Supporting Information

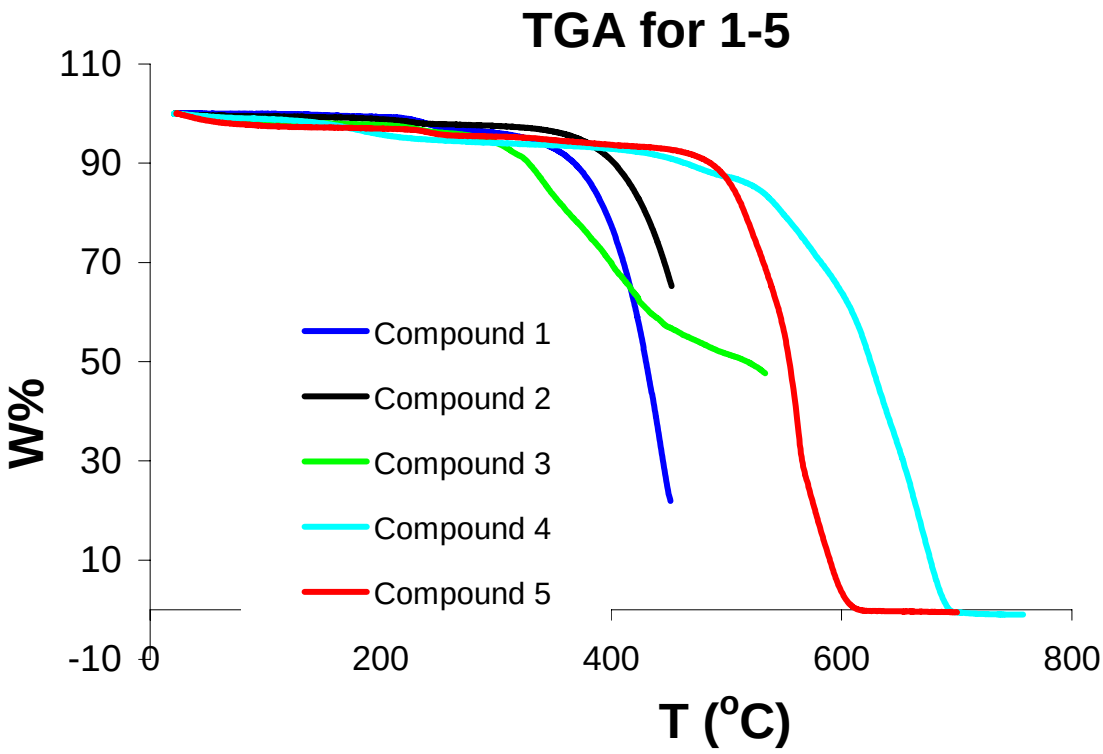
Linear and Star-shaped Benzimidazolyl Derivatives: Syntheses, Photophysical Properties and Use as Highly Efficient Electron Transport Materials in OLEDs

Wade White,[†] Zachary M. Hudson, [†] Xiaodong Feng, [‡] Sijin Han, [‡] Zheng-Hong Lu, [‡] Suning Wang*[†]

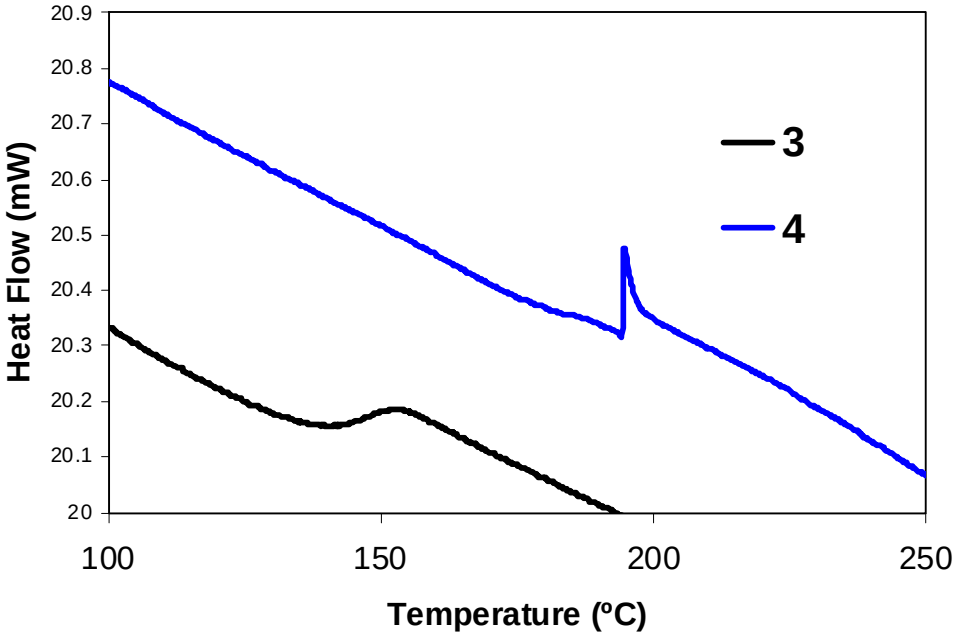
[†]Department of Chemistry, Queen's University, Kingston, Ontario, K7L 3N6, Canada

[‡]Department of Materials Science and Engineering, University of Toronto, Toronto, Ontario, M5S 3E4, Canada

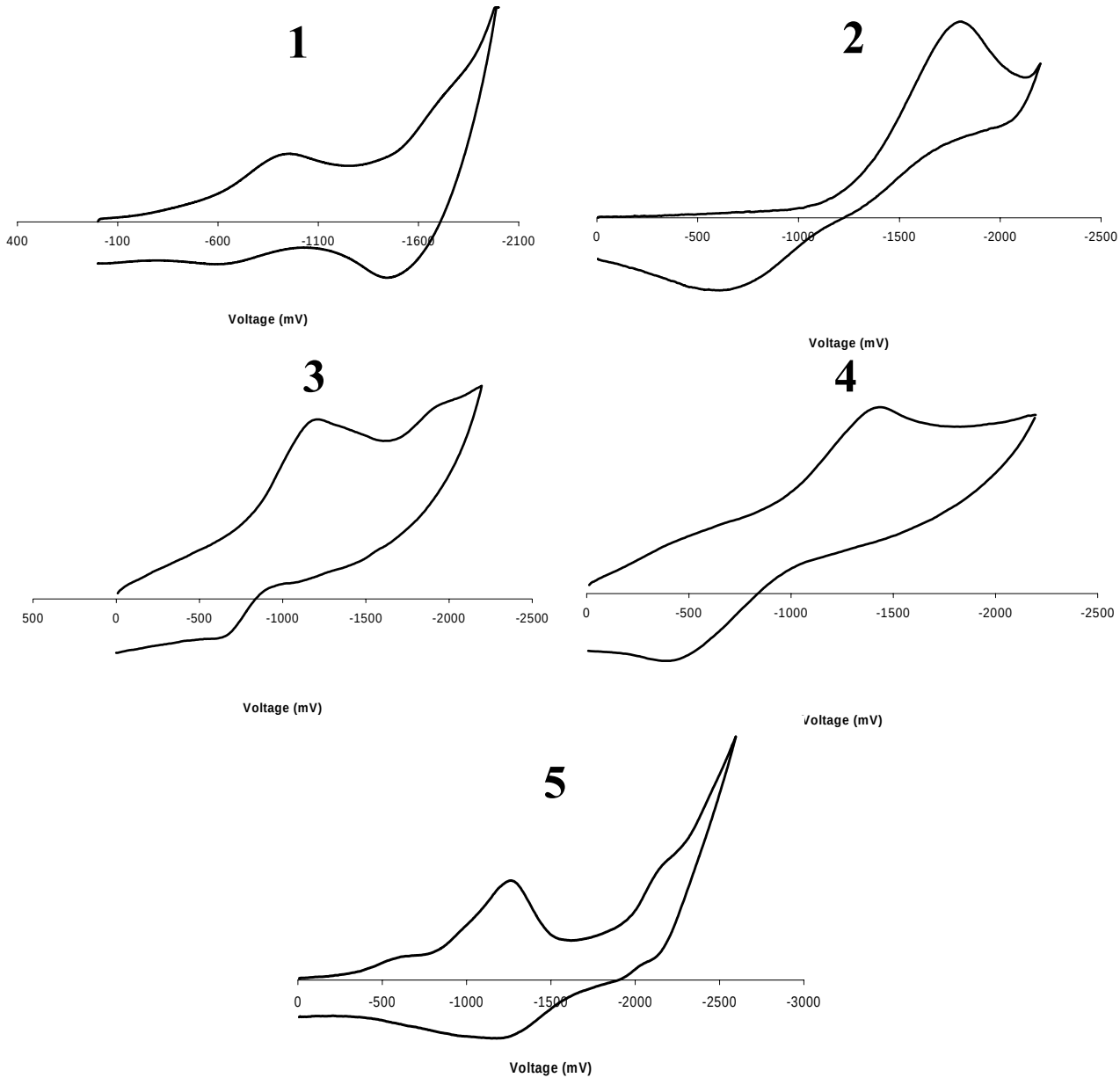
S1. Thermogravimetric analyses for compounds **1-5**



