## Supporting Information

## Blue Luminescent Rigid Molecular Rods bearing *N*-7-azaindole and 2,2 - dipyridylamine, and their Zn(II) and Ag(I) complexes.

Youngjin Kang, Corey Seward, Datong Song, and Suning Wang\* Department of Chemistry, Queen's University, Kingston, Ontario K7L 3N6, Canada



Figure 1. Enhanced phosphorescent emission spectra of 5-10 in CH<sub>2</sub>Cl<sub>2</sub> solution at 77K were obtained from time-resolved spectrometer.



Figure 2. A diagram showing the intermolecular stacking of 6. View bisecting the a- and c-axes. Arrows show  $\pi$  stacking interactions



Figure 3. Herringbone-type packing of compound 8



Figure 4. Variable temperature <sup>1</sup>H NMR spectrum of compound **10** in CD<sub>3</sub>CN

Fig 5. Excitation and emission spectra of 7 ( $[M] = 9.0 \times 10^{-5}$ ) at room temperature in CH<sub>3</sub>CN with increasing concentration of CF<sub>3</sub>COOH.



Table 1. Crystal data and structure refinement for  ${\bf 6}$ 

Empirical formula	$C_{31}H_{21}N_5$	
Formula weight	463.53	
Temperature	293(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 9.6666(17) Å	$\alpha = 90^{\circ}$ .
	b = 9.9118(17)  Å	$\beta = 95.814(3)^{\circ}$ .
	c = 25.086(4)  Å	$\gamma = 90^{\circ}$ .
Volume	2391.2(7) Å <sup>3</sup>	•
Z	4	
Density (calculated)	1.288 Mg/m <sup>3</sup>	
Absorption coefficient	0.078 mm <sup>-1</sup>	
F(000)	968	
Crystal size	.2 x .2 x .2 mm <sup>3</sup>	
Theta range for data collection	2.35 to 28.28°.	
Index ranges	-12<=h<=11, -12<=k<=12, -33<=	l<=32
Reflections collected	16958	
Independent reflections	5692 [R(int) = 0.0437]	
Completeness to theta = $28.28^{\circ}$	95.9 %	
Absorption correction	Empirical	
Max. and min. transmission	1.000 and 0.631	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	5692 / 0 / 325	
Goodness-of-fit on F <sup>2</sup>	0.828	
Final R indices [I>2sigma(I)]	R1 = 0.0466, wR2 = 0.1000	
R indices (all data)	R1 = 0.1417, $wR2 = 0.1262$	
Largest diff. peak and hole	0.137 and -0.171 e.Å <sup>-3</sup>	

Table 2. Atomic coordinates (x $10^4$ ) and equivalent isotropic displacement parameters (Å <sup>2</sup> x $10^3$ )	for <b>6</b> .	U(eq) is
defined as one third of the trace of the orthogonalized U <sup>ij</sup> tensor.		

	Х	У	Z	U(eq)
N(1)	10531(2)	-3469(2)	-1600(1)	71(1)
N(2)	11980(2)	-5039(2)	-1077(1)	98(1)
N(3)	-726(2)	-586(2)	1632(1)	79(1)
N(4)	2450(2)	-3316(2)	1956(1)	65(1)
N(5)	1084(2)	-1935(2)	1382(1)	58(1)
C(1)	10603(3)	-2864(2)	-2093(1)	91(1)
C(2)	11773(3)	-3222(3)	-2306(1)	96(1)
C(3)	13711(3)	-4857(3)	-1921(1)	104(1)
C(4)	14045(3)	-5670(4)	-1494(1)	133(1)
C(5)	13154(3)	-5748(4)	-1087(1)	142(1)
C(6)	12502(2)	-4101(3)	-1937(1)	79(1)
C(7)	11706(2)	-4256(3)	-1499(1)	73(1)
C(8)	9414(2)	-3306(2)	-1275(1)	61(1)
C(9)	8102(2)	-3078(2)	-1517(1)	68(1)
C(10)	7013(2)	-2883(2)	-1214(1)	68(1)
C(11)	7214(2)	-2915(2)	-660(1)	58(1)
C(12)	8537(2)	-3158(2)	-420(1)	69(1)
C(13)	9643(2)	-3346(2)	-723(1)	71(1)
C(14)	6071(2)	-2708(2)	-345(1)	64(1)
C(15)	5146(2)	-2543(2)	-72(1)	62(1)
C(16)	4075(2)	-2369(2)	282(1)	54(1)
C(17)	3958(2)	-1173(2)	559(1)	63(1)
C(18)	2971(2)	-1030(2)	915(1)	61(1)

C(19)	2102(2)	-2082(2)	1006(1)	55(1)
C(20)	2189(2)	-3264(2)	725(1)	69(1)
C(21)	3166(2)	-3407(2)	365(1)	67(1)
C(22)	-68(2)	-1082(2)	1237(1)	59(1)
C(23)	-445(2)	-781(2)	708(1)	79(1)
C(24)	-1568(3)	33(3)	582(1)	100(1)
C(25)	-2296(3)	526(3)	973(1)	96(1)
C(26)	-1842(3)	198(3)	1489(1)	93(1)
C(27)	1189(2)	-2796(2)	1831(1)	54(1)
C(28)	72(2)	-3116(2)	2112(1)	70(1)
C(29)	282(3)	-4002(3)	2529(1)	83(1)
C(30)	1548(3)	-4584(2)	2652(1)	83(1)
C(31)	2583(2)	-4208(2)	2358(1)	77(1)

Table 3. Bond lengths [Å] and angles  $[\circ]$  for **6**.

N(1)-C(7)	1.380(3)
N(1)-C(1)	1.383(3)
N(1)-C(8)	1.427(2)
N(2)-C(7)	1.317(3)
N(2)-C(5)	1.337(3)
N(3)-C(22)	1.324(2)
N(3)-C(26)	1.349(3)
N(4)-C(27)	1.331(2)
N(4)-C(31)	1.337(2)
N(5)-C(27)	1.408(2)
N(5)-C(22)	1.415(2)
N(5)-C(19)	1.439(2)
C(1)-C(2)	1.346(3)
C(2)-C(6)	1.407(3)
C(3)-C(4)	1.352(4)
C(3)-C(6)	1.386(3)
C(4)-C(5)	1.403(4)
C(6)-C(7)	1.411(3)
C(8)-C(9)	1.368(3)
C(8)-C(13)	1.380(3)
C(9)-C(10)	1.374(2)
C(10)-C(11)	1.382(3)
C(11)-C(12)	1.379(3)
C(11)-C(14)	1.438(3)
C(12)-C(13)	1.387(3)
C(14)-C(15)	1.190(2)
C(15)-C(16)	1.442(3)
C(16)-C(21)	1.382(3)
C(16)-C(17)	1.385(3)
C(17)-C(18)	1.378(2)
C(18)-C(19)	1.372(2)
C(19)-C(20)	1.374(2)
C(20)-C(21)	1.378(2)
C(22)-C(23)	1.374(3)
C(23)-C(24)	1.364(3)
C(24)-C(25)	1.355(3)
C(25)-C(26)	1.362(3)
C(27)-C(28)	1.385(2)
C(28)-C(29)	1.365(3)
C(29)-C(30)	1.360(3)
C(30)-C(31)	1.355(3)

