Electronic Supplementary Material (ESI) for CrystEngComm

N-Substituted pyridazines as building blocks in novel supramolecular architectures

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Supplementary Information

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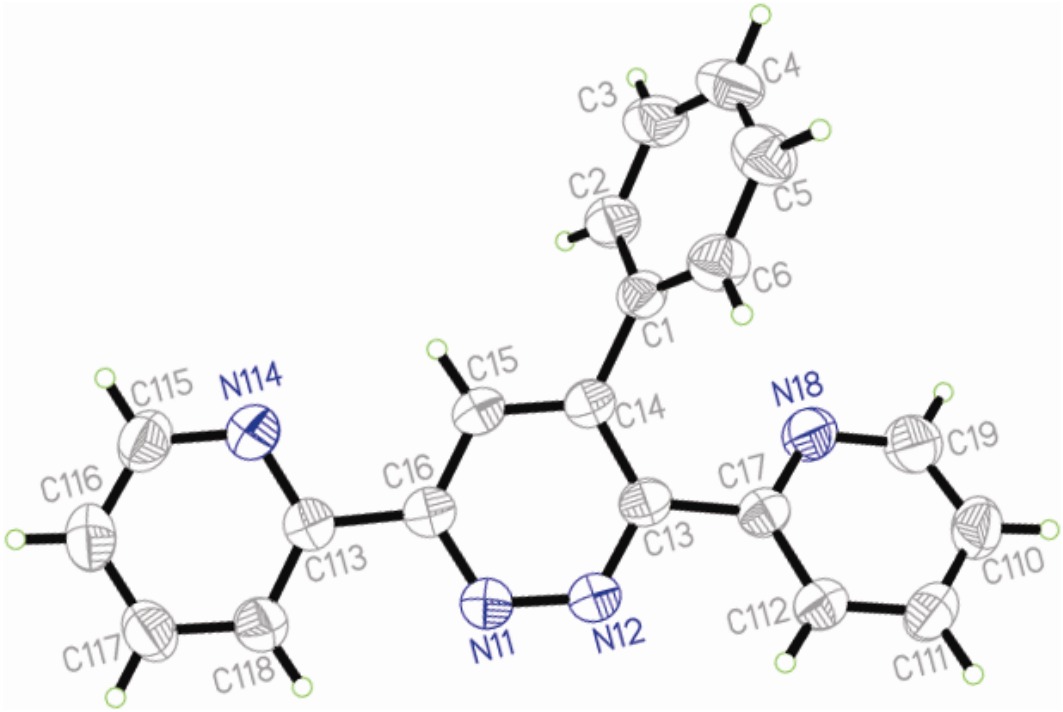
Crystallographic information for **1**



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

Identification code	1	
Empirical formula	C20 H14 N4	
Formula weight	310.35	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 6.164(6) Å	α= 90°.
	b = 14.713(1) Å	β= 95.380(1)°.
	c = 17.365(1) Å	γ = 90°.
Volume	1567.9(15) $Å^3$	
Z	4	
Density (calculated)	1.315 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	648	
Crystal size	0.22 x 0.16 x 0.12 mm^3	
Theta range for data collection	1.82 to 24.96°.	
Index ranges	-7<=h<=7, -17<=k<=17, -20<=l<=20	
Reflections collected	16199	
Independent reflections	2735 [R(int) = 0.0365]	
Completeness to theta = 24.96°	99.6 %	
Absorption correction	Multi scan	
Max. and min. transmission	0.9904 and 0.9824	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2735 / 0 / 217	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0404, wR2 = 0.0974	
R indices (all data)	R1 = 0.0539, wR2 = 0.1043	
Largest diff. peak and hole	0.151 and -0.155 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	741(2)	8427(1)	350(1)	39(1)
C(2)	-940(3)	8387(1)	-240(1)	49(1)
C(3)	-636(3)	8703(1)	-973(1)	58(1)
C(4)	1332(3)	9077(1)	-1122(1)	59(1)
C(5)	3002(3)	9132(1)	-539(1)	58(1)
C(6)	2712(3)	8808(1)	193(1)	51(1)
C(13)	1611(2)	7457(1)	1578(1)	39(1)
C(14)	360(2)	8120(1)	1145(1)	37(1)
C(15)	-1289(2)	8512(1)	1515(1)	40(1)
C(16)	-1584(2)	8275(1)	2275(1)	39(1)
C(17)	3387(2)	6905(1)	1278(1)	40(1)
C(19)	4816(3)	6220(1)	260(1)	65(1)
C(110)	6612(3)	5914(1)	714(1)	60(1)
C(111)	6758(3)	6102(1)	1492(1)	52(1)
C(112)	5127(2)	6605(1)	1781(1)	44(1)
C(113)	-3367(2)	8676(1)	2695(1)	40(1)
C(115)	-6316(3)	9624(1)	2646(1)	58(1)
C(116)	-6703(3)	9429(1)	3397(1)	58(1)
C(117)	-5349(3)	8821(1)	3804(1)	60(1)
C(118)	-3656(3)	8438(1)	3449(1)	50(1)
N(11)	-290(2)	7671(1)	2671(1)	47(1)
N(12)	1283(2)	7258(1)	2315(1)	46(1)
N(18)	3198(2)	6706(1)	521(1)	54(1)
N(114)	-4685(2)	9265(1)	2287(1)	52(1)

Table 3. Bond lengths [Å] and angles [°] for 1.

C(1)-C(6)	1.388(2)
C(1)-C(2)	1.389(2)
C(1)-C(14)	1.492(2)
C(2)-C(3)	1.384(2)
C(3)-C(4)	1.378(3)
C(4)-C(5)	1.377(3)
C(5)-C(6)	1.384(2)
C(13)-N(12)	1.3461(18)
C(13)-C(14)	1.415(2)
C(13)-C(17)	1.497(2)
C(14)-C(15)	1.380(2)
C(15)-C(16)	1.392(2)
C(16)-N(11)	1.3410(19)
C(16)-C(113)	1.496(2)
C(17)-N(18)	1.3412(19)
C(17)-C(112)	1.389(2)
C(19)-N(18)	1.340(2)
C(19)-C(110)	1.373(3)
C(110)-C(111)	1.374(3)
C(111)-C(112)	1.380(2)
C(113)-N(114)	1.343(2)
C(113)-C(118)	1.383(2)
C(115)-N(114)	1.340(2)
C(115)-C(116)	1.378(2)
C(116)-C(117)	1.373(3)
C(117)-C(118)	1.381(2)
N(11)-N(12)	1.3433(19)
C(6)-C(1)-C(2)	118.57(15)
C(6)-C(1)-C(14)	121.43(13)
C(2)-C(1)-C(14)	119.89(14)
C(3)-C(2)-C(1)	120.54(16)
C(4)-C(3)-C(2)	120.23(17)
C(5)-C(4)-C(3)	119.79(16)

C(4)-C(5)-C(6)	120.14(17)
C(5)-C(6)-C(1)	120.71(16)
N(12)-C(13)-C(14)	122.24(14)
N(12)-C(13)-C(17)	113.11(13)
C(14)-C(13)-C(17)	124.65(13)
C(15)-C(14)-C(13)	115.38(13)
C(15)-C(14)-C(1)	119.40(13)
C(13)-C(14)-C(1)	125.20(13)
C(14)-C(15)-C(16)	120.28(14)
N(11)-C(16)-C(15)	121.87(14)
N(11)-C(16)-C(113)	116.08(13)
C(15)-C(16)-C(113)	122.05(14)
N(18)-C(17)-C(112)	122.53(14)
N(18)-C(17)-C(13)	117.44(13)
C(112)-C(17)-C(13)	120.03(14)
N(18)-C(19)-C(110)	124.49(17)
C(19)-C(110)-C(111)	118.24(17)
C(110)-C(111)-C(112)	118.87(16)
C(111)-C(112)-C(17)	119.17(16)
N(114)-C(113)-C(118)	122.48(15)
N(114)-C(113)-C(16)	115.65(13)
C(118)-C(113)-C(16)	121.85(14)
N(114)-C(115)-C(116)	124.16(17)
C(117)-C(116)-C(115)	118.17(16)
C(116)-C(117)-C(118)	119.01(17)
C(117)-C(118)-C(113)	119.26(16)
C(16)-N(11)-N(12)	118.96(13)
N(11)-N(12)-C(13)	121.17(13)
C(19)-N(18)-C(17)	116.67(15)
C(115)-N(114)-C(113)	116.91(15)

Symmetry transformations used to generate equivalent atoms:

