7)-C(8)-H(8A)	109.5

C(7)-C(8)-H(8B)	109.5	C(14)-C(15)-H(15)	127.1
H(8A)-C(8)-H(8B)	109.5	N(2)-C(15)-H(15)	127.1
C(7)-C(8)-H(8C)	109.5	N(3)-C(16)-C(17)	124.8(2)
H(8A)-C(8)-H(8C)	109.5	N(3)-C(16)-N(2)	113.38(19)
H(8B)-C(8)-H(8C)	109.5	C(17)-C(16)-N(2)	121.6(2)
C(7)-C(9)-H(9A)	109.5	C(18)-C(17)-C(16)	115.5(2)
C(7)-C(9)-H(9B)	109.5	C(18)-C(17)-C(36)	121.4(2)
H(9A)-C(9)-H(9B)	109.5	C(16)-C(17)-C(36)	123.0(2)
C(7)-C(9)-H(9C)	109.5	C(17)-C(18)-C(19)	122.1(2)
H(9A)-C(9)-H(9C)	109.5	C(17)-C(18)-H(18)	118.9
H(9B)-C(9)-H(9C)	109.5	C(19)-C(18)-H(18)	118.9
C(6)-C(10)-C(11)	110.3(2)	C(18)-C(19)-C(20)	115.6(2)
C(6)-C(10)-C(12)	111.8(2)	C(18)-C(19)-C(37)	121.7(2)
C(11)-C(10)-C(12)	109.5(2)	C(20)-C(19)-C(37)	122.6(2)
C(6)-C(10)-H(10)	108.4	N(3)-C(20)-C(19)	124.7(2)
C(11)-C(10)-H(10)	108.4	N(3)-C(20)-N(4)	114.4(2)
C(12)-C(10)-H(10)	108.4	C(19)-C(20)-N(4)	120.7(2)
C(10)-C(11)-H(11A)	109.5	N(5)-C(21)-N(4)	103.72(19)
C(10)-C(11)-H(11B)	109.5	N(5)-C(21)-Ag(1)#1	130.72(16)
H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-Ag(1)#1	125.42(17)
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	106.0(2)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	127.0
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	127.0
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	106.6(2)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	126.7
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.7
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	123.1(2)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	117.9(2)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	118.8(2)
N(1)-C(13)-N(2)	103.55(19)	C(26)-C(25)-C(24)	117.4(2)
N(1)-C(13)-Ag(1)	128.58(17)	C(26)-C(25)-C(30)	120.7(2)
N(2)-C(13)-Ag(1)	127.11(16)	C(24)-C(25)-C(30)	121.9(2)
C(15)-C(14)-N(1)	107.1(2)	C(27)-C(26)-C(25)	120.9(2)
C(15)-C(14)-H(14)	126.4	C(27)-C(26)-H(26)	119.5
N(1)-C(14)-H(14)	126.4	C(25)-C(26)-H(26)	119.5
C(14)-C(15)-N(2)	105.8(2)	C(28)-C(27)-C(26)	120.2(2)

C(28)-C(27)-H(27)	119.9	H(34A)-C(34)-H(34C)	109.5
C(26)-C(27)-H(27)	119.9	H(34B)-C(34)-H(34C)	109.5
C(27)-C(28)-C(29)	121.6(2)	C(33)-C(35)-H(35A)	109.5
C(27)-C(28)-H(28)	119.2	C(33)-C(35)-H(35B)	109.5
C(29)-C(28)-H(28)	119.2	H(35A)-C(35)-H(35B)	109.5
C(28)-C(29)-C(24)	116.7(2)	C(33)-C(35)-H(35C)	109.5
C(28)-C(29)-C(33)	121.2(2)	H(35A)-C(35)-H(35C)	109.5
C(24)-C(29)-C(33)	122.1(2)	H(35B)-C(35)-H(35C)	109.5
C(31)-C(30)-C(25)	109.8(2)	C(17)-C(36)-H(36A)	109.5
C(31)-C(30)-C(32)	110.8(3)	C(17)-C(36)-H(36B)	109.5
C(25)-C(30)-C(32)	113.1(2)	H(36A)-C(36)-H(36B)	109.5
C(31)-C(30)-H(30)	107.7	C(17)-C(36)-H(36C)	109.5
C(25)-C(30)-H(30)	107.7	H(36A)-C(36)-H(36C)	109.5
C(32)-C(30)-H(30)	107.7	H(36B)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31A)	109.5	C(19)-C(37)-H(37A)	109.5
C(30)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37B)	109.5
H(31A)-C(31)-H(31B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(30)-C(31)-H(31C)	109.5	C(19)-C(37)-H(37C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32A)	109.5	F(2)-C(75)-F(3)	107.6(3)
C(30)-C(32)-H(32B)	109.5	F(2)-C(75)-F(1)	107.0(3)
H(32A)-C(32)-H(32B)	109.5	F(3)-C(75)-F(1)	106.6(3)
C(30)-C(32)-H(32C)	109.5	F(2)-C(75)-S(1)	111.5(2)
H(32A)-C(32)-H(32C)	109.5	F(3)-C(75)-S(1)	111.1(2)
H(32B)-C(32)-H(32C)	109.5	F(1)-C(75)-S(1)	112.7(2)
C(29)-C(33)-C(34)	110.4(2)	O(7)-C(77)-C(78)	109.0(3)
C(29)-C(33)-C(35)	112.8(2)	O(7)-C(77)-H(77A)	109.9
C(34)-C(33)-C(35)	109.8(2)	C(78)-C(77)-H(77A)	109.9
C(29)-C(33)-H(33)	107.9	O(7)-C(77)-H(77B)	109.9
C(34)-C(33)-H(33)	107.9	C(78)-C(77)-H(77B)	109.9
C(35)-C(33)-H(33)	107.9	H(77A)-C(77)-H(77B)	108.3
C(33)-C(34)-H(34A)	109.5	C(77)-C(78)-C(79)	103.6(3)
C(33)-C(34)-H(34B)	109.5	C(77)-C(78)-H(78A)	111.0
H(34A)-C(34)-H(34B)	109.5	C(79)-C(78)-H(78A)	111.0
C(33)-C(34)-H(34C)	109.5	C(77)-C(78)-H(78B)	111.0

C(79)-C(78)-H(78B)	111.0
H(78A)-C(78)-H(78B)	109.0
C(78)-C(79)-C(80)	101.9(3)
C(78)-C(79)-H(79A)	111.4
C(80)-C(79)-H(79A)	111.4
C(78)-C(79)-H(79B)	111.4
C(80)-C(79)-H(79B)	111.4
H(79A)-C(79)-H(79B)	109.3
O(7)-C(80)-C(79)	104.0(3)
O(7)-C(80)-H(80A)	111.0
C(79)-C(80)-H(80A)	111.0
O(7)-C(80)-H(80B)	111.0
C(79)-C(80)-H(80B)	111.0
H(80A)-C(80)-H(80B)	109.0
C(13)-N(1)-C(14)	111.50(19)
C(13)-N(1)-C(1)	126.7(2)
C(14)-N(1)-C(1)	121.05(19)
C(13)-N(2)-C(15)	112.00(19)
C(13)-N(2)-C(16)	126.33(19)
C(15)-N(2)-C(16)	121.67(19)
C(20)-N(3)-C(16)	117.2(2)
C(21)-N(4)-C(22)	111.95(19)
C(21)-N(4)-C(20)	125.71(19)
C(22)-N(4)-C(20)	122.33(19)
C(21)-N(5)-C(23)	111.69(19)
C(21)-N(5)-C(24)	125.92(19)
C(23)-N(5)-C(24)	122.31(19)
C(77)-O(7)-C(80)	102.7(3)
O(3)-S(1)-O(2)	115.89(18)
O(3)-S(1)-O(1)	115.67(16)
O(2)-S(1)-O(1)	113.56(14)
O(3)-S(1)-C(75)	103.65(17)
O(2)-S(1)-C(75)	102.93(13)
O(1)-S(1)-C(75)	102.62(13)
C(13)-Ag(1)-C(21)#1	173.42(9)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2,-y,-z+1

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **$6^{Me}(OTf)^-_2$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(1)	25(1)	13(1)	7(1)	-4(1)	-2(1)
C(2)	25(1)	23(1)	18(1)	5(1)	-6(1)	-3(1)
C(3)	35(2)	25(1)	23(1)	10(1)	-10(1)	-6(1)
C(4)	31(2)	34(1)	18(1)	13(1)	-11(1)	-7(1)
C(5)	28(1)	34(1)	16(1)	5(1)	-9(1)	-6(1)
C(6)	17(1)	27(1)	19(1)	6(1)	-6(1)	-4(1)
C(7)	42(2)	22(1)	20(1)	4(1)	-12(1)	-5(1)
C(8)	74(3)	41(2)	45(2)	-12(2)	-29(2)	15(2)
C(9)	57(2)	49(2)	31(2)	4(1)	-14(2)	-29(2)
C(10)	29(1)	25(1)	22(1)	3(1)	-11(1)	-7(1)
C(11)	35(2)	38(2)	40(2)	6(1)	-9(1)	-16(1)
C(12)	42(2)	30(2)	31(2)	-2(1)	-14(1)	-1(1)
C(13)	16(1)	14(1)	14(1)	3(1)	-2(1)	-2(1)
C(14)	13(1)	31(1)	18(1)	7(1)	-4(1)	-3(1)
C(15)	13(1)	27(1)	19(1)	5(1)	-1(1)	-4(1)
C(16)	13(1)	17(1)	11(1)	2(1)	-1(1)	0(1)
C(17)	18(1)	17(1)	17(1)	3(1)	-2(1)	-4(1)
C(18)	21(1)	20(1)	21(1)	2(1)	-7(1)	-7(1)
C(19)	20(1)	21(1)	15(1)	3(1)	-6(1)	-3(1)
C(20)	16(1)	14(1)	13(1)	4(1)	-2(1)	-2(1)
C(21)	14(1)	19(1)	12(1)	3(1)	-2(1)	-2(1)
C(22)	15(1)	22(1)	18(1)	3(1)	-2(1)	-2(1)
C(23)	13(1)	23(1)	16(1)	2(1)	-1(1)	-2(1)
C(24)	14(1)	14(1)	18(1)	6(1)	-2(1)	-2(1)

C(25)	20(1)	21(1)	19(1)	5(1)	-6(1)	-2(1)
C(26)	29(1)	21(1)	27(1)	1(1)	-9(1)	-5(1)
C(27)	31(2)	16(1)	33(1)	7(1)	-10(1)	-3(1)
C(28)	26(1)	22(1)	28(1)	9(1)	-14(1)	-1(1)
C(29)	16(1)	21(1)	17(1)	3(1)	-3(1)	-3(1)
C(30)	29(1)	20(1)	25(1)	4(1)	-14(1)	-5(1)
C(31)	50(2)	61(2)	26(2)	6(2)	-13(2)	-1(2)
C(32)	39(2)	62(2)	63(2)	27(2)	-32(2)	-18(2)
C(33)	25(1)	22(1)	22(1)	5(1)	-11(1)	-6(1)
C(34)	33(2)	44(2)	24(1)	6(1)	-11(1)	-18(1)
C(35)	32(2)	39(2)	20(1)	2(1)	-7(1)	-11(1)
C(36)	39(2)	19(1)	26(1)	6(1)	-13(1)	-12(1)
C(37)	39(2)	29(1)	26(1)	8(1)	-21(1)	-12(1)
C(75)	53(2)	32(2)	29(2)	7(1)	-16(2)	-10(1)
C(77)	35(2)	35(2)	41(2)	-1(1)	-2(1)	-13(1)
C(78)	52(2)	62(2)	39(2)	-17(2)	5(2)	-27(2)
C(79)	95(3)	37(2)	25(2)	-8(1)	7(2)	-15(2)
C(80)	70(3)	58(2)	70(3)	14(2)	-48(2)	-17(2)
N(1)	15(1)	21(1)	13(1)	5(1)	-4(1)	-3(1)
N(2)	14(1)	17(1)	13(1)	3(1)	-3(1)	-2(1)
N(3)	14(1)	16(1)	13(1)	2(1)	-2(1)	-2(1)
N(4)	15(1)	15(1)	14(1)	4(1)	-4(1)	-3(1)
N(5)	14(1)	15(1)	14(1)	4(1)	-1(1)	-2(1)
O(1)	53(1)	30(1)	21(1)	2(1)	-2(1)	-12(1)
O(2)	54(2)	59(1)	23(1)	15(1)	-11(1)	-27(1)
O(3)	27(1)	69(2)	117(3)	-22(2)	-25(2)	10(1)
O(7)	53(2)	64(2)	51(2)	4(1)	-9(1)	-25(1)
F(1)	72(2)	37(1)	58(1)	-13(1)	-29(1)	-6(1)
F(2)	167(3)	51(1)	50(1)	31(1)	-57(2)	-57(2)
F(3)	34(1)	58(1)	78(2)	3(1)	1(1)	-19(1)
S(1)	21(1)	30(1)	23(1)	0(1)	-4(1)	-1(1)
Ag(1)	14(1)	18(1)	14(1)	3(1)	-2(1)	-2(1)

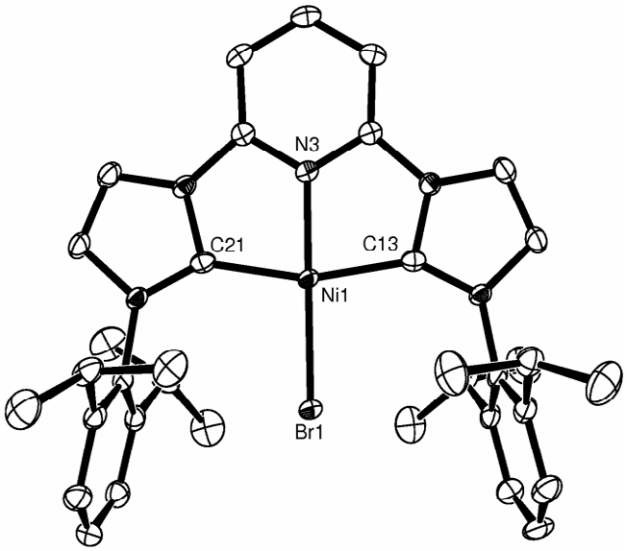


Table 1. Crystal data and structure refinement for **3(PF$_6$)$^-$**.