C(7)-N(1)-C(1)	107.16(18)
C(7)-N(1)-C(8)	127.94(19)
C(1)-N(1)-C(8)	124.89(19)
C(7)-N(2)-C(5)	113.4(2)
C(22)-N(3)-C(26)	116.6(2)
C(27)-N(4)-C(31)	116.76(18)
C(27)-N(5)-C(22)	123.95(15)
C(27)-N(5)-C(19)	117.67(16)
C(22)-N(5)-C(19)	117.67(15)
C(2) - C(1) - N(1)	111 1(2)
C(1) - C(2) - C(6)	1067(2)
C(4) - C(3) - C(6)	100.7(2) 118 5(3)
C(3) C(4) C(5)	110.5(3)
N(2) C(5) C(4)	119.0(3) 124.7(3)
N(2) - C(3) - C(4)	124.7(3) 125.0(2)
C(3) - C(0) - C(2)	155.9(2)
C(3) - C(6) - C(7)	116.3(3)
C(2)-C(6)-C(7)	107.7(2)
N(2)-C(7)-N(1)	125.1(2)
N(2)-C(7)-C(6)	127.5(2)
N(1)-C(7)-C(6)	107.4(2)
C(9)-C(8)-C(13)	119.79(18)
C(9)-C(8)-N(1)	119.09(19)
C(13)-C(8)-N(1)	121.1(2)
C(8)-C(9)-C(10)	120.4(2)
C(9)-C(10)-C(11)	121.0(2)
C(12)-C(11)-C(10)	118.24(18)
C(12)-C(11)-C(14)	120.94(19)
C(10)-C(11)-C(14)	120.8(2)
C(11) - C(12) - C(13)	121.1(2)
C(8)-C(13)-C(12)	119.5(2)
C(15)-C(14)-C(11)	178 4(2)
C(14)-C(15)-C(16)	176.9(2)
C(21)-C(16)-C(17)	11846(17)
C(21) C(16) C(15)	120.76(18)
C(21)- $C(10)$ - $C(15)$	120.70(18) 120.76(18)
C(17)-C(10)-C(15) C(18) C(17) C(16)	120.70(18) 120.64(10)
C(10) - C(17) - C(10)	120.04(19)
C(19) - C(18) - C(17)	120.55(18)
C(18) - C(19) - C(20)	119.52(17)
C(18) - C(19) - N(5)	120.1/(17)
C(20) - C(19) - N(5)	120.29(17)
C(19)-C(20)-C(21)	120.30(19)
C(20)-C(21)-C(16)	120.70(19)
N(3)-C(22)-C(23)	122.7(2)
N(3)-C(22)-N(5)	117.06(18)
C(23)-C(22)-N(5)	120.20(18)
C(24)-C(23)-C(22)	118.7(2)
C(25)-C(24)-C(23)	120.3(2)
C(24)-C(25)-C(26)	117.4(2)
N(3)-C(26)-C(25)	124.2(2)
N(4)-C(27)-C(28)	122.24(19)
N(4)-C(27)-N(5)	114.44(17)
C(28)-C(27)-N(5)	123.28(19)
C(29)-C(28)-C(27)	118.3(2)
C(30)-C(29)-C(28)	120.6(2)
C(31)-C(30)-C(29)	117.1(2)
N(4)-C(31)-C(30)	124.9(2)

Table 4.	Anisotropic displacement parameters (Å	$A^2 x 10^3$ ) for <b>6</b> .	The anisotropic	displacement factor	exponent
takes the	form: $-2\pi^2$ [ h <sup>2</sup> a <sup>*2</sup> U <sup>11</sup> + + 2 h k a <sup>*</sup> b <sup>*</sup> U	U <sup>12</sup> ]			

	$U^{11}$	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	$U^{12}$
N(1)	63(1)	78(1)	78(1)	-2(1)	36(1)	4(1)
N(2)	76(2)	152(2)	68(1)	-9(1)	12(1)	41(1)
N(3)	77(1)	90(1)	75(1)	-8(1)	30(1)	20(1)
N(4)	58(1)	74(1)	66(1)	-2(1)	15(1)	2(1)
N(5)	58(1)	66(1)	54(1)	1(1)	26(1)	8(1)
C(1)	90(2)	91(2)	101(2)	22(2)	55(2)	10(1)
C(2)	89(2)	100(2)	108(2)	10(2)	61(2)	5(2)
C(3)	60(2)	161(3)	93(2)	-36(2)	21(2)	7(2)
C(4)	78(2)	233(4)	89(2)	-28(2)	12(2)	69(2)
C(5)	107(2)	240(4)	80(2)	-1(2)	7(2)	89(3)
C(6)	53(2)	106(2)	83(2)	-24(2)	33(1)	0(1)
C(7)	56(2)	97(2)	68(2)	-17(1)	15(1)	3(1)
C(8)	60(1)	59(1)	68(1)	-9(1)	33(1)	-5(1)
C(9)	67(2)	75(2)	67(1)	3(1)	29(1)	3(1)
C(10)	61(1)	74(2)	73(1)	5(1)	30(1)	10(1)
C(11)	61(1)	51(1)	68(1)	-2(1)	33(1)	1(1)
C(12)	67(2)	81(2)	63(1)	-13(1)	24(1)	-5(1)
C(13)	55(1)	85(2)	76(2)	-16(1)	22(1)	-1(1)
C(14)	70(2)	58(1)	67(1)	5(1)	31(1)	6(1)
C(15)	66(1)	64(1)	60(1)	9(1)	25(1)	10(1)
C(16)	54(1)	61(1)	52(1)	6(1)	21(1)	9(1)
C(17)	62(1)	66(2)	66(1)	0(1)	25(1)	-9(1)
C(18)	67(1)	56(1)	62(1)	-8(1)	25(1)	-4(1)
C(19)	55(1)	60(1)	52(1)	-2(1)	24(1)	1(1)
C(20)	79(2)	58(1)	77(1)	-10(1)	41(1)	-10(1)
C(21)	80(2)	55(1)	73(1)	-9(1)	37(1)	1(1)
C(22)	55(1)	65(1)	62(1)	-4(1)	20(1)	0(1)
C(23)	67(2)	108(2)	63(1)	3(1)	17(1)	16(1)
C(24)	81(2)	136(3)	82(2)	18(2)	11(2)	20(2)
C(25)	70(2)	102(2)	116(2)	15(2)	15(2)	18(1)
C(26)	78(2)	99(2)	107(2)	-8(2)	38(2)	23(2)
C(27)	53(1)	62(1)	49(1)	-10(1)	16(1)	-3(1)
C(28)	58(1)	92(2)	66(1)	7(1)	27(1)	2(1)
C(29)	90(2)	97(2)	69(2)	7(1)	37(1)	-7(2)
C(30)	97(2)	94(2)	58(1)	9(1)	13(1)	4(2)
C(31)	72(2)	87(2)	71(2)	-1(1)	8(1)	9(1)
Table 5.	Hydrogen co	oordinates ( x 10 <sup>4</sup>	) and isotropic	displacemen	t parameters (Å <sup>2</sup>	$^{2}x 10^{3}$ ) for <b>6</b> .
		X	· 1	у	Z	Ú(eq)
H(1A)		9931	-228	35	-2257	109
		12047	204	2	2622	115

H(1A)	9931	-2285	-2257	109
H(2A)	12047	-2943	-2633	115
H(3)	14280	-4807	-2198	125
H(4)	14860	-6174	-1471	160
H(5)	13397	-6335	-804	171
H(9A)	7947	-3055	-1889	82
H(10A)	6127	-2726	-1383	81
H(12A)	8689	-3196	-48	83
H(13A)	10533	-3497	-556	85
H(17A)	4552	-459	505	76
H(18A)	2892	-216	1094	73
H(20A)	1585	-3971	777	83
H(21A)	3214	-4210	176	81

H(23A)	55	-1126	441	95
H(24A)	-1836	251	226	120
H(25A)	-3076	1067	893	115
H(26A)	-2334	536	1759	111
H(28A)	-799	-2736	2019	84
H(29A)	-447	-4210	2730	100
H(30A)	1697	-5213	2927	99
H(31A)	3451	-4602	2441	92

Table 6. Crystal data and structure refinement for **8**.

mpirical formula	$C_{36} H_{24} N_6$	
Formula weight	540.61	
Temperature	296(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 5.8339(10) Å	$\alpha = 90^{\circ}$ .
	b = 16.952(3) Å	$\beta = 99.643(3)^{\circ}$ .
	c = 14.493(3)  Å	$\gamma = 90^{\circ}$ .
Volume	1413.0(4) Å <sup>3</sup>	
Ζ	2	
Density (calculated)	1.271 Mg/m <sup>3</sup>	
Absorption coefficient	0.077 mm <sup>-1</sup>	
F(000)	564	
Crystal size	.2 x .2 x .5 mm <sup>3</sup>	
Theta range for data collection	1.86 to 28.28°.	
Index ranges	-6<=h<=7, -22<=k<=22, -19<=l<=	=19
Reflections collected	10191	
Independent reflections	3355 [R(int) = 0.0901]	
Completeness to theta = $28.28^{\circ}$	95.6 %	
Absorption correction	Empirical	
Max. and min. transmission	0.2881 and 0.1880	
Refinement method	Full-matrix least-squares on F <sup>2</sup>	
Data / restraints / parameters	3355 / 0 / 190	
Goodness-of-fit on F <sup>2</sup>	0.842	
Final R indices [I>2sigma(I)]	R1 = 0.0544, wR2 = 0.1065	
R indices (all data)	R1 = 0.1994, $wR2 = 0.1427$	
Largest diff. peak and hole	0.147 and -0.174 e.Å <sup>-3</sup>	