S2. DSC diagrams of **3** and **4.**

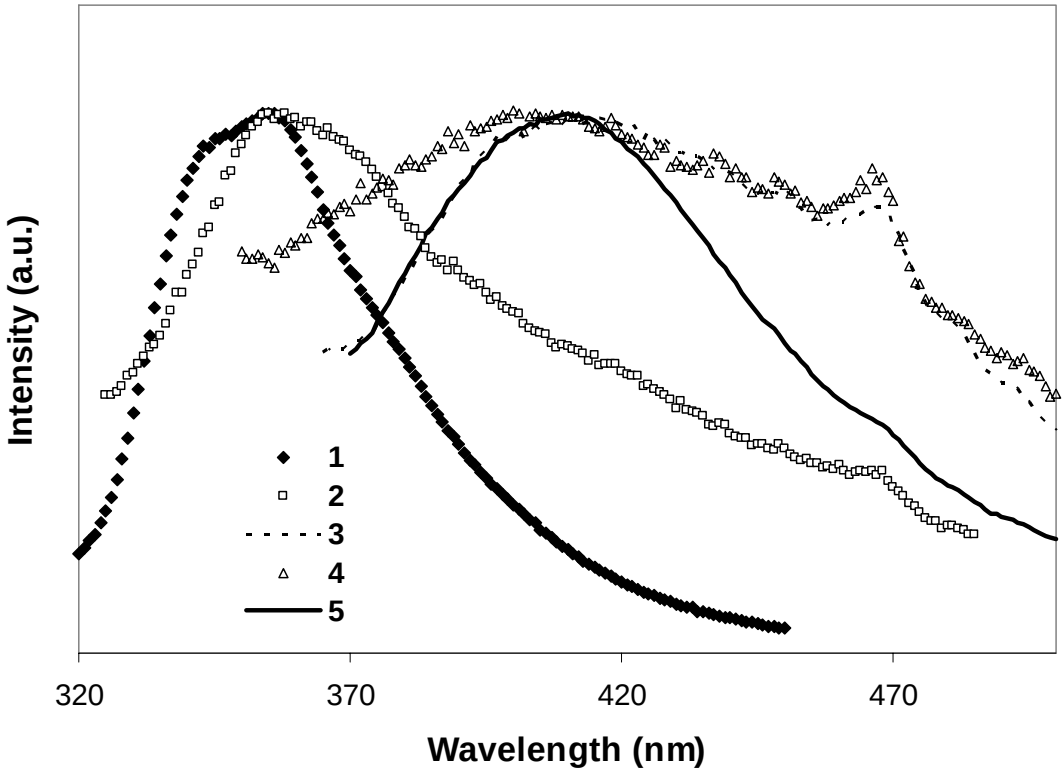


S3. Cyclic voltammetry diagrams for compounds **1-5**

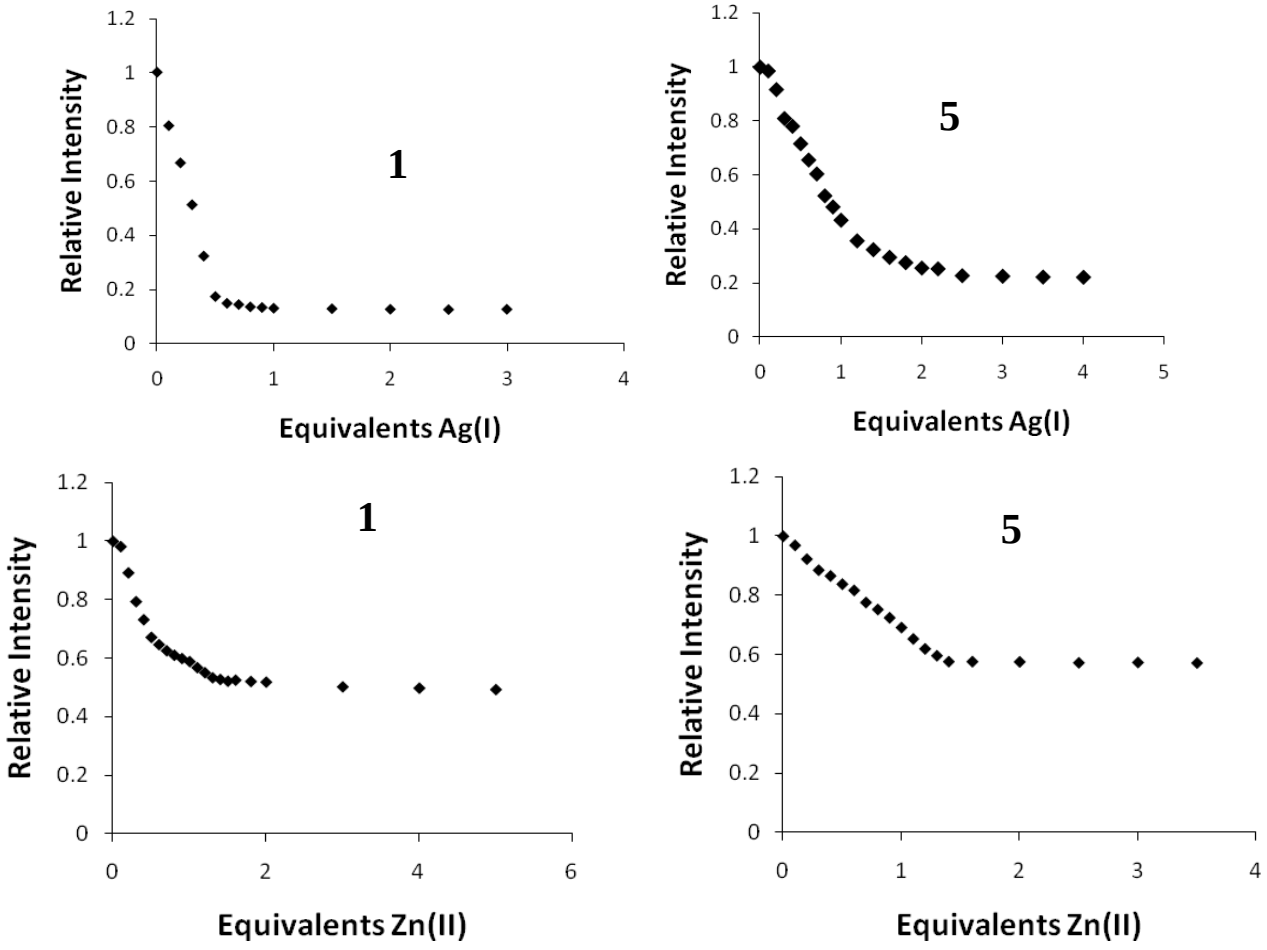


Cyclic voltammetry experiments for **1**, **2** and **4** were obtained in acetonitrile. Due to poor solubility, the corresponding diagrams for compounds **3** and **5** were performed in DMF.

S4. Solid state emission spectra of compounds **1 – 5**.



S5. Stern-Volmer plots for the fluorescent titrations of **1** and **5** with $AgNO_3$ and $Zn(O_2CCF_3)$.



S6. Crystal structural data for compounds **2** and **5**

Crystal data and structure refinement for 2.

Table 1. Crystal data and structure refinement for compound 2.