Identification code	**3(PF$_6$)$^-$**	
Empirical formula	C35 H41 Br F6 N5 Ni P	
Formula weight	815.32	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 35.7904(8) Å	α= 90°.
	b = 8.6403(2) Å	β= 99.3100(10)°.
	c = 23.4502(5) Å	γ = 90°.
Volume	7156.2(3) Å^3	
Z	8	
Density (calculated)	1.514 Mg/m^3	
Absorption coefficient	1.768 mm^{-1}	
F(000)	3344	
Crystal size	0.12 x 0.12 x 0.04 mm^3	
Theta range for data collection	2.92 to 27.52°.	
Index ranges	-42<=h<=46, -11<=k<=11, -30<=l<=30	
Reflections collected	41758	
Independent reflections	8207 [R(int) = 0.0568]	
Completeness to theta = 27.52°	99.6 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9326 and 0.8159	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8207 / 0 / 450
Goodness-of-fit on F^2	1.020
Final R indices [I>2sigma(I)]	R1 = 0.0394, wR2 = 0.0722
R indices (all data)	R1 = 0.0583, wR2 = 0.0781
Largest diff. peak and hole	0.383 and -0.382 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3(PF$_6$)$^-$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1157(1)	738(3)	2388(1)	18(1)
C(2)	1194(1)	-872(3)	2374(1)	19(1)
C(3)	898(1)	-1739(3)	2531(1)	26(1)
C(4)	589(1)	-1026(4)	2702(1)	28(1)
C(5)	562(1)	564(3)	2713(1)	26(1)
C(6)	845(1)	1495(3)	2550(1)	20(1)
C(7)	1539(1)	-1667(3)	2206(1)	24(1)
C(8)	1797(1)	-2268(4)	2738(2)	45(1)
C(9)	1433(1)	-2982(4)	1774(1)	36(1)
C(10)	809(1)	3248(3)	2527(1)	23(1)
C(11)	593(1)	3746(4)	1939(1)	37(1)
C(12)	620(1)	3922(4)	3010(1)	41(1)
C(13)	1531(1)	2154(3)	1732(1)	15(1)
C(14)	1739(1)	2285(3)	2695(1)	22(1)
C(15)	1980(1)	3143(3)	2448(1)	20(1)
C(16)	2006(1)	3640(3)	1395(1)	16(1)
C(17)	2326(1)	4528(3)	1415(1)	18(1)
C(18)	2426(1)	4963(3)	890(1)	21(1)
C(19)	2214(1)	4502(3)	371(1)	20(1)
C(20)	1899(1)	3613(3)	399(1)	16(1)
C(21)	1351(1)	2117(3)	88(1)	16(1)

C(22)	1633(1)	3081(3)	-649(1)	21(1)
C(23)	1330(1)	2242(3)	-883(1)	22(1)
C(24)	829(1)	675(3)	-536(1)	18(1)
C(25)	882(1)	-921(3)	-483(1)	19(1)
C(26)	562(1)	-1849(3)	-622(1)	24(1)
C(27)	210(1)	-1193(4)	-797(1)	27(1)
C(28)	165(1)	389(4)	-832(1)	26(1)
C(29)	476(1)	1373(3)	-700(1)	20(1)
C(30)	1272(1)	-1620(3)	-278(1)	26(1)
C(31)	1254(1)	-3136(4)	54(1)	39(1)
C(32)	1490(1)	-1869(4)	-783(2)	41(1)
C(33)	429(1)	3127(3)	-695(1)	25(1)
C(34)	416(1)	3687(3)	-78(1)	30(1)
C(35)	78(1)	3707(4)	-1102(1)	37(1)
N(1)	1465(1)	1691(2)	2255(1)	16(1)
N(2)	1850(1)	3053(2)	1861(1)	16(1)
N(3)	1794(1)	3212(2)	900(1)	15(1)
N(4)	1642(1)	2991(2)	-60(1)	16(1)
N(5)	1160(1)	1668(3)	-428(1)	17(1)
F(1)	2434(1)	1049(2)	793(1)	29(1)
F(2)	2392(1)	483(2)	1724(1)	27(1)
F(3)	1948(1)	-417(2)	1004(1)	34(1)
F(4)	2369(1)	-2064(2)	1514(1)	26(1)
F(5)	2407(1)	-1513(2)	577(1)	35(1)
F(6)	2852(1)	-607(2)	1294(1)	32(1)
P(1)	2396(1)	-517(1)	1148(1)	19(1)
Ni(1)	1372(1)	1946(1)	911(1)	14(1)
Br(1)	858(1)	412(1)	930(1)	20(1)

Table 3. Bond lengths [Å] and angles [°] for **3(PF$_6$)$^-$**.

C(1)-C(6)	1.398(3)	C(14)-N(1)	1.401(3)
C(1)-C(2)	1.399(4)	C(14)-H(14)	0.9500
C(1)-N(1)	1.450(3)	C(15)-N(2)	1.380(3)
C(2)-C(3)	1.394(4)	C(15)-H(15)	0.9500
C(2)-C(7)	1.518(3)	C(16)-N(3)	1.334(3)
C(3)-C(4)	1.383(4)	C(16)-C(17)	1.373(3)
C(3)-H(3)	0.9500	C(16)-N(2)	1.399(3)
C(4)-C(5)	1.378(4)	C(17)-C(18)	1.388(4)
C(4)-H(4)	0.9500	C(17)-H(17)	0.9500
C(5)-C(6)	1.395(4)	C(18)-C(19)	1.384(4)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.521(4)	C(19)-C(20)	1.376(3)
C(7)-C(8)	1.521(4)	C(19)-H(19)	0.9500
C(7)-C(9)	1.528(4)	C(20)-N(3)	1.336(3)
C(7)-H(7)	1.0000	C(20)-N(4)	1.403(3)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.345(3)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.376(3)
C(8)-H(8C)	0.9800	C(21)-Ni(1)	1.925(2)
C(9)-H(9A)	0.9800	C(22)-C(23)	1.347(4)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.378(3)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(12)	1.526(4)	C(23)-N(5)	1.401(3)
C(10)-C(11)	1.530(4)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.394(4)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.397(3)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.452(3)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.393(4)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.525(3)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.385(4)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(1)	1.347(3)	C(27)-C(28)	1.376(4)
C(13)-N(2)	1.377(3)	C(27)-H(27)	0.9500
C(13)-Ni(1)	1.925(2)	C(28)-C(29)	1.394(4)
C(14)-C(15)	1.339(4)	C(28)-H(28)	0.9500

C(29)-C(33)	1.525(4)	C(2)-C(3)-H(3)	119.5
C(30)-C(31)	1.530(4)	C(5)-C(4)-C(3)	120.7(3)
C(30)-C(32)	1.536(4)	C(5)-C(4)-H(4)	119.6
C(30)-H(30)	1.0000	C(3)-C(4)-H(4)	119.6
C(31)-H(31A)	0.9800	C(4)-C(5)-C(6)	120.9(2)
C(31)-H(31B)	0.9800	C(4)-C(5)-H(5)	119.5
C(31)-H(31C)	0.9800	C(6)-C(5)-H(5)	119.5
C(32)-H(32A)	0.9800	C(5)-C(6)-C(1)	116.9(3)
C(32)-H(32B)	0.9800	C(5)-C(6)-C(10)	121.5(2)
C(32)-H(32C)	0.9800	C(1)-C(6)-C(10)	121.6(2)
C(33)-C(35)	1.534(4)	C(2)-C(7)-C(8)	110.7(2)
C(33)-C(34)	1.535(4)	C(2)-C(7)-C(9)	112.6(2)
C(33)-H(33)	1.0000	C(8)-C(7)-C(9)	110.0(3)
C(34)-H(34A)	0.9800	C(2)-C(7)-H(7)	107.8
C(34)-H(34B)	0.9800	C(8)-C(7)-H(7)	107.8
C(34)-H(34C)	0.9800	C(9)-C(7)-H(7)	107.8
C(35)-H(35A)	0.9800	C(7)-C(8)-H(8A)	109.5
C(35)-H(35B)	0.9800	C(7)-C(8)-H(8B)	109.5
C(35)-H(35C)	0.9800	H(8A)-C(8)-H(8B)	109.5
N(3)-Ni(1)	1.8667(19)	C(7)-C(8)-H(8C)	109.5
F(1)-P(1)	1.6047(17)	H(8A)-C(8)-H(8C)	109.5
F(2)-P(1)	1.6065(16)	H(8B)-C(8)-H(8C)	109.5
F(3)-P(1)	1.5883(16)	C(7)-C(9)-H(9A)	109.5
F(4)-P(1)	1.6003(16)	C(7)-C(9)-H(9B)	109.5
F(5)-P(1)	1.5973(17)	H(9A)-C(9)-H(9B)	109.5
F(6)-P(1)	1.6112(16)	C(7)-C(9)-H(9C)	109.5
Ni(1)-Br(1)	2.2746(4)	H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.5
C(6)-C(1)-C(2)	123.6(2)	C(6)-C(10)-C(12)	113.6(2)
C(6)-C(1)-N(1)	117.5(2)	C(6)-C(10)-C(11)	109.8(2)
C(2)-C(1)-N(1)	118.8(2)	C(12)-C(10)-C(11)	110.0(2)
C(3)-C(2)-C(1)	116.7(2)	C(6)-C(10)-H(10)	107.7
C(3)-C(2)-C(7)	120.6(2)	C(12)-C(10)-H(10)	107.7
C(1)-C(2)-C(7)	122.7(2)	C(11)-C(10)-H(10)	107.7
C(4)-C(3)-C(2)	121.1(3)	C(10)-C(11)-H(11A)	109.5
C(4)-C(3)-H(3)	119.5	C(10)-C(11)-H(11B)	109.5

H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-Ni(1)	112.66(17)
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	105.3(2)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	127.3
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	127.3
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	107.5(2)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	126.3
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.3
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	123.8(2)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	118.2(2)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	118.0(2)
N(1)-C(13)-N(2)	103.2(2)	C(26)-C(25)-C(24)	117.0(2)
N(1)-C(13)-Ni(1)	144.78(19)	C(26)-C(25)-C(30)	121.4(2)
N(2)-C(13)-Ni(1)	111.90(16)	C(24)-C(25)-C(30)	121.6(2)
C(15)-C(14)-N(1)	107.9(2)	C(27)-C(26)-C(25)	120.6(3)
C(15)-C(14)-H(14)	126.0	C(27)-C(26)-H(26)	119.7
N(1)-C(14)-H(14)	126.0	C(25)-C(26)-H(26)	119.7
C(14)-C(15)-N(2)	105.3(2)	C(28)-C(27)-C(26)	121.0(3)
C(14)-C(15)-H(15)	127.3	C(28)-C(27)-H(27)	119.5
N(2)-C(15)-H(15)	127.3	C(26)-C(27)-H(27)	119.5
N(3)-C(16)-C(17)	122.6(2)	C(27)-C(28)-C(29)	120.9(3)
N(3)-C(16)-N(2)	109.7(2)	C(27)-C(28)-H(28)	119.6
C(17)-C(16)-N(2)	127.7(2)	C(29)-C(28)-H(28)	119.6
C(16)-C(17)-C(18)	117.1(2)	C(28)-C(29)-C(24)	116.8(3)
C(16)-C(17)-H(17)	121.5	C(28)-C(29)-C(33)	121.6(2)
C(18)-C(17)-H(17)	121.5	C(24)-C(29)-C(33)	121.5(2)
C(19)-C(18)-C(17)	121.2(2)	C(25)-C(30)-C(31)	112.8(2)
C(19)-C(18)-H(18)	119.4	C(25)-C(30)-C(32)	111.4(2)
C(17)-C(18)-H(18)	119.4	C(31)-C(30)-C(32)	109.9(2)
C(20)-C(19)-C(18)	117.1(2)	C(25)-C(30)-H(30)	107.5
C(20)-C(19)-H(19)	121.4	C(31)-C(30)-H(30)	107.5
C(18)-C(19)-H(19)	121.4	C(32)-C(30)-H(30)	107.5
N(3)-C(20)-C(19)	122.5(2)	C(30)-C(31)-H(31A)	109.5
N(3)-C(20)-N(4)	109.4(2)	C(30)-C(31)-H(31B)	109.5
C(19)-C(20)-N(4)	128.2(2)	H(31A)-C(31)-H(31B)	109.5
N(5)-C(21)-N(4)	103.1(2)	C(30)-C(31)-H(31C)	109.5
N(5)-C(21)-Ni(1)	144.17(18)	H(31A)-C(31)-H(31C)	109.5