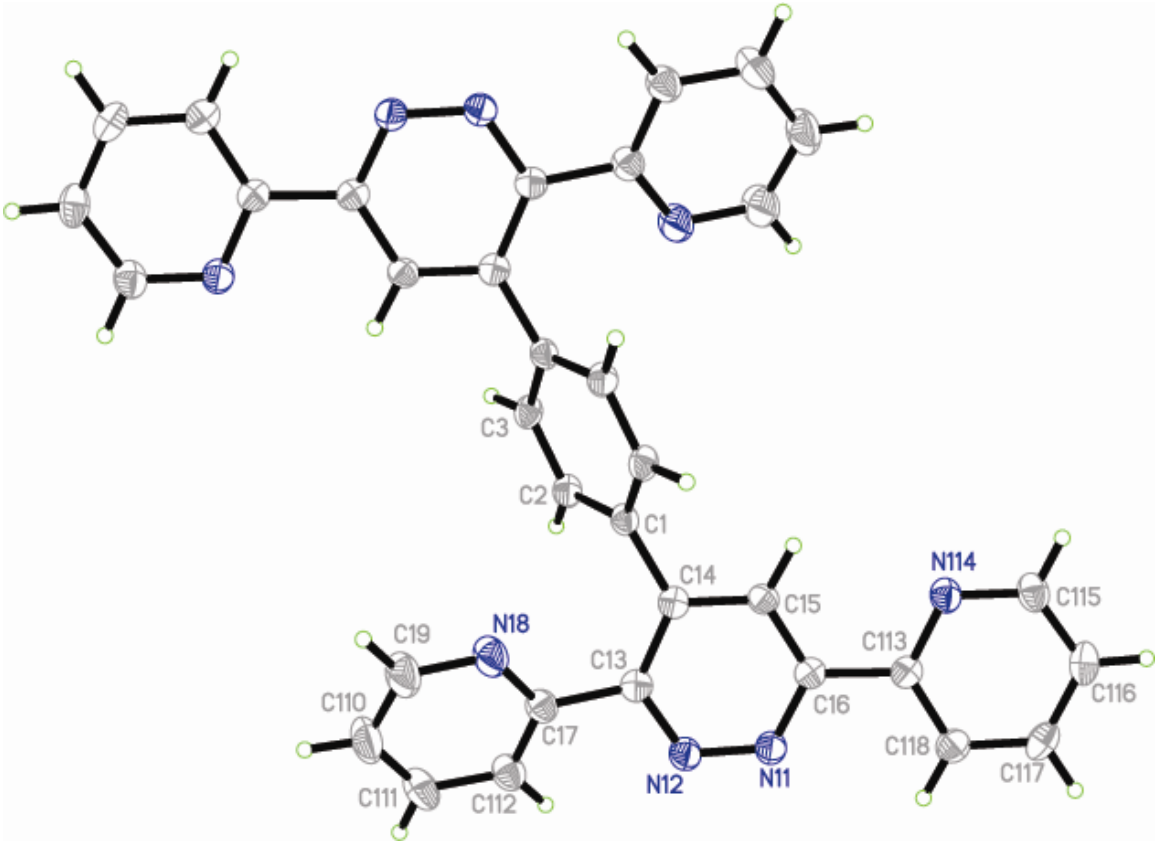
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	43(1)	36(1)	39(1)	0(1)	2(1)	5(1)
C(2)	48(1)	55(1)	44(1)	1(1)	-1(1)	1(1)
C(3)	71(1)	64(1)	39(1)	2(1)	-6(1)	2(1)
C(4)	89(2)	49(1)	40(1)	4(1)	12(1)	-2(1)
C(5)	64(1)	55(1)	58(1)	5(1)	16(1)	-10(1)
C(6)	48(1)	56(1)	49(1)	4(1)	-1(1)	-5(1)
C(13)	38(1)	39(1)	40(1)	0(1)	-3(1)	-3(1)
C(14)	36(1)	37(1)	38(1)	-1(1)	-2(1)	-3(1)
C(15)	39(1)	38(1)	42(1)	3(1)	-3(1)	1(1)
C(16)	39(1)	37(1)	40(1)	-1(1)	0(1)	-4(1)
C(17)	41(1)	34(1)	44(1)	2(1)	2(1)	-2(1)
C(19)	83(1)	65(1)	49(1)	-6(1)	11(1)	22(1)
C(110)	58(1)	54(1)	72(1)	4(1)	20(1)	15(1)
C(111)	41(1)	47(1)	68(1)	9(1)	2(1)	5(1)
C(112)	42(1)	43(1)	47(1)	3(1)	0(1)	-1(1)
C(113)	40(1)	38(1)	42(1)	-4(1)	2(1)	-5(1)
C(115)	47(1)	58(1)	69(1)	4(1)	8(1)	11(1)
C(116)	54(1)	54(1)	69(1)	-7(1)	20(1)	4(1)
C(117)	72(1)	58(1)	52(1)	-1(1)	21(1)	3(1)
C(118)	57(1)	48(1)	47(1)	0(1)	7(1)	4(1)
N(11)	46(1)	53(1)	42(1)	2(1)	4(1)	6(1)
N(12)	45(1)	51(1)	41(1)	4(1)	2(1)	6(1)
N(18)	63(1)	54(1)	44(1)	-5(1)	1(1)	14(1)
N(114)	47(1)	56(1)	52(1)	4(1)	5(1)	8(1)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(2)	-2281	8146	-142	59
H(3)	-1763	8662	-1367	70
H(4)	1530	9291	-1614	71
H(5)	4329	9387	-637	70
H(6)	3849	8846	583	62
H(15)	-2207	8937	1257	48
H(19)	4716	6081	-265	78
H(110)	7701	5588	500	72
H(111)	7935	5894	1818	63
H(112)	5191	6741	2305	53
H(115)	-7247	10031	2371	69
H(116)	-7849	9701	3623	70
H(117)	-5568	8670	4311	72
H(118)	-2720	8024	3714	60

Crystallographic information for **2**



Crystal data and structure refinement for **2**.

Identification code	**2**	
Empirical formula	C34 H22 N8	
Formula weight	542.60	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Trigonal	
Space group	R -3	
Unit cell dimensions	a = 36.000(1) Å	α= 90°.
	b = 36.000(1) Å	β= 90°.
	c = 6.213(5) Å	γ = 120°.
Volume	6973(6) $Å^3$	
Z	9	
Density (calculated)	1.163 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	2538	
Crystal size	0.22 x 0.16 x 0.12 mm^3	
Theta range for data collection	1.96 to 25.00°.	
Index ranges	-42<=h<=42, -42<=k<=42, -7<=l<=7	
Reflections collected	23138	
Independent reflections	2723 [R(int) = 0.0436]	
Completeness to theta = 25.00°	99.2 %	
Absorption correction	Multi scan	
Max. and min. transmission	0.9914 and 0.9842	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2723 / 0 / 194	
Goodness-of-fit on F^2	1.038	
Final R indices [I>2sigma(I)]	R1 = 0.0408, wR2 = 0.1077	
R indices (all data)	R1 = 0.0498, wR2 = 0.1125	
Largest diff. peak and hole	0.240 and -0.160 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	3681(1)	1616(1)	6086(2)	22(1)
C(2)	3491(1)	1485(1)	8101(2)	25(1)
C(3)	3149(1)	1538(1)	8676(2)	24(1)
C(13)	4417(1)	1656(1)	6442(2)	23(1)
C(14)	4022(1)	1525(1)	5374(2)	22(1)
C(15)	3949(1)	1275(1)	3576(2)	22(1)
C(16)	4243(1)	1151(1)	2969(2)	22(1)
C(17)	4575(1)	1950(1)	8327(2)	26(1)
C(19)	4573(1)	2492(1)	10235(3)	46(1)
C(110)	4852(1)	2492(1)	11754(3)	44(1)
C(111)	5002(1)	2211(1)	11507(3)	39(1)
C(112)	4863(1)	1935(1)	9762(2)	31(1)
C(113)	4175(1)	882(1)	1030(2)	23(1)
C(115)	3749(1)	540(1)	-1869(2)	30(1)
C(116)	4031(1)	417(1)	-2644(2)	31(1)
C(117)	4400(1)	532(1)	-1482(2)	30(1)
C(118)	4475(1)	768(1)	384(2)	28(1)
N(11)	4600(1)	1267(1)	4099(2)	27(1)
N(12)	4686(1)	1524(1)	5799(2)	27(1)
N(18)	4432(1)	2228(1)	8535(2)	37(1)
N(114)	3813(1)	767(1)	-69(2)	26(1)

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

C(1)-C(2)	1.392(2)
C(1)-C(3)#1	1.3930(19)
C(1)-C(14)	1.4869(18)
C(2)-C(3)	1.3803(19)
C(3)-C(1)#1	1.3930(19)
C(13)-N(12)	1.3361(18)
C(13)-C(14)	1.4168(19)
C(13)-C(17)	1.489(2)
C(14)-C(15)	1.374(2)
C(15)-C(16)	1.3911(19)
C(16)-N(11)	1.3343(18)
C(16)-C(113)	1.489(2)
C(17)-N(18)	1.3413(18)
C(17)-C(112)	1.389(2)
C(19)-N(18)	1.339(2)
C(19)-C(110)	1.377(2)
C(110)-C(111)	1.372(2)
C(111)-C(112)	1.383(2)
C(113)-N(114)	1.3413(18)
C(113)-C(118)	1.3915(19)
C(115)-N(114)	1.335(2)
C(115)-C(116)	1.379(2)
C(116)-C(117)	1.382(2)
C(117)-C(118)	1.382(2)
N(11)-N(12)	1.3338(17)
C(2)-C(1)-C(3)#1	118.54(13)
C(2)-C(1)-C(14)	121.02(11)
C(3)#1-C(1)-C(14)	120.13(12)
C(3)-C(2)-C(1)	120.62(12)
C(2)-C(3)-C(1)#1	120.84(13)
N(12)-C(13)-C(14)	121.73(12)
N(12)-C(13)-C(17)	113.53(11)
C(14)-C(13)-C(17)	124.73(12)
C(15)-C(14)-C(13)	115.62(12)

C(15)-C(14)-C(1)	118.37(12)
C(13)-C(14)-C(1)	125.94(12)
C(14)-C(15)-C(16)	120.05(12)
N(11)-C(16)-C(15)	121.69(12)
N(11)-C(16)-C(113)	116.58(12)
C(15)-C(16)-C(113)	121.73(12)
N(18)-C(17)-C(112)	122.68(13)
N(18)-C(17)-C(13)	116.90(12)
C(112)-C(17)-C(13)	120.41(12)
N(18)-C(19)-C(110)	124.05(15)
C(111)-C(110)-C(19)	118.49(15)
C(110)-C(111)-C(112)	118.94(15)
C(111)-C(112)-C(17)	118.88(14)
N(114)-C(113)-C(118)	122.74(13)
N(114)-C(113)-C(16)	115.43(12)
C(118)-C(113)-C(16)	121.81(12)
N(114)-C(115)-C(116)	123.94(13)
C(115)-C(116)-C(117)	118.22(14)
C(118)-C(117)-C(116)	119.12(13)
C(117)-C(118)-C(113)	118.66(13)
N(12)-N(11)-C(16)	119.20(11)
N(11)-N(12)-C(13)	121.57(11)
C(19)-N(18)-C(17)	116.94(13)
C(115)-N(114)-C(113)	117.32(12)

Symmetry transformations used to generate equivalent atoms:

#1 -x+2/3,-y+1/3,-z+4/3

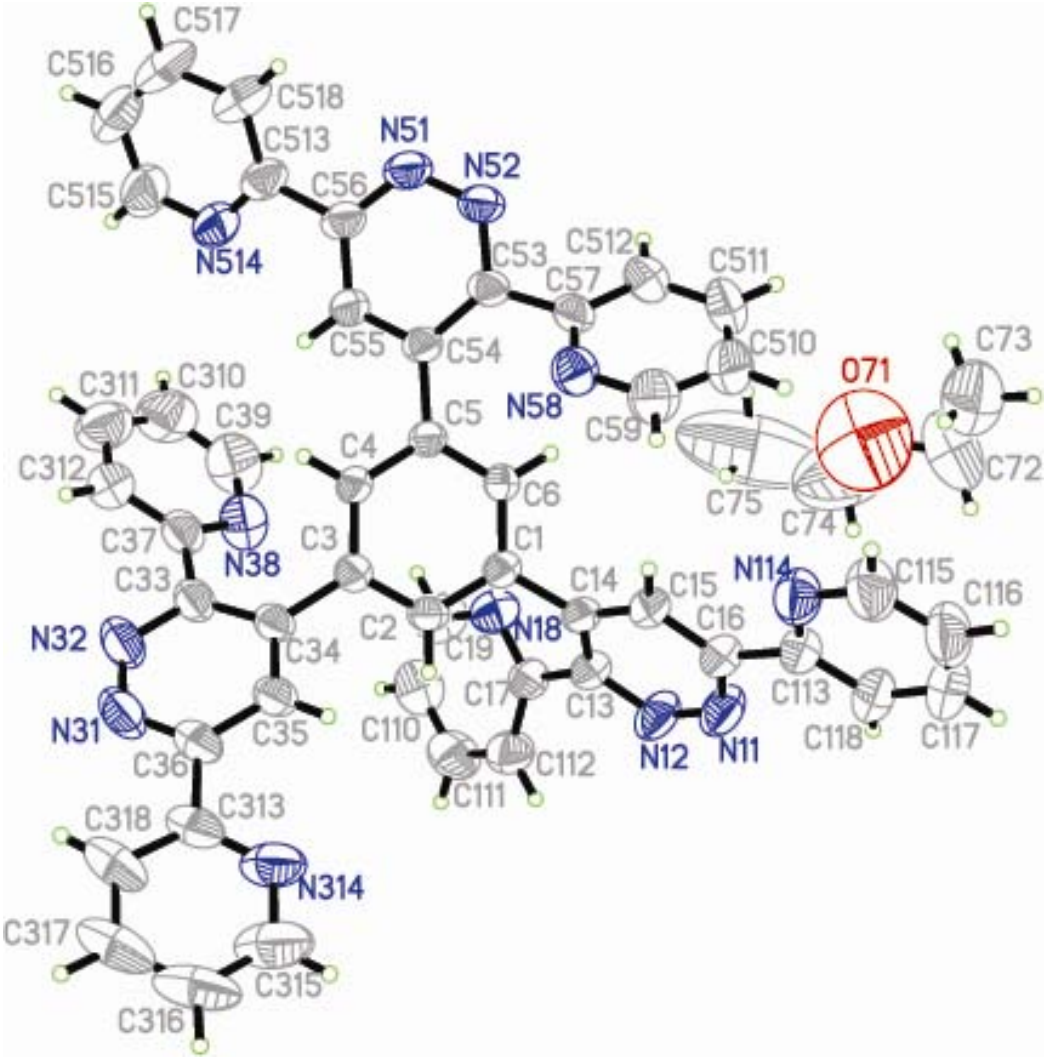
Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 2. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	25(1)	20(1)	22(1)	-3(1)	-4(1)	13(1)
C(2)	33(1)	27(1)	21(1)	-2(1)	-5(1)	21(1)
C(3)	31(1)	27(1)	18(1)	0(1)	0(1)	17(1)
C(13)	27(1)	21(1)	23(1)	3(1)	-1(1)	14(1)
C(14)	27(1)	21(1)	21(1)	3(1)	0(1)	13(1)
C(15)	24(1)	25(1)	20(1)	2(1)	-2(1)	14(1)
C(16)	25(1)	23(1)	21(1)	4(1)	1(1)	13(1)
C(17)	27(1)	22(1)	27(1)	-1(1)	-2(1)	11(1)
C(19)	52(1)	35(1)	58(1)	-21(1)	-18(1)	27(1)
C(110)	51(1)	35(1)	44(1)	-18(1)	-14(1)	19(1)
C(111)	43(1)	36(1)	34(1)	-6(1)	-15(1)	17(1)
C(112)	34(1)	28(1)	31(1)	-2(1)	-6(1)	17(1)
C(113)	27(1)	23(1)	22(1)	4(1)	2(1)	14(1)
C(115)	40(1)	29(1)	24(1)	-1(1)	-6(1)	20(1)
C(116)	47(1)	26(1)	21(1)	0(1)	2(1)	19(1)
C(117)	38(1)	28(1)	31(1)	2(1)	9(1)	21(1)
C(118)	29(1)	29(1)	30(1)	0(1)	1(1)	17(1)
N(11)	30(1)	33(1)	24(1)	-3(1)	-4(1)	20(1)
N(12)	30(1)	31(1)	26(1)	-2(1)	-4(1)	18(1)
N(18)	42(1)	29(1)	46(1)	-12(1)	-13(1)	22(1)
N(114)	33(1)	28(1)	23(1)	-1(1)	-4(1)	19(1)

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

	x	y	z	U(eq)
H(2A)	3596	1359	9090	30
H(3A)	3025	1450	10064	29
H(15A)	3696	1187	2746	27
H(19A)	4475	2691	10403	55
H(11B)	4938	2682	12947	53
H(11C)	4964	1739	9549	37
H(11D)	3494	458	-2663	36
H(11E)	3972	258	-3942	37
H(11F)	4599	451	-1961	37
H(11G)	4727	851	1211	34
H(111)	5196(6)	2201(5)	12520(30)	45(5)

Crystallographic information for **3**.



Crystal data and structure refinement for **3**.

Identification code	3	
Empirical formula	C52 H40 N12 O	
Formula weight	848.96	
Temperature	123(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P -1	
Unit cell dimensions	a = 12.676(1) Å	α= 73.300(2)°.
	b = 13.597(1) Å	β= 76.270(2)°.
	c = 13.826(1) Å	γ = 78.950(2)°.
Volume	2197.7(3) $Å^3$	
Z	2	
Density (calculated)	1.283 Mg/m^3	
Absorption coefficient	0.081 mm^{-1}	
F(000)	888	
Crystal size	0.20 x 0.16 x 0.10 mm^3	
Theta range for data collection	1.57 to 25.15°.	
Index ranges	-15<=h<=15, -16<=k<=16, -16<=l<=16	
Reflections collected	23851	
Independent reflections	7857 [R(int) = 0.0273]	
Completeness to theta = 25.15°	99.6 %	
Absorption correction	Multi scan	
Max. and min. transmission	0.9919 and 0.9840	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	7857 / 0 / 586	
Goodness-of-fit on F^2	1.025	
Final R indices [I>2sigma(I)]	R1 = 0.0640, wR2 = 0.1902	
R indices (all data)	R1 = 0.0782, wR2 = 0.2066	
Largest diff. peak and hole	0.712 and -0.286 $e.Å^{-3}$	

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

	x	y	z	U(eq)
C(1)	8349(2)	5104(2)	3085(2)	39(1)
C(2)	8064(2)	6171(2)	2805(2)	42(1)
C(3)	7206(2)	6655(2)	3400(2)	39(1)
C(4)	6621(2)	6053(2)	4282(2)	38(1)
C(5)	6897(2)	4988(2)	4587(1)	37(1)
C(6)	7773(2)	4518(2)	3975(1)	38(1)
C(13)	10310(2)	4838(2)	2084(2)	49(1)
C(14)	9228(2)	4594(2)	2393(2)	43(1)
C(15)	8995(2)	3885(2)	1969(2)	49(1)
C(16)	9809(2)	3476(2)	1261(2)	53(1)
C(17)	10718(2)	5529(2)	2530(2)	49(1)
C(19)	10733(2)	6017(2)	3971(2)	71(1)
C(33)	6598(2)	8460(2)	3734(2)	50(1)
C(34)	6887(2)	7793(2)	3067(2)	44(1)
C(35)	6826(2)	8255(2)	2055(2)	49(1)
C(36)	6470(2)	9310(2)	1757(2)	54(1)
C(37)	6722(2)	8141(2)	4828(2)	54(1)
C(39)	7696(3)	7142(3)	6032(3)	88(1)
C(53)	6083(2)	3365(2)	5807(2)	42(1)
C(54)	6278(2)	4406(2)	5579(2)	39(1)
C(55)	5883(2)	4883(2)	6370(2)	45(1)
C(56)	5305(2)	4351(2)	7302(2)	48(1)
C(57)	6381(2)	2714(2)	5058(2)	46(1)
C(59)	6420(2)	2583(2)	3444(2)	68(1)
C(72)	10374(13)	-395(5)	2837(8)	320(9)
C(73)	9334(5)	-787(5)	2933(5)	140(2)
C(74)	10734(10)	740(10)	3399(6)	228(5)
C(75)	10136(9)	1548(11)	4008(9)	323(9)
C(110)	11389(2)	6761(2)	3425(3)	74(1)
C(111)	11734(2)	6872(2)	2394(3)	77(1)
C(112)	11395(2)	6248(2)	1930(2)	67(1)

C(113)	9604(2)	2699(2)	787(2)	56(1)
C(115)	8373(3)	1758(2)	639(3)	83(1)
C(116)	9134(3)	1289(2)	-34(3)	88(1)
C(117)	10178(3)	1534(3)	-282(3)	90(1)
C(118)	10425(3)	2246(2)	127(2)	74(1)
C(310)	6999(4)	7528(3)	6806(3)	93(1)
C(311)	6144(3)	8246(3)	6563(2)	89(1)
C(312)	5990(3)	8564(2)	5562(2)	70(1)
C(313)	6421(2)	9848(2)	667(2)	61(1)
C(315)	6937(3)	9798(3)	-1008(3)	106(1)
C(316)	6364(3)	10758(4)	-1335(3)	106(1)
C(317)	5809(3)	11270(3)	-624(3)	96(1)
C(318)	5833(3)	10822(2)	388(3)	78(1)
C(510)	6926(3)	1598(2)	3634(3)	77(1)
C(511)	7147(3)	1139(2)	4592(3)	83(1)
C(512)	6876(2)	1706(2)	5332(2)	68(1)
C(513)	4788(2)	4871(2)	8139(2)	55(1)
C(515)	4787(3)	6168(3)	8885(2)	81(1)
C(516)	3875(3)	5923(3)	9596(2)	85(1)
C(517)	3393(3)	5124(3)	9568(2)	90(1)
C(518)	3858(2)	4569(3)	8830(2)	76(1)
N(11)	10799(2)	3777(2)	954(2)	70(1)
N(12)	11049(2)	4452(2)	1380(2)	68(1)
N(18)	10397(2)	5398(2)	3543(2)	60(1)
N(31)	6142(2)	9888(2)	2433(2)	70(1)
N(32)	6220(2)	9461(2)	3415(2)	68(1)
N(38)	7584(2)	7451(2)	5048(2)	71(1)
N(51)	5188(2)	3361(2)	7487(1)	56(1)
N(52)	5591(2)	2866(1)	6740(1)	52(1)
N(58)	6136(2)	3154(2)	4127(2)	55(1)
N(114)	8584(2)	2454(2)	1052(2)	71(1)
N(314)	6967(2)	9332(2)	-17(2)	82(1)
N(514)	5256(2)	5663(2)	8153(2)	68(1)
O(71)	9862(4)	445(6)	3285(5)	228(3)

