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Azines Possessing Extreme Push/Pull Donors/Acceptors

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Supporting Information

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General procedures

An MBraun UL-99-245 dry box and standard Schlenk techniques on a double manifold vacuum line were used in the manipulation of air and moisture sensitive compounds. NMR spectra were recorded on a Bruker AMX 400 or a Varian AS 500 spectrometer in five millimeter quartz tubes. ^{1}H and $^{13}C\{^{1}H\}$ chemical shifts are reported in parts per million (ppm) downfield from tetramethylsilane (TMS) and are calibrated to the residual signal of the solvent. Infrared spectra were obtained using a Bomem MB spectrometer with the % transmittance values reported in cm^{-1}. Melting points were measured using a Mel-Temp apparatus and are uncorrected. The high resolution mass spectra were obtained using a Kratos Concept double focussing mass specrometer. Samples were run by electron impact and exact mass was obtained by peak matching using perfluorokerosene as a mass reference.

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Synthesis of azines:

Note: Compounds **1**, **2**, **3**, **4**, and **6** were prepared on similar scales and followed the same procedure as used for **2**. (J. M. Hopkins, M. Bowdridge, K. N. Robertson, T. S. Cameron, H. A. Jenkins and J. A. C. Clyburne, *J. Org. Chem*, 2001, **66**, 5713-5716.). Compound **10** was prepared following a literature procedure (H.H. Szmant and C. J. McGinnis *J. Am. Chem. Soc.* 1950, **72**, 2890-2892).

Compound 1

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.22 (s, 12H), 2.42 (s, 6H), 6.47 (dt, J_1 = 7.7 Hz, J_2 = 1.1 Hz, 1H), 6.49 (s, 2H), 6.94 - 6.99 (m, 2H), 7.03 (s,4H), 7.11 (td, J_1 = 7.4 Hz, J_2 = 1.1 Hz, 1H), 7.16 (td, J_1 = 7.4 Hz, J_2 = 1.1 Hz, 1H), 7.51 (dt, J_1 = 7.4 Hz, J_2 = 1.1 Hz, 1H), 7.56 (dt, J_1 = 7.7 Hz, J_2 = 1.1 Hz, 1H), 7.97 (dt, J_1 = 7.7 Hz, J_2 = 1.1 Hz, 1H)

Preparation of 2:

A solution of 1,3-*bis*-(2,4,6-trimethylphenyl)-imidazol-2-ylidene (0.22 g, 0.72 mmol) in 20 mL of tetrahydrofuran (THF) was added to a stirred solution of 2,7-dibromo-9-diazofluorene (0.25 g, 0.73 mmol) in 25 mL of THF at room temperature. The dark red solution was stirred for 3.5 h. Solvent was removed *in vacuo* and the red solid was recrystallised from dichloromethane and hexane to produce red/orange crystals of **2**.

Characterisation Data

Compound 2

Red crystals ; Yield 0.4 g (79%) m.p. 260-262°C.

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^{1}H NMR (400 MHz, $CDCl_3$) δ 2.21 (s, 12H), 2.45 (s, 6H), 6.57 (d, J = 1.9, 1H), 6.58 (s, 2H),7.08 (s, 4H), 7.21 (dd, J_1 = 7.8 Hz, J_2= 1.9 Hz, 1 H), 7.27 (dd, J_1 = 7.8 Hz, J_2 = 1.9 Hz, 1H), 7.34 (d, J = 7.8 Hz, 1H), 7.39 (d, J = 7.8 Hz, 1H), 8.10 (d, J = 1.9 Hz, 1H).

^{13}C NMR (400 MHz, $CDCl_3$) δ 18.3, 21.6, 120.3, 120.6, 120.8, 123.4, 128.8, 129.4, 129.9, 130.2, 132.3, 136.0, 136.7, 140.8, 143.5, 150.0

HRMS–EI (m/z): $[M]^+$ calculated for $C_{34}H_{30}N_4Br_2$, 652.0837; found 652.0848.

Compound 3

Orange crystals ; Yield: 1.0 g (74%), m.p. 180-182 °C.

The crystal contains two isomeric forms of the molecule (determined by X-ray crystallography). The ^{1}H NMR intergrations are consistent with two isomers being present in *ca* equal amounts.

^{1}H NMR (400 MHz, $CDCl_3$) δ 2.21 (s, 24 H), 2.42 (d, J = 4.3 Hz, 12H), 6.06 (dd, J_1= 9.8, J_2 = 2.4 Hz, 1 H), 6.48 (d, J = 7.6 Hz, 1H), 6.53 (d, J = 5.2 Hz, 4H), 6.75 – 6.86 (m, 2H), 6.92 – 6.99 (m, 2H), 7.04 (s, 8H), 7.08 – 7.17 (m, 2H), 7.41 – 7.52 (m, 4H), 7.61(dd, J_1= 10.1 Hz, J_2 = 2.4 Hz, 1 H), 7.91 (d,1H)

^{13}C NMR ($CDCl_3$) the spectra obtained are complex due to the presence of two isomers in solutions as well as complex coupling between carbon and fluorine.

HRMS–EI (m/z) : $[M]^+$ calculated for $C_{34}H_{31}N_4F$, 514.2533; found 514.2532.

Compound 4

Orange crystals ; Yield: 1.00 g (74.1 %), m.p. 180-182 °C.

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^{1}H NMR (500 MHz, $CDCl_3$) δ 2.21 (s, 12H), 2.44 (s, 6H), 6.39 (d, J = 2.1 Hz, 1H), 6.58 (broad s, 2H), 7.05 (dd, J_1 = 7.9 Hz, J_2 = 2.1 Hz, 1H), 7.07 (s, 4H), 7.11 (dd, J_1 = 7.9 Hz, J_2 = 2.1 Hz, 1H), 7.38 (d, J = 7.9 Hz, 1H), 7.43 (d, J = 7.9 Hz, 1H), 7.91 (d, J = 2.1 Hz, 1H).

^{13}C NMR (400 MHz, $CDCl_3$) δ 18.4, 21.5, 119.9, 120.2, 120.5, 126.0, 127.1, 127.4, 129.4, 129.6, 132.2, 132.4, 132.9, , 135.7, 136.3, 140.7, 143.8, 149.9.

HRMS–EI (*m*/*z*): $[M]^+$ calculated for $C_{34}H_{30}N_4Cl_2$, 564.1848; found 564.1848.

Compound 6

Yield (0.81g, 29%), m.p. 167-169˚C.

^{1}H NMR (500 MHz, $CDCl_3$) δ 2.15 (s, 12H), 2.34 (s, 6H), 5.50-5.53 (m, 1H), 6.19-6.23 (m, 1H), 6.23-6.24 (m, 1H), 6.26-6.27 (m, 1H), 6.49 (s, 2H), 6.93 (s, 4H).

^{13}C NMR (500 MHz, $CDCl_3$) δ 18.1, 21.0, 107.2, 116.4, 124.2, 128.5, 128.6, 130.5, 134.2,135.4, 138.1, 150.3, 158.9.

HRMS–EI (*m*/*z*): $[M]^+$ calculated for $C_{26}H_{28}N_4$, 396.2314; found 396.2313.

Compound 5

Prepared as for compound **2** except using 1,3-bis(isopropyl)-4,5-dimethylimidazole-2-ylidene

Reddish-orange crystals; Yield: 0.96 g, 48%. m.p. 151-153˚C:

^{1}H NMR (500 MHz, C_6D_6) δ 1.25 (d, J = 7 Hz, 12H), 1.53 (s, 6H), 5.35 (broad, 2 H), 7.25 (t, J = 8 Hz, 1H), 7.28 (t, J = 8, 1H), 7.37 (t, J = 8 Hz, 1H), 7.50 (t, J = 8 Hz, 1H), 7.74 (d, J = 8 Hz, 1H), 7.78 (d, J = 8 Hz, 1 H), 8.24 (d, J = 8 Hz, 1H), 9.41 (d, J = 8 Hz, 1H)

^{13}C NMR (500 MHz, C_6D_6) δ 9.8, 21.4, 48.2, 118.4, 119.8, 119.9, 125.8, 126.8, 126.9, 127.1, 127.2, 128.3, 132.3, 138.3, 139.5, 140.7, 143.3, 152.8.

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MS *m*/*z* (relative intensity): 100% (373).

HRMS–EI (*m*/*z*) : $[M]^+$ calculated for $C_{24}H_{28}N_4$, 372.2314; found 372.2313.

Preparation and Characterisation Data of Compound 7

A solution of fluorenone hydrazone (0.418 g, 2 mmol) and pyridine (0.15 ml, 2 mmol) in methanol (25 mL) was added dropwise to a solution of 2-methylthio-1,3 dithiolium iodide (0.6 g, 2 mmol) in methanol (20 mL) at 0˚C under nitrogen. During the addition, an orange solid precipitated. The mixture was allowed to stir at room temperature for 2-3 hours. The solid was filtered, washed with cold methanol and dried. Recrystallisation from ether/benzene/hexane afforded reddish brown crystals (0.271 g, 46%) m.p. 150-152 ˚C.

^{1}H NMR ($CDCl_3$) δ 6.65 (d, *J* = 7.3 Hz,1 H), 6.73 (*J* = 7.0 Hz, 1H), 7.26-7.31 (m, 2H), 7.35-7.42 (m, 2H), 7.57-7.64 (m, 2H), 7.91 (d, *J* = 7.3 Hz, 1H), 8.53 (d, *J* = 7.3 Hz, 1H).

^{13}C NMR (400 MHz, $CDCl_3$) δ 117.2, 120.0, 120.1, 120.3, 120.4, 123.1, 128.4, 130.1, 130.8, 131.2, 131.5, 131.6, 136.7, 141.5, 142.5, 155.1.

IR (KBr): 649, 726, 789, 930, 1093, 1306, 1431, 1594, 2921, 3053 cm^{-1}.

MS *m*/*z* (relative intensity): 295 (M^+: 100%).

HRMS–EI (*m*/*z*) : $[M]^+$ calculated for $C_{16}H_{10}N_2S_2$, 294.0285; found 294.0286

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

Identification code	**2**	
Empirical formula	C34 H30 Br2 N4	
Formula weight	654.44	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.1477(7) Å	α= 90°.
	b = 20.9731(13) Å	β= 113.242(2)°.
	c = 14.0060(8) Å	γ = 90°.
Volume	3008.9(3) $Å^3$	
Z	4	
Density (calculated)	1.445 Mg/m^3	
Absorption coefficient	2.724 mm^{-1}	
F(000)	1328	
Crystal size	0.4 x 0.3 x 0.1 mm^3	
Theta range for data collection	1.86 to 27.53°.	
Index ranges	-14<=h<=14, -27<=k<=27, -18<=l<=18	
Reflections collected	28975	
Independent reflections	6935 [R(int) = 0.1293]	
Completeness to theta = 27.53°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6935 / 0 / 361	
Goodness-of-fit on F^2	1.039	
Final R indices [I>2sigma(I)]	R1 = 0.0845, wR2 = 0.1859	
R indices (all data)	R1 = 0.1996, wR2 = 0.2282	
Largest diff. peak and hole	2.164 and -0.784 $e.Å^{-3}$	

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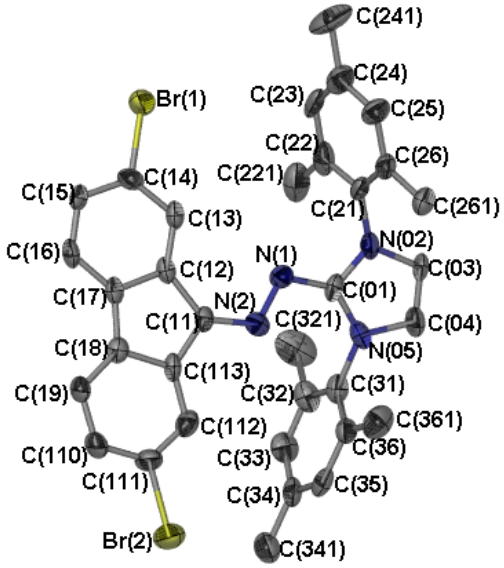

ORTEP Diagram of **2**

Hydrogen atoms are removed for clarity. Thermal ellipsoids are shown at 50%probability level.

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

	x	y	z	U(eq)
C(01)	3267(7)	851(3)	1859(6)	39(2)
C(03)	2031(7)	421(4)	2611(6)	46(2)
C(04)	1354(8)	385(4)	1585(6)	51(2)
C(11)	5106(7)	1566(3)	722(5)	35(2)
C(12)	6507(7)	1674(3)	1436(5)	36(2)
C(13)	7166(7)	1550(3)	2467(6)	40(2)
C(14)	8482(8)	1716(4)	2921(5)	45(2)
C(15)	9133(7)	2007(3)	2365(6)	41(2)
C(16)	8436(7)	2139(3)	1321(6)	44(2)
C(17)	7114(7)	1979(3)	839(6)	38(2)
C(18)	6170(7)	2057(3)	-217(6)	39(2)
C(19)	6248(8)	2329(4)	-1087(6)	45(2)
C(21)	4221(7)	874(4)	3787(6)	45(2)
C(22)	5407(9)	546(4)	4129(7)	58(2)
C(23)	6344(8)	737(5)	5107(7)	64(3)
C(24)	6104(9)	1195(4)	5706(7)	60(2)
C(25)	4909(8)	1492(4)	5319(7)	56(2)
C(26)	3961(7)	1335(4)	4355(6)	45(2)
C(31)	1796(7)	590(3)	7(6)	43(2)
C(32)	2360(8)	93(4)	-332(6)	52(2)
C(33)	2050(8)	33(4)	-1378(6)	56(2)
C(34)	1172(8)	442(4)	-2106(6)	48(2)
C(35)	643(7)	931(4)	-1733(6)	47(2)
C(36)	926(7)	1012(4)	-677(6)	42(2)
C(110)	5138(8)	2341(4)	-2018(6)	54(2)
C(111)	3992(8)	2079(4)	-2062(6)	50(2)
C(112)	3863(8)	1804(4)	-1237(6)	49(2)
C(113)	4946(7)	1800(3)	-288(6)	37(2)
C(221)	5685(9)	23(5)	3514(8)	77(3)
C(241)	7129(10)	1359(5)	6765(8)	96(4)

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C(261)	2668(7)	1687(4)	3941(6)	54(2)
C(321)	3356(11)	-344(4)	452(7)	85(3)
C(341)	855(9)	365(4)	-3253(6)	66(3)
C(361)	348(9)	1549(4)	-311(7)	69(3)
N(1)	4357(6)	1135(3)	1827(4)	42(2)
N(2)	4088(6)	1318(3)	863(4)	40(2)
N(02)	3243(6)	703(3)	2783(5)	44(2)
N(05)	2128(6)	655(3)	1105(5)	43(2)
Br(1)	9423(1)	1539(1)	4355(1)	56(1)
Br(2)	2498(1)	2098(1)	-3348(1)	75(1)

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

C(01)-N(02)	1.342(9)
C(01)-N(05)	1.356(9)
C(01)-N(1)	1.370(9)
C(03)-C(04)	1.335(10)
C(03)-N(02)	1.405(9)
C(04)-N(05)	1.406(9)
C(11)-N(2)	1.331(9)
C(11)-C(113)	1.440(10)
C(11)-C(12)	1.503(10)
C(12)-C(13)	1.363(10)
C(12)-C(17)	1.419(9)
C(13)-C(14)	1.393(10)
C(14)-C(15)	1.398(10)
C(14)-Br(1)	1.900(7)
C(15)-C(16)	1.385(10)
C(16)-C(17)	1.398(10)
C(17)-C(18)	1.447(10)
C(18)-C(19)	1.378(9)
C(18)-C(113)	1.434(9)
C(19)-C(110)	1.400(11)
C(21)-C(26)	1.354(10)
C(21)-C(22)	1.397(11)
C(21)-N(02)	1.444(9)
C(22)-C(23)	1.414(12)
C(22)-C(221)	1.501(12)
C(23)-C(24)	1.371(13)
C(24)-C(25)	1.372(12)
C(24)-C(241)	1.511(12)
C(25)-C(26)	1.386(10)
C(26)-C(261)	1.517(10)
C(31)-C(36)	1.383(10)
C(31)-C(32)	1.395(10)
C(31)-N(05)	1.438(9)

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C(32)-C(33)	1.371(11)
C(32)-C(321)	1.521(11)
C(33)-C(34)	1.396(11)
C(34)-C(35)	1.384(10)
C(34)-C(341)	1.511(10)
C(35)-C(36)	1.396(10)
C(36)-C(361)	1.485(10)
C(110)-C(111)	1.370(11)
C(111)-C(112)	1.348(10)
C(111)-Br(2)	1.912(8)
C(112)-C(113)	1.399(10)
N(1)-N(2)	1.319(7)

N(02)-C(01)-N(05)	108.2(6)
N(02)-C(01)-N(1)	119.3(7)
N(05)-C(01)-N(1)	132.5(7)
C(04)-C(03)-N(02)	107.8(6)
C(03)-C(04)-N(05)	107.4(7)
N(2)-C(11)-C(113)	119.8(6)
N(2)-C(11)-C(12)	133.0(6)
C(113)-C(11)-C(12)	107.2(6)
C(13)-C(12)-C(17)	121.9(7)
C(13)-C(12)-C(11)	131.3(6)
C(17)-C(12)-C(11)	106.8(6)
C(12)-C(13)-C(14)	117.8(7)
C(13)-C(14)-C(15)	122.7(7)
C(13)-C(14)-Br(1)	118.5(6)
C(15)-C(14)-Br(1)	118.9(6)
C(16)-C(15)-C(14)	118.5(7)
C(15)-C(16)-C(17)	120.5(7)
C(16)-C(17)-C(12)	118.7(7)
C(16)-C(17)-C(18)	132.1(6)
C(12)-C(17)-C(18)	109.2(6)
C(19)-C(18)-C(113)	119.0(7)
C(19)-C(18)-C(17)	132.5(7)

C(113)-C(18)-C(17)	108.4(6)
C(18)-C(19)-C(110)	119.4(7)
C(26)-C(21)-C(22)	122.9(8)
C(26)-C(21)-N(02)	119.7(7)
C(22)-C(21)-N(02)	117.4(8)
C(21)-C(22)-C(23)	115.5(8)
C(21)-C(22)-C(221)	123.0(9)
C(23)-C(22)-C(221)	121.5(8)
C(24)-C(23)-C(22)	122.9(8)
C(25)-C(24)-C(23)	118.0(9)
C(25)-C(24)-C(241)	121.7(10)
C(23)-C(24)-C(241)	120.3(9)
C(24)-C(25)-C(26)	121.7(9)
C(21)-C(26)-C(25)	119.0(7)
C(21)-C(26)-C(261)	121.0(7)
C(25)-C(26)-C(261)	120.0(7)
C(36)-C(31)-C(32)	122.0(7)
C(36)-C(31)-N(05)	119.6(6)
C(32)-C(31)-N(05)	118.3(7)
C(33)-C(32)-C(31)	118.3(8)
C(33)-C(32)-C(321)	121.4(7)
C(31)-C(32)-C(321)	120.2(7)
C(32)-C(33)-C(34)	122.3(8)
C(35)-C(34)-C(33)	117.4(7)
C(35)-C(34)-C(341)	121.6(8)
C(33)-C(34)-C(341)	121.0(7)
C(34)-C(35)-C(36)	122.6(7)
C(31)-C(36)-C(35)	117.4(7)
C(31)-C(36)-C(361)	121.8(7)
C(35)-C(36)-C(361)	120.8(7)
C(111)-C(110)-C(19)	120.0(7)
C(112)-C(111)-C(110)	123.1(7)
C(112)-C(111)-Br(2)	118.0(6)
C(110)-C(111)-Br(2)	118.9(6)
C(111)-C(112)-C(113)	118.2(7)

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C(112)-C(113)-C(18)	120.2(6)
C(112)-C(113)-C(11)	131.4(6)
C(18)-C(113)-C(11)	108.4(6)
N(2)-N(1)-C(01)	108.3(6)
N(1)-N(2)-C(11)	113.8(6)
C(01)-N(02)-C(03)	108.4(6)
C(01)-N(02)-C(21)	125.9(6)
C(03)-N(02)-C(21)	125.3(6)
C(01)-N(05)-C(04)	108.2(6)
C(01)-N(05)-C(31)	129.0(6)
C(04)-N(05)-C(31)	121.6(6)

Symmetry transformations used to generate equivalent atoms:

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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(01)	28(4)	33(4)	61(5)	-6(4)	23(4)	-1(3)
C(03)	30(4)	61(5)	56(5)	3(4)	26(4)	-11(4)
C(04)	50(5)	54(5)	62(6)	8(4)	34(5)	-8(4)
C(11)	33(4)	32(4)	47(4)	-5(3)	23(3)	-1(3)
C(12)	42(4)	29(4)	47(4)	2(3)	29(4)	1(3)
C(13)	38(4)	36(4)	56(5)	1(4)	31(4)	0(4)
C(14)	49(5)	52(5)	33(4)	10(4)	15(4)	25(4)
C(15)	29(4)	50(5)	50(5)	0(4)	22(4)	6(3)
C(16)	45(5)	43(5)	59(5)	8(4)	37(4)	-1(4)
C(17)	40(4)	34(4)	52(5)	0(3)	31(4)	2(3)
C(18)	39(4)	33(4)	49(4)	-2(3)	22(4)	0(3)
C(19)	44(5)	47(5)	50(5)	6(4)	25(4)	-17(4)
C(21)	22(4)	63(5)	46(5)	17(4)	11(4)	0(4)
C(22)	54(6)	52(5)	85(7)	24(5)	43(5)	7(4)
C(23)	23(4)	90(7)	76(6)	43(6)	16(5)	3(5)
C(24)	48(6)	55(5)	70(6)	16(5)	16(5)	-8(5)
C(25)	42(5)	55(5)	62(5)	14(4)	9(4)	2(4)
C(26)	35(4)	52(5)	49(5)	9(4)	19(4)	-6(4)
C(31)	44(5)	30(4)	62(5)	1(4)	29(4)	0(4)
C(32)	67(6)	34(4)	67(6)	0(4)	39(5)	-2(4)
C(33)	65(6)	47(5)	64(6)	-10(4)	34(5)	8(4)
C(34)	40(5)	53(5)	60(5)	-9(4)	31(4)	-12(4)
C(35)	28(4)	43(5)	69(6)	7(4)	17(4)	-6(3)
C(36)	39(4)	46(5)	46(5)	-6(4)	22(4)	-4(4)
C(110)	56(5)	63(6)	47(5)	7(4)	25(4)	-23(4)
C(111)	50(5)	54(5)	40(4)	7(4)	11(4)	-2(4)
C(112)	40(5)	48(5)	58(5)	-8(4)	19(4)	-12(4)
C(113)	37(4)	29(4)	58(5)	-5(3)	32(4)	-6(3)
C(221)	67(7)	68(7)	111(8)	21(6)	52(6)	10(5)
C(241)	58(6)	77(7)	100(8)	17(6)	-24(6)	-21(5)

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C(261)	38(5)	65(6)	62(5)	0(4)	22(4)	1(4)
C(321)	129(10)	45(6)	89(7)	8(5)	50(7)	46(6)
C(341)	69(6)	73(6)	63(6)	-5(5)	36(5)	-12(5)
C(361)	54(6)	63(6)	88(7)	-15(5)	25(5)	13(5)
N(1)	37(4)	45(4)	42(4)	3(3)	13(3)	7(3)
N(2)	48(4)	35(3)	39(4)	0(3)	20(3)	9(3)
N(02)	39(4)	48(4)	53(4)	7(3)	28(3)	-1(3)
N(05)	57(4)	39(4)	48(4)	1(3)	36(4)	0(3)
Br(1)	49(1)	71(1)	50(1)	13(1)	20(1)	13(1)
Br(2)	61(1)	94(1)	56(1)	9(1)	7(1)	-18(1)

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

	x	y	z	U(eq)
H(03)	1750	284	3120	56
H(04)	523	213	1250	62
H(13)	6751	1361	2855	48
H(15)	10014	2111	2688	50
H(16)	8851	2334	939	53
H(19)	7030	2503	-1055	54
H(23)	7161	543	5354	76
H(25)	4731	1805	5714	68
H(33)	2438	-291	-1609	67
H(35)	76	1217	-2205	57
H(110)	5179	2527	-2608	64
H(112)	3076	1622	-1298	58
H(22A)	4938	-40	2876	115
H(22B)	5871	-365	3910	115
H(22C)	6424	138	3362	115
H(24A)	6808	1691	7072	143
H(24B)	7908	1501	6693	143
H(24C)	7322	988	7201	143
H(26A)	2656	1994	4445	81
H(26B)	1968	1388	3809	81
H(26C)	2562	1901	3307	81
H(32A)	3448	-230	1141	128
H(32B)	4183	-299	396	128
H(32C)	3067	-778	314	128
H(34A)	1315	3	-3360	98
H(34B)	1117	742	-3511	98
H(34C)	-67	302	-3619	98
H(36A)	-226	1788	-898	104
H(36B)	1032	1822	133	104

H(36C)	-136	1383	69	104

Table 1. Crystal data and structure refinement for **3**.