Table 7. Atomic coordinates (x  $10^4$ ) and equivalent isotropic displacement parameters (Å<sup>2</sup>x  $10^3$ ) for **8**. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	Х	у	Z	U(eq)
N(1)	-12096(4)	-1006(2)	4000(2)	59(1)
N(2)	-10982(4)	-3428(2)	2617(2)	77(1)
N(3)	-11475(4)	-2184(1)	3280(2)	55(1)
C(1)	-11794(4)	-1782(2)	4095(2)	52(1)
C(2)	-11768(5)	-2172(2)	4940(2)	75(1)
C(3)	-12098(7)	-1744(3)	5703(3)	94(1)
C(4)	-12449(6)	-934(3)	5615(3)	88(1)
C(5)	-12395(5)	-600(2)	4772(3)	71(1)
C(6)	-12253(5)	-2969(2)	3099(2)	50(1)
C(7)	-14210(5)	-3234(2)	3394(2)	54(1)
C(8)	-14893(5)	-3988(2)	3213(2)	64(1)
C(9)	-13601(6)	-4472(2)	2745(2)	71(1)
C(10)	-11709(6)	-4165(2)	2439(2)	75(1)
C(11)	-10249(5)	-1800(2)	2631(2)	47(1)

C(12)	-11239(5)	-1738(2)	1699(2)	53(1)
C(13)	-10080(5)	-1354(2)	1072(2)	55(1)
C(14)	-7893(5)	-1023(2)	1376(2)	46(1)
C(15)	-6924(5)	-1101(2)	2313(2)	53(1)
C(16)	-8079(5)	-1480(2)	2935(2)	53(1)
C(17)	-6686(5)	-594(2)	755(2)	54(1)
C(18)	-5613(5)	-220(2)	272(2)	54(1)

Table 9. Bond lengths [Å] and angles  $[\circ]$  for **8**.

N(1)-C(1)	1.332(3)
N(1)-C(5)	1.349(3)
N(2)-C(10)	1.332(3)
N(2)-C(6)	1.348(3)
N(3)-C(1)	1.403(3)
N(3)-C(6)	1.416(3)
N(3)-C(11)	1.431(3)
C(1)-C(2)	1.389(4)
C(2)-C(3)	1.363(4)
C(3)-C(4)	1.391(4)
C(4)-C(5)	1.352(4)
C(6)-C(7)	1.361(3)
C(7)-C(8)	1.351(4)
C(8)-C(9)	1.369(4)
C(9)-C(10)	1.360(4)
C(11)-C(16)	1.380(3)
C(11)-C(12)	1.380(4)
C(12)-C(13)	1.382(3)
C(13)-C(14)	1.396(4)
C(14)-C(15)	1.387(3)
C(14)-C(17)	1.432(4)
C(15)-C(16)	1.371(3)
C(17)-C(18)	1.196(3)
	1 071(5)
C(18)-C(18)#1	1.3/1(5)
C(18)-C(18)#1	1.3/1(5)
C(18)-C(18)#1 C(1)-N(1)-C(5) C(10) N(2) C(6)	1.3/1(5) 116.9(3) 117.2(3)
C(18)-C(18)#1 C(1)-N(1)-C(5) C(10)-N(2)-C(6) C(1) N(2) C(6)	1.371(5) 116.9(3) 117.2(3) 121.9(2)
C(18)-C(18)#1 C(1)-N(1)-C(5) C(10)-N(2)-C(6) C(1)-N(3)-C(6) C(1)-N(3)-C(11)	1.371(5) 116.9(3) 117.2(3) 121.9(2)
C(18)-C(18)#1 C(1)-N(1)-C(5) C(10)-N(2)-C(6) C(1)-N(3)-C(6) C(1)-N(3)-C(11) C(6) N(3) C(11)	1.371(5) 116.9(3) 117.2(3) 121.9(2) 119.0(2)
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$	1.371(5) 116.9(3) 117.2(3) 121.9(2) 119.0(2) 119.1(2) 122.9(3)
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$	1.371(5) 116.9(3) 117.2(3) 121.9(2) 119.0(2) 119.1(2) 122.9(3) 115.3(3)
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$	1.371(5) 116.9(3) 117.2(3) 121.9(2) 119.0(2) 119.1(2) 122.9(3) 115.3(3) 121.8(3)
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$	1.371(5) 116.9(3) 117.2(3) 121.9(2) 119.0(2) 119.1(2) 122.9(3) 115.3(3) 121.8(3) 118.6(3)
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(1)-C(2)$	1.371(5) $116.9(3)$ $117.2(3)$ $121.9(2)$ $119.0(2)$ $119.1(2)$ $122.9(3)$ $115.3(3)$ $121.8(3)$ $118.6(3)$ $119.3(4)$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$	1.371(5) $116.9(3)$ $117.2(3)$ $121.9(2)$ $119.0(2)$ $119.1(2)$ $122.9(3)$ $115.3(3)$ $121.8(3)$ $118.6(3)$ $119.3(4)$ $118.1(3)$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$	$\begin{array}{c} 1.371(5) \\ 116.9(3) \\ 117.2(3) \\ 121.9(2) \\ 119.0(2) \\ 119.1(2) \\ 122.9(3) \\ 115.3(3) \\ 121.8(3) \\ 118.6(3) \\ 119.3(4) \\ 118.1(3) \\ 124.1(3) \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-C(7)$	$\begin{array}{c} 1.371(5) \\ 116.9(3) \\ 117.2(3) \\ 121.9(2) \\ 119.0(2) \\ 119.1(2) \\ 122.9(3) \\ 115.3(3) \\ 121.8(3) \\ 118.6(3) \\ 119.3(4) \\ 118.1(3) \\ 124.1(3) \\ 122.4(3) \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(1)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-N(3)$	$\begin{array}{c} 1.371(5) \\ 116.9(3) \\ 117.2(3) \\ 121.9(2) \\ 119.0(2) \\ 119.1(2) \\ 122.9(3) \\ 115.3(3) \\ 121.8(3) \\ 118.6(3) \\ 119.3(4) \\ 118.1(3) \\ 124.1(3) \\ 122.4(3) \\ 116.8(2) \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(1)$ $C(6)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$	$\begin{array}{c} 1.371(5) \\ 116.9(3) \\ 117.2(3) \\ 121.9(2) \\ 119.0(2) \\ 119.1(2) \\ 122.9(3) \\ 115.3(3) \\ 121.8(3) \\ 118.6(3) \\ 119.3(4) \\ 118.1(3) \\ 124.1(3) \\ 122.4(3) \\ 116.8(2) \\ 120.8(3) \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(8)-C(7)-C(6)$	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 124.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(8)-C(7)-C(6)$ $C(7)-C(6)-C(9)$	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\\ 119.6(3)\\ \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-C(7)$ $C(10)-C(9)-C(8)$	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 124.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\\ 119.6(3)\\ 118.5(3)\end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-R(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $C(7)-C(6)$ $C(7)-C(6)$ $C(7)-C(6)$ $C(7)-C(8)-C(9)$ $C(10)-C(9)-C(8)$ $N(2)-C(10)-C(9)$	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 124.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\\ 119.6(3)\\ 118.5(3)\\ 123.1(3)\\ \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-C(7)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(1)-C(9)-C(8)$ $N(2)-C(10)-C(9)$ $C(16)-C(11)-C(12)$	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 124.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\\ 119.6(3)\\ 118.5(3)\\ 123.1(3)\\ 119.6(3)\\ \end{array}$
C(18)-C(18)#1 $C(1)-N(1)-C(5)$ $C(10)-N(2)-C(6)$ $C(1)-N(3)-C(11)$ $C(6)-N(3)-C(11)$ $N(1)-C(1)-C(2)$ $N(1)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(2)-C(1)-N(3)$ $C(3)-C(2)-C(1)$ $C(2)-C(3)-C(4)$ $C(5)-C(4)-C(3)$ $N(1)-C(5)-C(4)$ $N(2)-C(6)-N(3)$ $C(7)-C(6)-N(3)$ $C(1)-C(9)-C(8)$ $N(2)-C(10)-C(9)$ $C(16)-C(11)-C(12)$ $C(16)-C(11)-N(3)$	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 124.1(3)\\ 124.1(3)\\ 124.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\\ 119.6(3)\\ 119.6(3)\\ 120.1(3)\\ \end{array}$
C(18)-C(18)#1 C(1)-N(1)-C(5) C(10)-N(2)-C(6) C(1)-N(3)-C(1) C(6)-N(3)-C(11) N(1)-C(1)-C(2) N(1)-C(1)-N(3) C(2)-C(1)-N(3) C(2)-C(1)-N(3) C(3)-C(2)-C(1) C(2)-C(3)-C(4) C(5)-C(4)-C(3) N(1)-C(5)-C(4) N(2)-C(6)-N(3) C(7)-C(6)-N(3) C(7)-C(6)-N(3) C(7)-C(6)-N(3) C(7)-C(6)-C(9) C(10)-C(9)-C(8) N(2)-C(10)-C(9) C(16)-C(11)-C(12) C(16)-C(11)-N(3) C(12)-C(11)-N(3)	$\begin{array}{c} 1.371(5)\\ 116.9(3)\\ 117.2(3)\\ 121.9(2)\\ 119.0(2)\\ 119.0(2)\\ 119.1(2)\\ 122.9(3)\\ 115.3(3)\\ 121.8(3)\\ 118.6(3)\\ 119.3(4)\\ 118.1(3)\\ 124.1(3)\\ 124.1(3)\\ 122.4(3)\\ 116.8(2)\\ 120.8(3)\\ 119.2(3)\\ 119.6(3)\\ 123.1(3)\\ 119.6(3)\\ 120.1(3)\\ 120.3(3)\\ \end{array}$

C(11) C(12) C(13)	120 6(3)	
C(11) - C(12) - C(13)	120.0(3)	
C(12)-C(13)-C(14)	120.2(3)	
C(15)-C(14)-C(13)	118.2(3)	
C(15)-C(14)-C(17)	120.1(3)	
C(13)-C(14)-C(17)	121.7(3)	
C(16)-C(15)-C(14)	121.5(3)	
C(15)-C(16)-C(11)	120.0(3)	
C(18)-C(17)-C(14)	176.9(3)	
C(17)-C(18)-C(18)#1	179.0(4)	

Symmetry transformations used to generate equivalent atoms: #1 -x-1,-y,-z

Table 10. Anisotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for **8**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2}U^{11} + ... + 2h k a^* b^* U^{12}]$ 

	$U^{11}$	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	$U^{12}$
N(1)	66(2)	54(2)	60(2)	-2(2)	21(1)	-3(1)
N(2)	79(2)	56(2)	103(2)	5(2)	40(2)	1(2)
N(3)	77(2)	42(2)	54(2)	-3(1)	36(1)	-12(1)
C(1)	54(2)	51(2)	55(2)	3(2)	17(2)	-9(2)
C(2)	109(3)	66(3)	53(2)	8(2)	25(2)	-9(2)
C(3)	133(3)	96(3)	58(3)	3(3)	28(2)	-25(3)
C(4)	98(3)	110(4)	64(3)	-23(3)	38(2)	-14(3)
C(5)	71(2)	71(3)	72(3)	-20(2)	19(2)	-3(2)
C(6)	60(2)	44(2)	50(2)	6(2)	19(2)	-2(2)
C(7)	60(2)	47(2)	63(2)	7(2)	33(2)	-2(2)
C(8)	65(2)	59(2)	73(2)	12(2)	23(2)	-18(2)
C(9)	88(3)	44(2)	81(3)	7(2)	14(2)	-13(2)
C(10)	97(3)	36(2)	100(3)	-3(2)	37(2)	3(2)
C(11)	58(2)	37(2)	51(2)	4(2)	26(2)	-3(2)
C(12)	55(2)	51(2)	58(2)	1(2)	21(2)	-11(2)
C(13)	65(2)	56(2)	47(2)	-1(2)	21(2)	-7(2)
C(14)	55(2)	38(2)	54(2)	5(2)	29(2)	-1(1)
C(15)	48(2)	52(2)	62(2)	8(2)	21(2)	-6(2)
C(16)	53(2)	54(2)	53(2)	8(2)	16(2)	-4(2)
C(17)	61(2)	50(2)	55(2)	2(2)	24(2)	-1(2)
C(18)	64(2)	50(2)	54(2)	7(2)	27(2)	-4(2)

Table 11. Hydrogen coordinates (  $x \ 10^4$ ) and isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for **8**.

	Х	У	Ζ	U(eq)
H(2)	-11531	-2714	4983	89
H(3)	-12088	-1991	6276	113
H(4)	-12714	-631	6122	106
H(5)	-12575	-56	4721	85
H(7)	-15067	-2901	3716	65
H(8)	-16234	-4177	3405	77
H(9)	-14007	-4999	2638	85
H(10)	-10883	-4486	2090	90
H(12)	-12697	-1955	1492	64
H(13)	-10760	-1317	446	66
H(15)	-5458	-890	2525	63
H(16)	-7399	-1521	3561	63

Table 12. Crystal data and structure refinement for 9	<b>)</b> .		
Empirical formula	$C_{42}H_{24}F_{12}N_6O_8Zn_2\ C_6H_6$		
Formula weight	1098.73		
Temperature	293(2) K		
Wavelength	0.71073 Å		
Crystal system	Triclinic		
Space group	P-1		
Unit cell dimensions	a = 11.140(15) Å	$\alpha = 112.04(2)^{\circ}$ .	
	b = 11.192(15)  Å	$\beta = 98.06(2)^{\circ}$ .	
	c = 11.500(15)  Å	$\gamma = 108.39(2)^{\circ}$ .	
Volume	1205(3) Å <sup>3</sup>	•	
Z	2		
Density (calculated)	1.622 Mg/m <sup>3</sup>		
Absorption coefficient	1.102 mm <sup>-1</sup>		
F(000)	592		
Crystal size	? x ? x ? mm <sup>3</sup>		
Theta range for data collection	2.00 to 28.37°.		
Index ranges	-14<=h<=14, -14<=k<=13, -15<=	l<=12	
Reflections collected	8657		
Independent reflections	5539 [R(int) = $0.0763$ ]		
Completeness to theta = $28.37^{\circ}$	91.9 %		
Absorption correction	Empirical		
Max. and min. transmission	1.000 and 0.658		
Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Data / restraints / parameters	5539 / 0 / 397		
Goodness-of-fit on F <sup>2</sup>	1.043		
Final R indices [I>2sigma(I)]	R1 = 0.0460, wR2 = 0.1169		
R indices (all data)	R1 = 0.0647, WR2 = 0.1293		
Largest diff. peak and hole	0.924 and -0.341 e.Å <sup>-3</sup>		

Table 13. Atomic coordinates (x  $10^4$ ) and equivalent isotropic displacement parameters (Å<sup>2</sup>x  $10^3$ ) for **9**. U(eq) is defined as one third of the trace of the orthogonalized U<sup>ij</sup> tensor.

	Х	У	Z	U(eq)
Zn(1)	4027(1)	2292(1)	-5643(1)	52(1)
O(1)	2674(2)	2845(2)	-6223(2)	64(1)
O(2)	1592(3)	2163(3)	-4996(3)	111(1)
O(3)	5456(2)	3157(3)	-6259(3)	92(1)
O(4)	4595(3)	1211(4)	-8051(4)	131(1)
N(1)	3503(2)	406(2)	-5662(2)	49(1)
N(2)	4899(2)	3253(2)	-3706(2)	48(1)
N(3)	3563(2)	1341(2)	-3413(2)	50(1)
C(1)	3260(2)	207(2)	-4633(2)	48(1)
C(2)	2670(3)	-1149(3)	-4765(3)	69(1)
C(3)	2351(3)	-2270(3)	-5944(4)	78(1)
C(4)	2630(3)	-2064(3)	-6996(3)	68(1)
C(5)	3208(2)	-725(3)	-6814(3)	60(1)
C(6)	4533(2)	2703(2)	-2902(2)	49(1)
C(7)	5112(3)	3491(3)	-1551(3)	66(1)
C(8)	6069(3)	4805(3)	-1065(3)	75(1)
C(9)	6453(3)	5359(3)	-1897(3)	73(1)
C(10)	5851(2)	4548(3)	-3197(3)	60(1)
C(11)	2775(2)	1054(3)	-2578(3)	53(1)
C(12)	3200(3)	682(3)	-1636(3)	64(1)
C(13)	2405(3)	397(3)	-881(3)	69(1)
C(14)	1195(3)	469(3)	-1065(3)	64(1)
C(15)	775(3)	827(3)	-2032(3)	70(1)
C(16)	1568(3)	1136(3)	-2787(3)	60(1)

C(17)	347(3)	132(3)	-312(3)	72(1)
C(18)	1772(2)	2712(3)	-5692(3)	60(1)
C(19)	841(3)	3379(3)	-5993(4)	76(1)
C(20)	5382(3)	2422(4)	-7355(3)	73(1)
C(21)	6390(3)	3039(4)	-7947(3)	77(1)
C(22)	-232(4)	-3930(5)	-10096(5)	112(1)
C(23)	396(4)	-4542(5)	-10876(5)	105(1)
C(24)	-624(4)	-4379(6)	-9212(5)	112(1)
F(1)	1368(13)	4661(10)	-5434(16)	144(5)
F(1A)	284(11)	3721(11)	-4944(11)	154(3)
F(2)	-266(6)	2886(10)	-5883(12)	121(3)
F(2A)	-108(10)	2579(9)	-6954(14)	186(6)
F(3)	565(8)	3068(11)	-7307(8)	127(3)
F(3A)	1380(10)	4579(11)	-5902(16)	125(6)
F(4)	7433(11)	2892(13)	-7618(14)	121(4)
F(4A)	7558(10)	3321(16)	-7363(12)	150(5)
F(5)	6762(10)	4468(10)	-7414(9)	119(3)
F(5A)	6281(13)	3982(14)	-8190(14)	150(5)
F(6)	6005(10)	2613(14)	-9171(9)	151(6)
F(6A)	6193(14)	2015(13)	-9128(11)	151(4)

Table 14. Bond lengths [Å] and angles [°] for **9**.