Identification code	compound 2	
Empirical formula	C27 H18 N6	
Formula weight	426.47	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2(1)	
Unit cell dimensions	a = 16.7951(9) Å	α= 90°.
	b = 16.5308(12) Å	β= 90°.
	c = 7.4080(5) Å	γ = 90°.
Volume	2056.7(2) $Å^3$	
Z	4	
Density (calculated)	1.377 Mg/m^3	
Absorption coefficient	0.085 mm^{-1}	
F(000)	888	
Crystal size	0.20 x 0.05 x 0.05 mm^3	
Theta range for data collection	2.43 to 27.05°.	
Index ranges	-21<=h<=17, -12<=k<=21, -9<=l<=9	
Reflections collected	7922	
Independent reflections	3955 [R(int) = 0.0562]	
Completeness to theta = 27.05°	99.4 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9957 and 0.9831	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3955 / 1 / 299	
Goodness-of-fit on F^2	1.029	
Final R indices [I>2sigma(I)]	R1 = 0.0449, wR2 = 0.0922	
R indices (all data)	R1 = 0.0667, wR2 = 0.1029	
Absolute structure parameter	4(3)	
Largest diff. peak and hole	0.174 and -0.255 $e.Å^{-3}$	

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

	x	y	z	U(eq)
N(1)	4444(1)	3529(1)	6491(3)	28(1)
N(2)	4340(1)	4727(1)	7917(3)	33(1)
N(3)	6846(1)	2242(1)	4422(3)	27(1)
N(4)	4260(1)	1281(1)	2262(3)	27(1)
N(5)	8051(1)	1728(1)	5071(4)	36(1)
N(6)	3155(1)	627(1)	1336(3)	34(1)
C(1)	3890(2)	4150(1)	8822(4)	29(1)
C(2)	3432(2)	4225(2)	10384(4)	38(1)
C(3)	3049(2)	3549(2)	11026(4)	41(1)
C(4)	3117(2)	2799(2)	10150(4)	37(1)
C(5)	3569(2)	2708(1)	8613(4)	31(1)
C(6)	3945(1)	3398(1)	7964(3)	26(1)
C(7)	4663(2)	4336(1)	6580(4)	33(1)
C(8)	8119(1)	2560(1)	4771(4)	29(1)
C(9)	8788(1)	3061(1)	4860(4)	35(1)
C(10)	8681(2)	3872(1)	4535(4)	38(1)
C(11)	7933(2)	4192(1)	4088(4)	37(1)
C(12)	7263(2)	3712(1)	3993(4)	33(1)
C(13)	7375(1)	2894(1)	4362(3)	27(1)
C(14)	7295(1)	1575(1)	4850(4)	33(1)
C(15)	3715(1)	643(1)	-64(4)	28(1)
C(16)	3643(2)	350(1)	-1824(4)	31(1)
C(17)	4286(2)	450(1)	-2966(4)	34(1)
C(18)	4981(2)	826(1)	-2372(3)	33(1)
C(19)	5057(1)	1134(1)	-658(4)	28(1)
C(20)	4410(1)	1042(1)	488(3)	24(1)
C(21)	3504(2)	1010(1)	2656(4)	31(1)
C(22)	4808(1)	2931(1)	5372(4)	28(1)
C(23)	4353(1)	2410(1)	4356(4)	26(1)
C(24)	4730(1)	1808(1)	3350(3)	24(1)
C(25)	5556(1)	1739(1)	3353(3)	26(1)

C(26)	5997(1)	2288(1)	4351(3)	26(1)
C(27)	5633(1)	2882(1)	5388(4)	28(1)

Table 3. Bond lengths [Å] and angles [°] for compound 2.

N(1)-C(7)	1.385(3)	C(10)-H(10A)	0.9500
N(1)-C(6)	1.392(3)	C(11)-C(12)	1.377(3)
N(1)-C(22)	1.428(3)	C(11)-H(11A)	0.9500
N(2)-C(7)	1.301(3)	C(12)-C(13)	1.394(3)
N(2)-C(1)	1.391(3)	C(12)-H(12A)	0.9500
N(3)-C(14)	1.372(3)	C(14)-H(14A)	0.9500
N(3)-C(13)	1.397(3)	C(15)-C(16)	1.396(4)
N(3)-C(26)	1.429(3)	C(15)-C(20)	1.402(3)
N(4)-C(21)	1.378(3)	C(16)-C(17)	1.382(4)
N(4)-C(20)	1.396(3)	C(16)-H(16A)	0.9500
N(4)-C(24)	1.425(3)	C(17)-C(18)	1.395(4)
N(5)-C(14)	1.305(3)	C(17)-H(17A)	0.9500
N(5)-C(8)	1.399(3)	C(18)-C(19)	1.374(4)
N(6)-C(21)	1.304(3)	C(18)-H(18A)	0.9500
N(6)-C(15)	1.401(3)	C(19)-C(20)	1.387(3)
C(1)-C(2)	1.396(4)	C(19)-H(19A)	0.9500
C(1)-C(6)	1.398(3)	C(21)-H(21A)	0.9500
C(2)-C(3)	1.374(4)	C(22)-C(23)	1.376(3)
C(2)-H(2A)	0.9500	C(22)-C(27)	1.387(3)
C(3)-C(4)	1.404(4)	C(23)-C(24)	1.395(3)
C(3)-H(3A)	0.9500	C(23)-H(23A)	0.9500
C(4)-C(5)	1.377(4)	C(24)-C(25)	1.394(3)
C(4)-H(4A)	0.9500	C(25)-C(26)	1.384(3)
C(5)-C(6)	1.391(3)	C(25)-H(25A)	0.9500
C(5)-H(5A)	0.9500	C(26)-C(27)	1.390(3)
C(7)-H(7A)	0.9500	C(27)-H(27A)	0.9500
C(8)-C(9)	1.397(3)		
C(8)-C(13)	1.400(3)	C(7)-N(1)-C(6)	105.8(2)
C(9)-C(10)	1.373(3)	C(7)-N(1)-C(22)	125.5(2)
C(9)-H(9A)	0.9500	C(6)-N(1)-C(22)	127.25(19)
C(10)-C(11)	1.404(4)	C(7)-N(2)-C(1)	104.58(19)

C(14)-N(3)-C(13)	106.12(18)	C(9)-C(10)-H(10A)	119.1
C(14)-N(3)-C(26)	126.82(18)	C(11)-C(10)-H(10A)	119.1
C(13)-N(3)-C(26)	126.31(17)	C(12)-C(11)-C(10)	121.8(2)
C(21)-N(4)-C(20)	105.9(2)	C(12)-C(11)-H(11A)	119.1
C(21)-N(4)-C(24)	126.1(2)	C(10)-C(11)-H(11A)	119.1
C(20)-N(4)-C(24)	127.3(2)	C(11)-C(12)-C(13)	116.0(2)
C(14)-N(5)-C(8)	104.44(19)	C(11)-C(12)-H(12A)	122.0
C(21)-N(6)-C(15)	104.10(19)	C(13)-C(12)-H(12A)	122.0
N(2)-C(1)-C(2)	129.6(2)	C(12)-C(13)-N(3)	132.1(2)
N(2)-C(1)-C(6)	110.8(2)	C(12)-C(13)-C(8)	123.0(2)
C(2)-C(1)-C(6)	119.6(2)	N(3)-C(13)-C(8)	104.90(18)
C(3)-C(2)-C(1)	118.2(2)	N(5)-C(14)-N(3)	114.1(2)
C(3)-C(2)-H(2A)	120.9	N(5)-C(14)-H(14A)	122.9
C(1)-C(2)-H(2A)	120.9	N(3)-C(14)-H(14A)	122.9
C(2)-C(3)-C(4)	121.3(3)	C(16)-C(15)-N(6)	128.8(2)
C(2)-C(3)-H(3A)	119.3	C(16)-C(15)-C(20)	120.5(2)
C(4)-C(3)-H(3A)	119.3	N(6)-C(15)-C(20)	110.6(2)
C(5)-C(4)-C(3)	121.7(2)	C(17)-C(16)-C(15)	117.6(2)
C(5)-C(4)-H(4A)	119.2	C(17)-C(16)-H(16A)	121.2
C(3)-C(4)-H(4A)	119.2	C(15)-C(16)-H(16A)	121.2
C(4)-C(5)-C(6)	116.5(2)	C(16)-C(17)-C(18)	121.0(2)
C(4)-C(5)-H(5A)	121.8	C(16)-C(17)-H(17A)	119.5
C(6)-C(5)-H(5A)	121.8	C(18)-C(17)-H(17A)	119.5
C(5)-C(6)-N(1)	132.2(2)	C(19)-C(18)-C(17)	122.3(3)
C(5)-C(6)-C(1)	122.8(2)	C(19)-C(18)-H(18A)	118.9
N(1)-C(6)-C(1)	105.0(2)	C(17)-C(18)-H(18A)	118.9
N(2)-C(7)-N(1)	113.9(2)	C(18)-C(19)-C(20)	116.9(2)
N(2)-C(7)-H(7A)	123.1	C(18)-C(19)-H(19A)	121.5
N(1)-C(7)-H(7A)	123.1	C(20)-C(19)-H(19A)	121.5
C(9)-C(8)-N(5)	129.9(2)	C(19)-C(20)-N(4)	133.3(2)
C(9)-C(8)-C(13)	119.7(2)	C(19)-C(20)-C(15)	121.7(2)
N(5)-C(8)-C(13)	110.4(2)	N(4)-C(20)-C(15)	104.9(2)
C(10)-C(9)-C(8)	117.7(2)	N(6)-C(21)-N(4)	114.5(2)
C(10)-C(9)-H(9A)	121.1	N(6)-C(21)-H(21A)	122.8
C(8)-C(9)-H(9A)	121.1	N(4)-C(21)-H(21A)	122.8
C(9)-C(10)-C(11)	121.7(2)	C(23)-C(22)-C(27)	121.5(2)