H(31B)-C(31)-H(31C)	109.5	C(22)-N(4)-C(20)	130.7(2)
C(30)-C(32)-H(32A)	109.5	C(21)-N(5)-C(23)	111.3(2)
C(30)-C(32)-H(32B)	109.5	C(21)-N(5)-C(24)	127.5(2)
H(32A)-C(32)-H(32B)	109.5	C(23)-N(5)-C(24)	121.2(2)
C(30)-C(32)-H(32C)	109.5	F(3)-P(1)-F(5)	90.65(10)
H(32A)-C(32)-H(32C)	109.5	F(3)-P(1)-F(4)	90.70(9)
H(32B)-C(32)-H(32C)	109.5	F(5)-P(1)-F(4)	90.68(9)
C(29)-C(33)-C(35)	113.5(2)	F(3)-P(1)-F(1)	90.54(9)
C(29)-C(33)-C(34)	109.9(2)	F(5)-P(1)-F(1)	90.27(9)
C(35)-C(33)-C(34)	109.6(2)	F(4)-P(1)-F(1)	178.44(10)
C(29)-C(33)-H(33)	107.9	F(3)-P(1)-F(2)	90.12(9)
C(35)-C(33)-H(33)	107.9	F(5)-P(1)-F(2)	179.23(10)
C(34)-C(33)-H(33)	107.9	F(4)-P(1)-F(2)	89.33(8)
C(33)-C(34)-H(34A)	109.5	F(1)-P(1)-F(2)	89.71(9)
C(33)-C(34)-H(34B)	109.5	F(3)-P(1)-F(6)	179.62(11)
H(34A)-C(34)-H(34B)	109.5	F(5)-P(1)-F(6)	89.58(9)
C(33)-C(34)-H(34C)	109.5	F(4)-P(1)-F(6)	89.61(9)
H(34A)-C(34)-H(34C)	109.5	F(1)-P(1)-F(6)	89.16(9)
H(34B)-C(34)-H(34C)	109.5	F(2)-P(1)-F(6)	89.65(9)
C(33)-C(35)-H(35A)	109.5	N(3)-Ni(1)-C(13)	81.46(9)
C(33)-C(35)-H(35B)	109.5	N(3)-Ni(1)-C(21)	80.92(9)
H(35A)-C(35)-H(35B)	109.5	C(13)-Ni(1)-C(21)	162.36(10)
C(33)-C(35)-H(35C)	109.5	N(3)-Ni(1)-Br(1)	179.64(7)
H(35A)-C(35)-H(35C)	109.5	C(13)-Ni(1)-Br(1)	98.24(7)
H(35B)-C(35)-H(35C)	109.5	C(21)-Ni(1)-Br(1)	99.38(7)
C(13)-N(1)-C(14)	111.0(2)		
C(13)-N(1)-C(1)	127.9(2)		
C(14)-N(1)-C(1)	121.1(2)		
C(13)-N(2)-C(15)	112.7(2)		
C(13)-N(2)-C(16)	117.0(2)		
C(15)-N(2)-C(16)	130.2(2)		
C(16)-N(3)-C(20)	119.4(2)		
C(16)-N(3)-Ni(1)	119.90(16)		
C(20)-N(3)-Ni(1)	120.51(17)		
C(21)-N(4)-C(22)	112.8(2)		
C(21)-N(4)-C(20)	116.5(2)		

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **3(PF$_6$)$^-$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	15(1)	25(2)	13(1)	5(1)	3(1)	-2(1)
C(2)	20(1)	24(2)	14(1)	4(1)	2(1)	-1(1)
C(3)	27(1)	25(2)	25(2)	3(1)	5(1)	-5(1)
C(4)	20(1)	35(2)	32(2)	6(1)	10(1)	-9(1)
C(5)	20(1)	33(2)	28(2)	5(1)	10(1)	1(1)
C(6)	18(1)	26(2)	16(1)	3(1)	4(1)	1(1)
C(7)	26(1)	21(2)	30(2)	5(1)	12(1)	2(1)
C(8)	27(2)	58(2)	48(2)	-5(2)	-1(1)	12(2)
C(9)	41(2)	32(2)	37(2)	-4(2)	7(1)	10(2)
C(10)	18(1)	29(2)	22(1)	2(1)	5(1)	3(1)
C(11)	44(2)	33(2)	31(2)	3(2)	-4(1)	10(2)
C(12)	54(2)	35(2)	39(2)	0(2)	26(2)	6(2)
C(13)	12(1)	14(1)	20(1)	-1(1)	4(1)	1(1)
C(14)	18(1)	31(2)	16(1)	-3(1)	1(1)	-2(1)
C(15)	18(1)	24(2)	17(1)	-4(1)	0(1)	-1(1)
C(16)	16(1)	13(1)	19(1)	-1(1)	5(1)	2(1)
C(17)	14(1)	17(1)	24(1)	-2(1)	3(1)	-1(1)
C(18)	16(1)	17(1)	31(2)	1(1)	9(1)	-2(1)
C(19)	20(1)	19(1)	23(1)	5(1)	10(1)	0(1)
C(20)	14(1)	16(1)	19(1)	1(1)	4(1)	2(1)
C(21)	11(1)	17(1)	22(1)	2(1)	5(1)	1(1)
C(22)	18(1)	28(2)	19(1)	5(1)	7(1)	-1(1)
C(23)	19(1)	31(2)	15(1)	3(1)	7(1)	-1(1)
C(24)	15(1)	24(2)	14(1)	0(1)	4(1)	-4(1)
C(25)	20(1)	23(2)	14(1)	0(1)	5(1)	1(1)
C(26)	31(1)	23(2)	19(1)	-3(1)	7(1)	-4(1)
C(27)	22(1)	36(2)	22(1)	-2(1)	3(1)	-11(1)
C(28)	16(1)	36(2)	27(2)	8(1)	2(1)	-1(1)
C(29)	16(1)	29(2)	17(1)	4(1)	5(1)	-1(1)
C(30)	24(1)	20(2)	31(2)	-6(1)	1(1)	3(1)
C(31)	40(2)	29(2)	46(2)	4(2)	4(2)	13(2)

C(32)	33(2)	41(2)	53(2)	0(2)	20(2)	10(2)
C(33)	18(1)	28(2)	30(2)	11(1)	6(1)	3(1)
C(34)	32(2)	24(2)	35(2)	8(1)	9(1)	9(1)
C(35)	33(2)	39(2)	39(2)	14(2)	5(1)	9(1)
N(1)	13(1)	19(1)	16(1)	2(1)	5(1)	-1(1)
N(2)	14(1)	18(1)	16(1)	-2(1)	4(1)	-1(1)
N(3)	14(1)	13(1)	17(1)	1(1)	4(1)	0(1)
N(4)	13(1)	19(1)	18(1)	3(1)	6(1)	0(1)
N(5)	14(1)	22(1)	15(1)	4(1)	5(1)	0(1)
F(1)	39(1)	21(1)	31(1)	9(1)	16(1)	7(1)
F(2)	35(1)	24(1)	25(1)	-4(1)	11(1)	2(1)
F(3)	22(1)	44(1)	35(1)	7(1)	2(1)	1(1)
F(4)	39(1)	19(1)	23(1)	5(1)	9(1)	-2(1)
F(5)	63(1)	24(1)	22(1)	-1(1)	16(1)	3(1)
F(6)	21(1)	36(1)	42(1)	9(1)	11(1)	7(1)
P(1)	20(1)	18(1)	19(1)	3(1)	7(1)	3(1)
Ni(1)	11(1)	17(1)	14(1)	2(1)	4(1)	-2(1)
Br(1)	15(1)	27(1)	18(1)	3(1)	4(1)	-7(1)

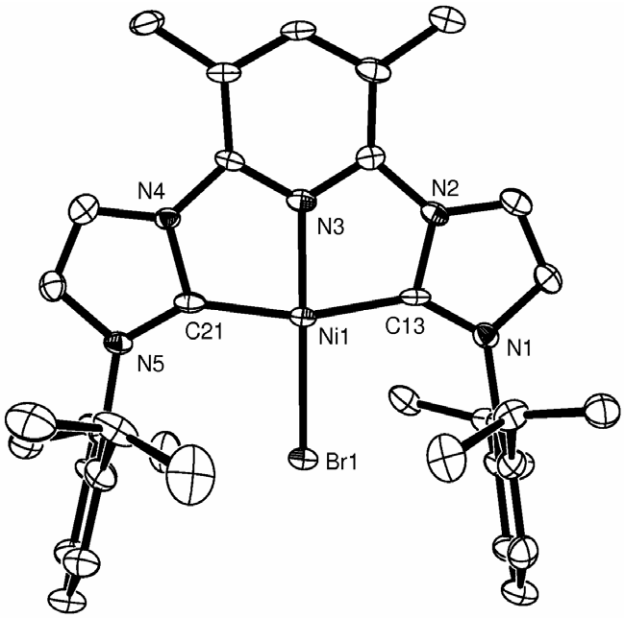


Table 1. Crystal data and structure refinement for $\mathbf{3^{Me}(AgI_2)^-}$.

Identification code	$\mathbf{3^{Me}(AgI_2)^-}$	
Empirical formula	C37 H45 Ag Br I2 N5 Ni	
Formula weight	1060.07	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 41.413(2) Å	α= 90°.
	b = 8.1837(4) Å	β= 104.661(2)°.
	c = 23.0900(11) Å	γ = 90°.
Volume	7570.7(6) Å^3	
Z	8	
Density (calculated)	1.860 Mg/m^3	
Absorption coefficient	3.735 mm^{-1}	
F(000)	4144	
Crystal size	0.40 x 0.14 x 0.14 mm^3	
Theta range for data collection	2.92 to 27.55°.	
Index ranges	-53<=h<=53, -10<=k<=10, -29<=l<=30	
Reflections collected	42239	
Independent reflections	8691 [R(int) = 0.0734]	
Completeness to theta = 27.55°	99.4 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.5908 and 0.3166
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	8691 / 0 / 434
Goodness-of-fit on F^2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0667, wR2 = 0.1858
R indices (all data)	R1 = 0.1067, wR2 = 0.2119
Largest diff. peak and hole	3.368 and -2.665 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3^{Me}(AgI$_2$)$^-$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	1157(2)	5013(9)	2303(3)	18(1)
C(2)	1222(2)	6675(10)	2359(3)	22(2)
C(3)	970(2)	7676(10)	2460(3)	26(2)
C(4)	670(2)	7011(10)	2499(4)	27(2)
C(5)	614(2)	5373(10)	2447(3)	22(2)
C(6)	858(2)	4296(9)	2354(3)	21(2)
C(7)	1548(2)	7435(10)	2290(3)	23(2)
C(8)	1759(2)	8075(11)	2882(4)	29(2)
C(9)	1479(2)	8781(11)	1819(4)	36(2)
C(10)	799(2)	2466(9)	2310(4)	23(2)
C(11)	526(2)	1902(11)	2587(5)	35(2)
C(12)	712(2)	1870(10)	1660(4)	29(2)
C(13)	1467(2)	3684(9)	1643(3)	19(2)
C(14)	1669(2)	3319(9)	2638(3)	21(2)
C(15)	1885(2)	2591(10)	2374(4)	24(2)
C(16)	1875(2)	2318(9)	1273(3)	16(1)
C(17)	2161(2)	1436(10)	1270(4)	23(2)
C(18)	2217(2)	1207(9)	703(4)	20(2)
C(19)	2007(2)	1775(9)	164(4)	20(2)

C(20)	1728(2)	2631(9)	228(3)	16(1)
C(21)	1229(2)	4154(9)	-34(3)	18(1)
C(22)	1413(2)	3290(10)	-838(4)	25(2)
C(23)	1135(2)	4122(9)	-1051(3)	21(2)
C(24)	735(2)	5711(9)	-638(3)	21(2)
C(25)	792(2)	7395(10)	-605(4)	24(2)
C(26)	512(2)	8392(10)	-721(4)	26(2)
C(27)	197(2)	7767(10)	-860(4)	29(2)
C(28)	149(2)	6068(10)	-890(4)	25(2)
C(29)	416(2)	5008(9)	-782(3)	19(2)
C(30)	1135(2)	8132(10)	-466(4)	33(2)
C(31)	1199(2)	8960(12)	-1013(5)	41(2)
C(32)	1194(3)	9293(14)	75(5)	51(3)
C(33)	361(2)	3171(9)	-803(4)	22(2)
C(34)	244(3)	2665(12)	-257(4)	39(2)
C(35)	105(2)	2663(11)	-1375(4)	32(2)
C(36)	2400(2)	783(11)	1808(4)	28(2)
C(37)	2100(2)	1503(11)	-409(4)	28(2)
N(1)	1415(2)	3989(7)	2186(3)	18(1)
N(2)	1757(1)	2779(7)	1768(3)	16(1)
N(3)	1666(1)	2885(7)	770(3)	16(1)
N(4)	1474(1)	3296(7)	-220(3)	16(1)
N(5)	1024(1)	4664(8)	-554(3)	18(1)
Ni(1)	1294(1)	4110(1)	808(1)	16(1)
Br(1)	841(1)	5645(1)	847(1)	23(1)
I(1)	2277(1)	6049(1)	1555(1)	55(1)
I(2)	2024(1)	6566(1)	-597(1)	49(1)
Ag(1)	2349(1)	6868(1)	534(1)	54(1)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{3^{Me}(AgI_2)^-}$.