Identification code	**3**	
Empirical formula	C37 H34 F N4	
Formula weight	553.68	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 10.5060(6) Å	α= 80.3250(10)°.
	b = 11.5012(7) Å	β= 81.3250(10)°.
	c = 25.6373(16) Å	γ = 89.4250(10)°.
Volume	3018.4(3) $Å^3$	
Z	4	
Density (calculated)	1.218 Mg/m^3	
Absorption coefficient	0.076 mm^{-1}	
F(000)	1172	
Crystal size	0.50 x 0.10 x 0.10 mm^3	
Theta range for data collection	0.82 to 27.49°.	
Index ranges	-13<=h<=13, -14<=k<=14, -33<=l<=33	
Reflections collected	26256	
Independent reflections	13150 [R(int) = 0.0234]	
Completeness to theta = 27.49°	94.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13150 / 0 / 769	
Goodness-of-fit on F^2	1.069	
Final R indices [I>2sigma(I)]	R1 = 0.0770, wR2 = 0.1807	
R indices (all data)	R1 = 0.0992, wR2 = 0.1929	
Largest diff. peak and hole	0.692 and -0.274 $e.Å^{-3}$	

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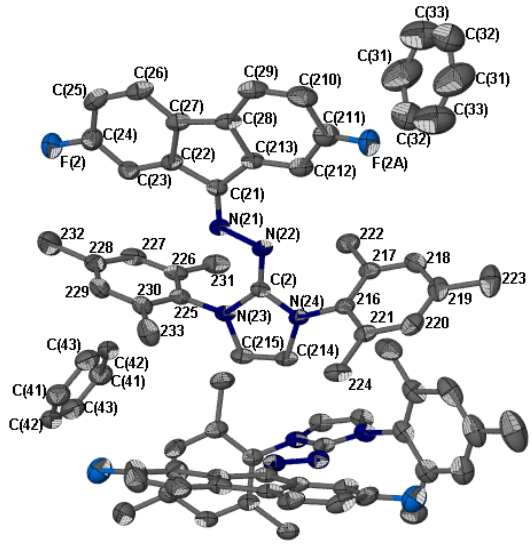
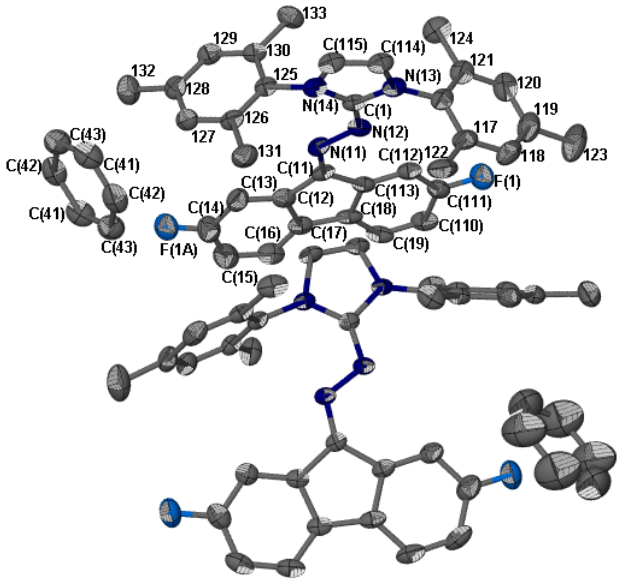


ORTEP Diagram of **3** (view 1)



ORTEP Diagram of **3** (view 2)

There is occupational disorder in regard to the position of the single F atom in each independent molecule, these diagrams indicate both possible positions. The actual occupancy of each position is indicated below.

F2 (64%) F2A (36%) F1 (21%) F1A (79%)

Hydrogen atoms are removed for clarity. Thermal ellipsoids are shown at 50% probability level.

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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)	-1334(2)	12169(2)	2779(1)	38(1)
C(11)	1325(2)	13755(2)	2119(1)	40(1)
C(12)	2142(3)	13948(2)	1602(1)	45(1)
C(13)	2031(3)	13596(3)	1121(1)	56(1)
C(14)	3004(4)	13846(3)	698(2)	69(1)
C(15)	4097(4)	14452(3)	749(1)	69(1)
C(16)	4217(3)	14840(3)	1220(1)	58(1)
C(17)	3256(3)	14593(2)	1652(1)	46(1)
C(18)	3122(2)	14845(2)	2195(1)	43(1)
C(19)	3938(3)	15448(2)	2445(1)	51(1)
C(110)	3595(3)	15554(2)	2973(1)	55(1)
C(111)	2408(3)	15049(2)	3249(1)	50(1)
C(112)	1603(2)	14457(2)	3011(1)	44(1)
C(113)	1938(2)	14340(2)	2484(1)	39(1)
C(114)	-2889(2)	10951(2)	3266(1)	45(1)
C(115)	-2930(2)	10905(2)	2755(1)	45(1)
1(16)	-1449(2)	12029(2)	3749(1)	45(1)
1(17)	-601(3)	11264(3)	3992(1)	54(1)
1(18)	-76(3)	11608(4)	4409(1)	69(1)
1(19)	-371(4)	12662(4)	4580(1)	72(1)
1(20)	-1250(3)	13387(3)	4335(1)	65(1)
1(21)	-1805(3)	13089(3)	3915(1)	52(1)
1(22)	-277(3)	10105(3)	3809(1)	67(1)
1(23)	256(5)	13042(5)	5022(2)	108(2)
1(24)	-2719(3)	13900(3)	3643(2)	65(1)
1(25)	-1869(2)	12047(2)	1874(1)	39(1)
1(26)	-1206(2)	11364(2)	1526(1)	43(1)
1(27)	-1055(3)	11807(2)	984(1)	48(1)
1(28)	-1554(3)	12888(2)	783(1)	47(1)
1(29)	-2264(3)	13503(2)	1146(1)	45(1)

1(30)	-2430(2)	13111(2)	1693(1)	41(1)
1(31)	-666(3)	10187(3)	1735(1)	58(1)
1(32)	-1315(4)	13386(3)	192(1)	69(1)
1(33)	-3169(3)	13821(2)	2076(1)	55(1)
C(2)	3836(2)	9652(2)	2571(1)	32(1)
C(21)	6402(2)	7831(2)	2403(1)	33(1)
C(22)	7169(2)	7303(2)	1983(1)	36(1)
C(23)	6986(3)	7248(2)	1466(1)	42(1)
C(24)	7885(3)	6667(2)	1160(1)	51(1)
C(25)	8957(3)	6142(2)	1348(1)	53(1)
C(26)	9144(2)	6197(2)	1865(1)	49(1)
C(27)	8262(2)	6775(2)	2185(1)	40(1)
C(28)	8185(2)	6955(2)	2738(1)	41(1)
C(29)	9021(3)	6632(2)	3108(1)	53(1)
C(210)	8708(3)	6880(3)	3616(1)	61(1)
C(211)	7568(3)	7450(3)	3761(2)	58(1)
C(212)	6730(3)	7798(2)	3396(1)	45(1)
C(213)	7043(2)	7564(2)	2883(1)	36(1)
C(214)	2290(2)	11006(2)	2659(1)	42(1)
C(215)	2439(2)	10830(2)	2158(1)	43(1)
2(16)	3269(2)	10203(2)	3477(1)	36(1)
2(17)	2904(2)	9169(2)	3837(1)	41(1)
2(18)	2965(3)	9162(3)	4372(1)	48(1)
2(19)	3356(3)	10144(3)	4559(1)	50(1)
2(20)	3716(2)	11150(3)	4189(1)	47(1)
2(21)	3684(2)	11204(2)	3647(1)	39(1)
2(22)	2426(3)	8099(2)	3652(1)	52(1)
2(23)	3345(3)	10122(4)	5150(1)	72(1)
2(24)	4101(3)	12314(2)	3256(1)	50(1)
2(25)	3679(2)	9452(2)	1620(1)	37(1)
2(26)	2982(2)	8451(2)	1590(1)	43(1)
2(27)	3287(3)	7943(2)	1135(1)	51(1)
2(28)	4243(3)	8406(3)	721(1)	54(1)
2(29)	4894(3)	9417(3)	765(1)	49(1)
2(30)	4627(2)	9965(2)	1211(1)	41(1)

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2(31)	1972(3)	7918(2)	2044(1)	56(1)
2(32)	4606(5)	7802(3)	241(1)	85(1)
2(33)	5366(3)	11046(3)	1267(1)	57(1)
N(11)	280(2)	13076(2)	2204(1)	42(1)
N(12)	-325(2)	12913(2)	2709(1)	43(1)
N(13)	-1914(2)	11745(2)	3285(1)	42(1)
N(14)	-1968(2)	11666(2)	2444(1)	40(1)
N(21)	5390(2)	8455(2)	2306(1)	34(1)
N(22)	4773(2)	8937(2)	2722(1)	35(1)
N(23)	3393(2)	9980(2)	2094(1)	37(1)
N(24)	3141(2)	10274(2)	2925(1)	35(1)
C(41)	-1093(3)	9337(3)	213(1)	64(1)
C(42)	14(4)	9109(3)	429(1)	61(1)
C(43)	1110(3)	9772(3)	219(1)	62(1)
C(31)	4289(6)	4438(6)	4720(3)	130(2)
C(32)	4239(6)	5613(6)	4671(2)	118(2)
C(33)	4923(7)	6188(5)	4960(3)	129(2)
F(1)	2095(2)	15162(2)	3756(1)	67(1)
F(1A)	2811(10)	13602(8)	258(4)	67(1)
F(2)	7710(3)	6570(3)	671(2)	65(1)
F(2A)	7364(5)	7739(5)	4204(2)	65(1)

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

C(1)-N(12)	1.341(3)
C(1)-N(13)	1.361(3)
C(1)-N(14)	1.365(3)
C(11)-N(11)	1.324(3)
C(11)-C(12)	1.451(4)
C(11)-C(113)	1.463(4)
C(12)-C(13)	1.382(4)
C(12)-C(17)	1.425(4)
C(13)-C(14)	1.368(5)
C(14)-F(1A)	1.253(12)
C(14)-C(15)	1.383(5)
C(15)-C(16)	1.380(5)
C(16)-C(17)	1.374(4)
C(17)-C(18)	1.456(4)
C(18)-C(19)	1.397(4)
C(18)-C(113)	1.424(3)
C(19)-C(110)	1.375(4)
C(110)-C(111)	1.416(4)
C(111)-F(1)	1.320(4)
C(111)-C(112)	1.361(4)
C(112)-C(113)	1.374(4)
C(114)-C(115)	1.326(4)
C(114)-N(13)	1.392(3)
C(115)-N(14)	1.402(3)
1(16)-1(17)	1.388(4)
1(16)-1(21)	1.388(4)
1(16)-N(13)	1.437(3)
1(17)-1(18)	1.389(5)
1(17)-1(22)	1.505(5)
1(18)-1(19)	1.374(5)
1(19)-1(20)	1.387(5)
1(19)-1(23)	1.520(5)
1(20)-1(21)	1.391(4)

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1(21)-1(24)	1.498(4)
1(25)-1(30)	1.391(3)
1(25)-1(26)	1.391(4)
1(25)-N(14)	1.441(3)
1(26)-1(27)	1.385(4)
1(26)-1(31)	1.507(4)
1(27)-1(28)	1.391(4)
1(28)-1(29)	1.387(4)
1(28)-1(32)	1.511(4)
1(29)-1(30)	1.383(4)
1(30)-1(33)	1.504(4)
C(2)-N(22)	1.337(3)
C(2)-N(23)	1.367(3)
C(2)-N(24)	1.370(3)
C(21)-N(21)	1.308(3)
C(21)-C(22)	1.459(3)
C(21)-C(213)	1.477(3)
C(22)-C(23)	1.379(4)
C(22)-C(27)	1.419(3)
C(23)-C(24)	1.377(4)
C(24)-F(2)	1.316(5)
C(24)-C(25)	1.385(4)
C(25)-C(26)	1.381(4)
C(26)-C(27)	1.384(4)
C(27)-C(28)	1.457(4)
C(28)-C(29)	1.391(4)
C(28)-C(213)	1.416(3)
C(29)-C(210)	1.372(4)
C(210)-C(211)	1.390(5)
C(211)-F(2A)	1.225(6)
C(211)-C(212)	1.389(4)
C(212)-C(213)	1.375(4)
C(214)-C(215)	1.320(4)
C(214)-N(24)	1.396(3)
C(215)-N(23)	1.404(3)

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2(16)-2(21)	1.392(3)
2(16)-2(17)	1.395(3)
2(16)-N(24)	1.430(3)
2(17)-2(18)	1.383(4)
2(17)-2(22)	1.507(4)
2(18)-2(19)	1.387(4)
2(19)-2(20)	1.383(4)
2(19)-2(23)	1.509(4)
2(20)-2(21)	1.388(4)
2(21)-2(24)	1.508(4)
2(25)-2(26)	1.389(3)
2(25)-2(30)	1.389(4)
2(25)-N(23)	1.440(3)
2(26)-2(27)	1.385(4)
2(26)-2(31)	1.503(4)
2(27)-2(28)	1.384(4)
2(28)-2(29)	1.384(4)
2(28)-2(32)	1.512(4)
2(29)-2(30)	1.386(4)
2(30)-2(33)	1.511(4)
N(11)-N(12)	1.336(3)
N(21)-N(22)	1.358(3)
C(41)-C(42)	1.365(5)
C(41)-C(43)#1	1.378(5)
C(42)-C(43)	1.375(5)
C(43)-C(41)#1	1.378(5)
C(31)-C(32)	1.337(8)
C(31)-C(33)#2	1.368(8)
C(32)-C(33)	1.355(8)
C(33)-C(31)#2	1.368(8)

N(12)-C(1)-N(13)	118.9(2)
N(12)-C(1)-N(14)	134.6(2)
N(13)-C(1)-N(14)	106.5(2)
N(11)-C(11)-C(12)	120.8(2)

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N(11)-C(11)-C(113)	131.1(2)
C(12)-C(11)-C(113)	107.9(2)
C(13)-C(12)-C(17)	119.9(3)
C(13)-C(12)-C(11)	132.3(3)
C(17)-C(12)-C(11)	107.7(2)
C(14)-C(13)-C(12)	119.8(3)
F(1A)-C(14)-C(13)	117.3(6)
F(1A)-C(14)-C(15)	122.0(5)
C(13)-C(14)-C(15)	120.4(4)
C(16)-C(15)-C(14)	121.0(3)
C(17)-C(16)-C(15)	119.7(3)
C(16)-C(17)-C(12)	119.2(3)
C(16)-C(17)-C(18)	132.4(3)
C(12)-C(17)-C(18)	108.4(2)
C(19)-C(18)-C(113)	120.5(3)
C(19)-C(18)-C(17)	131.0(2)
C(113)-C(18)-C(17)	108.5(2)
C(110)-C(19)-C(18)	119.8(3)
C(19)-C(110)-C(111)	118.4(3)
F(1)-C(111)-C(112)	120.0(3)
F(1)-C(111)-C(110)	117.4(3)
C(112)-C(111)-C(110)	122.6(3)
C(111)-C(112)-C(113)	119.7(3)
C(112)-C(113)-C(18)	119.1(2)
C(112)-C(113)-C(11)	133.5(2)
C(18)-C(113)-C(11)	107.4(2)
C(115)-C(114)-N(13)	107.8(2)
C(114)-C(115)-N(14)	108.0(2)
1(17)-1(16)-1(21)	122.7(3)
1(17)-1(16)-N(13)	118.5(3)
1(21)-1(16)-N(13)	118.7(2)
1(16)-1(17)-1(18)	117.4(3)
1(16)-1(17)-1(22)	120.7(3)
1(18)-1(17)-1(22)	121.9(3)
1(19)-1(18)-1(17)	122.2(3)

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1(18)-1(19)-1(20)	118.6(3)
1(18)-1(19)-1(23)	121.2(4)
1(20)-1(19)-1(23)	120.2(4)
1(19)-1(20)-1(21)	121.8(3)
1(16)-1(21)-1(20)	117.4(3)
1(16)-1(21)-1(24)	121.4(3)
1(20)-1(21)-1(24)	121.2(3)
1(30)-1(25)-1(26)	122.3(3)
1(30)-1(25)-N(14)	118.0(2)
1(26)-1(25)-N(14)	119.6(2)
1(27)-1(26)-1(25)	117.6(2)
1(27)-1(26)-1(31)	121.4(2)
1(25)-1(26)-1(31)	121.0(3)
1(26)-1(27)-1(28)	122.3(3)
1(29)-1(28)-1(27)	117.7(3)
1(29)-1(28)-1(32)	121.0(3)
1(27)-1(28)-1(32)	121.4(3)
1(30)-1(29)-1(28)	122.5(2)
1(29)-1(30)-1(25)	117.5(2)
1(29)-1(30)-1(33)	121.1(2)
1(25)-1(30)-1(33)	121.4(2)
N(22)-C(2)-N(23)	133.1(2)
N(22)-C(2)-N(24)	120.6(2)
N(23)-C(2)-N(24)	106.26(19)
N(21)-C(21)-C(22)	120.7(2)
N(21)-C(21)-C(213)	132.2(2)
C(22)-C(21)-C(213)	107.1(2)
C(23)-C(22)-C(27)	120.1(2)
C(23)-C(22)-C(21)	131.4(2)
C(27)-C(22)-C(21)	108.5(2)
C(24)-C(23)-C(22)	118.1(3)
F(2)-C(24)-C(23)	119.2(3)
F(2)-C(24)-C(25)	117.9(3)
C(23)-C(24)-C(25)	122.8(3)
C(26)-C(25)-C(24)	119.2(3)

C(25)-C(26)-C(27)	119.6(3)
C(26)-C(27)-C(22)	120.1(3)
C(26)-C(27)-C(28)	132.1(2)
C(22)-C(27)-C(28)	107.8(2)
C(29)-C(28)-C(213)	119.9(3)
C(29)-C(28)-C(27)	130.6(2)
C(213)-C(28)-C(27)	109.4(2)
C(210)-C(29)-C(28)	119.3(3)
C(29)-C(210)-C(211)	120.4(3)
F(2A)-C(211)-C(212)	119.6(4)
F(2A)-C(211)-C(210)	118.8(4)
C(212)-C(211)-C(210)	121.3(3)
C(213)-C(212)-C(211)	118.7(3)
C(212)-C(213)-C(28)	120.3(2)
C(212)-C(213)-C(21)	132.6(2)
C(28)-C(213)-C(21)	107.1(2)
C(215)-C(214)-N(24)	107.9(2)
C(214)-C(215)-N(23)	108.3(2)
2(21)-2(16)-2(17)	121.6(2)
2(21)-2(16)-N(24)	118.5(2)
2(17)-2(16)-N(24)	119.8(2)
2(18)-2(17)-2(16)	118.0(2)
2(18)-2(17)-2(22)	120.7(2)
2(16)-2(17)-2(22)	121.3(2)
2(17)-2(18)-2(19)	122.3(3)
2(20)-2(19)-2(18)	117.9(3)
2(20)-2(19)-2(23)	121.3(3)
2(18)-2(19)-2(23)	120.8(3)
2(19)-2(20)-2(21)	122.2(3)
2(20)-2(21)-2(16)	118.0(2)
2(20)-2(21)-2(24)	120.5(2)
2(16)-2(21)-2(24)	121.5(2)
2(26)-2(25)-2(30)	122.8(2)
2(26)-2(25)-N(23)	118.3(2)
2(30)-2(25)-N(23)	119.0(2)