C(23)-C(22)-N(1)	120.9(2)	C(26)-C(25)-H(25A)	120.7
C(27)-C(22)-N(1)	117.6(2)	C(24)-C(25)-H(25A)	120.7
C(22)-C(23)-C(24)	119.1(2)	C(25)-C(26)-C(27)	121.6(2)
C(22)-C(23)-H(23A)	120.4	C(25)-C(26)-N(3)	121.2(2)
C(24)-C(23)-H(23A)	120.4	C(27)-C(26)-N(3)	117.2(2)
C(25)-C(24)-C(23)	120.6(2)	C(22)-C(27)-C(26)	118.4(2)
C(25)-C(24)-N(4)	120.2(2)	C(22)-C(27)-H(27A)	120.8
C(23)-C(24)-N(4)	119.2(2)	C(26)-C(27)-H(27A)	120.8
C(26)-C(25)-C(24)	118.7(2)		

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

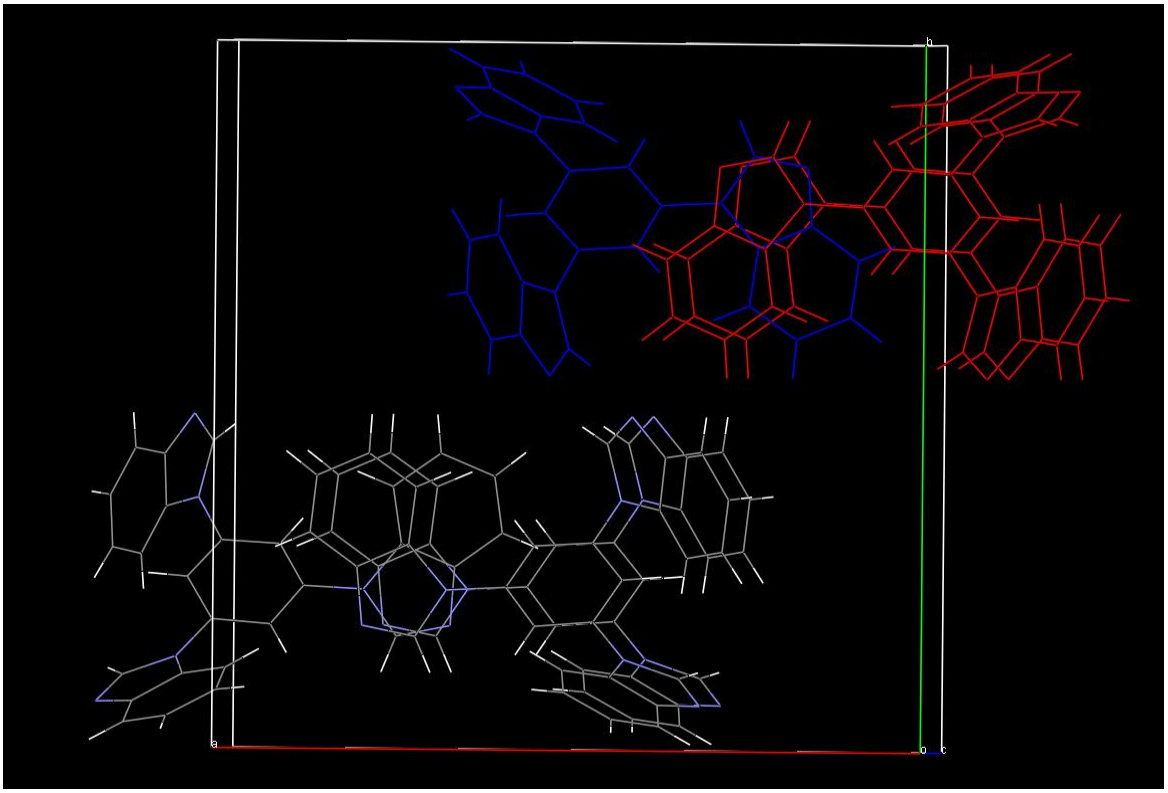
	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(1)	28(1)	26(1)	29(1)	-2(1)	4(1)	1(1)
N(2)	36(1)	26(1)	38(1)	-2(1)	5(1)	2(1)
N(3)	22(1)	28(1)	30(1)	-2(1)	-2(1)	-1(1)
N(4)	22(1)	31(1)	26(1)	-1(1)	1(1)	-1(1)
N(5)	27(1)	33(1)	48(1)	-4(1)	-7(1)	1(1)
N(6)	26(1)	39(1)	37(1)	-1(1)	-1(1)	-4(1)
C(1)	30(1)	28(1)	29(1)	-1(1)	-2(1)	5(1)
C(2)	41(2)	35(1)	37(2)	-3(1)	7(2)	8(1)
C(3)	40(2)	48(2)	35(2)	5(1)	11(2)	10(1)
C(4)	33(1)	38(1)	38(2)	10(1)	7(2)	2(1)
C(5)	32(2)	27(1)	35(1)	1(1)	-2(1)	4(1)
C(6)	23(1)	30(1)	26(1)	2(1)	-1(1)	4(1)
C(7)	35(2)	29(1)	35(2)	4(1)	5(1)	2(1)
C(8)	27(1)	32(1)	28(2)	-2(1)	-2(1)	-1(1)
C(9)	28(1)	43(1)	34(2)	-7(1)	-3(1)	-5(1)
C(10)	39(2)	41(1)	34(2)	-5(1)	6(1)	-15(1)
C(11)	46(2)	31(1)	35(2)	2(1)	9(1)	-6(1)
C(12)	35(2)	33(1)	31(1)	1(1)	2(1)	0(1)
C(13)	28(1)	30(1)	23(1)	-4(1)	-2(1)	-3(1)
C(14)	29(2)	29(1)	40(2)	-1(1)	-5(1)	2(1)
C(15)	28(1)	23(1)	32(1)	1(1)	-5(1)	-1(1)

C(16)	32(2)	26(1)	36(2)	-2(1)	-9(1)	0(1)
C(17)	44(2)	32(1)	25(1)	-3(1)	-8(1)	9(1)
C(18)	36(2)	34(1)	28(1)	2(1)	3(1)	7(1)
C(19)	23(1)	30(1)	30(1)	2(1)	-1(1)	2(1)
C(20)	23(1)	23(1)	25(1)	1(1)	-1(1)	4(1)
C(21)	24(1)	36(1)	33(1)	3(1)	5(1)	-3(1)
C(22)	29(1)	28(1)	26(1)	2(1)	2(1)	5(1)
C(23)	23(1)	30(1)	26(1)	3(1)	-2(1)	0(1)
C(24)	22(1)	28(1)	23(1)	2(1)	-2(1)	-2(1)
C(25)	25(1)	26(1)	26(1)	-2(1)	-2(1)	0(1)
C(26)	24(1)	28(1)	26(1)	2(1)	-2(1)	1(1)
C(27)	30(1)	28(1)	26(1)	-1(1)	-2(1)	-2(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for compound 2.

	x	y	z	U(eq)
H(2A)	3386	4730	10988	45
H(3A)	2731	3590	12083	49
H(4A)	2845	2344	10630	44
H(5A)	3621	2199	8027	38
H(7A)	5016	4581	5742	40
H(9A)	9299	2848	5136	42
H(10A)	9126	4226	4615	45
H(11A)	7886	4754	3845	45
H(12A)	6755	3927	3694	40
H(14A)	7074	1049	4975	39
H(16A)	3169	92	-2222	38
H(17A)	4253	261	-4175	40
H(18A)	5419	870	-3179	39
H(19A)	5530	1398	-275	33
H(21A)	3258	1094	3795	37
H(23A)	3789	2459	4340	32
H(25A)	5813	1324	2683	31
H(27A)	5941	3247	6091	34

Unit cell packing diagram of **2** projected down the c axis:



Crystal data and structure refinement for 5.