Zn(1)-O(1)	1.928(3)
Zn(1)-O(3)	1.958(3)
Zn(1)-N(1)	1.995(3)
Zn(1)-N(2)	2.000(3)
O(1)-C(18)	1.245(3)
O(2)-C(18)	1.182(4)
O(3)-C(20)	1.192(4)
O(4)-C(20)	1.219(5)
N(1)-C(1)	1.331(3)
N(1)-C(5)	1.350(3)
N(2)-C(6)	1.331(3)
N(2)-C(10)	1.337(3)
N(3)-C(6)	1.396(3)
N(3)-C(1)	1.397(3)
N(3)-C(11)	1.444(3)
C(1)-C(2)	1.389(4)
C(2)-C(3)	1.358(5)
C(3)-C(4)	1.372(5)
C(4)-C(5)	1.349(4)
C(6)-C(7)	1.393(4)
C(7)-C(8)	1.356(4)
C(8)-C(9)	1.369(5)
C(9)-C(10)	1.351(4)
C(11)-C(16)	1.370(4)
C(11)-C(12)	1.375(4)
C(12)-C(13)	1.373(4)
C(13)-C(14)	1.368(4)
C(14)-C(15)	1.386(4)
C(14)-C(17)	1.426(3)
C(15)-C(16)	1.379(3)
C(17)-C(17)#1	1.171(5)
C(18)-C(19)	1.527(4)
C(19)-F(2A)	1.214(8)
C(19)-F(1)	1.219(11)

C(19)-F(2)	1.227(6)
C(19)-F(3A)	1.242(9)
C(19)-F(3)	1.381(8)
C(19)-F(1A)	1.413(8)
C(20)-C(21)	1.510(4)
C(21)-F(5A)	1.225(10)
C(21)-F(4)	1.250(9)
C(21)-F(4A)	1.257(10)
C(21)-F(6)	1.261(9)
C(21)-F(6A)	1.340(12)
C(21)-F(5)	1.371(11)
C(22)-C(23)	1.334(7)
C(22)-C(24)	1.359(7)
C(23)-C(24)#2	1.347(7)
C(24)-C(23)#2	1.347(7)
O(1)-Zn(1)-O(3)	101.79(13)
O(1)-Zn(1)-N(1)	119.34(10)
O(3)-Zn(1)-N(1)	126.56(10)
O(1)-Zn(1)-N(2)	115.34(10)
O(3)-Zn(1)-N(2)	101.05(12)
N(1)-Zn(1)-N(2)	91.18(10)
C(18)-O(1)-Zn(1)	114.53(19)
C(20)-O(3)-Zn(1)	113.1(2)
C(1)-N(1)-C(5)	119.0(2)
C(1)-N(1)-Zn(1)	122.14(15)
C(5)-N(1)-Zn(1)	118.18(19)
C(6)-N(2)-C(10)	119.0(2)
C(6)-N(2)-Zn(1)	123.50(17)
C(10)-N(2)-Zn(1)	117.41(17)
C(6)-N(3)-C(1)	128.21(18)
C(6)-N(3)-C(11)	116.3(2)
C(1)-N(3)-C(11)	115.48(19)
N(1)-C(1)-C(2)	120.0(2)
N(1)-C(1)-N(3)	121.4(2)
C(2)-C(1)-N(3)	118.6(2)
C(3)-C(2)-C(1)	119.8(3)
C(2)-C(3)-C(4)	120.2(3)
C(5)-C(4)-C(3)	117.7(3)
C(4)-C(5)-N(1)	123.3(3)
N(2)-C(6)-C(7)	120.0(2)
N(2)-C(6)-N(3)	120.0(2)
C(7)-C(6)-N(3)	120.0(2)
C(8)-C(7)-C(6)	119.6(3)
C(7)-C(8)-C(9)	120.2(3)
C(10)-C(9)-C(8)	117.6(3)
N(2)-C(10)-C(9)	123.7(3)
C(16)-C(11)-C(12)	121.3(2)
C(16)-C(11)-N(3)	117.1(2)
C(12)-C(11)-N(3)	121.6(2)
C(13)-C(12)-C(11)	119.4(3)
C(14)-C(13)-C(12)	120.6(3)
C(13)-C(14)-C(15)	119.1(2)
C(13)-C(14)-C(17)	120.9(3)
C(15)-C(14)-C(17)	120.0(3)
C(16)-C(15)-C(14)	121.0(3)
C(11)-C(16)-C(15)	118.4(3)

C(17)#1-C(17)-C(14)	179.4(4)
O(2)-C(18)-O(1)	127.3(3)
O(2)-C(18)-C(19)	119.2(3)
O(1)-C(18)-C(19)	113.5(3)
F(2A)-C(19)-F(1)	131.2(8)
F(1)-C(19)-F(2)	114.1(8)
F(2A)-C(19)-F(3A)	114.9(9)
F(2)-C(19)-F(3A)	125.1(6)
F(1)-C(19)-F(3)	103.7(8)
F(2)-C(19)-F(3)	102.3(6)
F(2A)-C(19)-F(1A)	104.2(8)
F(3A)-C(19)-F(1A)	98.5(7)
F(2A)-C(19)-C(18)	113.7(4)
F(1)-C(19)-C(18)	112.0(7)
F(2)-C(19)-C(18)	114.7(4)
F(3A)-C(19)-C(18)	115.9(5)
F(3)-C(19)-C(18)	108.8(4)
F(1A)-C(19)-C(18)	107.3(5)
O(3)-C(20)-O(4)	127.3(3)
O(3)-C(20)-C(21)	116.9(3)
O(4)-C(20)-C(21)	115.8(3)
F(5A)-C(21)-F(4)	127.4(9)
F(5A)-C(21)-F(4A)	113.1(9)
F(4)-C(21)-F(6)	111.1(9)
F(4A)-C(21)-F(6)	121.7(8)
F(5A)-C(21)-F(6A)	103.7(7)
F(4A)-C(21)-F(6A)	102.0(9)
F(4)-C(21)-F(5)	104.4(8)
F(6)-C(21)-F(5)	105.1(7)
F(6A)-C(21)-F(5)	135.9(6)
F(5A)-C(21)-C(20)	115.9(5)
F(4)-C(21)-C(20)	110.2(6)
F(4A)-C(21)-C(20)	113.4(6)
F(6)-C(21)-C(20)	115.9(5)
F(6A)-C(21)-C(20)	107.0(6)
F(5)-C(21)-C(20)	109.4(5)
C(23)-C(22)-C(24)	120.5(4)
C(22)-C(23)-C(24)#2	119.3(5)
C(23)#2-C(24)-C(22)	120.3(4)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z #2 -x,-y-1,-z-2

Table 15. Anisotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for **9**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2$ [h<sup>2</sup> a<sup>\*2</sup>U<sup>11</sup> + ... + 2 h k a<sup>\*</sup> b<sup>\*</sup> U<sup>12</sup>]

	$U^{11}$	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	$U^{12}$
Zn(1)	53(1)	58(1)	63(1)	40(1)	28(1)	24(1)
O(1)	60(1)	74(1)	87(1)	55(1)	33(1)	33(1)
O(2)	105(2)	165(3)	165(3)	139(2)	83(2)	82(2)
O(3)	83(1)	131(2)	91(2)	71(2)	51(1)	44(1)
O(4)	121(2)	125(2)	138(3)	78(2)	44(2)	14(2)
N(1)	51(1)	52(1)	59(1)	34(1)	30(1)	23(1)
N(2)	46(1)	54(1)	60(1)	35(1)	27(1)	21(1)
N(3)	53(1)	55(1)	58(1)	35(1)	34(1)	22(1)
C(1)	44(1)	52(1)	63(1)	34(1)	30(1)	23(1)

C(2)	82(2)	59(1)	85(2)	46(1)	48(2)	26(1)
C(3)	85(2)	53(1)	105(2)	39(2)	49(2)	24(1)
C(4)	68(2)	56(1)	78(2)	25(1)	33(1)	24(1)
C(5)	65(1)	61(1)	64(2)	31(1)	33(1)	28(1)
C(6)	46(1)	58(1)	60(1)	34(1)	30(1)	25(1)
C(7)	70(2)	78(2)	59(2)	35(1)	36(1)	27(1)
C(8)	70(2)	75(2)	61(2)	18(1)	24(1)	20(1)
C(9)	60(2)	61(2)	82(2)	23(1)	27(1)	11(1)
C(10)	56(1)	56(1)	77(2)	37(1)	31(1)	19(1)
C(11)	56(1)	59(1)	62(1)	37(1)	36(1)	23(1)
C(12)	61(1)	81(2)	74(2)	52(1)	34(1)	30(1)
C(13)	79(2)	84(2)	64(2)	50(1)	37(1)	30(1)
C(14)	76(2)	67(1)	65(2)	38(1)	47(1)	25(1)
C(15)	66(2)	87(2)	86(2)	50(2)	53(1)	37(1)
C(16)	63(1)	78(2)	69(2)	50(1)	41(1)	35(1)
C(17)	83(2)	71(2)	69(2)	36(1)	47(1)	22(1)
C(18)	50(1)	61(1)	82(2)	46(1)	23(1)	20(1)
C(19)	53(2)	72(2)	118(3)	55(2)	29(2)	26(1)
C(20)	59(2)	116(3)	79(2)	67(2)	33(1)	43(2)
C(21)	73(2)	115(3)	80(2)	67(2)	43(2)	45(2)
C(22)	95(3)	108(3)	143(4)	71(3)	19(3)	41(2)
C(23)	77(2)	130(3)	113(3)	73(3)	27(2)	26(2)
C(24)	88(2)	137(4)	124(3)	60(3)	37(2)	56(2)
F(1)	123(8)	61(5)	207(10)	27(5)	3(6)	48(5)
F(1A)	175(8)	186(8)	235(10)	142(7)	153(7)	138(7)
F(2)	57(3)	141(7)	224(10)	125(7)	74(5)	46(4)
F(2A)	107(7)	104(5)	237(13)	-5(7)	-73(7)	59(5)
F(3)	117(6)	211(11)	120(5)	110(7)	37(5)	104(7)
F(3A)	80(5)	112(8)	267(16)	146(11)	80(8)	54(5)
F(4)	92(7)	168(6)	211(12)	139(7)	102(7)	93(6)
F(4A)	52(3)	284(14)	119(5)	122(7)	30(3)	34(5)
F(5)	121(5)	113(4)	156(7)	90(5)	80(5)	34(4)
F(5A)	201(12)	195(12)	223(13)	180(11)	158(11)	140(10)
F(6)	139(7)	216(12)	75(5)	95(7)	23(4)	11(8)
F(6A)	207(9)	194(9)	106(6)	79(5)	93(7)	113(7)

Table 16. Hydrogen coordinates (  $x \ 10^4$ ) and isotropic displacement parameters (Å<sup>2</sup>x 10<sup>3</sup>) for **9**.

	Х	У	Z	U(eq)
H(4)	2494	-1290	-4049	83
H(3)	1942	-3179	-6039	94
H(2)	2429	-2820	-7806	81
H(1)	3412	-574	-7517	72
H(7)	4845	3118	-986	79
H(8)	6465	5332	-164	90
H(9)	7105	6260	-1579	88
H(10)	6112	4912	-3770	72
H(12)	4019	623	-1512	77
H(13)	2693	152	-238	83
H(15)	-54	859	-2174	84
H(16)	1291	1394	-3422	72
H(22)	-402	-3190	-10157	134
H(23)	672	-4226	-11474	125
H(24)	-1052	-3939	-8665	134

Table 17. Crystal data and structure refinement for 10.

Empirical formula	$C_{72} H_{48} F_6 N_{12} O_4 Ag_2 -2 CH_3 CN$		
Formula weight	1473.64		
Temperature	293(2) K		
Wavelength	0.71073 Å		
Crystal system	Monoclinic		
Space group	P2(1)/c		
Unit cell dimensions	a = 21.686(6)  Å	$\alpha = 90^{\circ}$ .	
	b = 8.772(2)  Å	β=101.773(4)°.	
	c = 18.378(5)  Å	$\gamma = 90^{\circ}$ .	
Volume	3422.6(16) Å <sup>3</sup>	-	
Z	4		
Density (calculated)	1.511 Mg/m <sup>3</sup>		
Absorption coefficient	0.651 mm <sup>-1</sup>		
F(000)	1576		
Crystal size	? x ? x ? mm <sup>3</sup>		
Theta range for data collection	1.92 to 28.31°.		
Index ranges	-28<=h<=27, -11<=k<=11, -22<=	l<=23	
Reflections collected	24091		
Independent reflections	8161 [R(int) = 0.0549]		
Completeness to theta = $28.31^{\circ}$	95.7 %		
Absorption correction	Empirical		
Max. and min. transmission	0.3097 and 0.2287		
Refinement method	Full-matrix least-squares on F <sup>2</sup>		
Data / restraints / parameters	8161 / 0 / 565		
Goodness-of-fit on F <sup>2</sup>	0.886		
Final R indices [I>2sigma(I)]	R1 = 0.0471, $wR2 = 0.1003$		
R indices (all data)	R1 = 0.1024, $wR2 = 0.1168$		
Largest diff. peak and hole	1.065 and -0.361 e.Å <sup>-3</sup>		

Table	18. Atomic coordinates (x 10 <sup>4</sup> ) and equivalent isotropic displacement parameters (Å <sup>2</sup> x 10 <sup>3</sup> )
for <b>10</b>	. U(eq) is defined as one third of the trace of the orthogonalized U <sup>ij</sup> tensor.

	Х	У	Z	U(eq)
Ag(1)	1405(1)	4587(1)	1663(1)	57(1)
O(1)	856(1)	4793(3)	2850(2)	79(1)
O(2)	300(1)	4745(4)	1702(2)	77(1)
N(1)	2106(1)	2837(3)	2212(2)	48(1)
N(2)	1954(1)	3321(4)	34(2)	54(1)
N(3)	2542(1)	2467(3)	1161(2)	48(1)
N(4)	1347(1)	6353(3)	746(2)	46(1)
N(5)	2899(1)	6205(4)	2263(2)	60(1)
N(6)	2398(1)	7139(3)	1108(2)	46(1)
N(42)	5434(3)	5484(11)	2281(5)	197(4)
C(1)	2579(2)	2265(4)	1926(2)	45(1)
C(2)	3082(2)	1513(5)	2366(2)	56(1)
C(3)	3100(2)	1318(5)	3103(2)	66(1)
C(4)	2603(2)	1856(6)	3396(3)	68(1)
C(5)	2130(2)	2599(5)	2940(2)	57(1)
C(6)	1961(2)	2497(4)	639(2)	46(1)
C(7)	1438(2)	1680(5)	752(2)	57(1)
C(8)	899(2)	1731(6)	210(3)	76(1)
C(9)	884(2)	2585(6)	-412(3)	77(2)
C(10)	1417(2)	3342(6)	-477(3)	70(1)
C(11)	3116(2)	2512(4)	891(2)	46(1)

C(12)	3600(2)	3470(4)	1216(2)	50(1)
C(13)	4160(2)	3489(5)	972(2)	57(1)
C(14)	4248(2)	2560(4)	389(2)	51(1)
C(15)	3758(2)	1621(5)	58(2)	58(1)
C(16)	3197(2)	1598(5)	302(2)	53(1)
C(17)	4832(2)	2588(4)	140(2)	59(1)
C(18)	1815(2)	7217(4)	604(2)	42(1)
C(19)	1733(2)	8150(4)	-19(2)	51(1)
C(20)	1173(2)	8136(5)	-519(2)	59(1)
C(21)	694(2)	7227(5)	-380(2)	60(1)
C(22)	798(2)	6400(5)	252(2)	57(1)
C(23)	2426(2)	7017(4)	1880(2)	46(1)
C(24)	1978(2)	7715(5)	2211(3)	61(1)
C(25)	2035(3)	7562(7)	2962(3)	80(2)
C(26)	2512(3)	6740(8)	3361(3)	89(2)
C(27)	2933(2)	6087(7)	2997(3)	80(1)
C(28)	2972(2)	7202(4)	842(2)	42(1)
C(29)	3023(2)	6442(4)	198(2)	49(1)
C(30)	3577(2)	6517(4)	-60(2)	53(1)
C(31)	4090(2)	7326(4)	315(2)	51(1)
C(32)	4035(2)	8070(5)	958(2)	59(1)
C(33)	3480(2)	8016(4)	1218(2)	54(1)
C(34)	4675(2)	7385(4)	56(2)	61(1)
C(35)	369(2)	4800(4)	2377(3)	56(1)
C(36)	-244(2)	4888(5)	2679(3)	68(1)
C(40)	4520(3)	6079(11)	2943(4)	185(4)
C(41)	5032(4)	5786(9)	2577(4)	130(3)
F(1)	-606(4)	6105(11)	2371(6)	75(3)
F(1A)	-172(4)	5761(13)	3296(6)	68(2)
F(1B)	-329(6)	6291(13)	2937(9)	121(4)
F(2)	-137(4)	4990(14)	3429(5)	71(2)
F(2A)	-387(4)	3390(9)	2882(6)	64(2)
F(2B)	-304(4)	4025(15)	3209(6)	93(3)
F(3)	-583(4)	3602(11)	2472(6)	80(2)
F(3A)	-767(5)	4552(17)	2147(6)	104(3)
F(3B)	-731(3)	5430(13)	2226(4)	54(2)

Table 19. Bond lengths [Å] and angles  $[\circ]$  for **10**.

Ag(1)-N(1)	2.248(3)
Ag(1)-N(4)	2.274(3)
Ag(1)-O(2)	2.416(3)
O(1)-C(35)	1.224(5)
O(2)-C(35)	1.220(5)
N(1)-C(1)	1.341(4)
N(1)-C(5)	1.344(4)
N(2)-C(6)	1.324(4)
N(2)-C(10)	1.338(5)
N(3)-C(1)	1.404(4)
N(3)-C(6)	1.419(4)
N(3)-C(11)	1.432(4)
N(4)-C(18)	1.335(4)
N(4)-C(22)	1.342(4)
N(5)-C(23)	1.326(4)
N(5)-C(27)	1.340(5)
N(6)-C(18)	1.408(4)
N(6)-C(23)	1.411(4)

N(6)-C(28)	1.429(4)
N(42)-C(41)	1.148(9)
C(1)-C(2)	1.386(5)
C(2)-C(3)	1.357(5)
C(3)-C(4)	1.382(6)
C(4)-C(5)	1.353(6)
C(6)-C(7)	1.392(5)
C(7)-C(8)	1.373(6)
C(8)-C(9)	1.362(7)
C(9)-C(10)	1.357(6)
C(11)-C(12)	1.381(5)
C(11)- $C(16)$	1.386(5)
C(12)- $C(13)$	1.378(5)
C(13)-C(14)	1 391(5)
C(14)-C(15)	1.391(5) 1.384(5)
C(14)-C(17)	1.301(5) 1.431(5)
C(15)-C(16)	1 380(5)
C(17) - C(34) = 1	1.196(5)
C(18) - C(19)	1 389(5)
C(10) C(20)	1.365(5)
C(20) C(21)	1.300(5) 1.374(6)
C(20)-C(21)	1.374(0)
C(21) - C(22)	1.3+9(5) 1.200(5)
C(23)-C(24)	1.390(3)
C(24) - C(25) C(25) - C(25)	1.308(0) 1.340(7)
C(25) - C(20)	1.349(7) 1.262(7)
C(20) - C(27)	1.303(7) 1.275(5)
C(28) - C(33)	1.373(3) 1.292(5)
C(28) - C(29)	1.303(3) 1.270(5)
C(29) - C(30)	1.379(5)
C(30) - C(31)	1.381(5)
C(31) - C(32)	1.377(5)
C(31)-C(34)	1.443(5)
C(32) - C(33)	1.385(5)
C(34) - C(17) = 1	1.190(5)
C(35)-C(36)	1.543(6)
C(36)-F(2B)	1.260(10)
C(36) - F(3B)	1.294(8)
C(36)-F(1B)	1.345(11)
C(36)-F(1A)	1.350(9)
C(36)-F(2)	1.353(9)
C(36)-F(3)	1.357(9)
C(36)-F(3A)	1.369(11)
C(36)-F(1)	1.377(9)
C(36)- $F(2A)$	1.417(9)
C(40)-C(41)	1.434(10)
N(1)-Ag(1)-N(4)	136.71(9)
N(1)-Ag(1)-O(2)	127.55(10)
N(4)-Ag(1)-O(2)	94.43(10)
C(35)-O(2)-Ag(1)	96.7(2)
C(1)-N(1)-C(5)	117.0(3)
C(1)-N(1)-Ag(1)	125.5(2)
C(5)-N(1)-Ag(1)	116.0(2)
C(6)-N(2)-C(10)	117.1(4)
C(1)-N(3)-C(6)	122.7(3)
C(1)-N(3)-C(11)	118.4(3)
C(6)-N(3)-C(11)	118.7(3)
	· · /

C(18)-N(4)-C(22)	117.0(3)
C(18)-N(4)-Ag(1)	127.1(2)
C(22)-N(4)-Ag(1)	115.5(2)
C(23)-N(5)-C(27)	117.0(4)
C(18)-N(6)-C(23)	121.0(3)
C(18)-N(6)-C(28)	120.0(3)
C(23)-N(6)-C(28)	119.0(3)
N(1)-C(1)-C(2)	121 6(3)
N(1) - C(1) - N(3)	116 9(3)
C(2)-C(1)-N(3)	1214(3)
C(3)-C(2)-C(1)	120.0(4)
C(2) - C(3) - C(4)	120.0(4) 118 7(4)
C(5)-C(4)-C(3)	118.7(4)
N(1) C(5) C(4)	124.2(4)
N(2) C(6) C(7)	124.2(4) 122.4(4)
N(2) - C(0) - C(7) N(2) - C(6) - N(3)	122.4(4) 115 7(2)
$\Gamma(2) - C(0) - \Gamma(3)$	113.7(3) 121.9(2)
C(7) - C(0) - N(5)	121.0(5)
C(8) - C(7) - C(6)	110.2(4)
C(9) - C(8) - C(7)	119.9(3)
C(10) - C(9) - C(8)	117.9(5)
N(2)-C(10)-C(9)	124.4(5)
C(12)-C(11)-C(16)	118.9(3)
C(12)-C(11)-N(3)	120.3(3)
C(16)-C(11)-N(3)	120.8(3)
C(13)-C(12)-C(11)	120.6(4)
C(12)-C(13)-C(14)	120.8(4)
C(15)-C(14)-C(13)	118.2(3)
C(15)-C(14)-C(17)	121.4(4)
C(13)-C(14)-C(17)	120.4(4)
C(16)-C(15)-C(14)	121.0(4)
C(15)-C(16)-C(11)	120.4(4)
C(34)#1-C(17)-C(14)	179.0(5)
N(4)-C(18)-C(19)	121.5(3)
N(4)-C(18)-N(6)	117.3(3)
C(19)-C(18)-N(6)	121.2(3)
C(20)-C(19)-C(18)	119.7(4)
C(19)-C(20)-C(21)	118.9(4)
C(22)-C(21)-C(20)	118.1(4)
N(4)-C(22)-C(21)	124.7(4)
N(5)-C(23)-C(24)	122.6(4)
N(5)-C(23)-N(6)	116.4(3)
C(24)-C(23)-N(6)	121.0(4)
C(25)-C(24)-C(23)	118.1(5)
C(26)-C(25)-C(24)	120.2(5)
C(25) - C(26) - C(27)	1183(5)
N(5)-C(27)-C(26)	123 8(5)
C(33) - C(28) - C(29)	119.0(3)
C(33) - C(28) - N(6)	120.8(3)
C(29) - C(28) - N(6)	120.0(3) 120.2(3)
C(20) C(20) C(28)	120.2(3) 120.0(4)
C(30) - C(29) - C(28)	120.0(4) 121.5(4)
C(29) - C(30) - C(31) C(32) - C(31) - C(30)	121.3(4) 118.0(2)
C(32) - C(31) - C(30)	110.0(3)
C(32)- $C(31)$ - $C(34)$	120.1(4)
C(31) - C(31) - C(34)	121.8(4)
C(31)-C(32)-C(33)	120.9(4)
C(28)-C(33)-C(32)	120.5(4)
C(17)#1- $C(34)$ - $C(31)$	178.1(5)

O(2)-C(35)-O(1)	129.0(4)
O(2)-C(35)-C(36)	115.6(4)
O(1)-C(35)-C(36)	115.3(4)
F(2B)-C(36)-F(3B)	121.2(6)
F(2B)-C(36)-F(1B)	103.5(8)
F(3B)-C(36)-F(1A)	105.7(7)
F(3B)-C(36)-F(2)	125.4(6)
F(1A)-C(36)-F(3)	132.1(6)
F(2)-C(36)-F(3)	108.1(7)
F(2B)-C(36)-F(3A)	102.8(7)
F(1B)-C(36)-F(3A)	107.2(8)
F(1A)-C(36)-F(3A)	131.2(7)
F(2)-C(36)-F(3A)	133.4(6)
F(2B)-C(36)-F(1)	130.0(7)
F(2)-C(36)-F(1)	109.4(6)
F(3)-C(36)-F(1)	107.4(7)
F(3B)-C(36)-F(2A)	108.5(6)
F(1B)-C(36)-F(2A)	134.7(8)
F(1A)-C(36)-F(2A)	107.5(7)
F(1)-C(36)-F(2A)	133.7(6)
F(2B)-C(36)-C(35)	118.7(6)
F(3B)-C(36)-C(35)	115.9(5)
F(1B)-C(36)-C(35)	111.3(6)
F(1A)-C(36)-C(35)	111.7(5)
F(2)-C(36)-C(35)	112.9(5)
F(3)-C(36)-C(35)	108.3(5)
F(3A)-C(36)-C(35)	112.3(5)
F(1)-C(36)-C(35)	110.6(5)
F(2A)-C(36)-C(35)	107.4(4)
N(42)-C(41)-C(40)	176.9(10)

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y+1,-z

Table 20. Anisotropic displacement parameters  $(Å^2 x \ 10^3)$  for **10**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [h^2 a^{*2}U^{11} + ... + 2hk a^* b^* U^{12}]$ 

	$U^{11}$	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	$U^{12}$
Ag(1)	48(1)	68(1)	59(1)	10(1)	18(1)	7(1)
O(1)	46(2)	101(2)	86(2)	-17(2)	4(2)	4(2)
O(2)	74(2)	106(2)	55(2)	-10(2)	26(2)	-12(2)
N(1)	43(2)	62(2)	43(2)	6(1)	21(1)	5(1)
N(2)	46(2)	77(2)	40(2)	1(2)	9(2)	6(2)
N(3)	34(2)	75(2)	39(2)	4(2)	15(1)	1(1)
N(4)	30(2)	58(2)	52(2)	5(1)	11(1)	3(1)
N(5)	45(2)	93(2)	40(2)	5(2)	8(2)	0(2)
N(6)	32(2)	73(2)	35(2)	2(1)	12(1)	-2(1)
N(42)	98(5)	327(11)	163(7)	-34(6)	17(5)	-42(6)
C(1)	44(2)	54(2)	40(2)	5(2)	17(2)	1(2)
C(2)	49(2)	72(3)	52(3)	11(2)	18(2)	13(2)
C(3)	60(3)	84(3)	55(3)	23(2)	10(2)	15(2)
C(4)	73(3)	94(3)	42(3)	13(2)	22(2)	6(2)
C(5)	58(3)	71(3)	48(3)	9(2)	25(2)	7(2)
C(6)	37(2)	61(2)	42(2)	-8(2)	15(2)	3(2)
C(7)	47(2)	65(2)	60(3)	-5(2)	19(2)	-5(2)
C(8)	40(3)	92(3)	97(4)	-32(3)	19(3)	-12(2)
C(9)	44(3)	119(4)	63(3)	-32(3)	0(3)	8(3)

C(10)	59(3)	104(4)	47(3)	-6(3)	9(2)	19(3)
C(11)	35(2)	63(2)	42(2)	9(2)	15(2)	4(2)
C(12)	43(2)	62(2)	48(2)	-5(2)	16(2)	3(2)
C(13)	40(2)	67(3)	62(3)	0(2)	11(2)	-5(2)
C(14)	35(2)	67(2)	55(2)	12(2)	19(2)	4(2)
C(15)	54(2)	71(3)	58(3)	-3(2)	28(2)	4(2)
C(16)	43(2)	67(2)	52(2)	-6(2)	19(2)	-8(2)
C(17)	47(2)	73(2)	63(3)	9(2)	22(2)	2(2)
C(18)	33(2)	57(2)	39(2)	-1(2)	14(2)	5(2)
C(19)	47(2)	58(2)	52(3)	3(2)	16(2)	-1(2)
C(20)	59(3)	75(3)	43(3)	8(2)	9(2)	17(2)
C(21)	39(2)	81(3)	55(3)	-2(2)	-3(2)	11(2)
C(22)	42(2)	69(3)	59(3)	2(2)	6(2)	-1(2)
C(23)	35(2)	62(2)	41(2)	-6(2)	11(2)	-11(2)
C(24)	54(3)	79(3)	54(3)	-8(2)	22(2)	-1(2)
C(25)	76(3)	115(4)	59(3)	-26(3)	35(3)	-19(3)
C(26)	76(4)	152(5)	37(3)	-5(3)	11(3)	-31(3)
C(27)	58(3)	129(4)	50(3)	11(3)	3(3)	-9(3)
C(28)	35(2)	54(2)	39(2)	5(2)	12(2)	0(2)
C(29)	40(2)	61(2)	47(2)	-4(2)	12(2)	-3(2)
C(30)	48(2)	70(2)	45(2)	-3(2)	18(2)	4(2)
C(31)	37(2)	63(2)	57(2)	11(2)	22(2)	3(2)
C(32)	42(2)	69(3)	68(3)	-9(2)	17(2)	-15(2)
C(33)	46(2)	67(2)	51(3)	-13(2)	18(2)	-7(2)
C(34)	41(2)	72(2)	73(3)	13(2)	24(2)	2(2)
C(35)	47(2)	60(2)	65(3)	-8(2)	23(2)	-5(2)
C(36)	66(3)	80(3)	55(3)	-3(2)	7(2)	-6(2)
C(40)	88(5)	315(12)	144(7)	-44(7)	6(5)	2(6)
C(41)	90(5)	172(7)	113(6)	-5(5)	-14(4)	-38(5)

Table 21.	Hydrogen coordinates ( x 10 <sup>4</sup>	) and isotropic	displacement param	eters ( $Å^2 x \ 10^3$ ) for <b>10</b> .
	Х	у	Z	U(eq)

3402(17)	1170(40)	2170(20)	61(11)
3480(18)	870(50)	3400(20)	75(13)
2618(17)	1770(40)	3830(20)	56(12)
1799(17)	3010(40)	3120(20)	64(11)
1491(13)	1140(30)	1166(17)	26(8)
540(20)	1240(50)	230(20)	88(15)
548(19)	2630(40)	-790(20)	72(13)
1460(20)	3890(50)	-900(30)	104(17)
3551(14)	4100(30)	1588(18)	43(9)
4469(19)	4150(50)	1170(20)	81(14)
3807(17)	880(40)	-290(20)	67(12)
2870(17)	930(40)	70(20)	63(11)
2027(17)	8780(40)	-60(20)	64(12)
1114(19)	8570(50)	-910(20)	74(15)
345(15)	7190(40)	-722(18)	47(10)
447(17)	5800(40)	377(19)	57(10)
1671(16)	8240(40)	1887(18)	48(11)
1770(20)	7910(50)	3190(20)	89(16)
2610(20)	6640(60)	3840(30)	111(19)
3290(20)	5650(50)	3220(20)	84(15)
2722(17)	5860(40)	-40(20)	62(12)
3575(16)	6000(40)	-490(20)	62(11)
4380(16)	8560(40)	1292(18)	55(10)
	$\begin{array}{c} 3402(17)\\ 3480(18)\\ 2618(17)\\ 1799(17)\\ 1491(13)\\ 540(20)\\ 548(19)\\ 1460(20)\\ 3551(14)\\ 4469(19)\\ 3807(17)\\ 2870(17)\\ 2027(17)\\ 1114(19)\\ 345(15)\\ 447(17)\\ 1671(16)\\ 1770(20)\\ 2610(20)\\ 3290(20)\\ 2722(17)\\ 3575(16)\\ 4380(16)\\ \end{array}$	$\begin{array}{rrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrrr$	$\begin{array}{cccccccccccccccccccccccccccccccccccc$

H(33)	3464(13)	8510(30)	1622(16)	27(8)
H(40A)	4134	6131	2581	277
H(40B)	4590	7030	3206	277
H(40C)	4495	5272	3289	277