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

C(1)-C(6)	1.385(3)
C(1)-C(2)	1.389(3)
C(1)-C(14)	1.488(3)
C(2)-C(3)	1.381(3)
C(3)-C(4)	1.391(3)
C(3)-C(34)	1.486(3)
C(4)-C(5)	1.386(3)
C(5)-C(6)	1.396(3)
C(5)-C(54)	1.491(3)
C(13)-N(12)	1.332(3)
C(13)-C(14)	1.410(3)
C(13)-C(17)	1.484(3)
C(14)-C(15)	1.370(3)
C(15)-C(16)	1.395(3)
C(16)-N(11)	1.329(3)
C(16)-C(113)	1.482(3)
C(17)-N(18)	1.331(3)
C(17)-C(112)	1.378(3)
C(19)-N(18)	1.336(3)
C(19)-C(110)	1.368(4)
C(33)-N(32)	1.334(3)
C(33)-C(34)	1.415(3)
C(33)-C(37)	1.487(3)
C(34)-C(35)	1.373(3)
C(35)-C(36)	1.391(3)
C(36)-N(31)	1.331(3)
C(36)-C(313)	1.484(3)
C(37)-N(38)	1.330(3)
C(37)-C(312)	1.380(4)
C(39)-N(38)	1.338(4)
C(39)-C(310)	1.377(5)
C(53)-N(52)	1.338(3)
C(53)-C(54)	1.415(3)
C(53)-C(57)	1.488(3)

C(54)-C(55)	1.376(3)
C(55)-C(56)	1.392(3)
C(56)-N(51)	1.327(3)
C(56)-C(513)	1.484(3)
C(57)-N(58)	1.337(3)
C(57)-C(512)	1.378(3)
C(59)-N(58)	1.334(3)
C(59)-C(510)	1.350(4)
C(72)-O(71)	1.428(9)
C(72)-C(73)	1.478(14)
C(74)-O(71)	1.303(10)
C(74)-C(75)	1.549(17)
C(110)-C(111)	1.361(4)
C(111)-C(112)	1.378(4)
C(113)-N(114)	1.338(4)
C(113)-C(118)	1.386(4)
C(115)-N(114)	1.331(4)
C(115)-C(116)	1.373(5)
C(116)-C(117)	1.367(5)
C(117)-C(118)	1.368(4)
C(310)-C(311)	1.348(5)
C(311)-C(312)	1.376(4)
C(313)-N(314)	1.323(4)
C(313)-C(318)	1.386(4)
C(315)-N(314)	1.340(4)
C(315)-C(316)	1.375(6)
C(316)-C(317)	1.350(6)
C(317)-C(318)	1.362(5)
C(510)-C(511)	1.362(5)
C(511)-C(512)	1.394(4)
C(513)-N(514)	1.332(4)
C(513)-C(518)	1.377(4)
C(515)-N(514)	1.344(3)
C(515)-C(516)	1.354(5)
C(516)-C(517)	1.358(5)
C(517)-C(518)	1.394(4)

N(11)-N(12)	1.340(3)
N(31)-N(32)	1.334(3)
N(51)-N(52)	1.340(3)
C(6)-C(1)-C(2)	119.67(18)
C(6)-C(1)-C(14)	120.57(18)
C(2)-C(1)-C(14)	119.66(17)
C(3)-C(2)-C(1)	120.77(18)
C(2)-C(3)-C(4)	118.81(18)
C(2)-C(3)-C(34)	119.91(18)
C(4)-C(3)-C(34)	121.21(17)
C(5)-C(4)-C(3)	121.66(17)
C(4)-C(5)-C(6)	118.39(17)
C(4)-C(5)-C(54)	118.39(17)
C(6)-C(5)-C(54)	123.15(17)
C(1)-C(6)-C(5)	120.69(18)
N(12)-C(13)-C(14)	122.5(2)
N(12)-C(13)-C(17)	114.9(2)
C(14)-C(13)-C(17)	122.62(19)
C(15)-C(14)-C(13)	115.92(19)
C(15)-C(14)-C(1)	120.28(19)
C(13)-C(14)-C(1)	123.71(19)
C(14)-C(15)-C(16)	119.3(2)
N(11)-C(16)-C(15)	122.1(2)
N(11)-C(16)-C(113)	116.3(2)
C(15)-C(16)-C(113)	121.5(2)
N(18)-C(17)-C(112)	122.7(2)
N(18)-C(17)-C(13)	115.6(2)
C(112)-C(17)-C(13)	121.7(2)
N(18)-C(19)-C(110)	123.4(3)
N(32)-C(33)-C(34)	122.1(2)
N(32)-C(33)-C(37)	113.6(2)
C(34)-C(33)-C(37)	124.26(19)
C(35)-C(34)-C(33)	115.74(19)
C(35)-C(34)-C(3)	119.79(19)
C(33)-C(34)-C(3)	124.44(19)
C(34)-C(35)-C(36)	119.6(2)

N(31)-C(36)-C(35)	122.0(2)
N(31)-C(36)-C(313)	116.6(2)
C(35)-C(36)-C(313)	121.4(2)
N(38)-C(37)-C(312)	122.5(2)
N(38)-C(37)-C(33)	116.3(2)
C(312)-C(37)-C(33)	121.2(2)
N(38)-C(39)-C(310)	123.7(3)
N(52)-C(53)-C(54)	122.4(2)
N(52)-C(53)-C(57)	112.77(18)
C(54)-C(53)-C(57)	124.83(18)
C(55)-C(54)-C(53)	115.25(18)
C(55)-C(54)-C(5)	119.14(18)
C(53)-C(54)-C(5)	125.57(18)
C(54)-C(55)-C(56)	119.9(2)
N(51)-C(56)-C(55)	122.0(2)
N(51)-C(56)-C(513)	116.78(19)
C(55)-C(56)-C(513)	121.2(2)
N(58)-C(57)-C(512)	122.7(2)
N(58)-C(57)-C(53)	116.62(18)
C(512)-C(57)-C(53)	120.6(2)
N(58)-C(59)-C(510)	124.5(3)
O(71)-C(72)-C(73)	94.3(9)
O(71)-C(74)-C(75)	97.1(9)
C(111)-C(110)-C(19)	118.7(3)
C(110)-C(111)-C(112)	119.2(3)
C(17)-C(112)-C(111)	118.6(3)
N(114)-C(113)-C(118)	122.5(2)
N(114)-C(113)-C(16)	115.6(2)
C(118)-C(113)-C(16)	121.9(2)
N(114)-C(115)-C(116)	124.0(3)
C(117)-C(116)-C(115)	118.2(3)
C(116)-C(117)-C(118)	119.5(3)
C(117)-C(118)-C(113)	118.8(3)
C(311)-C(310)-C(39)	118.3(3)
C(310)-C(311)-C(312)	119.5(3)
C(311)-C(312)-C(37)	118.9(3)

N(314)-C(313)-C(318)	122.3(3)
N(314)-C(313)-C(36)	115.6(2)
C(318)-C(313)-C(36)	122.1(3)
N(314)-C(315)-C(316)	123.6(4)
C(317)-C(316)-C(315)	118.6(3)
C(316)-C(317)-C(318)	119.2(3)
C(317)-C(318)-C(313)	119.4(4)
C(59)-C(510)-C(511)	118.5(3)
C(510)-C(511)-C(512)	119.4(3)
C(57)-C(512)-C(511)	117.9(3)
N(514)-C(513)-C(518)	122.7(2)
N(514)-C(513)-C(56)	115.9(2)
C(518)-C(513)-C(56)	121.4(3)
N(514)-C(515)-C(516)	124.0(4)
C(515)-C(516)-C(517)	118.4(3)
C(516)-C(517)-C(518)	119.5(3)
C(513)-C(518)-C(517)	118.1(3)
C(16)-N(11)-N(12)	119.2(2)
C(13)-N(12)-N(11)	120.7(2)
C(17)-N(18)-C(19)	117.4(2)
C(36)-N(31)-N(32)	119.4(2)
N(31)-N(32)-C(33)	121.0(2)
C(37)-N(38)-C(39)	117.0(3)
C(56)-N(51)-N(52)	119.32(18)
C(53)-N(52)-N(51)	120.83(19)
C(59)-N(58)-C(57)	117.0(2)
C(115)-N(114)-C(113)	117.1(3)
C(313)-N(314)-C(315)	116.9(3)
C(513)-N(514)-C(515)	117.2(3)
C(74)-O(71)-C(72)	99.0(9)

Symmetry transformations used to generate equivalent atoms:

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for 3. 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)	36(1)	42(1)	37(1)	-10(1)	-2(1)	-5(1)
C(2)	41(1)	42(1)	36(1)	-4(1)	-2(1)	-8(1)
C(3)	39(1)	37(1)	40(1)	-8(1)	-6(1)	-4(1)
C(4)	36(1)	38(1)	37(1)	-9(1)	-3(1)	0(1)
C(5)	35(1)	38(1)	34(1)	-6(1)	-5(1)	-4(1)
C(6)	37(1)	35(1)	39(1)	-9(1)	-4(1)	-2(1)
C(13)	44(1)	52(1)	46(1)	-13(1)	3(1)	-6(1)
C(14)	41(1)	43(1)	37(1)	-7(1)	0(1)	-3(1)
C(15)	45(1)	50(1)	47(1)	-15(1)	2(1)	-7(1)
C(16)	51(1)	54(1)	49(1)	-17(1)	0(1)	-4(1)
C(17)	38(1)	52(1)	53(1)	-14(1)	-3(1)	-3(1)
C(19)	71(2)	92(2)	62(2)	-23(2)	-21(1)	-19(2)
C(33)	51(1)	38(1)	59(1)	-10(1)	-9(1)	-7(1)
C(34)	41(1)	37(1)	48(1)	-4(1)	-5(1)	-8(1)
C(35)	49(1)	41(1)	51(1)	-4(1)	-6(1)	-9(1)
C(36)	51(1)	42(1)	62(1)	3(1)	-13(1)	-11(1)
C(37)	64(2)	41(1)	59(1)	-11(1)	-12(1)	-12(1)
C(39)	106(3)	88(2)	81(2)	-21(2)	-45(2)	-3(2)
C(53)	35(1)	40(1)	43(1)	-1(1)	-5(1)	-2(1)
C(54)	35(1)	39(1)	37(1)	-3(1)	-5(1)	-1(1)
C(55)	46(1)	43(1)	37(1)	-6(1)	-2(1)	-1(1)
C(56)	42(1)	53(1)	37(1)	-2(1)	-4(1)	0(1)
C(57)	41(1)	38(1)	54(1)	-6(1)	-2(1)	-9(1)
C(59)	75(2)	72(2)	68(2)	-26(1)	-17(1)	-16(1)
C(72)	530(20)	96(5)	271(11)	-74(6)	117(13)	-89(8)
C(73)	141(4)	122(4)	156(5)	-57(4)	-6(4)	-5(3)
C(74)	237(11)	346(15)	131(6)	-70(7)	-14(6)	-123(10)
C(75)	270(12)	408(18)	287(13)	132(12)	-157(11)	-244(14)
C(110)	71(2)	75(2)	89(2)	-26(2)	-34(2)	-12(2)
C(111)	71(2)	69(2)	92(2)	-14(2)	-14(2)	-28(2)
C(112)	62(2)	70(2)	65(2)	-16(1)	3(1)	-21(1)

C(113)	62(2)	52(1)	52(1)	-18(1)	-5(1)	-2(1)
C(115)	88(2)	73(2)	98(2)	-36(2)	-18(2)	-15(2)
C(116)	120(3)	66(2)	90(2)	-39(2)	-25(2)	-8(2)
C(117)	106(3)	81(2)	89(2)	-51(2)	-3(2)	-2(2)
C(118)	80(2)	71(2)	71(2)	-36(2)	3(1)	-4(1)
C(310)	119(3)	103(3)	62(2)	-16(2)	-26(2)	-25(2)
C(311)	104(3)	100(3)	62(2)	-24(2)	1(2)	-26(2)
C(312)	74(2)	61(2)	67(2)	-16(1)	-1(1)	-9(1)
C(313)	54(1)	55(1)	64(2)	11(1)	-14(1)	-18(1)
C(315)	97(3)	130(3)	61(2)	14(2)	-5(2)	-18(2)
C(316)	99(3)	118(3)	74(2)	44(2)	-32(2)	-38(2)
C(317)	92(2)	73(2)	105(3)	37(2)	-45(2)	-29(2)
C(318)	82(2)	50(1)	93(2)	17(1)	-38(2)	-16(1)
C(510)	92(2)	65(2)	81(2)	-35(2)	-4(2)	-19(2)
C(511)	97(2)	41(1)	101(2)	-22(2)	-2(2)	-1(1)
C(512)	80(2)	43(1)	67(2)	-5(1)	-6(1)	0(1)
C(513)	54(1)	65(2)	35(1)	-5(1)	-5(1)	5(1)
C(515)	104(2)	78(2)	53(2)	-23(1)	-6(2)	5(2)
C(516)	79(2)	108(3)	55(2)	-30(2)	-4(2)	21(2)
C(517)	61(2)	137(3)	57(2)	-30(2)	14(1)	0(2)
C(518)	55(2)	109(2)	52(2)	-21(2)	8(1)	-10(2)
N(11)	58(1)	83(2)	73(1)	-42(1)	15(1)	-16(1)
N(12)	50(1)	84(2)	72(1)	-40(1)	16(1)	-16(1)
N(18)	57(1)	73(1)	52(1)	-15(1)	-9(1)	-15(1)
N(31)	90(2)	38(1)	75(2)	-3(1)	-23(1)	-3(1)
N(32)	91(2)	38(1)	72(1)	-10(1)	-19(1)	-3(1)
N(38)	81(2)	68(1)	72(2)	-24(1)	-31(1)	2(1)
N(51)	54(1)	57(1)	41(1)	0(1)	1(1)	-6(1)
N(52)	50(1)	47(1)	47(1)	1(1)	-2(1)	-7(1)
N(58)	58(1)	53(1)	57(1)	-15(1)	-15(1)	-7(1)
N(114)	71(2)	68(1)	81(2)	-34(1)	-8(1)	-11(1)
N(314)	74(2)	91(2)	55(1)	12(1)	-7(1)	-7(1)
N(514)	83(2)	68(1)	44(1)	-15(1)	2(1)	-3(1)
O(71)	139(4)	254(7)	299(8)	-75(6)	-67(4)	-8(4)

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

	x	y	z	U(eq)
H(2)	8455	6564	2209	50
H(4)	6031	6373	4677	46
H(6)	7970	3805	4168	45
H(15)	8301	3678	2152	58
H(19)	10510	5938	4677	86
H(35)	7020	7864	1572	59
H(39)	8277	6638	6204	106
H(55)	6002	5559	6284	54
H(59)	6260	2884	2792	82
H(72A)	10870	-887	3237	384
H(72B)	10743	-165	2127	384
H(73A)	8991	-981	3646	210
H(73B)	9482	-1381	2654	210
H(73C)	8855	-256	2562	210
H(74A)	11176	1053	2745	274
H(74B)	11180	180	3794	274
H(75A)	9683	2071	3600	485
H(75B)	10667	1863	4169	485
H(75C)	9688	1210	4635	485
H(110)	11595	7183	3752	89
H(111)	12193	7363	2007	92
H(112)	11619	6311	1226	80
H(115)	7667	1579	818	99
H(116)	8945	817	-314	105
H(117)	10716	1219	-726	108
H(118)	11130	2423	-35	89
H(310)	7114	7299	7479	111
H(311)	5663	8524	7069	107
H(312)	5402	9056	5383	84
H(315)	7326	9452	-1502	127

H(316)	6358	11048	-2031	127
H(317)	5414	11921	-824	116
H(318)	5460	11166	888	93
H(510)	7118	1240	3123	92
H(511)	7476	455	4750	99
H(512)	7023	1413	5990	81
H(515)	5108	6721	8904	97
H(516)	3586	6292	10092	102
H(517)	2757	4948	10037	108
H(518)	3550	4011	8805	91

Hydrogen bond table:

	1			**2**			**3**		
C-H···N	2.83	3.66	149	2.53	3.32	142	2.55	3.48	178
	3.00	3.79	143	2.57	3.28	134	2.62	3.37	139
	3.03	3.61	122	2.68	3.51	149	2.72	3.47	138
				2.90	3.78	158	2.75	3.51	140
							2.75	3.53	142
							2.76	3.31	119
							2.88	3.61	137
							2.91	3.81	162
							2.92	3.80	157
							2.93	3.75	148
							2.99	3.76	139

Torsion angles

1	
N11 – C16 – C113 – C118	0.16
C15 – C16 – C113 – N114	1.21
N2 – C13 – C17 – C112	-30.39
C14 – C13 – C17 – N18	-30.84
C13 – C14 – C1 – C6	-58.82
C15 – C14 – C1 – C12	-56.75
2	
N114 – C113 – C16 – C15	0.29
C118 – C113 – C16 – N11	2.12
C112 – C17 – C13 – N12	25. 76
N18 – C17 – C13 – C14	25.71
C15 – C14 – C1 – C3	54.67
C13 – C14- C1 – C2	57.92
3	
N38 – C37 – C33 – C34	34.92
N312 – C37 – C33 – N32	35.75
N31 – C36 – C313 – C318	-14.95
C35 – C36 – C313 – N314	-15.38
C33 – C34 – C3 – C4	44.46
C35 – C34 – C3 – C2	43.47
N514 – C513 – C56 – C55	-27.21
C518 – C513 – C56 – N51	-29.64
C512 – C57 – C53 – N52	-45.44
N58 – C57 – C53 – C54	-45.30
C6 – C5 – C54 – C53	-32.17
C4 – C5 – C54 – C55	-31.67
N18 – C17 – C13 – C14	41.11
C112 – C17 – C13 – N12	41.39
N114 – C113 – C16 – C15	2.56
C118 – C113 – C16 – N11	5.28
C2 –C1 – C14 – C13	58.39
C6 – C1 – C14 – C15	58.51

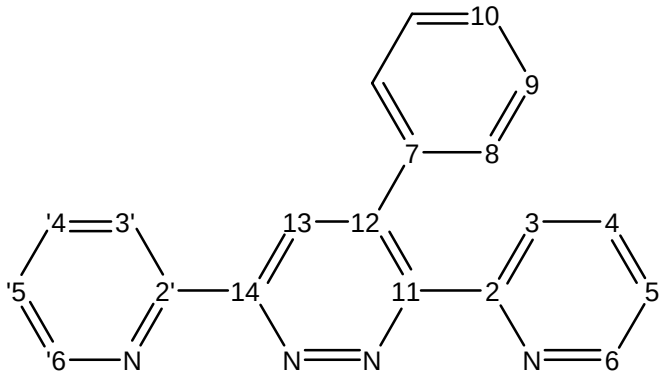
Synthesis and spectral analysis:

Phenylacetylene was purchased from Aldrich chemicals and used without further purification. The synthetic details and spectroscopic reports for di- and tri-acetylenes (by Sonogashira coupling), 3,6-di(2-pyridyl)-1,2,4,5-tetrazine and **3** are previously reported.[1-4]

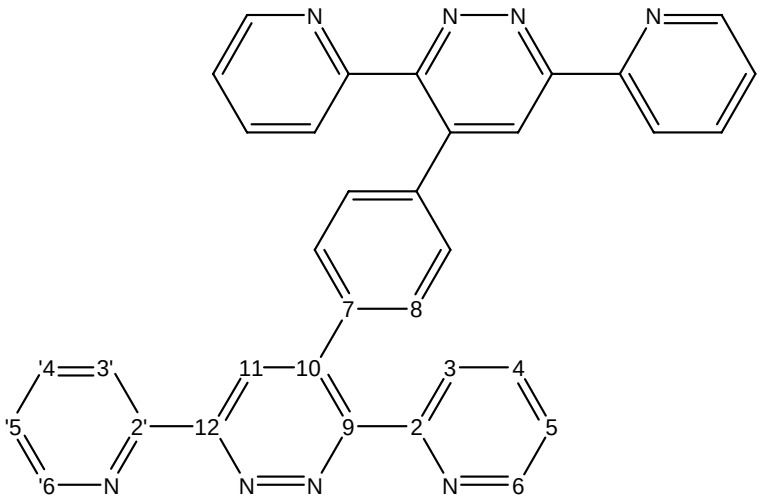
Single crystals of **1**, **2** and **3** were carefully chosen after they were viewed through a polarizing microscope. The crystals were glued to a thin glass fiber using NIH immersion oil and mounted on a diffractometer equipped with an APEX CCD area detector. The data collections were carried out at 123K and no extraordinary methods were employed, except that the crystals were smeared in the immersion oil to protect them from ambient laboratory conditions. The intensity data were processed using Bruker's suite of data processing programs (SAINT), and absorption corrections were applied using SADABS.[5] The structure solution of all the complexes was carried out by direct methods, and refinements were performed by full-matrix least-squares on F^2 using the SHELXTL-PLUS suite of programs.[6] All the non-hydrogen atoms were refined anisotropically and the hydrogen atoms obtained from Fourier maps were refined isotropically. In the case of **2**, the electron density associated with the disordered solvent water molecules were removed from the reflection file using SQUEEZE option in PLATON and refined. The resulting *****.sqf file was appended to the CIF file. Intermolecular interactions were computed using the PLATON program.[7]

Thermogravimetric analyses of **1-3** were carried out using Perkin-Elmer Pyris 1 TG analyzer under inert atmosphere with a heating rate of 5 ^{o}C/min. Absorbance spectra were obtained on a Shimidzu UV/Vis spectrometer recorded in the range 230-800 nm, using chloroform as the solvent.

4-Phenyl-3,6-di(2-pyridyl) pyridazine, **1**: Phenylacetylene (0.102g, 1 mmol) in toluene (5 mL) was added to a solution of 3,6-di(2-pyridyl)-1,2,4,5-tetrazine (Bptz) (0.236g, 1 mmol) in toluene (5 mL). The reaction mixture was stirred for 15 minutes and was heated in a pressure tube at 140 ^{o}C for 48 hours. The resultant yellow solution was brought to room temperature and the solvent was removed under vacuum. The product was purified by column chromatography (Silica 60; ethyl acetate (90%), methanol (10%). Yield: 0.27g (88%). ^{1}H-NMR ($CDCl_3$, δ/ppm, J/Hz): 8.83 (d, 1H, H^3, J = 8.03), 8.75 (d, 1H, H^6, J = 4.52), 8.69 (s, 1H, H^{13}), 8.50 (dd, 1H, $H^{6'}$, J = 4.52, J = 1.01), 8.00-7.90 (m, 2H, $H^{3',4}$), 7.82 (dt, 1H, $H^{4'}$, J = 7.53, J = 2.01), 7.44 (m, 1H, H^5), 7.34 (m, 3H, $H^{5',9}$), 7.30 (m, 3H, $H^{8,10}$). ^{13}C NMR ($CDCl_3$, δ/ppm): 158.41 (1C, C^q), 157.76 (1C, C^q), 155.85 (1C, C^{11}), 153.41 (1C, C^{14}), 149.49 (1C, C^6), 149.07 (1C, $C^{6'}$), 140.55 (1C, C^{12}), 137.24 (1C, $C^{3'}$), 136.97 (1C, C^7), 136.57 (1C, $C^{4'}$), 128.94 (2C, C^9), 128.45 (3C, $C^{8,10}$), 125.68 (1C, C^{13}), 124.92 (1C, C^4), 124.84 (1C, C^5), 123.39 (1C, $C^{5'}$) and 121.92 (1C, C^3). ESI-MS (CH_3OH); calculated for $C_{20}H_{15}N_4$: $[MH]^+$ 311.1297, found: 311.1299.



1,4-Benzene-bis(3,6-di(2-pyridyl)pyridazine), **2**: The 3,6-di(2-pyridyl)-1,2,4,5-tetrazine (Bptz) (0.472g, 2 mmol) was dissolved in toluene (5 mL) to give a deep purple solution to which 1,4-benzene-diacetylene (0.126g, 1 mmol) in toluene (5 mL) was added. The resultant solution was stirred for 15 minutes and transferred to a pressure tube (25 mL) and the reaction mixture was heated at 160 ^{o}C for 48 hours, during which time, the reaction mixture turned yellow. After cooling to room temperature, the solvent was removed under vacuum and the product was purified by column chromatography (silica gel 60; CH_2Cl_2 (70%), acetone (30%)). Yield: 0.41g (76%). ^{1}H-NMR ($CDCl_3$, δ/ppm, J/Hz): 8.84 (d, 2H, H^3 J = 8.03), 8.79 (d, 2H, H^6 J = 4.52), 8.72 (s, 2H, H^{11}), 8.53 (d, 2H, $H^{6'}$ J = 4.52), 8.00-7.96 (m, 4H, H^4, $H^{3'}$), 7.89 (dt, 2H, $H^{4'}$ J = 7.53, J = 1.50), 7.48 (m, 2H, H^5), 7.35 (m, 2H, $H^{5'}$), 7.27 (s, 4H, H^8). ^{13}C NMR ($CDCl_3$, δ/ppm): 157.58 (2C C^q), 157.15 (2C C^q), 154.90 (2C C^q), 152.67 (2C C^q), 148.86 (2C C^6), 148.42 (2C $C^{6'}$), 139.42 (2C C^{10}), 137.11 (2C C^4), 136.67 (2C $C^{4'}$), 136.58 (2C C^7), 128.66 (2C C^8), 125.19 (2C C^{11}), 124.58 (2C C^5), 124.52 (2C $C^{3'}$), 123.20 (2C $C^{5'}$), 121.68 (2C C^3). ESI-MS (CH_3OH); calculated for $C_{34}H_{22}N_8$: $[MH]^+$ 543.2046, found: 543. 2067



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(1) M. J. Plater, J. P. Sinclair, S. Aiken, T. Gelbrich, M. B. Hursthouse, *Tetrahedron* 2004, **60**, 6385.

(2) E. Weber, M. Hecker, E. Koepp, W. Orlia, M. Czugler, I. Csöregh, *J. Chem. Soc., Perkin Trans.II* 1988, 1251.

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(7) A. L. Speck, PLATON. *Acta Crystallogr., Sect. A*, 1990, **A46**, C34.

Additional figures for **1**

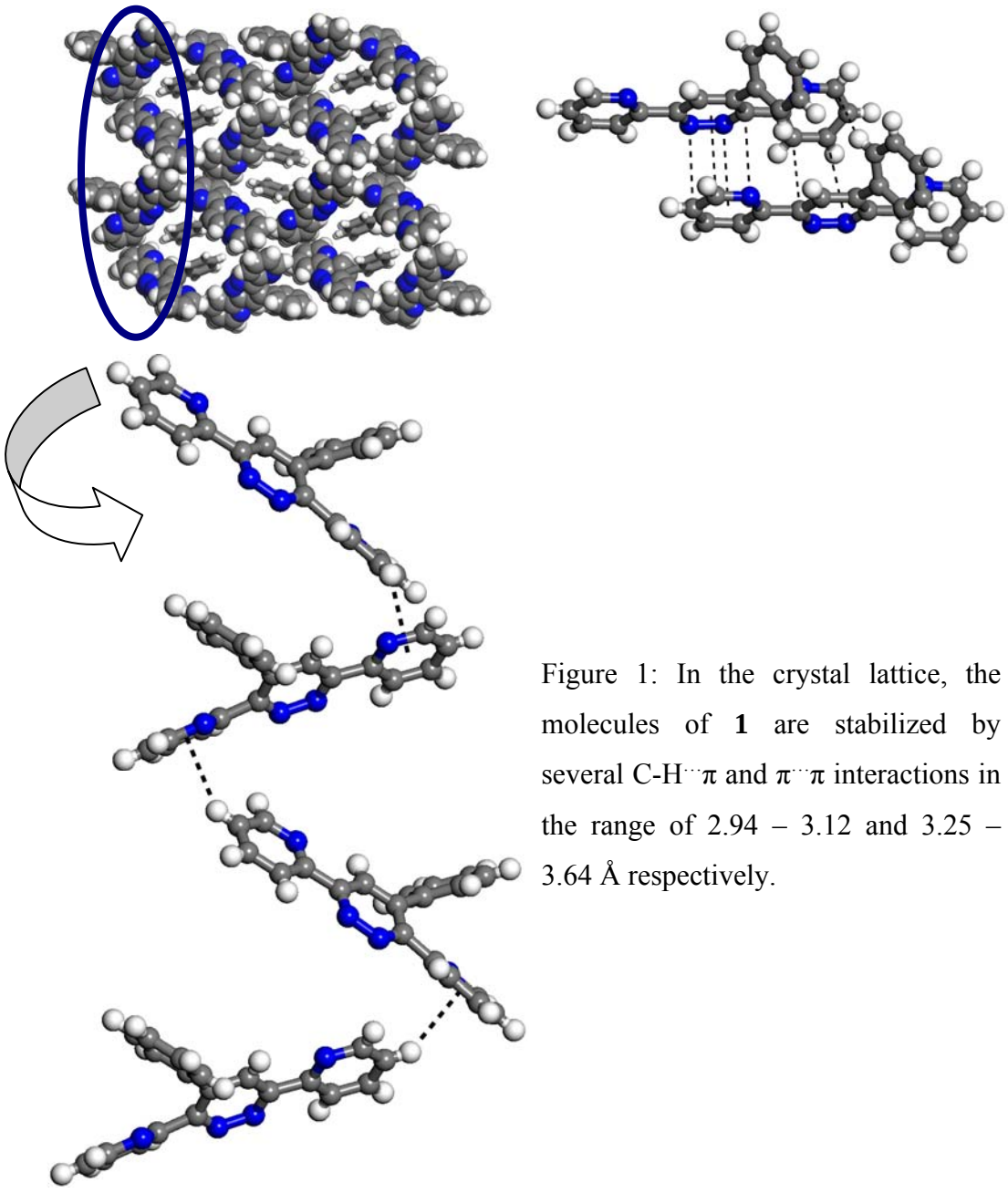


Figure 1: In the crystal lattice, the molecules of **1** are stabilized by several C-H···π and π···π interactions in the range of 2.94 – 3.12 and 3.25 – 3.64 Å respectively.

Additional figures for **2**

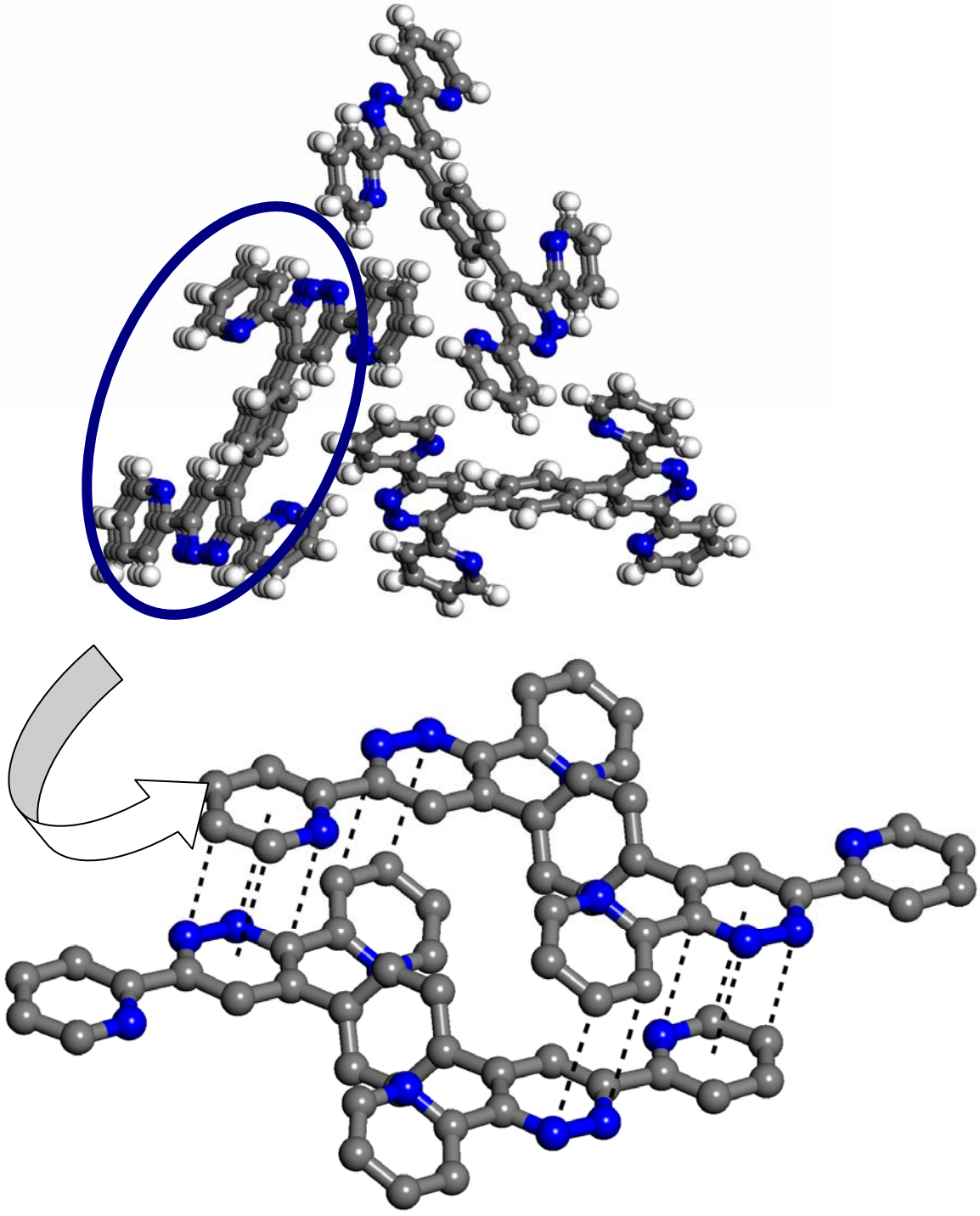


Figure 2: Each side of the triangular units are made of ligand **2**, stabilized by several π···π interactions in the range of 3.37 – 3.56 Å

Additional figures for **3**

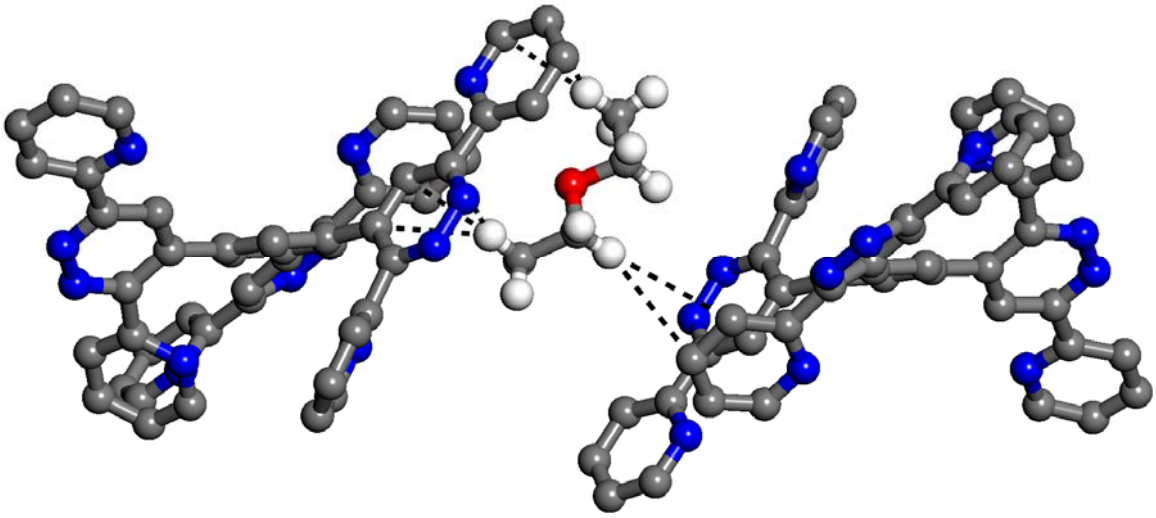


Figure 3: In the crystal structure of **3**, the solvent (ether) plays a major role in the stabilization of the framework, through the formation of several C-H···π interactions (2.97 – 3.43 Å)

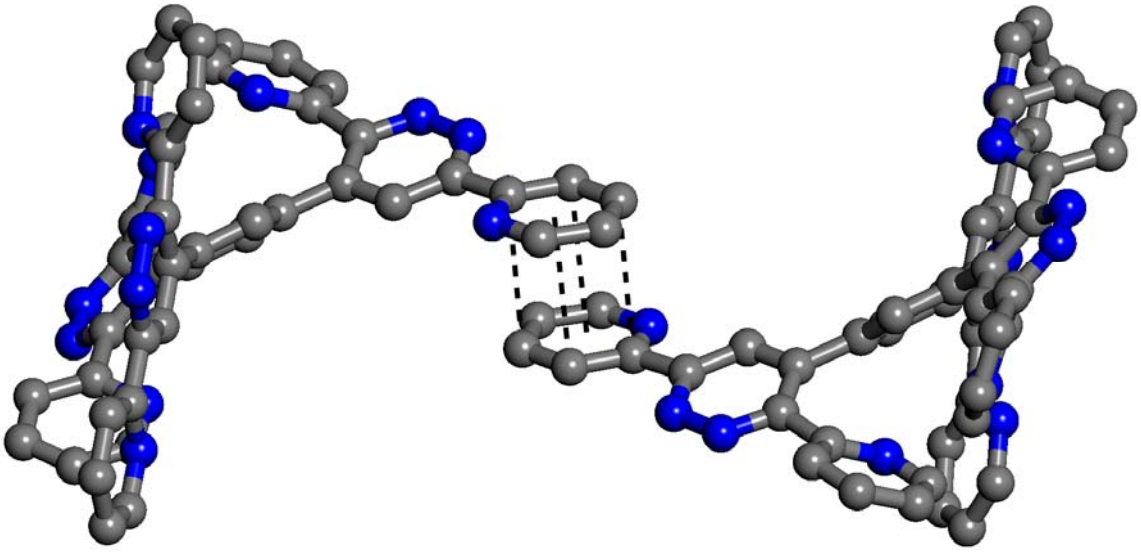
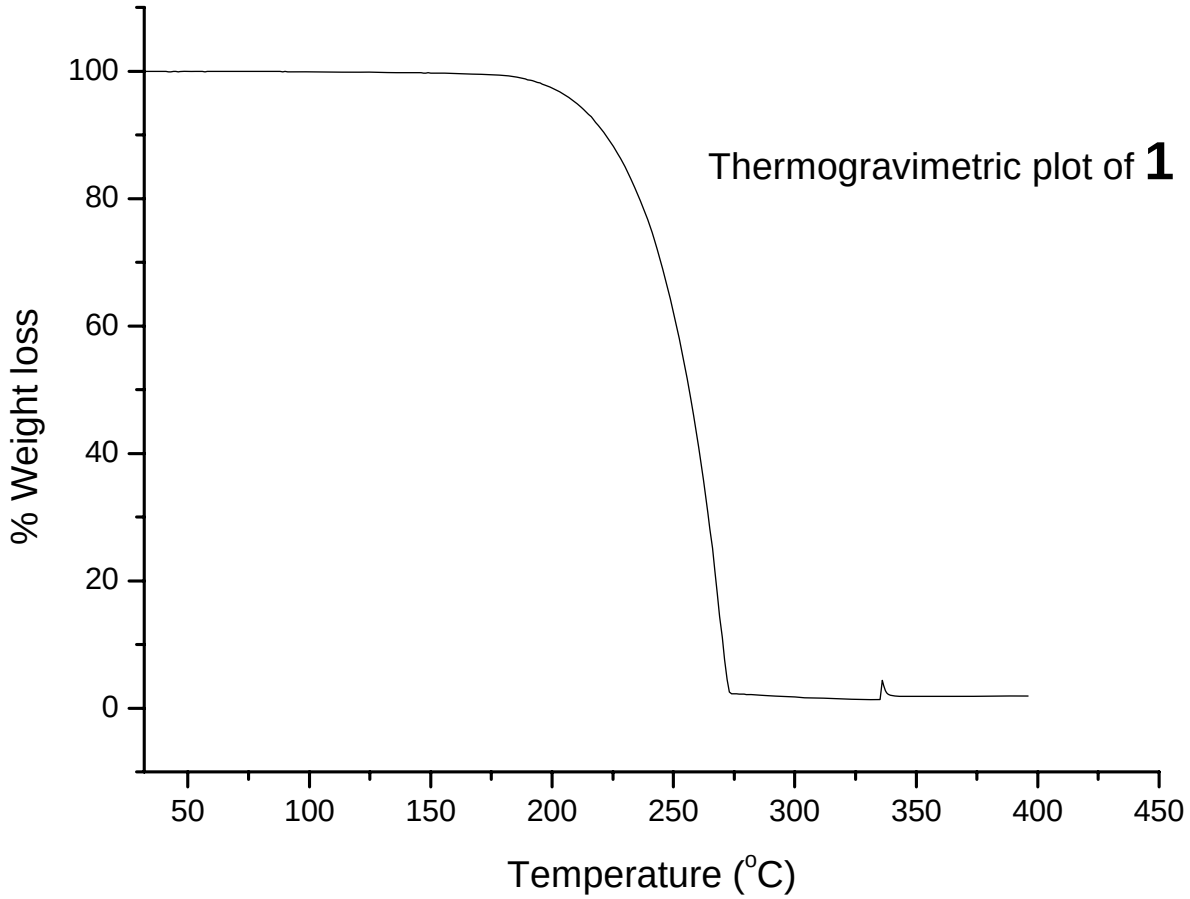
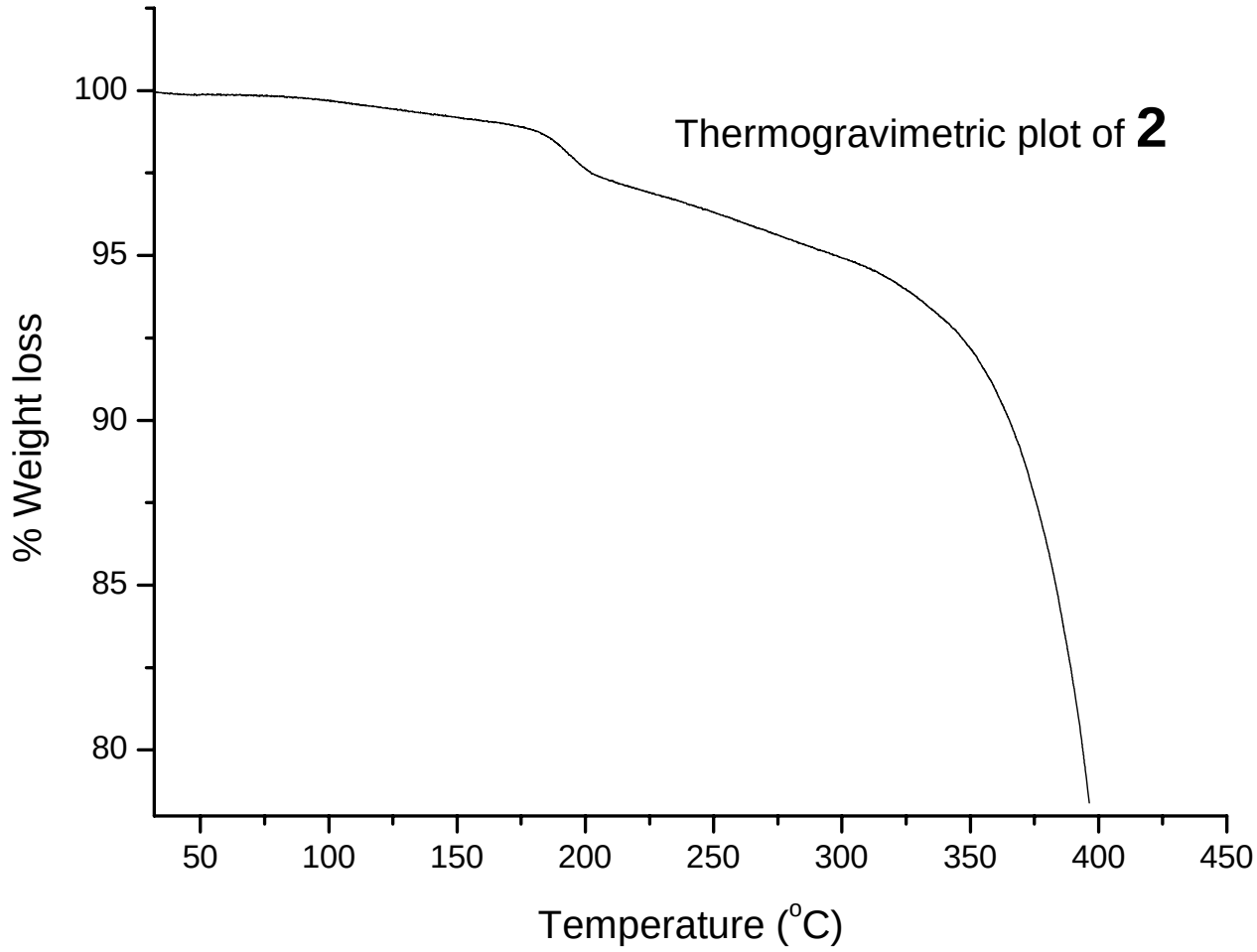
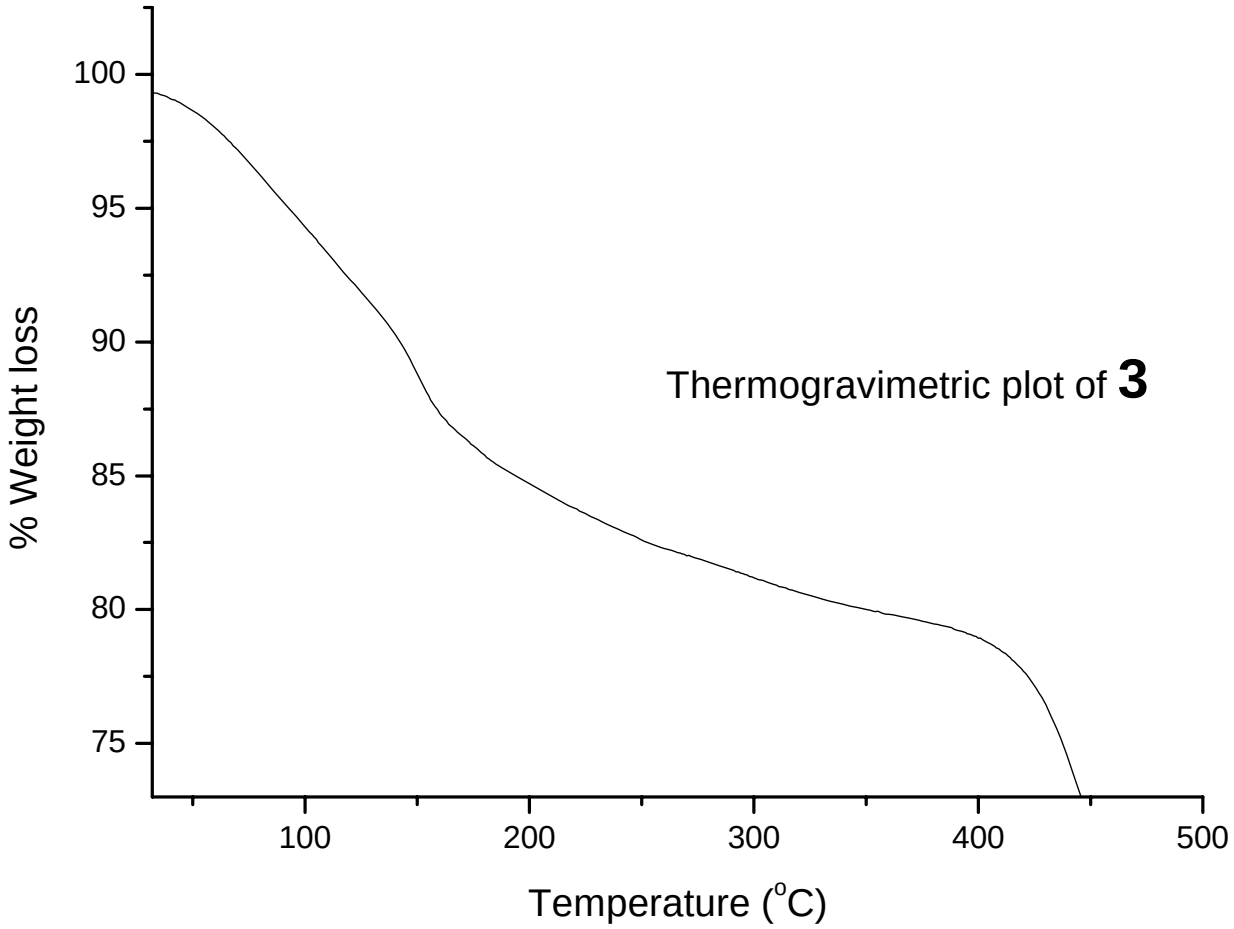


Figure 4: In addition to several C-H…N hydrogen bonds formed by the pyridazine and 2-pyridyl rings, the system is stabilized by π…π interactions in the range 3.45 – 3.50 Å.







Thermogravimetric plot of **3**