C(1)-C(2)	1.386(11)	C(14)-N(1)	1.392(9)
C(1)-C(6)	1.401(10)	C(14)-H(14)	0.9500
C(1)-N(1)	1.437(9)	C(15)-N(2)	1.373(10)
C(2)-C(3)	1.390(11)	C(15)-H(15)	0.9500
C(2)-C(7)	1.533(10)	C(16)-N(3)	1.344(9)
C(3)-C(4)	1.383(11)	C(16)-C(17)	1.388(10)
C(3)-H(3)	0.9500	C(16)-N(2)	1.403(9)
C(4)-C(5)	1.360(11)	C(17)-C(18)	1.399(11)
C(4)-H(4)	0.9500	C(17)-C(36)	1.480(11)
C(5)-C(6)	1.400(10)	C(18)-C(19)	1.406(11)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.517(11)	C(19)-C(20)	1.392(10)
C(7)-C(8)	1.517(11)	C(19)-C(37)	1.485(11)
C(7)-C(9)	1.522(12)	C(20)-N(3)	1.354(9)
C(7)-H(7)	1.0000	C(20)-N(4)	1.388(9)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.351(9)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.386(9)
C(8)-H(8C)	0.9800	C(21)-Ni(1)	1.895(8)
C(9)-H(9A)	0.9800	C(22)-C(23)	1.323(11)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.386(10)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(11)	1.507(11)	C(23)-N(5)	1.411(9)
C(10)-C(12)	1.531(11)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.397(11)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.401(10)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.442(9)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.387(11)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.500(11)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.363(11)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(1)	1.348(10)	C(27)-C(28)	1.403(12)
C(13)-N(2)	1.378(9)	C(27)-H(27)	0.9500
C(13)-Ni(1)	1.911(8)	C(28)-C(29)	1.379(10)
C(14)-C(15)	1.342(11)	C(28)-H(28)	0.9500

C(29)-C(33)	1.520(10)	C(1)-C(2)-C(3)	117.3(7)
C(30)-C(31)	1.515(14)	C(1)-C(2)-C(7)	122.9(7)
C(30)-C(32)	1.539(14)	C(3)-C(2)-C(7)	119.7(7)
C(30)-H(30)	1.0000	C(4)-C(3)-C(2)	120.2(8)
C(31)-H(31A)	0.9800	C(4)-C(3)-H(3)	119.9
C(31)-H(31B)	0.9800	C(2)-C(3)-H(3)	119.9
C(31)-H(31C)	0.9800	C(5)-C(4)-C(3)	121.2(7)
C(32)-H(32A)	0.9800	C(5)-C(4)-H(4)	119.4
C(32)-H(32B)	0.9800	C(3)-C(4)-H(4)	119.4
C(32)-H(32C)	0.9800	C(4)-C(5)-C(6)	121.4(7)
C(33)-C(34)	1.519(12)	C(4)-C(5)-H(5)	119.3
C(33)-C(35)	1.526(11)	C(6)-C(5)-H(5)	119.3
C(33)-H(33)	1.0000	C(5)-C(6)-C(1)	115.9(7)
C(34)-H(34A)	0.9800	C(5)-C(6)-C(10)	121.4(7)
C(34)-H(34B)	0.9800	C(1)-C(6)-C(10)	122.6(7)
C(34)-H(34C)	0.9800	C(8)-C(7)-C(9)	110.8(7)
C(35)-H(35A)	0.9800	C(8)-C(7)-C(2)	111.6(6)
C(35)-H(35B)	0.9800	C(9)-C(7)-C(2)	110.9(7)
C(35)-H(35C)	0.9800	C(8)-C(7)-H(7)	107.8
C(36)-H(36A)	0.9800	C(9)-C(7)-H(7)	107.8
C(36)-H(36B)	0.9800	C(2)-C(7)-H(7)	107.8
C(36)-H(36C)	0.9800	C(7)-C(8)-H(8A)	109.5
C(37)-H(37A)	0.9800	C(7)-C(8)-H(8B)	109.5
C(37)-H(37B)	0.9800	H(8A)-C(8)-H(8B)	109.5
C(37)-H(37C)	0.9800	C(7)-C(8)-H(8C)	109.5
N(3)-Ni(1)	1.860(6)	H(8A)-C(8)-H(8C)	109.5
Ni(1)-Br(1)	2.2761(11)	H(8B)-C(8)-H(8C)	109.5
I(1)-Ag(1)	2.5404(12)	C(7)-C(9)-H(9A)	109.5
I(2)-Ag(1)	2.6278(12)	C(7)-C(9)-H(9B)	109.5
I(2)-Ag(1)#1	2.8691(13)	H(9A)-C(9)-H(9B)	109.5
Ag(1)-I(2)#1	2.8691(13)	C(7)-C(9)-H(9C)	109.5
Ag(1)-Ag(1)#1	3.2064(19)	H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.5
C(2)-C(1)-C(6)	123.9(7)	C(11)-C(10)-C(6)	113.5(7)
C(2)-C(1)-N(1)	117.0(6)	C(11)-C(10)-C(12)	107.7(7)
C(6)-C(1)-N(1)	119.1(7)	C(6)-C(10)-C(12)	112.0(7)

C(11)-C(10)-H(10)	107.8	N(3)-C(20)-N(4)	110.1(6)
C(6)-C(10)-H(10)	107.8	N(3)-C(20)-C(19)	122.2(6)
C(12)-C(10)-H(10)	107.8	N(4)-C(20)-C(19)	127.7(7)
C(10)-C(11)-H(11A)	109.5	N(5)-C(21)-N(4)	103.1(6)
C(10)-C(11)-H(11B)	109.5	N(5)-C(21)-Ni(1)	144.2(5)
H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-Ni(1)	112.6(5)
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	107.0(7)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	126.5
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	126.5
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	107.1(7)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	126.5
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	126.5
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	123.6(7)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	117.2(6)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	119.1(7)
N(1)-C(13)-N(2)	103.9(6)	C(26)-C(25)-C(24)	116.7(7)
N(1)-C(13)-Ni(1)	142.7(5)	C(26)-C(25)-C(30)	120.2(7)
N(2)-C(13)-Ni(1)	113.3(5)	C(24)-C(25)-C(30)	123.0(7)
C(15)-C(14)-N(1)	107.3(7)	C(27)-C(26)-C(25)	121.9(8)
C(15)-C(14)-H(14)	126.3	C(27)-C(26)-H(26)	119.1
N(1)-C(14)-H(14)	126.3	C(25)-C(26)-H(26)	119.1
C(14)-C(15)-N(2)	106.5(6)	C(26)-C(27)-C(28)	119.9(7)
C(14)-C(15)-H(15)	126.7	C(26)-C(27)-H(27)	120.0
N(2)-C(15)-H(15)	126.7	C(28)-C(27)-H(27)	120.0
N(3)-C(16)-C(17)	122.6(7)	C(29)-C(28)-C(27)	121.2(7)
N(3)-C(16)-N(2)	109.4(6)	C(29)-C(28)-H(28)	119.4
C(17)-C(16)-N(2)	128.0(7)	C(27)-C(28)-H(28)	119.4
C(16)-C(17)-C(18)	114.8(7)	C(28)-C(29)-C(24)	116.8(7)
C(16)-C(17)-C(36)	125.1(7)	C(28)-C(29)-C(33)	120.6(7)
C(18)-C(17)-C(36)	120.1(7)	C(24)-C(29)-C(33)	122.6(6)
C(17)-C(18)-C(19)	124.9(7)	C(25)-C(30)-C(31)	111.0(7)
C(17)-C(18)-H(18)	117.6	C(25)-C(30)-C(32)	111.8(8)
C(19)-C(18)-H(18)	117.6	C(31)-C(30)-C(32)	112.0(8)
C(20)-C(19)-C(18)	114.6(7)	C(25)-C(30)-H(30)	107.2
C(20)-C(19)-C(37)	125.5(7)	C(31)-C(30)-H(30)	107.2
C(18)-C(19)-C(37)	119.8(6)	C(32)-C(30)-H(30)	107.2

C(30)-C(31)-H(31A)	109.5	C(19)-C(37)-H(37A)	109.5
C(30)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37B)	109.5
H(31A)-C(31)-H(31B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(30)-C(31)-H(31C)	109.5	C(19)-C(37)-H(37C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32A)	109.5	C(13)-N(1)-C(14)	110.9(6)
C(30)-C(32)-H(32B)	109.5	C(13)-N(1)-C(1)	125.8(6)
H(32A)-C(32)-H(32B)	109.5	C(14)-N(1)-C(1)	123.0(6)
C(30)-C(32)-H(32C)	109.5	C(15)-N(2)-C(13)	111.3(6)
H(32A)-C(32)-H(32C)	109.5	C(15)-N(2)-C(16)	132.6(6)
H(32B)-C(32)-H(32C)	109.5	C(13)-N(2)-C(16)	115.9(6)
C(34)-C(33)-C(29)	108.7(7)	C(16)-N(3)-C(20)	120.9(6)
C(34)-C(33)-C(35)	110.2(7)	C(16)-N(3)-Ni(1)	120.3(5)
C(29)-C(33)-C(35)	111.3(6)	C(20)-N(3)-Ni(1)	118.7(5)
C(34)-C(33)-H(33)	108.9	C(21)-N(4)-C(22)	111.5(6)
C(29)-C(33)-H(33)	108.9	C(21)-N(4)-C(20)	116.3(6)
C(35)-C(33)-H(33)	108.9	C(22)-N(4)-C(20)	132.2(6)
C(33)-C(34)-H(34A)	109.5	C(21)-N(5)-C(23)	111.3(6)
C(33)-C(34)-H(34B)	109.5	C(21)-N(5)-C(24)	128.1(6)
H(34A)-C(34)-H(34B)	109.5	C(23)-N(5)-C(24)	120.5(6)
C(33)-C(34)-H(34C)	109.5	N(3)-Ni(1)-C(21)	82.2(3)
H(34A)-C(34)-H(34C)	109.5	N(3)-Ni(1)-C(13)	81.1(3)
H(34B)-C(34)-H(34C)	109.5	C(21)-Ni(1)-C(13)	163.3(3)
C(33)-C(35)-H(35A)	109.5	N(3)-Ni(1)-Br(1)	178.99(19)
C(33)-C(35)-H(35B)	109.5	C(21)-Ni(1)-Br(1)	97.2(2)
H(35A)-C(35)-H(35B)	109.5	C(13)-Ni(1)-Br(1)	99.5(2)
C(33)-C(35)-H(35C)	109.5	Ag(1)-I(2)-Ag(1)#1	71.21(4)
H(35A)-C(35)-H(35C)	109.5	I(1)-Ag(1)-I(2)	138.28(5)
H(35B)-C(35)-H(35C)	109.5	I(1)-Ag(1)-I(2)#1	112.84(4)
C(17)-C(36)-H(36A)	109.5	I(2)-Ag(1)-I(2)#1	108.79(4)
C(17)-C(36)-H(36B)	109.5	I(1)-Ag(1)-Ag(1)#1	163.53(6)
H(36A)-C(36)-H(36B)	109.5	I(2)-Ag(1)-Ag(1)#1	57.90(3)
C(17)-C(36)-H(36C)	109.5	I(2)#1-Ag(1)-Ag(1)#1	50.88(3)
H(36A)-C(36)-H(36C)	109.5		
H(36B)-C(36)-H(36C)	109.5		

Symmetry transformations used to generate equivalent atoms:

#1 -x+1/2,-y+3/2,-z

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for $\mathbf{3^{Me}(AgI_2)^-}$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	16(3)	19(4)	17(3)	2(3)	3(3)	5(3)
C(2)	23(4)	23(4)	21(4)	0(3)	8(3)	0(3)
C(3)	32(4)	20(4)	25(4)	-3(3)	6(3)	-1(3)
C(4)	17(4)	21(4)	39(5)	-2(4)	4(3)	2(3)
C(5)	15(3)	24(4)	27(4)	-1(3)	4(3)	0(3)
C(6)	18(3)	18(4)	24(4)	2(3)	1(3)	3(3)
C(7)	23(4)	21(4)	30(4)	-1(3)	13(3)	-4(3)
C(8)	21(4)	37(5)	31(4)	1(4)	8(3)	-1(3)
C(9)	38(5)	32(5)	36(5)	7(4)	9(4)	-13(4)
C(10)	18(3)	18(4)	32(4)	0(3)	5(3)	-1(3)
C(11)	30(4)	25(5)	54(6)	-1(4)	18(4)	-2(4)
C(12)	24(4)	21(4)	36(5)	0(4)	-4(3)	1(3)
C(13)	12(3)	18(4)	28(4)	-1(3)	7(3)	6(3)
C(14)	16(3)	20(4)	23(4)	1(3)	0(3)	-4(3)
C(15)	14(3)	24(4)	30(4)	2(3)	1(3)	0(3)
C(16)	12(3)	13(3)	24(4)	-4(3)	5(3)	-5(3)
C(17)	11(3)	21(4)	36(4)	-2(3)	3(3)	-2(3)
C(18)	14(3)	14(4)	35(4)	3(3)	13(3)	3(3)
C(19)	13(3)	15(4)	33(4)	0(3)	9(3)	3(3)
C(20)	11(3)	13(3)	25(4)	4(3)	4(3)	2(3)
C(21)	10(3)	16(4)	28(4)	1(3)	8(3)	1(3)

C(22)	25(4)	27(4)	25(4)	-1(3)	10(3)	0(3)
C(23)	22(4)	22(4)	20(4)	2(3)	6(3)	-2(3)
C(24)	17(3)	22(4)	24(4)	-3(3)	7(3)	3(3)
C(25)	27(4)	18(4)	28(4)	6(3)	6(3)	0(3)
C(26)	23(4)	21(4)	36(4)	3(3)	9(3)	3(3)
C(27)	21(4)	25(4)	40(5)	0(4)	7(3)	9(3)
C(28)	15(3)	25(4)	34(4)	-2(3)	4(3)	-2(3)
C(29)	18(3)	13(4)	23(4)	6(3)	2(3)	4(3)
C(30)	22(4)	21(4)	50(5)	5(4)	-4(4)	1(3)
C(31)	20(4)	41(6)	64(7)	8(5)	14(4)	-4(4)
C(32)	45(6)	49(7)	55(6)	-8(5)	7(5)	-33(5)
C(33)	18(3)	14(4)	32(4)	3(3)	3(3)	0(3)
C(34)	55(6)	28(5)	34(5)	3(4)	11(4)	-7(4)
C(35)	30(4)	27(5)	36(5)	-8(4)	4(4)	1(4)
C(36)	19(4)	28(4)	37(5)	3(4)	5(3)	5(3)
C(37)	23(4)	32(5)	33(4)	-1(4)	15(3)	8(3)
N(1)	19(3)	14(3)	19(3)	0(2)	2(2)	1(2)
N(2)	13(3)	13(3)	22(3)	3(2)	3(2)	0(2)
N(3)	11(3)	13(3)	26(3)	1(2)	6(2)	-2(2)
N(4)	17(3)	12(3)	19(3)	2(2)	7(2)	4(2)
N(5)	11(3)	19(3)	23(3)	-1(3)	3(2)	1(2)
Ni(1)	12(1)	15(1)	21(1)	1(1)	5(1)	3(1)
Br(1)	19(1)	26(1)	25(1)	1(1)	6(1)	9(1)
I(1)	57(1)	57(1)	55(1)	-12(1)	21(1)	-24(1)
I(2)	35(1)	46(1)	61(1)	-3(1)	5(1)	3(1)
Ag(1)	67(1)	41(1)	56(1)	-3(1)	21(1)	19(1)

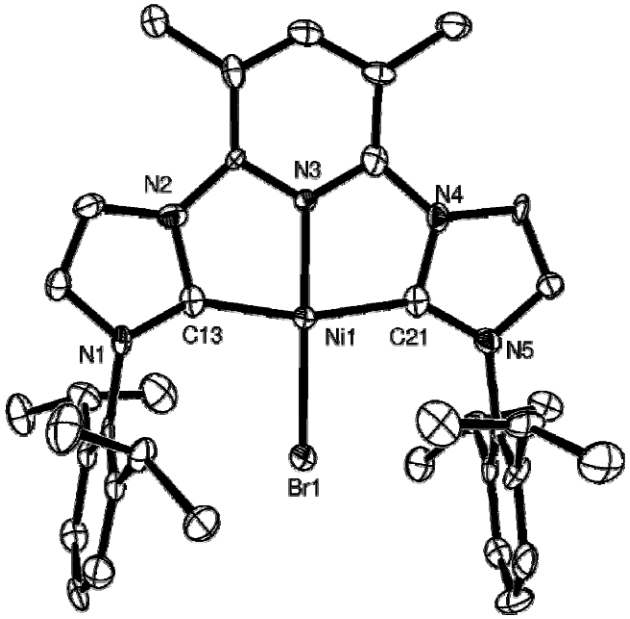


Table 1. Crystal data and structure refinement for $\mathbf{3^{Me}(OTf)^-}$.

Identification code	$\mathbf{3^{Me}(OTf)^-}$	
Empirical formula	C38 H45 Br F3 N5 Ni O3 S	
Formula weight	847.47	
Temperature	120(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.6147(3) Å	α= 101.802(2)°.
	b = 14.2268(7) Å	β= 98.787(3)°.
	c = 16.2224(8) Å	γ = 96.327(3)°.
Volume	1902.67(15) Å^3	
Z	2	
Density (calculated)	1.479 Mg/m^3	
Absorption coefficient	1.673 mm^{-1}	
F(000)	876	
Crystal size	0.42 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.95 to 25.02°.	
Index ranges	-10<=h<=10, -16<=k<=16, -19<=l<=19	
Reflections collected	27224	
Independent reflections	6686 [R(int) = 0.1479]	
Completeness to theta = 25.02°	99.4 %	
Absorption correction	Semi-empirical from equivalents	

Max. and min. transmission	0.9835 and 0.5400
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	6686 / 0 / 461
Goodness-of-fit on F^2	1.126
Final R indices [I>2sigma(I)]	R1 = 0.1050, wR2 = 0.1744
R indices (all data)	R1 = 0.1853, wR2 = 0.2085
Largest diff. peak and hole	0.654 and -0.664 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **3^{Me}(OTf)$^-$**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	305(11)	344(7)	2558(6)	18(2)
C(2)	-1240(10)	513(7)	2653(6)	19(2)
C(3)	-2404(10)	119(7)	1956(6)	22(2)
C(4)	-2079(12)	-444(7)	1208(7)	27(2)
C(5)	-535(11)	-608(7)	1144(7)	26(2)
C(6)	678(10)	-199(7)	1824(6)	19(2)
C(7)	-1593(11)	1147(7)	3457(7)	26(2)
C(8)	-3158(12)	763(8)	3700(7)	33(3)
C(9)	-1563(13)	2199(9)	3393(8)	42(3)
C(10)	2404(11)	-347(7)	1760(6)	21(2)
C(11)	2765(12)	-343(8)	860(6)	29(3)
C(12)	2830(13)	-1243(8)	2047(8)	39(3)
C(13)	2552(10)	1581(7)	3448(6)	17(2)
C(14)	1841(10)	291(7)	3975(6)	21(2)
C(15)	3016(11)	845(7)	4567(6)	23(2)
C(16)	4584(10)	2478(7)	4582(6)	16(2)
C(17)	5560(10)	2778(7)	5379(6)	21(2)
C(18)	6553(10)	3636(7)	5525(6)	21(2)
C(19)	6634(10)	4230(7)	4941(6)	20(2)
C(20)	5615(10)	3858(7)	4155(6)	21(2)

C(21)	4367(10)	3726(7)	2722(6)	17(2)
C(22)	6291(10)	5063(7)	3225(6)	17(2)
C(23)	5691(11)	5041(7)	2415(6)	22(2)
C(24)	3605(11)	3976(7)	1243(6)	18(2)
C(25)	2165(10)	4320(7)	1119(6)	18(2)
C(26)	1286(11)	4046(7)	278(6)	23(2)
C(27)	1855(12)	3483(8)	-376(7)	30(3)
C(28)	3339(12)	3184(7)	-211(7)	29(2)
C(29)	4261(11)	3426(7)	598(6)	21(2)
C(30)	1535(10)	4937(7)	1830(6)	20(2)
C(31)	-255(11)	4678(8)	1782(7)	31(3)
C(32)	1944(11)	6010(7)	1838(7)	29(3)
C(33)	5866(11)	3057(8)	792(6)	26(2)
C(34)	5639(11)	2054(8)	972(8)	36(3)
C(35)	6831(13)	3116(10)	74(7)	41(3)
C(36)	5593(11)	2165(8)	6052(7)	26(2)
C(37)	7775(12)	5142(8)	5148(7)	29(3)
C(38)	1390(11)	2284(8)	6926(7)	29(3)
N(1)	1570(9)	746(6)	3305(5)	20(2)
N(2)	3462(8)	1651(6)	4249(5)	19(2)
N(3)	4630(8)	3018(5)	3994(5)	13(2)
N(4)	5481(8)	4253(6)	3424(5)	18(2)
N(5)	4532(8)	4230(6)	2110(5)	21(2)
O(1)	115(7)	3608(5)	6333(4)	29(2)
O(2)	1789(8)	2698(5)	5492(5)	34(2)
O(3)	-813(8)	1930(5)	5605(5)	34(2)
F(1)	1861(7)	1415(4)	6691(4)	39(2)
F(2)	376(7)	2180(5)	7448(4)	40(2)
F(3)	2666(7)	2889(5)	7359(4)	44(2)
S(1)	507(3)	2673(2)	5972(2)	23(1)
Ni(1)	3210(1)	2616(1)	2947(1)	16(1)
Br(1)	1390(1)	2184(1)	1714(1)	27(1)

Table 3. Bond lengths [Å] and angles [°] for $\mathbf{3^{Me}(OTf)^-}$.

C(1)-C(6)	1.384(13)	C(14)-N(1)	1.379(12)
C(1)-C(2)	1.404(13)	C(14)-H(14)	0.9500
C(1)-N(1)	1.469(11)	C(15)-N(2)	1.390(13)
C(2)-C(3)	1.367(13)	C(15)-H(15)	0.9500
C(2)-C(7)	1.520(14)	C(16)-N(3)	1.344(11)
C(3)-C(4)	1.395(14)	C(16)-C(17)	1.387(13)
C(3)-H(3)	0.9500	C(16)-N(2)	1.393(11)
C(4)-C(5)	1.391(13)	C(17)-C(18)	1.367(13)
C(4)-H(4)	0.9500	C(17)-C(36)	1.528(14)
C(5)-C(6)	1.377(13)	C(18)-C(19)	1.397(14)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.540(12)	C(19)-C(20)	1.399(13)
C(7)-C(9)	1.520(16)	C(19)-C(37)	1.484(13)
C(7)-C(8)	1.536(13)	C(20)-N(3)	1.341(12)
C(7)-H(7)	1.0000	C(20)-N(4)	1.407(12)
C(8)-H(8A)	0.9800	C(21)-N(5)	1.354(12)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.392(11)
C(8)-H(8C)	0.9800	C(21)-Ni(1)	1.901(9)
C(9)-H(9A)	0.9800	C(22)-C(23)	1.328(13)
C(9)-H(9B)	0.9800	C(22)-N(4)	1.401(12)
C(9)-H(9C)	0.9800	C(22)-H(22)	0.9500
C(10)-C(12)	1.507(14)	C(23)-N(5)	1.391(12)
C(10)-C(11)	1.540(13)	C(23)-H(23)	0.9500
C(10)-H(10)	1.0000	C(24)-C(25)	1.384(13)
C(11)-H(11A)	0.9800	C(24)-C(29)	1.404(13)
C(11)-H(11B)	0.9800	C(24)-N(5)	1.460(12)
C(11)-H(11C)	0.9800	C(25)-C(26)	1.409(13)
C(12)-H(12A)	0.9800	C(25)-C(30)	1.510(13)
C(12)-H(12B)	0.9800	C(26)-C(27)	1.380(14)
C(12)-H(12C)	0.9800	C(26)-H(26)	0.9500
C(13)-N(1)	1.336(11)	C(27)-C(28)	1.395(14)
C(13)-N(2)	1.390(12)	C(27)-H(27)	0.9500
C(13)-Ni(1)	1.897(10)	C(28)-C(29)	1.382(14)
C(14)-C(15)	1.336(13)	C(28)-H(28)	0.9500