Table 3.1. Crystal data and structure refinement for Compound 5.

Identification code	Compound 5/CH_2Cl_2	
Empirical formula	C85 H56 Cl2 N12	
Formula weight	1316.32	
Temperature	180(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 13.2011(16) Å	α= 90°.
	b = 9.2379(11) Å	β= 93.0210(10)°.
	c = 56.398(7) Å	γ = 90°.
Volume	6868.2(14) $Å^3$	
Z	4	
Density (calculated)	1.273 Mg/m^3	
Absorption coefficient	0.152 mm^{-1}	
F(000)	2736	
Crystal size	0.35 x 0.20 x 0.06 mm^3	
Theta range for data collection	1.45 to 24.21°.	
Index ranges	-15<=h<=15, -10<=k<=10, -64<=l<=64	
Reflections collected	59676	
Independent reflections	10992 [R(int) = 0.0420]	
Completeness to theta = 24.21°	99.2 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.9910 and 0.9488	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10992 / 1 / 895	
Goodness-of-fit on F^2	1.086	
Final R indices [I>2sigma(I)]	R1 = 0.0950, wR2 = 0.2432	
R indices (all data)	R1 = 0.1140, wR2 = 0.2554	
Largest diff. peak and hole	0.671 and -1.088 $e.Å^{-3}$	

Table 3.2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for Compound 5. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	7994(2)	5479(3)	1705(1)	149(1)
Cl(2)	6968(2)	4792(4)	1249(1)	165(1)
C(1)	5782(3)	9060(5)	1237(1)	33(1)
C(2)	6345(3)	9190(4)	1033(1)	29(1)
C(3)	7315(3)	9788(4)	1051(1)	29(1)
C(4)	7766(3)	10157(5)	1278(1)	33(1)
C(5)	7207(3)	10016(5)	1480(1)	36(1)
C(6)	6207(3)	9497(5)	1458(1)	35(1)
C(7)	4728(3)	8452(4)	1219(1)	32(1)
C(8)	3987(3)	9054(5)	1063(1)	34(1)
C(9)	3022(3)	8477(5)	1042(1)	35(1)
C(10)	2783(3)	7296(5)	1181(1)	36(1)
C(11)	3509(3)	6681(5)	1336(1)	41(1)
C(12)	4474(3)	7257(5)	1354(1)	38(1)
C(13)	1157(4)	6559(6)	1349(1)	59(1)
C(14)	270(4)	5936(5)	1038(1)	56(1)
C(15)	-491(4)	5488(6)	867(2)	78(2)
C(16)	-255(6)	5481(6)	635(2)	83(2)
C(17)	688(5)	5838(6)	562(1)	71(2)
C(18)	1452(4)	6257(5)	725(1)	55(1)
C(19)	1216(4)	6322(5)	962(1)	46(1)
C(20)	5936(3)	8652(4)	797(1)	29(1)
C(21)	5786(3)	9564(4)	600(1)	31(1)
C(22)	5406(3)	9028(5)	385(1)	32(1)
C(23)	5187(3)	7564(4)	358(1)	29(1)
C(24)	5333(3)	6643(4)	550(1)	33(1)
C(25)	5691(3)	7181(5)	767(1)	35(1)
C(26)	5105(3)	7461(5)	-82(1)	34(1)
C(27)	3799(3)	6171(4)	-159(1)	33(1)
C(28)	2982(3)	5411(5)	-265(1)	41(1)
C(29)	2350(3)	4682(5)	-120(1)	46(1)

C(30)	2517(3)	4684(5)	124(1)	46(1)
C(31)	3320(3)	5443(5)	237(1)	40(1)
C(32)	3948(3)	6185(4)	88(1)	30(1)
C(33)	7916(3)	10089(4)	839(1)	31(1)
C(34)	8374(3)	8994(5)	714(1)	33(1)
C(35)	9027(3)	9311(4)	537(1)	32(1)
C(36)	9222(3)	10745(4)	482(1)	31(1)
C(37)	8742(3)	11851(4)	603(1)	35(1)
C(38)	8100(3)	11511(5)	778(1)	36(1)
C(39)	9762(3)	12143(4)	132(1)	33(1)
C(40)	11214(3)	11233(4)	79(1)	32(1)
C(41)	12162(3)	10857(5)	-6(1)	37(1)
C(42)	12696(3)	9779(5)	110(1)	41(1)
C(43)	12336(3)	9109(5)	311(1)	43(1)
C(44)	11407(3)	9456(5)	397(1)	38(1)
C(45)	10853(3)	10517(4)	272(1)	30(1)
C(46)	8836(3)	10695(5)	1293(1)	33(1)
C(47)	9614(3)	9825(5)	1218(1)	39(1)
C(48)	10591(3)	10351(5)	1217(1)	43(1)
C(49)	10798(3)	11740(5)	1293(1)	36(1)
C(50)	10042(3)	12601(5)	1374(1)	37(1)
C(51)	9066(3)	12082(5)	1376(1)	37(1)
C(52)	12431(4)	12733(5)	1472(1)	49(1)
C(53)	13334(3)	12942(5)	1173(1)	42(1)
C(54)	14090(4)	13181(6)	1014(1)	57(1)
C(55)	13878(5)	12887(6)	778(1)	61(2)
C(56)	12938(4)	12359(6)	697(1)	53(1)
C(57)	12177(4)	12129(5)	848(1)	45(1)
C(58)	12393(3)	12414(5)	1088(1)	37(1)
C(59)	7669(3)	10367(5)	1720(1)	42(1)
C(60)	8472(4)	9538(6)	1817(1)	52(1)
C(61)	8804(4)	9712(8)	2050(1)	69(2)
C(62)	8367(4)	10740(9)	2186(1)	73(2)
C(63)	7613(4)	11651(8)	2089(1)	65(2)
C(64)	7271(4)	11465(6)	1856(1)	48(1)
C(65)	8813(5)	12079(13)	2554(1)	127(4)

C(66)	9143(7)	10351(19)	2806(1)	141(5)
C(67)	9418(8)	9620(20)	3010(2)	167(7)
C(68)	9376(9)	8040(20)	2985(2)	162(7)
C(69)	9055(6)	7359(14)	2771(1)	127(4)
C(70)	8797(6)	8190(15)	2568(1)	113(4)
C(71)	8886(5)	9665(13)	2598(1)	93(3)
C(72)	5633(3)	9425(5)	1680(1)	36(1)
C(73)	4898(4)	10435(6)	1722(1)	47(1)
C(74)	4484(4)	10532(6)	1944(1)	55(1)
C(75)	4796(4)	9578(6)	2122(1)	50(1)
C(76)	5487(4)	8512(6)	2079(1)	53(1)
C(77)	5910(4)	8455(6)	1857(1)	47(1)
C(78)	3426(4)	9893(9)	2406(1)	81(2)
C(79)	4224(5)	9697(7)	2740(1)	69(2)
C(80)	4524(6)	9645(7)	2980(1)	74(2)
C(81)	5542(6)	9515(8)	3042(1)	82(2)
C(82)	6256(6)	9467(10)	2871(1)	97(2)
C(83)	5980(5)	9500(9)	2629(1)	83(2)
C(84)	4954(4)	9594(7)	2569(1)	61(2)
C(85)	7868(9)	5971(9)	1426(2)	142(4)
N(1)	1782(3)	6705(4)	1166(1)	43(1)
N(2)	251(3)	6096(5)	1284(1)	68(1)
N(3)	4798(2)	7051(4)	134(1)	30(1)
N(4)	4546(3)	6983(4)	-264(1)	37(1)
N(5)	9906(2)	11114(4)	305(1)	32(1)
N(6)	10512(2)	12266(4)	-9(1)	34(1)
N(7)	11819(3)	12283(4)	1286(1)	41(1)
N(8)	13334(3)	13139(5)	1418(1)	50(1)
N(9)	8680(4)	10859(9)	2432(1)	100(2)
N(10)	9113(5)	11923(13)	2780(1)	127(4)
N(11)	4404(4)	9686(6)	2353(1)	64(1)
N(12)	3269(4)	9871(8)	2632(1)	91(2)

Table 3.3. Bond lengths [Å] and angles [°] for Compound 5.