2(27)-2(26)-2(25)	117.4(3)
2(27)-2(26)-2(31)	121.5(3)
2(25)-2(26)-2(31)	121.0(3)
2(28)-2(27)-2(26)	122.0(3)
2(29)-2(28)-2(27)	118.5(3)
2(29)-2(28)-2(32)	120.5(3)
2(27)-2(28)-2(32)	121.0(3)
2(28)-2(29)-2(30)	122.1(3)
2(29)-2(30)-2(25)	117.3(2)
2(29)-2(30)-2(33)	122.1(3)
2(25)-2(30)-2(33)	120.5(2)
C(11)-N(11)-N(12)	114.0(2)
N(11)-N(12)-C(1)	111.5(2)
C(1)-N(13)-C(114)	109.2(2)
C(1)-N(13)-1(16)	122.2(2)
C(114)-N(13)-1(16)	128.3(2)
C(1)-N(14)-C(115)	108.5(2)
C(1)-N(14)-1(25)	125.4(2)
C(115)-N(14)-1(25)	124.8(2)
C(21)-N(21)-N(22)	115.6(2)
C(2)-N(22)-N(21)	111.40(19)
C(2)-N(23)-C(215)	108.5(2)
C(2)-N(23)-2(25)	127.56(19)
C(215)-N(23)-2(25)	123.3(2)
C(2)-N(24)-C(214)	109.0(2)
C(2)-N(24)-2(16)	125.94(19)
C(214)-N(24)-2(16)	125.0(2)
C(42)-C(41)-C(43)#1	120.0(3)
C(41)-C(42)-C(43)	120.2(3)
C(42)-C(43)-C(41)#1	119.8(3)
C(32)-C(31)-C(33)#2	120.4(5)
C(31)-C(32)-C(33)	120.1(5)
C(32)-C(33)-C(31)#2	119.4(5)

Symmetry transformations used to generate equivalent atoms:

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

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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)	29(1)	30(1)	55(2)	-7(1)	-10(1)	4(1)
C(11)	34(1)	31(1)	56(2)	-3(1)	-16(1)	8(1)
C(12)	45(2)	32(1)	53(2)	6(1)	-5(1)	7(1)
C(13)	64(2)	56(2)	53(2)	-7(1)	-20(2)	9(2)
C(14)	83(3)	71(2)	49(2)	0(2)	-6(2)	9(2)
C(15)	71(2)	68(2)	58(2)	5(2)	3(2)	1(2)
C(16)	51(2)	46(2)	68(2)	7(1)	1(2)	0(1)
C(17)	41(1)	31(1)	61(2)	3(1)	-8(1)	4(1)
C(18)	27(1)	24(1)	73(2)	2(1)	-4(1)	4(1)
C(19)	36(1)	34(1)	79(2)	-9(1)	3(1)	3(1)
C(110)	45(2)	39(2)	87(2)	-23(2)	-13(2)	5(1)
C(111)	51(2)	43(2)	59(2)	-18(1)	-9(1)	18(1)
C(112)	37(1)	32(1)	65(2)	-10(1)	-12(1)	6(1)
C(113)	34(1)	28(1)	54(2)	-3(1)	-5(1)	10(1)
C(114)	34(1)	39(1)	59(2)	3(1)	-7(1)	-7(1)
C(115)	35(1)	33(1)	64(2)	-2(1)	-10(1)	-9(1)
1(16)	35(1)	51(2)	47(2)	0(1)	-7(1)	-11(1)
1(17)	31(1)	69(2)	56(2)	9(2)	-4(1)	-3(1)
1(18)	43(2)	101(3)	57(2)	15(2)	-16(1)	-12(2)
1(19)	64(2)	100(3)	50(2)	0(2)	-13(2)	-29(2)
1(20)	65(2)	71(2)	59(2)	-12(2)	-7(2)	-23(2)
1(21)	45(2)	51(2)	56(2)	-4(1)	-7(1)	-14(1)
1(22)	42(2)	73(2)	76(2)	9(2)	-5(2)	16(2)
1(23)	102(3)	158(5)	67(3)	-6(3)	-35(2)	-46(3)
1(24)	72(2)	46(2)	82(2)	-14(2)	-22(2)	0(2)
1(25)	35(1)	32(1)	50(2)	-8(1)	-11(1)	-2(1)
1(26)	41(1)	35(1)	60(2)	-15(1)	-20(1)	3(1)
1(27)	50(2)	43(2)	57(2)	-23(1)	-15(1)	7(1)
1(28)	54(2)	40(1)	52(2)	-10(1)	-16(1)	-2(1)
1(29)	48(2)	31(1)	58(2)	-4(1)	-14(1)	3(1)

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1(30)	37(1)	32(1)	55(2)	-5(1)	-8(1)	0(1)
1(31)	66(2)	45(2)	68(2)	-15(1)	-24(2)	20(1)
1(32)	94(3)	59(2)	56(2)	-14(2)	-14(2)	6(2)
1(33)	59(2)	39(2)	60(2)	-1(1)	4(1)	12(1)
C(2)	33(1)	24(1)	39(1)	-2(1)	-7(1)	0(1)
C(21)	33(1)	25(1)	42(1)	-4(1)	-10(1)	-2(1)
C(22)	33(1)	26(1)	48(1)	-4(1)	-3(1)	-2(1)
C(23)	46(1)	31(1)	46(2)	-3(1)	-6(1)	-1(1)
C(24)	62(2)	39(1)	51(2)	-10(1)	3(1)	-4(1)
C(25)	46(2)	38(1)	71(2)	-15(1)	10(1)	2(1)
C(26)	33(1)	35(1)	78(2)	-12(1)	-5(1)	4(1)
C(27)	33(1)	27(1)	60(2)	-7(1)	-9(1)	-2(1)
C(28)	31(1)	25(1)	68(2)	-7(1)	-14(1)	2(1)
C(29)	45(2)	37(1)	82(2)	-13(1)	-28(2)	10(1)
C(210)	66(2)	50(2)	78(2)	-12(2)	-45(2)	11(2)
C(211)	71(2)	50(2)	64(2)	-19(2)	-31(2)	7(2)
C(212)	47(2)	38(1)	56(2)	-12(1)	-19(1)	6(1)
C(213)	35(1)	25(1)	51(2)	-7(1)	-15(1)	2(1)
C(214)	36(1)	33(1)	54(2)	-2(1)	-9(1)	11(1)
C(215)	38(1)	36(1)	55(2)	-1(1)	-15(1)	12(1)
2(16)	29(1)	34(1)	42(1)	-5(1)	-3(1)	10(1)
2(17)	32(1)	35(1)	51(2)	-3(1)	1(1)	7(1)
2(18)	39(1)	51(2)	47(2)	5(1)	1(1)	7(1)
2(19)	33(1)	72(2)	45(2)	-12(1)	-2(1)	8(1)
2(20)	36(1)	51(2)	59(2)	-23(1)	-6(1)	5(1)
2(21)	28(1)	36(1)	55(2)	-10(1)	-5(1)	8(1)
2(22)	55(2)	34(1)	63(2)	-6(1)	5(1)	-2(1)
2(23)	56(2)	112(3)	49(2)	-22(2)	1(2)	2(2)
2(24)	46(2)	33(1)	73(2)	-6(1)	-14(1)	3(1)
2(25)	38(1)	31(1)	42(1)	-2(1)	-15(1)	6(1)
2(26)	40(1)	32(1)	57(2)	-1(1)	-20(1)	6(1)
2(27)	64(2)	33(1)	64(2)	-7(1)	-33(2)	5(1)
2(28)	80(2)	44(2)	43(2)	-9(1)	-27(2)	17(2)
2(29)	56(2)	51(2)	39(2)	1(1)	-13(1)	8(1)
2(30)	43(1)	41(1)	39(1)	-1(1)	-14(1)	2(1)

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2(31)	45(2)	38(2)	82(2)	-1(1)	-12(2)	-3(1)
2(32)	149(4)	57(2)	53(2)	-15(2)	-24(2)	14(2)
2(33)	61(2)	61(2)	46(2)	-3(1)	-8(1)	-22(2)
N(11)	41(1)	36(1)	51(1)	-5(1)	-15(1)	5(1)
N(12)	33(1)	40(1)	52(1)	-3(1)	-3(1)	3(1)
N(13)	33(1)	38(1)	53(1)	-1(1)	-8(1)	-4(1)
N(14)	35(1)	29(1)	54(1)	-4(1)	-10(1)	-2(1)
N(21)	30(1)	28(1)	43(1)	-5(1)	-7(1)	1(1)
N(22)	31(1)	28(1)	45(1)	-7(1)	-6(1)	3(1)
N(23)	36(1)	30(1)	44(1)	-2(1)	-9(1)	6(1)
N(24)	32(1)	31(1)	43(1)	-4(1)	-5(1)	7(1)
C(41)	65(2)	48(2)	73(2)	-9(2)	3(2)	-2(2)
C(42)	88(2)	38(2)	52(2)	-6(1)	-2(2)	8(2)
C(43)	67(2)	52(2)	70(2)	-18(2)	-14(2)	12(2)
C(31)	109(4)	121(5)	186(6)	-75(4)	-54(4)	23(4)
C(32)	128(5)	125(5)	101(4)	-13(3)	-33(3)	48(4)
C(33)	137(5)	78(3)	175(6)	-18(4)	-39(4)	9(3)
F(1)	75(2)	65(1)	67(2)	-27(1)	-11(1)	0(1)
F(1A)	75(2)	65(1)	67(2)	-27(1)	-11(1)	0(1)
F(2)	88(2)	66(2)	44(1)	-16(1)	-8(1)	8(1)
F(2A)	88(2)	66(2)	44(1)	-16(1)	-8(1)	8(1)

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

	x	y	z	U(eq)
H(13A)	1281	13181	1084	68
H(15A)	4775	14603	455	83
H(16A)	4962	15276	1246	69
H(19A)	4727	15784	2249	61
H(11A)	4142	15956	3150	66
H(11B)	815	14128	3209	53
H(11C)	-3429	10518	3565	55
H(11D)	-3510	10439	2623	54
H(18A)	506	11097	4582	83
H(20A)	-1478	14107	4458	78
H(12A)	-740	10027	3512	100
H(12B)	-532	9457	4106	100
H(12C)	652	10078	3689	100
H(12D)	327	9681	4026	100
H(12E)	119	10251	3432	100
H(12F)	-1065	9630	3849	100
H(23A)	850	12432	5148	162
H(23B)	-410	13154	5320	162
H(23C)	733	13785	4884	162
H(12G)	-2853	14597	3817	97
H(12H)	-3544	13488	3669	97
H(12I)	-2357	14144	3265	97
H(12J)	-2983	13556	3350	97
H(12K)	-2292	14665	3499	97
H(12L)	-3479	14009	3902	97
H(27A)	-594	11359	740	57
H(29A)	-2650	14221	1014	55
H(13B)	-868	10027	2126	87
H(13C)	270	10204	1628	87

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H(13D)	-1050	9567	1587	87
H(13E)	-230	9838	1434	87
H(13F)	-1369	9661	1933	87
H(13G)	-49	10298	1974	87
H(32A)	-1739	14149	129	103
H(32B)	-1663	12840	-7	103
H(32C)	-386	13495	72	103
H(33A)	-3487	14537	1874	82
H(33B)	-2602	14039	2315	82
H(33C)	-3899	13350	2287	82
H(23D)	6260	7600	1326	50
H(25A)	9556	5750	1124	63
H(26A)	9873	5840	2001	59
H(29B)	9800	6244	3009	63
H(21A)	9273	6660	3871	73
H(21B)	5955	8191	3498	54
H(21C)	1706	11537	2812	50
H(21D)	1979	11211	1887	52
H(18B)	2731	8460	4621	58
H(20B)	3995	11827	4311	57
H(22D)	2219	7464	3960	78
H(22E)	3096	7838	3389	78
H(22F)	1652	8300	3487	78
H(23E)	3066	9339	5347	108
H(23F)	2749	10716	5272	108
H(23G)	4213	10298	5214	108
H(22A)	4358	12916	3450	76
H(22B)	3384	12604	3068	76
H(22C)	4831	12142	2995	76
H(22G)	4024	12192	2892	76
H(22H)	4998	12504	3274	76
H(22I)	3551	12966	3347	76
H(27B)	2827	7256	1105	62
H(29C)	5544	9746	481	59
H(31D)	1585	7223	1952	84

H(31E)	1304	8500	2110	84
H(31F)	2369	7685	2368	84
H(32D)	5300	8252	-7	127
H(32E)	3854	7762	59	127
H(32F)	4898	7003	358	127
H(23H)	5034	11294	1609	85
H(23I)	5263	11685	972	85
H(23J)	6281	10859	1257	85
H(23K)	6018	11264	950	85
H(23L)	5788	10874	1587	85
H(23M)	4771	11700	1301	85
H(41A)	-1850	8881	360	76
H(42A)	26	8491	725	73
H(43A)	1878	9616	371	74
H(31G)	3774	4036	4530	156
H(32G)	3723	6046	4434	141
H(33G)	4856	7018	4941	155
H(14)	2919	13614	375	250(100)
H(111)	2192	15117	3612	2000(500)
H(211)	7359	7577	4114	310(120)
H(24)	7750	6613	810	0(20)

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Table 1. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	C34 H30 Cl2 N4	
Formula weight	565.52	
Temperature	173(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	a = 10.5020(5) Å	α= 90°.
	b = 11.0120(5) Å	β= 90°.
	c = 25.2110(12) Å	γ = 90°.
Volume	2915.6(2) Å^3	
Z	4	
Density (calculated)	1.288 Mg/m^3	
Absorption coefficient	0.253 mm^{-1}	
F(000)	1184	
Crystal size	0.2 x 0.2 x 0.4 mm^3	
Theta range for data collection	2.02 to 20.00°.	
Index ranges	-10<=h<=10, -10<=k<=10, -24<=l<=24	
Reflections collected	11349	
Independent reflections	2700 [R(int) = 0.0456]	
Completeness to theta = 20.00°	99.8 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2700 / 2030 / 495	
Goodness-of-fit on F^2	1.067	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.0901	
R indices (all data)	R1 = 0.0540, wR2 = 0.0933	
Absolute structure parameter	0.24(12)	
Largest diff. peak and hole	0.111 and -0.144 e.Å^{-3}	

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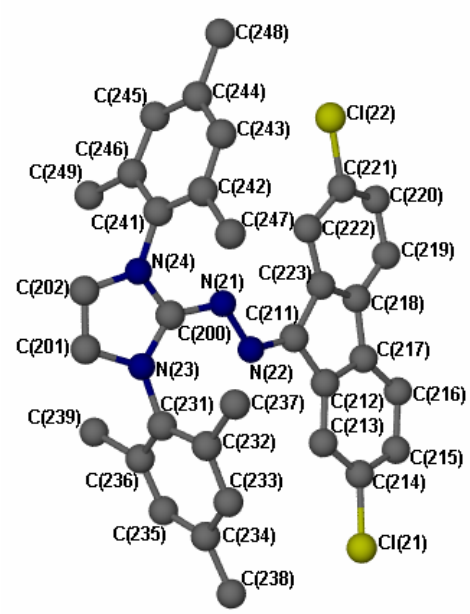
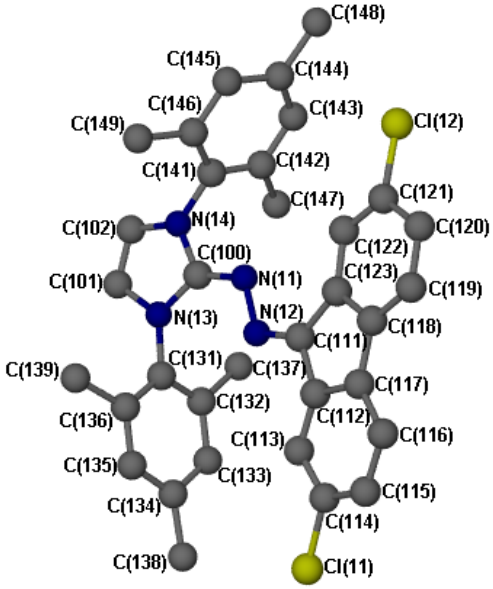


Ball and Stick Diagram of **4** (view 1)



Ball and Stick Digram of **4** (view 2)

These are the two components used to model the occupational disorder in the structure. The refined percentages of each component are listed below.

65% 35%

Please note that because of the poor quality of the data, in combination with twinning and occupational disorder, the structural parameters for 4 must be treated with caution, however the connectivity, arrangement and structure of the molecule is clearly determined. Hydrogen atoms have been removed for clarity.

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

	x	y	z	U(eq)
N(11)	12640(5)	10500(5)	3408(2)	29(1)
N(12)	12054(5)	10105(5)	2961(2)	28(1)
C(100)	13608(9)	11260(9)	3309(3)	27(2)
N(13)	14111(8)	11762(9)	2852(3)	33(2)
C(101)	15079(11)	12576(10)	3012(3)	33(2)
C(102)	15130(10)	12568(10)	3539(3)	31(2)
N(14)	14199(9)	11798(9)	3715(3)	33(2)
C(111)	11025(6)	9452(7)	3047(2)	26(1)

C(112)	10265(6)	9055(7)	2610(2)	27(1)
C(113)	10475(7)	9041(7)	2068(2)	35(2)
C(114)	9561(6)	8532(7)	1749(2)	34(1)
Cl(11)	9876(2)	8430(2)	1071(1)	61(1)
C(115)	8433(8)	8060(9)	1942(3)	46(2)
C(116)	8193(8)	8071(11)	2485(3)	38(2)
C(117)	9152(6)	8519(8)	2825(2)	30(1)
C(118)	9206(6)	8565(8)	3396(2)	26(1)
C(119)	8406(8)	8178(9)	3781(2)	33(2)
C(120)	8733(7)	8218(8)	4310(3)	35(2)
C(121)	9894(7)	8759(8)	4453(2)	44(2)
Cl(12)	10341(2)	8731(2)	5121(1)	68(1)
C(122)	10725(7)	9171(7)	4080(3)	36(2)
C(123)	10389(6)	9098(7)	3543(2)	26(1)
C(131)	13808(12)	11458(11)	2313(3)	31(2)
C(132)	14287(19)	10360(14)	2133(4)	39(2)
C(133)	13928(12)	10002(13)	1621(4)	41(2)
C(134)	13215(10)	10742(11)	1286(3)	41(2)
C(135)	12865(12)	11834(10)	1493(3)	40(2)
C(136)	13104(9)	12213(10)	1994(3)	30(2)
C(137)	15040(20)	9560(20)	2499(5)	44(3)
C(138)	12911(12)	10284(13)	749(3)	60(2)
C(139)	12700(20)	13479(14)	2179(5)	54(3)
C(141)	14013(16)	11400(12)	4249(3)	33(2)
C(142)	14460(20)	10274(15)	4417(4)	38(2)
C(143)	14240(20)	9912(15)	4927(4)	44(2)
C(144)	13500(20)	10586(16)	5268(5)	46(2)
C(145)	13096(14)	11752(12)	5112(3)	39(2)
C(146)	13300(20)	12153(15)	4587(4)	34(2)
C(147)	15335(10)	9526(11)	4070(4)	44(2)
C(148)	13200(30)	10161(19)	5829(5)	72(3)
C(149)	12826(13)	13365(11)	4427(3)	37(2)
N(21)	12691(10)	10509(11)	3033(4)	29(1)
N(22)	12066(9)	10118(11)	3476(4)	28(1)
C(200)	13580(20)	11380(20)	3112(5)	27(2)

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N(23)	14188(19)	11817(18)	3560(6)	33(2)
C(201)	15040(20)	12731(19)	3375(7)	33(2)
C(202)	15040(20)	12720(20)	2848(7)	31(2)
N(24)	14207(18)	11826(16)	2696(6)	33(2)
C(211)	11033(11)	9479(14)	3402(4)	26(1)
C(212)	10327(13)	9028(16)	3849(4)	26(1)
C(213)	10578(13)	9023(15)	4401(4)	36(2)
C(214)	9671(13)	8493(17)	4737(4)	44(2)
Cl(21)	10003(5)	8388(6)	5420(2)	68(1)
C(215)	8531(13)	7992(17)	4555(4)	35(2)
C(216)	8276(17)	7990(20)	4004(5)	33(2)
C(217)	9201(14)	8487(18)	3658(4)	26(1)
C(218)	9131(13)	8630(20)	3087(4)	30(1)
C(219)	8419(17)	8150(20)	2695(5)	38(2)
C(220)	8616(16)	8300(20)	2160(5)	46(2)
C(221)	9854(13)	8691(16)	2032(4)	34(1)
Cl(22)	10224(4)	8799(4)	1367(2)	61(1)
C(222)	10640(14)	9237(16)	2391(4)	35(2)
C(223)	10351(11)	9064(14)	2930(4)	27(1)
C(231)	13970(30)	11480(20)	4106(7)	33(2)
C(232)	14440(50)	10340(30)	4264(9)	38(2)
C(233)	14110(40)	10020(30)	4785(9)	44(2)
C(234)	13460(50)	10760(30)	5139(11)	46(2)
C(235)	13020(30)	11840(20)	4933(7)	39(2)
C(236)	13300(50)	12240(30)	4442(9)	34(2)
C(237)	15040(20)	9510(20)	3863(7)	44(2)
C(238)	13140(60)	10330(40)	5681(11)	72(3)
C(239)	12800(30)	13450(20)	4223(7)	37(2)
C(241)	14010(20)	11430(20)	2161(6)	31(2)
C(242)	14410(40)	10290(30)	1981(8)	39(2)
C(243)	14170(30)	9950(20)	1474(7)	41(2)
C(244)	13500(20)	10680(20)	1133(7)	41(2)
C(245)	13020(30)	11800(20)	1308(6)	40(2)
C(246)	13350(20)	12221(18)	1821(6)	30(2)
C(247)	15150(40)	9470(40)	2348(12)	44(3)

C(248)	13130(30)	10270(30)	572(6)	60(2)
C(249)	12830(50)	13400(30)	2023(12)	54(3)

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Table 3. Bond lengths [Å] and angles [°] for **4**.

N(11)-C(100)	1.340(6)
N(11)-N(12)	1.358(6)
N(12)-C(111)	1.316(6)
C(100)-N(14)	1.335(9)
C(100)-N(13)	1.384(8)
N(13)-C(101)	1.414(9)
N(13)-C(131)	1.434(10)
C(101)-C(102)	1.330(6)
C(102)-N(14)	1.368(9)
N(14)-C(141)	1.431(9)
C(111)-C(112)	1.429(7)
C(111)-C(123)	1.470(7)
C(112)-C(113)	1.386(7)
C(112)-C(117)	1.416(8)
C(113)-C(114)	1.371(7)
C(114)-C(115)	1.382(7)
C(114)-Cl(11)	1.745(6)
C(115)-C(116)	1.392(8)
C(116)-C(117)	1.412(7)
C(117)-C(118)	1.442(6)
C(118)-C(119)	1.352(7)
C(118)-C(123)	1.423(8)
C(119)-C(120)	1.378(8)
C(120)-C(121)	1.404(8)
C(121)-C(122)	1.360(8)
C(121)-Cl(12)	1.748(6)
C(122)-C(123)	1.401(8)
C(131)-C(136)	1.374(13)
C(131)-C(132)	1.387(13)
C(132)-C(133)	1.401(12)
C(132)-C(137)	1.504(14)
C(133)-C(134)	1.391(14)
C(134)-C(135)	1.361(11)

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C(134)-C(138)	1.479(10)
C(135)-C(136)	1.353(10)
C(136)-C(139)	1.530(13)
C(141)-C(142)	1.392(13)
C(141)-C(146)	1.403(13)
C(142)-C(143)	1.365(11)
C(142)-C(147)	1.514(14)
C(143)-C(144)	1.372(14)
C(144)-C(145)	1.409(12)
C(144)-C(148)	1.525(11)
C(145)-C(146)	1.414(10)
C(146)-C(149)	1.481(12)
N(21)-C(200)	1.347(10)
N(21)-N(22)	1.365(10)
N(22)-C(211)	1.306(10)
C(200)-N(24)	1.337(13)
C(200)-N(23)	1.387(13)
N(23)-C(201)	1.422(13)
N(23)-C(231)	1.444(14)
C(201)-C(202)	1.330(12)
C(202)-N(24)	1.370(14)
N(24)-C(241)	1.434(14)
C(211)-C(223)	1.461(10)
C(211)-C(212)	1.438(9)
C(212)-C(217)	1.409(12)
C(212)-C(213)	1.417(10)
C(213)-C(214)	1.403(10)
C(214)-C(215)	1.396(10)
C(214)-Cl(21)	1.759(10)
C(215)-C(216)	1.413(10)
C(216)-C(217)	1.416(10)
C(217)-C(218)	1.450(9)
C(218)-C(219)	1.351(12)
C(218)-C(223)	1.421(12)
C(219)-C(220)	1.374(13)

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C(220)-C(221)	1.407(13)
C(221)-C(222)	1.366(12)
C(221)-Cl(22)	1.724(10)
C(222)-C(223)	1.406(11)
C(231)-C(236)	1.384(18)
C(231)-C(232)	1.404(18)
C(232)-C(233)	1.409(16)
C(232)-C(237)	1.502(18)
C(233)-C(234)	1.384(19)
C(234)-C(235)	1.381(16)
C(234)-C(238)	1.485(15)
C(235)-C(236)	1.342(14)
C(236)-C(239)	1.537(17)
C(241)-C(242)	1.395(18)
C(241)-C(246)	1.404(18)
C(242)-C(243)	1.358(16)
C(242)-C(247)	1.511(19)
C(243)-C(244)	1.368(19)
C(244)-C(245)	1.408(17)
C(244)-C(248)	1.536(15)
C(245)-C(246)	1.419(14)
C(246)-C(249)	1.499(17)

C(100)-N(11)-N(12)	112.9(6)
C(111)-N(12)-N(11)	114.1(5)
N(14)-C(100)-N(11)	119.2(6)
N(14)-C(100)-N(13)	106.5(4)
N(11)-C(100)-N(13)	134.0(6)
C(100)-N(13)-C(101)	106.9(6)
C(100)-N(13)-C(131)	127.7(7)
C(101)-N(13)-C(131)	125.2(7)
C(102)-C(101)-N(13)	108.0(7)
C(101)-C(102)-N(14)	107.4(7)
C(100)-N(14)-C(102)	111.1(6)
C(100)-N(14)-C(141)	121.4(8)

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C(102)-N(14)-C(141)	126.4(8)
N(12)-C(111)-C(112)	119.8(5)
N(12)-C(111)-C(123)	131.3(5)
C(112)-C(111)-C(123)	108.7(4)
C(113)-C(112)-C(117)	120.3(6)
C(113)-C(112)-C(111)	132.5(6)
C(117)-C(112)-C(111)	107.1(5)
C(114)-C(113)-C(112)	118.1(6)
C(113)-C(114)-C(115)	123.3(6)
C(113)-C(114)-Cl(11)	117.8(5)
C(115)-C(114)-Cl(11)	118.8(5)
C(114)-C(115)-C(116)	119.8(6)
C(115)-C(116)-C(117)	118.1(7)
C(116)-C(117)-C(112)	120.1(5)
C(116)-C(117)-C(118)	130.3(6)
C(112)-C(117)-C(118)	109.6(6)
C(119)-C(118)-C(123)	119.0(5)
C(119)-C(118)-C(117)	132.9(6)
C(123)-C(118)-C(117)	108.0(5)
C(118)-C(119)-C(120)	122.0(6)
C(119)-C(120)-C(121)	118.6(5)
C(122)-C(121)-C(120)	121.4(6)
C(122)-C(121)-Cl(12)	119.9(5)
C(120)-C(121)-Cl(12)	118.2(5)
C(121)-C(122)-C(123)	119.2(6)
C(122)-C(123)-C(118)	119.7(6)
C(122)-C(123)-C(111)	133.8(5)
C(118)-C(123)-C(111)	106.5(5)
C(136)-C(131)-C(132)	122.0(8)
C(136)-C(131)-N(13)	122.3(9)
C(132)-C(131)-N(13)	115.7(9)
C(131)-C(132)-C(133)	116.7(10)
C(131)-C(132)-C(137)	120.2(9)
C(133)-C(132)-C(137)	122.8(10)
C(134)-C(133)-C(132)	122.6(9)

C(135)-C(134)-C(133)	115.5(8)
C(135)-C(134)-C(138)	126.4(10)
C(133)-C(134)-C(138)	118.1(9)
C(136)-C(135)-C(134)	125.4(9)
C(135)-C(136)-C(131)	117.4(8)
C(135)-C(136)-C(139)	121.0(9)
C(131)-C(136)-C(139)	121.3(9)
C(142)-C(141)-C(146)	121.4(8)
C(142)-C(141)-N(14)	120.9(9)
C(146)-C(141)-N(14)	117.6(9)
C(143)-C(142)-C(141)	119.3(10)
C(143)-C(142)-C(147)	119.3(9)
C(141)-C(142)-C(147)	120.9(9)
C(142)-C(143)-C(144)	121.8(9)
C(143)-C(144)-C(145)	119.3(8)
C(143)-C(144)-C(148)	122.3(10)
C(145)-C(144)-C(148)	118.2(10)
C(144)-C(145)-C(146)	119.9(9)
C(141)-C(146)-C(145)	117.7(8)
C(141)-C(146)-C(149)	123.2(7)
C(145)-C(146)-C(149)	119.0(8)
C(200)-N(21)-N(22)	115.8(11)
C(211)-N(22)-N(21)	116.9(9)
N(24)-C(200)-N(21)	119.3(11)
N(24)-C(200)-N(23)	106.2(9)
N(21)-C(200)-N(23)	133.5(11)
C(200)-N(23)-C(201)	105.8(9)
C(200)-N(23)-C(231)	127.9(15)
C(201)-N(23)-C(231)	126.3(15)
C(202)-C(201)-N(23)	108.7(11)
C(201)-C(202)-N(24)	106.6(11)
C(200)-N(24)-C(202)	111.2(11)
C(200)-N(24)-C(241)	123.6(13)
C(202)-N(24)-C(241)	125.2(13)
N(22)-C(211)-C(223)	133.8(9)

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N(22)-C(211)-C(212)	120.1(9)
C(223)-C(211)-C(212)	106.1(8)
C(217)-C(212)-C(213)	119.4(9)
C(217)-C(212)-C(211)	108.1(8)
C(213)-C(212)-C(211)	132.5(10)
C(214)-C(213)-C(212)	118.0(10)
C(215)-C(214)-C(213)	123.2(10)
C(215)-C(214)-Cl(21)	117.8(8)
C(213)-C(214)-Cl(21)	118.9(8)
C(214)-C(215)-C(216)	119.2(10)
C(217)-C(216)-C(215)	118.3(11)
C(216)-C(217)-C(212)	121.9(9)
C(216)-C(217)-C(218)	128.4(11)
C(212)-C(217)-C(218)	109.5(9)
C(219)-C(218)-C(223)	115.3(10)
C(219)-C(218)-C(217)	135.2(13)
C(223)-C(218)-C(217)	105.5(10)
C(218)-C(219)-C(220)	125.9(14)
C(219)-C(220)-C(221)	113.7(11)
C(222)-C(221)-C(220)	122.7(10)
C(222)-C(221)-Cl(22)	118.6(9)
C(220)-C(221)-Cl(22)	117.0(9)
C(221)-C(222)-C(223)	116.9(11)
C(222)-C(223)-C(218)	120.6(10)
C(222)-C(223)-C(211)	129.6(9)
C(218)-C(223)-C(211)	108.7(8)
C(236)-C(231)-C(232)	122.9(13)
C(236)-C(231)-N(23)	120.6(15)
C(232)-C(231)-N(23)	116.4(15)
C(231)-C(232)-C(233)	113.8(15)
C(231)-C(232)-C(237)	120.2(14)
C(233)-C(232)-C(237)	125.2(17)
C(234)-C(233)-C(232)	125.0(16)
C(235)-C(234)-C(233)	115.5(14)
C(235)-C(234)-C(238)	122.9(18)

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C(233)-C(234)-C(238)	121.2(18)
C(236)-C(235)-C(234)	123.6(16)
C(235)-C(236)-C(231)	118.8(15)
C(235)-C(236)-C(239)	122.6(15)
C(231)-C(236)-C(239)	118.4(13)
C(242)-C(241)-C(246)	120.5(12)
C(242)-C(241)-N(24)	122.4(15)
C(246)-C(241)-N(24)	117.1(15)
C(243)-C(242)-C(241)	120.1(15)
C(243)-C(242)-C(247)	120.4(17)
C(241)-C(242)-C(247)	119.5(17)
C(242)-C(243)-C(244)	121.4(16)
C(243)-C(244)-C(245)	120.3(14)
C(243)-C(244)-C(248)	122.6(15)
C(245)-C(244)-C(248)	116.7(15)
C(244)-C(245)-C(246)	118.8(15)
C(241)-C(246)-C(245)	118.3(14)
C(241)-C(246)-C(249)	120.7(15)
C(245)-C(246)-C(249)	120.2(16)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
N(11)	14(2)	22(2)	50(3)	-5(3)	-3(3)	-3(2)
N(12)	14(3)	25(2)	45(2)	-4(3)	-3(3)	-3(2)
C(100)	21(2)	16(3)	43(4)	9(4)	-6(4)	2(2)
N(13)	26(3)	26(3)	47(4)	1(3)	6(3)	-5(2)
C(101)	36(4)	15(4)	48(5)	13(5)	0(5)	-9(3)
C(102)	27(3)	18(4)	49(5)	18(4)	-14(4)	-7(3)
N(14)	32(3)	24(3)	42(4)	-3(3)	9(3)	-7(2)
C(111)	11(2)	14(2)	53(3)	-6(4)	6(3)	-2(2)
C(112)	18(2)	21(3)	43(3)	9(4)	-6(3)	5(2)
C(113)	44(4)	10(4)	50(3)	3(4)	6(3)	-14(3)
C(114)	39(4)	13(3)	51(3)	3(4)	-9(3)	-1(3)
Cl(11)	67(1)	61(1)	55(1)	-3(1)	-5(1)	-16(1)
C(115)	42(3)	31(5)	65(4)	-6(5)	-10(4)	-12(3)
C(116)	17(3)	34(4)	62(4)	10(5)	-12(4)	9(3)
C(117)	26(3)	15(3)	50(3)	1(4)	-1(3)	-4(2)
C(118)	15(2)	16(3)	48(4)	25(5)	-3(4)	1(2)
C(119)	25(3)	18(4)	57(4)	10(5)	6(4)	-12(3)
C(120)	30(3)	27(4)	47(4)	9(4)	23(3)	5(3)
C(121)	35(4)	45(5)	52(4)	2(4)	10(3)	-8(3)
Cl(12)	64(1)	90(2)	52(2)	-4(1)	7(1)	-9(1)
C(122)	21(3)	32(4)	55(3)	8(5)	-1(3)	7(3)
C(123)	16(3)	14(3)	48(3)	2(4)	-2(3)	-2(2)
C(131)	18(4)	27(3)	47(4)	-7(4)	14(4)	-2(3)
C(132)	25(5)	37(3)	57(6)	-9(4)	11(6)	4(2)
C(133)	38(6)	37(3)	46(6)	-15(4)	31(5)	-5(3)
C(134)	36(5)	58(4)	30(5)	-8(4)	33(4)	0(3)
C(135)	41(4)	43(3)	36(5)	5(4)	28(5)	0(3)
C(136)	24(4)	26(3)	40(5)	2(4)	27(4)	-5(3)
C(137)	30(4)	20(4)	82(8)	-12(7)	7(7)	1(3)
C(138)	63(6)	92(5)	26(5)	-7(5)	41(5)	0(4)

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C(139)	52(6)	35(4)	73(9)	-12(4)	13(7)	9(3)
C(141)	34(3)	23(3)	41(4)	4(3)	2(4)	-1(2)
C(142)	30(3)	17(3)	68(7)	12(5)	-10(8)	-6(3)
C(143)	33(5)	38(4)	60(6)	15(4)	-25(6)	5(3)
C(144)	41(3)	43(5)	53(6)	14(4)	-19(6)	-5(4)
C(145)	42(3)	46(4)	28(5)	-5(5)	-11(6)	8(3)
C(146)	39(3)	36(4)	27(6)	1(4)	-8(7)	-1(3)
C(147)	26(5)	34(4)	72(7)	6(5)	-21(4)	13(4)
C(148)	84(4)	76(7)	55(8)	22(5)	-11(9)	-13(5)
C(149)	54(3)	37(4)	21(7)	-2(5)	-5(6)	7(3)
N(21)	14(2)	22(2)	50(3)	-5(3)	-3(3)	-3(2)
N(22)	14(3)	25(2)	45(2)	-4(3)	-3(3)	-3(2)
C(200)	21(2)	16(3)	43(4)	9(4)	-6(4)	2(2)
N(23)	26(3)	26(3)	47(4)	1(3)	6(3)	-5(2)
C(201)	36(4)	15(4)	48(5)	13(5)	0(5)	-9(3)
C(202)	27(3)	18(4)	49(5)	18(4)	-14(4)	-7(3)
N(24)	32(3)	24(3)	42(4)	-3(3)	9(3)	-7(2)
C(211)	11(2)	14(2)	53(3)	-6(4)	6(3)	-2(2)
C(212)	16(3)	14(3)	48(3)	2(4)	-2(3)	-2(2)
C(213)	21(3)	32(4)	55(3)	8(5)	-1(3)	7(3)
C(214)	35(4)	45(5)	52(4)	2(4)	10(3)	-8(3)
Cl(21)	64(1)	90(2)	52(2)	-4(1)	7(1)	-9(1)
C(215)	30(3)	27(4)	47(4)	9(4)	23(3)	5(3)
C(216)	25(3)	18(4)	57(4)	10(5)	6(4)	-12(3)
C(217)	15(2)	16(3)	48(4)	25(5)	-3(4)	1(2)
C(218)	26(3)	15(3)	50(3)	1(4)	-1(3)	-4(2)
C(219)	17(3)	34(4)	62(4)	10(5)	-12(4)	9(3)
C(220)	42(3)	31(5)	65(4)	-6(5)	-10(4)	-12(3)
C(221)	39(4)	13(3)	51(3)	3(4)	-9(3)	-1(3)
Cl(22)	67(1)	61(1)	55(1)	-3(1)	-5(1)	-16(1)
C(222)	44(4)	10(4)	50(3)	3(4)	6(3)	-14(3)
C(223)	18(2)	21(3)	43(3)	9(4)	-6(3)	5(2)
C(231)	34(3)	23(3)	41(4)	4(3)	2(4)	-1(2)
C(232)	30(3)	17(3)	68(7)	12(5)	-10(8)	-6(3)
C(233)	33(5)	38(4)	60(6)	15(4)	-25(6)	5(3)

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C(234)	41(3)	43(5)	53(6)	14(4)	-19(6)	-5(4)
C(235)	42(3)	46(4)	28(5)	-5(5)	-11(6)	8(3)
C(236)	39(3)	36(4)	27(6)	1(4)	-8(7)	-1(3)
C(237)	26(5)	34(4)	72(7)	6(5)	-21(4)	13(4)
C(238)	84(4)	76(7)	55(8)	22(5)	-11(9)	-13(5)
C(239)	54(3)	37(4)	21(7)	-2(5)	-5(6)	7(3)
C(241)	18(4)	27(3)	47(4)	-7(4)	14(4)	-2(3)
C(242)	25(5)	37(3)	57(6)	-9(4)	11(6)	4(2)
C(243)	38(6)	37(3)	46(6)	-15(4)	31(5)	-5(3)
C(244)	36(5)	58(4)	30(5)	-8(4)	33(4)	0(3)
C(245)	41(4)	43(3)	36(5)	5(4)	28(5)	0(3)
C(246)	24(4)	26(3)	40(5)	2(4)	27(4)	-5(3)
C(247)	30(4)	20(4)	82(8)	-12(7)	7(7)	1(3)
C(248)	63(6)	92(5)	26(5)	-7(5)	41(5)	0(4)
C(249)	52(6)	35(4)	73(9)	-12(4)	13(7)	9(3)

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

	x	y	z	U(eq)
H(101)	15589	13037	2787	40
H(102)	15695	13005	3749	38
H(113)	11214	9368	1923	42
H(115)	7836	7735	1709	55
H(116)	7423	7791	2620	45
H(119)	7612	7875	3686	40
H(120)	8196	7893	4567	42
H(122)	11505	9497	4180	43
H(133)	14177	9241	1500	49
H(134)	12426	12364	1271	48
H(37A)	15334	8856	2308	66
H(37B)	14508	9299	2788	66
H(37C)	15756	9997	2635	66
H(38A)	12790	10958	513	90
H(38B)	12146	9808	763	90
H(38C)	13600	9789	624	90
H(39A)	12014	13766	1963	80
H(39B)	13412	14025	2149	80
H(39C)	12433	13441	2542	80
H(143)	14593	9189	5046	52
H(145)	12691	12256	5355	47
H(47A)	15879	10057	3870	66
H(47B)	14836	9043	3831	66
H(47C)	15846	9004	4288	66
H(48A)	12321	9909	5845	108
H(48B)	13333	10816	6073	108
H(48C)	13736	9490	5920	108
H(49A)	13533	13887	4348	56
H(49B)	12337	13709	4712	56

H(49C)	12298	13286	4118	56
H(201)	15514	13249	3588	40
H(202)	15505	13226	2626	38
H(21A)	11322	9361	4537	43
H(21B)	7948	7664	4792	42
H(21C)	7520	7671	3873	40
H(21D)	7733	7666	2796	45
H(22A)	7990	8157	1907	55
H(22B)	11333	9702	2285	42
H(233)	14331	9244	4901	52
H(235)	12509	12326	5146	47
H(37D)	15474	8861	4043	66
H(37E)	15632	9952	3649	66
H(37F)	14384	9170	3640	66
H(39D)	12239	10382	5734	108
H(38E)	13567	10833	5938	108
H(38F)	13414	9505	5723	108
H(39D)	12107	13729	4439	56
H(39E)	12510	13336	3865	56
H(39F)	13473	14038	4228	56
H(243)	14454	9194	1357	49
H(245)	12487	12257	1090	48
H(47D)	15471	8789	2153	66
H(47E)	14604	9192	2627	66
H(47F)	15852	9915	2499	66
H(48D)	12216	10217	548	90
H(48E)	13493	9488	500	90
H(48F)	13434	10849	318	90
H(49D)	13229	14062	1837	80
H(49E)	13005	13472	2395	80
H(49F)	11929	13427	1965	80

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

Identification code	**5**	
Empirical formula	C24 H28 N4	
Formula weight	372.50	
Temperature	173(2) K	
Wavelength	0.71069 Å	
Crystal system	Orthorhombic	
Space group	Pbca	
Unit cell dimensions	a = 11.0490(6) Å	α= 90°.
	b = 18.8681(10) Å	β= 90°.
	c = 19.8287(10) Å	γ = 90°.
Volume	4133.8(4) $Å^3$	
Z	8	
Density (calculated)	1.197 Mg/m^3	
Absorption coefficient	0.072 mm^{-1}	
F(000)	1600	
Crystal size	0.40 x 0.30 x 0.20 mm^3	
Theta range for data collection	2.05 to 27.54°.	
Index ranges	-13<=h<=14, -24<=k<=24, -25<=l<=25	
Reflections collected	38365	
Independent reflections	4770 [R(int) = 0.1136]	
Completeness to theta = 27.54°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	4770 / 0 / 269	
Goodness-of-fit on F^2	1.006	
Final R indices [I>2sigma(I)]	R1 = 0.0600, wR2 = 0.1244	
R indices (all data)	R1 = 0.1237, wR2 = 0.1495	
Largest diff. peak and hole	0.240 and -0.267 e.$Å^{-3}$	

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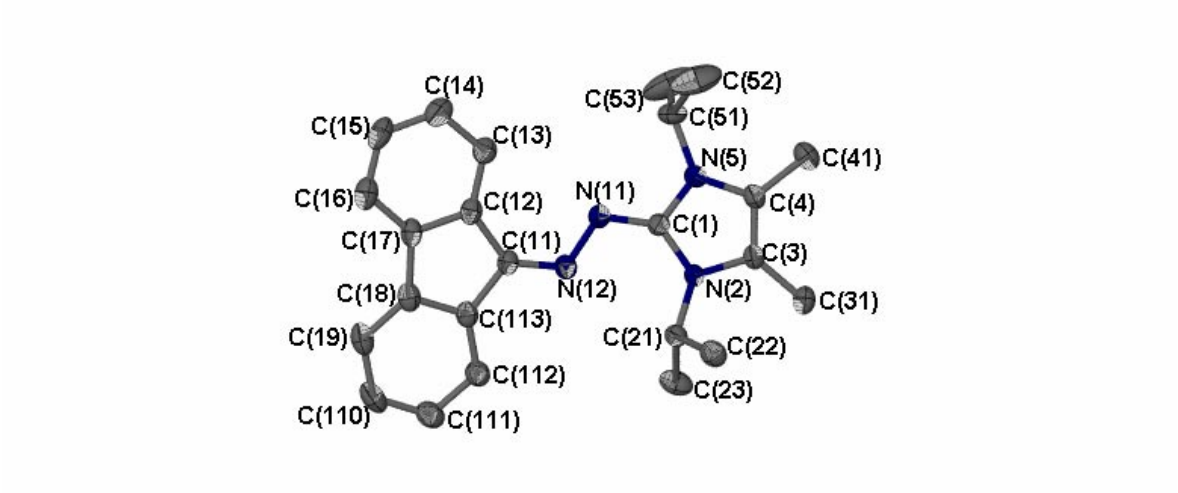

ORTEP Diagram of **5**
Hydrogen atoms are removed for clarity. Thermal ellipsoids are shown at 50% probability level.

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

	x	y	z	U(eq)
C(1)	10796(2)	1054(1)	914(1)	31(1)
C(3)	12241(2)	290(1)	579(1)	31(1)
C(4)	12649(2)	946(1)	460(1)	34(1)
C(11)	7843(2)	1281(1)	1426(1)	32(1)
C(12)	7613(2)	2005(1)	1667(1)	33(1)
C(13)	8315(2)	2618(1)	1664(1)	38(1)
C(14)	7825(2)	3241(1)	1920(1)	45(1)
C(15)	6657(2)	3257(1)	2172(1)	49(1)
C(16)	5946(2)	2656(1)	2174(1)	47(1)
C(17)	6419(2)	2030(1)	1924(1)	36(1)
C(18)	5871(2)	1326(1)	1848(1)	38(1)
C(19)	4741(2)	1066(2)	2032(1)	45(1)
C(21)	10436(2)	-222(1)	1243(1)	32(1)
C(22)	11224(2)	-541(1)	1790(1)	41(1)
C(23)	9907(2)	-765(1)	764(1)	48(1)
C(31)	12808(2)	-400(1)	383(1)	41(1)
C(41)	13826(2)	1164(1)	153(1)	47(1)
C(51)	11776(2)	2205(1)	661(1)	49(1)
C(52)	12662(4)	2502(2)	1142(2)	93(1)
C(53)	11688(4)	2509(2)	-17(2)	100(2)
C(110)	4463(2)	370(2)	1881(1)	49(1)
C(111)	5293(2)	-68(2)	1555(1)	46(1)
C(112)	6432(2)	181(1)	1388(1)	39(1)
C(113)	6725(2)	882(1)	1533(1)	33(1)
N(2)	11085(2)	349(1)	876(1)	29(1)
N(5)	11760(2)	1420(1)	672(1)	35(1)
N(11)	9806(2)	1399(1)	1128(1)	34(1)
N(12)	8814(2)	982(1)	1176(1)	33(1)

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

C(1)-N(11)	1.341(3)
C(1)-N(5)	1.359(3)
C(1)-N(2)	1.370(3)
C(3)-C(4)	1.338(3)
C(3)-N(2)	1.410(3)
C(3)-C(31)	1.497(3)
C(4)-N(5)	1.394(3)
C(4)-C(41)	1.494(3)
C(11)-N(12)	1.310(3)
C(11)-C(113)	1.461(3)
C(11)-C(12)	1.470(3)
C(12)-C(13)	1.392(3)
C(12)-C(17)	1.415(3)
C(13)-C(14)	1.391(3)
C(14)-C(15)	1.384(4)
C(15)-C(16)	1.380(4)
C(16)-C(17)	1.384(3)
C(17)-C(18)	1.467(3)
C(18)-C(19)	1.390(3)
C(18)-C(113)	1.408(3)
C(19)-C(110)	1.381(4)
C(21)-N(2)	1.485(3)
C(21)-C(23)	1.515(3)
C(21)-C(22)	1.516(3)
C(51)-C(53)	1.463(4)
C(51)-C(52)	1.477(4)
C(51)-N(5)	1.481(3)
C(110)-C(111)	1.393(4)
C(111)-C(112)	1.385(3)
C(112)-C(113)	1.393(3)
N(11)-N(12)	1.353(2)
N(11)-C(1)-N(5)	120.23(19)

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N(11)-C(1)-N(2)	132.8(2)
N(5)-C(1)-N(2)	106.95(18)
C(4)-C(3)-N(2)	107.85(18)
C(4)-C(3)-C(31)	128.12(19)
N(2)-C(3)-C(31)	123.78(19)
C(3)-C(4)-N(5)	107.63(18)
C(3)-C(4)-C(41)	128.4(2)
N(5)-C(4)-C(41)	124.0(2)
N(12)-C(11)-C(113)	121.71(19)
N(12)-C(11)-C(12)	131.7(2)
C(113)-C(11)-C(12)	106.52(18)
C(13)-C(12)-C(17)	119.6(2)
C(13)-C(12)-C(11)	132.3(2)
C(17)-C(12)-C(11)	108.0(2)
C(14)-C(13)-C(12)	118.9(2)
C(15)-C(14)-C(13)	120.9(3)
C(16)-C(15)-C(14)	121.0(2)
C(15)-C(16)-C(17)	119.0(2)
C(16)-C(17)-C(12)	120.6(2)
C(16)-C(17)-C(18)	130.8(2)
C(12)-C(17)-C(18)	108.51(19)
C(19)-C(18)-C(113)	120.5(2)
C(19)-C(18)-C(17)	131.6(2)
C(113)-C(18)-C(17)	107.91(19)
C(110)-C(19)-C(18)	118.7(2)
N(2)-C(21)-C(23)	111.67(19)
N(2)-C(21)-C(22)	111.20(17)
C(23)-C(21)-C(22)	113.67(19)
C(53)-C(51)-C(52)	119.3(3)
C(53)-C(51)-N(5)	113.8(2)
C(52)-C(51)-N(5)	112.2(2)
C(19)-C(110)-C(111)	121.2(2)
C(112)-C(111)-C(110)	120.5(3)
C(111)-C(112)-C(113)	119.0(2)
C(112)-C(113)-C(18)	120.1(2)

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C(112)-C(113)-C(11)	130.9(2)
C(18)-C(113)-C(11)	109.0(2)
C(1)-N(2)-C(3)	108.11(17)
C(1)-N(2)-C(21)	124.31(17)
C(3)-N(2)-C(21)	125.85(17)
C(1)-N(5)-C(4)	109.41(17)
C(1)-N(5)-C(51)	121.60(19)
C(4)-N(5)-C(51)	128.99(19)
C(1)-N(11)-N(12)	113.59(18)
C(11)-N(12)-N(11)	116.09(18)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **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}
C(1)	28(1)	29(1)	36(1)	-3(1)	-3(1)	0(1)
C(3)	26(1)	37(1)	30(1)	1(1)	0(1)	1(1)
C(4)	27(1)	40(1)	36(1)	2(1)	1(1)	-1(1)
C(11)	29(1)	36(1)	32(1)	0(1)	-2(1)	5(1)
C(12)	31(1)	39(1)	29(1)	-3(1)	-5(1)	6(1)
C(13)	35(1)	41(1)	38(1)	-3(1)	-6(1)	3(1)
C(14)	49(2)	42(1)	45(2)	-8(1)	-12(1)	6(1)
C(15)	49(2)	48(2)	52(2)	-15(1)	-9(1)	19(1)
C(16)	41(2)	58(2)	44(2)	-7(1)	0(1)	13(1)
C(17)	29(1)	46(1)	33(1)	-3(1)	-4(1)	7(1)
C(18)	32(1)	51(2)	30(1)	2(1)	-2(1)	5(1)
C(19)	30(1)	66(2)	39(1)	2(1)	1(1)	4(1)
C(21)	29(1)	31(1)	35(1)	4(1)	0(1)	-2(1)
C(22)	40(1)	47(1)	36(1)	7(1)	2(1)	-3(1)
C(23)	52(2)	51(2)	42(2)	3(1)	-8(1)	-19(1)
C(31)	34(1)	44(1)	44(1)	-3(1)	3(1)	7(1)
C(41)	37(1)	53(2)	53(2)	3(1)	9(1)	-5(1)
C(51)	47(2)	31(1)	67(2)	3(1)	-1(1)	-7(1)
C(52)	158(4)	43(2)	79(2)	-15(2)	-25(2)	-11(2)
C(53)	198(5)	40(2)	62(2)	7(2)	-24(3)	11(2)
C(110)	30(1)	70(2)	48(2)	13(1)	-2(1)	-9(1)
C(111)	37(1)	51(2)	49(2)	8(1)	-9(1)	-8(1)
C(112)	34(1)	42(1)	41(1)	2(1)	-3(1)	-1(1)
C(113)	29(1)	41(1)	30(1)	1(1)	-3(1)	3(1)
N(2)	24(1)	30(1)	34(1)	1(1)	2(1)	1(1)
N(5)	30(1)	31(1)	45(1)	0(1)	2(1)	-3(1)
N(11)	29(1)	33(1)	41(1)	-1(1)	0(1)	2(1)
N(12)	28(1)	36(1)	35(1)	-1(1)	-2(1)	0(1)

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

	x	y	z	U(eq)
H(13)	9110(20)	2610(1)	1491(5)	45
H(14)	8334(13)	3694(12)	1922(1)	54
H(15)	6337(9)	3694(12)	2349(5)	59
H(16)	5160(20)	2672(1)	2342(5)	57
H(19)	4172(16)	1360(8)	2256(6)	54
H(21)	9751(17)	4(6)	1471(6)	38
H(22A)	11914	-784	1584	62
H(22B)	10748	-882	2053	62
H(22C)	11518	-164	2088	62
H(23A)	9352	-530	450	73
H(23B)	9466	-1125	1021	73
H(23C)	10562	-991	509	73
H(31A)	13584	-310	159	61
H(31B)	12269	-654	73	61
H(31C)	12942	-688	787	61
H(41A)	14259	743	-7	71
H(41B)	14318	1409	491	71
H(41C)	13673	1483	-228	71
H(51)	10950(20)	2338(4)	877(6)	58
H(52A)	13482	2442	961	140
H(52B)	12596	2253	1574	140
H(52C)	12497	3007	1209	140
H(53A)	12413	2385	-276	150
H(53B)	11622	3025	16	150
H(53C)	10970	2319	-244	150
H(110)	3680(20)	184(5)	2003(4)	59
H(111)	5062(6)	-569(13)	1441(3)	55
H(112)	7021(15)	-130(8)	1171(6)	47

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Table 1. Crystal data and structure refinement for **6**

Identification code	**6**	
Empirical formula	C52 H56 N8	
Formula weight	793.05	
Temperature	173(2) K	
Wavelength	0.71069 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.4223(6) Å	α= 79.4400(10)°.
	b = 15.6479(10) Å	β= 82.2910(10)°.
	c = 16.0880(10) Å	γ = 74.5940(10)°.
Volume	2238.9(2) $Å^3$	
Z	2	
Density (calculated)	1.176 Mg/m^3	
Absorption coefficient	0.071 mm^{-1}	
F(000)	848	
Crystal size	0.40 x 0.40 x 0.30 mm^3	
Theta range for data collection	1.73 to 27.60°.	
Index ranges	-12<=h<=12, -20<=k<=20, -20<=l<=20	
Reflections collected	22193	
Independent reflections	10308 [R(int) = 0.0562]	
Completeness to theta = 27.60°	99.2 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	10308 / 0 / 541	
Goodness-of-fit on F^2	0.946	
Final R indices [I>2sigma(I)]	R1 = 0.0650, wR2 = 0.1357	
R indices (all data)	R1 = 0.1587, wR2 = 0.1699	
Largest diff. peak and hole	0.219 and -0.162 $e.Å^{-3}$	

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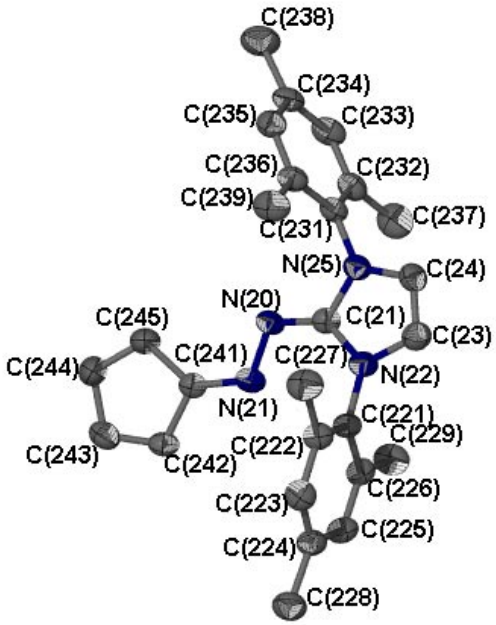

ORTEP Diagram of **6**
Hydrogen atoms have been removed for clarity. Thermal ellipsoids are shown at 50% probability level.

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

	x	y	z	U(eq)
C(11)	5989(3)	2087(2)	5656(2)	40(1)
C(13)	7234(3)	2061(2)	6755(2)	55(1)
C(14)	7891(3)	1329(2)	6414(2)	55(1)
C(21)	6743(3)	1944(2)	751(2)	40(1)
C(23)	4974(3)	1785(2)	1801(2)	51(1)
C(24)	6218(3)	1222(2)	2045(2)	51(1)
C(121)	5241(3)	3436(2)	6409(2)	39(1)
C(122)	3974(3)	3550(2)	6954(2)	42(1)
C(123)	3258(3)	4422(2)	7075(2)	43(1)
C(124)	3795(3)	5146(2)	6676(2)	44(1)
C(125)	5079(3)	4992(2)	6149(2)	45(1)
C(126)	5846(3)	4133(2)	6008(2)	43(1)
C(127)	3392(3)	2769(2)	7395(2)	62(1)
C(128)	2970(3)	6089(2)	6804(2)	57(1)
C(129)	7277(3)	3975(2)	5458(2)	59(1)
C(131)	7468(3)	669(2)	5181(2)	41(1)
C(132)	8317(3)	813(2)	4427(2)	44(1)
C(133)	8570(3)	179(2)	3885(2)	46(1)
C(134)	8019(3)	-573(2)	4095(2)	49(1)
C(135)	7203(3)	-697(2)	4861(2)	55(1)
C(136)	6899(3)	-74(2)	5421(2)	49(1)
C(137)	8973(3)	1606(2)	4200(2)	67(1)
C(138)	8278(4)	-1250(2)	3497(2)	72(1)
C(139)	6008(4)	-234(2)	6256(2)	70(1)
C(141)	2988(3)	3158(2)	4583(2)	44(1)
C(142)	1559(3)	3778(2)	4666(2)	57(1)
C(143)	973(4)	3951(2)	3928(2)	72(1)
C(144)	2008(4)	3456(2)	3335(2)	73(1)
C(145)	3213(3)	2979(2)	3719(2)	57(1)
C(221)	4237(3)	2999(2)	591(2)	40(1)

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C(222)	4184(3)	3838(2)	776(2)	45(1)
C(223)	3231(3)	4576(2)	357(2)	50(1)
C(224)	2341(3)	4488(2)	-220(2)	47(1)
C(225)	2392(3)	3638(2)	-360(2)	48(1)
C(226)	3336(3)	2879(2)	36(2)	42(1)
C(227)	5161(3)	3947(2)	1395(2)	63(1)
C(228)	1361(3)	5303(2)	-699(2)	62(1)
C(229)	3419(3)	1969(2)	-160(2)	59(1)
C(231)	8854(3)	847(2)	1408(2)	41(1)
C(232)	9304(3)	-19(2)	1213(2)	46(1)
C(233)	10785(3)	-447(2)	1221(2)	52(1)
C(234)	11804(3)	-46(2)	1416(2)	49(1)
C(235)	11307(3)	818(2)	1614(2)	49(1)
C(236)	9851(3)	1279(2)	1607(2)	44(1)
C(237)	8232(4)	-473(2)	975(2)	68(1)
C(238)	13431(3)	-504(2)	1377(2)	75(1)
C(239)	9348(3)	2229(2)	1781(2)	63(1)
C(241)	7542(3)	3130(2)	-1152(2)	38(1)
C(242)	6847(3)	3758(2)	-1847(2)	43(1)
C(243)	7872(3)	4099(2)	-2330(2)	55(1)
C(244)	9265(3)	3701(2)	-1979(2)	77(1)
C(245)	9076(3)	3125(2)	-1275(2)	65(1)
N(10)	5120(2)	2266(1)	5035(1)	42(1)
N(11)	3847(2)	2878(1)	5202(1)	42(1)
N(12)	6058(2)	2533(1)	6294(1)	43(1)
N(15)	7133(2)	1339(1)	5734(1)	46(1)
N(20)	7589(2)	2195(1)	80(1)	41(1)
N(21)	6784(2)	2736(1)	-538(1)	40(1)
N(22)	5272(2)	2237(1)	997(1)	43(1)
N(25)	7324(2)	1313(1)	1400(1)	43(1)

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Table 3. Bond lengths [Å] and angles [°] for **6**.

C(11)-N(10)	1.321(3)
C(11)-N(12)	1.360(3)
C(11)-N(15)	1.363(3)
C(13)-C(14)	1.327(3)
C(13)-N(12)	1.381(3)
C(14)-N(15)	1.380(3)
C(21)-N(20)	1.318(3)
C(21)-N(25)	1.361(3)
C(21)-N(22)	1.368(3)
C(23)-C(24)	1.324(4)
C(23)-N(22)	1.387(3)
C(24)-N(25)	1.385(3)
C(121)-C(122)	1.375(3)
C(121)-C(126)	1.380(3)
C(121)-N(12)	1.449(3)
C(122)-C(123)	1.389(3)
C(122)-C(127)	1.493(4)
C(123)-C(124)	1.379(4)
C(124)-C(125)	1.372(4)
C(124)-C(128)	1.511(3)
C(125)-C(126)	1.391(3)
C(126)-C(129)	1.499(3)
C(131)-C(132)	1.378(3)
C(131)-C(136)	1.378(4)
C(131)-N(15)	1.444(3)
C(132)-C(133)	1.392(3)
C(132)-C(137)	1.496(4)
C(133)-C(134)	1.379(4)
C(134)-C(135)	1.373(4)
C(134)-C(138)	1.510(4)
C(135)-C(136)	1.395(4)
C(136)-C(139)	1.504(4)
C(141)-N(11)	1.306(3)

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C(141)-C(142)	1.441(4)
C(141)-C(145)	1.445(4)
C(142)-C(143)	1.329(4)
C(143)-C(144)	1.443(4)
C(144)-C(145)	1.340(4)
C(221)-C(226)	1.379(3)
C(221)-C(222)	1.385(3)
C(221)-N(22)	1.438(3)
C(222)-C(223)	1.385(4)
C(222)-C(227)	1.504(4)
C(223)-C(224)	1.379(4)
C(224)-C(225)	1.376(4)
C(224)-C(228)	1.509(4)
C(225)-C(226)	1.386(4)
C(226)-C(229)	1.494(4)
C(231)-C(232)	1.390(3)
C(231)-C(236)	1.393(4)
C(231)-N(25)	1.433(3)
C(232)-C(233)	1.379(4)
C(232)-C(237)	1.502(4)
C(233)-C(234)	1.373(4)
C(234)-C(235)	1.389(4)
C(234)-C(238)	1.507(4)
C(235)-C(236)	1.370(3)
C(236)-C(239)	1.502(3)
C(241)-N(21)	1.299(3)
C(241)-C(245)	1.431(4)
C(241)-C(242)	1.448(3)
C(242)-C(243)	1.320(4)
C(243)-C(244)	1.437(4)
C(244)-C(245)	1.336(4)
N(10)-N(11)	1.351(3)
N(20)-N(21)	1.354(3)

N(10)-C(11)-N(12)	133.1(2)

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N(10)-C(11)-N(15)	121.4(2)
N(12)-C(11)-N(15)	105.5(2)
C(14)-C(13)-N(12)	108.0(2)
C(13)-C(14)-N(15)	107.4(2)
N(20)-C(21)-N(25)	121.1(2)
N(20)-C(21)-N(22)	132.6(2)
N(25)-C(21)-N(22)	106.1(2)
C(24)-C(23)-N(22)	108.3(2)
C(23)-C(24)-N(25)	107.7(2)
C(122)-C(121)-C(126)	123.4(2)
C(122)-C(121)-N(12)	118.9(2)
C(126)-C(121)-N(12)	117.5(2)
C(121)-C(122)-C(123)	117.1(2)
C(121)-C(122)-C(127)	121.4(2)
C(123)-C(122)-C(127)	121.5(2)
C(124)-C(123)-C(122)	121.9(2)
C(125)-C(124)-C(123)	118.6(2)
C(125)-C(124)-C(128)	120.8(3)
C(123)-C(124)-C(128)	120.6(3)
C(124)-C(125)-C(126)	122.0(3)
C(121)-C(126)-C(125)	116.9(2)
C(121)-C(126)-C(129)	121.8(2)
C(125)-C(126)-C(129)	121.2(3)
C(132)-C(131)-C(136)	123.0(2)
C(132)-C(131)-N(15)	118.2(2)
C(136)-C(131)-N(15)	118.7(2)
C(131)-C(132)-C(133)	117.4(3)
C(131)-C(132)-C(137)	121.8(2)
C(133)-C(132)-C(137)	120.8(3)
C(134)-C(133)-C(132)	121.7(3)
C(135)-C(134)-C(133)	118.8(2)
C(135)-C(134)-C(138)	119.8(3)
C(133)-C(134)-C(138)	121.4(3)
C(134)-C(135)-C(136)	121.7(3)
C(131)-C(136)-C(135)	117.4(3)

C(131)-C(136)-C(139)	122.4(2)
C(135)-C(136)-C(139)	120.2(3)
N(11)-C(141)-C(142)	122.6(3)
N(11)-C(141)-C(145)	130.9(3)
C(142)-C(141)-C(145)	106.4(2)
C(143)-C(142)-C(141)	108.5(3)
C(142)-C(143)-C(144)	108.4(3)
C(145)-C(144)-C(143)	109.6(3)
C(144)-C(145)-C(141)	107.1(3)
C(226)-C(221)-C(222)	122.1(2)
C(226)-C(221)-N(22)	119.8(2)
C(222)-C(221)-N(22)	118.1(2)
C(223)-C(222)-C(221)	118.0(2)
C(223)-C(222)-C(227)	121.0(3)
C(221)-C(222)-C(227)	121.0(2)
C(224)-C(223)-C(222)	121.7(3)
C(225)-C(224)-C(223)	118.2(3)
C(225)-C(224)-C(228)	120.9(3)
C(223)-C(224)-C(228)	120.9(3)
C(224)-C(225)-C(226)	122.4(3)
C(221)-C(226)-C(225)	117.5(2)
C(221)-C(226)-C(229)	121.3(2)
C(225)-C(226)-C(229)	121.1(2)
C(232)-C(231)-C(236)	121.9(2)
C(232)-C(231)-N(25)	119.2(2)
C(236)-C(231)-N(25)	118.9(2)
C(233)-C(232)-C(231)	117.8(3)
C(233)-C(232)-C(237)	120.5(3)
C(231)-C(232)-C(237)	121.7(3)
C(234)-C(233)-C(232)	122.3(3)
C(233)-C(234)-C(235)	118.1(3)
C(233)-C(234)-C(238)	121.6(3)
C(235)-C(234)-C(238)	120.2(3)
C(236)-C(235)-C(234)	122.2(3)
C(235)-C(236)-C(231)	117.8(2)

C(235)-C(236)-C(239)	121.4(3)
C(231)-C(236)-C(239)	120.8(2)
N(21)-C(241)-C(245)	131.4(2)
N(21)-C(241)-C(242)	122.0(2)
C(245)-C(241)-C(242)	106.4(2)
C(243)-C(242)-C(241)	108.1(2)
C(242)-C(243)-C(244)	108.5(3)
C(245)-C(244)-C(243)	109.7(3)
C(244)-C(245)-C(241)	107.2(3)
C(11)-N(10)-N(11)	111.6(2)
C(141)-N(11)-N(10)	115.4(2)
C(11)-N(12)-C(13)	109.4(2)
C(11)-N(12)-C(121)	127.2(2)
C(13)-N(12)-C(121)	122.5(2)
C(11)-N(15)-C(14)	109.7(2)
C(11)-N(15)-C(131)	124.0(2)
C(14)-N(15)-C(131)	126.2(2)
C(21)-N(20)-N(21)	111.9(2)
C(241)-N(21)-N(20)	114.8(2)
C(21)-N(22)-C(23)	108.6(2)
C(21)-N(22)-C(221)	127.0(2)
C(23)-N(22)-C(221)	123.4(2)
C(21)-N(25)-C(24)	109.3(2)
C(21)-N(25)-C(231)	124.3(2)
C(24)-N(25)-C(231)	126.4(2)

Symmetry transformations used to generate equivalent atoms:

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Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$)for **6**. 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(11)	45(2)	33(1)	42(2)	-10(1)	-5(1)	-4(1)
C(13)	60(2)	49(2)	55(2)	-21(2)	-23(2)	9(2)
C(14)	55(2)	46(2)	59(2)	-18(2)	-24(2)	12(1)
C(21)	42(2)	35(2)	42(2)	-13(1)	-6(1)	-4(1)
C(23)	45(2)	61(2)	45(2)	-9(2)	-1(1)	-9(2)
C(24)	52(2)	58(2)	41(2)	0(1)	-2(1)	-12(2)
C(121)	41(2)	34(2)	42(2)	-14(1)	-12(1)	-1(1)
C(122)	45(2)	38(2)	44(2)	-12(1)	-8(1)	-6(1)
C(123)	41(2)	40(2)	47(2)	-18(1)	-7(1)	-1(1)
C(124)	54(2)	32(2)	45(2)	-13(1)	-18(1)	-1(1)
C(125)	55(2)	36(2)	46(2)	-5(1)	-14(1)	-12(1)
C(126)	45(2)	46(2)	40(2)	-11(1)	-11(1)	-6(1)
C(127)	72(2)	47(2)	69(2)	-19(2)	9(2)	-17(2)
C(128)	76(2)	36(2)	58(2)	-18(1)	-19(2)	2(1)
C(129)	57(2)	66(2)	53(2)	-10(2)	-1(2)	-14(2)
C(131)	42(2)	34(2)	45(2)	-13(1)	-8(1)	2(1)
C(132)	45(2)	30(1)	49(2)	-5(1)	-7(1)	2(1)
C(133)	45(2)	45(2)	42(2)	-9(1)	-3(1)	2(1)
C(134)	47(2)	52(2)	52(2)	-22(1)	-5(1)	-9(1)
C(135)	64(2)	46(2)	59(2)	-17(2)	2(2)	-21(2)
C(136)	50(2)	48(2)	47(2)	-12(1)	-1(1)	-9(1)
C(137)	80(2)	40(2)	73(2)	-6(2)	3(2)	-9(2)
C(138)	80(2)	73(2)	76(2)	-42(2)	0(2)	-24(2)
C(139)	81(2)	76(2)	58(2)	-18(2)	13(2)	-31(2)
C(141)	45(2)	37(2)	52(2)	-8(1)	-10(1)	-8(1)
C(142)	45(2)	55(2)	72(2)	-16(2)	-12(2)	-4(2)
C(143)	56(2)	63(2)	97(3)	-5(2)	-33(2)	-9(2)
C(144)	82(3)	76(2)	65(2)	-5(2)	-34(2)	-17(2)
C(145)	65(2)	53(2)	54(2)	-11(2)	-16(2)	-11(2)
C(221)	38(2)	40(2)	41(2)	-11(1)	-5(1)	-3(1)

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C(222)	45(2)	46(2)	45(2)	-14(1)	-6(1)	-6(1)
C(223)	56(2)	43(2)	52(2)	-18(1)	-1(2)	-7(1)
C(224)	40(2)	46(2)	49(2)	-9(1)	-4(1)	-1(1)
C(225)	40(2)	56(2)	48(2)	-14(1)	-9(1)	-6(1)
C(226)	39(2)	46(2)	42(2)	-16(1)	0(1)	-5(1)
C(227)	70(2)	59(2)	69(2)	-19(2)	-21(2)	-16(2)
C(228)	56(2)	55(2)	65(2)	-5(2)	-8(2)	0(2)
C(229)	70(2)	54(2)	59(2)	-18(2)	-16(2)	-13(2)
C(231)	45(2)	39(2)	34(1)	-5(1)	-5(1)	-2(1)
C(232)	58(2)	40(2)	38(2)	-7(1)	-6(1)	-8(1)
C(233)	64(2)	37(2)	49(2)	-12(1)	-9(2)	3(2)
C(234)	48(2)	50(2)	40(2)	-3(1)	-7(1)	5(1)
C(235)	51(2)	50(2)	46(2)	-7(1)	-10(1)	-11(1)
C(236)	48(2)	39(2)	41(2)	-9(1)	-9(1)	-2(1)
C(237)	86(2)	58(2)	68(2)	-17(2)	-17(2)	-24(2)
C(238)	63(2)	69(2)	75(2)	-10(2)	-7(2)	13(2)
C(239)	71(2)	44(2)	75(2)	-18(2)	-20(2)	-7(2)
C(241)	42(2)	32(1)	40(2)	-11(1)	-6(1)	-5(1)
C(242)	45(2)	42(2)	41(2)	-10(1)	-13(1)	-4(1)
C(243)	63(2)	52(2)	48(2)	1(1)	-13(2)	-13(2)
C(244)	50(2)	87(3)	84(3)	25(2)	-12(2)	-24(2)
C(245)	46(2)	68(2)	72(2)	15(2)	-14(2)	-10(2)
N(10)	44(1)	35(1)	46(1)	-12(1)	-10(1)	-2(1)
N(11)	41(1)	34(1)	50(1)	-11(1)	-5(1)	-5(1)
N(12)	43(1)	39(1)	45(1)	-13(1)	-11(1)	3(1)
N(15)	48(1)	38(1)	49(1)	-17(1)	-11(1)	5(1)
N(20)	44(1)	36(1)	39(1)	-4(1)	-7(1)	-2(1)
N(21)	45(1)	35(1)	38(1)	-12(1)	-7(1)	0(1)
N(22)	43(1)	44(1)	38(1)	-9(1)	-6(1)	-3(1)
N(25)	43(1)	41(1)	42(1)	-4(1)	-5(1)	-5(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **6**.

	x	y	z	U(eq)
H(13)	7516	2227	7222	66
H(14)	8713	889	6599	66
H(23)	4057	1863	2114	61
H(24)	6330	835	2558	62
H(123)	2392	4521	7436	51
H(125)	5447	5478	5879	54
H(12A)	2502	2979	7745	93
H(12B)	4116	2367	7744	93
H(12C)	3182	2460	6981	93
H(12D)	4032	2225	7235	93
H(12E)	2417	2837	7236	93
H(12F)	3352	2744	7999	93
H(12G)	2104	6070	7190	85
H(12H)	2682	6435	6269	85
H(12I)	3598	6361	7035	85
H(12J)	3486	6508	6473	85
H(12K)	2908	6142	7394	85
H(12L)	1991	6216	6628	85
H(12M)	7512	4538	5236	89
H(12N)	7186	3687	4996	89
H(12O)	8050	3597	5788	89
H(12P)	7653	3343	5444	89
H(12Q)	7980	4195	5684	89
H(12R)	7115	4284	4892	89
H(133)	9125	265	3367	56
H(135)	6844	-1209	5011	65
H(13A)	9525	1589	3654	100
H(13B)	9618	1592	4619	100
H(13C)	8196	2148	4181	100

H(13D)	8701	1963	4649	100
H(13E)	8608	1961	3684	100
H(13F)	10030	1404	4122	100
H(13G)	8865	-1068	2993	108
H(13H)	7346	-1286	3346	108
H(13I)	8789	-1828	3770	108
H(13J)	7802	-1720	3746	108
H(13K)	9321	-1502	3394	108
H(13L)	7878	-960	2969	108
H(13M)	5712	-784	6300	106
H(13N)	5146	255	6291	106
H(13O)	6597	-276	6712	106
H(13P)	5925	247	6568	106
H(13Q)	6491	-792	6578	106
H(13R)	5040	-261	6156	106
H(142)	1121	4017	5154	69
H(143)	52	4327	3814	86
H(144)	1861	3466	2773	88
H(145)	4039	2603	3475	68
H(223)	3190	5145	468	60
H(225)	1771	3571	-733	57
H(22A)	4976	4571	1443	95
H(22B)	6178	3728	1197	95
H(22C)	4952	3614	1940	95
H(22D)	5762	3371	1610	95
H(22E)	4560	4214	1857	95
H(22F)	5786	4328	1113	95
H(22G)	827	5116	-1072	93
H(22H)	1957	5679	-1026	93
H(22I)	674	5632	-303	93
H(22J)	1479	5835	-529	93
H(22K)	348	5273	-575	93
H(22L)	1631	5319	-1297	93
H(22M)	2712	2017	-555	89
H(22N)	3203	1586	353	89

H(22O)	4395	1720	-405	89
H(22P)	4161	1531	150	89
H(22Q)	3670	1963	-758	89
H(22R)	2478	1828	1	89
H(233)	11105	-1026	1091	62
H(235)	11985	1092	1755	58
H(23A)	7256	-83	1002	102
H(23B)	8243	-1020	1363	102
H(23C)	8513	-608	408	102
H(23D)	8752	-1057	847	102
H(23E)	7765	-121	486	102
H(23F)	7495	-533	1441	102
H(23G)	13965	-122	1533	112
H(23H)	13776	-621	810	112
H(23I)	13588	-1059	1763	112
H(23J)	13588	-1080	1204	112
H(23K)	13777	-580	1927	112
H(23L)	13964	-142	974	112
H(23M)	8299	2438	1751	94
H(23N)	9839	2603	1366	94
H(23O)	9583	2253	2338	94
H(23P)	10182	2425	1885	94
H(23Q)	8641	2260	2271	94
H(23R)	8898	2610	1299	94
H(242)	5852	3897	-1938	51
H(243)	7719	4526	-2816	66
H(244)	10162	3826	-2208	92
H(245)	9806	2785	-930	78

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

Identification code	p212121	
Empirical formula	C16 H10 N2 S2	
Formula weight	294.38	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P2(1)2(1)2(1)	
Unit cell dimensions	a = 8.6383(4) Å	α= 90°.
	b = 10.1038(5) Å	β= 90°.
	c = 15.5131(7) Å	γ = 90°.
Volume	1353.98(11) $Å^3$	
Z	4	
Density (calculated)	1.444 Mg/m^3	
Absorption coefficient	0.382 mm^{-1}	
F(000)	608	
Crystal size	0.30 x 0.30 x 0.30 mm^3	
Theta range for data collection	2.41 to 27.55°.	
Index ranges	-11<=h<=11, -13<=k<=13, -20<=l<=20	
Reflections collected	12173	
Independent reflections	3112 [R(int) = 0.0835]	
Completeness to theta = 27.55°	99.9 %	
Absorption correction	None	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	3112 / 55 / 242	
Goodness-of-fit on F^2	1.211	
Final R indices [I>2sigma(I)]	R1 = 0.0482, wR2 = 0.0936	
R indices (all data)	R1 = 0.0538, wR2 = 0.0974	
Absolute structure parameter	0.00(11)	
Largest diff. peak and hole	0.275 and -0.270 $e.Å^{-3}$	

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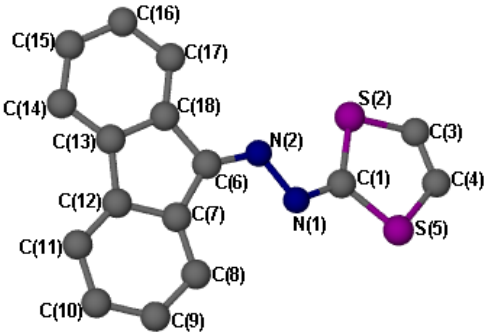
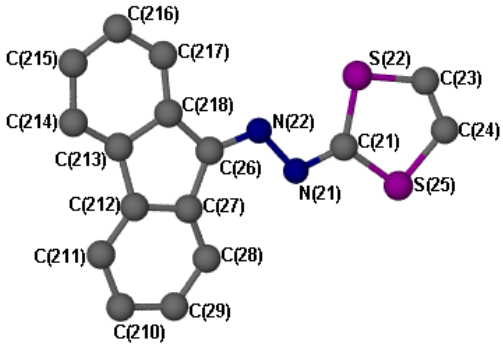


ORTEP Diagram of **7** (view 1)



ORTEP Diagram of **7** (view 2)

These are the two components used to model the occupational disorder in the structure. The refined percentages of each component are listed below.

(75%) (25%)

Hydrogen atoms are removed for clarity.

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

	x	y	z	U(eq)
C(1)	196(4)	8105(3)	8425(2)	19(1)
C(3)	2819(6)	7852(4)	9182(3)	27(1)
C(4)	3005(5)	7285(5)	8422(3)	24(1)
C(6)	-3272(6)	9573(8)	8709(5)	21(1)
C(7)	-4266(9)	9641(10)	7938(4)	21(1)
C(8)	-4097(5)	9116(6)	7117(3)	21(1)
C(9)	-5261(8)	9376(7)	6513(4)	29(1)
C(10)	-6526(13)	10175(17)	6701(7)	35(2)
C(11)	-6691(19)	10690(20)	7532(8)	28(1)
C(12)	-5548(6)	10459(5)	8132(5)	20(1)
C(13)	-5479(11)	10789(12)	9060(4)	20(1)
C(14)	-6441(14)	11558(14)	9567(6)	22(1)
C(15)	-6022(12)	11733(11)	10426(6)	27(1)
C(16)	-4712(10)	11187(7)	10780(4)	27(1)
C(17)	-3711(9)	10463(6)	10268(4)	25(1)
C(18)	-4101(9)	10262(10)	9408(4)	21(1)
N(1)	-1219(4)	8385(3)	8194(2)	26(1)
N(2)	-1936(4)	9041(3)	8876(2)	24(1)
S(2)	1028(1)	8554(1)	9408(1)	25(1)
S(5)	1409(1)	7218(1)	7740(1)	27(1)
C(21)	249(11)	8363(10)	8926(6)	19(1)
C(23)	2602(15)	7297(18)	8209(10)	27(1)
C(24)	3055(17)	7542(15)	8999(10)	24(1)
C(26)	-3380(20)	9420(30)	8527(15)	21(1)
C(27)	-4030(30)	10210(30)	9240(13)	21(1)
C(28)	-3680(30)	10260(20)	10100(13)	21(1)
C(29)	-4620(40)	10990(30)	10652(15)	29(1)
C(210)	-6010(40)	11590(40)	10400(20)	35(2)
C(211)	-6390(50)	11440(50)	9530(20)	28(1)
C(212)	-5420(30)	10810(30)	8958(13)	20(1)

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C(213)	-5740(20)	10280(20)	8100(14)	20(1)
C(214)	-6820(60)	10710(70)	7510(20)	22(1)
C(215)	-6710(40)	10240(50)	6670(18)	27(1)
C(216)	-5510(20)	9500(20)	6358(13)	27(1)
C(217)	-4410(20)	9160(20)	6948(12)	25(1)
C(218)	-4370(30)	9650(40)	7776(13)	21(1)
N(21)	-1105(11)	8900(10)	9123(6)	26(1)
N(22)	-2020(11)	8880(11)	8400(7)	24(1)
S(22)	750(4)	7733(3)	7916(2)	25(1)
S(25)	1666(4)	8209(3)	9707(2)	27(1)

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

C(1)-N(1)	1.306(4)
C(1)-S(5)	1.741(3)
C(1)-S(2)	1.745(3)
C(3)-C(4)	1.321(6)
C(3)-S(2)	1.738(5)
C(4)-S(5)	1.739(4)
C(6)-N(2)	1.299(5)
C(6)-C(18)	1.474(6)
C(6)-C(7)	1.475(6)
C(7)-C(8)	1.387(7)
C(7)-C(12)	1.415(7)
C(8)-C(9)	1.400(6)
C(9)-C(10)	1.390(10)
C(10)-C(11)	1.395(10)
C(11)-C(12)	1.376(9)
C(12)-C(13)	1.478(6)
C(13)-C(14)	1.383(8)
C(13)-C(18)	1.411(8)
C(14)-C(15)	1.393(9)
C(15)-C(16)	1.374(9)
C(16)-C(17)	1.383(7)
C(17)-C(18)	1.391(7)
N(1)-N(2)	1.394(4)
C(21)-N(21)	1.324(11)
C(21)-S(25)	1.730(9)
C(21)-S(22)	1.746(9)
C(23)-C(24)	1.310(14)
C(23)-S(22)	1.721(12)
C(24)-S(25)	1.760(12)
C(26)-N(22)	1.312(14)
C(26)-C(218)	1.461(17)
C(26)-C(27)	1.479(17)
C(27)-C(28)	1.370(18)

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C(27)-C(212)	1.413(19)
C(28)-C(29)	1.392(17)
C(29)-C(210)	1.40(2)
C(210)-C(211)	1.40(2)
C(211)-C(212)	1.38(2)
C(212)-C(213)	1.461(14)
C(213)-C(214)	1.38(2)
C(213)-C(218)	1.438(19)
C(214)-C(215)	1.39(2)
C(215)-C(216)	1.37(2)
C(216)-C(217)	1.365(15)
C(217)-C(218)	1.380(18)
N(21)-N(22)	1.372(11)

N(1)-C(1)-S(5)	120.5(3)
N(1)-C(1)-S(2)	124.7(3)
S(5)-C(1)-S(2)	114.8(2)
C(4)-C(3)-S(2)	117.7(4)
C(3)-C(4)-S(5)	117.6(4)
N(2)-C(6)-C(18)	118.7(5)
N(2)-C(6)-C(7)	134.3(5)
C(18)-C(6)-C(7)	107.0(4)
C(8)-C(7)-C(12)	120.1(5)
C(8)-C(7)-C(6)	131.8(5)
C(12)-C(7)-C(6)	108.0(5)
C(7)-C(8)-C(9)	117.9(5)
C(10)-C(9)-C(8)	122.2(6)
C(11)-C(10)-C(9)	119.4(7)
C(12)-C(11)-C(10)	119.3(9)
C(11)-C(12)-C(7)	121.0(7)
C(11)-C(12)-C(13)	130.5(8)
C(7)-C(12)-C(13)	107.9(6)
C(14)-C(13)-C(18)	120.1(7)
C(14)-C(13)-C(12)	131.0(7)
C(18)-C(13)-C(12)	108.8(6)

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C(13)-C(14)-C(15)	117.4(8)
C(16)-C(15)-C(14)	123.1(6)
C(15)-C(16)-C(17)	119.8(6)
C(16)-C(17)-C(18)	118.5(6)
C(17)-C(18)-C(13)	121.1(5)
C(17)-C(18)-C(6)	131.0(5)
C(13)-C(18)-C(6)	107.9(5)
C(1)-N(1)-N(2)	108.1(3)
C(6)-N(2)-N(1)	116.1(4)
C(3)-S(2)-C(1)	94.8(2)
C(4)-S(5)-C(1)	94.91(19)
N(21)-C(21)-S(25)	120.0(7)
N(21)-C(21)-S(22)	125.2(8)
S(25)-C(21)-S(22)	114.8(5)
C(24)-C(23)-S(22)	118.5(13)
C(23)-C(24)-S(25)	116.9(13)
N(22)-C(26)-C(218)	118.1(17)
N(22)-C(26)-C(27)	132.6(15)
C(218)-C(26)-C(27)	106.7(11)
C(28)-C(27)-C(212)	118.3(16)
C(28)-C(27)-C(26)	131.6(18)
C(212)-C(27)-C(26)	108.9(15)
C(27)-C(28)-C(29)	119.2(19)
C(28)-C(29)-C(210)	124(2)
C(211)-C(210)-C(29)	115(2)
C(212)-C(211)-C(210)	122(2)
C(211)-C(212)-C(27)	121.1(19)
C(211)-C(212)-C(213)	130(2)
C(27)-C(212)-C(213)	106.7(18)
C(214)-C(213)-C(218)	117.8(19)
C(214)-C(213)-C(212)	128(2)
C(218)-C(213)-C(212)	108.9(17)
C(213)-C(214)-C(215)	118(2)
C(216)-C(215)-C(214)	125(2)
C(215)-C(216)-C(217)	116(2)

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C(216)-C(217)-C(218)	123.3(18)
C(217)-C(218)-C(213)	117.6(16)
C(217)-C(218)-C(26)	134.3(17)
C(213)-C(218)-C(26)	105.9(14)
C(21)-N(21)-N(22)	108.3(8)
C(26)-N(22)-N(21)	113.0(11)
C(23)-S(22)-C(21)	95.0(6)
C(21)-S(25)-C(24)	94.6(7)

Symmetry transformations used to generate equivalent atoms:

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	22(2)	20(2)	15(2)	-3(1)	1(2)	5(1)
C(3)	20(2)	28(2)	32(2)	7(2)	-1(2)	0(2)
C(4)	12(2)	22(2)	37(3)	1(2)	1(2)	3(2)
C(6)	19(2)	16(3)	28(4)	-1(2)	-1(2)	-4(2)
C(7)	24(2)	18(2)	21(3)	7(2)	1(2)	-4(2)
C(8)	18(2)	20(2)	26(2)	1(2)	-3(2)	-2(2)
C(9)	41(3)	24(2)	20(3)	3(2)	-2(2)	-6(2)
C(10)	36(4)	32(3)	36(3)	2(2)	-11(3)	-10(3)
C(11)	26(4)	22(3)	36(3)	4(2)	-5(2)	-3(3)
C(12)	15(2)	14(2)	32(2)	0(2)	2(2)	-12(2)
C(13)	23(2)	22(2)	16(2)	4(2)	0(2)	1(2)
C(14)	21(2)	19(4)	27(2)	1(2)	4(2)	-1(2)
C(15)	26(2)	23(3)	32(2)	-3(2)	10(2)	-5(2)
C(16)	33(2)	27(3)	22(3)	-4(2)	0(2)	-9(2)
C(17)	23(2)	25(3)	27(3)	-5(2)	-6(2)	-2(2)
C(18)	18(2)	22(2)	24(3)	3(3)	0(2)	-3(2)
N(1)	21(2)	30(2)	25(2)	-4(1)	1(1)	6(1)
N(2)	20(1)	28(2)	24(2)	-1(2)	2(2)	3(1)
S(2)	20(1)	30(1)	26(1)	-2(1)	-2(1)	2(1)
S(5)	24(1)	30(1)	28(1)	-1(1)	3(1)	7(1)
C(21)	22(2)	20(2)	15(2)	-3(1)	1(2)	5(1)
C(23)	20(2)	28(2)	32(2)	7(2)	-1(2)	0(2)
C(24)	12(2)	22(2)	37(3)	1(2)	1(2)	3(2)
C(26)	19(2)	16(3)	28(4)	-1(2)	-1(2)	-4(2)
C(27)	24(2)	18(2)	21(3)	7(2)	1(2)	-4(2)
C(28)	18(2)	20(2)	26(2)	1(2)	-3(2)	-2(2)
C(29)	41(3)	24(2)	20(3)	3(2)	-2(2)	-6(2)
C(210)	36(4)	32(3)	36(3)	2(2)	-11(3)	-10(3)
C(211)	26(4)	22(3)	36(3)	4(2)	-5(2)	-3(3)
C(212)	15(2)	14(2)	32(2)	0(2)	2(2)	-12(2)

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C(213)	23(2)	22(2)	16(2)	4(2)	0(2)	1(2)
C(214)	21(2)	19(4)	27(2)	1(2)	4(2)	-1(2)
C(215)	26(2)	23(3)	32(2)	-3(2)	10(2)	-5(2)
C(216)	33(2)	27(3)	22(3)	-4(2)	0(2)	-9(2)
C(217)	23(2)	25(3)	27(3)	-5(2)	-6(2)	-2(2)
C(218)	18(2)	22(2)	24(3)	3(3)	0(2)	-3(2)
N(21)	21(2)	30(2)	25(2)	-4(1)	1(1)	6(1)
N(22)	20(1)	28(2)	24(2)	-1(2)	2(2)	3(1)
S(22)	20(1)	30(1)	26(1)	-2(1)	-2(1)	2(1)
S(25)	24(1)	30(1)	28(1)	-1(1)	3(1)	7(1)

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Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **7**.

	x	y	z	U(eq)
H(3)	3620	7875	9582	32
H(4)	3955	6934	8257	28
H(8)	-3238	8607	6973	26
H(9)	-5186	9002	5966	34
H(10)	-7255	10367	6279	42
H(11)	-7564	11176	7678	34
H(14)	-7333	11942	9343	27
H(15)	-6660	12244	10777	32
H(16)	-4498	11303	11363	32
H(17)	-2798	10119	10493	30
H(23)	3266	6896	7816	32
H(24)	4063	7372	9178	28
H(28)	-2817	9820	10313	26
H(29)	-4317	11078	11224	34
H(210)	-6634	12062	10782	42
H(211)	-7333	11774	9331	34
H(214)	-7601	11302	7667	27
H(215)	-7512	10446	6292	32
H(216)	-5449	9252	5783	32
H(217)	-3650	8556	6783	30

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Table 1. Crystal data and structure refinement for **10**.

Identification code	l03	
Empirical formula	C13 H8 N	
Formula weight	178.20	
Temperature	173(2) K	
Wavelength	0.71069 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 11.1600(4) Å	α= 90.000(5)°.
	b = 5.9650(2) Å	β= 121.071(2)°.
	c = 15.3604(2) Å	γ = 90.000(5)°.
Volume	875.83(4) $Å^3$	
Z	4	
Density (calculated)	1.351 Mg/m^3	
Absorption coefficient	0.080 mm^{-1}	
F(000)	372	
Crystal size	0.30 x 0.30 x 0.05 mm^3	
Theta range for data collection	2.13 to 28.25°.	
Index ranges	0<=h<=14, -7<=k<=0, -20<=l<=16	
Reflections collected	2115	
Independent reflections	2115 [R(int) = 0.0000]	
Completeness to theta = 28.25°	98.5 %	
Absorption correction	None	
Max. and min. transmission	0.9960 and 0.9765	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	2115 / 0 / 135	
Goodness-of-fit on F^2	1.087	
Final R indices [I>2sigma(I)]	R1 = 0.0726, wR2 = 0.2092	
R indices (all data)	R1 = 0.1073, wR2 = 0.2470	
Largest diff. peak and hole	0.554 and -0.671 $e.Å^{-3}$	

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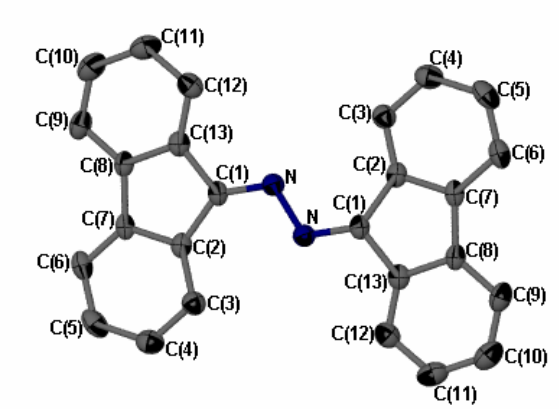

ORTEP Diagram of **10**

Hydrogen atoms are removed for clarity. Thermal ellipsoids are shown at 50% probability level.

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

	x	y	z	U(eq)
C(1)	425(3)	2810(4)	5804(2)	30(1)
C(2)	-831(3)	1530(4)	5616(2)	31(1)
C(3)	-2245(3)	1927(5)	4990(2)	37(1)
C(4)	-3188(3)	383(5)	4974(2)	43(1)
C(5)	-2731(3)	-1539(5)	5570(2)	46(1)
C(6)	-1308(3)	-1966(5)	6205(2)	39(1)
C(7)	-363(3)	-407(4)	6234(2)	30(1)
C(8)	1173(3)	-380(4)	6834(2)	31(1)
C(9)	2143(3)	-1855(5)	7548(2)	42(1)
C(10)	3551(4)	-1344(6)	8022(2)	51(1)
C(11)	4003(3)	611(6)	7798(2)	49(1)
C(12)	3054(3)	2103(5)	7084(2)	40(1)
C(13)	1642(3)	1593(4)	6602(2)	32(1)
N	623(2)	4569(4)	5391(2)	33(1)

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Table 3. Bond lengths [Å] and angles [°] for **10**.

C(1)-N	1.303(3)
C(1)-C(13)	1.468(4)
C(1)-C(2)	1.488(4)
C(2)-C(3)	1.380(4)
C(2)-C(7)	1.414(3)
C(3)-C(4)	1.389(4)
C(4)-C(5)	1.390(5)
C(5)-C(6)	1.392(5)
C(6)-C(7)	1.389(4)
C(7)-C(8)	1.468(4)
C(8)-C(9)	1.387(4)
C(8)-C(13)	1.407(4)
C(9)-C(10)	1.383(5)
C(10)-C(11)	1.383(5)
C(11)-C(12)	1.385(4)
C(12)-C(13)	1.385(4)
N-N#1	1.384(4)

N-C(1)-C(13)	119.2(2)
N-C(1)-C(2)	134.3(2)
C(13)-C(1)-C(2)	106.4(2)
C(3)-C(2)-C(7)	120.1(2)
C(3)-C(2)-C(1)	132.2(2)
C(7)-C(2)-C(1)	107.7(2)
C(2)-C(3)-C(4)	118.8(3)
C(3)-C(4)-C(5)	121.2(3)
C(4)-C(5)-C(6)	120.7(3)
C(7)-C(6)-C(5)	118.2(3)
C(6)-C(7)-C(2)	120.9(3)
C(6)-C(7)-C(8)	130.4(2)
C(2)-C(7)-C(8)	108.6(2)
C(9)-C(8)-C(13)	119.4(3)
C(9)-C(8)-C(7)	132.1(2)

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C(13)-C(8)-C(7)	108.5(2)
C(10)-C(9)-C(8)	119.2(3)
C(9)-C(10)-C(11)	121.1(3)
C(10)-C(11)-C(12)	120.7(3)
C(11)-C(12)-C(13)	118.5(3)
C(12)-C(13)-C(8)	121.2(3)
C(12)-C(13)-C(1)	130.2(3)
C(8)-C(13)-C(1)	108.6(2)
C(1)-N-N#1	112.0(3)

Symmetry transformations used to generate equivalent atoms:

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

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	41(1)	24(1)	31(1)	-1(1)	22(1)	0(1)
C(2)	42(1)	26(1)	28(1)	-2(1)	20(1)	1(1)
C(3)	38(1)	35(2)	36(1)	-3(1)	19(1)	-4(1)
C(4)	39(2)	50(2)	40(2)	-9(1)	20(1)	-5(1)
C(5)	55(2)	40(2)	55(2)	-15(1)	37(2)	-18(1)
C(6)	57(2)	30(1)	42(1)	-3(1)	33(1)	-7(1)
C(7)	47(2)	23(1)	31(1)	-2(1)	26(1)	0(1)
C(8)	44(1)	26(1)	29(1)	0(1)	23(1)	2(1)
C(9)	57(2)	32(1)	38(1)	5(1)	26(1)	10(1)
C(10)	54(2)	51(2)	45(2)	4(1)	22(2)	17(2)
C(11)	38(2)	55(2)	48(2)	-4(1)	18(1)	10(1)
C(12)	43(2)	36(2)	46(2)	-7(1)	26(1)	-5(1)
C(13)	43(2)	27(1)	32(1)	-3(1)	23(1)	1(1)
N	32(1)	29(1)	34(1)	-2(1)	16(1)	-1(1)

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

	x	y	z	U(eq)
H(3)	-2585(12)	3300(50)	4555(15)	44
H(4)	-4210(40)	659(11)	4527(16)	52
H(5)	-3390(30)	-2560(40)	5544(3)	55
H(6)	-1009(12)	-3220(50)	6585(15)	47
H(9)	1816(12)	-3320(50)	7725(6)	50
H(10)	4280(30)	-2440(40)	8550(20)	62
H(11)	4970(40)	933(15)	8137(14)	59
H(12)	3360(12)	3430(50)	6931(6)	48

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Atomic Coordinates for **1 (Optimized Geometry with constraints on heavy atoms)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	2.368957	-1.674860	-0.046781
2	7	0	0.318144	-2.409784	0.077128
3	7	0	0.715206	-0.000594	-0.198569
4	7	0	-0.600541	0.087208	-0.563970
5	6	0	2.426974	-3.055310	0.140827
6	6	0	1.175165	-3.501950	0.216026
7	6	0	1.063278	-1.273628	-0.085966
8	6	0	3.489829	-0.781746	-0.183325
9	6	0	3.878324	-0.379920	-1.449958
10	6	0	4.950771	0.494543	-1.546591
11	6	0	5.620453	0.962169	-0.428836
12	6	0	5.198405	0.525882	0.815548
13	6	0	4.125485	-0.332776	0.969669
14	6	0	3.163009	-0.867980	-2.680098
15	6	0	6.776406	1.930171	-0.561723
16	6	0	3.648495	-0.776515	2.333873
17	6	0	-1.098353	-2.464711	0.346229
18	6	0	-1.556155	-2.021439	1.580092
19	6	0	-2.920873	-2.081452	1.824386
20	6	0	-3.811874	-2.565838	0.877581
21	6	0	-3.306675	-3.004629	-0.342910
22	6	0	-1.952196	-2.953184	-0.636571
23	6	0	-0.608679	-1.432047	2.594761
24	6	0	-5.296083	-2.573244	1.146622
25	6	0	-1.435031	-3.295322	-2.004496
26	6	0	-1.175807	1.247975	-0.408222
27	6	0	-2.576240	1.441829	-0.809096
28	6	0	-3.481192	0.575868	-1.403292
29	6	0	-4.759282	1.015653	-1.665596
30	6	0	-5.141943	2.307369	-1.335093
31	6	0	-4.256848	3.179098	-0.723655
32	6	0	-2.959800	2.750472	-0.467226
33	6	0	-1.811488	3.423963	0.152246
34	6	0	-1.687164	4.697851	0.684892
35	6	0	-0.477805	5.073534	1.237859
36	6	0	0.591609	4.187449	1.272161
37	6	0	0.480966	2.907684	0.747580
38	6	0	-0.726895	2.517152	0.180691
39	1	0	3.372158	-3.572706	0.186102
40	1	0	0.783359	-4.495866	0.364202
41	1	0	5.271707	0.818972	-2.534753
42	1	0	5.715781	0.880105	1.705648
43	1	0	3.678456	-0.538585	-3.586980
44	1	0	2.138364	-0.478545	-2.711536
45	1	0	3.095204	-1.961725	-2.706500

46	1	0	7.461694	1.855341	0.288900
47	1	0	6.419221	2.967612	-0.603706
48	1	0	7.348752	1.747427	-1.477405
49	1	0	4.244652	-0.308578	3.123020
50	1	0	3.717005	-1.863076	2.461801
51	1	0	2.600270	-0.498455	2.491514
52	1	0	-3.298608	-1.727123	2.781327
53	1	0	-3.994452	-3.376345	-1.100447
54	1	0	0.262064	-2.076019	2.764432
55	1	0	-1.111980	-1.285684	3.555204
56	1	0	-0.234278	-0.457660	2.258172
57	1	0	-5.510894	-2.629510	2.218894
58	1	0	-5.792121	-3.418010	0.656079
59	1	0	-5.764212	-1.654994	0.767561
60	1	0	-2.239934	-3.666337	-2.646324
61	1	0	-0.646139	-4.056360	-1.983366
62	1	0	-1.006022	-2.401882	-2.475145
63	1	0	-3.174155	-0.434472	-1.653604
64	1	0	-5.474669	0.347983	-2.140565
65	1	0	-6.155743	2.638762	-1.548681
66	1	0	-4.573121	4.186731	-0.462621
67	1	0	-2.524783	5.391476	0.665715
68	1	0	-0.362927	6.070739	1.656686
69	1	0	1.533785	4.502913	1.714480
70	1	0	1.316496	2.218234	0.766916

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Atomic Coordinates for **2 (Optimized Geometry with constraints on heavy atoms)**

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.709613	-2.121724	-0.006259
2	6	0	-1.528271	-4.194747	-0.013545
3	6	0	-0.203254	-4.298186	0.115068
4	6	0	0.542104	1.036875	-0.128918
5	6	0	-0.483514	2.121728	0.043818
6	6	0	-1.834794	2.064530	0.209343
7	6	0	-2.526156	3.268489	0.327041
8	6	0	-1.891033	4.512804	0.264690
9	6	0	-0.519650	4.544885	0.072339
10	6	0	0.208177	3.357465	-0.050239
11	6	0	1.618498	3.100747	-0.249175
12	6	0	2.701940	3.934738	-0.421083
13	6	0	-3.166902	-2.288784	-0.305767
14	6	0	-3.772389	-1.578920	0.733519
15	6	0	-5.050596	-1.048103	0.444275
16	6	0	-5.688758	-1.251774	-0.752306
17	6	0	-5.031994	-1.971764	-1.718345
18	6	0	-3.764297	-2.490576	-1.503879
19	6	0	1.687558	-2.731605	0.488137
20	6	0	1.964320	-2.389041	1.811371
21	6	0	3.265410	-2.130567	2.157810
22	6	0	4.313824	-2.228240	1.241769
23	6	0	3.990430	-2.561607	-0.061979
24	6	0	2.682639	-2.835337	-0.466158
25	6	0	3.971991	3.378927	-0.612649
26	6	0	4.130612	2.018261	-0.615723
27	6	0	3.107740	1.157020	-0.445336
28	6	0	1.819966	1.681353	-0.286505
29	6	0	-3.128348	-1.383869	2.075058
30	6	0	-7.079378	-0.704966	-0.977205
31	6	0	-3.055368	-3.245896	-2.612021
32	6	0	0.830647	-2.228625	2.812782
33	6	0	5.736862	-1.930068	1.653639
34	6	0	2.379481	-3.173356	-1.880322
35	7	0	-0.766212	-0.753841	-0.041015
36	7	0	0.462020	-0.291258	-0.168793
37	7	0	-1.849706	-2.827531	-0.063689
38	7	0	0.321403	-2.993644	0.122298
39	35	0	-4.408757	3.210785	0.577578
40	35	0	5.880581	1.292025	-0.870008
41	1	0	-2.299194	-4.947557	-0.050019
42	1	0	0.443592	-5.154172	0.221085
43	1	0	-2.359391	1.119897	0.240828
44	1	0	-2.466164	5.426684	0.362088
45	1	0	-0.013774	5.506445	0.013578

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46	1	0	2.592169	5.016640	-0.413209
47	1	0	-5.546205	-0.472093	1.223831
48	1	0	-5.506600	-2.140044	-2.682664
49	1	0	3.489353	-1.852626	3.186030
50	1	0	4.783035	-2.627286	-0.805277
51	1	0	4.829346	4.028512	-0.753145
52	1	0	3.257859	0.083870	-0.452263
53	1	0	-2.755450	-2.330198	2.484268
54	1	0	-3.843085	-0.964007	2.788661
55	1	0	-2.274697	-0.701534	2.000099
56	1	0	-7.437728	-0.920941	-1.988417
57	1	0	-7.101510	0.382347	-0.836583
58	1	0	-7.795143	-1.138046	-0.267850
59	1	0	-3.583225	-3.114026	-3.560952
60	1	0	-3.002128	-4.323521	-2.415878
61	1	0	-2.028235	-2.890995	-2.746841
62	1	0	0.158909	-3.094426	2.813948
63	1	0	0.229322	-1.342814	2.577915
64	1	0	1.226518	-2.106805	3.825272
65	1	0	5.822661	-1.811082	2.737877
66	1	0	6.081791	-1.001781	1.180844
67	1	0	6.421139	-2.728730	1.343565
68	1	0	3.293237	-3.217306	-2.480059
69	1	0	1.720203	-2.419734	-2.330318
70	1	0	1.869697	-4.139531	-1.982434

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Atomic Coordinates for **3**(Optimized geometry with constraints on heavy atoms)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.247436	-0.592010	0.133922
2	6	0	0.321165	-2.750046	0.294743
3	6	0	-1.003415	-2.701351	0.230405
4	6	0	2.205598	-1.150455	0.073212
5	6	0	2.970697	-0.920168	1.192226
6	6	0	4.326012	-0.689464	0.995440
7	6	0	4.892288	-0.702815	-0.262254
8	6	0	4.086464	-0.961567	-1.342676
9	6	0	2.724656	-1.206652	-1.204466
10	6	0	2.368677	-0.914674	2.558536
11	6	0	6.364561	-0.415404	-0.445385
12	6	0	1.870152	-1.539268	-2.390640
13	6	0	-2.709708	-0.859555	0.035176
14	6	0	-3.219987	-0.590397	-1.216022
15	6	0	-4.495160	-0.037259	-1.281611
16	6	0	-5.236197	0.212837	-0.145676
17	6	0	-4.695969	-0.097141	1.077941
18	6	0	-3.413645	-0.633404	1.197820
19	6	0	-2.454510	-0.900408	-2.463450
20	6	0	-6.610772	0.833507	-0.224281
21	6	0	-2.857576	-0.966577	2.554438
22	6	0	0.870307	2.612647	0.185050
23	6	0	1.985904	3.423843	0.602781
24	6	0	1.766167	4.675439	0.213008
25	6	0	0.504261	4.719633	-0.484735
26	6	0	-0.041088	3.496010	-0.505290
27	7	0	-0.324754	0.720076	0.005283
28	7	0	0.814719	1.326235	0.402915
29	7	0	0.798442	-1.455019	0.238441
30	7	0	-1.363840	-1.373480	0.128177
31	1	0	0.997183	-3.586254	0.381600
32	1	0	-1.745432	-3.483986	0.249011
33	1	0	4.954498	-0.500802	1.863895
34	1	0	4.521627	-0.993087	-2.340064
35	1	0	1.800244	-1.829040	2.765129
36	1	0	1.675202	-0.070227	2.657911
37	1	0	3.139972	-0.816022	3.328435
38	1	0	6.756471	-0.885741	-1.353351
39	1	0	6.953240	-0.776104	0.405015
40	1	0	6.547768	0.663686	-0.532278
41	1	0	1.368220	-2.507430	-2.278134
42	1	0	2.472601	-1.578544	-3.303028

43	1	0	1.085298	-0.787879	-2.543942
44	1	0	-4.918869	0.186081	-2.258718
45	1	0	-5.272833	0.082424	1.982889
46	1	0	-2.121292	-1.944410	-2.491492
47	1	0	-1.558067	-0.272236	-2.538956
48	1	0	-3.066166	-0.718706	-3.351976
49	1	0	-7.266440	0.456039	0.567582
50	1	0	-7.091578	0.632096	-1.187399
51	1	0	-6.557520	1.924182	-0.109261
52	1	0	-2.612887	-2.031489	2.648974
53	1	0	-3.577069	-0.717734	3.339496
54	1	0	-1.934723	-0.408796	2.754626
55	1	0	2.839200	3.032266	1.144441
56	1	0	2.415023	5.529865	0.374639
57	1	0	0.075557	5.616415	-0.922742
58	1	0	-0.979869	3.188945	-0.945280

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Atomic Coordinates for **4** (optimized geometry with constraints on heavy atoms)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.759289	0.059013	-0.021667
2	6	0	3.701759	-1.077461	-0.023623
3	6	0	3.994086	0.217706	-0.188741
4	6	0	-1.677599	-0.095301	-0.160362
5	6	0	-2.300500	1.208521	0.109911
6	6	0	-1.770134	2.485722	0.272669
7	6	0	-2.637314	3.551236	0.489765
8	6	0	-4.006415	3.354155	0.538636
9	6	0	-4.549147	2.097345	0.368298
10	6	0	-3.702640	1.022992	0.156431
11	6	0	-3.993271	-0.393769	-0.086698
12	6	0	-5.191382	-1.097739	-0.115286
13	6	0	1.571960	-2.370327	0.637610
14	6	0	2.117741	-2.791786	1.988132
15	6	0	1.517699	-3.496198	-0.374687
16	6	0	4.629567	-2.250147	-0.092210
17	6	0	5.335806	0.849595	-0.369097
18	6	0	2.571812	2.384700	-0.299663
19	6	0	3.068825	3.124661	0.877835
20	6	0	2.833835	2.912843	-1.638973
21	6	0	-5.159215	-2.448729	-0.401963
22	6	0	-3.955806	-3.104670	-0.652166
23	6	0	-2.754205	-2.418916	-0.588913
24	6	0	-2.769766	-1.055101	-0.307742
25	7	0	2.302330	-1.191551	0.107675
26	7	0	2.793828	0.925932	-0.177527
27	7	0	0.495689	0.507911	-0.026566
28	7	0	-0.423033	-0.463078	-0.236855
29	1	0	-0.699704	2.634736	0.242204
30	1	0	-2.232435	4.552104	0.621141
31	1	0	-4.664596	4.203862	0.707233
32	1	0	-5.627262	1.955273	0.399677
33	1	0	-6.137886	-0.595837	0.071950
34	1	0	0.554980	-2.009029	0.769835
35	1	0	3.088432	-3.291721	1.933515
36	1	0	1.420686	-3.501153	2.449758
37	1	0	2.208778	-1.933799	2.662639
38	1	0	1.106859	-3.135803	-1.322762
39	1	0	0.859762	-4.290491	-0.002510
40	1	0	2.495517	-3.948518	-0.565777
41	1	0	5.645093	-1.904779	-0.299759
42	1	0	4.353364	-2.936712	-0.899781
43	1	0	4.674107	-2.830775	0.833932

44	1	0	6.114537	0.084618	-0.381403
45	1	0	5.577230	1.543842	0.444206
46	1	0	5.412002	1.409217	-1.308689
47	1	0	1.480367	2.414104	-0.204452
48	1	0	4.163085	3.193557	0.933820
49	1	0	2.713657	2.663014	1.804442
50	1	0	2.691853	4.154438	0.856298
51	1	0	3.898127	2.954763	-1.907549
52	1	0	2.452617	3.938393	-1.714953
53	1	0	2.320968	2.316254	-2.400143
54	1	0	-6.089750	-3.010795	-0.439632
55	1	0	-3.961201	-4.167303	-0.882646
56	1	0	-1.810803	-2.926034	-0.772663

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Atomic Coordinates for **5** (optimized geometry with constraints on heavy atoms)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.666555	-0.099723	0.000235
2	7	0	-0.528103	0.476287	-0.000338
3	7	0	0.528113	-0.476294	-0.000339
4	6	0	1.666546	0.099727	0.000238
5	1	0	-1.778545	-1.187129	0.000688
6	1	0	-2.555958	0.527329	0.000268
7	1	0	2.555961	-0.527309	0.000259
8	1	0	1.778522	1.187134	0.000682

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Atomic Coordinates for **6** (optimized geometry with constraints on heavy atoms)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.666263	0.138561	-0.443528
2	7	0	0.675122	-0.268828	-0.411413
3	6	0	-1.508260	-0.704572	0.018346
4	6	0	-2.939001	-0.290798	-0.027466
5	6	0	-3.950063	-1.098872	0.475067
6	6	0	-5.273656	-0.682379	0.471598
7	6	0	-5.601072	0.552035	-0.052448
8	6	0	-4.604289	1.363733	-0.579800
9	6	0	-3.294993	0.949925	-0.559856
10	6	0	-1.144319	-2.035634	0.599856
11	6	0	1.499090	0.643128	-0.059196
12	6	0	2.939231	0.276094	-0.056488
13	6	0	3.865038	0.990350	0.687904
14	6	0	5.197500	0.616450	0.724482
15	6	0	5.629274	-0.472770	-0.010952
16	6	0	4.722575	-1.185778	-0.769983
17	6	0	3.391166	-0.826923	-0.790145
18	6	0	1.087221	2.021014	0.366513
19	1	0	-3.711000	-2.069514	0.898985
20	1	0	-6.044451	-1.329907	0.881135
21	1	0	-6.635787	0.886385	-0.058461
22	1	0	-4.859058	2.333537	-1.000049
23	1	0	-2.511819	1.583673	-0.961043
24	1	0	-0.093552	-2.253698	0.409492
25	1	0	-1.761472	-2.832382	0.170164
26	1	0	-1.309926	-2.050501	1.685026
27	1	0	3.543925	1.845972	1.275450
28	1	0	5.900553	1.184826	1.327900
29	1	0	6.676726	-0.763725	0.007650
30	1	0	5.056209	-2.039282	-1.355549
31	1	0	2.673190	-1.390499	-1.376601
32	1	0	0.966511	2.079185	1.456829
33	1	0	0.122624	2.270097	-0.078678
34	1	0	1.832659	2.767688	0.077748

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Atomic Coordinates for **7** (optimized geometry with constraints on heavy atoms)
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	6.715102	-0.331633	-0.115791
2	7	0	-0.078367	-0.091937	-0.355515
3	7	0	-1.449326	0.177471	-0.334515
4	8	0	-7.823058	0.004401	0.014034
5	6	0	0.638422	0.843338	0.068164
6	6	0	2.119872	0.605885	0.011184
7	6	0	3.002782	1.394112	0.738182
8	6	0	4.374255	1.146452	0.712647
9	6	0	4.846128	0.084895	-0.031923
10	6	0	4.006931	-0.719437	-0.773693
11	6	0	2.645284	-0.447912	-0.732110
12	6	0	0.136457	2.123907	0.647527
13	6	0	-2.210952	-0.785070	0.075662
14	6	0	-3.674595	-0.535711	0.064589
15	6	0	-4.556967	-1.464644	0.645071
16	6	0	-5.917290	-1.244845	0.620559
17	6	0	-6.425222	-0.118749	0.008496
18	6	0	-5.561096	0.810847	-0.558369
19	6	0	-4.198768	0.598744	-0.535870
20	6	0	-1.674156	-2.108181	0.567566
21	6	0	-8.397589	0.972958	-0.501650
22	1	0	2.640892	2.219544	1.342787
23	1	0	5.058604	1.765738	1.282350
24	1	0	4.395780	-1.540677	-1.364143
25	1	0	1.958769	-1.069948	-1.297749
26	1	0	-0.892586	2.297373	0.329934
27	1	0	0.141878	2.088643	1.745363
28	1	0	0.760766	2.970338	0.345158
29	1	0	-4.176274	-2.356471	1.129960
30	1	0	-6.608923	-1.953209	1.066917
31	1	0	-5.957017	1.701173	-1.037193
32	1	0	-3.524573	1.316327	-0.989454
33	1	0	-0.630836	-2.215629	0.269667
34	1	0	-1.723572	-2.171543	1.662611
35	1	0	-2.256025	-2.943770	0.165524
36	1	0	-8.146932	1.963341	-0.055381
37	1	0	-8.223673	1.097854	-1.595608
38	1	0	-9.487489	0.864584	-0.386309

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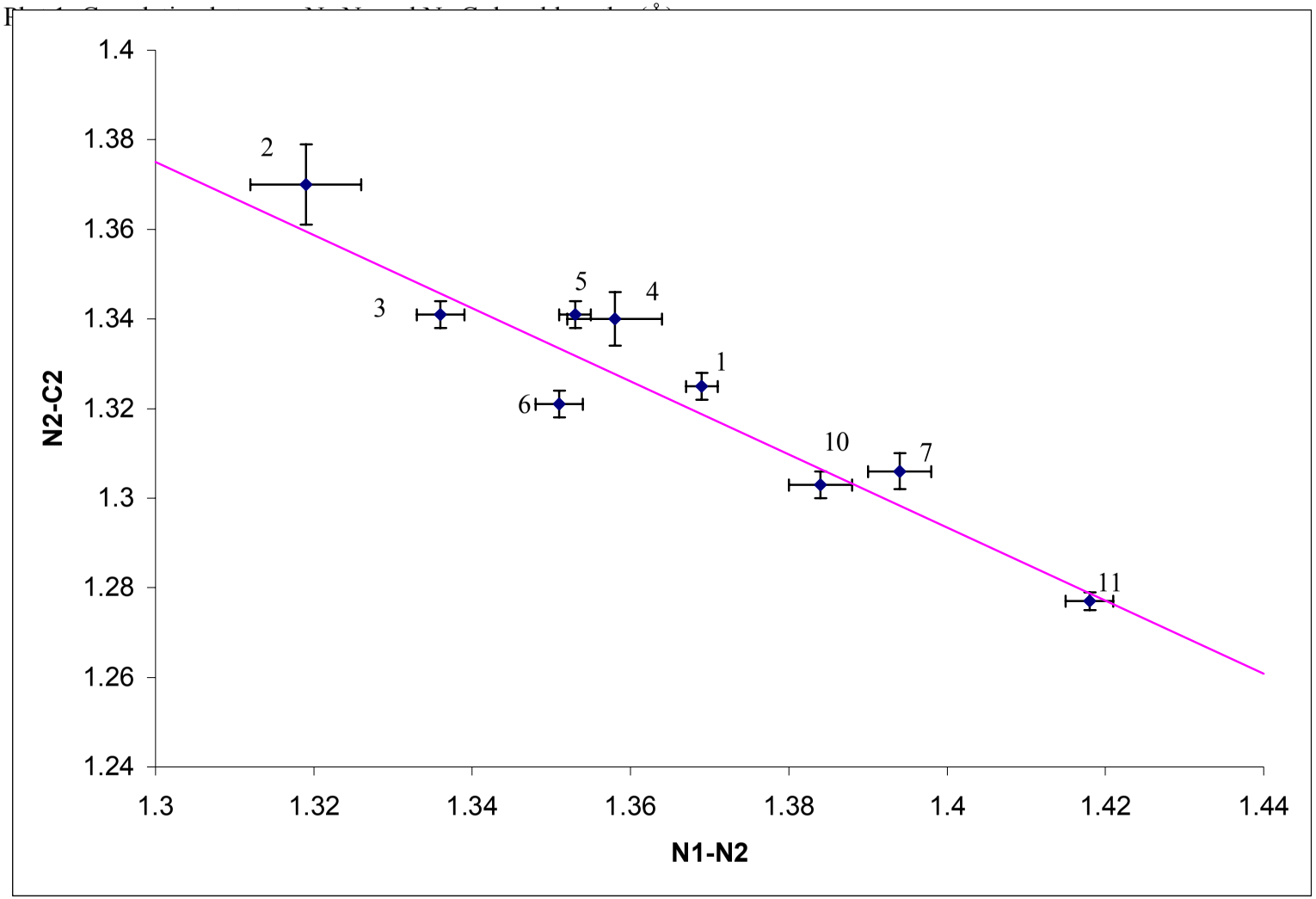

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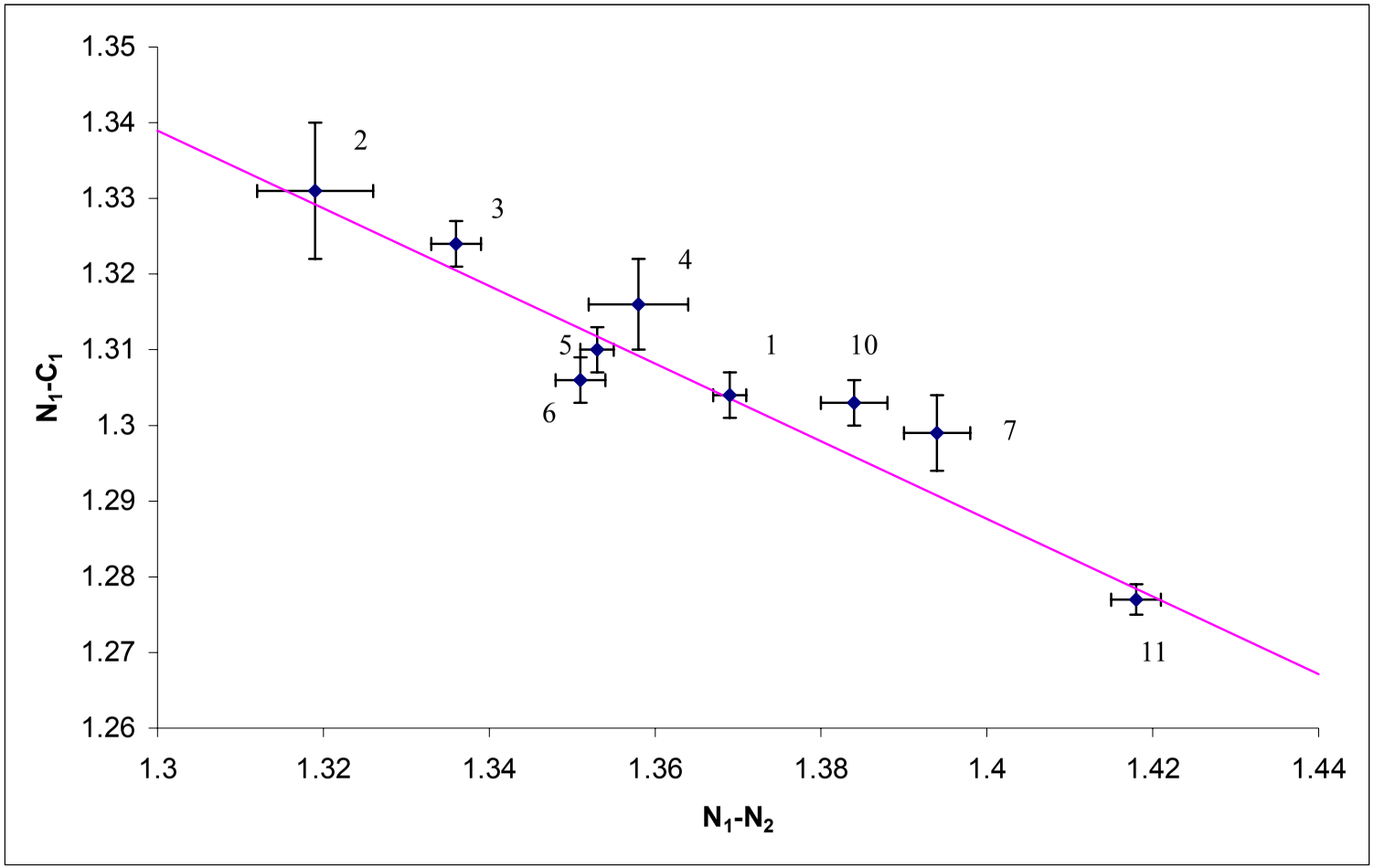

Plot 2: Correlation between N_1-N_2 and N_1-C_1 bond lengths (Å).

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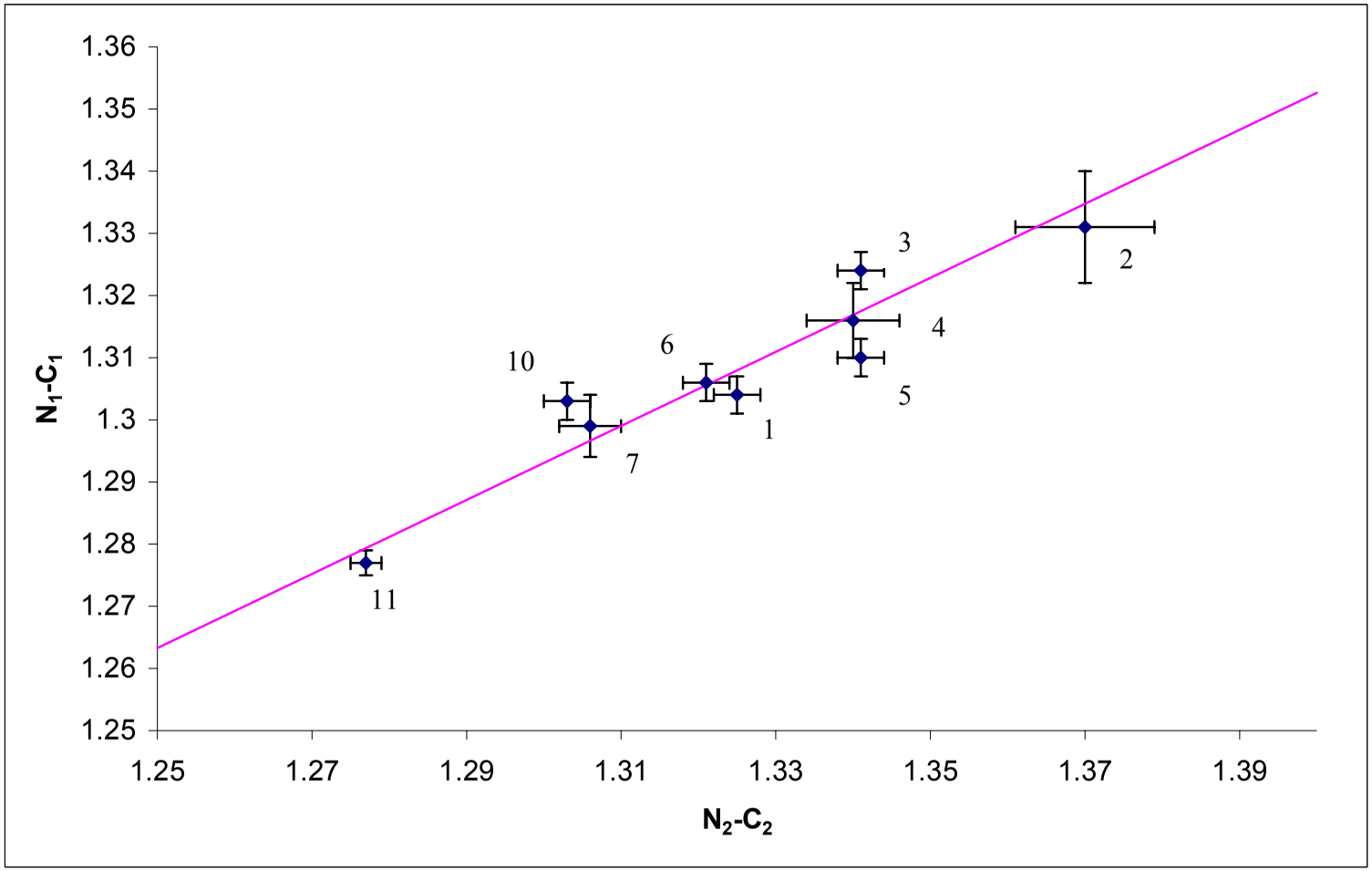

Plot 3: Correlation between N_2-C_2 and N_1-C_1 bond lengths (Å)

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Surface Second Harmonic Generation studies:

Surface SHG experiments were conducted on spin cast films of submonolayer coverage in a total internal reflection geometry. Experiments were conducted under nonresonant conditions with a fundamental frequency of 1300 nm, and SHG detection at 650 nm to avoid resonantly enhanced signals that would skew the relative ranking of the second order response. Kikteva, T.; Star, D.; Zhao, Z.; Baisley, T. L.; Leach, G. W. J. Phys. Chem. B 1999, 103, 1124-1133.

Note that direct comparison of the calculated β_{tot} values with experimental surface SHG intensities are complicated since the calculated β_{tot} values are a measure of the total intrinsic quadratic hyperpolarizability and represent a sum of hyperpolarizability tensor components, while the surface SHG results reflect the macroscopic, orientation-averaged nonlinear susceptibilities which weight various components of the hyperpolarizability tensor according to their orientation at the surface. Nevertheless, both experiment and calculation show similar trends. (T. Kikteva, D. Star, G. W. Leach, *J. Phys. Chem. B*, 2000, **104**, 2860)

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Table.1 Hyperpolarisability Calculations at B3LYP/6-31+G* level (for 6-31G* optimised molecular geometry)

Compounds	**Dipole Moment (μ) in D (in 10^{-18}esu)**	**β_{tot}/esu (10^{-30})**	**β_{vec}/esu (10^{-30})**	**$\mu\beta_{vec}$ (10^{-48})**
1	5.12 (2.02)	28.7	-28.3	-57.0
2	5.21 (2.05)	30.9	-30.7	-63.0
3	5.53 (2.18)	26.0	-25.0	-54.5
4	5.30 (2.09)	28.7	-28.5	-59.5
6	5.30 (2.09)	20.1	-19.7	-41.2
5	6.73 (2.65)	45.5	-45.3	-120.0
7	1.85 (0.73)	17.7	-14.9	-10.8