C(29)-C(33)	1.543(13)	C(6)-C(1)-N(1)	119.2(8)
C(30)-C(32)	1.525(14)	C(2)-C(1)-N(1)	116.8(8)
C(30)-C(31)	1.531(12)	C(3)-C(2)-C(1)	115.9(9)
C(30)-H(30)	1.0000	C(3)-C(2)-C(7)	121.7(8)
C(31)-H(31A)	0.9800	C(1)-C(2)-C(7)	122.3(8)
C(31)-H(31B)	0.9800	C(2)-C(3)-C(4)	121.8(9)
C(31)-H(31C)	0.9800	C(2)-C(3)-H(3)	119.1
C(32)-H(32A)	0.9800	C(4)-C(3)-H(3)	119.1
C(32)-H(32B)	0.9800	C(5)-C(4)-C(3)	120.5(9)
C(32)-H(32C)	0.9800	C(5)-C(4)-H(4)	119.7
C(33)-C(34)	1.512(15)	C(3)-C(4)-H(4)	119.7
C(33)-C(35)	1.541(14)	C(6)-C(5)-C(4)	119.4(9)
C(33)-H(33)	1.0000	C(6)-C(5)-H(5)	120.3
C(34)-H(34A)	0.9800	C(4)-C(5)-H(5)	120.3
C(34)-H(34B)	0.9800	C(5)-C(6)-C(1)	118.4(9)
C(34)-H(34C)	0.9800	C(5)-C(6)-C(10)	120.4(9)
C(35)-H(35A)	0.9800	C(1)-C(6)-C(10)	121.3(8)
C(35)-H(35B)	0.9800	C(2)-C(7)-C(9)	112.0(9)
C(35)-H(35C)	0.9800	C(2)-C(7)-C(8)	112.9(8)
C(36)-H(36A)	0.9800	C(9)-C(7)-C(8)	110.6(8)
C(36)-H(36B)	0.9800	C(2)-C(7)-H(7)	107.0
C(36)-H(36C)	0.9800	C(9)-C(7)-H(7)	107.0
C(37)-H(37A)	0.9800	C(8)-C(7)-H(7)	107.0
C(37)-H(37B)	0.9800	C(7)-C(8)-H(8A)	109.5
C(37)-H(37C)	0.9800	C(7)-C(8)-H(8B)	109.5
C(38)-F(2)	1.323(11)	H(8A)-C(8)-H(8B)	109.5
C(38)-F(3)	1.324(11)	C(7)-C(8)-H(8C)	109.5
C(38)-F(1)	1.342(12)	H(8A)-C(8)-H(8C)	109.5
C(38)-S(1)	1.833(12)	H(8B)-C(8)-H(8C)	109.5
N(3)-Ni(1)	1.877(7)	C(7)-C(9)-H(9A)	109.5
O(1)-S(1)	1.437(7)	C(7)-C(9)-H(9B)	109.5
O(2)-S(1)	1.447(7)	H(9A)-C(9)-H(9B)	109.5
O(3)-S(1)	1.428(7)	C(7)-C(9)-H(9C)	109.5
Ni(1)-Br(1)	2.2717(15)	H(9A)-C(9)-H(9C)	109.5
		H(9B)-C(9)-H(9C)	109.5
C(6)-C(1)-C(2)	124.0(9)	C(12)-C(10)-C(11)	111.5(9)

C(12)-C(10)-C(6)	112.2(8)	C(18)-C(19)-C(37)	121.3(9)
C(11)-C(10)-C(6)	112.1(8)	C(20)-C(19)-C(37)	124.8(9)
C(12)-C(10)-H(10)	106.9	N(3)-C(20)-C(19)	122.4(9)
C(11)-C(10)-H(10)	106.9	N(3)-C(20)-N(4)	110.0(8)
C(6)-C(10)-H(10)	106.9	C(19)-C(20)-N(4)	127.6(9)
C(10)-C(11)-H(11A)	109.5	N(5)-C(21)-N(4)	103.4(8)
C(10)-C(11)-H(11B)	109.5	N(5)-C(21)-Ni(1)	143.3(7)
H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-Ni(1)	113.3(7)
C(10)-C(11)-H(11C)	109.5	C(23)-C(22)-N(4)	106.2(8)
H(11A)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22)	126.9
H(11B)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22)	126.9
C(10)-C(12)-H(12A)	109.5	C(22)-C(23)-N(5)	108.3(9)
C(10)-C(12)-H(12B)	109.5	C(22)-C(23)-H(23)	125.9
H(12A)-C(12)-H(12B)	109.5	N(5)-C(23)-H(23)	125.9
C(10)-C(12)-H(12C)	109.5	C(25)-C(24)-C(29)	125.1(9)
H(12A)-C(12)-H(12C)	109.5	C(25)-C(24)-N(5)	117.3(8)
H(12B)-C(12)-H(12C)	109.5	C(29)-C(24)-N(5)	117.6(8)
N(1)-C(13)-N(2)	104.2(8)	C(24)-C(25)-C(26)	115.9(9)
N(1)-C(13)-Ni(1)	143.6(7)	C(24)-C(25)-C(30)	123.1(9)
N(2)-C(13)-Ni(1)	112.0(6)	C(26)-C(25)-C(30)	121.1(8)
C(15)-C(14)-N(1)	108.0(9)	C(27)-C(26)-C(25)	121.4(9)
C(15)-C(14)-H(14)	126.0	C(27)-C(26)-H(26)	119.3
N(1)-C(14)-H(14)	126.0	C(25)-C(26)-H(26)	119.3
C(14)-C(15)-N(2)	106.2(9)	C(26)-C(27)-C(28)	119.9(10)
C(14)-C(15)-H(15)	126.9	C(26)-C(27)-H(27)	120.1
N(2)-C(15)-H(15)	126.9	C(28)-C(27)-H(27)	120.1
N(3)-C(16)-C(17)	120.6(8)	C(29)-C(28)-C(27)	121.7(10)
N(3)-C(16)-N(2)	109.4(8)	C(29)-C(28)-H(28)	119.1
C(17)-C(16)-N(2)	129.9(9)	C(27)-C(28)-H(28)	119.1
C(18)-C(17)-C(16)	116.7(9)	C(28)-C(29)-C(24)	116.0(9)
C(18)-C(17)-C(36)	121.0(9)	C(28)-C(29)-C(33)	121.9(9)
C(16)-C(17)-C(36)	122.2(8)	C(24)-C(29)-C(33)	122.0(9)
C(17)-C(18)-C(19)	125.0(9)	C(25)-C(30)-C(32)	110.3(8)
C(17)-C(18)-H(18)	117.5	C(25)-C(30)-C(31)	113.3(8)
C(19)-C(18)-H(18)	117.5	C(32)-C(30)-C(31)	110.0(8)
C(18)-C(19)-C(20)	113.9(9)	C(25)-C(30)-H(30)	107.7

C(32)-C(30)-H(30)	107.7	H(36A)-C(36)-H(36C)	109.5
C(31)-C(30)-H(30)	107.7	H(36B)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31A)	109.5	C(19)-C(37)-H(37A)	109.5
C(30)-C(31)-H(31B)	109.5	C(19)-C(37)-H(37B)	109.5
H(31A)-C(31)-H(31B)	109.5	H(37A)-C(37)-H(37B)	109.5
C(30)-C(31)-H(31C)	109.5	C(19)-C(37)-H(37C)	109.5
H(31A)-C(31)-H(31C)	109.5	H(37A)-C(37)-H(37C)	109.5
H(31B)-C(31)-H(31C)	109.5	H(37B)-C(37)-H(37C)	109.5
C(30)-C(32)-H(32A)	109.5	F(2)-C(38)-F(3)	108.9(9)
C(30)-C(32)-H(32B)	109.5	F(2)-C(38)-F(1)	106.7(9)
H(32A)-C(32)-H(32B)	109.5	F(3)-C(38)-F(1)	106.7(8)
C(30)-C(32)-H(32C)	109.5	F(2)-C(38)-S(1)	112.7(7)
H(32A)-C(32)-H(32C)	109.5	F(3)-C(38)-S(1)	111.9(8)
H(32B)-C(32)-H(32C)	109.5	F(1)-C(38)-S(1)	109.7(7)
C(34)-C(33)-C(35)	112.9(9)	C(13)-N(1)-C(14)	111.4(8)
C(34)-C(33)-C(29)	111.3(8)	C(13)-N(1)-C(1)	126.6(8)
C(35)-C(33)-C(29)	111.0(9)	C(14)-N(1)-C(1)	122.0(8)
C(34)-C(33)-H(33)	107.1	C(13)-N(2)-C(15)	110.2(7)
C(35)-C(33)-H(33)	107.1	C(13)-N(2)-C(16)	117.1(8)
C(29)-C(33)-H(33)	107.1	C(15)-N(2)-C(16)	132.7(8)
C(33)-C(34)-H(34A)	109.5	C(20)-N(3)-C(16)	121.5(8)
C(33)-C(34)-H(34B)	109.5	C(20)-N(3)-Ni(1)	119.4(7)
H(34A)-C(34)-H(34B)	109.5	C(16)-N(3)-Ni(1)	119.1(6)
C(33)-C(34)-H(34C)	109.5	C(21)-N(4)-C(22)	110.9(8)
H(34A)-C(34)-H(34C)	109.5	C(21)-N(4)-C(20)	115.5(8)
H(34B)-C(34)-H(34C)	109.5	C(22)-N(4)-C(20)	133.6(8)
C(33)-C(35)-H(35A)	109.5	C(21)-N(5)-C(23)	111.3(8)
C(33)-C(35)-H(35B)	109.5	C(21)-N(5)-C(24)	125.0(8)
H(35A)-C(35)-H(35B)	109.5	C(23)-N(5)-C(24)	123.7(8)
C(33)-C(35)-H(35C)	109.5	O(3)-S(1)-O(1)	115.5(4)
H(35A)-C(35)-H(35C)	109.5	O(3)-S(1)-O(2)	115.7(4)
H(35B)-C(35)-H(35C)	109.5	O(1)-S(1)-O(2)	114.8(4)
C(17)-C(36)-H(36A)	109.5	O(3)-S(1)-C(38)	102.7(5)
C(17)-C(36)-H(36B)	109.5	O(1)-S(1)-C(38)	102.4(4)
H(36A)-C(36)-H(36B)	109.5	O(2)-S(1)-C(38)	102.9(4)
C(17)-C(36)-H(36C)	109.5	N(3)-Ni(1)-C(13)	82.0(4)

N(3)-Ni(1)-C(21)	81.5(4)	C(13)-Ni(1)-Br(1)	98.0(3)
C(13)-Ni(1)-C(21)	163.2(4)	C(21)-Ni(1)-Br(1)	98.6(3)
N(3)-Ni(1)-Br(1)	176.6(2)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **$3^{Me}(OTf)^-$**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	30(4)	7(4)	16(4)	6(3)	4(3)	-6(3)
C(2)	23(3)	14(4)	21(4)	8(3)	5(3)	-1(3)
C(3)	14(4)	22(6)	34(6)	10(5)	5(4)	6(4)
C(4)	34(6)	15(6)	29(6)	4(5)	5(5)	-11(4)
C(5)	29(5)	22(6)	25(6)	3(5)	7(4)	5(4)
C(6)	23(3)	14(4)	21(4)	8(3)	5(3)	-1(3)
C(7)	18(5)	26(6)	31(6)	0(5)	1(4)	6(4)
C(8)	33(6)	23(6)	46(7)	5(5)	22(5)	3(5)
C(9)	35(6)	43(8)	46(8)	2(6)	15(6)	1(5)
C(10)	28(5)	24(6)	16(5)	5(4)	14(4)	5(4)
C(11)	32(6)	33(7)	23(6)	6(5)	9(5)	5(5)
C(12)	34(6)	38(7)	55(8)	26(6)	11(6)	16(5)
C(13)	18(3)	11(4)	22(4)	3(3)	8(3)	8(3)
C(14)	23(5)	23(6)	21(6)	8(5)	10(4)	2(4)
C(15)	24(5)	29(6)	15(6)	6(5)	0(4)	4(4)
C(16)	16(4)	19(6)	14(5)	10(4)	-2(4)	-3(4)
C(17)	17(5)	18(6)	29(6)	8(5)	10(4)	2(4)
C(18)	13(4)	30(6)	19(6)	-1(5)	2(4)	7(4)
C(19)	12(4)	27(6)	19(6)	0(5)	-1(4)	6(4)
C(20)	11(4)	27(6)	28(6)	11(5)	8(4)	6(4)
C(21)	18(3)	11(4)	22(4)	3(3)	8(3)	8(3)
C(22)	17(4)	18(6)	24(6)	16(4)	4(4)	3(4)
C(23)	26(5)	25(6)	13(6)	1(4)	4(4)	-4(4)
C(24)	30(4)	7(4)	16(4)	6(3)	4(3)	-6(3)
C(25)	18(5)	19(6)	23(6)	11(4)	9(4)	-1(4)
C(26)	21(5)	20(6)	28(6)	6(5)	4(4)	2(4)
C(27)	37(6)	32(7)	18(6)	6(5)	-4(5)	10(5)
C(28)	49(6)	13(6)	26(6)	8(5)	11(5)	1(5)
C(29)	31(5)	23(6)	16(6)	10(4)	9(4)	8(4)
C(30)	26(5)	20(6)	15(5)	8(4)	-2(4)	5(4)
C(31)	25(5)	40(7)	31(7)	8(5)	16(5)	5(5)

C(32)	23(5)	30(7)	30(7)	-2(5)	3(4)	6(4)
C(33)	28(5)	35(7)	13(6)	-4(5)	4(4)	9(5)
C(34)	23(5)	37(7)	48(8)	1(6)	15(5)	15(5)
C(35)	34(6)	59(9)	30(7)	1(6)	14(5)	10(6)
C(36)	25(5)	26(6)	27(6)	9(5)	4(4)	-3(4)
C(37)	31(5)	29(7)	23(6)	2(5)	-5(5)	0(5)
C(38)	23(5)	23(6)	39(7)	-1(5)	13(5)	2(4)
N(1)	25(4)	12(5)	23(5)	8(4)	3(4)	0(3)
N(2)	17(4)	26(5)	14(4)	3(4)	2(3)	3(3)
N(3)	17(4)	13(4)	8(4)	-1(3)	4(3)	0(3)
N(4)	20(4)	19(5)	18(5)	5(4)	9(3)	-1(3)
N(5)	16(4)	21(5)	23(5)	7(4)	-3(3)	0(3)
O(1)	31(4)	24(4)	32(4)	2(3)	5(3)	8(3)
O(2)	36(4)	33(5)	40(5)	14(4)	23(3)	5(3)
O(3)	27(4)	34(5)	33(5)	-1(4)	1(3)	-9(3)
F(1)	46(4)	25(4)	52(4)	17(3)	12(3)	10(3)
F(2)	44(4)	52(4)	27(4)	13(3)	16(3)	3(3)
F(3)	38(4)	36(4)	49(4)	14(3)	-13(3)	-9(3)
S(1)	24(1)	20(2)	23(2)	2(1)	6(1)	1(1)
Ni(1)	17(1)	17(1)	15(1)	5(1)	0(1)	-1(1)
Br(1)	30(1)	25(1)	24(1)	10(1)	-5(1)	-7(1)

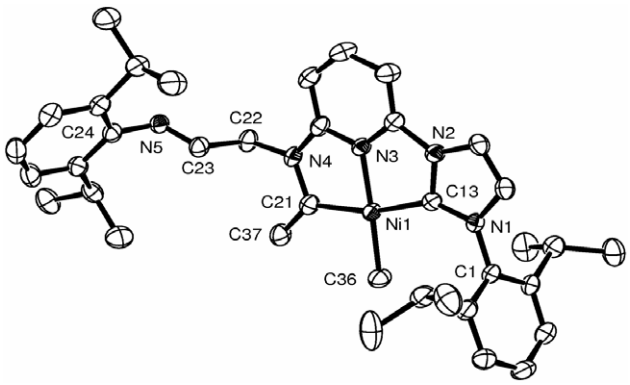


Table 1. Crystal data and structure refinement for **7**.

Identification code	**7**	
Empirical formula	C41 H57 N5 Ni O	
Formula weight	694.63	
Temperature	120(2) K	
Wavelength	0.6709 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.907(2) Å	α= 111.24(3)°.
	b = 13.813(3) Å	β= 93.82(3)°.
	c = 15.330(3) Å	γ = 99.87(3)°.
Volume	1907.3(7) Å^3	
Z	2	
Density (calculated)	1.210 Mg/m^3	
Absorption coefficient	0.546 mm^{-1}	
F(000)	748	
Crystal size	0.02 x 0.02 x 0.01 mm^3	
Theta range for data collection	2.37 to 28.33°.	
Index ranges	-13<=h<=13, -18<=k<=18, -19<=l<=20	
Reflections collected	18662	
Independent reflections	9332 [R(int) = 0.0377]	
Completeness to theta = 27.50°	98.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9946 and 0.9892	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9332 / 0 / 444	
Goodness-of-fit on F^2	1.024	
Final R indices [I>2sigma(I)]	R1 = 0.0498, wR2 = 0.1154	

R indices (all data)	R1 = 0.0797, wR2 = 0.1286
Largest diff. peak and hole	0.459 and -0.407 e.Å^{-3}

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^{2}x 10^3) for **7**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	-1906(2)	1831(2)	4085(2)	24(1)
C(2)	-2594(2)	2496(2)	3804(2)	26(1)
C(3)	-4019(2)	2166(2)	3550(2)	32(1)
C(4)	-4714(2)	1220(2)	3565(2)	36(1)
C(5)	-4002(3)	577(2)	3840(2)	36(1)
C(6)	-2578(2)	867(2)	4103(2)	30(1)
C(7)	-1830(3)	3542(2)	3795(2)	33(1)
C(8)	-1953(4)	4454(2)	4693(2)	53(1)
C(9)	-2307(3)	3739(2)	2921(2)	47(1)
C(10)	-1804(3)	141(2)	4384(2)	40(1)
C(11)	-2465(4)	-218(3)	5111(2)	62(1)
C(12)	-1701(3)	-813(3)	3520(2)	52(1)
C(13)	275(2)	2655(2)	5224(2)	24(1)
C(14)	484(2)	1909(2)	3656(2)	28(1)
C(15)	1770(2)	2298(2)	4117(2)	28(1)
C(16)	2665(2)	3218(2)	5864(2)	26(1)
C(17)	4068(2)	3356(2)	5884(2)	35(1)
C(18)	4847(3)	3824(2)	6785(2)	39(1)
C(19)	4244(3)	4119(2)	7595(2)	35(1)
C(20)	2793(2)	3939(2)	7502(2)	28(1)
C(21)	500(2)	3798(2)	7903(2)	29(1)
C(22)	2611(3)	4618(2)	9186(2)	34(1)
C(23)	2785(2)	3778(2)	9564(2)	31(1)
C(24)	3713(2)	3127(2)	10601(2)	29(1)
C(25)	4636(2)	2460(2)	10255(2)	32(1)

C(26)	4680(3)	1650(2)	10588(2)	39(1)
C(27)	3851(3)	1519(2)	11248(2)	43(1)
C(28)	2983(3)	2209(2)	11597(2)	40(1)
C(29)	2898(3)	3029(2)	11294(2)	32(1)
C(30)	5553(2)	2595(2)	9536(2)	33(1)
C(31)	4967(3)	1797(3)	8538(2)	48(1)
C(32)	7034(3)	2532(2)	9803(2)	45(1)
C(33)	1933(3)	3778(2)	11662(2)	35(1)
C(34)	488(3)	3326(2)	11098(2)	47(1)
C(35)	1827(3)	4064(2)	12709(2)	49(1)
C(36)	-1866(2)	2917(2)	6491(2)	35(1)
C(37)	-319(3)	3884(2)	8575(2)	38(1)
C(38)	7810(4)	10568(3)	1255(2)	59(1)
C(39)	8604(3)	9716(3)	945(2)	55(1)
C(40)	10497(3)	9129(3)	1444(2)	57(1)
C(41)	11642(3)	9410(3)	2221(2)	55(1)
N(1)	-417(2)	2137(1)	4335(1)	24(1)
N(2)	1643(2)	2747(2)	5065(1)	25(1)
N(3)	2047(2)	3493(1)	6639(1)	24(1)
N(4)	1980(2)	4158(2)	8198(1)	28(1)
N(5)	3649(2)	3970(2)	10277(1)	29(1)
Ni(1)	114(1)	3208(1)	6541(1)	24(1)
O(1)	9752(2)	9940(1)	1630(1)	40(1)

Table 3. Bond lengths [Å] and angles [°] for **7**.

C(1)-C(6)	1.393(3)	C(14)-N(1)	1.400(3)
C(1)-C(2)	1.399(3)	C(14)-H(14)	0.9500
C(1)-N(1)	1.448(3)	C(15)-N(2)	1.382(3)
C(2)-C(3)	1.390(3)	C(15)-H(15)	0.9500
C(2)-C(7)	1.517(3)	C(16)-N(3)	1.334(3)
C(3)-C(4)	1.378(4)	C(16)-C(17)	1.367(3)
C(3)-H(3)	0.9500	C(16)-N(2)	1.407(3)
C(4)-C(5)	1.382(4)	C(17)-C(18)	1.400(4)
C(4)-H(4)	0.9500	C(17)-H(17)	0.9500
C(5)-C(6)	1.387(3)	C(18)-C(19)	1.371(4)
C(5)-H(5)	0.9500	C(18)-H(18)	0.9500
C(6)-C(10)	1.521(3)	C(19)-C(20)	1.405(3)
C(7)-C(9)	1.521(3)	C(19)-H(19)	0.9500
C(7)-C(8)	1.522(4)	C(20)-N(3)	1.342(3)
C(7)-H(7)	1.0000	C(20)-N(4)	1.359(3)
C(8)-H(8A)	0.9800	C(21)-C(37)	1.337(3)
C(8)-H(8B)	0.9800	C(21)-N(4)	1.449(3)
C(8)-H(8C)	0.9800	C(21)-Ni(1)	1.930(2)
C(9)-H(9A)	0.9800	C(22)-N(4)	1.459(3)
C(9)-H(9B)	0.9800	C(22)-C(23)	1.502(3)
C(9)-H(9C)	0.9800	C(22)-H(22A)	0.9900
C(10)-C(12)	1.517(4)	C(22)-H(22B)	0.9900
C(10)-C(11)	1.517(4)	C(23)-N(5)	1.259(3)
C(10)-H(10)	1.0000	C(23)-H(23)	0.9500
C(11)-H(11A)	0.9800	C(24)-C(25)	1.402(3)
C(11)-H(11B)	0.9800	C(24)-C(29)	1.408(3)
C(11)-H(11C)	0.9800	C(24)-N(5)	1.431(3)
C(12)-H(12A)	0.9800	C(25)-C(26)	1.394(4)
C(12)-H(12B)	0.9800	C(25)-C(30)	1.516(3)
C(12)-H(12C)	0.9800	C(26)-C(27)	1.387(4)
C(13)-N(1)	1.356(3)	C(26)-H(26)	0.9500
C(13)-N(2)	1.386(3)	C(27)-C(28)	1.381(4)
C(13)-Ni(1)	1.912(2)	C(27)-H(27)	0.9500
C(14)-C(15)	1.335(3)	C(28)-C(29)	1.383(4)

C(28)-H(28)	0.9500	C(40)-H(40B)	0.9900
C(29)-C(33)	1.514(4)	C(41)-H(41A)	0.9800
C(30)-C(32)	1.523(3)	C(41)-H(41B)	0.9800
C(30)-C(31)	1.528(4)	C(41)-H(41C)	0.9800
C(30)-H(30)	1.0000	N(3)-Ni(1)	1.8725(19)
C(31)-H(31A)	0.9800		
C(31)-H(31B)	0.9800	C(6)-C(1)-C(2)	123.2(2)
C(31)-H(31C)	0.9800	C(6)-C(1)-N(1)	118.24(19)
C(32)-H(32A)	0.9800	C(2)-C(1)-N(1)	118.5(2)
C(32)-H(32B)	0.9800	C(3)-C(2)-C(1)	116.9(2)
C(32)-H(32C)	0.9800	C(3)-C(2)-C(7)	121.2(2)
C(33)-C(35)	1.523(3)	C(1)-C(2)-C(7)	121.8(2)
C(33)-C(34)	1.524(4)	C(4)-C(3)-C(2)	121.2(2)
C(33)-H(33)	1.0000	C(4)-C(3)-H(3)	119.4
C(34)-H(34A)	0.9800	C(2)-C(3)-H(3)	119.4
C(34)-H(34B)	0.9800	C(3)-C(4)-C(5)	120.4(2)
C(34)-H(34C)	0.9800	C(3)-C(4)-H(4)	119.8
C(35)-H(35A)	0.9800	C(5)-C(4)-H(4)	119.8
C(35)-H(35B)	0.9800	C(4)-C(5)-C(6)	120.9(2)
C(35)-H(35C)	0.9800	C(4)-C(5)-H(5)	119.5
C(36)-Ni(1)	1.924(2)	C(6)-C(5)-H(5)	119.5
C(36)-H(36A)	0.9800	C(5)-C(6)-C(1)	117.4(2)
C(36)-H(36B)	0.9800	C(5)-C(6)-C(10)	120.3(2)
C(36)-H(36C)	0.9800	C(1)-C(6)-C(10)	122.3(2)
C(37)-H(37A)	0.9500	C(2)-C(7)-C(9)	113.1(2)
C(37)-H(37B)	0.9500	C(2)-C(7)-C(8)	110.1(2)
C(38)-C(39)	1.481(4)	C(9)-C(7)-C(8)	111.0(2)
C(38)-H(38A)	0.9800	C(2)-C(7)-H(7)	107.5
C(38)-H(38B)	0.9800	C(9)-C(7)-H(7)	107.5
C(38)-H(38C)	0.9800	C(8)-C(7)-H(7)	107.5
C(39)-O(1)	1.405(3)	C(7)-C(8)-H(8A)	109.5
C(39)-H(39A)	0.9900	C(7)-C(8)-H(8B)	109.5
C(39)-H(39B)	0.9900	H(8A)-C(8)-H(8B)	109.5
C(40)-O(1)	1.401(3)	C(7)-C(8)-H(8C)	109.5
C(40)-C(41)	1.480(4)	H(8A)-C(8)-H(8C)	109.5
C(40)-H(40A)	0.9900	H(8B)-C(8)-H(8C)	109.5

C(7)-C(9)-H(9A)	109.5	C(16)-C(17)-C(18)	115.6(2)
C(7)-C(9)-H(9B)	109.5	C(16)-C(17)-H(17)	122.2
H(9A)-C(9)-H(9B)	109.5	C(18)-C(17)-H(17)	122.2
C(7)-C(9)-H(9C)	109.5	C(19)-C(18)-C(17)	122.3(2)
H(9A)-C(9)-H(9C)	109.5	C(19)-C(18)-H(18)	118.9
H(9B)-C(9)-H(9C)	109.5	C(17)-C(18)-H(18)	118.9
C(12)-C(10)-C(11)	110.4(2)	C(18)-C(19)-C(20)	117.9(2)
C(12)-C(10)-C(6)	110.5(2)	C(18)-C(19)-H(19)	121.0
C(11)-C(10)-C(6)	112.2(2)	C(20)-C(19)-H(19)	121.0
C(12)-C(10)-H(10)	107.9	N(3)-C(20)-N(4)	112.1(2)
C(11)-C(10)-H(10)	107.9	N(3)-C(20)-C(19)	119.8(2)
C(6)-C(10)-H(10)	107.9	N(4)-C(20)-C(19)	128.1(2)
C(10)-C(11)-H(11A)	109.5	C(37)-C(21)-N(4)	117.9(2)
C(10)-C(11)-H(11B)	109.5	C(37)-C(21)-Ni(1)	132.2(2)
H(11A)-C(11)-H(11B)	109.5	N(4)-C(21)-Ni(1)	109.84(16)
C(10)-C(11)-H(11C)	109.5	N(4)-C(22)-C(23)	111.8(2)
H(11A)-C(11)-H(11C)	109.5	N(4)-C(22)-H(22A)	109.3
H(11B)-C(11)-H(11C)	109.5	C(23)-C(22)-H(22A)	109.3
C(10)-C(12)-H(12A)	109.5	N(4)-C(22)-H(22B)	109.3
C(10)-C(12)-H(12B)	109.5	C(23)-C(22)-H(22B)	109.3
H(12A)-C(12)-H(12B)	109.5	H(22A)-C(22)-H(22B)	107.9
C(10)-C(12)-H(12C)	109.5	N(5)-C(23)-C(22)	121.7(2)
H(12A)-C(12)-H(12C)	109.5	N(5)-C(23)-H(23)	119.2
H(12B)-C(12)-H(12C)	109.5	C(22)-C(23)-H(23)	119.2
N(1)-C(13)-N(2)	102.15(18)	C(25)-C(24)-C(29)	122.1(2)
N(1)-C(13)-Ni(1)	145.66(17)	C(25)-C(24)-N(5)	119.1(2)
N(2)-C(13)-Ni(1)	112.06(15)	C(29)-C(24)-N(5)	118.8(2)
C(15)-C(14)-N(1)	107.1(2)	C(26)-C(25)-C(24)	117.7(2)
C(15)-C(14)-H(14)	126.5	C(26)-C(25)-C(30)	120.4(2)
N(1)-C(14)-H(14)	126.5	C(24)-C(25)-C(30)	121.9(2)
C(14)-C(15)-N(2)	106.3(2)	C(27)-C(26)-C(25)	121.0(3)
C(14)-C(15)-H(15)	126.9	C(27)-C(26)-H(26)	119.5
N(2)-C(15)-H(15)	126.9	C(25)-C(26)-H(26)	119.5
N(3)-C(16)-C(17)	123.5(2)	C(28)-C(27)-C(26)	119.9(3)
N(3)-C(16)-N(2)	108.82(19)	C(28)-C(27)-H(27)	120.0
C(17)-C(16)-N(2)	127.6(2)	C(26)-C(27)-H(27)	120.0

C(27)-C(28)-C(29)	121.6(2)	C(33)-C(35)-H(35A)	109.5
C(27)-C(28)-H(28)	119.2	C(33)-C(35)-H(35B)	109.5
C(29)-C(28)-H(28)	119.2	H(35A)-C(35)-H(35B)	109.5
C(28)-C(29)-C(24)	117.6(2)	C(33)-C(35)-H(35C)	109.5
C(28)-C(29)-C(33)	121.9(2)	H(35A)-C(35)-H(35C)	109.5
C(24)-C(29)-C(33)	120.4(2)	H(35B)-C(35)-H(35C)	109.5
C(25)-C(30)-C(32)	111.6(2)	Ni(1)-C(36)-H(36A)	109.5
C(25)-C(30)-C(31)	111.7(2)	Ni(1)-C(36)-H(36B)	109.5
C(32)-C(30)-C(31)	111.0(2)	H(36A)-C(36)-H(36B)	109.5
C(25)-C(30)-H(30)	107.4	Ni(1)-C(36)-H(36C)	109.5
C(32)-C(30)-H(30)	107.4	H(36A)-C(36)-H(36C)	109.5
C(31)-C(30)-H(30)	107.4	H(36B)-C(36)-H(36C)	109.5
C(30)-C(31)-H(31A)	109.5	C(21)-C(37)-H(37A)	120.0
C(30)-C(31)-H(31B)	109.5	C(21)-C(37)-H(37B)	120.0
H(31A)-C(31)-H(31B)	109.5	H(37A)-C(37)-H(37B)	120.0
C(30)-C(31)-H(31C)	109.5	C(39)-C(38)-H(38A)	109.5
H(31A)-C(31)-H(31C)	109.5	C(39)-C(38)-H(38B)	109.5
H(31B)-C(31)-H(31C)	109.5	H(38A)-C(38)-H(38B)	109.5
C(30)-C(32)-H(32A)	109.5	C(39)-C(38)-H(38C)	109.5
C(30)-C(32)-H(32B)	109.5	H(38A)-C(38)-H(38C)	109.5
H(32A)-C(32)-H(32B)	109.5	H(38B)-C(38)-H(38C)	109.5
C(30)-C(32)-H(32C)	109.5	O(1)-C(39)-C(38)	109.7(2)
H(32A)-C(32)-H(32C)	109.5	O(1)-C(39)-H(39A)	109.7
H(32B)-C(32)-H(32C)	109.5	C(38)-C(39)-H(39A)	109.7
C(29)-C(33)-C(35)	113.6(2)	O(1)-C(39)-H(39B)	109.7
C(29)-C(33)-C(34)	111.3(2)	C(38)-C(39)-H(39B)	109.7
C(35)-C(33)-C(34)	109.2(2)	H(39A)-C(39)-H(39B)	108.2
C(29)-C(33)-H(33)	107.5	O(1)-C(40)-C(41)	110.3(2)
C(35)-C(33)-H(33)	107.5	O(1)-C(40)-H(40A)	109.6
C(34)-C(33)-H(33)	107.5	C(41)-C(40)-H(40A)	109.6
C(33)-C(34)-H(34A)	109.5	O(1)-C(40)-H(40B)	109.6
C(33)-C(34)-H(34B)	109.5	C(41)-C(40)-H(40B)	109.6
H(34A)-C(34)-H(34B)	109.5	H(40A)-C(40)-H(40B)	108.1
C(33)-C(34)-H(34C)	109.5	C(40)-C(41)-H(41A)	109.5
H(34A)-C(34)-H(34C)	109.5	C(40)-C(41)-H(41B)	109.5
H(34B)-C(34)-H(34C)	109.5	H(41A)-C(41)-H(41B)	109.5

C(40)-C(41)-H(41C)	109.5	C(20)-N(4)-C(21)	116.45(19)
H(41A)-C(41)-H(41C)	109.5	C(20)-N(4)-C(22)	119.84(19)
H(41B)-C(41)-H(41C)	109.5	C(21)-N(4)-C(22)	123.3(2)
C(13)-N(1)-C(14)	112.06(19)	C(23)-N(5)-C(24)	117.7(2)
C(13)-N(1)-C(1)	125.67(18)	N(3)-Ni(1)-C(13)	81.50(9)
C(14)-N(1)-C(1)	122.26(18)	N(3)-Ni(1)-C(36)	177.77(10)
C(15)-N(2)-C(13)	112.47(19)	C(13)-Ni(1)-C(36)	100.58(11)
C(15)-N(2)-C(16)	130.25(19)	N(3)-Ni(1)-C(21)	82.68(10)
C(13)-N(2)-C(16)	117.19(19)	C(13)-Ni(1)-C(21)	164.05(10)
C(16)-N(3)-C(20)	120.9(2)	C(36)-Ni(1)-C(21)	95.21(11)
C(16)-N(3)-Ni(1)	120.41(15)	C(40)-O(1)-C(39)	114.0(2)
C(20)-N(3)-Ni(1)	118.68(16)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **7**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	26(1)	25(1)	19(1)	6(1)	-2(1)	4(1)
C(2)	31(1)	27(1)	20(1)	7(1)	1(1)	7(1)
C(3)	33(1)	34(1)	30(1)	11(1)	-1(1)	12(1)
C(4)	24(1)	41(2)	35(1)	10(1)	-4(1)	2(1)
C(5)	34(1)	34(1)	38(1)	15(1)	-2(1)	-2(1)
C(6)	31(1)	28(1)	31(1)	13(1)	-5(1)	2(1)
C(7)	37(1)	28(1)	36(1)	14(1)	2(1)	10(1)
C(8)	79(2)	29(2)	42(2)	7(1)	2(2)	5(2)
C(9)	66(2)	40(2)	41(2)	22(1)	7(1)	13(1)
C(10)	35(1)	31(1)	53(2)	24(1)	-11(1)	-4(1)
C(11)	110(3)	48(2)	40(2)	24(2)	8(2)	33(2)
C(12)	63(2)	55(2)	61(2)	37(2)	22(2)	33(2)
C(13)	25(1)	21(1)	26(1)	9(1)	2(1)	5(1)
C(14)	34(1)	29(1)	22(1)	9(1)	6(1)	10(1)
C(15)	33(1)	30(1)	24(1)	10(1)	9(1)	10(1)
C(16)	27(1)	21(1)	28(1)	9(1)	-1(1)	5(1)
C(17)	27(1)	38(1)	37(1)	10(1)	5(1)	7(1)
C(18)	24(1)	42(2)	45(2)	11(1)	-2(1)	5(1)
C(19)	31(1)	35(1)	33(1)	9(1)	-9(1)	3(1)
C(20)	30(1)	24(1)	29(1)	10(1)	-3(1)	7(1)
C(21)	33(1)	25(1)	28(1)	9(1)	-1(1)	7(1)
C(22)	42(1)	31(1)	23(1)	7(1)	-4(1)	6(1)
C(23)	35(1)	30(1)	24(1)	8(1)	-1(1)	3(1)
C(24)	30(1)	31(1)	23(1)	9(1)	-2(1)	2(1)
C(25)	30(1)	35(1)	28(1)	10(1)	-3(1)	5(1)
C(26)	39(1)	41(2)	38(1)	16(1)	0(1)	13(1)
C(27)	53(2)	44(2)	38(2)	24(1)	1(1)	10(1)
C(28)	48(2)	46(2)	30(1)	20(1)	7(1)	9(1)
C(29)	34(1)	37(1)	25(1)	11(1)	1(1)	4(1)
C(30)	31(1)	36(1)	31(1)	10(1)	4(1)	9(1)
C(31)	46(2)	57(2)	31(1)	7(1)	8(1)	6(1)

C(32)	36(1)	50(2)	52(2)	21(1)	10(1)	14(1)
C(33)	42(1)	35(1)	28(1)	11(1)	12(1)	7(1)
C(34)	42(2)	49(2)	49(2)	14(1)	10(1)	12(1)
C(35)	65(2)	48(2)	34(2)	15(1)	17(1)	12(2)
C(36)	27(1)	45(2)	30(1)	10(1)	5(1)	10(1)
C(37)	41(1)	46(2)	24(1)	10(1)	4(1)	10(1)
C(38)	61(2)	45(2)	68(2)	19(2)	-14(2)	14(2)
C(39)	48(2)	57(2)	48(2)	8(2)	-7(1)	15(2)
C(40)	49(2)	55(2)	47(2)	-7(2)	-4(1)	23(2)
C(41)	49(2)	64(2)	42(2)	5(2)	-3(1)	23(2)
N(1)	26(1)	23(1)	22(1)	9(1)	0(1)	6(1)
N(2)	25(1)	24(1)	24(1)	8(1)	1(1)	4(1)
N(3)	24(1)	21(1)	25(1)	7(1)	-1(1)	4(1)
N(4)	31(1)	29(1)	22(1)	8(1)	-4(1)	6(1)
N(5)	28(1)	35(1)	22(1)	10(1)	3(1)	6(1)
Ni(1)	23(1)	27(1)	22(1)	8(1)	1(1)	6(1)
O(1)	39(1)	37(1)	34(1)	5(1)	-2(1)	8(1)