Cl(1)-C(85)	1.635(10)	C(22)-C(23)	1.390(6)
Cl(2)-C(85)	1.864(12)	C(23)-C(24)	1.379(6)
C(1)-C(6)	1.397(6)	C(23)-N(3)	1.422(5)
C(1)-C(2)	1.410(6)	C(24)-C(25)	1.384(6)
C(1)-C(7)	1.500(6)	C(26)-N(4)	1.306(5)
C(2)-C(3)	1.394(6)	C(26)-N(3)	1.359(5)
C(2)-C(20)	1.492(5)	C(27)-N(4)	1.394(5)
C(3)-C(4)	1.421(6)	C(27)-C(32)	1.395(6)
C(3)-C(33)	1.499(5)	C(27)-C(28)	1.396(6)
C(4)-C(5)	1.397(6)	C(28)-C(29)	1.375(7)
C(4)-C(46)	1.496(6)	C(29)-C(30)	1.380(7)
C(5)-C(6)	1.404(6)	C(30)-C(31)	1.396(6)
C(5)-C(59)	1.491(6)	C(31)-C(32)	1.392(6)
C(6)-C(72)	1.499(6)	C(32)-N(3)	1.391(5)
C(7)-C(12)	1.391(6)	C(33)-C(38)	1.383(6)
C(7)-C(8)	1.396(6)	C(33)-C(34)	1.389(6)
C(8)-C(9)	1.380(6)	C(34)-C(35)	1.380(6)
C(9)-C(10)	1.388(6)	C(35)-C(36)	1.389(6)
C(10)-C(11)	1.385(6)	C(36)-C(37)	1.397(6)
C(10)-N(1)	1.429(5)	C(36)-N(5)	1.423(5)
C(11)-C(12)	1.379(6)	C(37)-C(38)	1.371(6)
C(13)-N(2)	1.306(7)	C(39)-N(6)	1.307(5)
C(13)-N(1)	1.363(6)	C(39)-N(5)	1.367(5)
C(14)-C(19)	1.390(7)	C(40)-C(45)	1.383(6)
C(14)-N(2)	1.396(8)	C(40)-N(6)	1.401(5)
C(14)-C(15)	1.418(8)	C(40)-C(41)	1.407(6)
C(15)-C(16)	1.357(10)	C(41)-C(42)	1.368(6)
C(16)-C(17)	1.374(10)	C(42)-C(43)	1.393(6)
C(17)-C(18)	1.384(8)	C(43)-C(44)	1.380(6)
C(18)-C(19)	1.389(7)	C(44)-C(45)	1.391(6)
C(19)-N(1)	1.384(6)	C(45)-N(5)	1.387(5)
C(20)-C(21)	1.399(6)	C(46)-C(47)	1.388(6)
C(20)-C(25)	1.405(6)	C(46)-C(51)	1.391(6)
C(21)-C(22)	1.383(6)	C(47)-C(48)	1.378(6)

C(48)-C(49)	1.376(6)	C(75)-N(11)	1.434(6)
C(49)-C(50)	1.373(6)	C(76)-C(77)	1.398(6)
C(49)-N(7)	1.441(5)	C(78)-N(12)	1.299(7)
C(50)-C(51)	1.376(6)	C(78)-N(11)	1.353(7)
C(52)-N(8)	1.301(6)	C(79)-N(12)	1.382(8)
C(52)-N(7)	1.355(6)	C(79)-C(80)	1.393(8)
C(53)-C(54)	1.392(7)	C(79)-C(84)	1.400(7)
C(53)-N(8)	1.395(6)	C(80)-C(81)	1.376(10)
C(53)-C(58)	1.396(6)	C(81)-C(82)	1.383(10)
C(54)-C(55)	1.372(8)	C(82)-C(83)	1.395(9)
C(55)-C(56)	1.388(8)	C(83)-C(84)	1.381(8)
C(56)-C(57)	1.368(7)	C(84)-N(11)	1.389(7)
C(57)-C(58)	1.391(6)		
C(58)-N(7)	1.389(6)	C(6)-C(1)-C(2)	120.0(4)
C(59)-C(64)	1.390(7)	C(6)-C(1)-C(7)	119.8(4)
C(59)-C(60)	1.395(7)	C(2)-C(1)-C(7)	120.2(3)
C(60)-C(61)	1.373(7)	C(3)-C(2)-C(1)	119.5(4)
C(61)-C(62)	1.368(9)	C(3)-C(2)-C(20)	119.2(3)
C(62)-C(63)	1.394(9)	C(1)-C(2)-C(20)	121.3(3)
C(62)-N(9)	1.429(7)	C(2)-C(3)-C(4)	120.2(4)
C(63)-C(64)	1.377(7)	C(2)-C(3)-C(33)	122.3(3)
C(65)-N(10)	1.323(10)	C(4)-C(3)-C(33)	117.4(3)
C(65)-N(9)	1.327(11)	C(5)-C(4)-C(3)	119.8(4)
C(66)-C(71)	1.362(12)	C(5)-C(4)-C(46)	121.4(4)
C(66)-C(67)	1.369(16)	C(3)-C(4)-C(46)	118.8(3)
C(66)-N(10)	1.460(15)	C(4)-C(5)-C(6)	119.5(4)
C(67)-C(68)	1.47(2)	C(4)-C(5)-C(59)	120.9(4)
C(68)-C(69)	1.407(15)	C(6)-C(5)-C(59)	119.6(4)
C(69)-C(70)	1.405(11)	C(1)-C(6)-C(5)	120.7(4)
C(70)-C(71)	1.376(13)	C(1)-C(6)-C(72)	122.3(4)
C(71)-N(9)	1.462(12)	C(5)-C(6)-C(72)	117.0(4)
C(72)-C(73)	1.376(7)	C(12)-C(7)-C(8)	118.7(4)
C(72)-C(77)	1.377(6)	C(12)-C(7)-C(1)	120.6(4)
C(73)-C(74)	1.393(7)	C(8)-C(7)-C(1)	120.7(4)
C(74)-C(75)	1.381(7)	C(9)-C(8)-C(7)	120.8(4)
C(75)-C(76)	1.372(7)	C(8)-C(9)-C(10)	119.4(4)

C(11)-C(10)-C(9)	120.5(4)	C(31)-C(32)-C(27)	122.7(4)
C(11)-C(10)-N(1)	119.2(4)	C(38)-C(33)-C(34)	118.6(4)
C(9)-C(10)-N(1)	120.3(4)	C(38)-C(33)-C(3)	118.8(4)
C(12)-C(11)-C(10)	119.7(4)	C(34)-C(33)-C(3)	122.3(4)
C(11)-C(12)-C(7)	120.9(4)	C(35)-C(34)-C(33)	121.1(4)
N(2)-C(13)-N(1)	113.5(5)	C(34)-C(35)-C(36)	119.6(4)
C(19)-C(14)-N(2)	110.1(5)	C(35)-C(36)-C(37)	119.6(4)
C(19)-C(14)-C(15)	118.7(6)	C(35)-C(36)-N(5)	121.2(4)
N(2)-C(14)-C(15)	131.2(6)	C(37)-C(36)-N(5)	119.2(4)
C(16)-C(15)-C(14)	117.8(6)	C(38)-C(37)-C(36)	119.8(4)
C(15)-C(16)-C(17)	123.2(6)	C(37)-C(38)-C(33)	121.3(4)
C(16)-C(17)-C(18)	120.4(7)	N(6)-C(39)-N(5)	114.3(4)
C(17)-C(18)-C(19)	117.4(6)	C(45)-C(40)-N(6)	110.8(4)
N(1)-C(19)-C(18)	132.3(4)	C(45)-C(40)-C(41)	120.0(4)
N(1)-C(19)-C(14)	105.2(5)	N(6)-C(40)-C(41)	129.2(4)
C(18)-C(19)-C(14)	122.5(5)	C(42)-C(41)-C(40)	117.6(4)
C(21)-C(20)-C(25)	117.7(4)	C(41)-C(42)-C(43)	121.5(4)
C(21)-C(20)-C(2)	122.3(4)	C(44)-C(43)-C(42)	122.0(4)
C(25)-C(20)-C(2)	120.0(4)	C(43)-C(44)-C(45)	116.1(4)
C(22)-C(21)-C(20)	120.8(4)	C(40)-C(45)-N(5)	105.3(4)
C(21)-C(22)-C(23)	120.4(4)	C(40)-C(45)-C(44)	122.8(4)
C(24)-C(23)-C(22)	119.8(4)	N(5)-C(45)-C(44)	131.8(4)
C(24)-C(23)-N(3)	121.3(4)	C(47)-C(46)-C(51)	119.0(4)
C(22)-C(23)-N(3)	118.8(4)	C(47)-C(46)-C(4)	120.1(4)
C(23)-C(24)-C(25)	119.9(4)	C(51)-C(46)-C(4)	120.9(4)
C(24)-C(25)-C(20)	121.3(4)	C(48)-C(47)-C(46)	120.3(4)
N(4)-C(26)-N(3)	115.2(4)	C(49)-C(48)-C(47)	119.8(4)
N(4)-C(27)-C(32)	110.6(4)	C(50)-C(49)-C(48)	120.6(4)
N(4)-C(27)-C(28)	129.5(4)	C(50)-C(49)-N(7)	120.3(4)
C(32)-C(27)-C(28)	119.9(4)	C(48)-C(49)-N(7)	119.1(4)
C(29)-C(28)-C(27)	118.0(4)	C(49)-C(50)-C(51)	119.9(4)
C(28)-C(29)-C(30)	121.5(4)	C(50)-C(51)-C(46)	120.4(4)
C(29)-C(30)-C(31)	122.2(4)	N(8)-C(52)-N(7)	115.0(4)
C(32)-C(31)-C(30)	115.7(4)	C(54)-C(53)-N(8)	130.8(4)
N(3)-C(32)-C(31)	132.2(4)	C(54)-C(53)-C(58)	119.4(5)
N(3)-C(32)-C(27)	105.1(3)	N(8)-C(53)-C(58)	109.8(4)

C(55)-C(54)-C(53)	118.3(5)	C(75)-C(76)-C(77)	119.0(5)
C(54)-C(55)-C(56)	121.5(5)	C(72)-C(77)-C(76)	121.5(5)
C(57)-C(56)-C(55)	121.5(5)	N(12)-C(78)-N(11)	114.7(6)
C(56)-C(57)-C(58)	117.2(5)	N(12)-C(79)-C(80)	129.8(6)
N(7)-C(58)-C(57)	132.3(4)	N(12)-C(79)-C(84)	110.4(5)
N(7)-C(58)-C(53)	105.6(4)	C(80)-C(79)-C(84)	119.7(6)
C(57)-C(58)-C(53)	122.1(4)	C(81)-C(80)-C(79)	118.3(6)
C(64)-C(59)-C(60)	119.2(4)	C(80)-C(81)-C(82)	121.2(6)
C(64)-C(59)-C(5)	120.6(4)	C(81)-C(82)-C(83)	121.9(7)
C(60)-C(59)-C(5)	120.1(4)	C(84)-C(83)-C(82)	116.3(6)
C(61)-C(60)-C(59)	120.4(5)	C(83)-C(84)-N(11)	132.8(5)
C(62)-C(61)-C(60)	119.8(5)	C(83)-C(84)-C(79)	122.5(5)
C(61)-C(62)-C(63)	120.7(5)	N(11)-C(84)-C(79)	104.6(5)
C(61)-C(62)-N(9)	119.2(6)	Cl(1)-C(85)-Cl(2)	112.5(5)
C(63)-C(62)-N(9)	120.0(6)	C(13)-N(1)-C(19)	106.6(4)
C(64)-C(63)-C(62)	119.5(5)	C(13)-N(1)-C(10)	126.0(4)
C(63)-C(64)-C(59)	120.1(5)	C(19)-N(1)-C(10)	127.1(4)
N(10)-C(65)-N(9)	115.6(11)	C(13)-N(2)-C(14)	104.6(4)
C(71)-C(66)-C(67)	122.7(16)	C(26)-N(3)-C(32)	105.6(3)
C(71)-C(66)-N(10)	111.9(10)	C(26)-N(3)-C(23)	126.6(3)
C(67)-C(66)-N(10)	125.4(12)	C(32)-N(3)-C(23)	127.4(3)
C(66)-C(67)-C(68)	113.7(13)	C(26)-N(4)-C(27)	103.5(3)
C(69)-C(68)-C(67)	122.5(12)	C(39)-N(5)-C(45)	106.0(3)
C(70)-C(69)-C(68)	120.1(13)	C(39)-N(5)-C(36)	126.6(3)
C(71)-C(70)-C(69)	115.4(9)	C(45)-N(5)-C(36)	127.4(3)
C(66)-C(71)-C(70)	125.4(11)	C(39)-N(6)-C(40)	103.6(3)
C(66)-C(71)-N(9)	103.3(11)	C(52)-N(7)-C(58)	105.6(4)
C(70)-C(71)-N(9)	131.2(7)	C(52)-N(7)-C(49)	127.3(4)
C(73)-C(72)-C(77)	118.5(4)	C(58)-N(7)-C(49)	127.1(4)
C(73)-C(72)-C(6)	120.5(4)	C(52)-N(8)-C(53)	104.1(4)
C(77)-C(72)-C(6)	120.6(4)	C(65)-N(9)-C(62)	126.2(8)
C(72)-C(73)-C(74)	120.9(5)	C(65)-N(9)-C(71)	107.1(7)
C(75)-C(74)-C(73)	119.6(5)	C(62)-N(9)-C(71)	126.6(7)
C(76)-C(75)-C(74)	120.4(4)	C(65)-N(10)-C(66)	102.1(8)
C(76)-C(75)-N(11)	119.1(5)	C(78)-N(11)-C(84)	106.0(4)
C(74)-C(75)-N(11)	120.5(5)	C(78)-N(11)-C(75)	127.3(5)

C(84)-N(11)-C(75)	126.7(5)	C(78)-N(12)-C(79)	104.2(5)

Table 3.4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for Compound 5. 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}
Cl(1)	148(2)	121(2)	179(3)	-7(2)	24(2)	5(2)
Cl(2)	120(2)	138(2)	231(4)	15(2)	-60(2)	19(2)
C(1)	32(2)	38(2)	29(2)	0(2)	1(2)	2(2)
C(2)	29(2)	29(2)	30(2)	0(2)	-1(2)	1(2)
C(3)	33(2)	28(2)	26(2)	0(2)	3(2)	4(2)
C(4)	30(2)	37(2)	31(2)	-1(2)	1(2)	-1(2)
C(5)	36(2)	44(3)	27(2)	-2(2)	-1(2)	-2(2)
C(6)	32(2)	40(2)	31(2)	1(2)	1(2)	2(2)
C(7)	36(2)	33(2)	26(2)	-1(2)	3(2)	-3(2)
C(8)	37(2)	35(2)	31(2)	2(2)	7(2)	0(2)
C(9)	30(2)	39(2)	38(2)	4(2)	3(2)	-2(2)
C(10)	32(2)	37(2)	41(2)	-4(2)	5(2)	0(2)
C(11)	45(3)	39(3)	39(2)	5(2)	9(2)	-7(2)
C(12)	38(2)	41(3)	36(2)	2(2)	2(2)	2(2)
C(13)	55(3)	54(3)	68(4)	7(3)	15(3)	-14(3)
C(14)	43(3)	39(3)	87(4)	17(3)	0(3)	-8(2)
C(15)	49(3)	39(3)	142(7)	17(4)	-19(4)	-18(3)
C(16)	100(6)	39(3)	106(6)	18(3)	-48(5)	-18(3)
C(17)	96(5)	36(3)	78(4)	7(3)	-33(4)	-15(3)
C(18)	62(3)	39(3)	61(3)	4(2)	-8(3)	-3(2)
C(19)	42(3)	32(2)	65(3)	11(2)	-6(2)	-2(2)
C(20)	24(2)	35(2)	29(2)	-2(2)	2(2)	1(2)
C(21)	30(2)	29(2)	35(2)	-1(2)	2(2)	-3(2)
C(22)	28(2)	34(2)	33(2)	6(2)	0(2)	0(2)
C(23)	28(2)	31(2)	28(2)	-1(2)	4(2)	0(2)
C(24)	39(2)	24(2)	35(2)	0(2)	3(2)	0(2)
C(25)	39(2)	34(2)	30(2)	1(2)	3(2)	1(2)
C(26)	34(2)	35(2)	32(2)	2(2)	1(2)	1(2)

C(27)	33(2)	30(2)	35(2)	0(2)	0(2)	3(2)
C(28)	39(2)	41(3)	42(3)	-5(2)	-10(2)	2(2)
C(29)	37(3)	39(3)	59(3)	-3(2)	-12(2)	-5(2)
C(30)	39(3)	41(3)	58(3)	4(2)	4(2)	-10(2)
C(31)	44(3)	35(2)	41(2)	0(2)	7(2)	-2(2)
C(32)	29(2)	27(2)	34(2)	-4(2)	1(2)	0(2)
C(33)	28(2)	33(2)	31(2)	-2(2)	-1(2)	-1(2)
C(34)	35(2)	30(2)	34(2)	0(2)	4(2)	-6(2)
C(35)	36(2)	29(2)	32(2)	-6(2)	8(2)	-1(2)
C(36)	31(2)	31(2)	31(2)	-1(2)	3(2)	-2(2)
C(37)	40(2)	26(2)	38(2)	0(2)	8(2)	-1(2)
C(38)	35(2)	34(2)	38(2)	-4(2)	11(2)	4(2)
C(39)	32(2)	30(2)	38(2)	-2(2)	2(2)	-2(2)
C(40)	31(2)	33(2)	32(2)	-3(2)	-1(2)	-6(2)
C(41)	32(2)	39(2)	40(2)	-1(2)	5(2)	-9(2)
C(42)	28(2)	37(2)	60(3)	-3(2)	8(2)	2(2)
C(43)	39(3)	36(2)	55(3)	1(2)	3(2)	5(2)
C(44)	39(2)	35(2)	39(2)	3(2)	5(2)	-2(2)
C(45)	27(2)	30(2)	33(2)	-3(2)	4(2)	-7(2)
C(46)	32(2)	38(2)	28(2)	0(2)	-2(2)	-1(2)
C(47)	38(2)	31(2)	48(3)	-5(2)	3(2)	-1(2)
C(48)	35(2)	43(3)	50(3)	-6(2)	8(2)	0(2)
C(49)	34(2)	41(3)	33(2)	3(2)	1(2)	-6(2)
C(50)	43(3)	36(2)	31(2)	-4(2)	-5(2)	-7(2)
C(51)	40(2)	38(2)	34(2)	-5(2)	0(2)	3(2)
C(52)	54(3)	50(3)	42(3)	-2(2)	3(2)	-16(2)
C(53)	43(3)	34(2)	49(3)	2(2)	1(2)	-12(2)
C(54)	48(3)	44(3)	79(4)	4(3)	16(3)	-15(2)
C(55)	77(4)	45(3)	64(4)	2(3)	33(3)	-11(3)
C(56)	71(4)	45(3)	43(3)	6(2)	13(3)	-7(3)
C(57)	55(3)	36(3)	45(3)	4(2)	0(2)	-4(2)
C(58)	38(2)	31(2)	42(3)	0(2)	5(2)	-2(2)
C(59)	37(2)	58(3)	31(2)	-2(2)	2(2)	-9(2)
C(60)	42(3)	77(4)	37(3)	4(2)	2(2)	3(3)
C(61)	43(3)	124(6)	39(3)	6(3)	-4(2)	8(3)
C(62)	45(3)	143(6)	30(3)	-9(3)	-2(2)	-15(4)

C(63)	50(3)	104(5)	42(3)	-20(3)	6(2)	-8(3)
C(64)	43(3)	67(3)	35(2)	-8(2)	0(2)	-5(2)
C(65)	70(5)	249(12)	62(4)	-73(6)	13(4)	-47(6)
C(66)	73(5)	302(17)	45(5)	-38(8)	-6(4)	-10(9)
C(67)	90(6)	370(20)	36(4)	11(9)	5(4)	59(12)
C(68)	102(7)	340(20)	48(5)	16(9)	2(4)	74(12)
C(69)	94(6)	225(12)	64(5)	33(6)	18(4)	43(7)
C(70)	81(5)	219(12)	40(4)	2(6)	2(3)	48(7)
C(71)	63(4)	180(9)	36(4)	-11(5)	5(3)	11(5)
C(72)	33(2)	44(3)	32(2)	-2(2)	3(2)	-3(2)
C(73)	44(3)	61(3)	37(3)	9(2)	3(2)	5(2)
C(74)	46(3)	76(4)	44(3)	3(3)	15(2)	13(3)
C(75)	47(3)	69(3)	34(2)	5(2)	13(2)	1(3)
C(76)	61(3)	65(3)	32(2)	8(2)	4(2)	3(3)
C(77)	50(3)	55(3)	35(2)	2(2)	4(2)	6(2)
C(78)	50(3)	143(7)	50(3)	9(4)	21(3)	15(4)
C(79)	89(5)	79(4)	41(3)	7(3)	19(3)	0(4)
C(80)	102(5)	74(4)	48(3)	1(3)	25(3)	1(4)
C(81)	105(6)	91(5)	49(4)	-3(3)	0(4)	7(4)
C(82)	97(5)	142(7)	52(4)	4(4)	-5(4)	-3(5)
C(83)	71(4)	131(6)	47(3)	4(4)	7(3)	0(4)
C(84)	67(4)	85(4)	34(3)	5(3)	13(3)	-1(3)
C(85)	208(11)	77(5)	152(9)	12(6)	113(8)	-19(6)
N(1)	35(2)	40(2)	53(2)	6(2)	7(2)	-9(2)
N(2)	51(3)	51(3)	105(4)	7(3)	27(3)	-17(2)
N(3)	32(2)	29(2)	29(2)	-1(1)	3(1)	-1(2)
N(4)	39(2)	42(2)	31(2)	5(2)	1(2)	1(2)
N(5)	34(2)	28(2)	33(2)	1(2)	7(2)	-2(2)
N(6)	29(2)	35(2)	40(2)	1(2)	3(2)	-2(2)
N(7)	41(2)	45(2)	38(2)	-3(2)	-1(2)	-11(2)
N(8)	48(2)	49(2)	53(3)	-1(2)	-5(2)	-16(2)
N(9)	53(3)	214(8)	33(3)	-25(4)	-2(2)	-9(4)
N(10)	76(4)	260(11)	45(4)	-49(6)	0(3)	-35(6)
N(11)	64(3)	93(4)	35(2)	8(2)	13(2)	8(3)
N(12)	75(4)	141(6)	60(3)	19(3)	28(3)	16(4)

Table 3.5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for Compound 5.

	x	y	z	U(eq)
H(8A)	4149	9872	970	41
H(9A)	2526	8884	934	43
H(11A)	3344	5866	1429	49
H(12A)	4972	6832	1460	46
H(13A)	1362	6773	1509	70
H(15A)	-1144	5202	912	93
H(16A)	-767	5217	519	100
H(17A)	817	5797	397	86
H(18A)	2111	6491	677	65
H(21A)	5947	10563	615	37
H(22A)	5295	9665	254	38
H(24A)	5188	5640	532	40
H(25A)	5772	6543	899	41
H(26A)	5684	8053	-101	41
H(28A)	2866	5397	-433	49
H(29A)	1787	4166	-189	55
H(30A)	2071	4151	218	55
H(31A)	3429	5453	405	48
H(34A)	8236	8012	750	39
H(35A)	9340	8552	454	38
H(37A)	8861	12834	564	41
H(38A)	7775	12268	859	43
H(39A)	9166	12719	116	40
H(41A)	12421	11334	-139	44
H(42A)	13328	9481	53	50
H(43A)	12742	8392	390	52
H(44A)	11161	8998	533	45
H(47A)	9473	8863	1167	47
H(48A)	11120	9757	1163	51
H(50A)	10193	13555	1428	44

H(51A)	8545	12674	1434	45
H(52A)	12217	12751	1631	58
H(54A)	14737	13538	1068	68
H(55A)	14386	13048	668	73
H(56A)	12821	12152	533	63
H(57A)	11529	11790	792	55
H(60A)	8792	8848	1721	62
H(61A)	9336	9122	2116	83
H(63A)	7337	12393	2182	78
H(64A)	6763	12089	1787	58
H(65A)	8700	13004	2483	152
H(67A)	9618	10093	3155	200
H(68A)	9573	7459	3118	194
H(69A)	9012	6333	2764	153
H(70A)	8576	7764	2421	136
H(73A)	4670	11074	1599	57
H(74A)	3990	11249	1972	66
H(76A)	5675	7823	2198	63
H(77A)	6399	7731	1828	56
H(78A)	2897	10043	2288	97
H(80A)	4039	9697	3098	89
H(81A)	5759	9457	3205	98
H(82A)	6955	9409	2920	117
H(83A)	6470	9460	2512	99
H(85A)	8540	5939	1356	170
H(85B)	7622	6983	1417	170

Unit cell packing diagram of **5** projected down the b axis: