JUSTUS-LIEBIG-
UNIVERSITÄT
GIESSEN

Bis(bis(8-quinoloyl)amide)metal(II) complexes for organic electronics

Elektronischer Anhang für die
Dissertation zur Erlangung des akademischen Grades
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am Fachbereich Chemie der Justus-Liebig-Universität Gießen

vorgelegt von

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Gutachter:

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2. Prof. Dr. Derck Schlettwein

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1 NMR-spectra

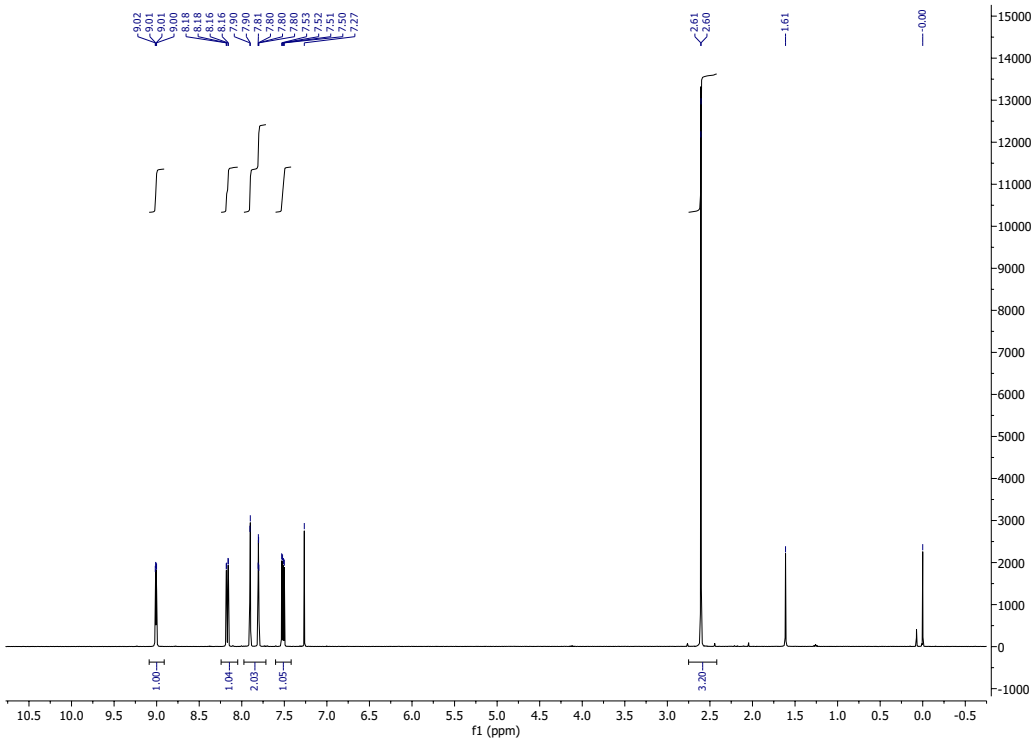

Figure 1: ^{1}H-NMR-spectrum of 6-methyl-8-nitro-quinoline **8b**

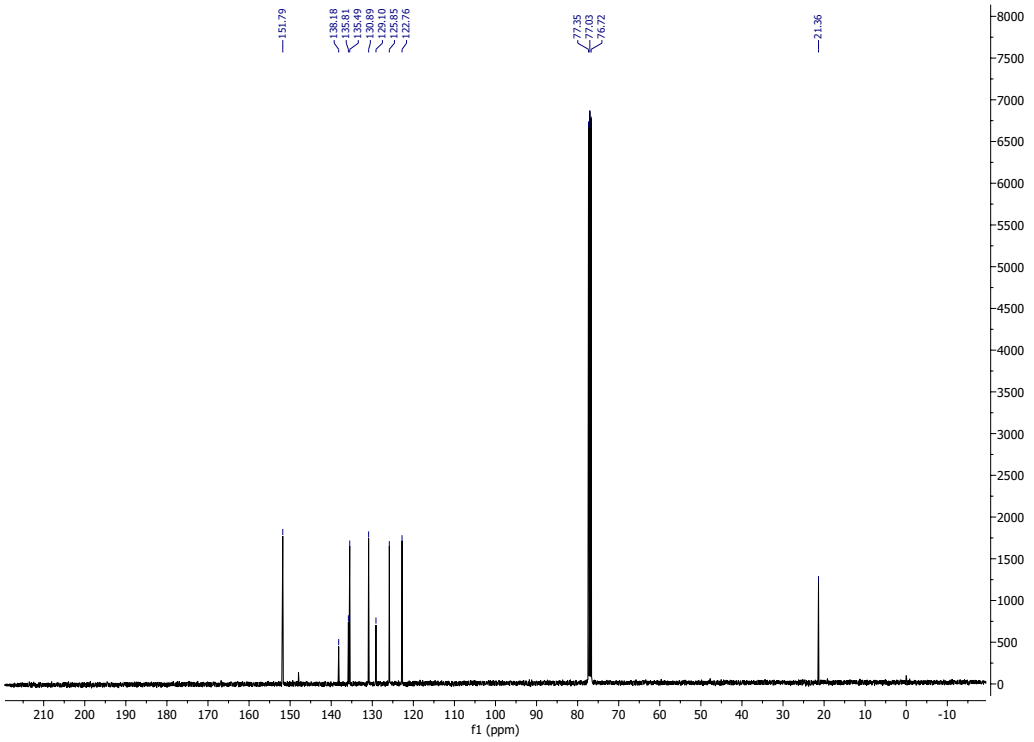

Figure 2: ^{13}C-NMR-spectrum of 6-methyl-8-nitro-quinoline **8b**

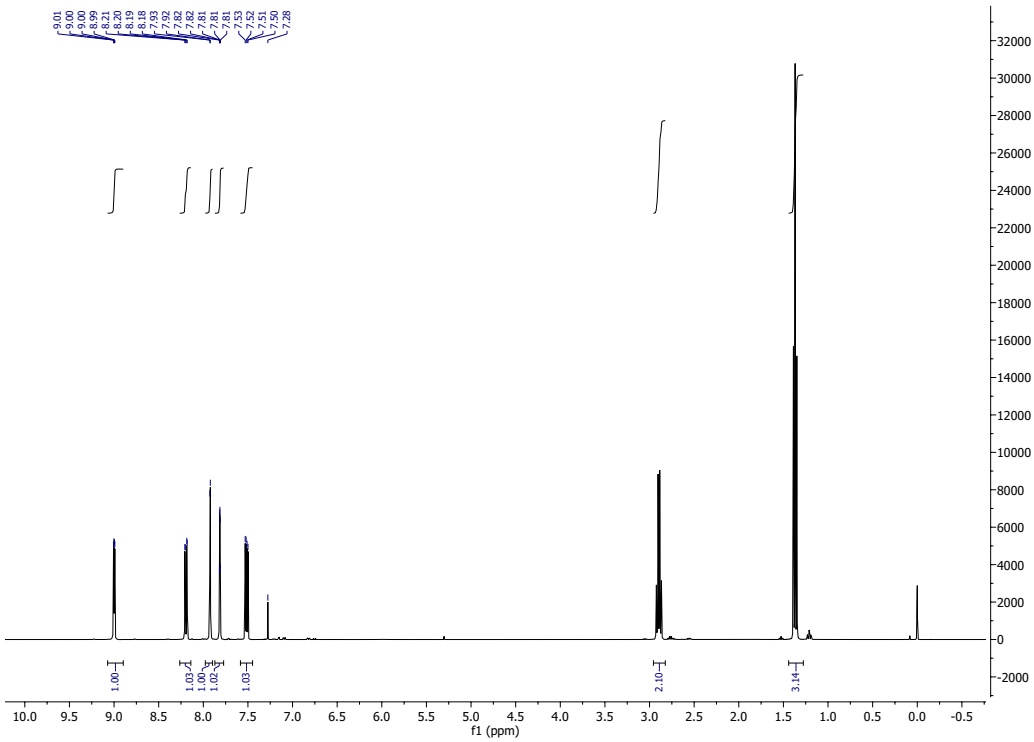

Figure 3: ^{1}H-NMR-spectrum of 6-ethyl-8-nitro-quinoline **8c**

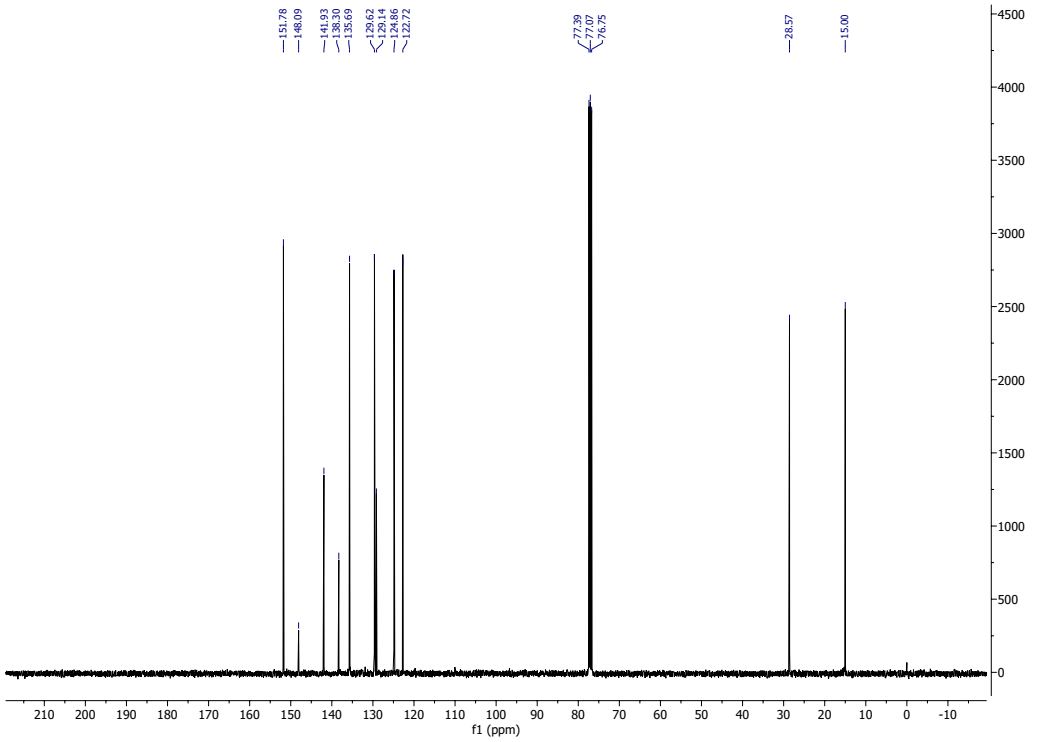

Figure 4: ^{13}C-NMR-spectrum of 6-ethyl-8-nitro-quinoline **8c**

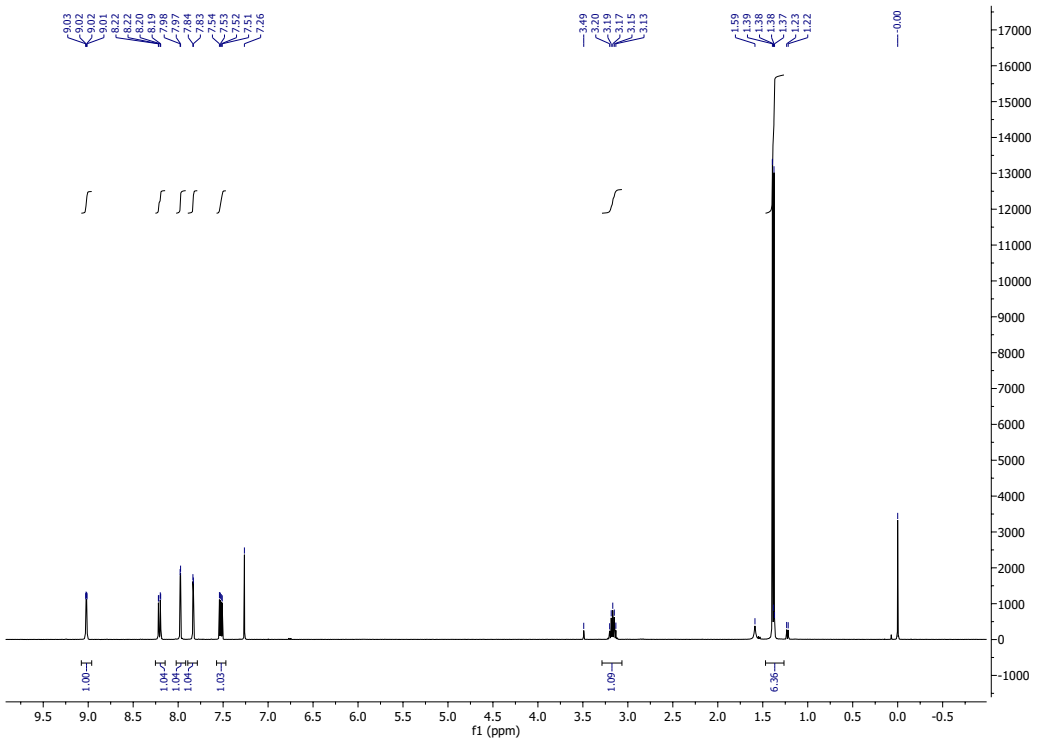

Figure 5: ^{1}H-NMR-spectrum of 6-(1-methylethyl)-8-nitro-quinoline **8d**

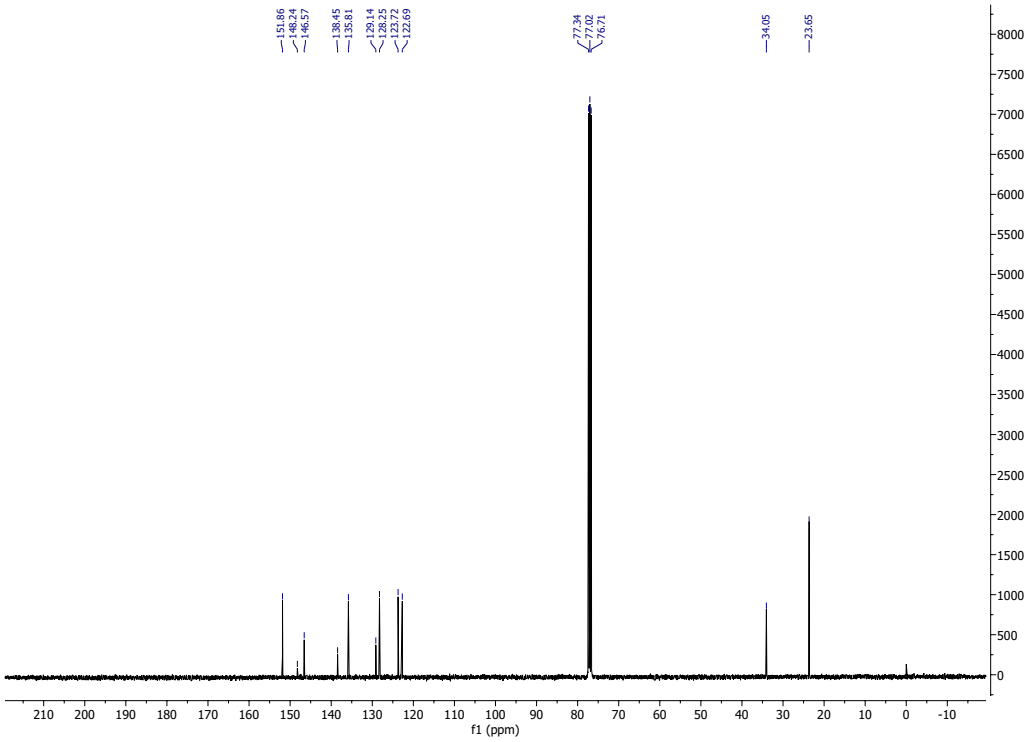

Figure 6: ^{13}C-NMR-spectrum of 6-(1-methylethyl)-8-nitro-quinoline **8d**

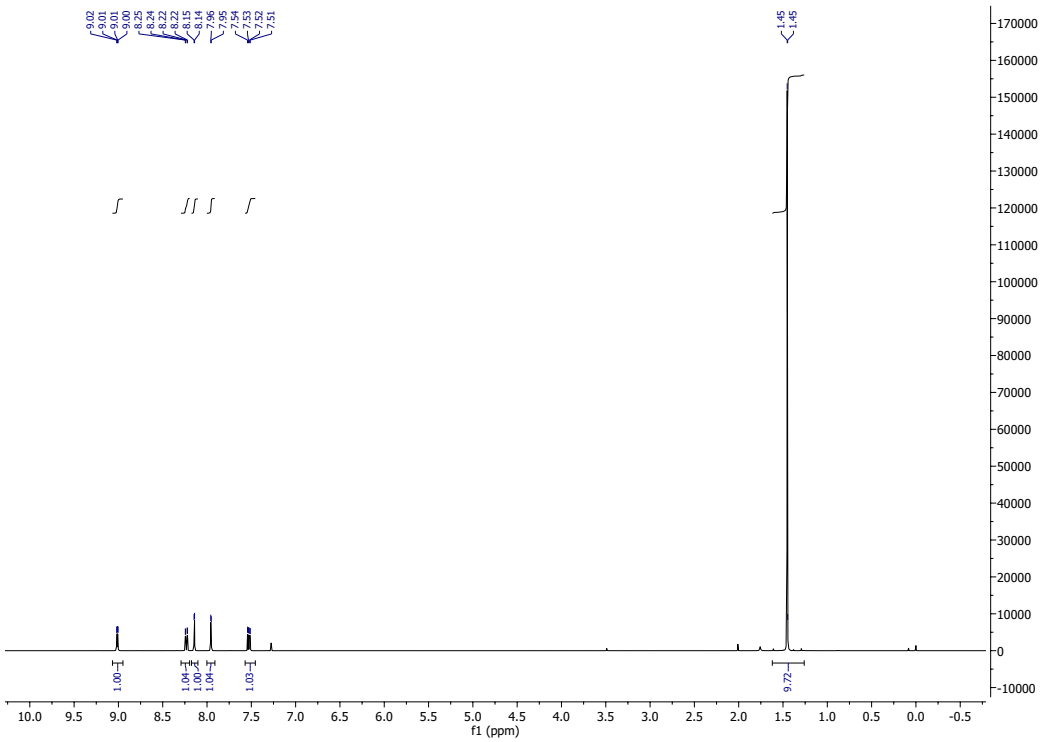

Figure 7: ^{1}H-NMR-spectrum of 6-(1,1-dimethylethyl)-8-nitro-quinoline **8e**

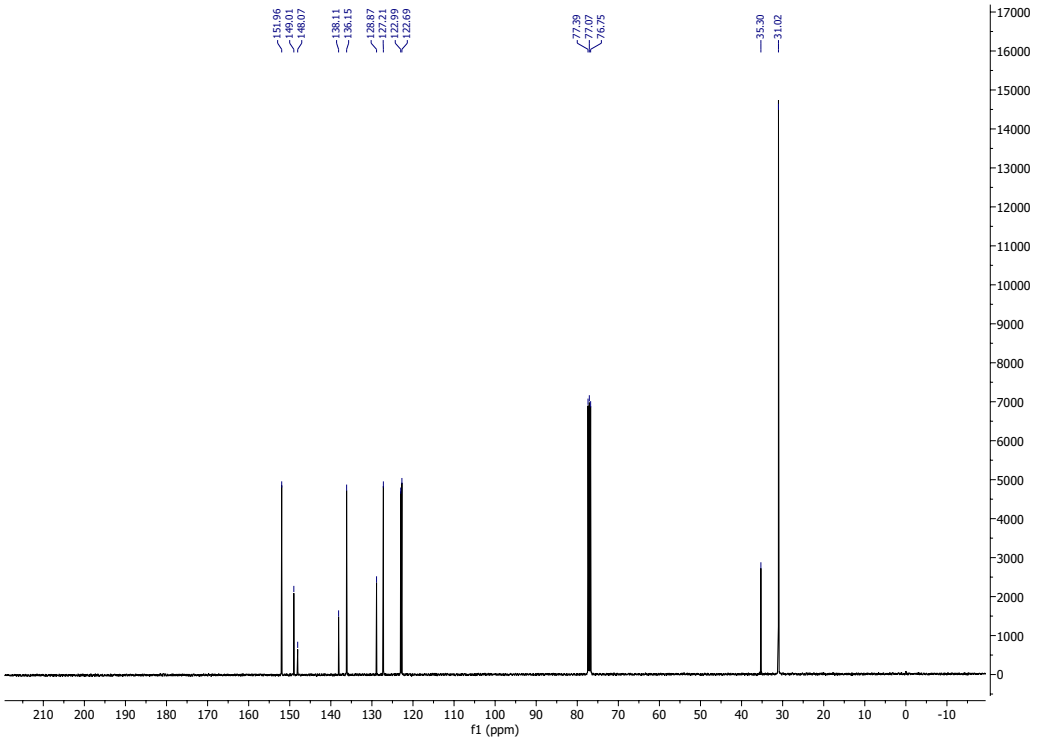

Figure 8: ^{13}C-NMR-spectrum of 6-(1,1-dimethylethyl)-8-nitro-quinoline **8e**

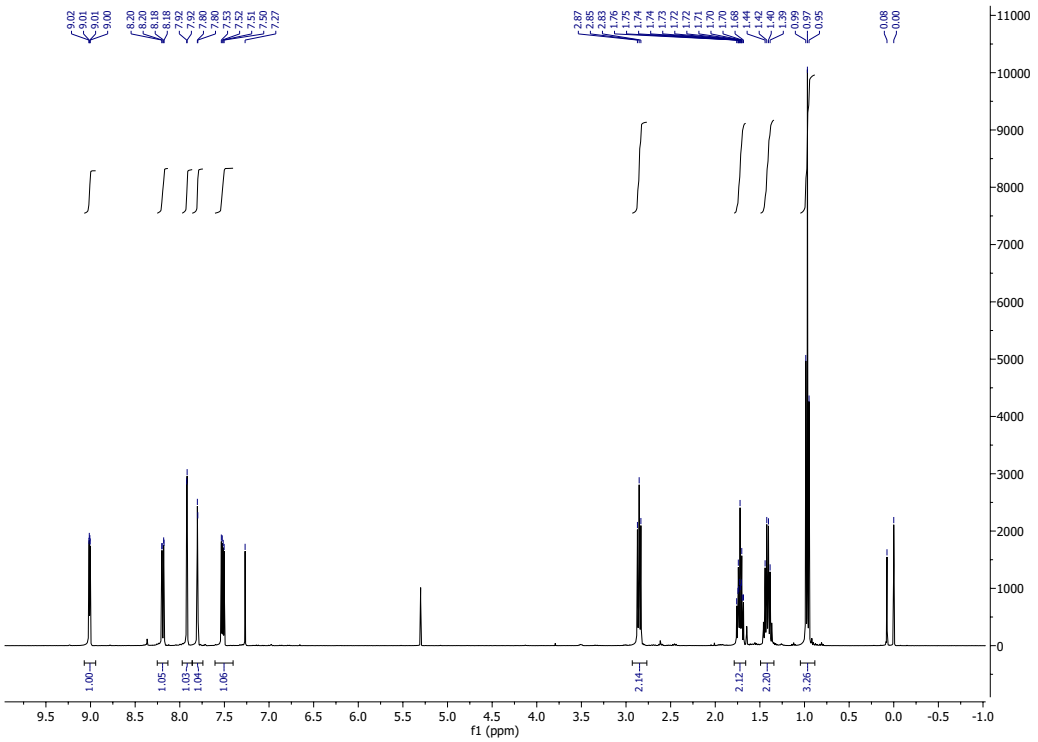

Figure 9: ^{1}H-NMR-spectrum of 6-butyl-8-nitro-quinoline **8f**

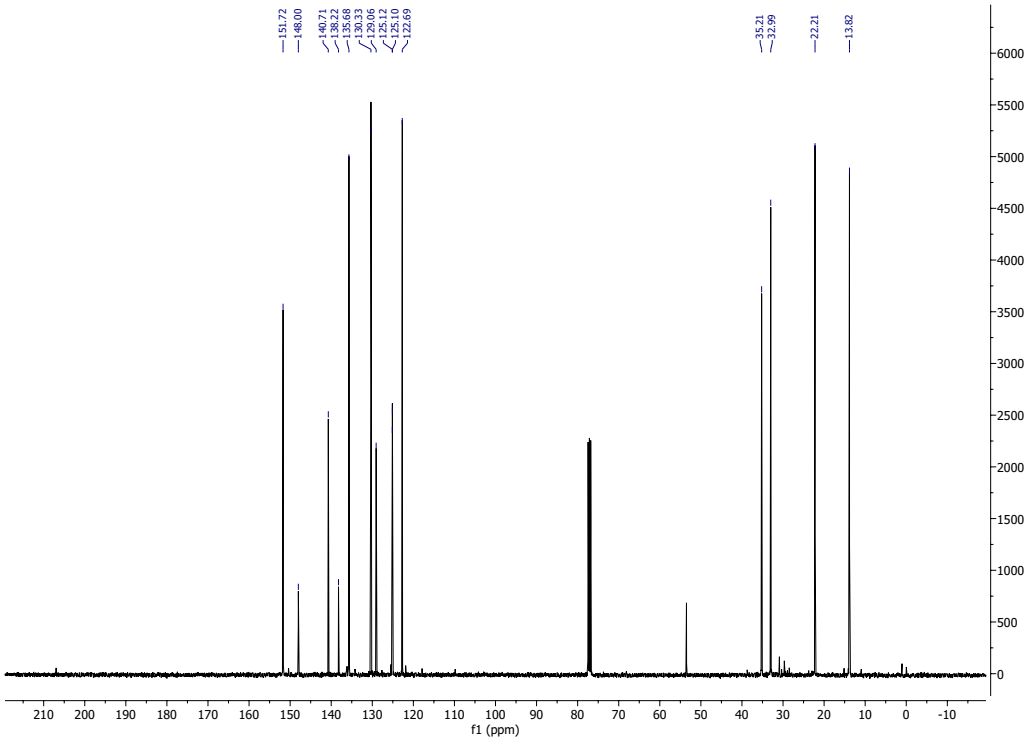

Figure 10: ^{13}C-NMR-spectrum of 6-butyl-8-nitro-quinoline **8f**

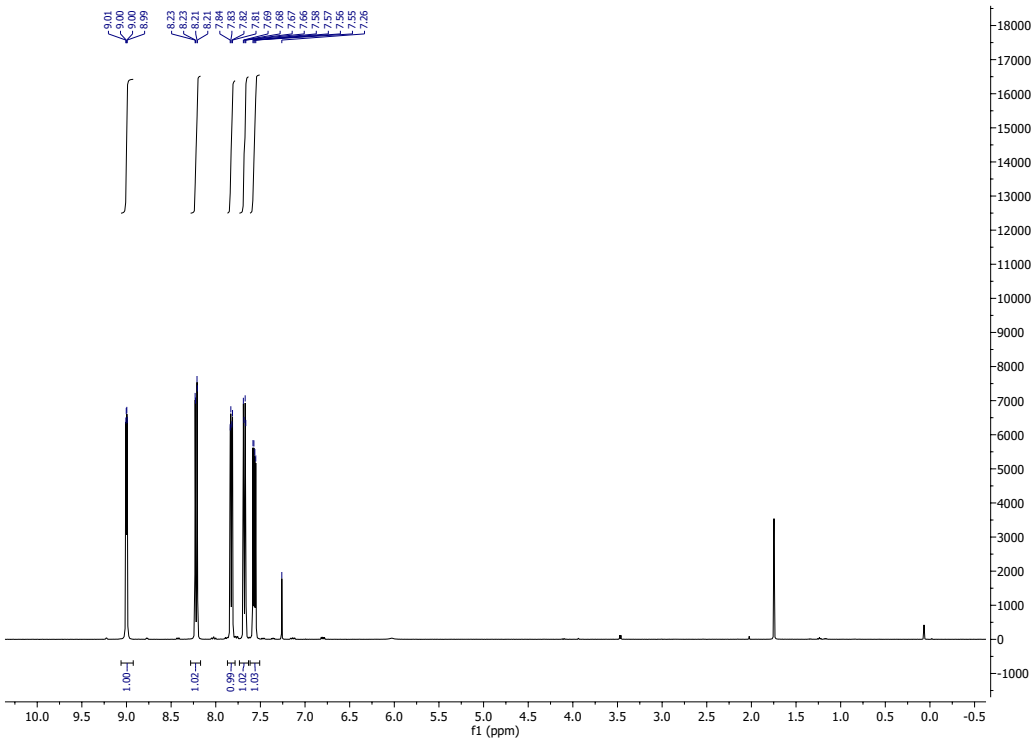

Figure 11: ^{1}H-NMR-spectrum of 6-fluoro-8-nitro-quinoline **8g**

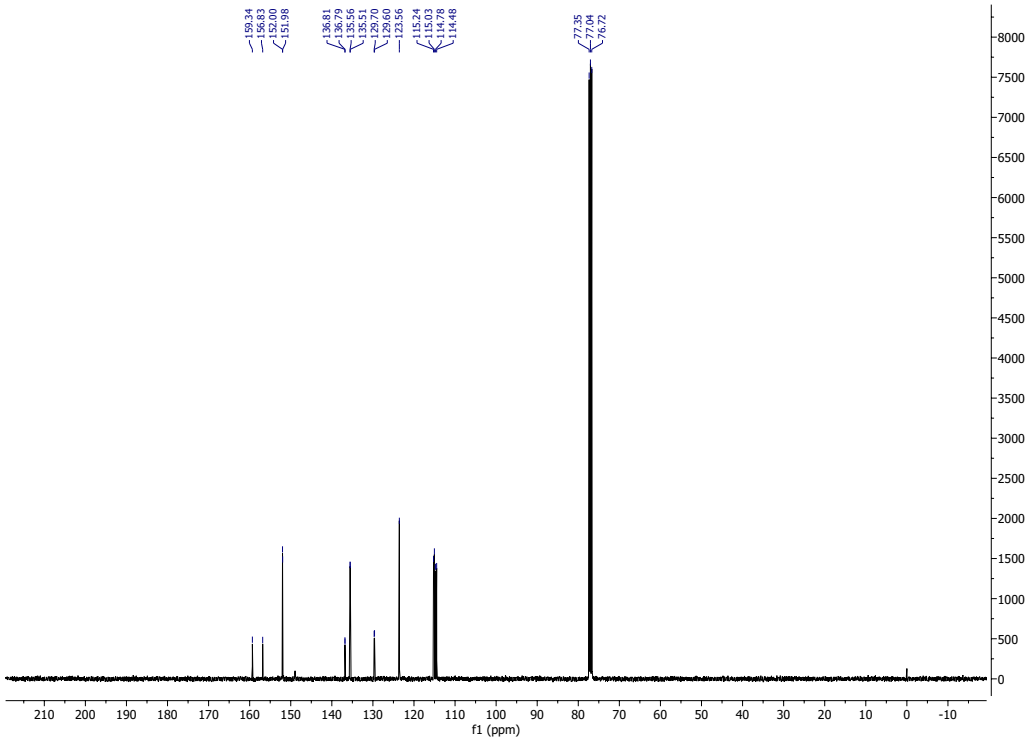

Figure 12: ^{13}C-NMR-spectrum of 6-fluoro-8-nitro-quinoline **8g**

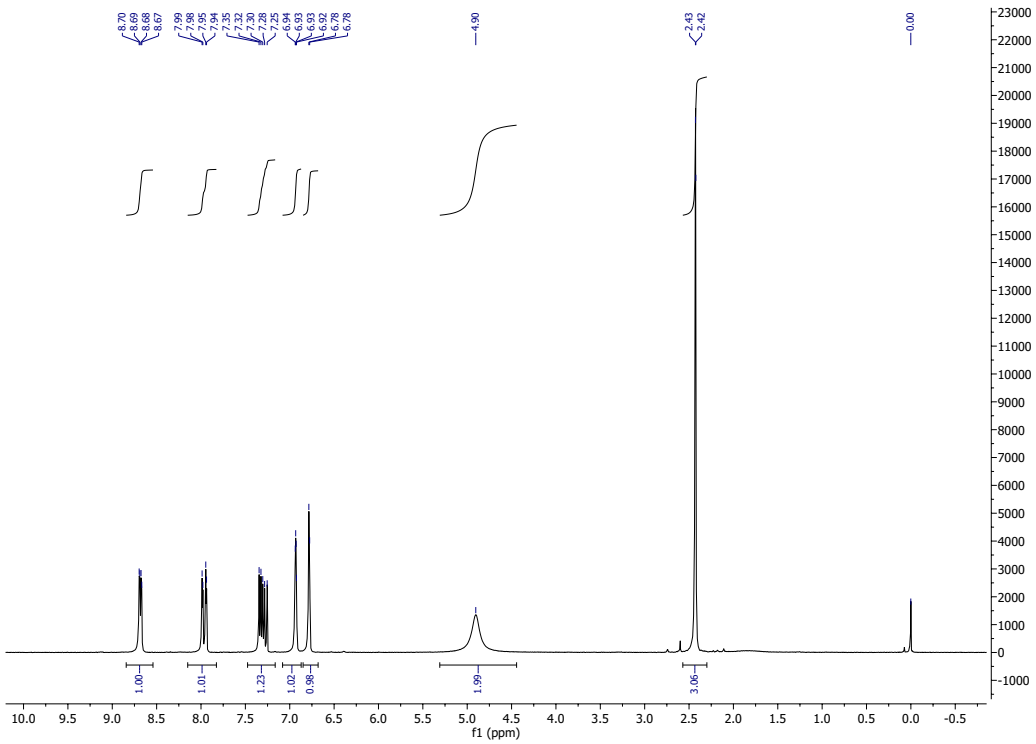

Figure 13: ^{1}H-NMR-spectrum of 8-amino-6-methyl-quinoline **7b**

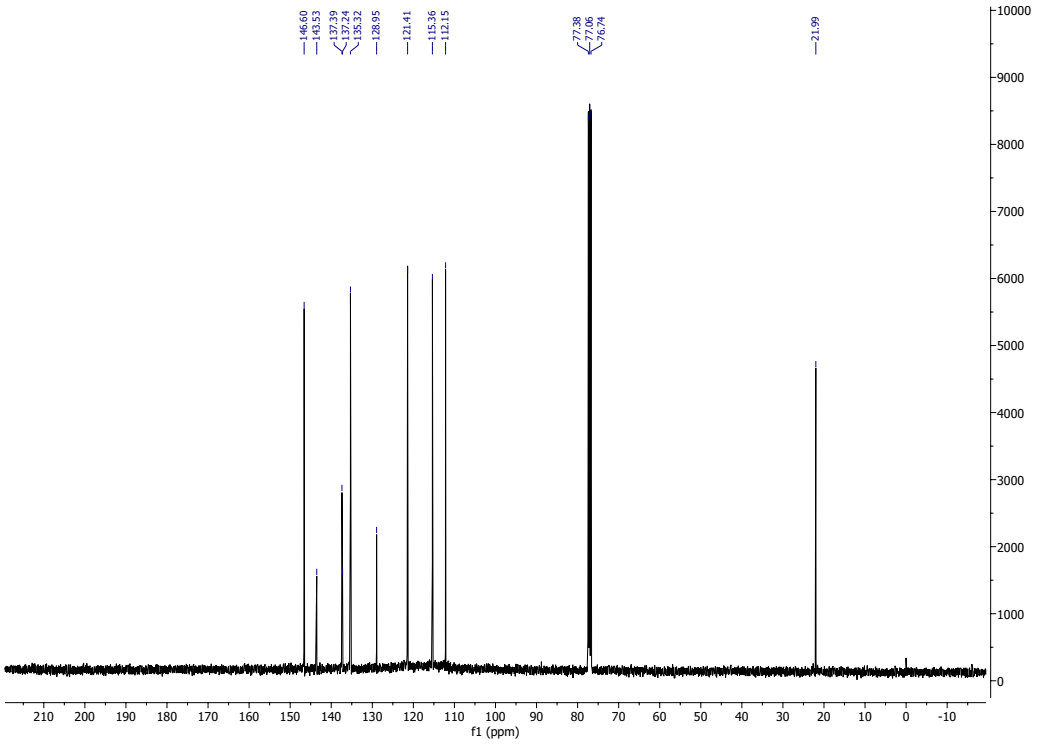

Figure 14: ^{13}C-NMR-spectrum of 8-amino-6-methyl-quinoline **7b**

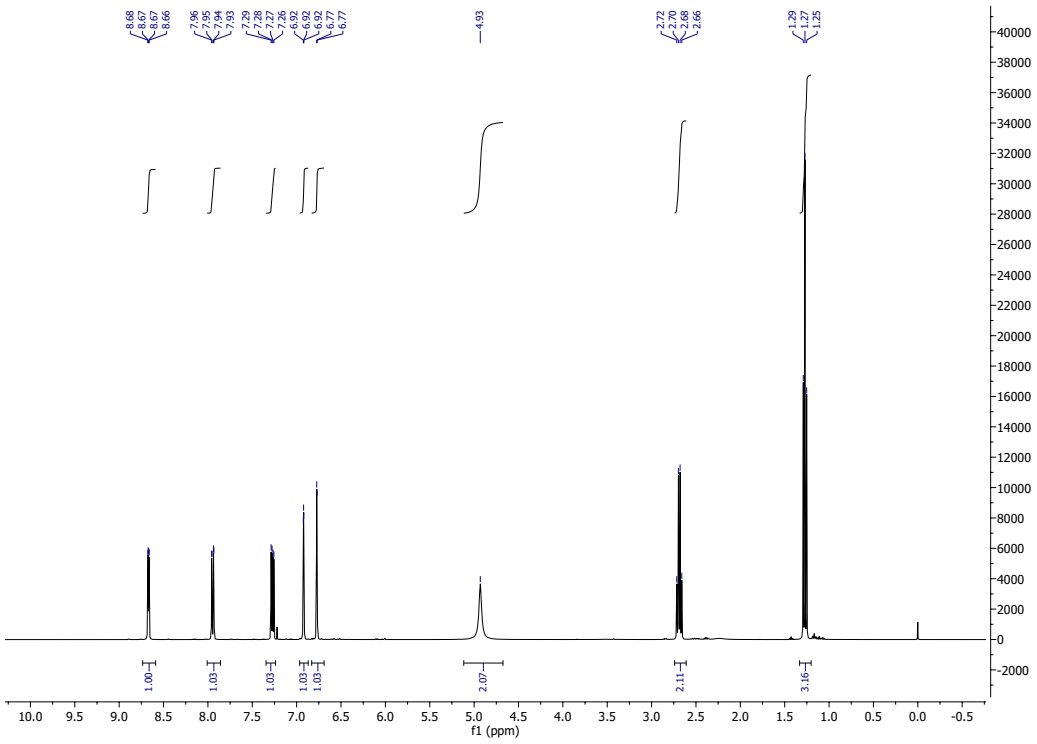

Figure 15: ^{1}H-NMR-spectrum of 8-amino-6-ethyl-quinoline **7c**

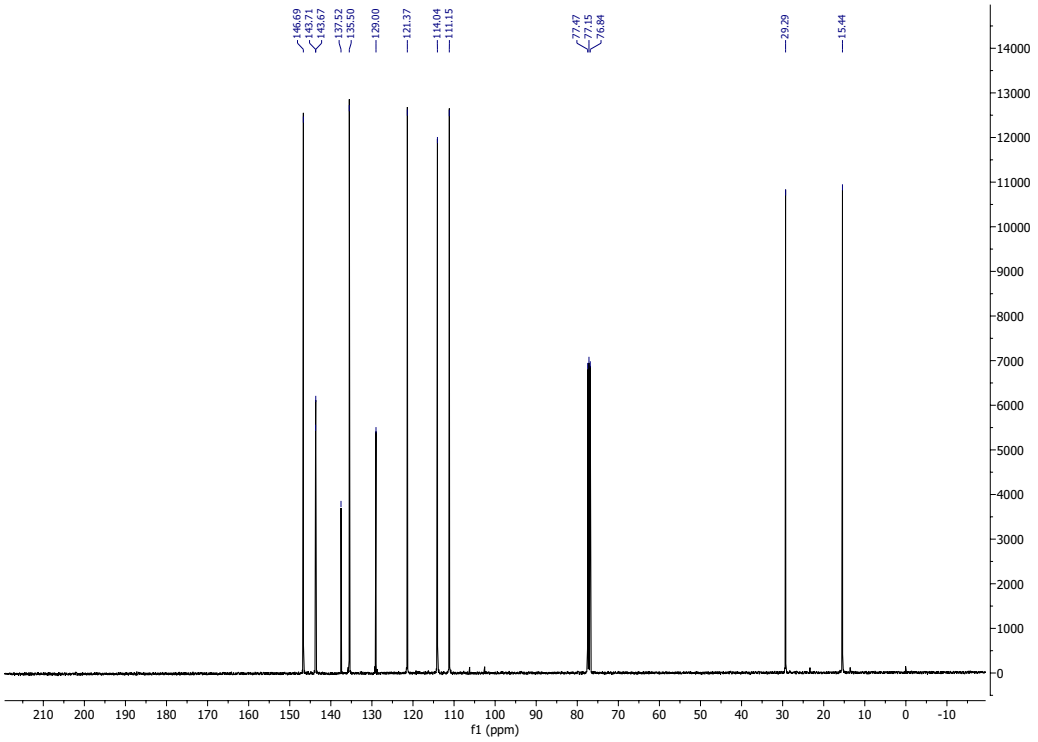

Figure 16: ^{13}C-NMR-spectrum of 8-amino-6-ethyl-quinoline **7c**

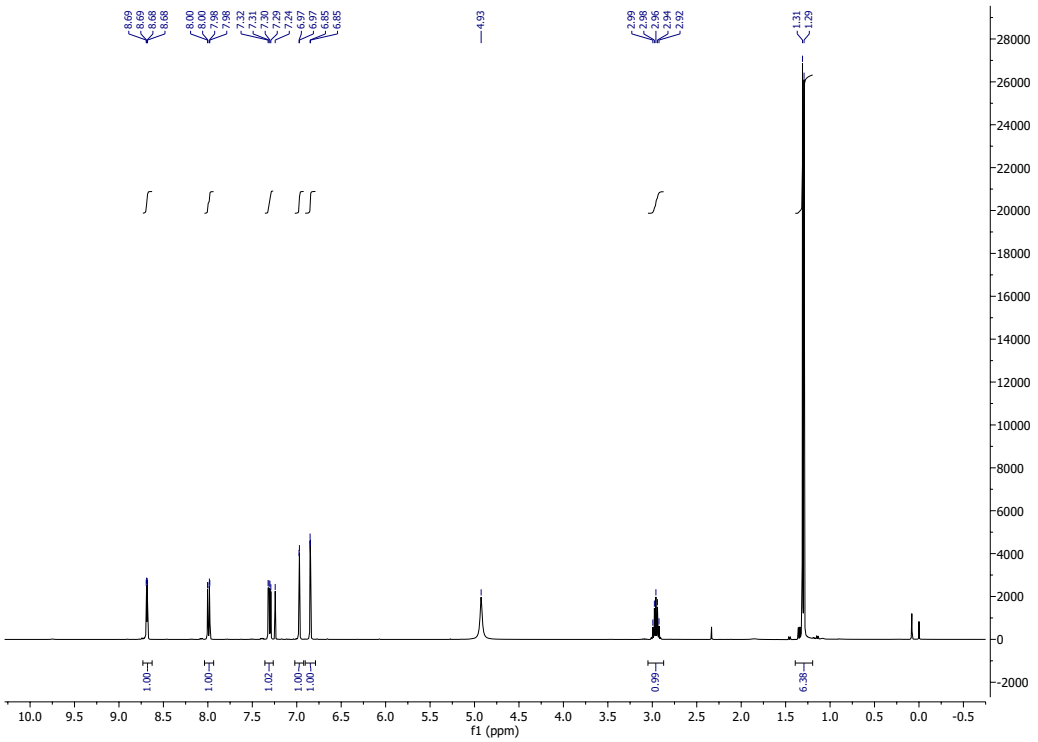

Figure 17: ^{1}H-NMR-spectrum of 8-amino-6-(1-methylethyl)-quinoline **7d**

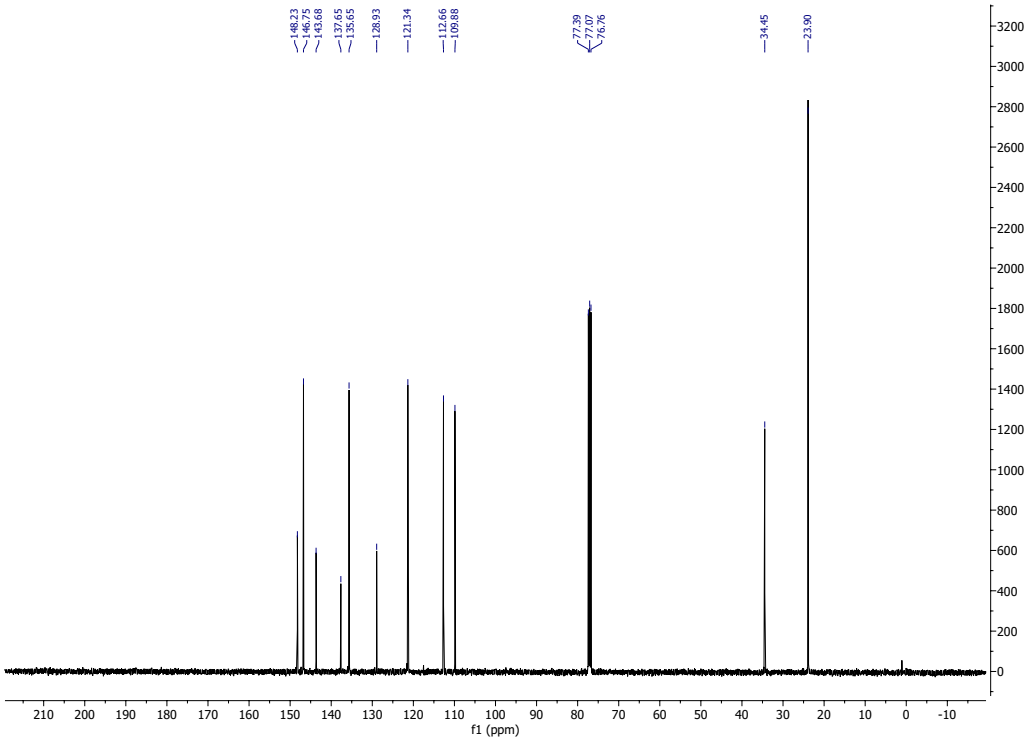

Figure 18: ^{13}C-NMR-spectrum of 8-amino-6-(1-methylethyl)-quinoline **7d**

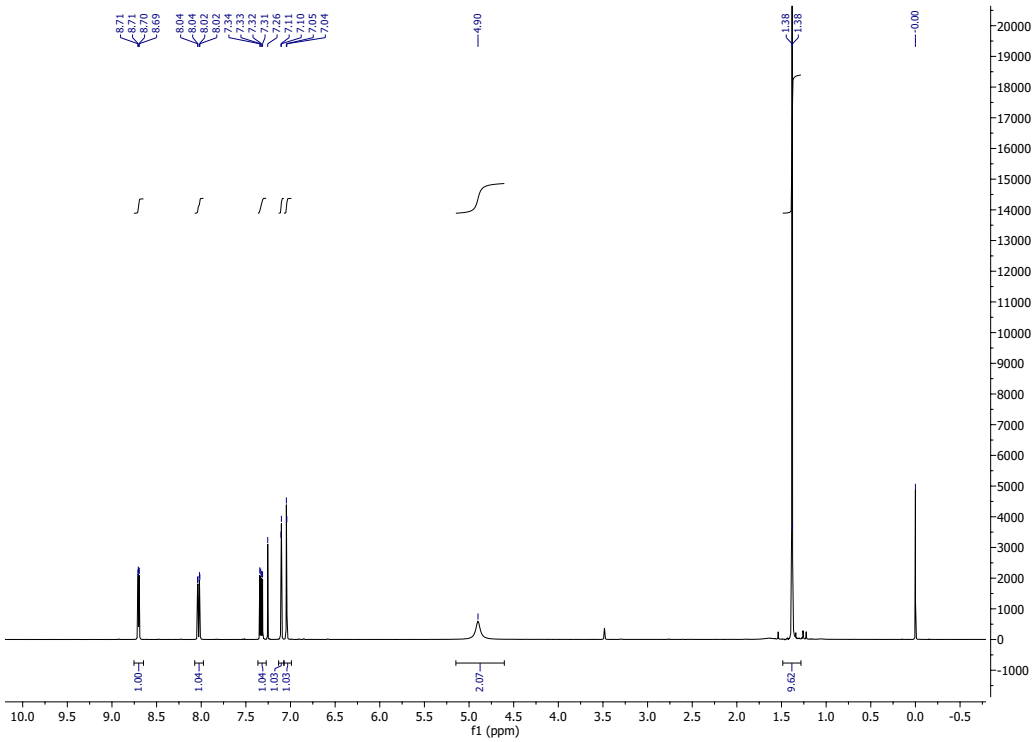

Figure 19: ^{1}H-NMR-spectrum of 8-amino-6-(1,1-dimethylethyl)-quinoline **7e**

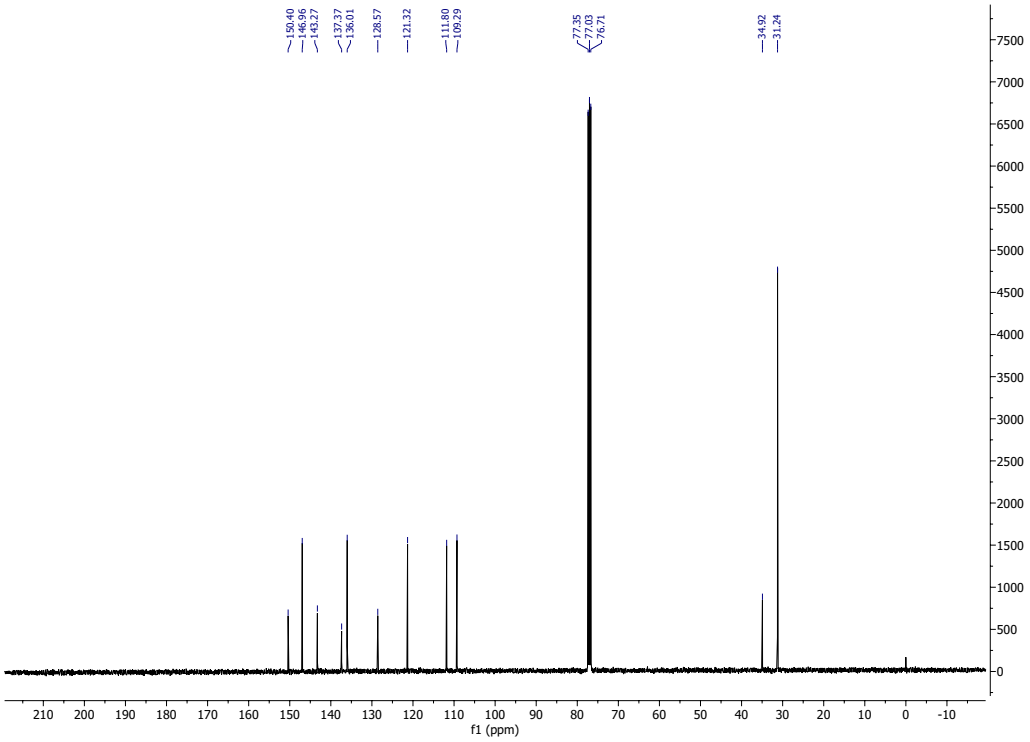

Figure 20: ^{13}C-NMR-spectrum of 8-amino-6-(1,1-dimethylethyl)-quinoline **7e**

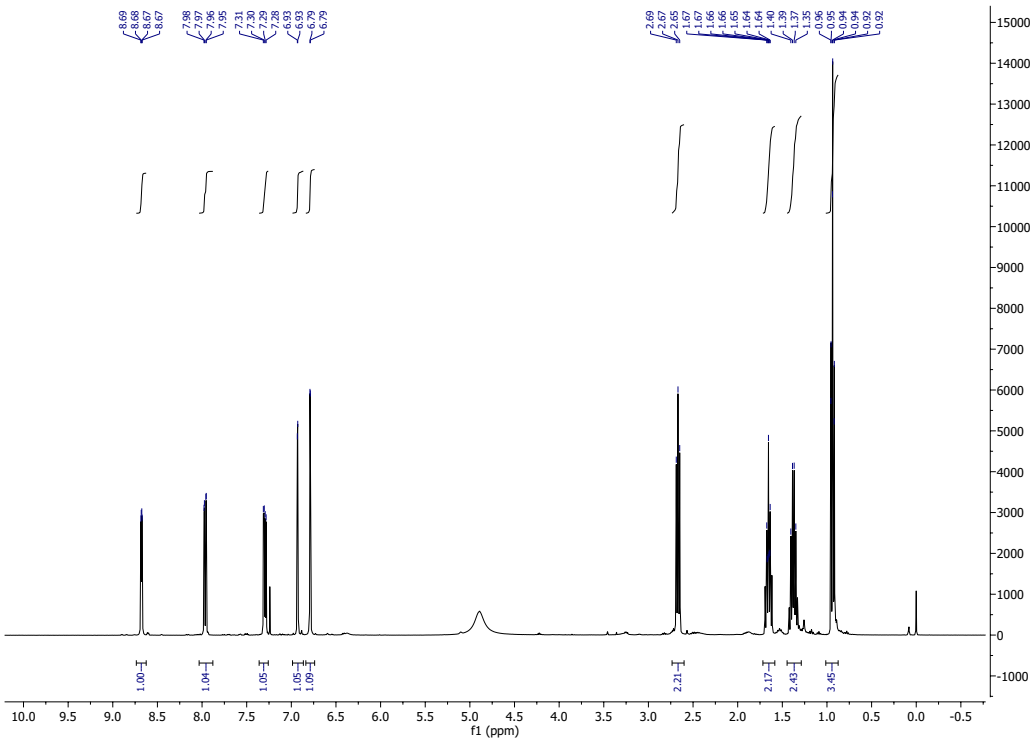

Figure 21: ^{1}H-NMR-spectrum of 8-amino-6-butyl-quinoline **7f**

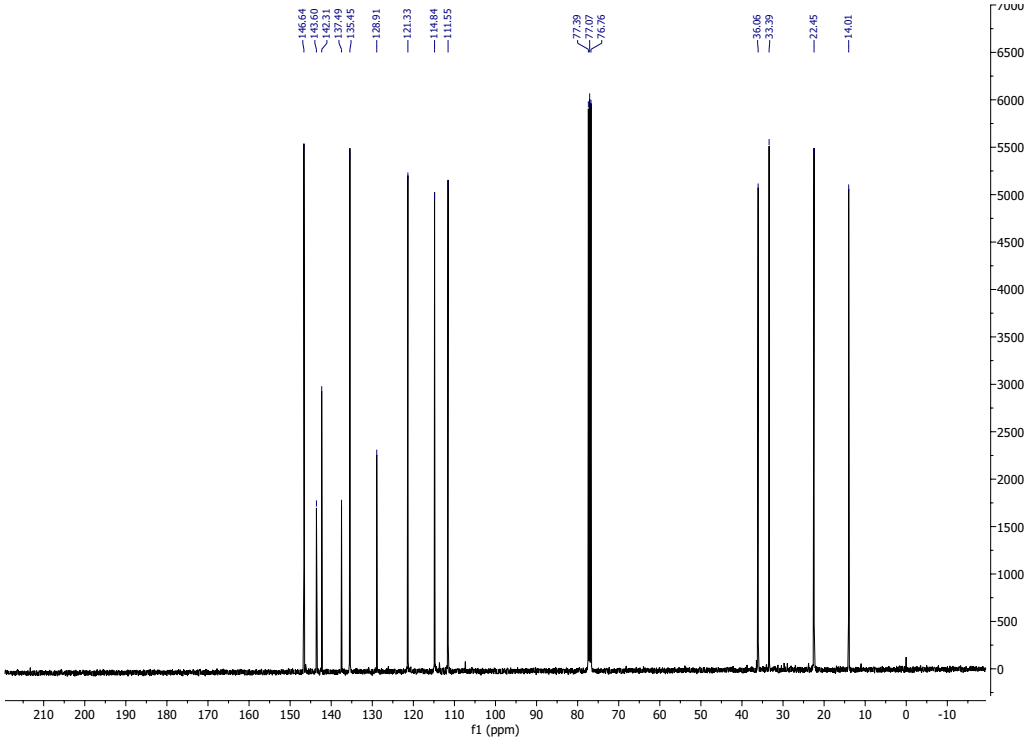

Figure 22: ^{13}C-NMR-spectrum of 8-amino-6-butyl-quinoline **7f**

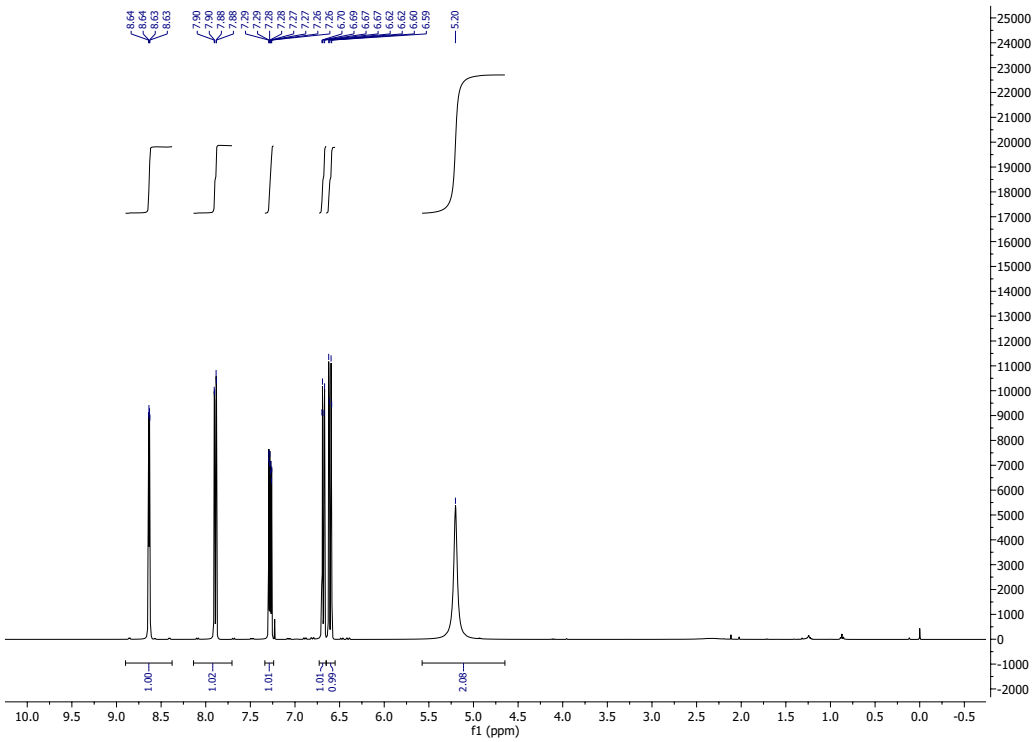

Figure 23: ^{1}H-NMR-spectrum of 8-amino-6-fluoro-quinoline **7g**

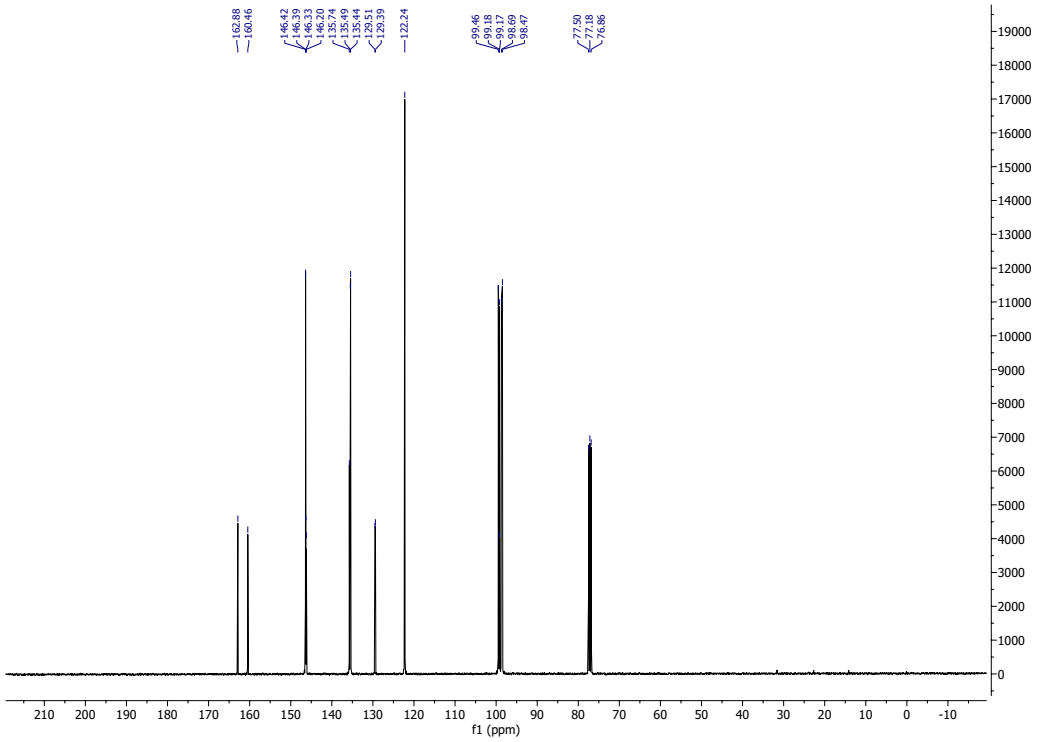

Figure 24: ^{13}C-NMR-spectrum of 8-amino-6-fluoro-quinoline **7g**

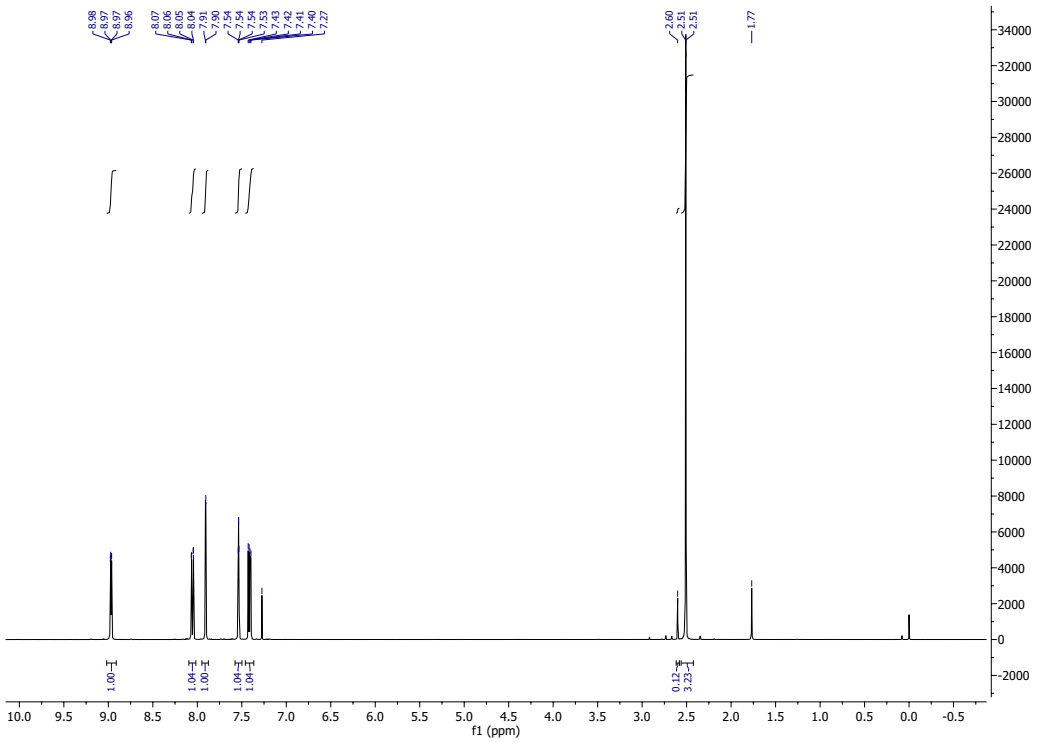

Figure 25: ^{1}H-NMR-spectrum of 8-bromo-6-methyl-quinoline **6b**

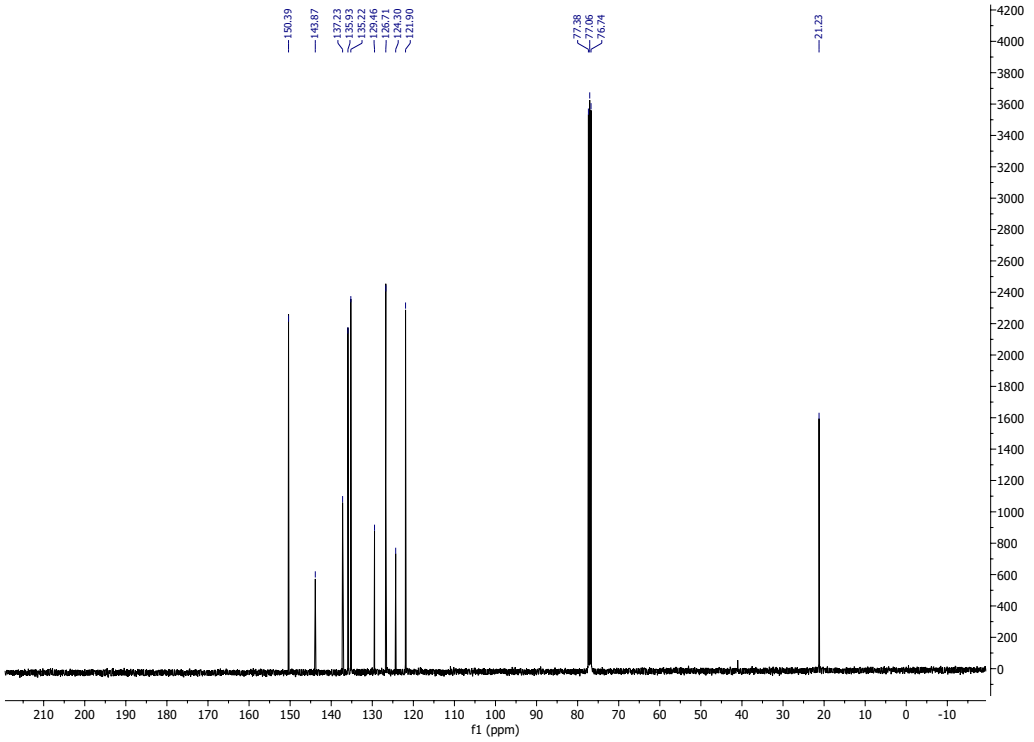

Figure 26: ^{13}C-NMR-spectrum of 8-bromo-6-methyl-quinoline **6b**

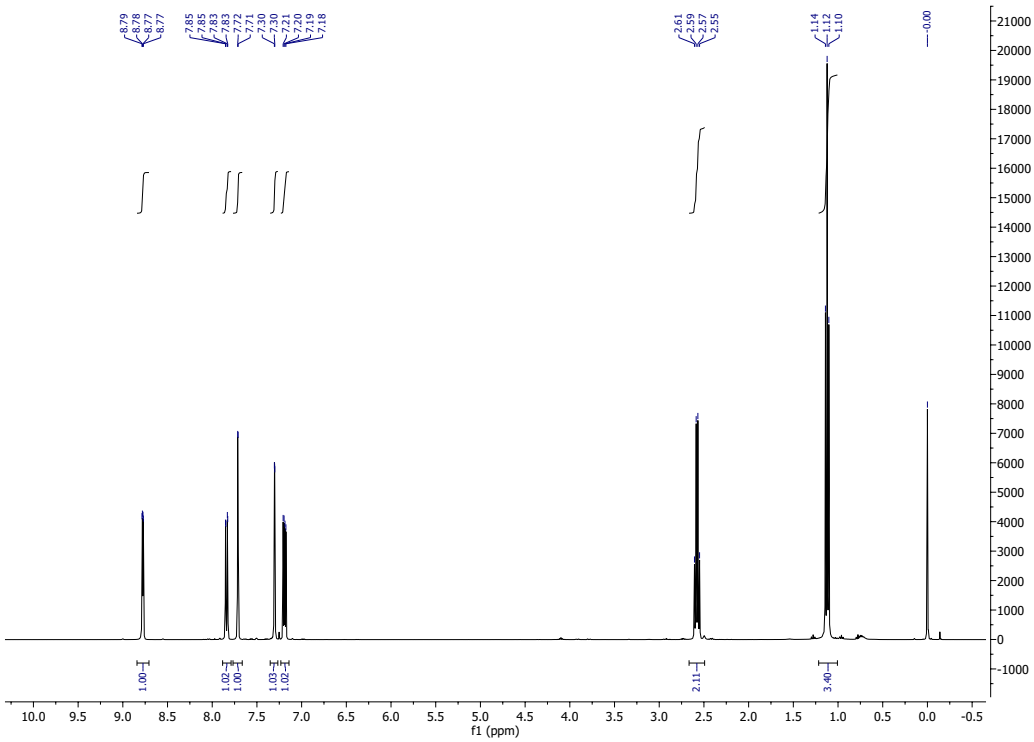

Figure 27: ^{1}H-NMR-spectrum of 8-bromo-6-ethyl-quinoline **6c**

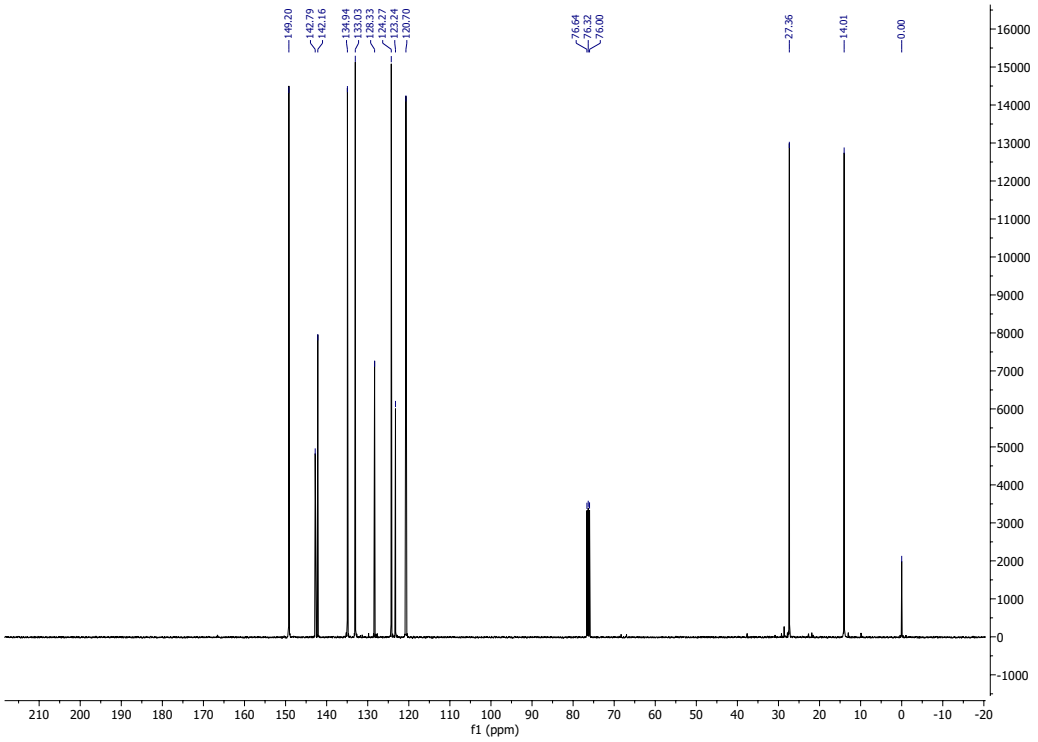

Figure 28: ^{13}C-NMR-spectrum of 8-bromo-6-ethyl-quinoline **6c**

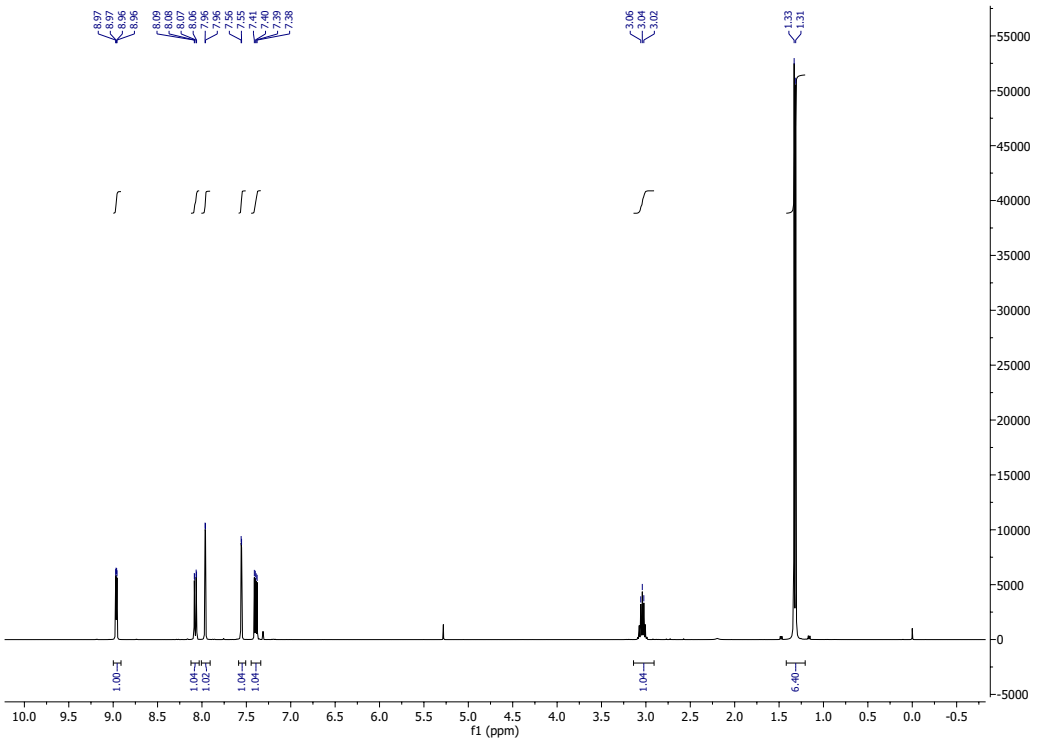

Figure 29: ^{1}H-NMR-spectrum of 8-bromo-6-(1-methylethyl)-quinoline **6d**

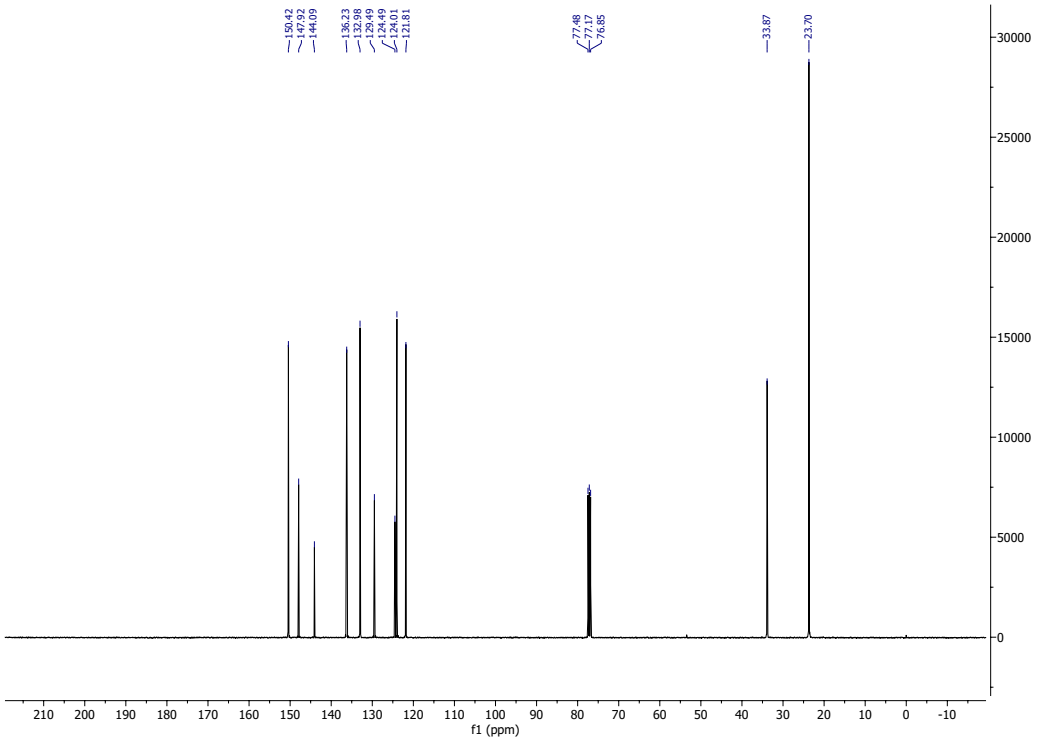

Figure 30: ^{13}C-NMR-spectrum of 8-bromo-6-(1-methylethyl)-quinoline **6d**

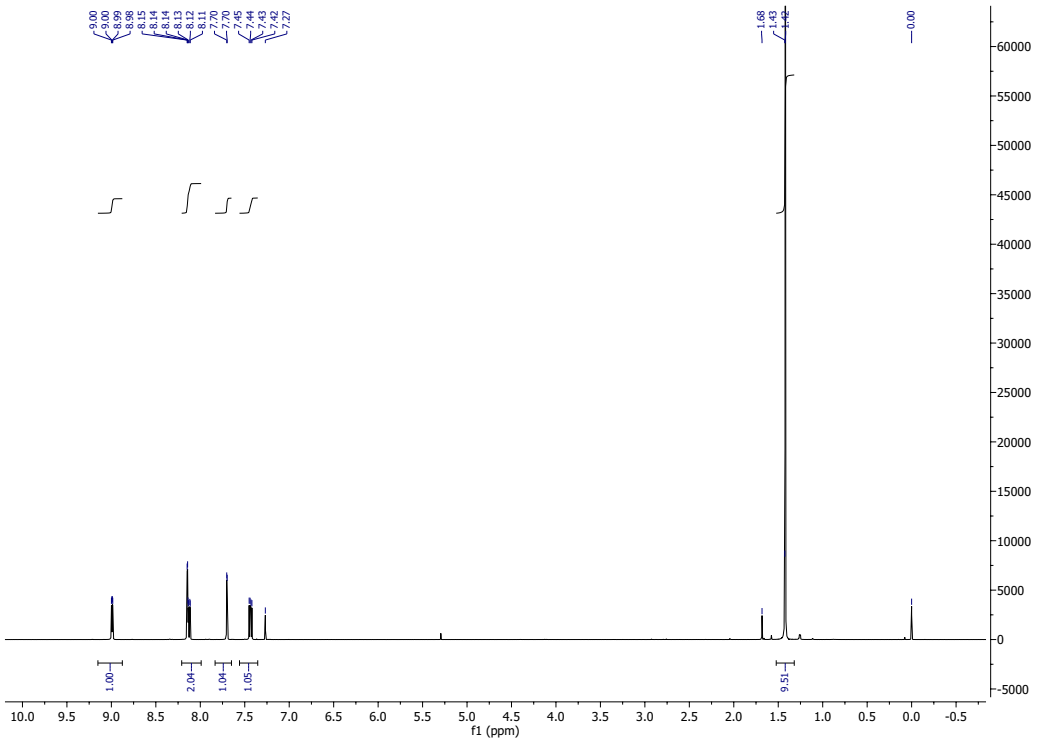

Figure 31: ^{1}H-NMR-spectrum of 8-bromo-6-(1,1-dimethylethyl)-quinoline **6e**

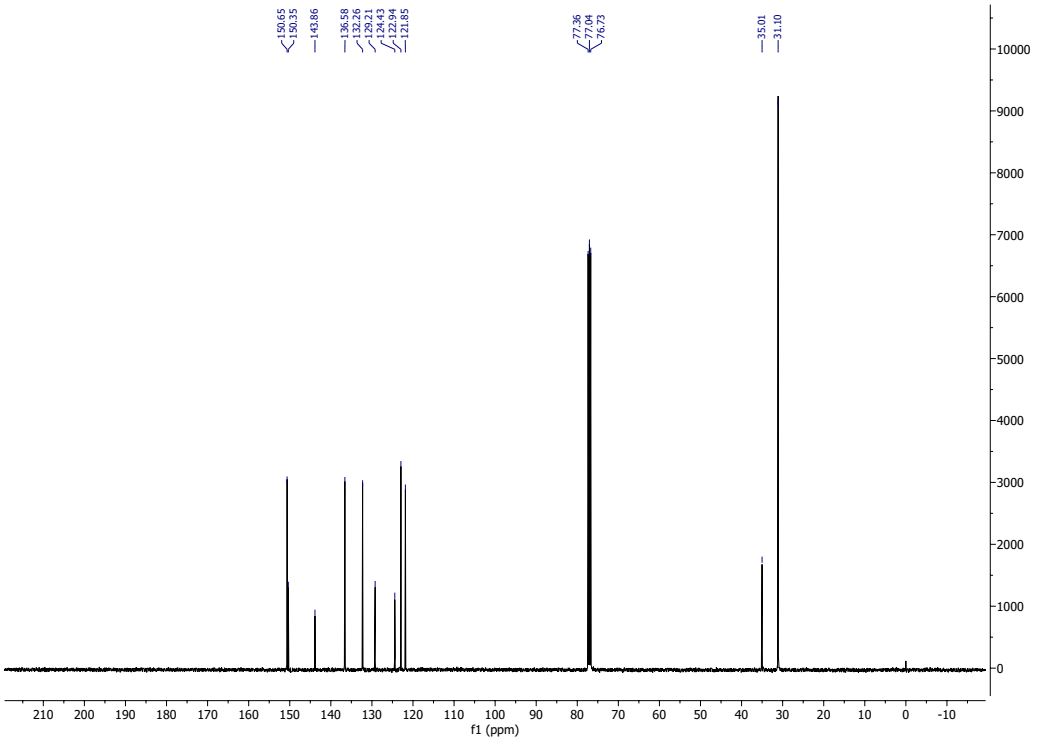

Figure 32: ^{13}C-NMR-spectrum of 8-bromo-6-(1,1-dimethylethyl)-quinoline **6e**

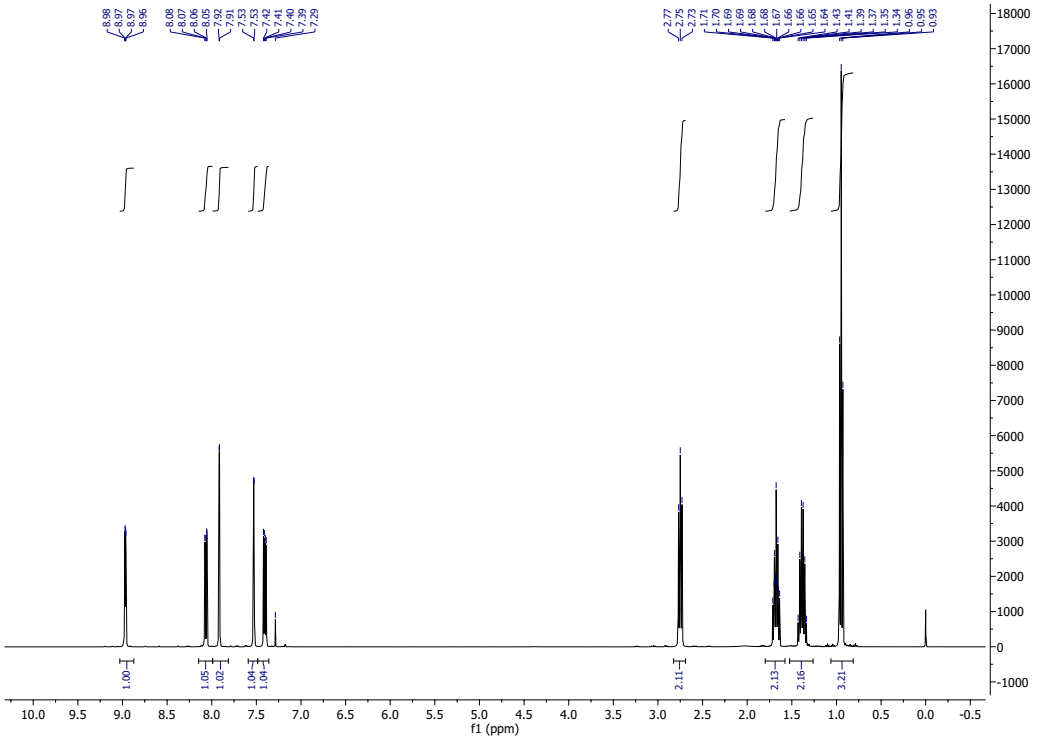

Figure 33: ^{1}H-NMR-spectrum of 8-bromo-6-butyl-quinoline **6f**

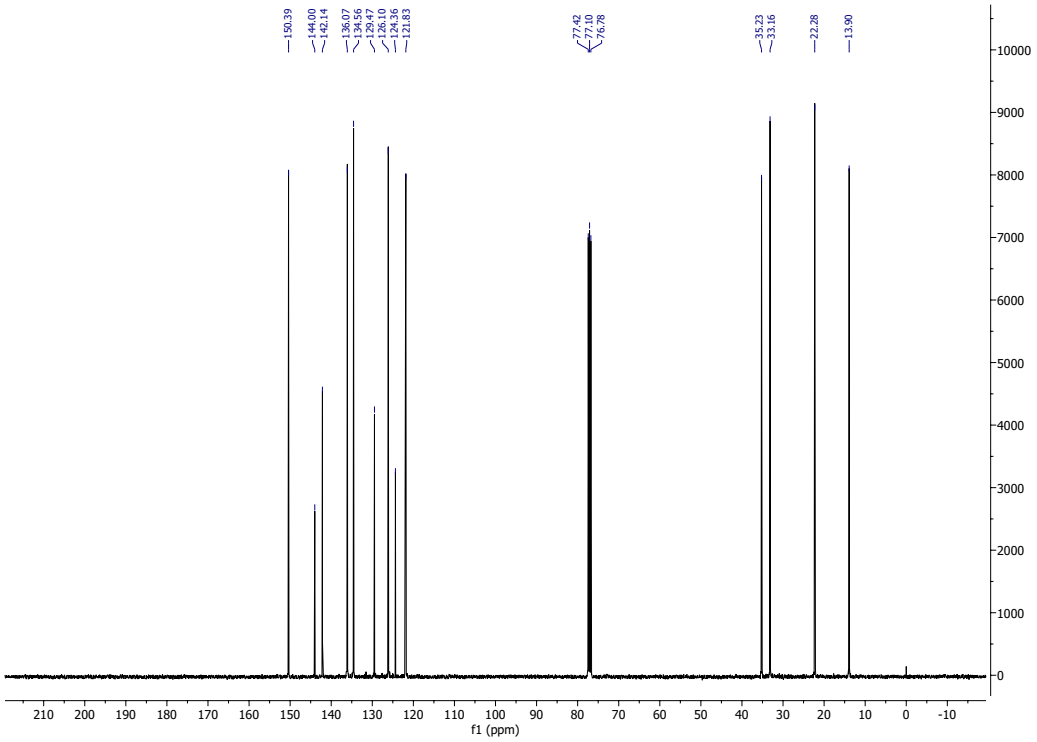

Figure 34: ^{13}C-NMR-spectrum of 8-bromo-6-butyl-quinoline **6f**

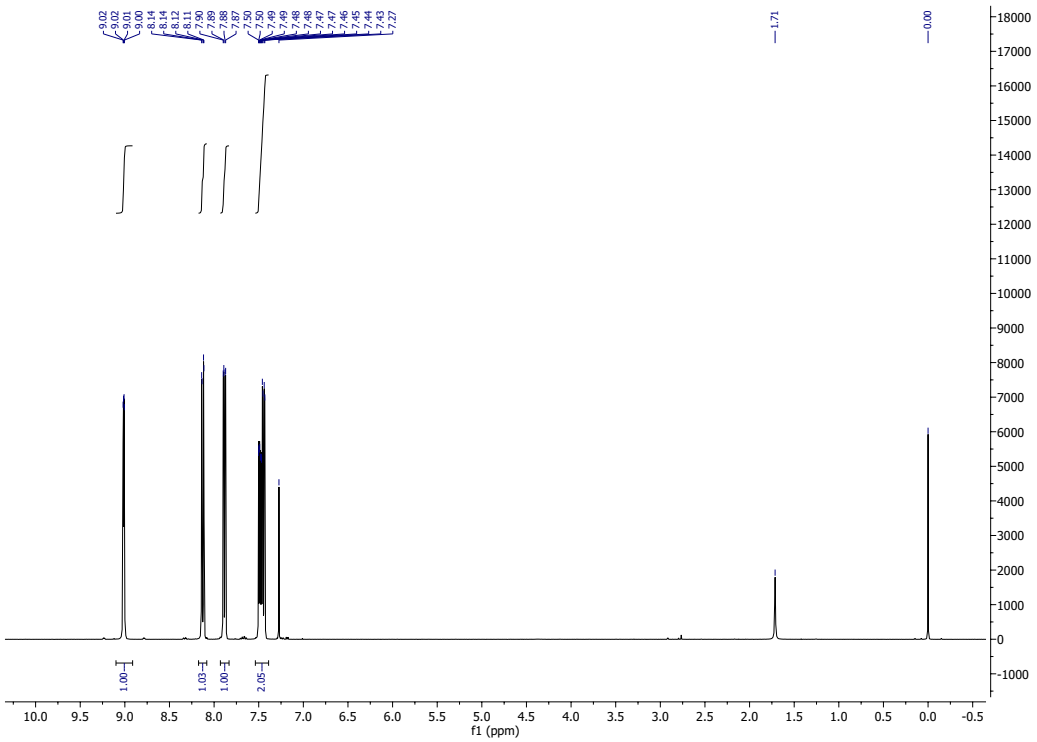

Figure 35: ^{1}H-NMR-spectrum of 8-bromo-6-fluoro-quinoline **6g**

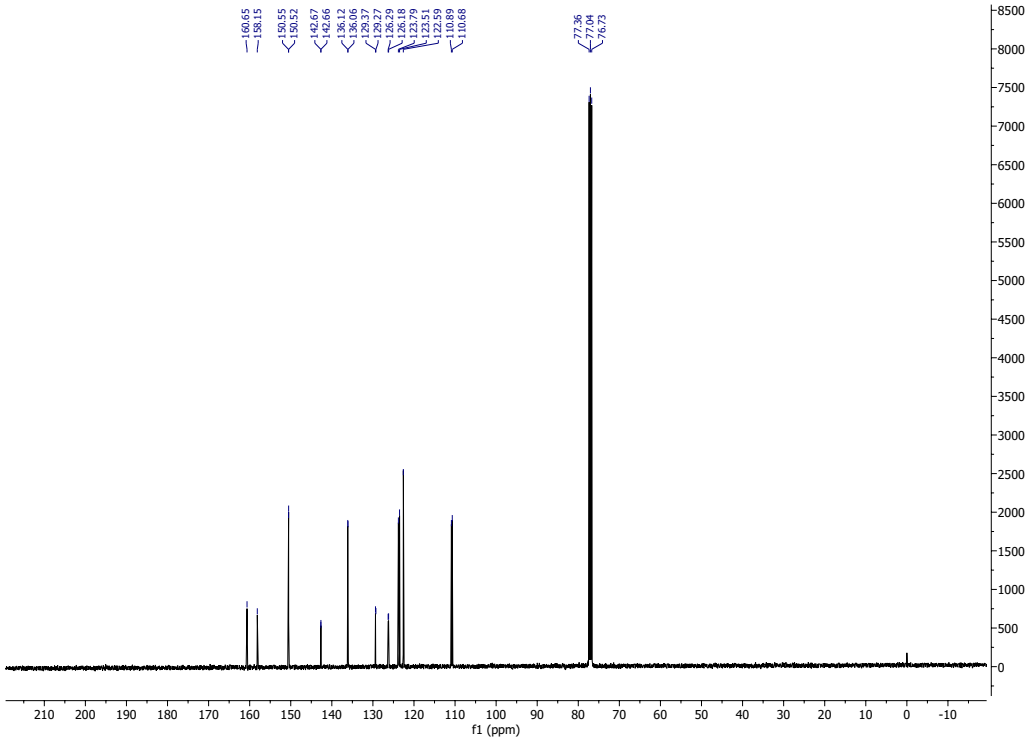

Figure 36: ^{13}C-NMR-spectrum of 8-bromo-6-fluoro-quinoline **6g**

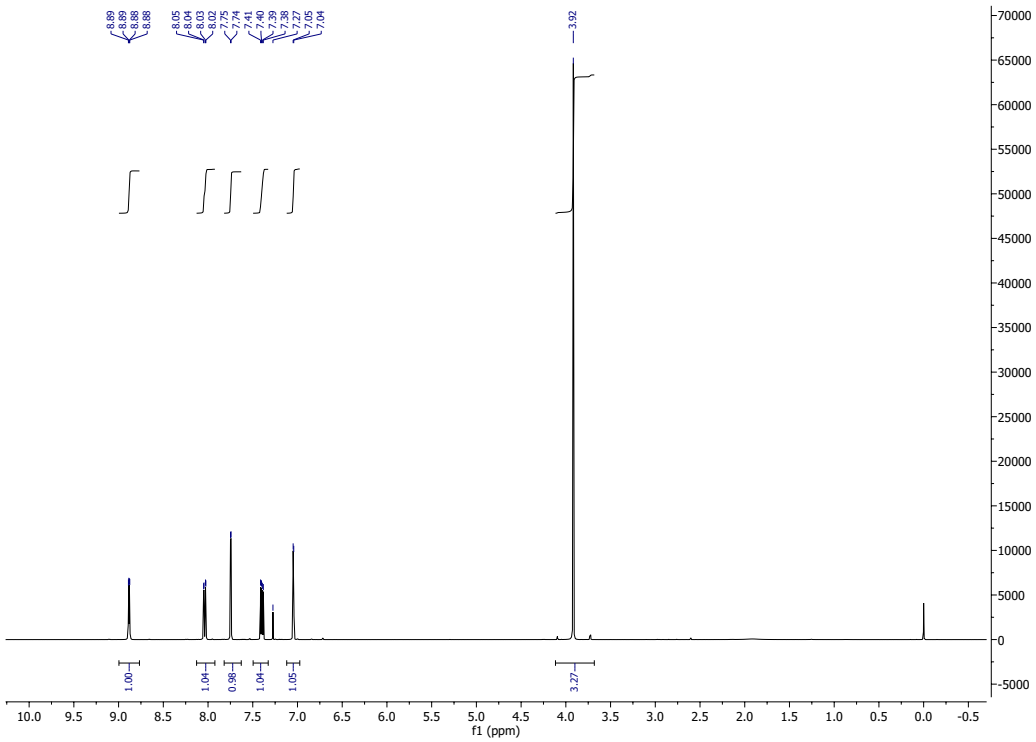

Figure 37: ^{1}H-NMR-spectrum of 8-bromo-6-methoxy-quinoline **6h**

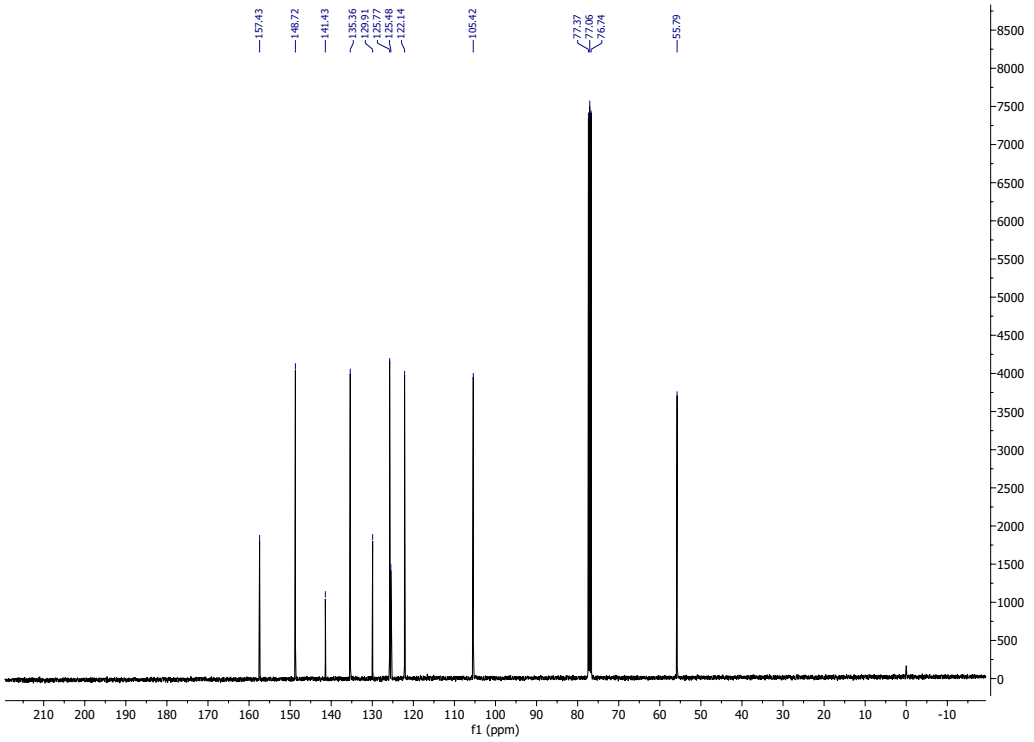

Figure 38: ^{13}C-NMR-spectrum of 8-bromo-6-methoxy-quinoline **6h**

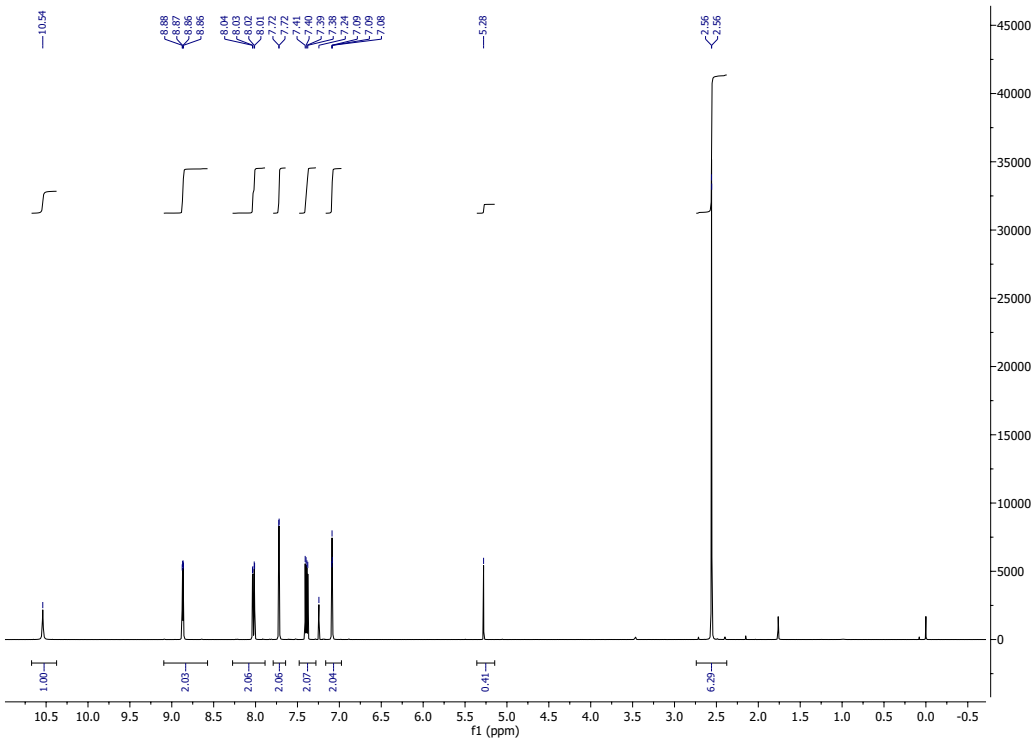

Figure 39: ^{1}H-NMR-spectrum of 6-Methyl-N-(6-methyl-8-quinolinyl)-8-quinolinamine **5b**

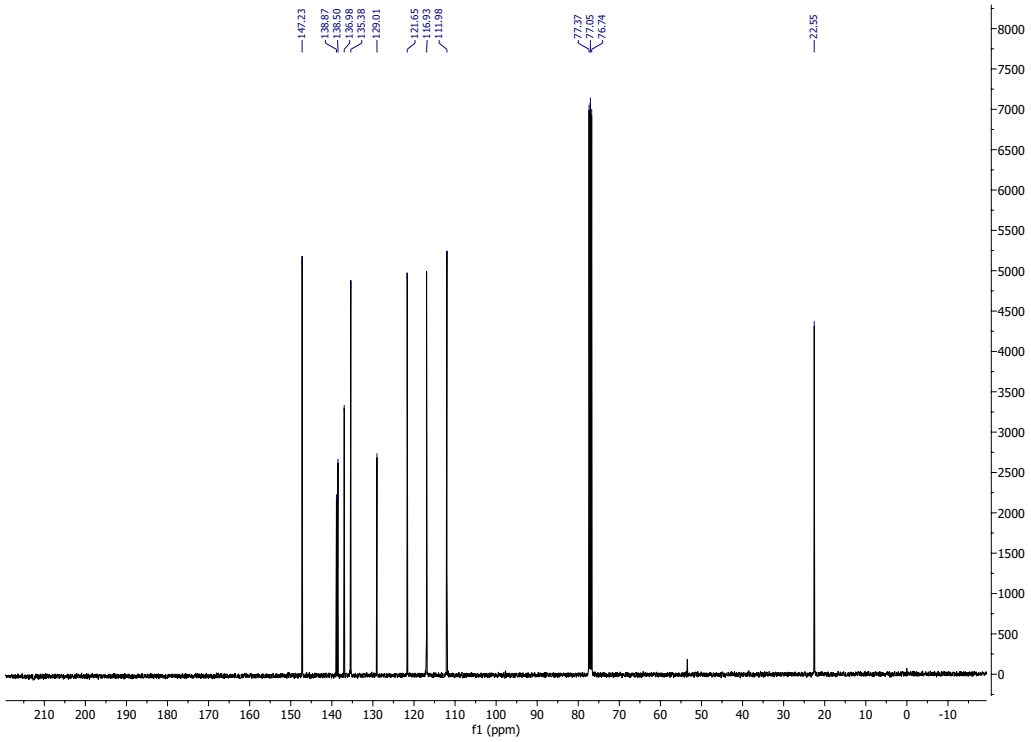

Figure 40: ^{13}C-NMR-spectrum of 6-Methyl-N-(6-methyl-8-quinolinyl)-8-quinolinamine **5b**

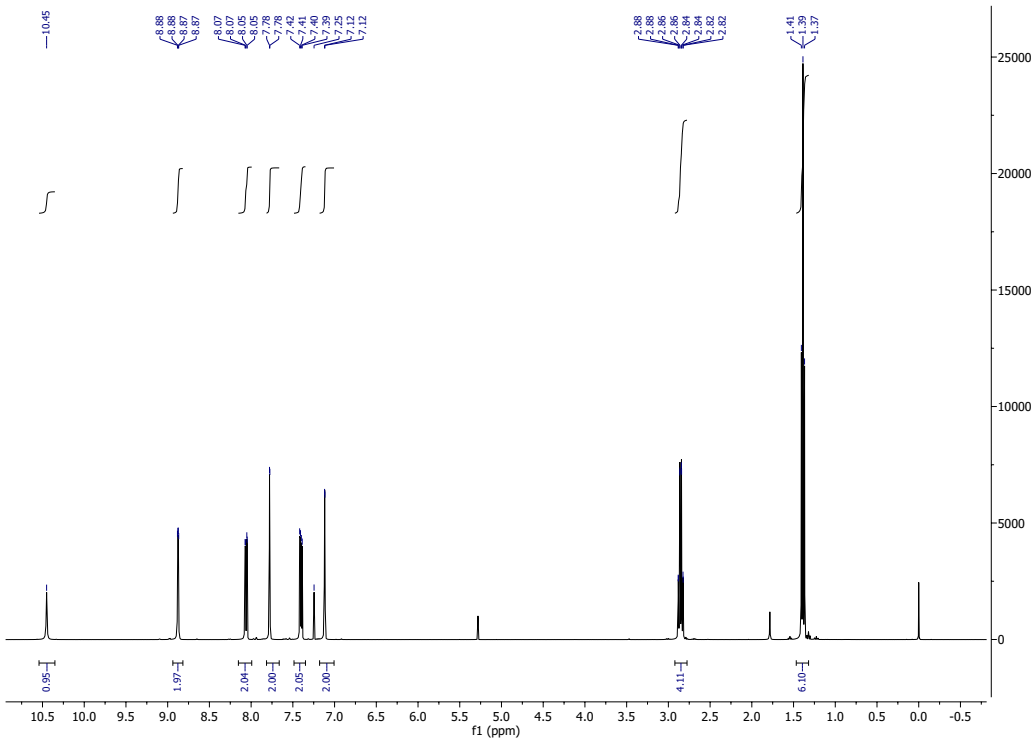

Figure 41: ^{1}H-NMR-spectrum of 6-ethyl-N-(6-methyl-8-quinolinyl)-8-quinolinamine **5c**

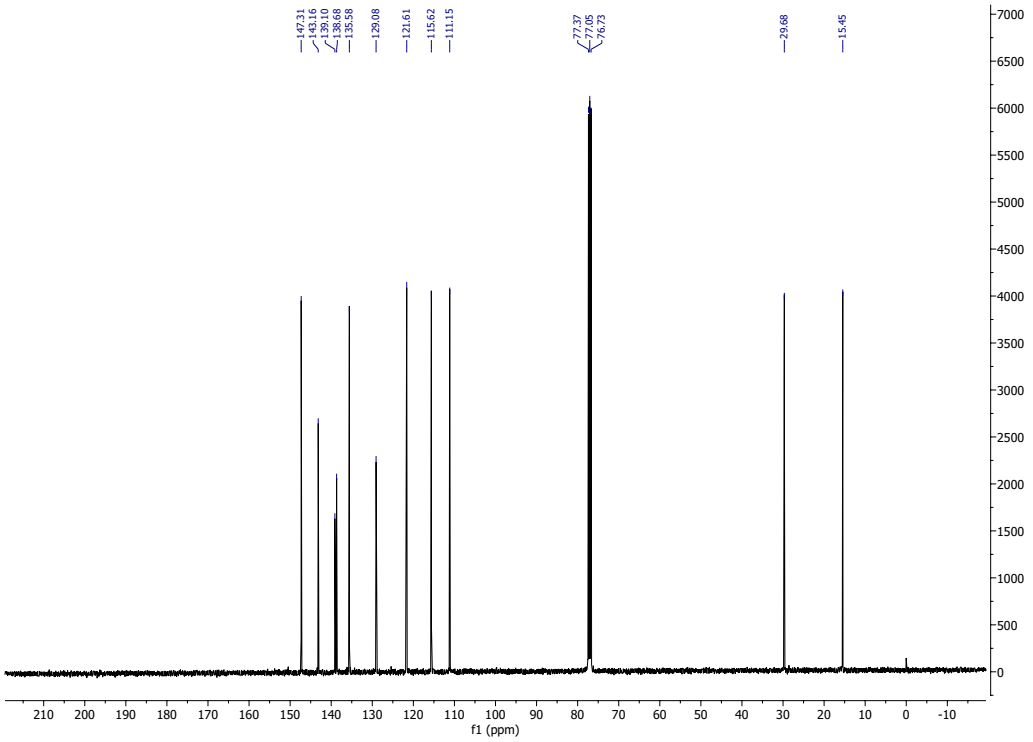

Figure 42: ^{13}C-NMR-spectrum of 6-ethyl-N-(6-methyl-8-quinolinyl)-8-quinolinamine **5c**

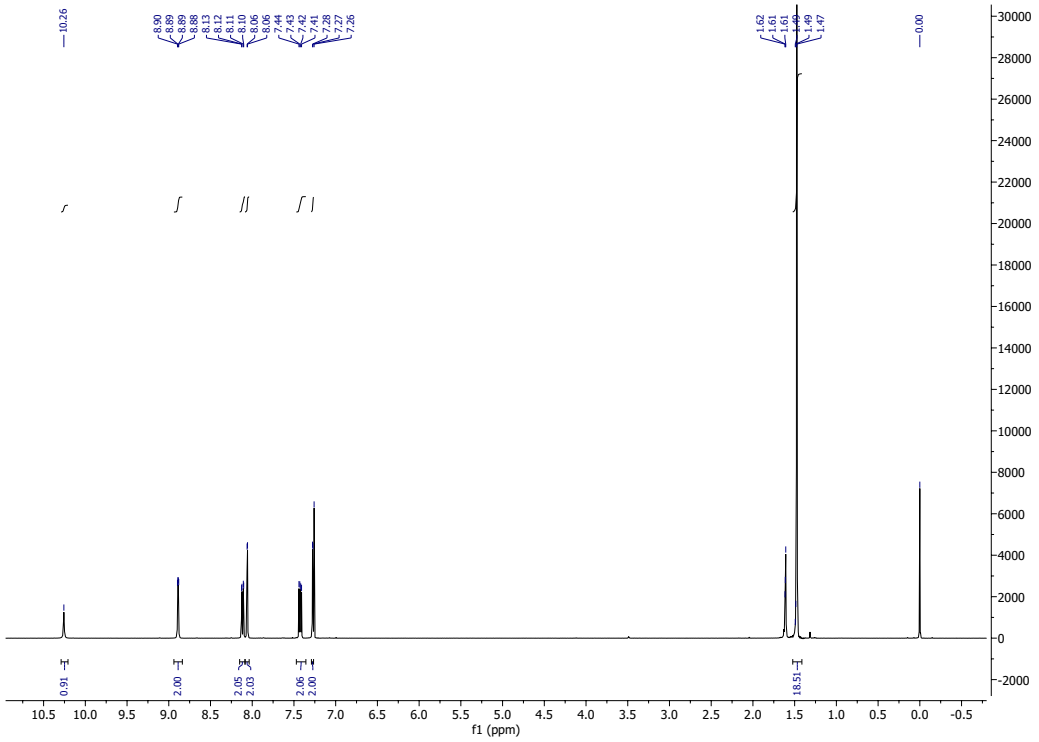

Figure 43: ^{1}H-NMR-spectrum of 6-(1,1-dimethylethyl)-N-(6-(1,1-dimethylethyl)-8-quinolinyl)-8-quinolinamine **5e**

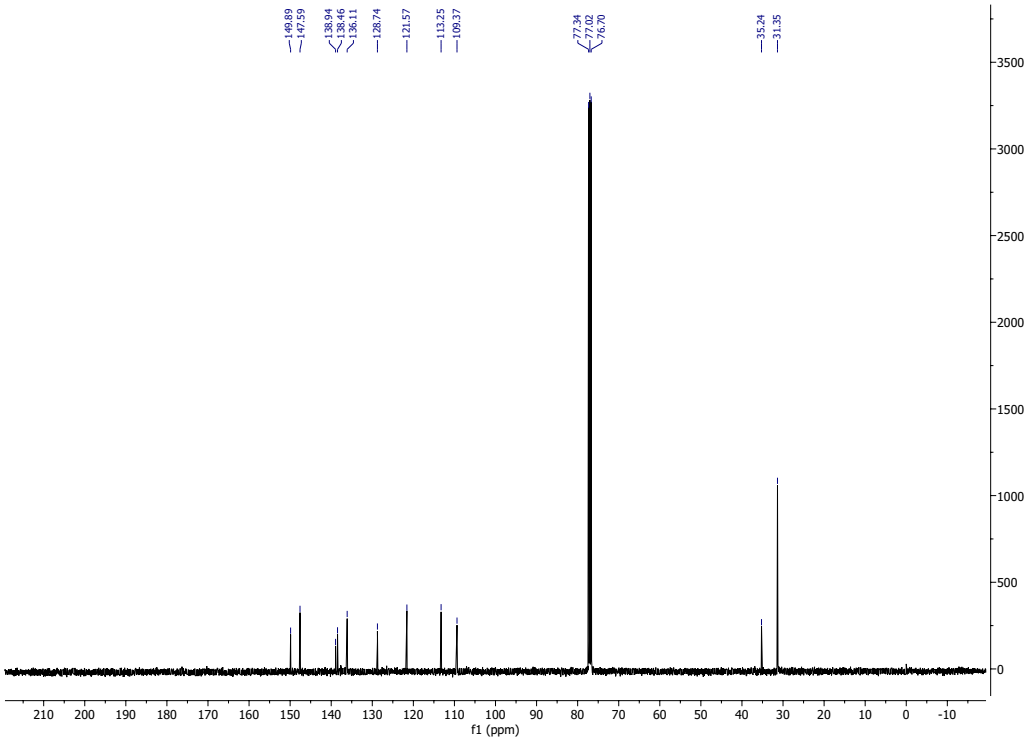

Figure 44: ^{13}C-NMR-spectrum of 6-(1,1-dimethylethyl)-N-(6-(1,1-dimethylethyl)-8-quinolinyl)-8-quinolinamine **5e**

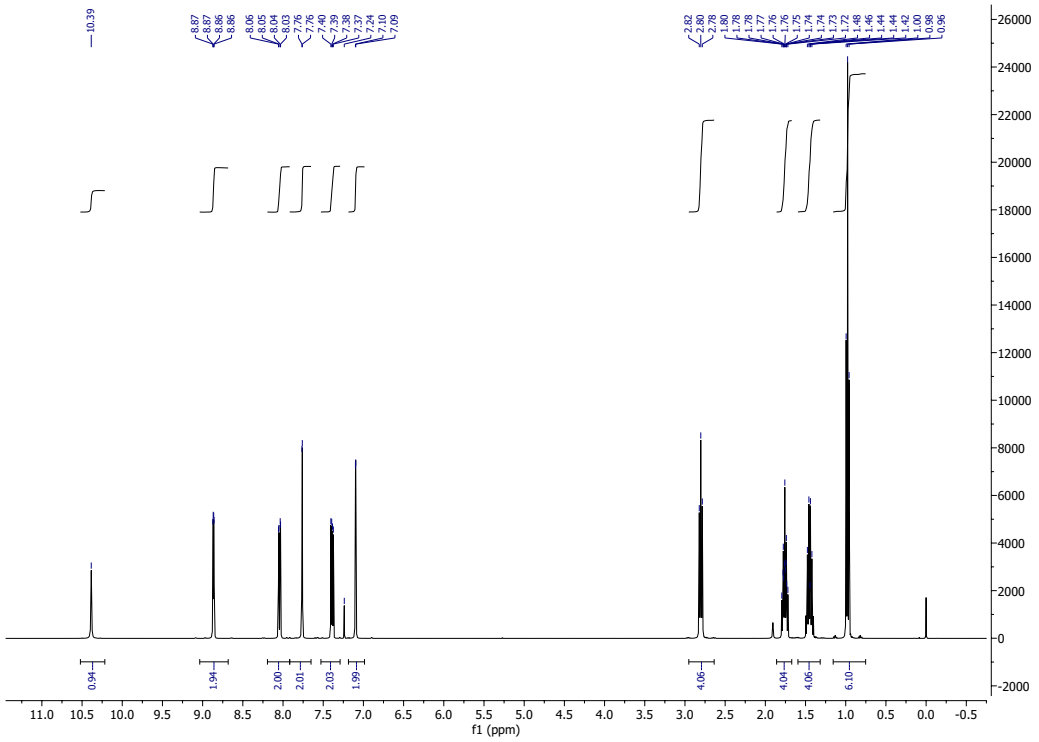

Figure 45: ^{1}H-NMR-spectrum of 6-Butyl-N-(6-butyl-8-quinolinyl)-8-quinolinamine **5f**

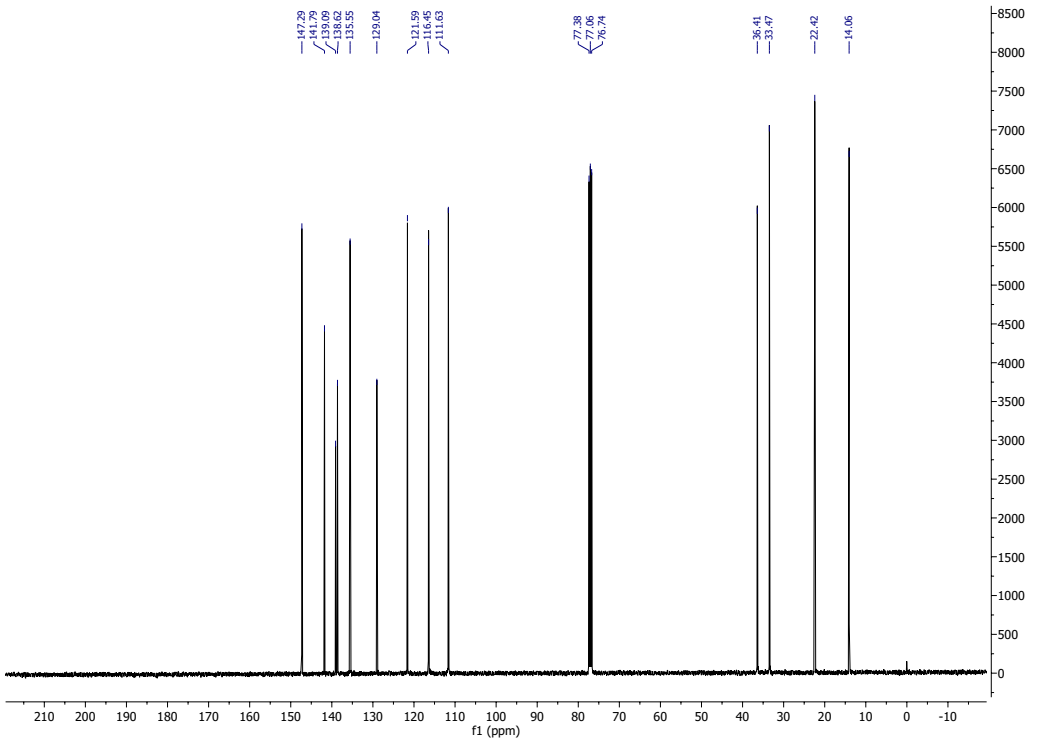

Figure 46: ^{13}C-NMR-spectrum of 6-Butyl-N-(6-butyl-8-quinolinyl)-8-quinolinamine **5f**

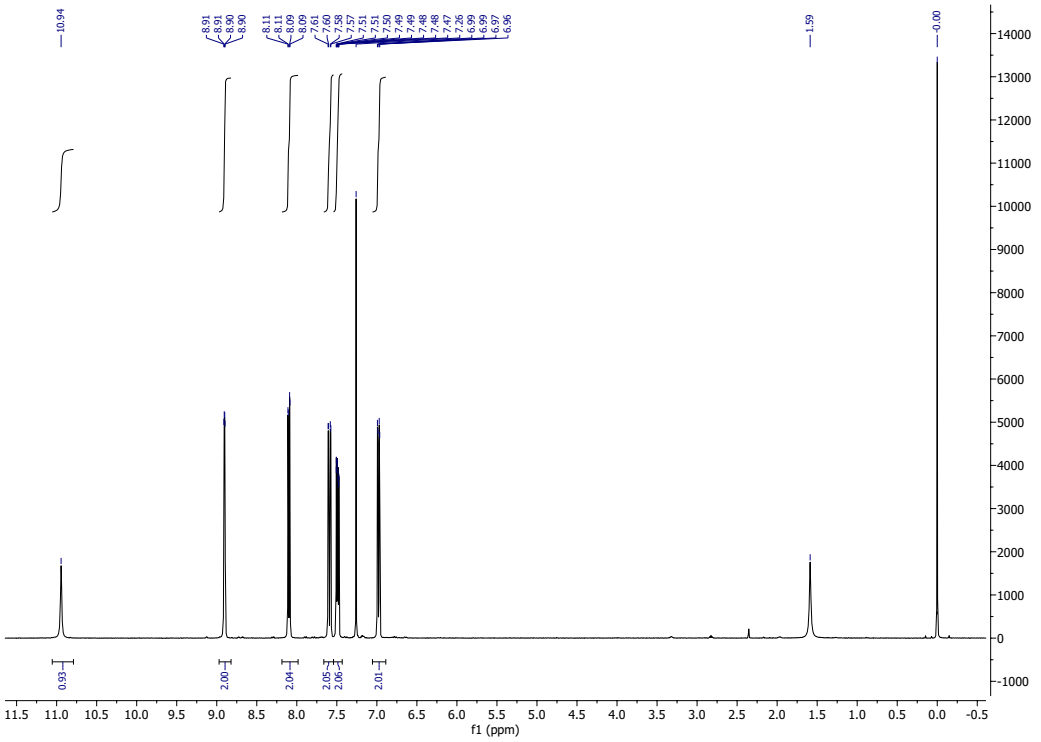

Figure 47: ^{1}H-NMR-spectrum of 6-fluoro-N-(6-fluoro-8-quinolinyl)-8-quinolinamine **5g**

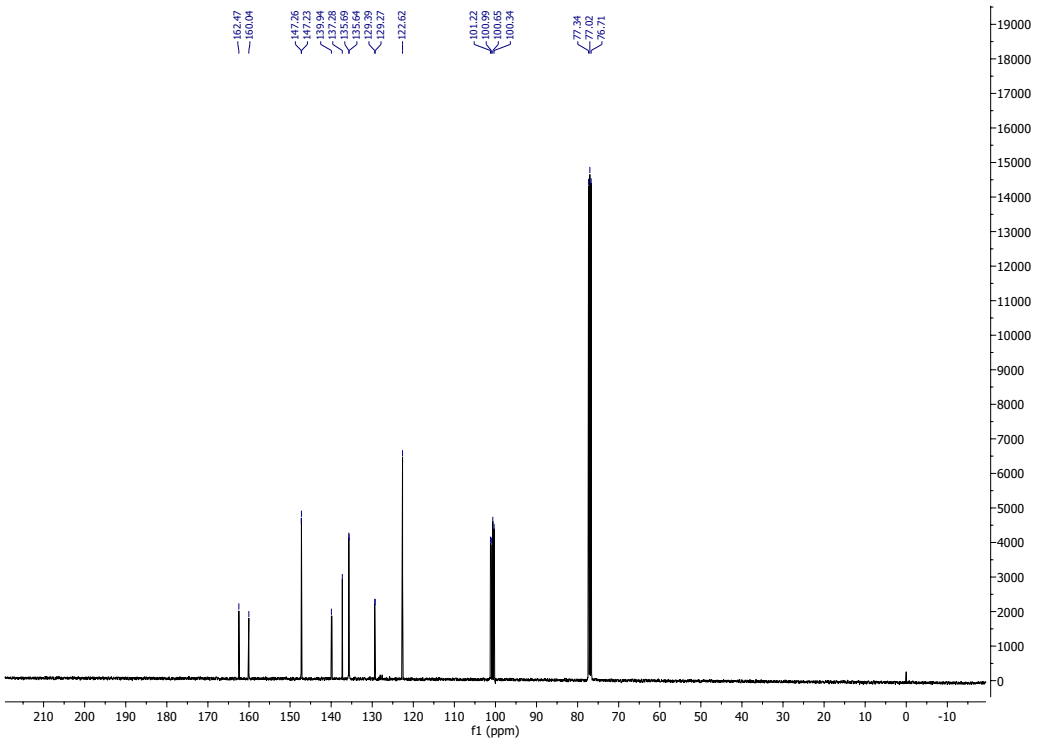

Figure 48: ^{13}C-NMR-spectrum of 6-fluoro-N-(6-fluoro-8-quinolinyl)-8-quinolinamine **5g**

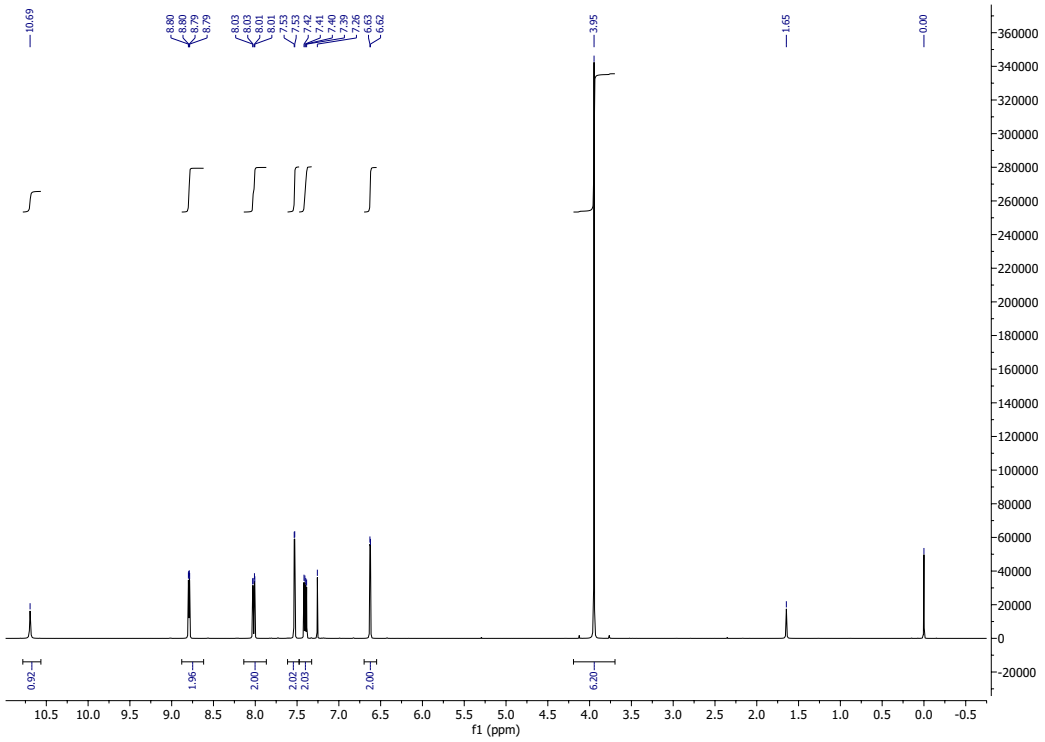

Figure 49: ^{1}H-NMR-spectrum of 6-methoxy-N-(6-methoxy-8-quinolinyl)-8-quinolinamine **5h**

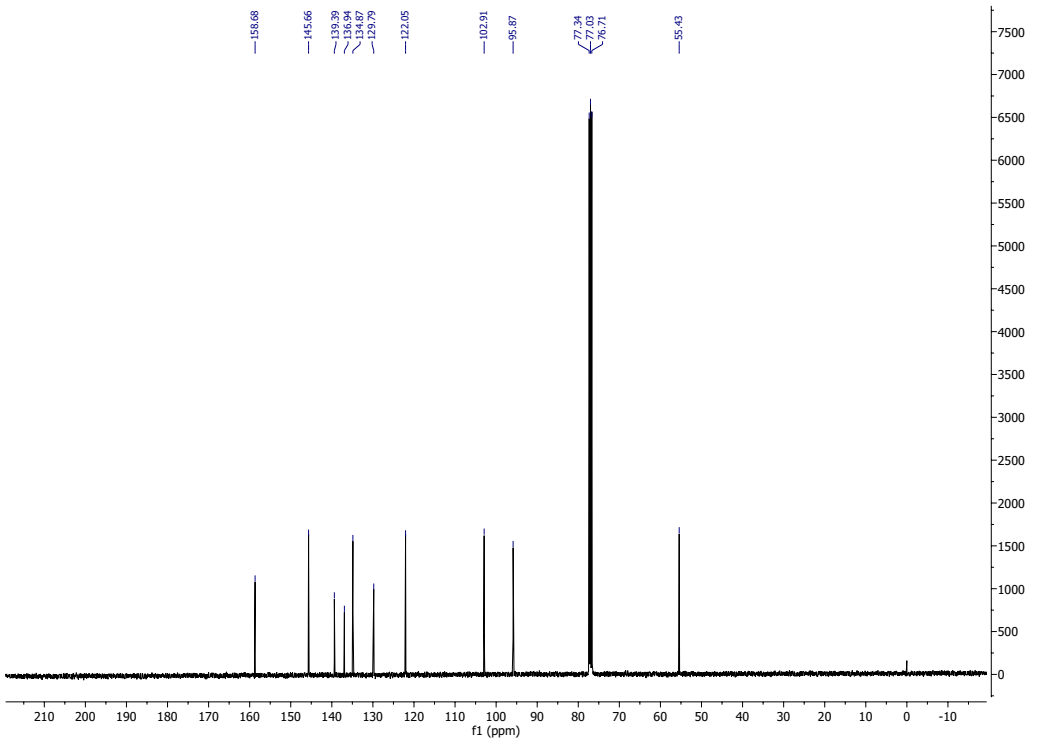

Figure 50: ^{13}C-NMR-spectrum of 6-methoxy-N-(6-methoxy-8-quinolinyl)-8-quinolinamine **5h**

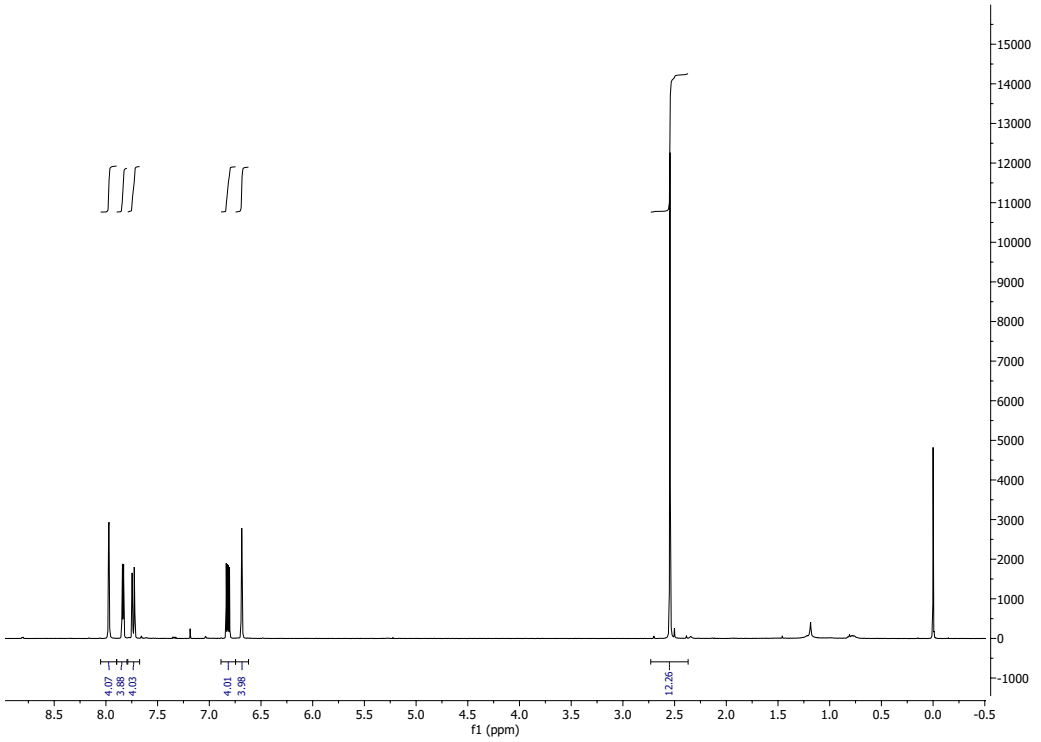

Figure 51: ^{1}H-NMR-spectrum of zinc complex **1b**

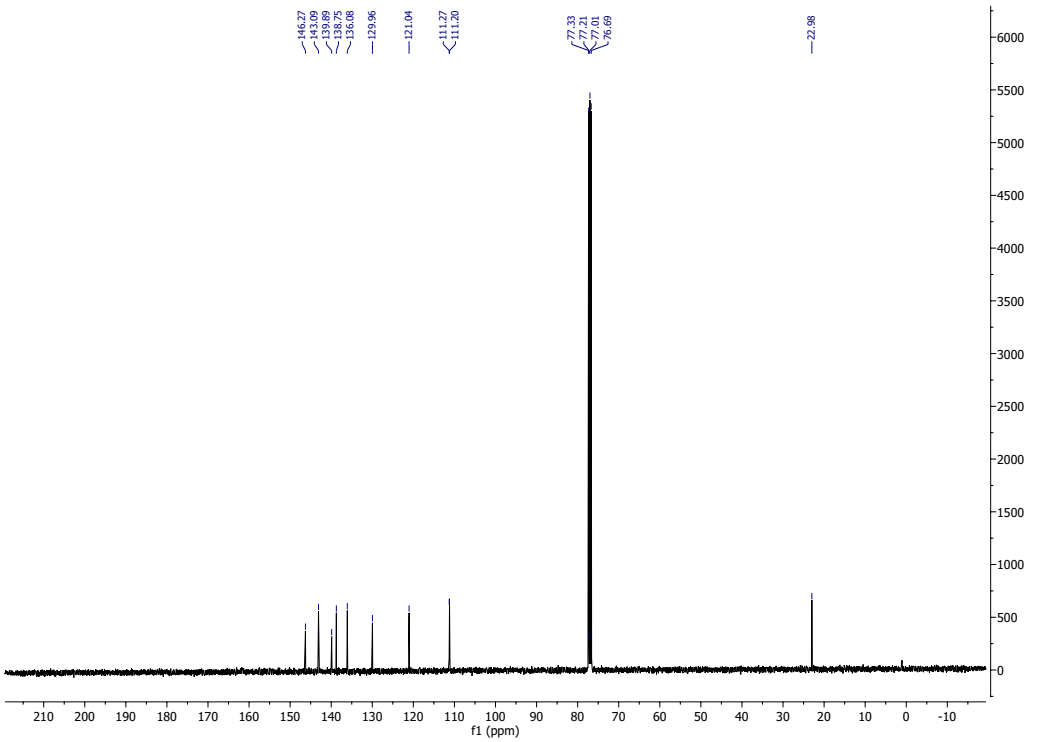

Figure 52: ^{13}C-NMR-spectrum of zinc complex **1b**

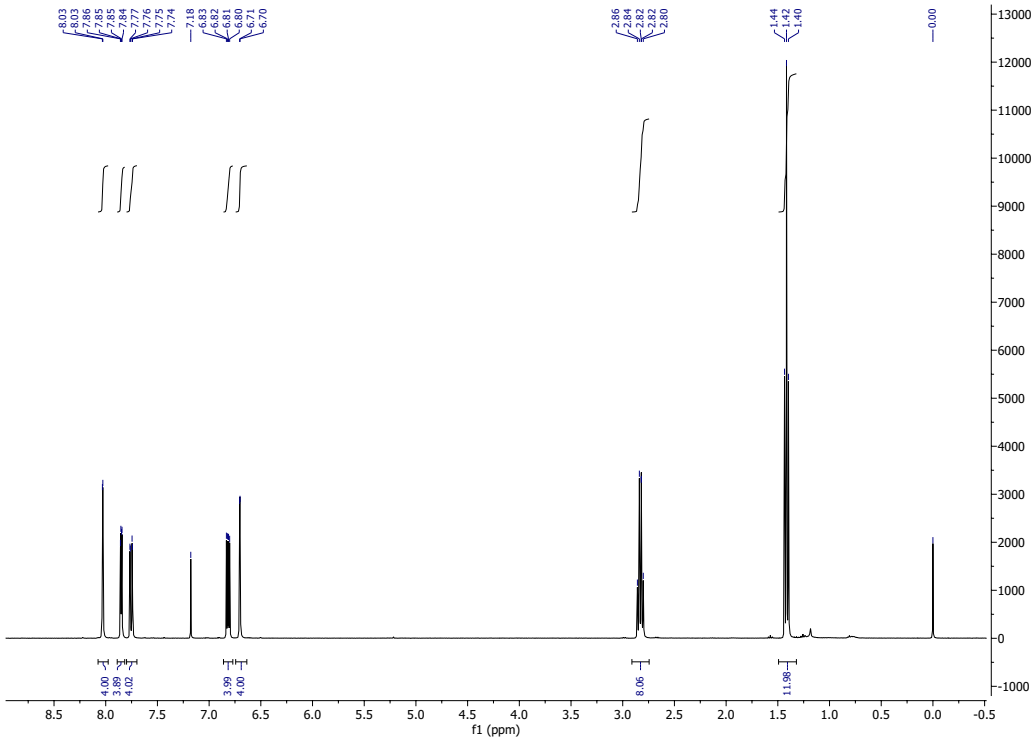

Figure 53: ^{1}H-NMR-spectrum of zinc complex **1c**

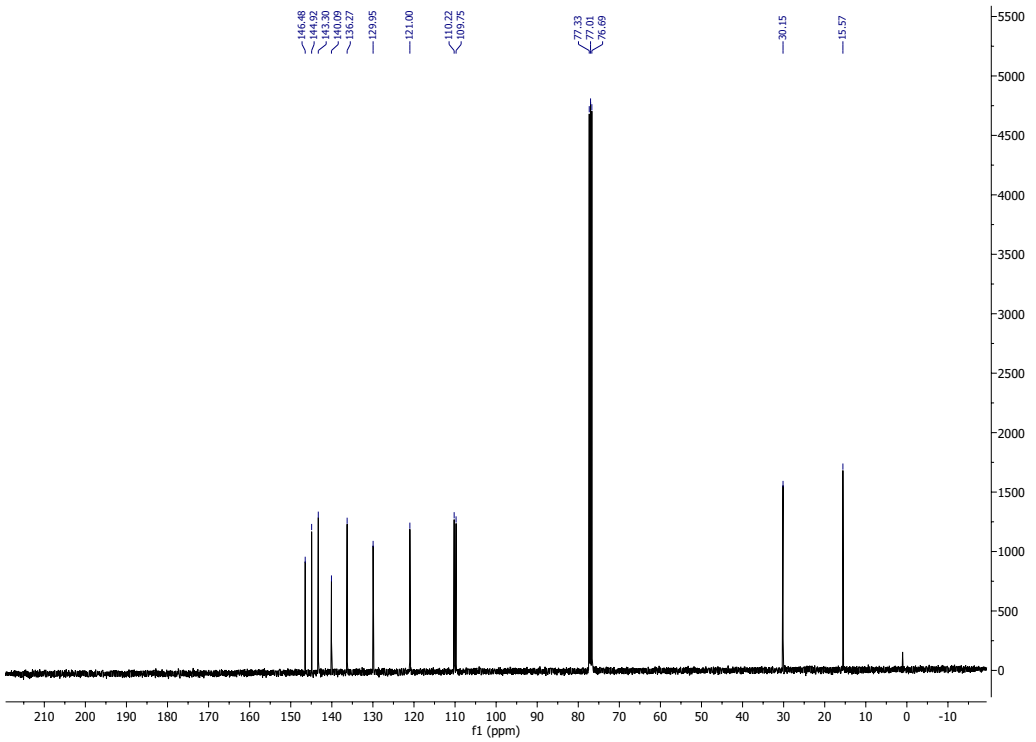

Figure 54: ^{13}C-NMR-spectrum of zinc complex **1c**

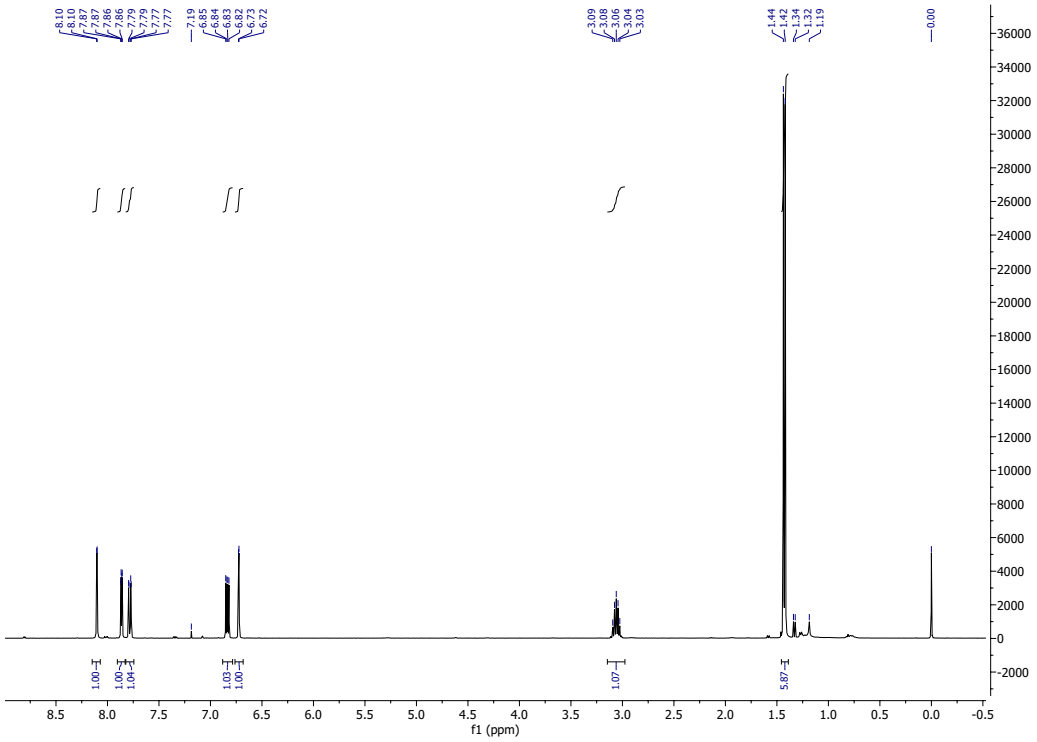

Figure 55: ^{1}H-NMR-spectrum of zinc complex **1d**

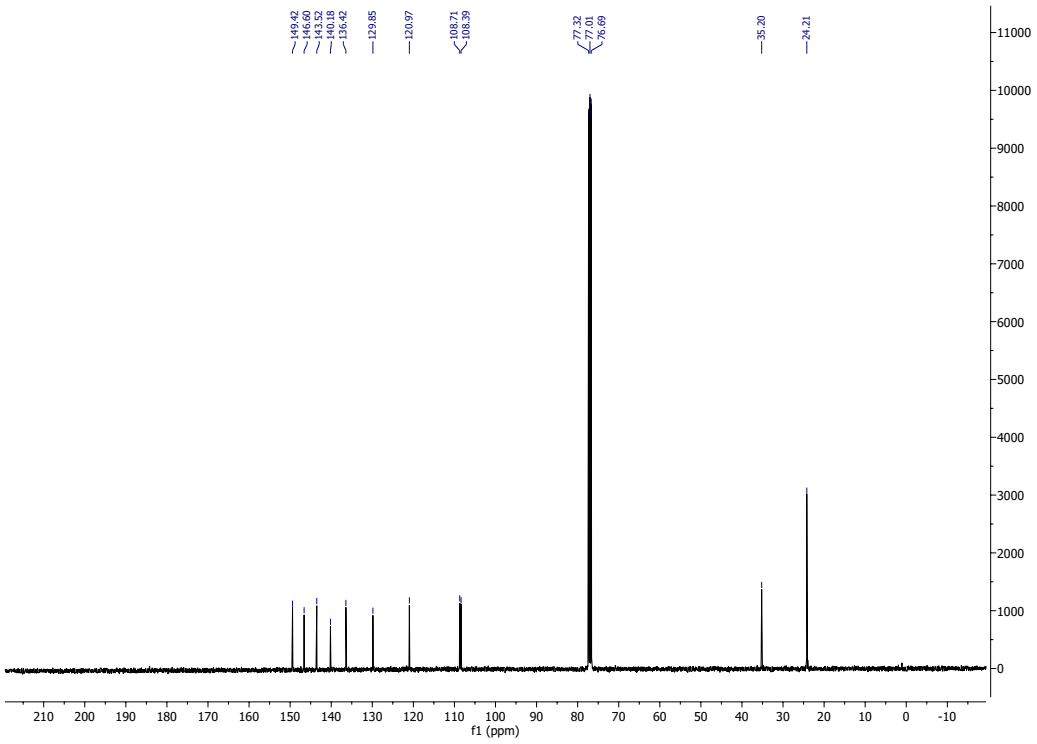

Figure 56: ^{13}C-NMR-spectrum of zinc complex **1d**

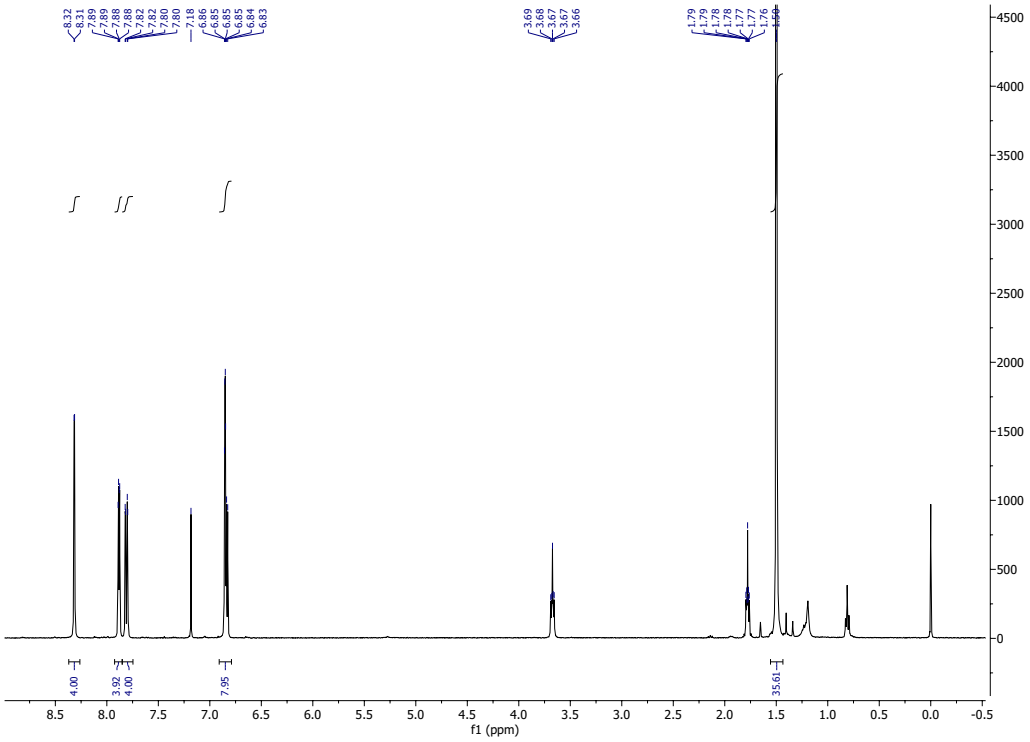

Figure 57: ^{1}H-NMR-spectrum of zinc complex **1e**

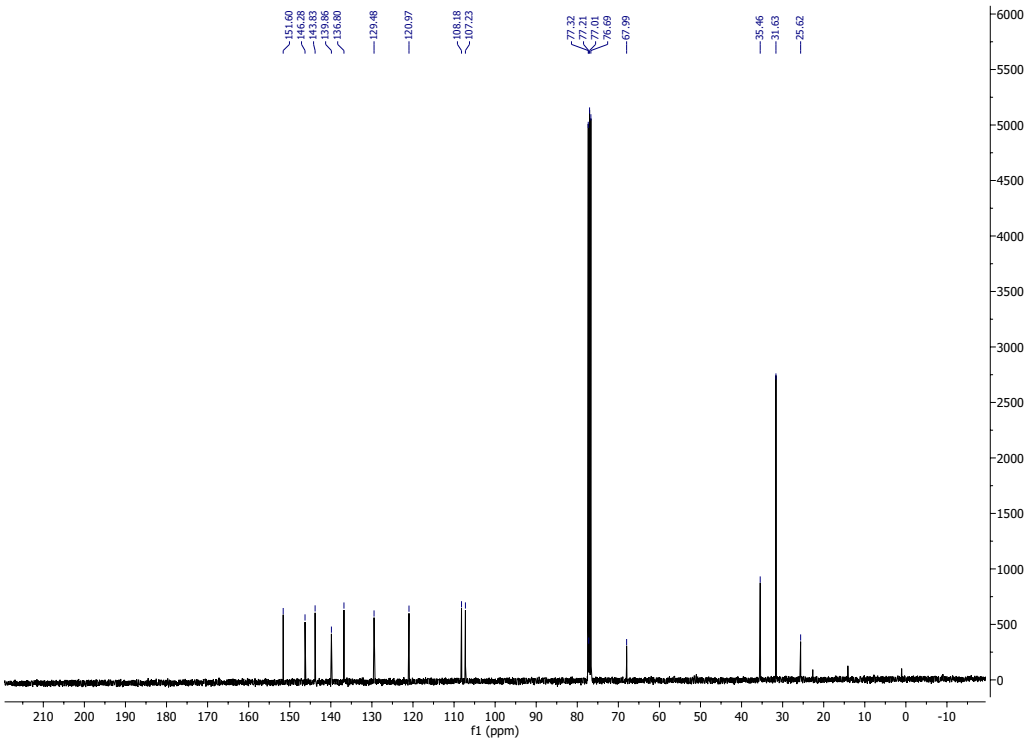

Figure 58: ^{13}C-NMR-spectrum of zinc complex **1e**

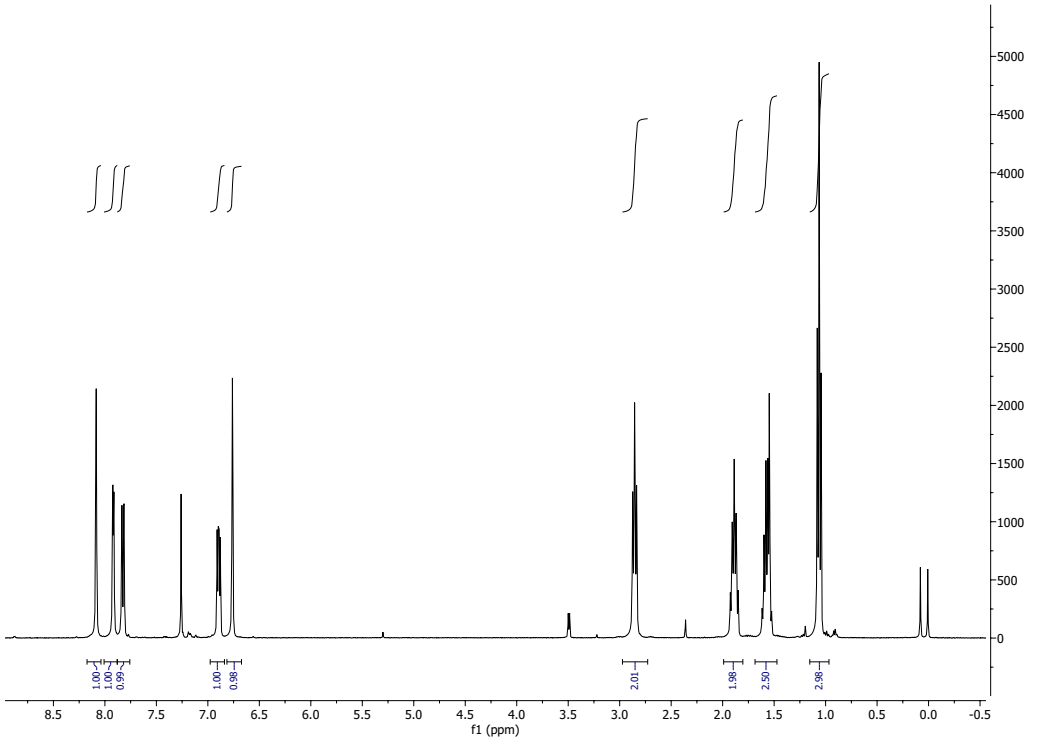

Figure 59: ^{1}H-NMR-spectrum of zinc complex **1f**

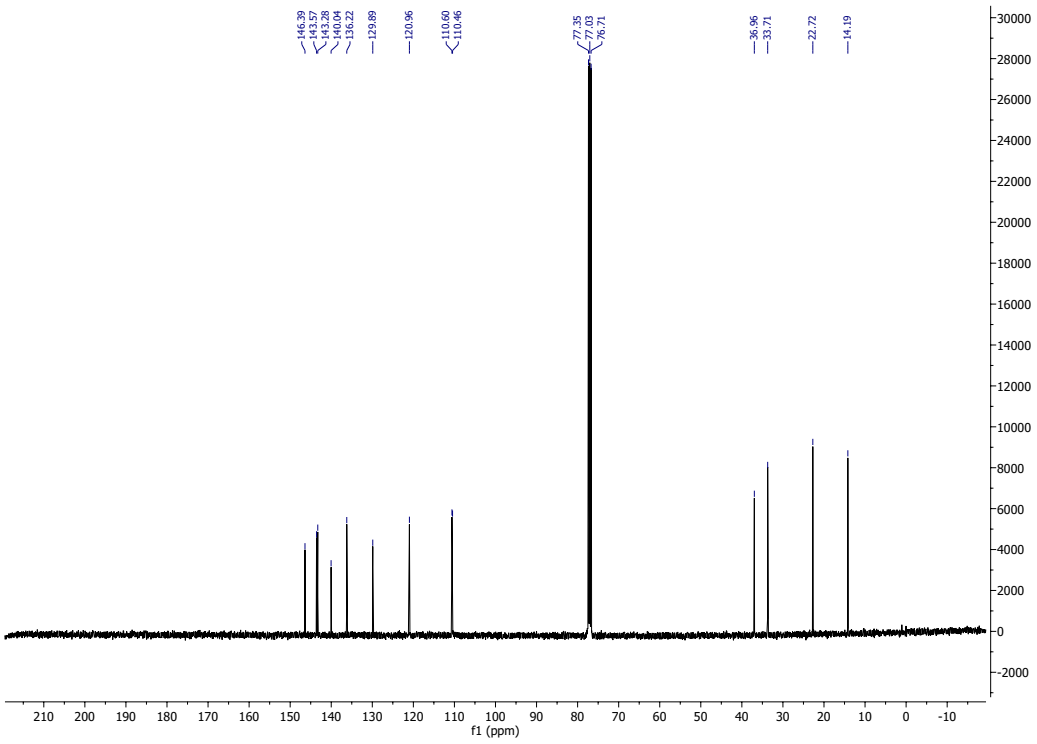

Figure 60: ^{13}C-NMR-spectrum of zinc complex **1f**

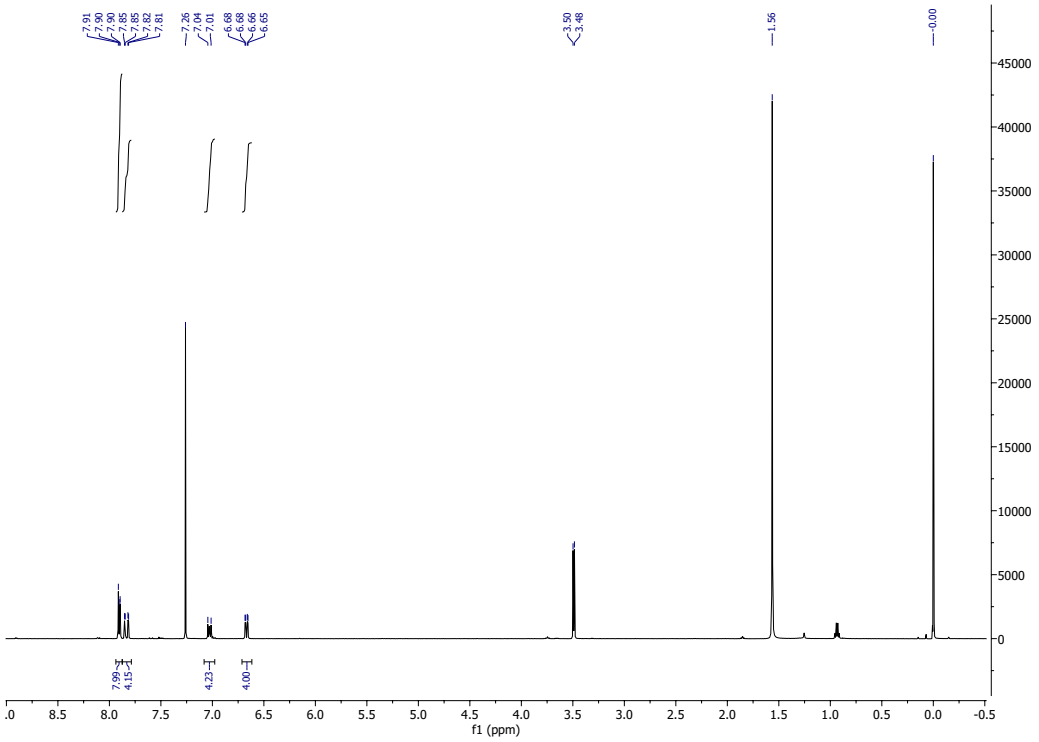

Figure 61: ^{1}H-NMR-spectrum of zinc complex **1g**

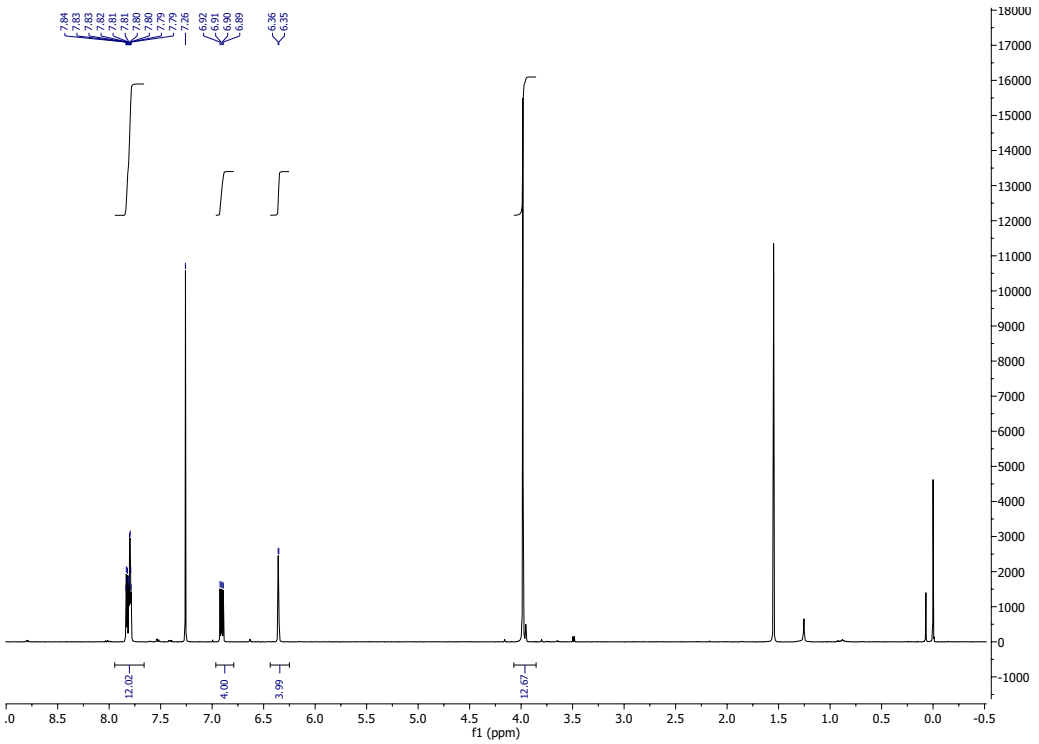

Figure 62: ^{1}H-NMR-spectrum of zinc complex **1h**

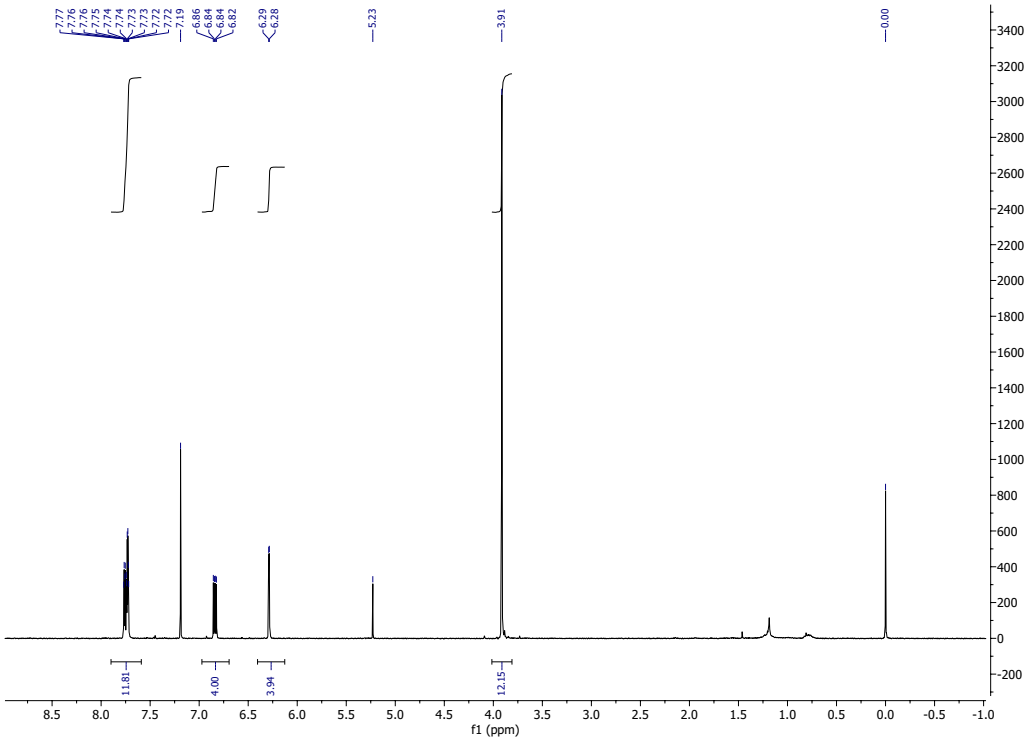

Figure 63: ^{13}C-NMR-spectrum of zinc complex **1h**

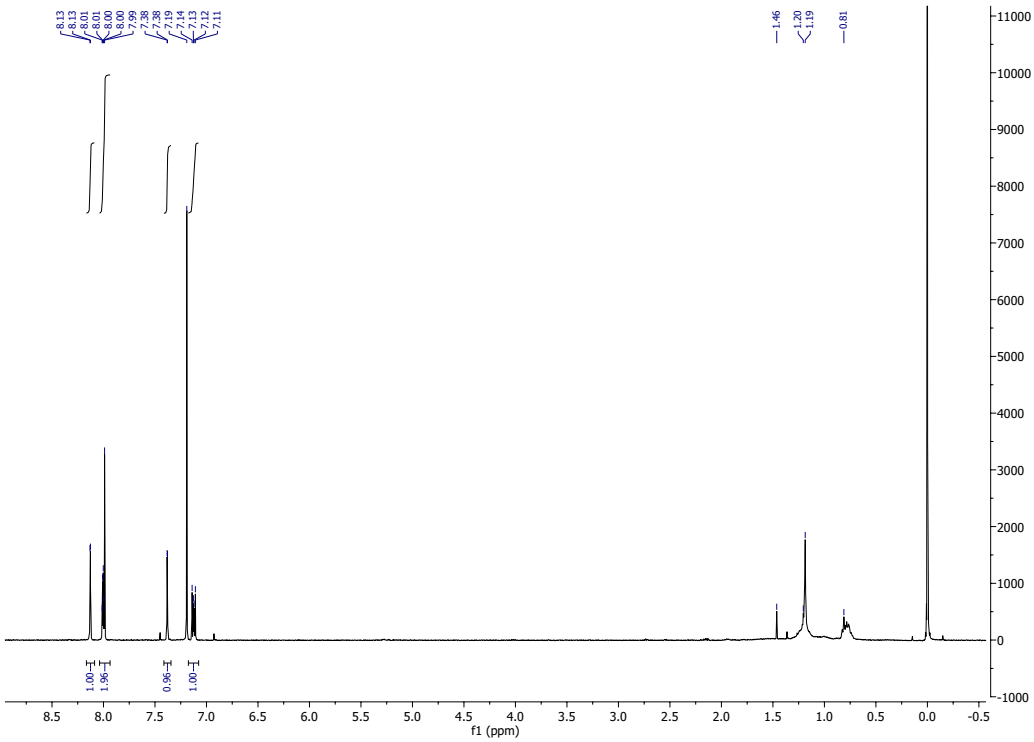

Figure 64: ^{1}H-NMR-spectrum of zinc complex **1i**

2 Crystallography

Crystallographic data were collected at low temperatures (100 K) using ϕ- and ω-scans on a BRUKER D8 Venture system equipped with dual IμS microfocus sources, a PHOTON100 detector and an OXFORD CRYOSYSTEMS 700 low temperature system. Mo-Kα radiation with wavelength 0.71073 Å or Cu-Kα radiation with wavelength 1.54178 Å and a collimating Quazar multilayer mirror were used. Semi-empirical absorption corrections from equivalents were applied using SADABS-2016/2[1] the space groups were determined by systematic absences using XPREP and the structures were solved by direct methods using SHELXT.[2] Refinement for all structures was performed against F2 on all data by full-matrix least squares using SHELXL. [3] All non-hydrogen atoms were refined anisotropically and C-H hydrogen atoms were positioned at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2x or 1.5x (CH3 hydrogens) the Ueq value of the atoms they are linked to. The crystallographic data were deposited at the Cambridge Crystallographic Data Centre as CCDC 1897889-1897893 and can be obtained free of charge. [4]

2.1 Zn-complex 1a

2.1.1 Crystals obtained by vapor diffusion

The unit cell of [Zn(BQA)2] was determined using 9567 reflections and the structure was solved in the hexagonal space group $P6_1$. Partial racemic twinning was found and the twin ratio was refined and converged to 0.035(9). The asymmetric unit contains one molecule of [Zn(BQA)2] as well as heavily disordered solvent molecules. The SQUEEZE [5] method as implemented in Platon[6] was used to include a model for the disordered solvent molecules. The obtained model was added as .fab-file to the refinement using SHELXL. SQUEEZE found one independent void with disordered solvent, located at 0.0 0.0 0.0, with a volume of 1179 Å^3. The equivalent of 279 electrons were identified in the void. This number of electrons corresponds to approximately 7 molecules of THF in the unit cell; however, there could also be n-hexane from the vapor diffusion in the crystal lattice which would change the amount of solvent molecules slightly.

Table 1: Crystal data and structure refinement for $Zn(BQA)_2$

CCDC No.	1897889
Empirical formula	C36 H24 N6 Zn
Formula weight	605.98
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Hexagonal
Space group	$P6_1$
Unit cell dimensions	a = 20.6945(4) Å $\alpha = 90°$.
	b = 20.6945(4) Å $\beta = 90°$.
	c = 13.5955(3) Å $\gamma = 120°$.
Volume	5042.4(2) $Å^3$
Z	6
Density (calculated)	1.197 Mg/m^3
Absorption coefficient	0.762 mm^{-1}
F(000)	1872
Crystal size	0.980 × 0.163 × 0.137 mm^3
Theta range for data collection	2.273 to 29.129°.
Index ranges	-28<=h<=28, -28<=k<=28, -18<=l<=18
Reflections collected	149185
Independent reflections	9051 [R(int) = 0.1439]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	9051 / 1 / 389
Goodness-of-fit on F2	0.980
Final R indices [I>2sigma(I)]	R1 = 0.0296, wR2 = 0.0645
R indices (all data)	R1 = 0.0377, wR2 = 0.0664
Absolute structure parameter	0.035(9)
Largest diff. peak and hole	0.342 and -0.302 e.$Å^{-3}$

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

	x	y	z	U(eq)
Zn(1)	755(1)	5084(1)	4934(1)	16(1)
N(1)	412(1)	5842(1)	4385(1)	19(1)
N(2)	1058(1)	5853(1)	6072(1)	17(1)
N(3)	1287(1)	4700(1)	5987(1)	17(1)
N(11)	1738(1)	5591(1)	3970(1)	17(1)
N(12)	500(1)	4282(1)	3863(1)	18(1)
N(13)	-345(1)	4188(1)	5380(1)	18(1)

Table 2 – continued from previous page

	x	y	z	U(eq)
C(1)	104(1)	5818(2)	3522(2)	24(1)
C(2)	-39(2)	6378(2)	3199(2)	30(1)
C(3)	128(2)	6963(2)	3802(2)	29(1)
C(4)	459(2)	7020(2)	4726(2)	24(1)
C(5)	607(1)	6442(1)	4996(2)	18(1)
C(6)	977(1)	6462(1)	5906(2)	18(1)
C(7)	1233(2)	7111(2)	6468(2)	25(1)
C(8)	1079(2)	7680(2)	6200(2)	28(1)
C(9)	694(2)	7641(2)	5364(2)	31(1)
C(10)	1306(1)	5697(1)	6920(2)	16(1)
C(11)	1387(1)	6008(1)	7863(2)	19(1)
C(12)	1659(2)	5780(2)	8659(2)	25(1)
C(13)	1864(1)	5253(2)	8571(2)	22(1)
C(14)	1762(1)	4889(2)	7653(2)	20(1)
C(15)	1462(1)	5090(1)	6854(2)	17(1)
C(16)	1923(2)	4306(2)	7501(2)	25(1)
C(17)	1758(2)	3937(2)	6625(2)	27(1)
C(18)	1416(1)	4145(2)	5887(2)	22(1)
C(21)	2351(1)	6243(1)	4076(2)	20(1)
C(22)	2922(1)	6546(2)	3367(2)	21(1)
C(23)	2824(1)	6156(2)	2513(2)	21(1)
C(24)	2167(1)	5462(1)	2359(2)	18(1)
C(25)	1634(1)	5189(1)	3128(2)	16(1)
C(26)	944(1)	4479(1)	3045(2)	16(1)
C(27)	809(2)	4127(2)	2130(2)	21(1)
C(28)	1337(2)	4417(2)	1367(2)	24(1)
C(29)	2010(2)	5060(2)	1467(2)	23(1)
C(30)	-90(1)	3587(1)	4042(2)	18(1)
C(31)	-281(2)	2912(2)	3594(2)	27(1)
C(32)	-929(2)	2241(2)	3855(2)	31(1)
C(33)	-1400(2)	2214(2)	4570(2)	32(1)
C(34)	-1220(2)	2873(2)	5105(2)	23(1)
C(35)	-558(1)	3548(1)	4860(2)	18(1)
C(36)	-1647(2)	2898(2)	5894(2)	29(1)
C(37)	-1419(2)	3538(2)	6412(2)	29(1)
C(38)	-759(2)	4179(2)	6131(2)	24(1)

Table 3: Selected bond lengths [Å] and angles [°] for complex **1a**

Zn(1)-N(12)	2.067(2)
Zn(1)-N(2)	2.080(2)
Zn(1)-N(1)	2.154(2)

Table 3 – continued from previous page

Zn(1)-N(3)	2.183(2)
Zn(1)-N(13)	2.183(2)
Zn(1)-N(11)	2.195(2)
N(12)-Zn(1)-N(2)	175.29(8)
N(12)-Zn(1)-N(1)	107.22(8)
N(2)-Zn(1)-N(1)	77.44(8)
N(12)-Zn(1)-N(3)	98.24(8)
N(2)-Zn(1)-N(3)	77.08(8)
N(1)-Zn(1)-N(3)	154.40(8)
N(12)-Zn(1)-N(13)	77.02(8)
N(2)-Zn(1)-N(13)	103.31(8)
N(1)-Zn(1)-N(13)	97.50(8)
N(3)-Zn(1)-N(13)	90.64(8)
N(12)-Zn(1)-N(11)	76.50(8)
N(2)-Zn(1)-N(11)	103.05(8)
N(1)-Zn(1)-N(11)	90.53(8)
N(3)-Zn(1)-N(11)	92.88(7)
N(13)-Zn(1)-N(11)	153.53(8)

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	15(1)	20(1)	11(1)	-1(1)	0(1)	7(1)
N(1)	14(1)	23(1)	16(1)	0(1)	0(1)	7(1)
N(2)	16(1)	21(1)	12(1)	-1(1)	-1(1)	8(1)
N(3)	17(1)	24(1)	12(1)	2(1)	4(1)	11(1)
N(11)	17(1)	19(1)	12(1)	0(1)	-2(1)	8(1)
N(12)	15(1)	22(1)	13(1)	-1(1)	0(1)	7(1)
N(13)	17(1)	22(1)	15(1)	2(1)	0(1)	11(1)
C(1)	20(1)	26(1)	22(1)	-1(1)	-6(1)	7(1)
C(2)	24(1)	30(2)	29(1)	3(1)	-8(1)	9(1)
C(3)	23(2)	30(2)	38(2)	6(1)	-3(1)	16(1)
C(4)	19(1)	26(1)	29(1)	3(1)	4(1)	12(1)
C(5)	11(1)	20(1)	20(1)	1(1)	3(1)	5(1)
C(6)	14(1)	21(1)	16(1)	1(1)	4(1)	7(1)
C(7)	26(1)	25(1)	20(1)	-2(1)	3(1)	11(1)
C(8)	35(2)	21(1)	26(1)	-2(1)	6(1)	12(1)
C(9)	37(2)	29(2)	34(2)	4(1)	6(1)	23(1)
C(10)	11(1)	20(1)	14(1)	0(1)	3(1)	4(1)
C(11)	17(1)	23(1)	16(1)	-3(1)	2(1)	9(1)
C(12)	21(1)	31(2)	13(1)	-3(1)	-1(1)	6(1)
C(13)	16(1)	31(2)	14(1)	1(1)	-2(1)	8(1)

Table 4 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(14)	15(1)	28(1)	16(1)	4(1)	3(1)	9(1)
C(15)	10(1)	23(1)	14(1)	1(1)	2(1)	6(1)
C(16)	23(1)	35(2)	20(1)	5(1)	0(1)	17(1)
C(17)	31(2)	36(2)	25(1)	1(1)	2(1)	24(1)
C(18)	23(1)	30(2)	17(1)	-1(1)	2(1)	15(1)
C(21)	19(1)	23(1)	17(1)	0(1)	-1(1)	10(1)
C(22)	15(1)	21(1)	24(1)	2(1)	0(1)	7(1)
C(23)	16(1)	27(1)	19(1)	9(1)	6(1)	12(1)
C(24)	18(1)	23(1)	16(1)	3(1)	3(1)	12(1)
C(25)	15(1)	21(1)	12(1)	1(1)	-1(1)	10(1)
C(26)	15(1)	21(1)	14(1)	0(1)	0(1)	10(1)
C(27)	20(1)	24(1)	15(1)	-3(1)	-2(1)	9(1)
C(28)	30(2)	33(2)	12(1)	-4(1)	0(1)	18(1)
C(29)	25(1)	34(2)	13(1)	1(1)	7(1)	16(1)
C(30)	18(1)	22(1)	13(1)	2(1)	-2(1)	9(1)
C(31)	31(2)	26(2)	21(1)	-3(1)	0(1)	13(1)
C(32)	37(2)	19(1)	27(1)	-3(1)	-4(1)	6(1)
C(33)	28(2)	23(2)	30(1)	4(1)	-3(1)	1(1)
C(34)	19(1)	26(1)	20(1)	6(1)	-2(1)	8(1)
C(35)	14(1)	22(1)	16(1)	4(1)	-1(1)	8(1)
C(36)	21(1)	31(2)	31(2)	14(1)	8(1)	10(1)
C(37)	27(2)	34(2)	29(2)	10(1)	12(1)	17(1)
C(38)	24(1)	27(2)	22(1)	5(1)	5(1)	15(1)

2.1.2 Crystals obtained by sublimation

The unit cell of complex **1a** obtained from sublimation was determined using 9782 reflections and the structure was solved in the monoclinic space group C2/c. The structure was refined as a pseudo merohedral twin. The twin ratio was refined and converged to 0.035(9). The asymmetric unit contains one molecule of **1a**.

Table 5: Crystal data and structure refinement for Zn-complex **1a**

CCDC No.	1897892
Empirical formula	C36 H24 N6 Zn
Formula weight	605.98
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	C2/c
Unit cell dimensions	a = 19.5616(9) Å $\alpha = 90°$.
	b = 13.4711(6) Å $\beta = 113.988(3)°$.
	c = 22.5945(14) Å $\gamma = 90°$.
Volume	5439.8(5) $Å^3$
Z	8
Density (calculated)	1.480 $Mg\,m^{-3}$
Absorption coefficient	1.556 mm^{-1}
F(000)	2496
Crystal size	0.058 x 0.057 x 0.036 mm^3
Theta range for data collection	2.140 to 72.109°.
Index ranges	-24<=h<=24, -16<=k<=15, -27<=l<=27
Reflections collected	95886
Independent reflections	5366 [R(int) = 0.1319]
Completeness to theta = 67.679°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	5366 / 0 / 389
Goodness-of-fit on F2	1.908
Final R indices [I>2sigma(I)]	R1 = 0.1157, wR2 = 0.3658
R indices (all data)	R1 = 0.1249, wR2 = 0.3765
Largest diff. peak and hole	1.425 and -1.875 e.$Å^{-3}$

Table 6: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	6618(1)	5680(1)	7012(1)	20(1)
N(1)	5642(3)	6657(4)	6626(3)	20(1)
N(2)	6909(3)	6715(4)	6465(3)	22(1)
N(3)	7705(3)	5175(4)	7101(3)	22(1)
N(21)	7092(3)	6199(4)	8012(3)	23(1)
N(22)	6308(3)	4575(4)	7496(3)	22(1)
N(23)	6053(3)	4608(4)	6241(3)	20(1)
C(1)	5003(4)	6554(5)	6686(4)	26(1)

Table 6 – continued from previous page

	x	y	z	U(eq)
C(2)	4407(4)	7241(6)	6418(4)	30(2)
C(3)	4499(4)	8047(6)	6085(4)	27(2)
C(4)	5173(4)	8198(5)	6025(3)	23(1)
C(5)	5334(4)	9043(5)	5728(3)	26(1)
C(6)	6016(5)	9131(5)	5716(4)	26(1)
C(7)	6576(4)	8390(5)	5953(3)	21(1)
C(8)	6446(4)	7514(5)	6227(3)	20(1)
C(9)	5742(4)	7453(5)	6294(3)	20(1)
C(11)	8096(5)	4427(5)	7456(4)	29(2)
C(12)	8758(5)	4088(6)	7422(4)	35(2)
C(13)	9006(4)	4542(6)	7000(4)	31(2)
C(14)	8593(4)	5330(5)	6603(3)	25(1)
C(15)	8792(4)	5786(6)	6140(4)	29(2)
C(16)	8353(5)	6540(6)	5769(4)	29(2)
C(17)	7718(4)	6885(5)	5852(3)	24(1)
C(18)	7501(4)	6474(5)	6323(3)	21(1)
C(19)	7944(4)	5642(5)	6683(3)	22(1)
C(21)	7504(5)	6991(6)	8248(4)	31(2)
C(22)	7782(5)	7256(7)	8907(5)	37(2)
C(23)	7626(4)	6655(7)	9327(4)	33(2)
C(24)	7183(4)	5786(6)	9095(4)	27(2)
C(25)	6960(5)	5170(6)	9493(4)	34(2)
C(26)	6464(6)	4411(6)	9207(4)	36(2)
C(27)	6211(5)	4201(5)	8540(4)	28(2)
C(28)	6463(4)	4723(5)	8133(3)	22(1)
C(29)	6924(4)	5584(5)	8421(3)	23(1)
C(31)	5923(4)	4694(5)	5624(4)	26(1)
C(32)	5565(5)	3943(6)	5168(4)	28(2)
C(33)	5369(5)	3092(5)	5387(4)	29(2)
C(34)	5529(4)	2954(6)	6048(4)	27(1)
C(35)	5416(5)	2041(6)	6307(4)	38(2)
C(36)	5636(6)	1968(6)	6969(4)	38(2)
C(37)	5925(5)	2782(5)	7383(4)	29(2)
C(38)	6027(4)	3715(5)	7154(3)	21(1)
C(39)	5864(4)	3764(5)	6470(3)	22(1)

Table 7: Selected bond lengths [Å] and angles [°] for complex **1a**

Zn(1)-N(22)	2.078(6)
Zn(1)-N(2)	2.090(6)
Zn(1)-N(3)	2.164(6)
Zn(1)-N(21)	2.180(6)

Table 7 – continued from previous page

Zn(1)-N(23)	2.184(6)
Zn(1)-N(1)	2.187(6)
N(22)-Zn(1)-N(2)	175.6(2)
N(22)-Zn(1)-N(3)	102.2(2)
N(2)-Zn(1)-N(3)	76.7(2)
N(22)-Zn(1)-N(21)	77.1(2)
N(2)-Zn(1)-N(21)	107.1(2)
N(3)-Zn(1)-N(21)	90.9(2)
N(22)-Zn(1)-N(23)	77.6(2)
N(2)-Zn(1)-N(23)	98.1(2)
N(3)-Zn(1)-N(23)	91.5(2)
N(21)-Zn(1)-N(23)	154.5(2)
N(22)-Zn(1)-N(1)	104.3(2)
N(2)-Zn(1)-N(1)	76.5(2)
N(3)-Zn(1)-N(1)	153.1(2)
N(21)-Zn(1)-N(1)	98.9(2)
N(23)-Zn(1)-N(1)	90.2(2)

Table 8: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	27(1)	13(1)	21(1)	1(1)	11(1)	0(1)
N(1)	24(3)	18(3)	20(3)	-4(2)	9(2)	-1(2)
N(2)	26(3)	16(3)	23(3)	4(2)	11(2)	1(2)
N(3)	27(3)	14(3)	23(3)	1(2)	9(2)	5(2)
N(21)	27(3)	17(3)	26(3)	-3(2)	12(2)	0(2)
N(22)	28(3)	15(2)	24(3)	3(2)	11(2)	0(2)
N(23)	24(3)	12(2)	23(3)	1(2)	8(2)	0(2)
C(1)	30(4)	21(3)	29(3)	-5(3)	13(3)	-3(3)
C(2)	25(3)	25(4)	42(4)	-8(3)	16(3)	-4(3)
C(3)	25(3)	25(3)	28(3)	-9(3)	7(3)	4(3)
C(4)	28(3)	16(3)	22(3)	-6(2)	7(3)	3(2)
C(5)	36(4)	16(3)	23(3)	-2(2)	9(3)	10(3)
C(6)	39(4)	8(3)	30(4)	2(2)	13(3)	2(3)
C(7)	22(3)	15(3)	28(3)	3(2)	11(3)	5(2)
C(8)	24(3)	14(3)	21(3)	-1(2)	8(2)	0(2)
C(9)	27(3)	11(3)	18(3)	-2(2)	6(2)	-1(2)
C(11)	40(4)	20(3)	21(3)	7(3)	8(3)	6(3)
C(12)	43(5)	28(4)	26(4)	7(3)	6(3)	14(3)
C(13)	30(4)	30(4)	26(4)	-1(3)	6(3)	9(3)
C(14)	27(3)	24(3)	24(3)	-3(3)	9(3)	5(3)
C(15)	24(3)	29(4)	34(4)	-4(3)	13(3)	3(3)

Table 8 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(16)	37(4)	27(4)	30(4)	5(3)	22(3)	3(3)
C(17)	26(3)	22(3)	26(3)	6(2)	13(3)	3(3)
C(18)	23(3)	13(3)	24(3)	0(2)	9(3)	-2(2)
C(19)	25(3)	18(3)	20(3)	-1(2)	4(3)	0(2)
C(21)	31(4)	26(4)	40(4)	-5(3)	19(3)	-3(3)
C(22)	27(4)	40(4)	43(5)	-18(4)	14(3)	-10(3)
C(23)	28(4)	41(4)	28(4)	-16(3)	8(3)	-2(3)
C(24)	28(3)	26(4)	25(4)	-5(3)	7(3)	10(3)
C(25)	47(5)	32(4)	20(3)	2(3)	12(3)	11(3)
C(26)	64(6)	24(4)	28(4)	2(3)	27(4)	4(3)
C(27)	41(4)	21(3)	29(4)	1(3)	19(3)	2(3)
C(28)	26(3)	16(3)	22(3)	0(2)	9(3)	3(2)
C(29)	27(3)	19(3)	21(3)	1(2)	7(3)	5(3)
C(31)	32(4)	18(3)	26(3)	2(3)	11(3)	4(3)
C(32)	38(4)	23(3)	22(3)	-3(3)	9(3)	5(3)
C(33)	34(4)	23(3)	28(4)	-8(3)	10(3)	-2(3)
C(34)	28(3)	22(3)	31(4)	-4(3)	13(3)	-2(3)
C(35)	53(5)	27(4)	33(4)	-8(3)	17(4)	-10(4)
C(36)	58(5)	22(4)	37(4)	1(3)	23(4)	-11(3)
C(37)	44(4)	16(3)	27(3)	0(3)	15(3)	-5(3)
C(38)	23(3)	15(3)	25(3)	0(2)	10(3)	0(2)
C(39)	21(3)	16(3)	29(3)	0(2)	10(3)	1(2)

2.2 Zn-complex 1b

Zinc-complex **1b** crystallized in the tetragonal space group $P\bar{4}2_1c$. The asymmetric unit contains one quarter of the molecule.

Table 9: Crystal data and structure refinement for Zn-complex **1b**

Identification code	D19227
Empirical formula	C40 H32 N6 Zn
Formula weight	662,08
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	$P\bar{4}2_1c$
Unit cell dimensions	a = 8.7393(3) Å $\alpha = 90°$.
	b = 8.7393(3) Å $\beta = 90°$.
	c = 20.1485(7) Å $\gamma = 90°$.
Volume	1538.85(12) $Å^3$
Z	2
Density (calculated)	1.429 $Mg\,m^{-3}$
Absorption coefficient	0.839 mm^{-1}
F(000)	688
Crystal size	0.186 x 0.169 x 0.168 mm^3
Theta range for data collection	2.540 to 30.033°.
Index ranges	-12<=h<=12, -12<=k<=12, -28<=l<=28
Reflections collected	42161
Independent reflections	2256 [R(int) = 0.0569]
Completeness to theta = 25.242°	99,90%
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2256 / 0 / 108
Goodness-of-fit on F2	1,044
Final R indices [I>2sigma(I)]	R1 = 0.0291, wR2 = 0.0683
R indices (all data)	R1 = 0.0355, wR2 = 0.0715
Absolute structure parameter	0.020(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.261 and -0.288 $e.Å^{-3}$

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

	x	y	z	U(eq)
Zn(1)	5000	5000	5000	12(1)
N(1)	7217(2)	4084(2)	5234(1)	13(1)
N(2)	5000	5000	6048(1)	13(1)
C(1)	8274(3)	3673(3)	4803(1)	17(1)
C(2)	9677(2)	3015(3)	4990(1)	21(1)
C(3)	9954(3)	2832(3)	5655(1)	21(1)

Table 10 – continued from previous page

	x	y	z	U(eq)
C(4)	8869(3)	3297(3)	6132(1)	17(1)
C(5)	7477(2)	3925(2)	5896(1)	14(1)
C(6)	6298(3)	4462(3)	6350(1)	14(1)
C(7)	6686(3)	4379(3)	7024(1)	20(1)
C(8)	8073(3)	3746(3)	7256(1)	20(1)
C(9)	9138(3)	3191(3)	6824(1)	22(1)
C(10)	8344(3)	3677(4)	7997(1)	28(1)

Table 11: Selected bond lengths [Å] and angles [°] for complex **1b**

Zn(1)-N(2)#1	2.1117(19)
Zn(1)-N(2)	2.1117(19)
Zn(1)-N(1)#1	2.1486(19)
Zn(1)-N(1)#2	2.1486(19)
Zn(1)-N(1)#3	2.1486(19)
Zn(1)-N(1)	2.1486(19)
N(2)#1-Zn(1)-N(2)	180.0
N(2)#1-Zn(1)-N(1)#1	77.35(5)
N(2)-Zn(1)-N(1)#1	102.65(5)
N(2)#1-Zn(1)-N(1)#2	77.35(5)
N(2)-Zn(1)-N(1)#2	102.65(5)
N(1)#1-Zn(1)-N(1)#2	154.70(10)
N(2)#1-Zn(1)-N(1)#3	102.65(5)
N(2)-Zn(1)-N(1)#3	77.35(5)
N(1)#1-Zn(1)-N(1)#3	92.75(2)
N(1)#2-Zn(1)-N(1)#3	92.75(2)
N(2)#1-Zn(1)-N(1)	102.65(5)
N(2)-Zn(1)-N(1)	77.35(5)
N(1)#1-Zn(1)-N(1)	92.75(2)
N(1)#2-Zn(1)-N(1)	92.75(2)
N(1)#3-Zn(1)-N(1)	154.70(10)

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

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	15(1)	15(1)	8(1)	0	0	0
N(1)	15(1)	14(1)	11(1)	0(1)	1(1)	-1(1)
N(2)	12(1)	19(1)	7(1)	0	0	0(2)
C(1)	20(1)	18(1)	12(1)	-1(1)	1(1)	-2(1)

Table 12 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2)	21(1)	24(1)	18(1)	-2(1)	6(1)	3(1)
C(3)	15(1)	28(1)	21(1)	1(1)	0(1)	4(1)
C(4)	15(1)	20(1)	17(1)	2(1)	-1(1)	0(1)
C(5)	13(1)	15(1)	13(1)	0(1)	0(1)	-1(1)
C(6)	13(1)	18(1)	12(1)	0(1)	1(1)	-1(1)
C(7)	17(1)	31(1)	11(1)	0(1)	1(1)	1(1)
C(8)	16(1)	29(1)	14(1)	2(1)	-2(1)	-2(1)
C(9)	17(1)	31(1)	17(1)	4(1)	-2(1)	3(1)
C(10)	21(1)	50(2)	14(1)	5(1)	-4(1)	2(1)

2.3 Zn-complex 1c

2.3.1 Crystals obtained from THF/n-hexane

When complex **1c** was crystallized from THF/n-hexane ths structure was solved in monoclinic space group $P2_1/n$. The asymmetric unit contains one molecule of **1c**. The structure was found to be heavily disordered. The disorder was refined with the help of same distance restraints, similarity restraints on anisotropic displacement parameters and advanced rigid bond restraints. Some atoms very close to each other were set to the same anisotropic displacement parameters. The disorder of one ligand was found to be over two, the other over three positions. The disorder ratio was allowed to refine freely and converged to 0.546(1) and 0.521(3):0.336(3):0.143(3) respectively. SQUEEZE found two independent voids with disordered solvent, located at 0.0 0.0 0.5 and 0.5 0.5 1.0 with volumes of 484 and 485 $Å^3$ respectively. The equivalent of 149 electrons were identified in each void. This number corresponds to approximately three molecules of THF for each void; however, there could also be n-hexane from the vapor diffusion in the crystal lattice which would change the amount of solvent molecules slightly.

Table 13: Crystal data and structure refinement for Zn-complex **1c**

Identification code	D19226_sq
Empirical formula	C44 H40 N6 Zn
Formula weight	718.19
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	$P2_1/n$
Unit cell dimensions	a = 12.2744(4) Å $\alpha = 90°$.
	b = 29.5813(11) Å $\beta = 90.0358(15)°$.
	c = 12.4028(4) Å $\gamma = 90°$.
Volume	4503.4(3) $Å^3$
Z	4
Density (calculated)	1.059 $Mg\,m^{-3}$
Absorption coefficient	0.578 mm^{-1}
F(000)	1504
Crystal size	0.350 x 0.226 x 0.196 mm^3
Theta range for data collection	2.334 to 25.025°.
Index ranges	-14<=h<=14, -35<=k<=35, -14<=l<=14
Reflections collected	82588
Independent reflections	7957 [R(int) = 0.0558]
Completeness to theta = 25.025°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	7957 / 4768 / 1099
Goodness-of-fit on F2	1.075
Final R indices [I>2sigma(I)]	R1 = 0.0688, wR2 = 0.1705
R indices (all data)	R1 = 0.0874, wR2 = 0.1829
Extinction coefficient	0.0033(3)
Largest diff. peak and hole	0.938 and -0.905 $e.Å^{-3}$

Table 14: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	4283(1)	7209(1)	3044(1)	44(1)
N(1)	2726(11)	7042(5)	2267(16)	36(3)
N(2)	4349(9)	6537(5)	2989(17)	42(3)
N(3)	5902(11)	7094(4)	3661(15)	36(2)
C(1)	1966(12)	7304(6)	1855(12)	45(1)
C(2)	964(10)	7142(5)	1485(9)	45(1)
C(3)	757(8)	6696(4)	1565(9)	45(1)

Table 14 – continued from previous page

	x	y	z	U(eq)
C(4)	1522(9)	6401(4)	2030(10)	45(2)
C(5)	2533(10)	6589(5)	2355(15)	41(3)
C(6)	3402(9)	6308(5)	2761(13)	42(3)
C(7)	3152(11)	5856(5)	2904(15)	57(3)
C(8)	2130(11)	5665(5)	2607(14)	70(3)
C(9)	1360(12)	5933(5)	2148(12)	64(3)
C(10)	2009(15)	5149(5)	2703(17)	97(5)
C(11)	1090(20)	4946(8)	2080(20)	163(9)
C(21)	6623(13)	7387(5)	4031(16)	42(3)
C(22)	7671(14)	7254(5)	4362(16)	52(3)
C(23)	7966(12)	6817(5)	4252(16)	56(3)
C(24)	7239(10)	6494(4)	3824(14)	51(3)
C(25)	6172(10)	6654(4)	3574(14)	39(2)
C(26)	5347(9)	6346(4)	3178(14)	43(3)
C(27)	5682(10)	5909(4)	2963(12)	54(3)
C(28)	6741(10)	5755(4)	3215(12)	63(3)
C(29)	7499(11)	6041(4)	3635(12)	62(3)
C(30)	7000(14)	5255(4)	3001(15)	93(4)
C(31)	6477(14)	4964(5)	3806(16)	93(4)
N(1A)	2661(15)	7036(6)	2470(20)	44(3)
N(2A)	4222(11)	6481(6)	3150(20)	48(3)
N(3A)	5854(14)	6993(5)	3807(19)	41(3)
C(1A)	1944(15)	7318(7)	2051(14)	45(1)
C(2A)	884(13)	7178(6)	1746(11)	45(1)
C(3A)	593(10)	6739(5)	1879(10)	45(1)
C(4A)	1343(12)	6425(6)	2303(14)	54(3)
C(5A)	2398(13)	6589(6)	2560(19)	46(3)
C(6A)	3218(12)	6287(6)	2980(17)	49(3)
C(7A)	2912(14)	5841(6)	3138(18)	59(4)
C(8A)	1863(14)	5674(6)	2870(18)	72(4)
C(9A)	1121(14)	5964(6)	2453(16)	64(4)
C(10A)	1679(15)	5171(6)	3056(18)	85(5)
C(11A)	646(16)	4984(8)	2557(18)	95(6)
C(21A)	6607(16)	7267(6)	4189(18)	42(3)
C(22A)	7656(16)	7121(6)	4505(18)	49(3)
C(23A)	7887(15)	6679(6)	4378(19)	57(3)
C(24A)	7107(13)	6376(5)	3981(17)	56(3)
C(25A)	6057(12)	6547(5)	3721(17)	45(3)
C(26A)	5181(11)	6258(5)	3346(16)	47(3)
C(27A)	5476(13)	5809(5)	3222(14)	59(3)
C(28A)	6526(13)	5643(5)	3447(16)	71(3)
C(29A)	7319(13)	5914(5)	3861(15)	66(3)
C(30A)	6750(15)	5135(5)	3327(15)	86(4)

Table 14 – continued from previous page

	x	y	z	U(eq)
C(31A)	6340(20)	4883(7)	4270(20)	128(8)
N(41)	3670(30)	7384(4)	4599(14)	38(3)
N(42)	4310(20)	7935(4)	3033(12)	41(2)
N(43)	4943(15)	7389(4)	1465(10)	40(2)
C(41)	3439(12)	7098(5)	5379(11)	42(3)
C(42)	3047(9)	7245(4)	6376(10)	44(2)
C(43)	2855(8)	7693(4)	6538(8)	41(2)
C(44)	3063(15)	8002(4)	5718(10)	42(2)
C(45)	3510(20)	7835(4)	4748(13)	39(2)
C(46)	3820(18)	8143(4)	3893(12)	42(2)
C(47)	3533(10)	8594(4)	4057(10)	50(3)
C(48)	3040(10)	8755(4)	5010(10)	57(3)
C(49)	2814(12)	8462(4)	5822(10)	47(2)
C(50)	2765(10)	9253(4)	5104(12)	76(3)
C(51)	3818(14)	9518(6)	5307(14)	94(5)
C(61)	5188(12)	7095(4)	701(10)	44(2)
C(62)	5602(9)	7231(4)	-319(9)	44(2)
C(63)	5780(8)	7679(4)	-461(8)	43(2)
C(64)	5543(10)	7999(4)	316(8)	45(2)
C(65)	5071(13)	7837(3)	1298(8)	39(2)
C(66)	4746(14)	8143(4)	2144(9)	45(2)
C(67)	5045(12)	8593(4)	1991(9)	66(3)
C(68)	5554(11)	8741(4)	1024(10)	71(2)
C(69)	5776(10)	8456(4)	208(10)	61(3)
C(70)	5830(12)	9246(4)	916(12)	95(3)
C(71)	5012(13)	9479(5)	304(13)	116(5)
N(41A)	3590(40)	7417(7)	4540(20)	38(3)
N(42A)	4320(30)	7894(6)	2861(18)	42(3)
N(43A)	4830(20)	7271(5)	1413(14)	40(3)
C(41A)	3240(20)	7168(7)	5341(17)	41(3)
C(42A)	2784(14)	7356(6)	6276(14)	40(3)
C(43A)	2648(14)	7807(6)	6345(13)	41(2)
C(44A)	3070(20)	8084(6)	5527(15)	39(3)
C(45A)	3560(40)	7876(6)	4620(20)	38(3)
C(46A)	3930(30)	8141(6)	3709(17)	41(3)
C(47A)	3804(18)	8605(6)	3832(15)	51(3)
C(48A)	3284(17)	8809(5)	4721(14)	56(3)
C(49A)	2980(20)	8556(6)	5576(16)	47(3)
C(50A)	3085(19)	9315(6)	4734(14)	74(4)
C(51A)	3570(20)	9513(9)	5761(18)	80(7)
C(61A)	5033(18)	6937(6)	743(14)	46(3)
C(62A)	5464(15)	7021(6)	-298(13)	50(3)
C(63A)	5689(16)	7456(6)	-565(13)	48(3)

Table 14 – continued from previous page

	x	y	z	U(eq)
C(64A)	5508(14)	7821(5)	120(12)	43(2)
C(65A)	5050(20)	7709(5)	1149(13)	40(3)
C(66A)	4790(20)	8054(5)	1919(14)	46(3)
C(67A)	5001(17)	8499(5)	1602(11)	61(3)
C(68A)	5418(17)	8616(5)	560(13)	66(3)
C(69A)	5713(15)	8276(5)	-121(12)	59(3)
C(70A)	5476(15)	9132(5)	255(15)	85(4)
C(71A)	6479(19)	9336(8)	630(20)	125(7)
N(41B)	3826(17)	7229(7)	4764(15)	38(3)
N(42B)	4230(30)	7846(8)	3280(20)	42(3)
N(43B)	5000(30)	7378(9)	1613(19)	41(4)
C(41B)	3689(16)	6906(8)	5471(16)	42(4)
C(42B)	3223(17)	6985(9)	6483(17)	46(4)
C(43B)	2940(20)	7415(8)	6749(18)	41(4)
C(44B)	3032(19)	7768(7)	6003(16)	38(3)
C(45B)	3540(20)	7662(7)	5001(16)	39(3)
C(46B)	3720(20)	8003(7)	4191(17)	40(3)
C(47B)	3380(20)	8437(7)	4464(18)	45(3)
C(48B)	2890(30)	8545(8)	5470(20)	48(3)
C(49B)	2749(19)	8217(7)	6217(17)	41(3)
C(50B)	2480(20)	9023(8)	5650(30)	60(4)
C(51B)	3310(30)	9337(13)	6150(40)	83(8)
C(61B)	5340(30)	7122(10)	810(20)	43(4)
C(62B)	5860(20)	7303(10)	-110(20)	48(4)
C(63B)	6030(20)	7756(10)	-100(20)	53(4)
C(64B)	5600(20)	8045(8)	673(18)	49(3)
C(65B)	5120(30)	7832(9)	1592(18)	43(3)
C(66B)	4730(30)	8093(8)	2492(19)	47(3)
C(67B)	4910(30)	8556(8)	2440(20)	58(4)
C(68B)	5390(30)	8766(8)	1530(20)	71(4)
C(69B)	5800(30)	8511(9)	710(20)	60(4)
C(70B)	5520(30)	9288(9)	1580(30)	93(5)
C(71B)	6090(50)	9402(18)	2590(40)	154(16)

Table 15: Selected bond lengths [Å] and angles [°] for complex **1c**

Zn(1)-N(42B)	1.91(2)
Zn(1)-N(2)	1.990(14)
Zn(1)-N(42A)	2.040(19)
Zn(1)-N(43B)	2.04(2)
Zn(1)-N(41A)	2.130(18)
Zn(1)-N(41)	2.134(11)

Table 15 – continued from previous page

Zn(1)-N(43A)	2.140(15)
Zn(1)-N(42)	2.147(12)
Zn(1)-N(3)	2.155(13)
Zn(1)-N(1A)	2.175(17)
Zn(1)-N(2A)	2.159(17)
Zn(1)-N(43)	2.185(11)
N(42B)-Zn(1)-N(43B)	84.5(9)
N(42A)-Zn(1)-N(41A)	79.5(6)
N(2)-Zn(1)-N(41)	106.7(7)
N(42A)-Zn(1)-N(43A)	78.6(5)
N(41A)-Zn(1)-N(43A)	157.4(8)
N(2)-Zn(1)-N(42)	176.1(7)
N(41)-Zn(1)-N(42)	76.6(4)
N(2)-Zn(1)-N(3)	79.5(4)
N(41)-Zn(1)-N(3)	92.5(11)
N(42)-Zn(1)-N(3)	98.5(9)
N(42A)-Zn(1)-N(1A)	102.5(14)
N(41A)-Zn(1)-N(1A)	89.3(17)
N(43A)-Zn(1)-N(1A)	89.9(10)
N(42A)-Zn(1)-N(2A)	177.1(11)
N(41A)-Zn(1)-N(2A)	102.7(9)
N(43A)-Zn(1)-N(2A)	99.0(8)
N(1A)-Zn(1)-N(2A)	75.8(6)
N(2)-Zn(1)-N(43)	101.4(6)
N(41)-Zn(1)-N(43)	151.9(4)
N(42)-Zn(1)-N(43)	75.3(3)
N(3)-Zn(1)-N(43)	90.8(7)

Table 16: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	27(1)	75(1)	30(1)	-4(1)	5(1)	-1(1)
N(1)	26(3)	68(4)	15(6)	-7(3)	7(3)	-2(3)
N(2)	32(3)	65(4)	29(6)	4(4)	-3(4)	-8(3)
N(3)	32(4)	58(5)	18(5)	14(4)	7(3)	-9(3)
C(1)	32(2)	86(2)	17(4)	-7(3)	2(2)	4(2)
C(2)	32(2)	86(2)	17(4)	-7(3)	2(2)	4(2)
C(3)	32(2)	86(2)	17(4)	-7(3)	2(2)	4(2)
C(4)	35(4)	77(4)	24(5)	-5(4)	1(4)	-10(3)
C(5)	31(4)	74(4)	19(6)	-6(4)	-1(4)	-5(3)
C(6)	36(4)	66(4)	24(6)	2(4)	4(4)	-10(3)
C(7)	47(6)	72(5)	53(8)	7(5)	-1(5)	-16(4)

Table 16 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(8)	57(6)	78(5)	75(8)	7(5)	-5(5)	-22(4)
C(9)	52(6)	82(5)	58(7)	0(5)	-9(5)	-23(5)
C(10)	85(9)	89(6)	117(11)	32(7)	-14(7)	-37(6)
C(11)	197(19)	110(12)	180(20)	-14(14)	-46(14)	-54(14)
C(21)	36(4)	60(6)	29(7)	12(5)	2(4)	-12(4)
C(22)	40(4)	75(7)	41(6)	20(6)	-7(4)	-17(5)
C(23)	33(4)	78(7)	56(6)	25(6)	-9(4)	-12(5)
C(24)	39(4)	66(5)	48(6)	24(5)	-2(4)	-6(4)
C(25)	33(4)	57(5)	28(5)	20(4)	1(3)	-10(3)
C(26)	39(4)	56(5)	35(6)	14(4)	6(4)	-7(3)
C(27)	49(5)	58(5)	56(7)	13(4)	3(4)	-10(4)
C(28)	58(5)	58(5)	72(7)	22(5)	12(5)	1(4)
C(29)	48(5)	67(6)	72(7)	32(5)	-4(5)	0(4)
C(30)	91(7)	65(5)	123(9)	41(5)	25(7)	3(5)
C(31)	91(7)	65(5)	123(9)	41(5)	25(7)	3(5)
N(1A)	33(5)	80(5)	19(8)	0(4)	6(5)	-1(4)
N(2A)	34(4)	75(6)	35(7)	4(5)	-2(5)	5(4)
N(3A)	35(5)	70(6)	17(6)	8(6)	4(4)	-3(5)
C(1A)	32(2)	86(2)	17(4)	-7(3)	2(2)	4(2)
C(2A)	32(2)	86(2)	17(4)	-7(3)	2(2)	4(2)
C(3A)	32(2)	86(2)	17(4)	-7(3)	2(2)	4(2)
C(4A)	38(5)	84(5)	40(7)	-7(5)	-1(5)	-2(4)
C(5A)	33(5)	82(5)	22(7)	1(5)	0(5)	2(4)
C(6A)	39(5)	79(5)	30(7)	-1(5)	-7(5)	-2(4)
C(7A)	51(7)	78(5)	48(8)	1(6)	-1(6)	1(5)
C(8A)	57(7)	79(5)	81(9)	-1(6)	-8(6)	-8(5)
C(9A)	40(6)	87(5)	65(9)	-2(6)	-1(6)	-6(5)
C(10A)	74(9)	80(6)	100(11)	8(7)	-8(8)	-19(6)
C(11A)	105(12)	77(9)	104(14)	-10(10)	-18(9)	-15(9)
C(21A)	38(5)	68(7)	20(6)	16(6)	7(4)	-4(5)
C(22A)	38(5)	77(8)	32(6)	17(7)	2(4)	-7(6)
C(23A)	44(6)	80(7)	47(7)	21(7)	-1(5)	4(5)
C(24A)	45(5)	75(7)	47(7)	14(6)	0(5)	3(5)
C(25A)	37(5)	69(6)	28(6)	7(6)	6(4)	2(4)
C(26A)	43(5)	69(6)	29(6)	-1(5)	-1(5)	2(4)
C(27A)	55(6)	69(6)	54(8)	4(6)	-3(6)	7(5)
C(28A)	64(6)	73(7)	77(8)	12(6)	1(6)	13(5)
C(29A)	51(6)	79(7)	68(8)	21(6)	1(6)	17(5)
C(30A)	84(9)	74(8)	101(11)	29(8)	27(8)	21(7)
C(31A)	159(17)	101(12)	124(16)	50(11)	39(13)	24(12)
N(41)	21(6)	69(4)	25(4)	3(3)	1(4)	5(4)
N(42)	34(4)	59(4)	28(5)	-1(3)	5(5)	-2(4)
N(43)	20(5)	67(4)	31(4)	-7(4)	-1(3)	-1(4)

Table 16 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	19(6)	71(5)	36(4)	8(4)	-2(4)	14(4)
C(42)	22(5)	73(5)	38(4)	18(4)	3(4)	18(4)
C(43)	27(4)	77(5)	17(4)	8(3)	-8(3)	15(4)
C(44)	26(4)	71(5)	28(5)	0(4)	2(4)	8(4)
C(45)	21(4)	70(4)	26(5)	2(4)	0(4)	3(4)
C(46)	27(5)	68(4)	30(5)	-4(4)	3(4)	0(4)
C(47)	38(6)	67(4)	46(6)	8(4)	12(4)	7(4)
C(48)	50(5)	70(5)	51(6)	-3(4)	16(4)	8(4)
C(49)	31(5)	72(5)	39(6)	-3(4)	7(4)	6(4)
C(50)	75(7)	76(6)	79(8)	2(6)	12(6)	16(5)
C(51)	102(10)	85(8)	94(12)	27(9)	-23(10)	5(7)
C(61)	27(5)	71(5)	33(4)	-9(4)	4(3)	-5(5)
C(62)	21(4)	84(6)	26(4)	-9(5)	-2(3)	-17(5)
C(63)	17(4)	90(5)	21(4)	0(4)	-11(3)	-13(4)
C(64)	31(4)	77(5)	28(4)	5(4)	-7(4)	-8(4)
C(65)	23(4)	65(4)	27(4)	1(4)	-5(4)	-4(4)
C(66)	36(4)	68(4)	31(5)	-1(4)	3(4)	-6(4)
C(67)	75(5)	76(5)	46(6)	-5(4)	15(5)	-21(4)
C(68)	78(5)	86(5)	49(5)	3(4)	10(5)	-31(5)
C(69)	54(5)	81(5)	49(6)	6(4)	13(5)	-19(5)
C(70)	105(7)	99(6)	81(7)	10(6)	5(6)	-52(6)
C(71)	142(11)	84(8)	122(11)	11(8)	-17(9)	-31(8)
N(41A)	21(6)	68(5)	26(5)	6(4)	-4(5)	1(5)
N(42A)	28(5)	73(5)	24(5)	-3(4)	4(5)	-6(5)
N(43A)	16(5)	78(6)	27(5)	-6(5)	-5(4)	-8(6)
C(41A)	18(7)	71(6)	34(5)	6(4)	-3(5)	2(5)
C(42A)	19(7)	78(6)	24(5)	13(5)	-8(5)	5(6)
C(43A)	27(4)	77(5)	17(4)	8(3)	-8(3)	15(4)
C(44A)	26(5)	71(5)	20(5)	6(4)	-6(4)	6(5)
C(45A)	22(5)	68(4)	25(5)	3(4)	-3(5)	3(5)
C(46A)	29(6)	70(5)	25(5)	4(4)	2(5)	0(5)
C(47A)	46(8)	72(5)	36(6)	12(5)	20(5)	7(6)
C(48A)	57(7)	72(5)	39(6)	12(5)	21(5)	13(5)
C(49A)	39(6)	72(5)	30(6)	5(5)	10(5)	12(5)
C(50A)	85(9)	75(6)	63(8)	7(6)	23(7)	7(7)
C(51A)	92(14)	61(10)	86(14)	14(10)	-9(11)	4(10)
C(61A)	25(6)	85(7)	29(5)	-11(5)	8(4)	-6(6)
C(62A)	31(6)	92(7)	25(5)	-7(6)	5(5)	-5(6)
C(63A)	27(6)	91(7)	27(5)	-8(6)	0(5)	-12(7)
C(64A)	15(4)	88(5)	25(5)	-4(5)	-5(4)	-11(5)
C(65A)	17(5)	79(5)	25(4)	-2(4)	-2(4)	-7(5)
C(66A)	32(5)	77(5)	28(5)	-1(4)	3(5)	-15(5)
C(67A)	65(5)	82(5)	35(6)	-6(5)	12(5)	-29(5)

Table 16 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(68A)	71(6)	88(6)	41(6)	-1(5)	15(5)	-31(5)
C(69A)	48(6)	93(6)	35(6)	1(5)	9(5)	-22(6)
C(70A)	100(8)	91(6)	64(7)	-2(6)	15(7)	-42(7)
C(71A)	118(13)	140(14)	118(15)	2(13)	10(12)	-70(12)
N(41B)	18(7)	72(6)	25(6)	5(5)	0(6)	8(6)
N(42B)	30(6)	71(6)	26(6)	-1(5)	5(5)	-5(6)
N(43B)	23(7)	73(6)	29(6)	-8(6)	-1(6)	-6(6)
C(41B)	21(8)	74(7)	31(6)	9(6)	-2(6)	6(7)
C(42B)	25(8)	78(7)	35(7)	11(7)	1(7)	9(8)
C(43B)	20(8)	78(7)	23(7)	9(6)	0(7)	8(7)
C(44B)	21(6)	72(6)	22(6)	6(5)	0(5)	9(6)
C(45B)	22(6)	70(6)	25(6)	6(5)	4(5)	5(6)
C(46B)	27(6)	68(5)	26(5)	3(5)	4(5)	2(5)
C(47B)	35(6)	70(5)	30(6)	3(5)	8(5)	3(5)
C(48B)	39(7)	73(6)	31(7)	5(5)	8(6)	12(6)
C(49B)	26(7)	73(6)	23(7)	1(6)	-5(6)	9(6)
C(50B)	58(8)	73(7)	49(8)	1(7)	13(7)	14(7)
C(51B)	86(16)	85(14)	77(17)	10(14)	-1(14)	-5(13)
C(61B)	26(7)	77(7)	26(6)	-8(6)	-1(6)	-8(7)
C(62B)	29(7)	89(7)	26(6)	-6(6)	2(6)	-9(7)
C(63B)	35(7)	91(6)	32(7)	-2(6)	17(6)	-13(7)
C(64B)	35(6)	82(5)	29(6)	-2(5)	3(5)	-13(5)
C(65B)	29(6)	73(5)	25(6)	-3(5)	1(5)	-9(5)
C(66B)	41(6)	71(5)	30(6)	-4(5)	7(6)	-9(6)
C(67B)	59(8)	75(6)	40(8)	-5(6)	16(7)	-18(7)
C(68B)	78(7)	84(6)	50(7)	-2(6)	19(7)	-30(6)
C(69B)	59(7)	83(6)	37(7)	1(6)	8(7)	-23(6)
C(70B)	110(11)	89(7)	80(10)	0(9)	26(10)	-39(9)
C(71B)	190(30)	160(30)	120(20)	-60(20)	20(20)	-70(30)

The structure of **1c** crystallized from $CDCl_3$ was solved in the tetragonal space group $I2_1/a$. The asymmetric unit contains one quarter of the molecule of **1c**. The structure was found to be heavily disordered over symmertry elements. The disorder was refined with the help of same distance restraints on 1,2 and 1,3 distances, similarity restraints on anisotropic displacement parameters and advanced rigid bond restraints. Some atoms very close to each other were set to the same anisotropic displacement parameters. One of the ethyl groups was observed to be disordered even further and splits into a second disorder. This disorder ratio was allowed to refine freely and converged to 0.74(1).

2.3.2 Crystals obtained from $CDCl_3$/n-hexane

Table 17: Crystal data and structure refinement for Zn-complex **1c**

Identification code	D19303
Empirical formula	C44 H40 N6 Zn
Formula weight	718.19
Temperature	200(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	$I2_1/a$
Unit cell dimensions	a = 16.4563(3) Å $\alpha = 90°$.
	b = 16.4563(3) Å $\beta = 90°$.
	c = 13.3651(3) Å $\gamma = 90°$.
Volume	3619.40(15) $Å^3$
Z	4
Density (calculated)	1.318 $Mg\,m^{-3}$
Absorption coefficient	0.719 mm^{-1}
F(000)	1504
Crystal size	0.469 x 0.321 x 0.272 mm^3
Theta range for data collection	1.963 to 30.014°.
Index ranges	-23<=h<=23, -23<=k<=23, -18<=l<=18
Reflections collected	90471
Independent reflections	2642 [R(int) = 0.0515]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	2642 / 443 / 226
Goodness-of-fit on F2	1.076
Final R indices [I>2sigma(I)]	R1 = 0.0272, wR2 = 0.0702
R indices (all data)	R1 = 0.0335, wR2 = 0.0740
Extinction coefficient	0.0038(3)
Largest diff. peak and hole	0.356 and -0.249 e.$Å^{-3}$

Table 18: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1c**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	5000	2500	8750	26(1)
N(1)	5000	2500	7218(1)	31(1)
N(2)	3777(8)	2913(13)	8339(8)	27(1)
C(1)	4411(7)	2893(10)	6691(8)	34(2)

Table 18 – continued from previous page

	x	y	z	U(eq)
C(2)	4334(9)	3144(13)	5709(9)	47(2)
C(3)	3655(7)	3592(7)	5400(7)	85(1)
C(4)	3004(7)	3738(9)	5970(8)	62(2)
C(5)	3048(7)	3502(11)	6980(8)	43(2)
C(6)	2386(8)	3648(12)	7618(9)	46(2)
C(7)	2409(7)	3399(12)	8578(8)	43(2)
C(8)	3138(6)	3044(8)	8907(8)	36(2)
C(9)	3750(7)	3099(10)	7352(7)	28(1)
C(10)	3575(11)	3783(6)	4289(8)	85(1)
C(11)	3717(5)	4680(4)	4168(5)	85(1)
N(22)	6250(8)	2147(13)	8437(8)	28(2)
C(21)	5664(6)	2091(9)	6820(7)	27(1)
C(22)	5712(8)	1817(13)	5836(9)	46(2)
C(23)	6400(4)	1428(4)	5410(5)	45(1)
C(24)	7041(5)	1255(9)	6076(7)	52(2)
C(25)	7032(7)	1474(11)	7097(7)	36(2)
C(26)	7653(8)	1369(13)	7817(9)	41(2)
C(27)	7557(8)	1618(12)	8780(8)	37(2)
C(28)	6843(5)	2012(7)	9083(7)	27(1)
C(29)	6338(7)	1888(11)	7476(8)	29(1)
C(30)	6359(9)	1078(5)	4346(6)	85(2)
C(31)	5866(5)	341(6)	4199(7)	97(3)
C(31A)	6523(18)	1712(10)	3670(10)	106(8)

Table 19: Selected bond lengths [Å] and angles [°] for complex **1c**

Zn(1)-N(1)#1	2.0479(14)
Zn(1)-N(1)	2.0479(14)
Zn(1)-N(22)	2.177(12)
Zn(1)-N(2)	2.195(11)
N(1)#1-Zn(1)-N(1)	180.0
N(1)#1-Zn(1)-N(22)	101.1(3)
N(1)-Zn(1)-N(22)	78.9(3)
N(1)#1-Zn(1)-N(2)	104.5(3)
N(1)-Zn(1)-N(2)	75.5(3)
N(22)-Zn(1)-N(2)	154.27(17)

Table 20: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1c**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	26(1)	26(1)	28(1)	0	0	0
N(1)	33(1)	32(1)	29(1)	0	0	5(1)
N(2)	24(2)	21(2)	37(3)	-2(2)	-1(2)	1(2)
C(1)	38(2)	32(2)	33(3)	-6(2)	4(2)	1(2)
C(2)	73(5)	42(3)	27(2)	0(2)	-9(2)	6(3)
C(3)	129(4)	69(2)	57(2)	18(2)	-20(2)	11(2)
C(4)	92(5)	41(4)	54(3)	3(3)	-43(3)	13(4)
C(5)	40(3)	30(3)	59(3)	-13(2)	-13(2)	5(2)
C(6)	32(3)	36(3)	69(5)	-6(4)	-20(3)	4(2)
C(7)	21(2)	42(3)	68(6)	-16(5)	-7(3)	2(2)
C(8)	36(2)	32(2)	39(3)	-2(2)	-5(2)	-8(2)
C(9)	30(3)	22(2)	30(2)	-1(2)	-10(2)	2(2)
C(10)	129(4)	69(2)	57(2)	18(2)	-20(2)	11(2)
C(11)	129(4)	69(2)	57(2)	18(2)	-20(2)	11(2)
N(22)	28(2)	26(4)	30(2)	2(2)	3(2)	-3(2)
C(21)	34(2)	27(2)	21(2)	-4(2)	7(2)	2(2)
C(22)	52(3)	53(5)	32(3)	-7(3)	2(2)	6(3)
C(23)	57(2)	40(2)	37(2)	-2(1)	26(2)	9(2)
C(24)	41(2)	50(4)	64(4)	-1(3)	21(3)	12(3)
C(25)	31(3)	30(3)	47(3)	0(3)	18(2)	5(2)
C(26)	28(2)	39(3)	57(4)	14(3)	11(2)	10(2)
C(27)	30(3)	38(2)	45(3)	15(2)	4(2)	2(2)
C(28)	21(2)	29(2)	33(3)	7(2)	-1(2)	4(1)
C(29)	23(2)	26(2)	39(3)	7(2)	-2(2)	0(1)
C(30)	129(5)	83(5)	42(2)	-10(3)	36(3)	30(4)
C(31)	108(6)	116(6)	68(4)	-55(4)	16(5)	5(5)
C(31A)	190(20)	90(11)	42(7)	-7(6)	10(9)	0(12)

2.4 Zn-complex 1d

Table 21: Crystal data and structure refinement for Zn-complex **1d**

Identification code	D19428
Empirical formula	C56 H64 N6 O2 Zn
Formula weight	918,5
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	Pn
Unit cell dimensions	a = 12.3210(13) Å $\alpha = 90°$. b = 15.5945(14) Å $\beta = 92.016(6)°$. c = 12.3986(11) Å $\gamma = 90°$.
Volume	2380.8(4) Å^{3}2380.8(4) Å^3
Z	2
Density (calculated)	1.281 Mg m^{-3}1.281 Mg m^{-3}
Absorption coefficient	0.565 mm^{-1}0.565 mm^{-1}
F(000)	976
Crystal size	0.191 x 0.138 x 0.074 mm^{3}0.191 x 0.138 x 0.074 mm^3
Theta range for data collection	2.099 to 32.032°.
Index ranges	-18<=h<=18, -23<=k<=23, -18<=l<=18
Reflections collected	245173
Independent reflections	16504 [R(int) = 0.0886]
Completeness to theta = 25.242°	0,995
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	16504 / 7824 / 1505
Goodness-of-fit on F2	1,118
Final R indices [I>2sigma(I)]	R1 = 0.0571, wR2 = 0.1256
R indices (all data)	R1 = 0.0790, wR2 = 0.1355
Absolute structure parameter	0.50(3)
Extinction coefficient	0.0066(6)
Largest diff. peak and hole	0.549 and -0.646 e.Å^{-3}

Table 22: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å$^2 \times 10^3$) for complex **1d**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	3365(1)	5476(1)	5028(1)	11(1)
N(1)	3289(7)	6790(5)	5040(8)	12(1)
N(2)	2667(6)	5784(5)	3400(6)	10(1)

Table 22 – continued from previous page

	x	y	z	U(eq)
N(3)	4093(6)	5824(6)	6652(6)	13(2)
C(1)	3075(6)	7201(7)	4057(8)	10(2)
C(2)	2719(8)	6653(6)	3197(8)	11(1)
C(3)	2313(8)	5258(7)	2630(8)	14(1)
C(4)	1978(10)	5555(7)	1595(9)	18(2)
C(5)	2061(9)	6412(7)	1363(9)	16(2)
C(6)	2447(9)	6988(7)	2181(9)	15(2)
C(7)	2547(14)	7883(9)	1961(13)	17(3)
C(8)	2931(16)	8400(9)	2779(12)	13(2)
C(9)	3232(12)	8054(8)	3795(11)	10(2)
C(10)	3030(16)	9375(9)	2667(13)	15(3)
C(11)	2930(30)	9697(16)	1500(16)	23(3)
C(12)	2185(18)	9813(12)	3359(18)	24(3)
C(13)	3446(6)	7198(6)	5992(7)	10(1)
C(14)	3912(8)	6666(6)	6866(8)	11(2)
C(15)	4539(7)	5335(7)	7404(8)	13(2)
C(16)	4859(9)	5636(7)	8432(9)	17(2)
C(17)	4692(8)	6483(7)	8677(8)	14(2)
C(18)	4173(7)	7030(6)	7898(8)	11(1)
C(19)	3911(12)	7901(8)	8099(11)	11(2)
C(20)	3410(16)	8391(9)	7323(11)	14(2)
C(21)	3167(14)	8030(9)	6290(11)	15(2)
C(22)	3171(15)	9339(9)	7433(13)	17(3)
C(23)	3320(20)	9658(14)	8590(16)	27(4)
C(24)	3870(18)	9862(15)	6670(17)	26(4)
N(31)	3412(7)	4145(4)	5009(7)	11(1)
N(32)	1822(6)	5144(5)	5675(6)	10(1)
N(33)	4963(6)	5225(6)	4420(7)	13(2)
C(31)	2576(6)	3719(6)	5481(6)	11(1)
C(32)	1698(7)	4270(6)	5803(8)	11(2)
C(33)	1048(8)	5674(7)	5956(9)	15(2)
C(34)	72(8)	5389(7)	6380(10)	17(2)
C(35)	-61(8)	4513(7)	6534(10)	16(2)
C(36)	770(7)	3934(6)	6278(8)	12(1)
C(37)	693(7)	3039(7)	6477(9)	14(2)
C(38)	1554(7)	2517(6)	6230(9)	16(2)
C(39)	2467(8)	2849(7)	5730(9)	17(2)
C(40)	1529(9)	1550(7)	6440(10)	24(2)
C(41)	870(20)	1080(16)	5562(19)	32(3)
C(42)	1110(20)	1337(14)	7552(14)	31(4)
C(43)	4270(6)	3780(6)	4528(6)	11(1)
C(44)	5118(8)	4378(6)	4236(9)	12(2)
C(45)	5693(9)	5790(7)	4171(10)	16(2)

Table 22 – continued from previous page

	x	y	z	U(eq)
C(46)	6691(9)	5550(7)	3741(12)	20(2)
C(47)	6883(8)	4708(7)	3528(10)	18(2)
C(48)	6095(7)	4082(7)	3758(9)	15(2)
C(49)	6248(8)	3204(7)	3547(9)	16(2)
C(50)	5410(8)	2641(7)	3738(9)	16(2)
C(51)	4444(7)	2920(6)	4218(9)	15(2)
C(52)	5560(9)	1706(7)	3428(9)	24(2)
C(53)	5194(19)	1080(14)	4312(16)	26(3)
C(54)	4946(18)	1497(15)	2363(14)	31(4)
Zn(1A)	2860(1)	5476(1)	4904(1)	11(1)
N(1A)	2944(9)	6796(8)	4902(10)	12(1)
N(2A)	2133(9)	5841(7)	3293(8)	12(2)
N(3A)	3588(9)	5789(7)	6527(8)	12(2)
C(1A)	2773(8)	7194(9)	3910(11)	13(2)
C(2A)	2332(11)	6685(8)	3052(11)	11(1)
C(3A)	1685(13)	5346(8)	2529(10)	15(2)
C(4A)	1346(12)	5662(8)	1501(11)	13(2)
C(5A)	1599(12)	6503(9)	1262(12)	16(2)
C(6A)	2087(13)	7043(9)	2035(12)	13(2)
C(7A)	2313(19)	7927(11)	1816(18)	12(3)
C(8A)	2810(20)	8398(12)	2629(18)	13(2)
C(9A)	3046(19)	8034(12)	3638(17)	10(2)
C(10A)	3070(20)	9354(13)	2470(20)	17(4)
C(11A)	3000(40)	9650(20)	1310(20)	23(5)
C(12A)	2380(30)	9904(17)	3200(30)	23(5)
C(13A)	3163(8)	7197(10)	5860(11)	10(1)
C(14A)	3522(11)	6639(8)	6743(10)	9(2)
C(15A)	3923(10)	5262(9)	7302(11)	13(2)
C(16A)	4263(12)	5539(9)	8331(12)	14(2)
C(17A)	4213(12)	6397(9)	8562(11)	15(2)
C(18A)	3803(11)	6984(9)	7781(11)	11(1)
C(19A)	3688(17)	7881(11)	7915(16)	13(3)
C(20A)	3300(20)	8420(11)	7123(15)	10(3)
C(21A)	3015(19)	8077(10)	6095(14)	8(3)
C(22A)	3210(20)	9392(12)	7240(20)	18(4)
C(23A)	3320(30)	9730(20)	8390(20)	22(5)
C(24A)	4100(30)	9820(20)	6560(30)	27(6)
N(31A)	2820(9)	4144(7)	4956(9)	11(1)
N(32A)	1291(8)	5235(7)	5531(8)	10(2)
N(33A)	4426(8)	5140(7)	4294(8)	12(2)
C(31A)	1932(9)	3790(8)	5441(7)	10(2)
C(32A)	1095(10)	4375(7)	5727(10)	9(2)
C(33A)	536(11)	5802(9)	5792(12)	13(2)

Table 22 – continued from previous page

	x	y	z	U(eq)
C(34A)	-466(11)	5586(8)	6215(11)	12(2)
C(35A)	-655(11)	4728(8)	6412(11)	12(2)
C(36A)	144(9)	4110(7)	6184(10)	9(2)
C(37A)	10(9)	3225(8)	6431(10)	11(2)
C(38A)	813(10)	2652(8)	6189(10)	11(2)
C(39A)	1766(10)	2930(8)	5720(11)	13(2)
C(40A)	677(10)	1702(8)	6463(11)	16(2)
C(41A)	1070(30)	1100(20)	5590(30)	32(3)
C(42A)	1300(30)	1509(19)	7545(19)	27(6)
C(43A)	3640(8)	3740(8)	4482(7)	11(1)
C(44A)	4529(10)	4281(7)	4139(10)	8(2)
C(45A)	5196(11)	5654(9)	3998(12)	12(2)
C(46A)	6169(12)	5367(9)	3560(13)	16(2)
C(47A)	6297(10)	4504(8)	3395(12)	14(2)
C(48A)	5478(10)	3932(7)	3672(10)	11(2)
C(49A)	5531(10)	3031(8)	3464(11)	12(2)
C(50A)	4673(9)	2517(7)	3715(10)	11(2)
C(51A)	3755(9)	2864(7)	4220(10)	10(2)
C(52A)	4695(9)	1561(7)	3483(10)	12(2)
C(53A)	5390(30)	1120(19)	4390(20)	30(6)
C(54A)	5180(30)	1350(19)	2395(16)	27(5)
Zn(1B)	3450(20)	5473(11)	5320(20)	11(1)
N(1B)	3270(90)	6783(18)	5170(40)	12(4)
N(2B)	2650(60)	5630(30)	3710(30)	12(4)
N(3B)	4110(60)	5970(30)	6870(30)	12(4)
C(1B)	3020(60)	7090(20)	4140(40)	11(4)
C(2B)	2700(50)	6470(30)	3350(30)	11(1)
C(3B)	2320(70)	5060(30)	2970(40)	16(6)
C(4B)	2060(70)	5250(40)	1890(40)	14(5)
C(5B)	2070(70)	6090(40)	1540(40)	14(5)
C(6B)	2420(60)	6730(30)	2300(40)	14(4)
C(7B)	2470(70)	7600(40)	1980(50)	11(5)
C(8B)	2800(80)	8200(30)	2740(50)	13(4)
C(9B)	3070(80)	7940(30)	3800(50)	10(2)
C(10B)	2910(90)	9150(30)	2510(70)	16(5)
C(11B)	3070(180)	9410(70)	1340(90)	23(3)
C(12B)	1990(140)	9680(60)	3000(130)	24(3)
C(13B)	3430(70)	7280(20)	6050(40)	13(4)
C(14B)	3900(60)	6820(30)	6990(40)	11(4)
C(15B)	4530(70)	5540(40)	7700(40)	13(2)
C(16B)	4760(80)	5920(50)	8690(40)	15(5)
C(17B)	4580(80)	6780(50)	8830(40)	15(5)
C(18B)	4110(60)	7270(40)	7970(40)	11(1)

Table 22 – continued from previous page

	x	y	z	U(eq)
C(19B)	3870(80)	8150(40)	8040(50)	12(5)
C(20B)	3430(90)	8600(30)	7190(60)	14(4)
C(21B)	3220(90)	8160(30)	6200(60)	15(2)
C(22B)	3190(120)	9550(40)	7250(90)	19(5)
C(23B)	3300(300)	9900(80)	8420(100)	27(4)
C(24B)	4000(200)	10060(60)	6570(180)	26(4)
N(31B)	3320(40)	4410(30)	4880(60)	10(4)
N(32B)	1680(30)	5390(30)	5430(50)	13(4)
N(33B)	4930(50)	5440(30)	4370(70)	12(5)
C(31B)	2490(30)	4000(30)	5410(40)	12(4)
C(32B)	1610(40)	4540(30)	5700(50)	11(4)
C(33B)	890(50)	5910(40)	5690(70)	15(2)
C(34B)	-50(50)	5650(50)	6210(90)	17(2)
C(35B)	-120(50)	4790(50)	6480(80)	14(5)
C(36B)	710(40)	4210(40)	6220(60)	12(1)
C(37B)	660(50)	3330(40)	6490(60)	12(5)
C(38B)	1510(60)	2810(40)	6210(60)	15(4)
C(39B)	2410(50)	3140(30)	5690(60)	13(5)
C(40B)	1530(70)	1850(40)	6470(80)	21(5)
C(41B)	630(130)	1340(60)	5900(120)	32(3)
C(42B)	1510(180)	1700(80)	7690(80)	31(4)
C(43B)	4210(40)	4000(30)	4520(40)	12(4)
C(44B)	5090(40)	4580(40)	4240(60)	12(4)
C(45B)	5690(70)	5980(40)	4120(110)	15(6)
C(46B)	6690(70)	5710(50)	3740(130)	16(5)
C(47B)	6880(70)	4860(50)	3600(120)	16(6)
C(48B)	6080(50)	4250(40)	3840(90)	13(5)
C(49B)	6200(60)	3350(40)	3730(80)	15(5)
C(50B)	5390(60)	2790(40)	3980(70)	15(5)
C(51B)	4410(50)	3120(30)	4370(60)	12(5)
C(52B)	5530(70)	1830(40)	3860(80)	18(5)
C(53B)	4950(130)	1290(60)	4700(90)	24(2)
C(54B)	5150(170)	1530(70)	2730(80)	21(12)
O(61)	9796(8)	8022(7)	3227(8)	30(2)
C(61)	9924(11)	8088(8)	4470(10)	20(2)
C(62)	9115(9)	7492(10)	4946(10)	26(2)
C(63)	8614(10)	6995(10)	4067(12)	32(3)
C(64)	9358(17)	7151(13)	3128(14)	35(3)
O(61A)	10070(8)	7342(7)	4696(9)	44(3)
C(61A)	9734(11)	6705(8)	3868(11)	34(3)
C(62A)	9190(20)	7115(12)	2918(17)	50(4)
C(63A)	9140(20)	8085(10)	3021(13)	82(4)
C(64A)	9800(20)	8130(12)	4154(17)	71(5)

Table 22 – continued from previous page

	x	y	z	U(eq)
O(71)	7129(8)	7500(7)	5008(7)	39(2)
C(71)	6251(17)	8002(12)	5493(16)	51(4)
C(72)	6523(13)	7996(10)	6708(14)	33(3)
C(73)	6941(17)	7048(11)	6796(15)	43(4)
C(74)	7603(10)	6980(9)	5812(11)	39(3)
O(71A)	6174(10)	7293(7)	5172(8)	31(3)
C(71A)	6400(20)	8169(11)	5549(19)	32(4)
O(72A)	6370(30)	8098(16)	6769(19)	51(5)
C(73A)	6910(20)	7194(14)	6919(15)	33(4)
C(74A)	6410(11)	6681(9)	5994(11)	23(3)

Table 23: Selected bond lengths [Å] and angles [°] for complex **1d**

Zn(1)-N(1)	2.051(8)
Zn(1)-N(31)	2.077(7)
Zn(1)-N(32)	2.152(8)
Zn(1)-N(33)	2.169(8)
Zn(1)-N(2)	2.219(8)
Zn(1)-N(3)	2.241(8)
N(1)-Zn(1)-N(31)	179.0(4)
N(1)-Zn(1)-N(32)	101.3(3)
N(31)-Zn(1)-N(32)	77.8(3)
N(1)-Zn(1)-N(33)	103.0(3)
N(31)-Zn(1)-N(33)	77.8(3)
N(32)-Zn(1)-N(33)	155.6(3)
N(1)-Zn(1)-N(2)	76.9(3)
N(31)-Zn(1)-N(2)	102.5(3)
N(32)-Zn(1)-N(2)	94.1(3)
N(33)-Zn(1)-N(2)	92.9(3)
N(1)-Zn(1)-N(3)	76.6(3)
N(31)-Zn(1)-N(3)	104.0(3)
N(32)-Zn(1)-N(3)	93.1(3)
N(33)-Zn(1)-N(3)	91.0(3)
N(2)-Zn(1)-N(3)	153.5(3)

Table 24: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1d**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	14(1)	9(1)	10(1)	0(1)	1(1)	0(1)

Table 24 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
N(1)	16(3)	11(1)	8(2)	0(3)	-1(2)	2(3)
N(2)	10(3)	11(3)	9(3)	0(2)	2(3)	-2(3)
N(3)	7(3)	18(4)	14(4)	0(3)	-1(3)	-1(3)
C(1)	6(3)	10(3)	13(3)	-3(3)	0(3)	1(3)
C(2)	11(4)	8(2)	13(3)	1(2)	1(3)	1(3)
C(3)	16(4)	12(3)	13(3)	2(3)	2(3)	-2(3)
C(4)	21(4)	18(4)	14(4)	-3(3)	-2(3)	-5(3)
C(5)	19(4)	15(3)	14(3)	0(3)	-6(3)	-3(3)
C(6)	21(5)	9(3)	16(4)	-4(3)	-1(3)	-1(3)
C(7)	27(7)	15(4)	9(5)	4(3)	-2(4)	1(4)
C(8)	18(4)	10(2)	11(4)	1(2)	0(3)	0(2)
C(9)	9(5)	11(2)	10(4)	-1(2)	-2(3)	-4(2)
C(10)	21(5)	13(4)	13(6)	3(4)	-6(4)	0(3)
C(11)	43(9)	10(5)	15(6)	-1(5)	1(6)	1(5)
C(12)	37(9)	11(6)	24(8)	-1(5)	4(5)	4(5)
C(13)	10(4)	10(2)	9(3)	1(2)	-1(3)	2(3)
C(14)	10(4)	13(3)	9(3)	3(2)	-1(3)	0(3)
C(15)	9(3)	16(3)	16(3)	2(3)	0(3)	3(3)
C(16)	16(4)	21(4)	14(4)	3(3)	-1(3)	4(3)
C(17)	14(4)	16(4)	12(3)	3(3)	-2(3)	-1(3)
C(18)	9(3)	15(3)	8(3)	-1(2)	-2(3)	-3(3)
C(19)	19(6)	10(4)	5(5)	-1(3)	-6(3)	0(3)
C(20)	19(4)	13(4)	9(4)	-4(3)	1(3)	1(3)
C(21)	20(5)	12(3)	12(5)	6(3)	-4(3)	1(3)
C(22)	22(5)	15(4)	12(6)	2(4)	-7(4)	1(3)
C(23)	55(9)	9(6)	17(7)	-7(5)	-8(6)	4(5)
C(24)	35(8)	16(6)	26(7)	-1(5)	-6(5)	-7(5)
N(31)	10(1)	10(1)	14(1)	0(3)	4(1)	1(3)
N(32)	12(3)	11(3)	8(3)	1(3)	0(3)	-1(2)
N(33)	11(3)	12(3)	16(4)	0(3)	-1(3)	-2(3)
C(31)	12(3)	12(3)	8(3)	0(3)	0(2)	0(2)
C(32)	8(3)	14(3)	11(4)	1(3)	-1(3)	1(3)
C(33)	13(3)	18(4)	14(4)	-2(3)	1(3)	2(3)
C(34)	12(3)	20(4)	19(4)	-2(3)	1(3)	5(3)
C(35)	12(4)	20(4)	16(4)	1(4)	3(3)	0(3)
C(36)	8(3)	17(3)	11(3)	0(3)	-2(2)	-1(2)
C(37)	12(3)	15(4)	15(4)	2(4)	0(3)	-2(3)
C(38)	17(4)	14(4)	18(4)	1(3)	5(3)	-4(3)
C(39)	18(4)	12(4)	22(5)	4(3)	3(3)	-1(3)
C(40)	26(4)	13(4)	32(5)	8(4)	4(4)	-1(3)
C(41)	49(9)	13(4)	33(4)	-4(3)	3(5)	-8(5)
C(42)	41(9)	18(8)	34(6)	13(5)	13(5)	4(6)
C(43)	12(2)	8(3)	13(3)	-1(3)	1(2)	0(2)

Table 24 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(44)	10(3)	15(3)	11(4)	0(3)	2(3)	2(3)
C(45)	14(4)	18(4)	16(4)	0(4)	1(3)	-1(3)
C(46)	11(4)	27(5)	20(5)	3(4)	0(3)	-3(3)
C(47)	8(3)	29(4)	17(5)	2(4)	1(3)	3(3)
C(48)	8(3)	22(4)	14(4)	-2(3)	3(3)	1(3)
C(49)	15(4)	19(4)	14(5)	0(3)	2(3)	3(3)
C(50)	18(4)	12(4)	18(5)	-3(3)	2(3)	1(3)
C(51)	14(3)	12(4)	19(4)	-3(3)	4(3)	3(3)
C(52)	28(4)	16(4)	27(5)	-2(3)	11(4)	1(3)
C(53)	30(7)	17(5)	32(7)	-3(5)	1(6)	-2(4)
C(54)	43(10)	26(9)	25(6)	-11(6)	-2(5)	1(7)
Zn(1A)	14(1)	9(1)	10(1)	0(1)	1(1)	0(1)
N(1A)	16(3)	11(1)	8(2)	0(3)	-1(2)	2(3)
N(2A)	22(5)	5(4)	9(4)	2(3)	2(4)	-1(4)
N(3A)	20(5)	5(4)	9(4)	0(3)	3(4)	0(4)
C(1A)	7(5)	15(4)	16(4)	9(3)	0(4)	3(4)
C(2A)	11(4)	8(2)	13(3)	1(2)	1(3)	1(3)
C(3A)	27(5)	5(4)	11(4)	-1(3)	-2(4)	-4(4)
C(4A)	17(5)	12(5)	10(5)	-3(4)	-3(4)	-1(4)
C(5A)	19(4)	15(3)	14(3)	0(3)	-6(3)	-3(3)
C(6A)	21(6)	7(4)	12(4)	4(3)	2(4)	-4(4)
C(7A)	24(8)	4(4)	9(6)	1(4)	0(5)	-2(4)
C(8A)	18(4)	10(2)	11(4)	1(2)	0(3)	0(2)
C(9A)	9(5)	11(2)	10(4)	-1(2)	-2(3)	-4(2)
C(10A)	28(7)	6(5)	18(8)	-2(5)	7(6)	-3(5)
C(11A)	35(10)	18(10)	16(9)	5(8)	4(9)	-1(8)
C(12A)	40(12)	11(7)	20(9)	1(6)	9(7)	-5(6)
C(13A)	10(4)	10(2)	9(3)	1(2)	-1(3)	2(3)
C(14A)	12(5)	10(4)	5(4)	-2(3)	-3(4)	2(4)
C(15A)	9(3)	16(3)	16(3)	2(3)	0(3)	3(3)
C(16A)	12(5)	12(5)	17(5)	5(4)	-1(4)	1(4)
C(17A)	18(5)	21(5)	7(4)	-1(4)	0(4)	-4(4)
C(18A)	9(3)	15(3)	8(3)	-1(2)	-2(3)	-3(3)
C(19A)	17(7)	16(5)	6(6)	-3(4)	-6(5)	-4(4)
C(20A)	13(5)	7(4)	11(6)	7(3)	1(5)	0(4)
C(21A)	15(6)	5(4)	3(5)	-1(3)	-4(4)	3(4)
C(22A)	33(7)	4(5)	16(8)	-3(5)	4(6)	2(5)
C(23A)	24(8)	21(10)	22(9)	-1(7)	-4(7)	-2(8)
C(24A)	43(13)	9(8)	31(10)	4(7)	16(8)	-8(8)
N(31A)	10(1)	10(1)	14(1)	0(3)	4(1)	1(3)
N(32A)	12(4)	7(4)	12(5)	-2(4)	2(4)	0(3)
N(33A)	15(4)	8(4)	11(5)	2(4)	3(4)	-1(3)
C(31A)	13(4)	9(4)	9(4)	3(3)	2(3)	-4(3)

Table 24 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(32A)	12(4)	7(4)	6(5)	-4(3)	0(3)	-3(3)
C(33A)	16(5)	7(5)	15(6)	-5(4)	2(4)	4(4)
C(34A)	19(5)	7(4)	12(5)	-2(4)	5(4)	2(4)
C(35A)	19(5)	10(4)	9(5)	0(4)	3(4)	3(4)
C(36A)	13(4)	6(4)	7(5)	-2(4)	1(3)	0(3)
C(37A)	13(5)	10(4)	9(5)	1(4)	3(3)	1(3)
C(38A)	18(5)	8(4)	6(5)	1(4)	4(4)	-1(4)
C(39A)	19(5)	8(4)	13(5)	2(4)	3(4)	1(4)
C(40A)	20(5)	10(5)	20(5)	8(4)	5(4)	-2(4)
C(41A)	49(9)	13(4)	33(4)	-4(3)	3(5)	-8(5)
C(42A)	37(13)	15(12)	29(8)	6(7)	-1(7)	-2(8)
C(43A)	12(2)	8(3)	13(3)	-1(3)	1(2)	0(2)
C(44A)	10(4)	6(4)	7(4)	1(3)	2(3)	2(3)
C(45A)	12(5)	8(4)	18(6)	-2(4)	2(4)	-2(3)
C(46A)	16(5)	15(5)	17(6)	3(4)	4(4)	-3(4)
C(47A)	13(5)	13(4)	18(6)	2(5)	5(4)	-4(4)
C(48A)	14(4)	8(4)	10(5)	3(4)	5(3)	2(3)
C(49A)	18(5)	5(4)	14(5)	-1(4)	10(4)	1(3)
C(50A)	17(5)	6(4)	11(5)	0(4)	1(3)	0(3)
C(51A)	16(5)	5(4)	9(5)	1(4)	6(4)	0(3)
C(52A)	14(5)	5(4)	15(5)	0(4)	6(4)	1(3)
C(53A)	50(15)	7(7)	31(9)	-1(6)	-22(8)	4(8)
C(54A)	47(13)	18(10)	19(7)	-3(6)	17(7)	12(8)
Zn(1B)	14(1)	9(1)	10(1)	0(1)	1(1)	0(1)
N(1B)	13(10)	13(8)	11(7)	3(6)	0(8)	1(8)
N(2B)	14(9)	9(6)	13(8)	2(6)	1(8)	1(7)
N(3B)	11(9)	15(7)	10(7)	0(6)	0(7)	1(7)
C(1B)	11(10)	10(6)	13(7)	1(6)	-1(8)	0(7)
C(2B)	11(4)	8(2)	13(3)	1(2)	1(3)	1(3)
C(3B)	21(12)	12(9)	14(9)	1(8)	0(10)	-1(10)
C(4B)	20(11)	10(8)	14(9)	2(9)	1(9)	-3(9)
C(5B)	19(10)	9(8)	12(8)	1(7)	-2(9)	-4(8)
C(6B)	19(9)	8(7)	14(7)	2(6)	-1(7)	-2(8)
C(7B)	17(11)	9(7)	9(9)	1(7)	-1(9)	-1(8)
C(8B)	17(10)	10(7)	12(7)	0(6)	-2(8)	-1(7)
C(9B)	9(5)	11(2)	10(4)	-1(2)	-2(3)	-4(2)
C(10B)	21(11)	12(8)	14(10)	-1(8)	-4(10)	-3(9)
C(11B)	43(9)	10(5)	15(6)	-1(5)	1(6)	1(5)
C(12B)	37(9)	11(6)	24(8)	-1(5)	4(5)	4(5)
C(13B)	14(9)	14(7)	10(7)	2(6)	-2(8)	1(7)
C(14B)	12(9)	12(7)	10(7)	0(6)	-2(8)	0(8)
C(15B)	9(3)	16(3)	16(3)	2(3)	0(3)	3(3)
C(16B)	12(12)	18(9)	13(9)	2(8)	-2(9)	1(10)

Table 24 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(17B)	12(12)	19(8)	12(9)	1(7)	-2(10)	1(9)
C(18B)	9(3)	15(3)	8(3)	-1(2)	-2(3)	-3(3)
C(19B)	13(11)	13(7)	9(9)	-3(7)	-4(9)	-4(8)
C(20B)	18(9)	14(7)	11(8)	1(6)	-2(8)	-1(8)
C(21B)	20(5)	12(3)	12(5)	6(3)	-4(3)	1(3)
C(22B)	27(11)	14(8)	15(10)	-1(8)	-4(10)	3(9)
C(23B)	55(9)	9(6)	17(7)	-7(5)	-8(6)	4(5)
C(24B)	35(8)	16(6)	26(7)	-1(5)	-6(5)	-7(5)
N(31B)	10(7)	10(7)	11(8)	1(7)	1(7)	1(6)
N(32B)	13(8)	11(7)	14(10)	-1(8)	0(7)	0(6)
N(33B)	12(8)	11(7)	14(10)	1(9)	2(8)	0(7)
C(31B)	12(7)	11(7)	13(9)	2(7)	2(7)	1(6)
C(32B)	10(7)	13(7)	9(9)	-1(7)	0(7)	0(6)
C(33B)	13(3)	18(4)	14(4)	-2(3)	1(3)	2(3)
C(34B)	12(3)	20(4)	19(4)	-2(3)	1(3)	5(3)
C(35B)	14(8)	17(7)	12(10)	-3(8)	0(8)	2(7)
C(36B)	8(3)	17(3)	11(3)	0(3)	-2(2)	-1(2)
C(37B)	12(9)	14(7)	9(10)	-2(8)	0(8)	-2(7)
C(38B)	16(8)	13(7)	16(9)	1(7)	3(8)	-1(6)
C(39B)	13(9)	12(8)	13(10)	1(9)	1(9)	1(8)
C(40B)	24(11)	13(8)	25(9)	1(9)	6(9)	0(8)
C(41B)	49(9)	13(4)	33(4)	-4(3)	3(5)	-8(5)
C(42B)	41(9)	18(8)	34(6)	13(5)	13(5)	4(6)
C(43B)	12(7)	9(7)	14(9)	-1(8)	3(7)	1(6)
C(44B)	11(7)	12(7)	12(9)	1(8)	3(8)	0(6)
C(45B)	12(9)	15(9)	16(12)	2(11)	1(10)	-4(8)
C(46B)	12(9)	18(9)	17(11)	2(10)	1(10)	-3(9)
C(47B)	12(10)	19(8)	17(12)	2(10)	1(10)	-3(8)
C(48B)	12(8)	15(7)	13(10)	0(8)	3(8)	1(7)
C(49B)	14(9)	15(7)	14(11)	-1(9)	4(10)	1(8)
C(50B)	17(8)	12(7)	17(10)	-4(8)	5(8)	1(7)
C(51B)	12(8)	11(7)	14(10)	-1(9)	3(9)	0(7)
C(52B)	22(11)	13(8)	19(10)	-5(9)	5(9)	1(9)
C(53B)	28(4)	16(4)	27(5)	-2(3)	11(4)	1(3)
C(54B)	30(30)	10(20)	22(12)	-7(15)	1(17)	0(20)
O(61)	32(5)	32(5)	27(4)	6(4)	9(3)	9(4)
C(61)	24(5)	13(4)	22(4)	-11(4)	0(3)	7(3)
C(62)	18(4)	34(6)	26(5)	0(5)	9(4)	2(4)
C(63)	21(5)	34(6)	40(6)	3(5)	7(4)	3(4)
C(64)	32(6)	41(7)	33(6)	-17(5)	6(5)	1(5)
O(61A)	24(4)	40(5)	66(6)	-25(4)	-4(4)	2(4)
C(61A)	39(6)	26(5)	38(6)	-14(4)	16(5)	-13(4)
C(62A)	53(9)	38(7)	60(8)	-4(6)	12(6)	-15(6)

Table 24 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(63A)	110(12)	58(7)	78(9)	-4(7)	17(8)	-7(9)
C(64A)	79(10)	44(7)	88(10)	-11(7)	-4(9)	-10(7)
O(71)	46(5)	41(5)	30(4)	-3(4)	3(3)	4(4)
C(71)	46(8)	48(9)	60(7)	-17(6)	-2(6)	2(6)
C(72)	18(4)	26(5)	56(7)	-5(5)	16(4)	-2(4)
C(73)	39(6)	26(5)	67(8)	18(6)	21(6)	11(5)
C(74)	39(6)	35(6)	42(6)	-6(4)	3(4)	10(4)
O(71A)	60(7)	17(4)	17(4)	-12(3)	-6(4)	-3(4)
C(71A)	37(8)	15(5)	43(7)	-11(5)	-5(6)	-6(5)
O(72A)	54(11)	45(8)	53(8)	-22(6)	-10(8)	7(7)
C(73A)	27(7)	42(8)	28(6)	-16(5)	-18(5)	-2(6)
C(74A)	23(5)	21(5)	25(5)	-7(4)	-9(4)	-3(4)

2.5 Zn-complex 1e

Zn-complex **1e** crystallized in triclinic space group $P\bar{1}$. The asymmetric unit contains two molecule of **1e** and three molecules of THF. The tructure was found to be disordered and the disorder was refined with the help of same distance restraints on 1,2 and 1,3 distances, similarity restraints on anisotropic displacement parameters and advanced rigid bond restraints. Some atoms very close to each other were set to the same anisotropic displacement parameters. One half of a ligand, five *tert*-butyl groups and two of the solvent molecules were found to be disordered. These disorder ratios were allowed to refine freely and converged to 0.582(6) for the disordered half of the ligand, 0.605(5), 0.729(6), 0.573(6), 0.865(5), 0.30(4) for the tert-butyl groups and 0.625(8), 0.67(3) for the solvent molecules.

Table 25: Crystal data and structure refinement for Zn-complex **1e**

Identification code	D19217
Empirical formula	C116 H136 N12 O3 Zn2
Formula weight	1877.10
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 16.9522(6) Å α = 103.8982(13)°. b = 17.4631(6) Å β = 92.6608(13)°. c = 17.8947(6) Å γ = 102.1000(13)°.
Volume	5002.0(3) $Å^3$
Z	2
Density (calculated)	1.246 $Mg\,m^{-3}$
Absorption coefficient	0.539 mm^{-1}
F(000)	2000
Crystal size	0.737 x 0.331 x 0.100 mm^3
Theta range for data collection	2.357 to 26.372°.
Index ranges	-21<=h<=21, -21<=k<=21, -22<=l<=22
Reflections collected	237694
Independent reflections	20454 [R(int) = 0.0685]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	20454 / 4277 / 1569
Goodness-of-fit on F2	1.031
Final R indices [I>2sigma(I)]	R1 = 0.0417, wR2 = 0.0963
R indices (all data)	R1 = 0.0613, wR2 = 0.1072
Extinction coefficient	n/a
Largest diff. peak and hole	0.569 and -0.483 $e.Å^{-3}$

Table 26: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1e**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	2376(1)	4894(1)	-32(1)	15(1)
N(1)	3484(1)	4767(1)	-529(1)	16(1)
N(2)	3030(1)	6100(1)	188(1)	17(1)
N(3)	1536(1)	5549(1)	511(1)	16(1)
C(1)	3657(1)	4084(1)	-907(1)	19(1)
C(2)	4385(1)	4064(1)	-1245(1)	21(1)
C(3)	4941(1)	4774(1)	-1161(1)	20(1)

Table 26 – continued from previous page

	x	y	z	U(eq)
C(4)	4784(1)	5513(1)	-745(1)	17(1)
C(5)	4027(1)	5482(1)	-443(1)	14(1)
C(6)	3810(1)	6218(1)	-22(1)	15(1)
C(7)	4424(1)	6920(1)	122(1)	18(1)
C(8)	5190(1)	6953(1)	-169(1)	20(1)
C(9)	5358(1)	6260(1)	-615(1)	19(1)
C(10)	5807(1)	7771(1)	26(1)	25(1)
C(11)	5989(1)	8098(1)	905(1)	31(1)
C(12)	5452(2)	8370(1)	-312(1)	32(1)
C(13)	6609(2)	7704(2)	-310(2)	46(1)
C(21)	811(1)	5237(1)	692(1)	18(1)
C(22)	304(1)	5718(1)	1056(1)	23(1)
C(23)	560(1)	6543(1)	1218(1)	22(1)
C(24)	1331(1)	6897(1)	1036(1)	19(1)
C(25)	1816(1)	6370(1)	692(1)	16(1)
C(26)	2632(1)	6682(1)	504(1)	17(1)
C(27)	2866(1)	7524(1)	663(1)	24(1)
C(28)	2386(1)	8059(1)	1016(1)	25(1)
C(29)	1630(1)	7745(1)	1203(1)	23(1)
C(30)	2737(1)	8977(1)	1191(2)	35(1)
C(31)	2153(2)	9474(2)	1600(3)	41(1)
C(32)	2898(4)	9204(2)	450(3)	76(2)
C(33)	3512(2)	9193(2)	1765(4)	71(2)
C(31A)	2631(9)	9364(7)	2016(7)	72(5)
C(32A)	2287(8)	9309(7)	611(9)	69(4)
C(33A)	3652(5)	9210(5)	1080(7)	36(3)
N(41)	1793(1)	4600(1)	-1229(1)	16(1)
N(42)	1787(1)	3682(1)	-244(1)	16(1)
N(43)	2646(1)	4605(1)	1059(1)	16(1)
C(41)	1790(1)	5082(1)	-1696(1)	23(1)
C(42)	1482(1)	4799(2)	-2476(1)	29(1)
C(43)	1198(1)	3987(2)	-2776(1)	29(1)
C(44)	1212(1)	3442(1)	-2307(1)	23(1)
C(45)	1506(1)	3785(1)	-1520(1)	16(1)
C(46)	1522(1)	3273(1)	-994(1)	16(1)
C(47)	1315(1)	2440(1)	-1329(1)	20(1)
C(48)	1041(1)	2095(1)	-2121(1)	24(1)
C(49)	965(1)	2594(1)	-2595(1)	27(1)
C(50)	808(1)	1167(1)	-2433(1)	32(1)
C(51)	1501(3)	827(3)	-2209(3)	48(1)
C(52)	701(3)	951(3)	-3346(2)	42(1)
C(53)	31(3)	888(3)	-2150(3)	49(1)
C(51A)	904(5)	660(3)	-1786(4)	39(2)

Table 26 – continued from previous page

	x	y	z	U(eq)
C(52A)	1294(5)	837(4)	-3051(4)	41(2)
C(53A)	-123(4)	852(4)	-2712(5)	44(2)
C(61)	3090(1)	5084(1)	1689(1)	18(1)
C(62)	3212(1)	4832(1)	2363(1)	22(1)
C(63)	2826(1)	4071(1)	2385(1)	23(1)
C(64)	2308(1)	3551(1)	1737(1)	19(1)
C(65)	2253(1)	3844(1)	1072(1)	15(1)
C(66)	1760(1)	3339(1)	376(1)	16(1)
C(67)	1306(1)	2597(1)	428(1)	19(1)
C(68)	1362(1)	2300(1)	1094(1)	24(1)
C(69)	1864(1)	2768(1)	1734(1)	24(1)
C(70)	869(2)	1443(1)	1054(1)	34(1)
C(71)	-44(8)	1360(20)	1001(18)	35(4)
C(72)	1055(18)	857(17)	308(12)	32(4)
C(73)	1170(19)	1160(20)	1741(15)	73(3)
C(71A)	-29(4)	1402(9)	835(9)	39(2)
C(72A)	1180(10)	823(9)	458(8)	50(3)
C(73A)	920(12)	1233(8)	1842(6)	73(3)
Zn(81)	2640(1)	5732(1)	5207(1)	18(1)
N(81)	3728(1)	5575(1)	4709(1)	18(1)
N(82)	2437(1)	4466(1)	4796(1)	18(1)
N(83)	1466(1)	5350(1)	5541(1)	21(1)
C(81)	4342(1)	6166(1)	4670(1)	23(1)
C(82)	5027(1)	6019(1)	4304(1)	30(1)
C(83)	5061(1)	5235(2)	3982(1)	30(1)
C(84)	4417(1)	4590(1)	4019(1)	23(1)
C(85)	3744(1)	4792(1)	4391(1)	18(1)
C(86)	3046(1)	4171(1)	4443(1)	19(1)
C(87)	3112(1)	3373(1)	4134(1)	24(1)
C(88)	3782(2)	3166(1)	3757(1)	26(1)
C(89)	4425(1)	3770(1)	3696(1)	27(1)
C(90)	3796(2)	2271(1)	3402(1)	36(1)
C(91)	2982(2)	1690(2)	3429(2)	45(1)
C(92)	4472(2)	2049(2)	3811(2)	47(1)
C(93)	3915(2)	2168(2)	2531(2)	49(1)
C(91A)	3080(9)	1742(12)	2920(12)	48(5)
C(92A)	3994(13)	1933(10)	4136(8)	38(4)
C(93A)	4611(8)	2165(10)	3001(11)	37(5)
C(101)	1035(1)	5821(2)	5939(1)	27(1)
C(102)	267(1)	5508(2)	6149(1)	34(1)
C(103)	-43(1)	4694(2)	5915(1)	36(1)
C(104)	397(1)	4175(2)	5475(1)	29(1)
C(105)	1176(1)	4532(1)	5306(1)	21(1)

Table 26 – continued from previous page

	x	y	z	U(eq)
C(106)	1670(1)	4042(1)	4871(1)	22(1)
C(107)	1302(2)	3222(1)	4586(1)	31(1)
C(108)	519(2)	2863(2)	4742(1)	38(1)
C(109)	85(1)	3332(2)	5196(1)	36(1)
C(110)	161(2)	1955(2)	4395(2)	51(1)
C(111)	-20(4)	1503(3)	5058(3)	54(2)
C(112)	-503(4)	1765(4)	3810(4)	52(2)
C(113)	856(3)	1458(3)	4018(4)	47(1)
C(11B)	-700(4)	1735(4)	4757(6)	75(3)
C(12B)	-139(7)	1931(5)	3546(5)	69(3)
C(13B)	662(4)	1507(4)	4544(5)	54(2)
N(121)	3135(1)	5949(1)	6404(1)	18(1)
N(122)	2854(1)	6984(1)	5603(1)	22(1)
C(121)	3251(1)	5408(1)	6777(1)	20(1)
C(122)	3562(1)	5619(1)	7555(1)	25(1)
C(123)	3737(1)	6412(1)	7952(1)	28(1)
C(124)	3584(1)	7005(1)	7586(1)	25(1)
C(125)	3289(1)	6743(1)	6792(1)	20(1)
C(126)	3116(1)	7314(1)	6372(1)	23(1)
C(127)	3206(2)	8102(1)	6816(1)	29(1)
C(128)	3523(2)	8374(1)	7604(1)	34(1)
C(129)	3716(2)	7832(1)	7979(1)	33(1)
C(130)	3634(2)	9279(2)	8006(2)	42(1)
C(131)	4153(3)	9513(2)	8787(2)	79(1)
C(132)	4114(2)	9791(2)	7527(2)	60(1)
C(133)	2807(2)	9460(2)	8112(2)	70(1)
N(123)	2231(6)	6048(3)	4194(4)	22(1)
C(141)	1923(18)	5566(6)	3510(7)	24(2)
C(142)	1661(7)	5838(6)	2888(6)	30(2)
C(143)	1721(5)	6642(5)	2988(4)	38(2)
C(144)	2042(4)	7192(4)	3712(4)	32(2)
C(145)	2278(5)	6865(4)	4318(4)	19(1)
C(146)	2623(6)	7378(4)	5069(5)	21(2)
C(147)	2751(4)	8210(4)	5132(4)	33(2)
C(148)	2494(4)	8547(3)	4553(3)	41(1)
C(149)	2136(4)	8042(3)	3854(3)	44(1)
C(150)	2624(5)	9478(3)	4740(3)	54(2)
C(151)	2293(5)	9798(3)	5515(4)	66(2)
C(152)	3545(6)	9838(4)	4830(6)	65(3)
C(153)	2205(6)	9757(4)	4126(4)	102(3)
N(23B)	2248(8)	6151(5)	4184(6)	22(1)
C(41B)	1970(30)	5696(9)	3476(10)	24(2)
C(42B)	1821(9)	6035(6)	2860(7)	21(2)

Table 26 – continued from previous page

	x	y	z	U(eq)
C(43B)	1986(6)	6860(6)	3007(5)	25(2)
C(44B)	2334(5)	7369(5)	3736(5)	23(2)
C(45B)	2484(8)	6972(6)	4318(7)	19(1)
C(46B)	2845(8)	7443(6)	5079(6)	17(2)
C(47B)	3102(5)	8267(5)	5167(5)	24(2)
C(48B)	2974(5)	8671(3)	4597(4)	31(2)
C(49B)	2578(5)	8221(4)	3899(4)	31(2)
C(50B)	3249(7)	9598(5)	4800(5)	42(2)
C(51B)	2823(7)	9971(4)	5480(4)	53(2)
C(52B)	4179(6)	9834(4)	5042(4)	52(2)
C(53B)	3094(7)	9945(4)	4119(4)	69(3)
O(1S)	520(1)	6941(1)	7787(1)	41(1)
C(1S)	185(2)	6411(2)	8245(2)	37(1)
C(2S)	719(2)	6677(2)	9011(2)	41(1)
C(3S)	1486(2)	7232(2)	8848(2)	46(1)
C(4S)	1375(2)	7120(2)	7981(2)	45(1)
O(11S)	5194(6)	11990(6)	7610(5)	42(2)
C(11S)	5071(7)	11577(6)	6815(5)	48(2)
C(12S)	5322(9)	12211(6)	6359(4)	46(2)
C(13S)	5738(9)	12976(6)	6986(7)	39(2)
C(14S)	5860(7)	12652(7)	7684(6)	39(2)
O(11T)	5449(18)	11885(13)	7618(10)	58(4)
C(11T)	5325(19)	11466(11)	6821(11)	57(5)
C(12T)	5606(14)	12064(10)	6351(8)	36(3)
C(13T)	5897(19)	12869(11)	6965(13)	43(5)
C(14T)	6064(17)	12589(14)	7682(13)	44(5)
O(21S)	3018(4)	11896(2)	6420(3)	71(2)
C(21S)	2909(6)	12239(7)	5786(5)	44(2)
C(22S)	2687(9)	13009(7)	6140(7)	45(3)
C(23S)	3225(8)	13319(4)	6924(6)	29(2)
C(24S)	3182(3)	12513(3)	7132(3)	32(1)
O(21T)	3566(5)	12143(3)	6108(4)	52(2)
C(21T)	2806(12)	12240(13)	5756(10)	64(5)
C(22T)	2776(14)	13089(10)	6152(12)	32(3)
C(23T)	3169(13)	13177(9)	6971(10)	47(4)
C(24T)	3477(7)	12416(6)	6911(5)	47(2)

Table 27: Selected bond lengths [Å] and angles [°] for complex **1e**

Zn(1)-N(42)	2.0777(16)
Zn(1)-N(2)	2.0969(16)
Zn(1)-N(3)	2.1358(16)

Table 27 – continued from previous page

Zn(1)-N(1)	2.1439(16)
Zn(1)-N(43)	2.1838(16)
Zn(1)-N(41)	2.2116(16)
N(42)-Zn(1)-N(2)	176.94(6)
N(42)-Zn(1)-N(3)	104.88(6)
N(2)-Zn(1)-N(3)	77.74(6)
N(42)-Zn(1)-N(1)	99.85(6)
N(2)-Zn(1)-N(1)	77.59(6)
N(3)-Zn(1)-N(1)	155.21(6)
N(42)-Zn(1)-N(43)	77.03(6)
N(2)-Zn(1)-N(43)	101.60(6)
N(3)-Zn(1)-N(43)	88.73(6)
N(1)-Zn(1)-N(43)	98.61(6)
N(42)-Zn(1)-N(41)	76.31(6)
N(2)-Zn(1)-N(41)	105.08(6)
N(3)-Zn(1)-N(41)	96.91(6)
N(1)-Zn(1)-N(41)	87.12(6)
N(43)-Zn(1)-N(41)	153.31(6)

Table 28: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1e**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	14(1)	14(1)	17(1)	4(1)	3(1)	3(1)
N(1)	16(1)	15(1)	16(1)	5(1)	0(1)	3(1)
N(2)	16(1)	16(1)	21(1)	5(1)	5(1)	5(1)
N(3)	15(1)	20(1)	15(1)	5(1)	2(1)	5(1)
C(1)	19(1)	15(1)	20(1)	1(1)	-1(1)	3(1)
C(2)	22(1)	17(1)	22(1)	0(1)	3(1)	7(1)
C(3)	16(1)	24(1)	18(1)	3(1)	5(1)	6(1)
C(4)	16(1)	19(1)	15(1)	4(1)	1(1)	5(1)
C(5)	14(1)	16(1)	13(1)	5(1)	0(1)	2(1)
C(6)	15(1)	18(1)	14(1)	5(1)	2(1)	6(1)
C(7)	18(1)	15(1)	19(1)	1(1)	2(1)	5(1)
C(8)	17(1)	19(1)	22(1)	5(1)	3(1)	1(1)
C(9)	15(1)	21(1)	23(1)	6(1)	7(1)	5(1)
C(10)	20(1)	17(1)	36(1)	3(1)	10(1)	1(1)
C(11)	25(1)	20(1)	41(1)	-1(1)	-4(1)	-1(1)
C(12)	36(1)	20(1)	38(1)	9(1)	11(1)	-1(1)
C(13)	25(1)	23(1)	79(2)	-1(1)	26(1)	-4(1)
C(21)	17(1)	20(1)	17(1)	4(1)	1(1)	3(1)
C(22)	13(1)	28(1)	25(1)	5(1)	3(1)	3(1)
C(23)	15(1)	28(1)	23(1)	3(1)	4(1)	9(1)

Table 28 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(24)	16(1)	23(1)	18(1)	3(1)	1(1)	7(1)
C(25)	15(1)	19(1)	15(1)	3(1)	1(1)	5(1)
C(26)	20(1)	17(1)	15(1)	5(1)	2(1)	3(1)
C(27)	17(1)	20(1)	36(1)	8(1)	8(1)	6(1)
C(28)	22(1)	19(1)	33(1)	4(1)	3(1)	8(1)
C(29)	22(1)	20(1)	27(1)	1(1)	4(1)	11(1)
C(30)	26(1)	19(1)	60(2)	4(1)	13(1)	7(1)
C(31)	33(2)	17(2)	68(3)	1(2)	9(2)	8(1)
C(32)	125(5)	22(2)	95(4)	26(2)	71(4)	21(3)
C(33)	33(2)	23(2)	139(5)	-8(3)	-10(3)	5(2)
C(31A)	80(10)	33(6)	75(7)	-22(5)	34(7)	-14(6)
C(32A)	54(7)	28(6)	121(10)	26(6)	-20(8)	3(5)
C(33A)	29(4)	15(4)	60(7)	10(4)	0(4)	-2(3)
N(41)	12(1)	22(1)	19(1)	9(1)	5(1)	7(1)
N(42)	17(1)	18(1)	14(1)	5(1)	1(1)	3(1)
N(43)	12(1)	18(1)	16(1)	4(1)	4(1)	5(1)
C(41)	18(1)	29(1)	29(1)	17(1)	6(1)	10(1)
C(42)	25(1)	44(1)	28(1)	23(1)	5(1)	14(1)
C(43)	28(1)	49(1)	17(1)	13(1)	2(1)	16(1)
C(44)	18(1)	36(1)	17(1)	6(1)	2(1)	12(1)
C(45)	12(1)	23(1)	17(1)	6(1)	3(1)	8(1)
C(46)	12(1)	21(1)	15(1)	4(1)	2(1)	5(1)
C(47)	18(1)	21(1)	21(1)	5(1)	3(1)	5(1)
C(48)	19(1)	26(1)	24(1)	-3(1)	1(1)	6(1)
C(49)	24(1)	37(1)	16(1)	-3(1)	-2(1)	11(1)
C(50)	34(1)	26(1)	27(1)	-5(1)	0(1)	5(1)
C(51)	68(3)	22(2)	51(3)	-2(2)	-8(2)	19(2)
C(52)	58(3)	27(2)	31(2)	-6(2)	3(2)	4(2)
C(53)	55(3)	23(2)	53(3)	-4(2)	19(3)	-10(2)
C(51A)	62(5)	16(3)	35(4)	6(2)	2(3)	1(3)
C(52A)	57(5)	19(3)	42(4)	0(3)	20(3)	4(3)
C(53A)	41(4)	27(3)	49(5)	-5(3)	-5(3)	-6(3)
C(61)	15(1)	19(1)	19(1)	1(1)	3(1)	4(1)
C(62)	20(1)	27(1)	16(1)	0(1)	-1(1)	6(1)
C(63)	26(1)	31(1)	15(1)	6(1)	2(1)	10(1)
C(64)	21(1)	24(1)	16(1)	6(1)	4(1)	8(1)
C(65)	14(1)	18(1)	15(1)	4(1)	5(1)	6(1)
C(66)	16(1)	18(1)	15(1)	5(1)	3(1)	6(1)
C(67)	18(1)	19(1)	20(1)	5(1)	3(1)	2(1)
C(68)	24(1)	22(1)	26(1)	11(1)	5(1)	2(1)
C(69)	29(1)	26(1)	21(1)	13(1)	4(1)	6(1)
C(70)	40(1)	26(1)	37(1)	18(1)	2(1)	-4(1)
C(71)	42(5)	29(8)	41(9)	15(6)	32(5)	8(5)

Table 28 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(72)	22(7)	11(5)	67(7)	13(6)	10(6)	8(4)
C(73)	83(7)	61(3)	64(3)	50(3)	-20(4)	-40(4)
C(71A)	37(2)	26(3)	50(5)	14(4)	15(2)	-10(2)
C(72A)	51(6)	23(3)	83(5)	24(3)	11(4)	9(3)
C(73A)	83(7)	61(3)	64(3)	50(3)	-20(4)	-40(4)
Zn(81)	22(1)	17(1)	15(1)	3(1)	3(1)	4(1)
N(81)	21(1)	19(1)	15(1)	4(1)	-1(1)	4(1)
N(82)	24(1)	17(1)	12(1)	4(1)	6(1)	3(1)
N(83)	21(1)	31(1)	14(1)	7(1)	0(1)	8(1)
C(81)	22(1)	20(1)	24(1)	5(1)	-3(1)	0(1)
C(82)	21(1)	31(1)	33(1)	10(1)	0(1)	-2(1)
C(83)	21(1)	41(1)	30(1)	10(1)	5(1)	9(1)
C(84)	25(1)	31(1)	17(1)	5(1)	0(1)	11(1)
C(85)	21(1)	21(1)	12(1)	5(1)	-1(1)	5(1)
C(86)	25(1)	21(1)	11(1)	5(1)	1(1)	5(1)
C(87)	32(1)	20(1)	20(1)	7(1)	2(1)	2(1)
C(88)	41(1)	23(1)	16(1)	2(1)	0(1)	13(1)
C(89)	31(1)	32(1)	20(1)	4(1)	3(1)	14(1)
C(90)	48(2)	25(1)	35(1)	-1(1)	5(1)	15(1)
C(91)	54(2)	20(1)	52(2)	-9(2)	-7(2)	13(1)
C(92)	53(2)	29(2)	57(2)	-2(2)	-9(2)	22(2)
C(93)	65(2)	42(2)	34(2)	-13(1)	2(2)	24(2)
C(91A)	42(8)	50(11)	44(11)	-9(9)	4(7)	15(7)
C(92A)	44(11)	18(8)	54(9)	9(7)	7(7)	13(8)
C(93A)	45(8)	18(8)	50(11)	5(7)	14(8)	12(7)
C(101)	27(1)	44(1)	16(1)	10(1)	3(1)	18(1)
C(102)	27(1)	65(2)	23(1)	22(1)	7(1)	23(1)
C(103)	19(1)	70(2)	27(1)	29(1)	5(1)	12(1)
C(104)	19(1)	49(1)	19(1)	17(1)	-4(1)	2(1)
C(105)	21(1)	31(1)	12(1)	9(1)	-2(1)	2(1)
C(106)	28(1)	24(1)	13(1)	7(1)	-3(1)	0(1)
C(107)	33(1)	31(1)	21(1)	4(1)	-2(1)	-5(1)
C(108)	37(1)	39(1)	26(1)	9(1)	-8(1)	-16(1)
C(109)	22(1)	54(2)	28(1)	23(1)	-6(1)	-13(1)
C(110)	52(2)	42(2)	38(2)	4(1)	-2(1)	-26(1)
C(111)	71(4)	32(3)	48(3)	9(2)	1(3)	-10(2)
C(112)	53(3)	41(3)	42(3)	4(3)	-14(3)	-21(3)
C(113)	57(3)	25(2)	44(3)	-3(2)	-4(3)	-9(2)
C(11B)	49(5)	29(4)	128(8)	-1(4)	31(5)	-14(3)
C(12B)	107(9)	24(4)	52(5)	-5(3)	-34(5)	-11(5)
C(13B)	58(4)	28(3)	66(6)	10(3)	-2(4)	-10(3)
N(121)	18(1)	18(1)	19(1)	4(1)	4(1)	3(1)
N(122)	26(1)	23(1)	17(1)	6(1)	4(1)	7(1)

Table 28 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(121)	20(1)	21(1)	20(1)	6(1)	4(1)	2(1)
C(122)	27(1)	28(1)	20(1)	12(1)	1(1)	3(1)
C(123)	33(1)	32(1)	18(1)	8(1)	-1(1)	1(1)
C(124)	30(1)	25(1)	18(1)	4(1)	2(1)	3(1)
C(125)	22(1)	19(1)	18(1)	4(1)	4(1)	3(1)
C(126)	27(1)	21(1)	19(1)	4(1)	5(1)	4(1)
C(127)	40(1)	21(1)	26(1)	6(1)	7(1)	9(1)
C(128)	49(2)	22(1)	26(1)	-1(1)	5(1)	6(1)
C(129)	52(2)	25(1)	17(1)	-2(1)	1(1)	4(1)
C(130)	70(2)	23(1)	28(1)	-3(1)	1(1)	9(1)
C(131)	140(4)	31(2)	52(2)	-14(1)	-29(2)	24(2)
C(132)	81(2)	29(2)	56(2)	-2(1)	7(2)	0(2)
C(133)	72(2)	30(2)	98(3)	-11(2)	14(2)	16(2)
N(123)	26(1)	23(1)	17(1)	6(1)	4(1)	7(1)
C(141)	19(3)	36(3)	18(1)	6(2)	5(2)	7(4)
C(142)	21(5)	52(4)	16(2)	11(3)	4(2)	2(3)
C(143)	36(5)	57(4)	24(3)	18(3)	-1(3)	8(3)
C(144)	29(4)	39(3)	31(3)	21(2)	2(3)	4(2)
C(145)	11(4)	28(2)	22(1)	12(1)	9(2)	6(2)
C(146)	17(5)	22(2)	26(2)	10(2)	11(2)	5(2)
C(147)	41(4)	25(2)	33(3)	10(2)	7(3)	6(3)
C(148)	53(4)	29(2)	43(3)	20(2)	2(3)	4(2)
C(149)	55(4)	40(3)	46(3)	27(2)	-2(3)	12(3)
C(150)	70(4)	30(2)	68(4)	31(2)	5(3)	5(3)
C(151)	82(5)	25(3)	98(5)	22(3)	30(4)	16(3)
C(152)	80(6)	33(4)	85(5)	24(4)	30(5)	0(4)
C(153)	169(9)	40(3)	101(6)	39(4)	-35(6)	23(4)
N(23B)	26(1)	23(1)	17(1)	6(1)	4(1)	7(1)
C(41B)	19(3)	36(3)	18(1)	6(2)	5(2)	7(4)
C(42B)	10(5)	35(5)	13(3)	4(3)	4(3)	0(4)
C(43B)	20(5)	33(4)	25(3)	11(3)	-2(3)	7(3)
C(44B)	22(4)	28(3)	19(3)	7(2)	0(3)	7(3)
C(45B)	11(4)	28(2)	22(1)	12(1)	9(2)	6(2)
C(46B)	9(6)	24(3)	19(3)	3(2)	5(3)	5(3)
C(47B)	32(4)	22(3)	20(3)	7(2)	4(3)	7(3)
C(48B)	45(4)	21(3)	27(3)	6(2)	0(3)	6(3)
C(49B)	42(4)	25(3)	31(3)	15(2)	0(3)	10(3)
C(50B)	65(7)	23(4)	37(4)	14(3)	6(4)	2(4)
C(51B)	89(7)	25(4)	48(4)	10(3)	9(4)	19(4)
C(52B)	73(6)	21(3)	51(4)	8(3)	3(4)	-11(3)
C(53B)	128(9)	35(4)	44(4)	21(3)	-4(5)	10(5)
O(1S)	49(1)	40(1)	37(1)	15(1)	-4(1)	11(1)
C(1S)	37(1)	39(1)	40(2)	13(1)	5(1)	11(1)

Table 28 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2S)	46(2)	46(2)	36(1)	15(1)	1(1)	18(1)
C(3S)	46(2)	41(2)	51(2)	14(1)	-10(1)	8(1)
C(4S)	44(2)	40(2)	53(2)	21(1)	4(1)	5(1)
O(11S)	47(4)	40(3)	35(2)	16(2)	6(2)	-2(2)
C(11S)	63(5)	36(3)	40(3)	12(2)	-2(3)	-1(3)
C(12S)	58(5)	42(4)	35(3)	16(2)	-1(3)	2(3)
C(13S)	42(5)	34(3)	40(3)	15(2)	3(3)	1(3)
C(14S)	36(4)	40(3)	34(3)	9(2)	1(2)	-2(3)
O(11T)	74(10)	49(6)	41(4)	13(4)	5(6)	-8(7)
C(11T)	95(12)	33(5)	39(5)	10(4)	5(7)	7(7)
C(12T)	45(8)	31(5)	28(4)	7(4)	-4(5)	6(5)
C(13T)	44(10)	42(6)	39(6)	13(5)	2(6)	-4(7)
C(14T)	54(10)	37(6)	38(5)	16(4)	1(6)	-5(6)
O(21S)	112(4)	35(2)	55(3)	2(2)	-36(3)	12(2)
C(21S)	51(4)	38(4)	34(4)	-4(3)	-6(3)	9(3)
C(22S)	42(5)	65(6)	27(4)	2(4)	-3(3)	25(5)
C(23S)	36(3)	27(2)	26(3)	12(2)	8(2)	5(2)
C(24S)	32(3)	33(2)	31(3)	10(2)	-1(2)	6(2)
O(21T)	71(5)	30(3)	50(3)	0(2)	-11(3)	14(3)
C(21T)	102(10)	41(8)	43(7)	5(6)	-37(7)	21(7)
C(22T)	36(6)	30(5)	29(7)	13(5)	4(5)	0(4)
C(23T)	36(7)	81(9)	22(5)	3(6)	-2(5)	23(7)
C(24T)	36(5)	59(6)	43(5)	21(4)	-8(4)	-1(4)

2.6 Zn-complex 1f

The structure of **1f** was solved in the tetragonal space group $I\bar{4}$. The asymmetric unit contains one quarter of a molecule of **1f**. The structure was found to be disordered and the disorder was refined with the help of same distance restraints on 1,2 and 1,3 distances, restraints to a common plane, similarity restraints on anisotropic displacement parameters and advanced rigid bond restraints. Some atoms very close to each other were set to the same anisotropic displacement parameters.

Table 29: Crystal data and structure refinement for Zn-complex **1f**

Identification code	D19091
Empirical formula	C52 H56 N6 Zn
Formula weight	830.39
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	$I\bar{4}$
Unit cell dimensions	a = 12.5654(3) Å $\alpha = 90°$.
	b = 12.5654(3) Å $\beta = 90°$.
	c = 13.2240(4) Å $\gamma = 90°$.
Volume	2087.93(12) $Å^3$
Z	2
Density (calculated)	1.321 $Mg\,m^{-3}$
Absorption coefficient	0.633 mm^{-1}
F(000)	880
Crystal size	0.239 x 0.193 x 0.170 mm^3
Theta range for data collection	2.236 to 34.337°.
Index ranges	-19<=h<=19, -19<=k<=19, -20<=l<=20
Reflections collected	20431
Independent reflections	4365 [R(int) = 0.0537]
Completeness to theta = 25.242°	100.0 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	4365 / 513 / 250
Goodness-of-fit on F2	1.043
Final R indices [I>2sigma(I)]	R1 = 0.0356, wR2 = 0.0690
R indices (all data)	R1 = 0.0429, wR2 = 0.0714
Absolute structure parameter	0.025(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.630 and -0.386 $e.Å^{-3}$

Table 30: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1f**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	5000	5000	0	14(1)
N(2)	5000	5000	1555(1)	19(1)
N(1)	6715(12)	4881(13)	320(10)	16(2)
C(1)	7501(6)	4830(7)	-308(7)	10(1)
C(2)	8522(11)	4541(13)	-46(10)	26(2)
C(3)	8731(10)	4215(15)	935(8)	22(2)

Table 30 – continued from previous page

	x	y	z	U(eq)
C(4)	7903(9)	4216(17)	1648(8)	17(2)
C(5)	8001(7)	3799(8)	2640(6)	18(1)
C(6)	7133(6)	3778(6)	3269(5)	16(1)
C(7)	6167(7)	4222(10)	2943(7)	20(1)
C(8)	5980(6)	4640(6)	1961(5)	16(1)
C(9)	6890(10)	4585(18)	1306(9)	14(2)
C(10)	7226(5)	3248(4)	4302(4)	21(1)
C(11)	7483(13)	3980(11)	5185(9)	30(3)
C(12)	7647(8)	3621(8)	6292(6)	25(1)
C(13)	8332(7)	4209(10)	7021(8)	38(2)
N(21)	3331(12)	5170(13)	425(10)	17(2)
C(21)	2499(10)	5262(9)	-172(10)	35(3)
C(22)	1474(9)	5574(13)	139(10)	23(2)
C(23)	1382(9)	5839(15)	1150(8)	25(2)
C(24)	2251(9)	5776(16)	1816(9)	20(2)
C(25)	2206(7)	6078(9)	2850(7)	24(2)
C(26)	3096(6)	6032(7)	3441(6)	24(2)
C(27)	4056(7)	5644(10)	3066(6)	18(1)
C(28)	4148(7)	5320(6)	2067(6)	16(1)
C(29)	3238(9)	5397(17)	1422(8)	14(2)
C(30)	3072(5)	6473(6)	4502(5)	36(2)
C(31)	2349(12)	5902(11)	5190(8)	20(2)
C(32)	2467(8)	6581(8)	6169(6)	25(1)
C(33)	2064(8)	5908(9)	7021(8)	42(3)

Table 31: Selected bond lengths [Å] and angles [°] for complex **1f**

Zn(1)-N(2)#1	2.0569(17)
Zn(1)-N(2)	2.0569(17)
Zn(1)-N(21)	2.181(16)
Zn(1)-N(1)	2.201(16)
N(2)#1-Zn(1)-N(2)	180.0
N(2)#1-Zn(1)-N(21)	104.9(3)
N(2)-Zn(1)-N(21)	75.1(3)
N(2)#1-Zn(1)-N(1)	101.1(3)
N(2)-Zn(1)-N(1)	78.9(3)
N(21)-Zn(1)-N(1)	153.93(15)

Table 32: Anisotropic displacement parameters (Å^2 × 10^3) for complex **1f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	15(1)	15(1)	13(1)	0	0	0
N(2)	19(1)	24(2)	15(1)	0	0	-1(1)
N(1)	19(4)	14(3)	13(2)	2(2)	-2(2)	-2(2)
C(1)	4(2)	10(2)	16(2)	-1(2)	2(2)	-2(1)
C(2)	20(3)	32(5)	25(4)	0(3)	0(2)	-5(2)
C(3)	13(3)	26(4)	28(3)	-5(3)	2(2)	-3(2)
C(4)	14(3)	18(3)	20(3)	-1(3)	-5(2)	-2(3)
C(5)	15(3)	18(3)	21(3)	-5(2)	-5(2)	-1(2)
C(6)	21(3)	13(2)	15(2)	1(2)	-6(2)	-2(2)
C(7)	17(3)	24(3)	18(2)	-1(2)	7(2)	-6(2)
C(8)	16(2)	18(1)	13(1)	3(2)	-5(1)	-6(1)
C(9)	11(2)	12(3)	20(3)	-3(2)	6(2)	-3(2)
C(10)	24(3)	15(2)	25(2)	6(2)	-7(2)	-2(2)
C(11)	44(6)	21(4)	23(4)	3(2)	8(3)	-1(3)
C(12)	38(2)	19(3)	17(2)	3(1)	-2(2)	4(2)
C(13)	51(5)	42(3)	20(2)	-8(2)	-5(3)	-4(4)
N(21)	16(3)	13(3)	23(4)	-1(3)	-3(2)	-1(2)
C(21)	39(4)	34(4)	31(5)	-4(3)	0(3)	-1(3)
C(22)	12(3)	20(3)	36(5)	2(3)	-1(3)	5(2)
C(23)	12(3)	24(3)	38(5)	-3(4)	5(3)	0(3)
C(24)	11(3)	15(3)	33(4)	1(4)	2(2)	-5(2)
C(25)	21(4)	22(3)	28(4)	-5(3)	11(3)	-2(3)
C(26)	23(3)	25(4)	24(3)	-5(2)	6(2)	-9(2)
C(27)	12(3)	30(4)	11(2)	-4(2)	0(2)	-8(2)
C(28)	16(2)	18(1)	13(1)	3(2)	-5(1)	-6(1)
C(29)	14(3)	13(3)	16(3)	-3(3)	7(2)	-3(3)
C(30)	32(3)	42(4)	34(3)	-21(3)	16(2)	-17(3)
C(31)	28(3)	17(3)	15(3)	-6(2)	1(2)	-4(2)
C(32)	38(2)	19(3)	17(2)	3(1)	-2(2)	4(2)
C(33)	61(7)	41(5)	25(3)	-3(3)	4(4)	26(5)

2.7 Zn-complex 1g

Zn-complex **1g** crystallized in the monoclinic space group $P2_1/c$ and the asymmetric unit contains one molecule of the complex.

Table 33: Crystal data and structure refinement for Zn-complex **1g**

Identification code	D19114
Empirical formula	C36 H20 F4 N6 Zn
Formula weight	677.95
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P21/c
Unit cell dimensions	a = 19.7659(7) Å $\alpha = 90°$.
	b = 16.3402(6) Å $\beta = 97.8502(13)°$.
	c = 8.6854(3) Å $\gamma = 90°$.
Volume	2778.91(17) $Å^3$
Z	4
Density (calculated)	1.620 $Mg\,m^{-3}$
Absorption coefficient	0.951 mm^{-1}
F(000)	1376
Crystal size	0.270 x 0.072 x 0.026 mm^3
Theta range for data collection	2.425 to 28.282°.
Index ranges	-26<=h<=26, -20<=k<=21, -11<=l<=11
Reflections collected	72569
Independent reflections	6897 [R(int) = 0.0566]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	6897 / 0 / 424
Goodness-of-fit on F2	1.037
Final R indices [I>2sigma(I)]	R1 = 0.0345, wR2 = 0.0714
R indices (all data)	R1 = 0.0507, wR2 = 0.0764
Extinction coefficient	n/a
Largest diff. peak and hole	0.355 and -0.471 $e.Å^{-3}$

Table 34: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1g**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	2581(1)	4778(1)	7226(1)	12(1)
F(1)	5868(1)	5344(1)	7220(1)	26(1)
F(2)	4375(1)	7522(1)	11543(1)	23(1)
N(1)	3354(1)	3906(1)	6674(2)	14(1)
N(2)	3498(1)	5365(1)	8021(2)	13(1)
N(3)	2266(1)	6006(1)	7929(2)	14(1)
C(1)	3246(1)	3188(1)	5982(2)	19(1)

Table 34 – continued from previous page

	x	y	z	U(eq)
C(2)	3770(1)	2732(1)	5450(2)	24(1)
C(3)	4415(1)	3044(1)	5631(2)	22(1)
C(4)	4551(1)	3818(1)	6342(2)	18(1)
C(5)	5201(1)	4189(1)	6491(2)	20(1)
C(6)	5255(1)	4951(1)	7119(2)	18(1)
C(7)	4730(1)	5382(1)	7678(2)	16(1)
C(8)	4082(1)	5029(1)	7606(2)	13(1)
C(9)	3996(1)	4229(1)	6876(2)	14(1)
C(11)	1643(1)	6318(1)	7760(2)	17(1)
C(12)	1490(1)	7074(1)	8413(2)	21(1)
C(13)	2004(1)	7491(1)	9299(2)	20(1)
C(14)	2675(1)	7175(1)	9518(2)	15(1)
C(15)	3227(1)	7560(1)	10460(2)	18(1)
C(16)	3840(1)	7180(1)	10601(2)	17(1)
C(17)	3982(1)	6454(1)	9850(2)	15(1)
C(18)	3464(1)	6063(1)	8870(2)	12(1)
C(19)	2786(1)	6423(1)	8772(2)	13(1)
F(21)	-187(1)	4348(1)	2138(2)	41(1)
F(22)	-208(1)	2971(1)	8869(2)	48(1)
N(21)	2381(1)	5122(1)	4850(2)	12(1)
N(22)	1595(1)	4313(1)	6565(2)	14(1)
N(23)	2388(1)	4155(1)	9268(2)	15(1)
C(21)	2806(1)	5512(1)	4061(2)	14(1)
C(22)	2611(1)	5818(1)	2561(2)	17(1)
C(23)	1954(1)	5697(1)	1879(2)	16(1)
C(24)	1491(1)	5255(1)	2663(2)	15(1)
C(25)	820(1)	5062(1)	1957(2)	21(1)
C(26)	449(1)	4587(1)	2801(2)	25(1)
C(27)	654(1)	4301(1)	4308(2)	23(1)
C(28)	1295(1)	4502(1)	5091(2)	14(1)
C(29)	1728(1)	4977(1)	4183(2)	12(1)
C(31)	2816(1)	4093(1)	10572(2)	18(1)
C(32)	2646(1)	3690(1)	11892(2)	22(1)
C(33)	2010(1)	3354(1)	11829(2)	23(1)
C(34)	1536(1)	3415(1)	10463(2)	20(1)
C(35)	864(1)	3105(1)	10350(2)	30(1)
C(36)	451(1)	3242(1)	9007(3)	29(1)
C(37)	635(1)	3640(1)	7699(2)	22(1)
C(38)	1301(1)	3930(1)	7709(2)	15(1)
C(39)	1752(1)	3826(1)	9170(2)	15(1)

Table 35: Selected bond lengths [Å] and angles [°] for complex **1g**

Zn(1)-N(2)	2.0830(15)
Zn(1)-N(22)	2.0980(15)
Zn(1)-N(21)	2.1228(15)
Zn(1)-N(23)	2.1246(15)
Zn(1)-N(1)	2.1888(15)
Zn(1)-N(3)	2.2106(15)
N(2)-Zn(1)-N(22)	172.48(6)
N(2)-Zn(1)-N(21)	103.80(6)
N(22)-Zn(1)-N(21)	77.69(6)
N(2)-Zn(1)-N(23)	101.07(6)
N(22)-Zn(1)-N(23)	77.78(6)
N(21)-Zn(1)-N(23)	155.12(6)
N(2)-Zn(1)-N(1)	76.77(6)
N(22)-Zn(1)-N(1)	110.69(6)
N(21)-Zn(1)-N(1)	90.11(5)
N(23)-Zn(1)-N(1)	94.66(6)
N(2)-Zn(1)-N(3)	75.89(6)
N(22)-Zn(1)-N(3)	96.79(6)
N(21)-Zn(1)-N(3)	90.37(5)
N(23)-Zn(1)-N(3)	96.60(5)
N(1)-Zn(1)-N(3)	151.95(6)

Table 36: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1g**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	10(1)	14(1)	11(1)	1(1)	2(1)	-1(1)
F(1)	11(1)	37(1)	32(1)	-4(1)	6(1)	-4(1)
F(2)	25(1)	24(1)	20(1)	-7(1)	3(1)	-10(1)
N(1)	14(1)	14(1)	14(1)	2(1)	3(1)	0(1)
N(2)	11(1)	14(1)	15(1)	-1(1)	3(1)	-1(1)
N(3)	15(1)	16(1)	10(1)	3(1)	4(1)	0(1)
C(1)	20(1)	16(1)	21(1)	1(1)	4(1)	-3(1)
C(2)	32(1)	15(1)	28(1)	-4(1)	10(1)	1(1)
C(3)	24(1)	19(1)	26(1)	-1(1)	11(1)	7(1)
C(4)	18(1)	20(1)	16(1)	4(1)	6(1)	5(1)
C(5)	14(1)	26(1)	20(1)	2(1)	6(1)	4(1)
C(6)	12(1)	27(1)	16(1)	3(1)	2(1)	-1(1)
C(7)	14(1)	18(1)	16(1)	0(1)	2(1)	-1(1)
C(8)	15(1)	15(1)	9(1)	1(1)	2(1)	1(1)
C(9)	14(1)	15(1)	12(1)	3(1)	3(1)	1(1)

Table 36 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(11)	15(1)	22(1)	14(1)	4(1)	3(1)	2(1)
C(12)	20(1)	24(1)	19(1)	5(1)	8(1)	9(1)
C(13)	28(1)	16(1)	18(1)	3(1)	10(1)	6(1)
C(14)	23(1)	14(1)	11(1)	2(1)	8(1)	0(1)
C(15)	29(1)	13(1)	14(1)	-1(1)	8(1)	-2(1)
C(16)	23(1)	17(1)	11(1)	0(1)	4(1)	-9(1)
C(17)	15(1)	17(1)	13(1)	2(1)	3(1)	-2(1)
C(18)	16(1)	13(1)	9(1)	2(1)	6(1)	-2(1)
C(19)	17(1)	14(1)	9(1)	2(1)	5(1)	-1(1)
F(21)	17(1)	70(1)	32(1)	14(1)	-9(1)	-17(1)
F(22)	41(1)	73(1)	32(1)	-3(1)	13(1)	-42(1)
N(21)	14(1)	11(1)	12(1)	-2(1)	3(1)	-1(1)
N(22)	13(1)	16(1)	13(1)	0(1)	4(1)	-2(1)
N(23)	18(1)	14(1)	14(1)	0(1)	4(1)	2(1)
C(21)	13(1)	15(1)	16(1)	-2(1)	5(1)	-2(1)
C(22)	20(1)	17(1)	16(1)	2(1)	7(1)	-2(1)
C(23)	22(1)	16(1)	12(1)	3(1)	3(1)	2(1)
C(24)	15(1)	15(1)	14(1)	0(1)	3(1)	3(1)
C(25)	18(1)	27(1)	17(1)	3(1)	-2(1)	1(1)
C(26)	11(1)	38(1)	24(1)	2(1)	-4(1)	-5(1)
C(27)	15(1)	33(1)	21(1)	6(1)	2(1)	-7(1)
C(28)	13(1)	15(1)	15(1)	0(1)	4(1)	0(1)
C(29)	13(1)	11(1)	13(1)	-2(1)	4(1)	1(1)
C(31)	21(1)	17(1)	17(1)	0(1)	2(1)	6(1)
C(32)	34(1)	18(1)	13(1)	1(1)	2(1)	9(1)
C(33)	42(1)	15(1)	15(1)	3(1)	10(1)	2(1)
C(34)	32(1)	13(1)	16(1)	-1(1)	9(1)	-4(1)
C(35)	45(1)	26(1)	21(1)	-1(1)	16(1)	-19(1)
C(36)	33(1)	32(1)	25(1)	-7(1)	13(1)	-22(1)
C(37)	23(1)	26(1)	18(1)	-4(1)	6(1)	-11(1)
C(38)	18(1)	12(1)	16(1)	-2(1)	7(1)	-3(1)
C(39)	20(1)	12(1)	15(1)	-1(1)	7(1)	0(1)

2.8 Zn-complex 1h

Zinc complex **1h** crystallized in the triclinic space group $P\bar{1}$. The asymmetric unit one molecule of **1h** and two molecules of DCM. the structure was refined as non-merohedral twin and the twin ratio was refined and converged to 0.0978(6). One of solvent molecules was found to be disordered over two positions, the disorder ratio was allowed to refine freely and convereged to 0.86(3). The disorder was refined with the help of same distance restraints on 1,2 and 1,3 distances, restraints to a similarity restraints on anisotropic

displacement parameters. Disordered atoms were set to the same anisotropic displacement parameters.

Table 37: Crystal data and structure refinement for Zn-complex **1h**

Identification code	D19084_5
Empirical formula	C42 H36 Cl4 N6 O4 Zn
Formula weight	895.94
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 8.7203(9) Å α = 65.707(3)°.
	b = 14.4963(14) Å β = 82.496(4)°.
	c = 17.3371(17) Å γ = 78.203(4)°.
Volume	1952.7(3) $Å^3$
Z	2
Density (calculated)	1.524 $Mg\,m^{-3}$
Absorption coefficient	0.955 mm^{-1}
F(000)	920
Crystal size	0.982 x 0.074 x 0.062 mm^3
Theta range for data collection	2.389 to 30.034°.
Index ranges	-12<=h<=12, -18<=k<=20, 0<=l<=24
Reflections collected	11434
Independent reflections	11434 [R(int) = ?]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	11434 / 423 / 535
Goodness-of-fit on F2	1.068
Final R indices [I>2sigma(I)]	R1 = 0.0507, wR2 = 0.0963
R indices (all data)	R1 = 0.0704, wR2 = 0.1030
Extinction coefficient	n/a
Largest diff. peak and hole	0.539 and -0.555 $e.Å^{-3}$

Table 38: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **1h**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Zn(1)	4825(1)	2926(1)	2690(1)	8(1)
O(1)	3195(2)	531(2)	453(1)	22(1)
O(2)	9591(2)	-765(2)	1856(1)	20(1)
N(1)	2689(2)	3106(2)	2112(1)	10(1)

Table 38 – continued from previous page

	x	y	z	U(eq)
N(2)	5387(2)	1845(2)	2137(1)	10(1)
N(3)	7185(2)	2246(2)	3052(1)	10(1)
C(1)	1385(3)	3758(2)	2126(2)	14(1)
C(2)	33(3)	3822(2)	1734(2)	17(1)
C(3)	66(3)	3178(2)	1330(2)	15(1)
C(4)	1440(3)	2476(2)	1303(2)	11(1)
C(5)	1525(3)	1819(2)	874(1)	11(1)
C(6)	2917(3)	1198(2)	852(2)	12(1)
C(7)	4253(3)	1176(2)	1251(2)	14(1)
C(8)	4230(3)	1783(2)	1703(1)	9(1)
C(9)	2753(3)	2468(2)	1711(1)	9(1)
C(10)	1938(3)	523(2)	4(2)	22(1)
C(11)	8008(3)	2472(2)	3521(2)	14(1)
C(12)	9520(3)	1941(2)	3772(2)	18(1)
C(13)	10169(3)	1174(2)	3504(2)	16(1)
C(14)	9339(3)	925(2)	2990(1)	10(1)
C(15)	9998(3)	146(2)	2691(2)	11(1)
C(16)	9109(3)	-41(2)	2195(2)	12(1)
C(17)	7575(3)	500(2)	1981(2)	12(1)
C(18)	6851(3)	1263(2)	2264(1)	8(1)
C(19)	7811(3)	1484(2)	2780(1)	9(1)
C(20)	11120(3)	-1362(2)	2060(2)	24(1)
O(21)	1591(3)	4633(2)	5613(1)	26(1)
O(22)	5199(3)	7416(2)	2717(1)	30(1)
N(21)	3859(2)	2097(2)	3938(1)	10(1)
N(22)	4283(2)	4044(2)	3207(1)	10(1)
N(23)	5570(2)	4264(2)	1679(1)	9(1)
C(21)	3720(3)	1114(2)	4272(2)	12(1)
C(22)	2981(3)	648(2)	5074(2)	14(1)
C(23)	2408(3)	1231(2)	5532(2)	13(1)
C(24)	2541(3)	2284(2)	5197(1)	10(1)
C(25)	1968(3)	2913(2)	5653(2)	15(1)
C(26)	2106(3)	3930(2)	5266(2)	16(1)
C(27)	2848(3)	4351(2)	4448(2)	15(1)
C(28)	3489(3)	3768(2)	3983(1)	10(1)
C(29)	3285(3)	2688(2)	4382(1)	9(1)
C(30)	895(4)	4278(2)	6452(2)	27(1)
C(31)	6176(3)	4329(2)	919(2)	12(1)
C(32)	6734(3)	5210(2)	325(2)	15(1)
C(33)	6660(3)	6029(2)	536(2)	14(1)
C(34)	6032(3)	5981(2)	1344(2)	11(1)
C(35)	5935(3)	6811(2)	1588(2)	14(1)
C(36)	5331(3)	6688(2)	2385(2)	18(1)

Table 38 – continued from previous page

	x	y	z	U(eq)
C(37)	4776(3)	5785(2)	2961(2)	17(1)
C(38)	4787(3)	4958(2)	2744(1)	10(1)
C(39)	5485(3)	5069(2)	1903(1)	9(1)
C(40)	5801(5)	8339(2)	2197(2)	36(1)
Cl(41)	3552(5)	8822(3)	4033(3)	39(1)
Cl(42)	1848(4)	7115(4)	4496(3)	25(1)
C(41)	3677(6)	7473(4)	4479(4)	19(1)
Cl(43)	3380(30)	8780(13)	4144(9)	23(4)
Cl(44)	2050(20)	6923(15)	4631(12)	25(1)
C(41A)	3800(30)	7460(20)	4340(40)	19(1)
Cl(51)	2478(1)	7571(1)	141(1)	23(1)
Cl(52)	84(1)	6555(1)	1368(1)	24(1)
C(51)	2126(3)	6539(2)	1105(2)	20(1)

Table 39: Selected bond lengths [Å] and angles [°] for complex **1h**

Zn(1)-N(2)	2.1002(19)
Zn(1)-N(22)	2.1043(19)
Zn(1)-N(3)	2.145(2)
Zn(1)-N(1)	2.148(2)
Zn(1)-N(21)	2.153(2)
Zn(1)-N(23)	2.162(2)
N(2)-Zn(1)-N(22)	178.20(8)
N(2)-Zn(1)-N(3)	77.70(7)
N(22)-Zn(1)-N(3)	102.44(8)
N(2)-Zn(1)-N(1)	77.55(8)
N(22)-Zn(1)-N(1)	102.34(8)
N(3)-Zn(1)-N(1)	155.22(7)
N(2)-Zn(1)-N(21)	104.52(8)
N(22)-Zn(1)-N(21)	77.27(8)
N(3)-Zn(1)-N(21)	92.50(8)
N(1)-Zn(1)-N(21)	92.34(7)
N(2)-Zn(1)-N(23)	101.23(8)
N(22)-Zn(1)-N(23)	76.97(8)
N(3)-Zn(1)-N(23)	92.43(7)
N(1)-Zn(1)-N(23)	93.68(7)
N(21)-Zn(1)-N(23)	154.24(7)

Table 40: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1h**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	9(1)	7(1)	8(1)	-4(1)	0(1)	-1(1)
O(1)	20(1)	25(1)	33(1)	-23(1)	-11(1)	1(1)
O(2)	16(1)	23(1)	27(1)	-19(1)	-6(1)	7(1)
N(1)	9(1)	10(1)	11(1)	-4(1)	0(1)	-1(1)
N(2)	8(1)	10(1)	12(1)	-5(1)	-2(1)	-1(1)
N(3)	11(1)	10(1)	12(1)	-6(1)	-2(1)	-2(1)
C(1)	12(1)	14(1)	15(1)	-8(1)	-1(1)	1(1)
C(2)	9(1)	20(1)	21(1)	-10(1)	-2(1)	4(1)
C(3)	10(1)	20(1)	16(1)	-7(1)	-2(1)	-1(1)
C(4)	8(1)	12(1)	10(1)	-3(1)	-1(1)	-2(1)
C(5)	11(1)	13(1)	9(1)	-2(1)	-4(1)	-6(1)
C(6)	14(1)	12(1)	15(1)	-8(1)	-2(1)	-2(1)
C(7)	10(1)	14(1)	21(1)	-11(1)	-5(1)	1(1)
C(8)	8(1)	9(1)	9(1)	-4(1)	-1(1)	-2(1)
C(9)	10(1)	9(1)	8(1)	-2(1)	0(1)	-3(1)
C(10)	24(1)	25(1)	28(1)	-17(1)	-11(1)	-4(1)
C(11)	14(1)	16(1)	16(1)	-10(1)	-3(1)	-1(1)
C(12)	16(1)	23(1)	22(1)	-14(1)	-9(1)	-1(1)
C(13)	10(1)	19(1)	21(1)	-10(1)	-8(1)	1(1)
C(14)	9(1)	10(1)	10(1)	-3(1)	0(1)	-3(1)
C(15)	10(1)	10(1)	12(1)	-3(1)	-1(1)	0(1)
C(16)	12(1)	12(1)	12(1)	-6(1)	1(1)	0(1)
C(17)	12(1)	12(1)	13(1)	-7(1)	-2(1)	-2(1)
C(18)	8(1)	9(1)	8(1)	-2(1)	0(1)	-3(1)
C(19)	9(1)	10(1)	8(1)	-4(1)	1(1)	-3(1)
C(20)	21(1)	25(1)	29(2)	-19(1)	-9(1)	11(1)
O(21)	41(1)	18(1)	20(1)	-12(1)	14(1)	-5(1)
O(22)	55(2)	18(1)	27(1)	-17(1)	19(1)	-23(1)
N(21)	9(1)	9(1)	10(1)	-3(1)	-1(1)	-2(1)
N(22)	12(1)	9(1)	10(1)	-4(1)	2(1)	-3(1)
N(23)	8(1)	9(1)	10(1)	-4(1)	-1(1)	1(1)
C(21)	11(1)	12(1)	14(1)	-5(1)	-3(1)	-3(1)
C(22)	16(1)	8(1)	15(1)	-1(1)	-2(1)	-7(1)
C(23)	14(1)	14(1)	10(1)	-1(1)	-1(1)	-6(1)
C(24)	10(1)	12(1)	9(1)	-3(1)	-1(1)	-3(1)
C(25)	16(1)	18(1)	11(1)	-6(1)	3(1)	-5(1)
C(26)	19(1)	15(1)	13(1)	-7(1)	3(1)	-2(1)
C(27)	18(1)	10(1)	15(1)	-4(1)	2(1)	-2(1)
C(28)	10(1)	8(1)	10(1)	-3(1)	-1(1)	-1(1)
C(29)	9(1)	9(1)	9(1)	-2(1)	-1(1)	-2(1)

Table 40 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(30)	36(2)	28(2)	17(1)	-13(1)	12(1)	-7(1)
C(31)	12(1)	14(1)	11(1)	-7(1)	-2(1)	-2(1)
C(32)	15(1)	19(1)	11(1)	-6(1)	2(1)	-4(1)
C(33)	15(1)	16(1)	11(1)	-3(1)	2(1)	-5(1)
C(34)	9(1)	11(1)	10(1)	-2(1)	-1(1)	-2(1)
C(35)	17(1)	10(1)	15(1)	-4(1)	4(1)	-7(1)
C(36)	24(1)	11(1)	22(1)	-9(1)	6(1)	-8(1)
C(37)	26(1)	14(1)	13(1)	-7(1)	6(1)	-9(1)
C(38)	11(1)	9(1)	10(1)	-4(1)	-1(1)	-3(1)
C(39)	9(1)	9(1)	9(1)	-2(1)	-1(1)	-1(1)
C(40)	61(2)	17(1)	37(2)	-16(1)	18(2)	-24(2)
Cl(41)	25(1)	21(1)	80(2)	-28(1)	-17(1)	2(1)
Cl(42)	30(1)	25(1)	25(1)	-12(1)	-5(1)	-8(1)
C(41)	18(1)	19(1)	19(3)	-11(1)	-3(1)	5(1)
Cl(43)	50(10)	12(4)	9(6)	1(3)	-9(3)	-11(5)
Cl(44)	30(1)	25(1)	25(1)	-12(1)	-5(1)	-8(1)
C(41A)	18(1)	19(1)	19(3)	-11(1)	-3(1)	5(1)
Cl(51)	20(1)	25(1)	23(1)	-10(1)	1(1)	-4(1)
Cl(52)	20(1)	23(1)	24(1)	-4(1)	-1(1)	-3(1)
C(51)	18(1)	18(1)	21(1)	-7(1)	-5(1)	3(1)

2.9 Zn-complex 1i

Table 41: Crystal data and structure refinement for Zn-complex **1i**

Identification code	D19376
Empirical formula	C46 H34 N10 Zn
Formula weight	792,2
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P21/n
Unit cell dimensions	a = 15.4507(5) Å
	b = 15.2554(5) Å α = 90°.
	c = 17.0199(5) Å β = 98.038(3)°.
Volume	3972.3(2) Å3 γ = 90°.
Z	4
Density (calculated)	1.325 Mg m^{-3}
Absorption coefficient	1.226 mm^{-1}
F(000)	1640
Crystal size	0.106 x 0.100 x 0.019 mm^3
Theta range for data collection	3.620 to 66.588°.
Index ranges	-18<=h<=18, -18<=k<=18, -20<=l<=20
Reflections collected	43368
Independent reflections	6925 [R(int) = 0.1441]
Completeness to theta = 66.588°	98,70%
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	6925 / 1044 / 573
Goodness-of-fit on F2	1,212
Final R indices [I>2sigma(I)]	R1 = 0.1153, wR2 = 0.2669
R indices (all data)	R1 = 0.1557, wR2 = 0.2870
Extinction coefficient	n/a
Largest diff. peak and hole	2.940 and -0.453 e.Å^{-3}

Table 42: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å^2 $\times$ 10^3) for complex **1i**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
FE1	6698(1)	3897(1)	8348(1)	22(1)
N(1)	5542(4)	3961(5)	7580(4)	22(1)
N(2)	6913(4)	2953(5)	7433(4)	24(2)
N(3)	3852(5)	3471(6)	4248(5)	47(2)

Table 42 – continued from previous page

	x	y	z	U(eq)
C(1)	7603(6)	2455(6)	7404(5)	32(2)
C(2)	7727(6)	1983(7)	6721(6)	41(2)
C(3)	7106(6)	2026(7)	6070(5)	38(2)
C(4)	6364(5)	2554(6)	6078(5)	26(2)
C(5)	5708(5)	2654(6)	5415(5)	30(2)
C(6)	5027(5)	3214(6)	5472(5)	28(2)
C(7)	4934(5)	3675(6)	6170(5)	25(2)
C(8)	5530(5)	3566(5)	6859(4)	20(2)
C(9)	6281(5)	3013(5)	6785(4)	22(2)
C(10)	4378(6)	3362(7)	4780(5)	35(2)
N(4)	5967(4)	4917(5)	8873(4)	24(1)
N(5)	1765(5)	4741(6)	7243(5)	46(2)
C(11)	6235(6)	5421(6)	9498(5)	28(2)
C(12)	5685(6)	6026(6)	9803(5)	31(2)
C(13)	4840(6)	6051(6)	9488(5)	32(2)
C(14)	4504(6)	5503(6)	8838(5)	27(2)
C(15)	3625(6)	5467(6)	8509(5)	31(2)
C(16)	3378(5)	4899(6)	7887(5)	30(2)
C(17)	3988(5)	4376(6)	7545(5)	26(2)
C(18)	4876(5)	4413(5)	7834(5)	22(2)
C(19)	5131(5)	4952(6)	8533(5)	24(2)
C(20)	2478(6)	4822(6)	7539(5)	33(2)
N(21)	7833(4)	3847(5)	9148(4)	22(1)
N(22)	7549(4)	4788(5)	7822(4)	25(1)
N(23)	11734(5)	4233(6)	9445(5)	39(2)
C(21)	7370(6)	5232(6)	7157(5)	32(2)
C(22)	8014(6)	5654(7)	6792(6)	39(2)
C(23)	8863(6)	5607(6)	7137(6)	36(2)
C(24)	9083(5)	5126(6)	7848(5)	30(2)
C(25)	9954(5)	5011(6)	8201(5)	31(2)
C(26)	10109(5)	4508(6)	8876(5)	26(2)
C(27)	9432(5)	4125(6)	9241(5)	25(2)
C(28)	8559(5)	4218(5)	8910(4)	22(2)
C(29)	8394(5)	4724(6)	8186(5)	23(2)
C(30)	11017(5)	4351(6)	9207(5)	30(2)
N(24)	6416(4)	2865(5)	9174(4)	23(1)
N(25)	9268(5)	3039(6)	12529(4)	42(2)
C(31)	5724(5)	2368(6)	9128(5)	26(2)
C(32)	5592(5)	1751(6)	9722(5)	30(2)
C(33)	6196(6)	1712(6)	10386(5)	31(2)
C(34)	6940(5)	2267(6)	10466(5)	25(2)
C(35)	7554(5)	2304(6)	11166(5)	30(2)
C(36)	8221(5)	2887(6)	11205(5)	28(2)

Table 42 – continued from previous page

	x	y	z	U(eq)
C(37)	8374(5)	3419(6)	10550(5)	25(2)
C(38)	7799(5)	3388(6)	9833(5)	23(2)
C(39)	7044(5)	2825(5)	9825(4)	19(2)
C(40)	8810(6)	2972(6)	11942(5)	30(2)
C(1S)	5420(20)	2390(20)	2293(15)	93(9)
C(2S)	5748(17)	2990(20)	3060(20)	90(7)
C(3S)	6716(15)	2987(17)	3331(14)	86(6)
C(4S)	7025(16)	3710(20)	4043(15)	89(7)
C(5S)	7988(16)	3580(20)	4399(15)	97(7)
C(6S)	8200(30)	4210(40)	5210(20)	170(18)
C(1T)	4900(30)	2290(30)	2280(20)	87(12)
C(2T)	5910(20)	2460(30)	2660(20)	78(8)
C(3T)	6020(20)	3220(30)	3230(30)	78(8)
C(4T)	7020(20)	3330(30)	3710(30)	95(9)
C(5T)	7080(30)	4130(30)	4270(30)	102(11)
C(6T)	8080(30)	4250(40)	4760(30)	108(14)

Table 43: Selected bond lengths [Å] and angles [°] for complex **1i**

FE1-N(1)	2.063(6)
FE1-N(21)	2.065(6)
FE1-N(22)	2.170(7)
FE1-N(2)	2.180(7)
FE1-N(4)	2.185(7)
FE1-N(24)	2.194(7)
N(1)-FE1-N(21)	178.1(3)
N(1)-FE1-N(22)	103.3(3)
N(21)-FE1-N(22)	77.7(3)
N(1)-FE1-N(2)	77.5(2)
N(21)-FE1-N(2)	104.3(3)
N(22)-FE1-N(2)	87.6(3)
N(1)-FE1-N(4)	76.9(3)
N(21)-FE1-N(4)	101.3(3)
N(22)-FE1-N(4)	95.7(3)
N(2)-FE1-N(4)	154.3(2)
N(1)-FE1-N(24)	102.0(3)
N(21)-FE1-N(24)	77.2(3)
N(22)-FE1-N(24)	154.2(2)
N(2)-FE1-N(24)	92.8(3)
N(4)-FE1-N(24)	95.1(3)
C(18)-N(1)-C(8)	126.4(6)
C(18)-N(1)-FE1	116.7(5)

Table 43 – continued from previous page

C(8)-N(1)-FE1	116.8(5)
C(1)-N(2)-C(9)	119.9(7)
C(1)-N(2)-FE1	127.8(5)
C(9)-N(2)-FE1	111.6(5)

Table 44: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **1i**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
FE1	17(1)	29(1)	17(1)	-1(1)	-3(1)	1(1)
N(1)	20(3)	29(4)	16(3)	-1(3)	-1(2)	0(3)
N(2)	23(3)	30(4)	18(3)	-1(3)	-5(2)	4(3)
N(3)	35(4)	69(6)	32(4)	10(4)	-10(3)	-6(4)
C(1)	27(4)	39(5)	27(4)	-3(4)	-3(3)	11(4)
C(2)	40(5)	45(6)	35(4)	-10(4)	-4(4)	21(4)
C(3)	42(5)	43(6)	29(4)	-9(4)	-1(3)	13(4)
C(4)	27(4)	33(5)	16(3)	-1(3)	0(3)	1(3)
C(5)	26(4)	42(5)	19(4)	-7(4)	-3(3)	-4(3)
C(6)	16(3)	48(5)	18(3)	1(3)	-5(3)	-3(3)
C(7)	12(3)	43(5)	21(3)	3(3)	-2(3)	3(3)
C(8)	17(3)	23(4)	18(3)	4(3)	-2(3)	-2(3)
C(9)	20(3)	26(4)	17(3)	-1(3)	-4(3)	0(3)
C(10)	27(4)	50(6)	25(4)	1(4)	-5(3)	-2(4)
N(4)	21(3)	30(4)	22(3)	-2(3)	1(2)	5(3)
N(5)	25(3)	69(6)	43(5)	4(4)	1(3)	11(4)
C(11)	30(4)	26(4)	24(4)	0(3)	-4(3)	4(3)
C(12)	37(4)	30(5)	25(4)	-4(4)	4(3)	3(4)
C(13)	35(4)	29(5)	31(4)	-4(4)	6(3)	9(4)
C(14)	32(4)	26(4)	24(4)	2(3)	2(3)	8(3)
C(15)	29(4)	33(5)	31(4)	5(3)	2(3)	13(4)
C(16)	20(3)	41(5)	29(4)	5(3)	4(3)	8(3)
C(17)	19(3)	36(5)	22(4)	4(3)	2(3)	-2(3)
C(18)	17(3)	24(4)	23(4)	6(3)	4(3)	2(3)
C(19)	22(3)	24(4)	25(4)	1(3)	1(3)	4(3)
C(20)	23(3)	45(6)	30(4)	8(4)	5(3)	11(4)
N(21)	18(3)	29(4)	17(3)	-2(3)	-2(2)	-3(3)
N(22)	23(3)	27(4)	23(3)	0(3)	-4(2)	0(3)
N(23)	22(3)	56(5)	37(4)	9(4)	-3(3)	-3(3)
C(21)	26(4)	38(5)	28(4)	7(4)	-8(3)	-2(4)
C(22)	35(4)	45(6)	35(5)	21(4)	-2(3)	0(4)
C(23)	29(4)	37(5)	40(5)	15(4)	1(3)	-4(4)
C(24)	27(4)	35(5)	24(4)	3(3)	-6(3)	-8(3)
C(25)	20(4)	34(5)	37(4)	4(4)	1(3)	-5(3)

Table 44 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(26)	20(3)	33(5)	24(4)	-2(3)	-2(3)	0(3)
C(27)	19(3)	34(5)	22(4)	-1(3)	0(3)	-2(3)
C(28)	19(3)	26(4)	20(4)	-3(3)	-1(3)	-3(3)
C(29)	23(3)	26(4)	19(3)	-2(3)	-2(3)	-1(3)
C(30)	24(3)	36(5)	29(4)	6(4)	0(3)	-2(3)
N(24)	23(3)	27(4)	19(3)	1(3)	-1(2)	3(3)
N(25)	37(4)	57(6)	28(4)	4(4)	-8(3)	-3(4)
C(31)	25(4)	32(5)	19(4)	-4(3)	0(3)	2(3)
C(32)	21(4)	35(5)	35(4)	0(4)	4(3)	-3(3)
C(33)	32(4)	33(5)	28(4)	7(4)	1(3)	-4(3)
C(34)	25(4)	30(4)	19(3)	1(3)	-1(3)	3(3)
C(35)	27(4)	40(5)	21(4)	6(4)	-1(3)	4(3)
C(36)	26(4)	37(5)	17(3)	3(3)	-6(3)	4(3)
C(37)	16(4)	36(5)	20(3)	2(3)	-4(3)	3(3)
C(38)	17(3)	29(4)	20(3)	1(3)	-3(3)	2(3)
C(39)	18(3)	22(4)	18(3)	-5(3)	-1(2)	6(3)
C(40)	26(4)	33(5)	28(4)	-1(4)	-6(3)	6(4)
C(1S)	150(30)	64(15)	75(15)	34(11)	39(16)	0(20)
C(2S)	105(14)	93(18)	83(14)	19(12)	47(12)	5(14)
C(3S)	101(13)	81(15)	86(14)	27(11)	49(10)	20(12)
C(4S)	103(11)	95(19)	81(15)	23(12)	56(10)	17(13)
C(5S)	98(12)	109(18)	93(15)	7(13)	48(11)	13(13)
C(6S)	190(30)	190(30)	140(30)	-50(30)	40(20)	-50(30)
C(1T)	100(20)	80(30)	90(20)	37(19)	39(17)	0(20)
C(2T)	86(18)	75(17)	88(19)	24(14)	61(14)	10(15)
C(3T)	89(17)	76(18)	84(17)	26(13)	60(13)	3(15)
C(4T)	102(16)	90(20)	100(20)	27(15)	40(15)	13(16)
C(5T)	115(18)	100(20)	100(20)	21(16)	35(16)	0(18)
C(6T)	100(20)	100(30)	130(30)	20(30)	40(20)	-10(20)

2.10 Fe-complex 2a

The unit cell of Fe-complex **2a** was determined using 9870 reflections and the structure was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of **2a** and heavily disordered solvent molecules. SQUEEZE was used to include a solvent model in the refinement. SQUEEZE identified one independent void with a size of 289 Å^3 at 0.0 0.5 0.5 in the unit cell. The equivalent of 98 electrons were found in the unit cell, which corresponds to about two molecules of DCM. The obtained model was added as .fab-file to the refinement using SHELXL.

Table 45: Crystal data and structure refinement for complex **2a**

Identification code	D18158_sq
Empirical formula	C36 H24 Fe N6
Formula weight	596.46
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 11.8578(15) Å α = 90.362(6)°.
	b = 12.2367(15) Å β = 101.553(5)°.
	c = 12.2682(15) Å γ = 116.949(5)°.
Volume	1545.0(3) $Å^3$
Z	2
Density (calculated)	1.282 $Mg\,m^{-3}$
Absorption coefficient	0.523 mm^{-1}
F(000)	616
Crystal size	0.664 x 0.375 x 0.006 mm^3
Theta range for data collection	2.299 to 26.732°.
Index ranges	-15<=h<=14, -15<=k<=15, -15<=l<=15
Reflections collected	43004
Independent reflections	6492 [R(int) = 0.0848]
Completeness to theta = 25.242°	99.3 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	6492 / 0 / 388
Goodness-of-fit on F2	1.078
Final R indices [I>2sigma(I)]	R1 = 0.0608, wR2 = 0.1245
R indices (all data)	R1 = 0.0816, wR2 = 0.1338
Extinction coefficient	n/a
Largest diff. peak and hole	0.693 and -0.908 $e.Å^{-3}$

Table 46: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2a**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Fe(1)	4779(1)	2422(1)	7462(1)	14(1)
N(1)	5083(3)	3996(2)	8153(2)	17(1)
N(2)	6637(3)	3127(2)	7937(2)	17(1)
N(3)	4924(3)	1020(2)	6889(2)	15(1)
N(21)	4359(3)	1638(2)	8803(2)	17(1)
N(22)	2917(3)	1727(2)	6977(2)	15(1)
N(23)	4738(3)	3020(2)	5996(2)	16(1)
C(1)	4218(4)	4381(3)	8218(3)	20(1)

Table 46 – continued from previous page

	x	y	z	U(eq)
C(2)	4571(4)	5563(3)	8728(3)	26(1)
C(3)	5836(4)	6331(3)	9188(3)	26(1)
C(4)	6795(4)	5959(3)	9143(3)	24(1)
C(5)	8133(4)	6698(3)	9593(3)	33(1)
C(6)	8986(4)	6259(4)	9494(4)	42(1)
C(7)	8566(4)	5068(4)	8959(3)	37(1)
C(8)	7267(3)	4300(3)	8497(3)	21(1)
C(9)	6373(3)	4764(3)	8606(2)	20(1)
C(10)	7168(3)	2409(3)	7629(3)	20(1)
C(11)	8442(4)	2633(4)	7780(3)	32(1)
C(12)	8753(4)	1736(4)	7379(3)	34(1)
C(13)	7823(4)	624(3)	6834(3)	28(1)
C(14)	6511(4)	338(3)	6660(2)	21(1)
C(15)	5479(4)	-799(3)	6137(3)	24(1)
C(16)	4230(4)	-1006(3)	6010(3)	25(1)
C(17)	3990(3)	-55(3)	6388(3)	20(1)
C(18)	6194(3)	1239(3)	7045(2)	16(1)
C(21)	5172(4)	1655(3)	9739(3)	22(1)
C(22)	4718(4)	1021(3)	10640(3)	28(1)
C(23)	3417(4)	354(3)	10569(3)	27(1)
C(24)	2529(4)	314(3)	9592(3)	24(1)
C(25)	1167(4)	-339(3)	9448(3)	29(1)
C(26)	393(4)	-324(3)	8471(3)	30(1)
C(27)	889(4)	338(3)	7604(3)	25(1)
C(28)	2220(3)	1022(3)	7704(2)	18(1)
C(29)	3050(3)	986(3)	8720(2)	17(1)
C(30)	2466(3)	2020(3)	5958(2)	18(1)
C(31)	1226(4)	1774(3)	5393(3)	27(1)
C(32)	1008(4)	2171(4)	4329(3)	34(1)
C(33)	1983(4)	2801(3)	3791(3)	31(1)
C(34)	3267(4)	3092(3)	4335(3)	22(1)
C(35)	4357(4)	3753(3)	3865(3)	26(1)
C(36)	5576(4)	4028(3)	4448(3)	24(1)
C(37)	5738(3)	3658(3)	5530(3)	19(1)
C(38)	3501(3)	2726(3)	5409(2)	18(1)

Table 47: Selected bond lengths [Å] and angles [°] for **2a**

Fe(1)-N(2)	1.922(3)
Fe(1)-N(22)	1.928(3)
Fe(1)-N(3)	1.942(2)
Fe(1)-N(1)	1.946(2)

Table 47 – continued from previous page

Fe(1)-N(23)	1.946(3)
Fe(1)-N(21)	1.947(3)
N(2)-Fe(1)-N(22)	179.48(12)
N(2)-Fe(1)-N(3)	83.29(11)
N(22)-Fe(1)-N(3)	96.97(11)
N(2)-Fe(1)-N(1)	82.95(11)
N(22)-Fe(1)-N(1)	96.79(11)
N(3)-Fe(1)-N(1)	166.24(12)
N(2)-Fe(1)-N(23)	96.58(12)
N(22)-Fe(1)-N(23)	82.97(11)
N(3)-Fe(1)-N(23)	90.82(10)
N(1)-Fe(1)-N(23)	90.86(10)
N(2)-Fe(1)-N(21)	97.46(12)
N(22)-Fe(1)-N(21)	82.99(11)
N(3)-Fe(1)-N(21)	90.31(10)
N(1)-Fe(1)-N(21)	91.37(10)
N(23)-Fe(1)-N(21)	165.95(12)

Table 48: Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2a**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	26(1)	9(1)	10(1)	1(1)	6(1)	10(1)
N(1)	33(2)	13(1)	10(1)	5(1)	11(1)	13(1)
N(2)	20(2)	14(1)	16(1)	-1(1)	2(1)	7(1)
N(3)	29(2)	9(1)	9(1)	4(1)	7(1)	9(1)
N(21)	35(2)	10(1)	13(1)	1(1)	6(1)	16(1)
N(22)	23(2)	12(1)	12(1)	4(1)	7(1)	9(1)
N(23)	28(2)	9(1)	16(1)	-1(1)	10(1)	9(1)
C(1)	35(2)	15(2)	16(1)	7(1)	14(1)	13(2)
C(2)	51(3)	18(2)	22(2)	7(1)	18(2)	22(2)
C(3)	57(3)	11(2)	16(2)	4(1)	17(2)	17(2)
C(4)	46(2)	14(2)	12(1)	1(1)	10(1)	13(2)
C(5)	50(3)	15(2)	26(2)	-6(1)	2(2)	10(2)
C(6)	40(3)	24(2)	45(2)	-12(2)	-7(2)	8(2)
C(7)	37(2)	23(2)	45(2)	-9(2)	-1(2)	14(2)
C(8)	31(2)	12(2)	16(2)	-1(1)	1(1)	8(2)
C(9)	36(2)	11(2)	12(1)	3(1)	8(1)	9(2)
C(10)	30(2)	17(2)	18(2)	2(1)	6(1)	14(2)
C(11)	31(2)	26(2)	37(2)	-3(2)	4(2)	14(2)
C(12)	31(2)	33(2)	47(2)	1(2)	11(2)	21(2)
C(13)	40(2)	29(2)	28(2)	5(2)	12(2)	25(2)
C(14)	40(2)	21(2)	12(1)	5(1)	8(1)	23(2)

Table 48 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(15)	46(2)	20(2)	16(2)	0(1)	7(2)	22(2)
C(16)	40(2)	13(2)	20(2)	-2(1)	2(2)	13(2)
C(17)	29(2)	15(2)	17(2)	-1(1)	4(1)	11(2)
C(18)	25(2)	16(2)	11(1)	3(1)	6(1)	12(1)
C(21)	41(2)	20(2)	13(1)	2(1)	5(1)	21(2)
C(22)	57(3)	27(2)	12(2)	4(1)	6(2)	31(2)
C(23)	55(3)	20(2)	18(2)	11(1)	19(2)	23(2)
C(24)	48(2)	17(2)	16(2)	5(1)	16(2)	20(2)
C(25)	42(2)	22(2)	28(2)	6(2)	21(2)	13(2)
C(26)	32(2)	23(2)	34(2)	5(2)	19(2)	9(2)
C(27)	30(2)	23(2)	26(2)	3(1)	10(2)	14(2)
C(28)	30(2)	15(2)	15(1)	4(1)	10(1)	14(2)
C(29)	30(2)	11(2)	14(1)	3(1)	10(1)	12(1)
C(30)	33(2)	13(2)	12(1)	2(1)	4(1)	13(2)
C(31)	30(2)	28(2)	23(2)	4(2)	2(2)	15(2)
C(32)	38(2)	34(2)	27(2)	1(2)	-6(2)	20(2)
C(33)	51(3)	29(2)	16(2)	0(2)	0(2)	24(2)
C(34)	44(2)	13(2)	13(1)	2(1)	6(1)	17(2)
C(35)	59(3)	16(2)	11(1)	5(1)	13(2)	22(2)
C(36)	46(2)	15(2)	19(2)	5(1)	16(2)	16(2)
C(37)	33(2)	13(2)	15(1)	4(1)	12(1)	12(2)
C(38)	32(2)	11(2)	12(1)	0(1)	6(1)	12(1)

2.11 Fe-complex 2d

The structure of **2d** was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one molecule of **2d** and one molecule of THF. The disorder was refined with the help of same distance restraints on 1,2 and 1,3 distances, similarity restraints on anisotropic displacement parameters and advanced rigid bond restraints. One ligand ligand was found to be completely disordered over two positions and half of the other ligand and additional isopropyl group and the THF molecule. These disorder ratios were allowed to refine freely and converged to 0.543(8) for the fully disordered ligand, 0.519(8) for the disordered half ligand 0.0552(7) for the isopropyl group and 0.51(2) for THF. To accommodate additional heavily disordered solvent SQUEEZE was used. SQUEEZE found one independent void with disordered solvent, located at 0.5 0.5 0.0, with a volume of 307 $Å^3$. The equivalent of 67 electrons were identified in the void. This number of electrons corresponds to approximately two molecules of THF in the unit cell; however, there could also be n-hexane from the vapor diffusion in the crystal lattice which would change the amount of solvent molecules slightly.

Table 49: Crystal data and structure refinement for **2d**

Identification code	D19354_sq
Empirical formula	C52 H56 Fe N6 O
Formula weight	836.87
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 12.0939(9) Å α = 88.663(2)°.
	b = 12.6103(10) Å β = 73.194(2)°.
	c = 16.4894(13) Å γ = 87.452(3)°.
Volume	2404.8(3) $Å^3$
Z	2
Density (calculated)	1.156 $Mg\,m^{-3}$
Absorption coefficient	0.355 mm^{-1}
F(000)	888
Crystal size	0.470 x 0.243 x 0.135 mm^3
Theta range for data collection	1.760 to 29.573°.
Index ranges	-16<=h<=16, -17<=k<=17, -22<=l<=22
Reflections collected	469999
Independent reflections	13479 [R(int) = 0.0728]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	13479 / 3130 / 937
Goodness-of-fit on F2	1.081
Final R indices [I>2sigma(I)]	R1 = 0.0700, wR2 = 0.1899
R indices (all data)	R1 = 0.0798, wR2 = 0.1966
Extinction coefficient	0.0128(11)
Largest diff. peak and hole	2.223 and -0.415 $e.Å^{-3}$

Table 50: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for D19354_sq. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Fe(1)	2797(1)	7526(1)	4336(1)	24(1)
N(2)	2367(16)	7456(10)	5506(10)	26(2)
N(1)	3429(17)	6085(12)	4364(7)	18(2)
C(1)	3920(18)	5403(13)	3745(8)	22(2)
C(2)	4200(20)	4340(14)	3902(8)	24(2)
C(3)	4044(16)	4005(11)	4715(8)	22(2)
C(4)	3556(17)	4703(11)	5396(6)	19(2)

Table 50 – continued from previous page

	x	y	z	U(eq)
C(5)	3300(20)	4402(10)	6261(7)	23(2)
C(6)	2767(18)	5109(10)	6900(7)	23(2)
C(7)	2500(20)	6164(12)	6669(8)	25(2)
C(8)	2650(20)	6496(11)	5838(7)	18(2)
C(9)	3246(15)	5753(9)	5188(7)	16(2)
C(10)	2536(11)	4789(10)	7825(7)	30(2)
C(11)	3479(15)	5118(16)	8195(9)	46(3)
C(12)	1344(13)	5178(13)	8386(11)	45(3)
N(3)	2202(11)	8969(10)	4486(7)	21(2)
C(21)	2136(12)	9699(10)	3910(6)	27(1)
C(22)	1649(8)	10722(7)	4126(5)	27(1)
C(23)	1173(7)	10968(6)	4957(5)	25(1)
C(24)	1162(9)	10198(7)	5596(5)	25(1)
C(25)	660(11)	10363(9)	6471(6)	29(2)
C(26)	697(11)	9565(9)	7047(6)	29(2)
C(27)	1299(12)	8594(8)	6768(7)	26(2)
C(28)	1828(11)	8366(8)	5921(7)	19(1)
C(29)	1717(13)	9201(9)	5329(6)	20(2)
C(30)	111(8)	9745(10)	7986(6)	39(2)
C(31)	-1163(5)	9486(6)	8219(4)	46(2)
C(32)	693(10)	9170(11)	8575(8)	50(3)
N(2A)	2347(16)	7440(12)	5620(12)	19(2)
N(1A)	3300(20)	6063(13)	4520(9)	19(2)
C(1A)	3760(20)	5386(16)	3892(10)	24(3)
C(2A)	4100(30)	4337(17)	4064(10)	33(3)
C(3A)	3900(20)	3992(14)	4873(10)	30(3)
C(4A)	3400(20)	4680(12)	5550(8)	23(2)
C(5A)	3240(30)	4421(15)	6407(9)	32(3)
C(6A)	2770(20)	5158(15)	7025(9)	35(3)
C(7A)	2420(30)	6188(16)	6816(9)	27(3)
C(8A)	2590(30)	6502(13)	5987(9)	23(2)
C(9A)	3084(18)	5726(13)	5339(8)	19(2)
C(10A)	2609(18)	4865(16)	7952(9)	52(4)
C(11A)	3590(20)	5270(20)	8244(15)	64(6)
C(12A)	1428(19)	5260(20)	8502(15)	61(5)
N(3A)	1980(12)	8930(11)	4617(8)	19(2)
C(21A)	1948(15)	9716(12)	4066(8)	27(1)
C(22A)	1387(10)	10719(9)	4348(6)	27(1)
C(23A)	916(8)	10893(8)	5184(6)	25(1)
C(24A)	990(11)	10095(9)	5781(6)	25(1)
C(25A)	492(14)	10210(10)	6661(7)	26(2)
C(26A)	574(15)	9398(11)	7210(7)	29(2)
C(27A)	1131(13)	8415(9)	6901(7)	20(2)

Table 50 – continued from previous page

	x	y	z	U(eq)
C(28A)	1636(14)	8255(10)	6043(8)	19(1)
C(29A)	1540(17)	9111(11)	5472(8)	20(2)
C(30A)	6(10)	9528(11)	8156(7)	42(3)
C(31A)	-937(7)	8729(8)	8480(5)	56(3)
C(32A)	890(14)	9438(14)	8640(11)	54(3)
N(41)	1381(2)	6973(2)	4196(1)	25(1)
N(42)	3219(2)	7605(2)	3115(1)	27(1)
C(41)	499(2)	6544(2)	4774(2)	28(1)
C(42)	-491(2)	6217(2)	4574(2)	33(1)
C(43)	-573(2)	6365(2)	3772(2)	37(1)
C(44)	341(2)	6818(2)	3137(2)	32(1)
C(45)	327(3)	7024(3)	2293(2)	39(1)
C(46)	1265(3)	7454(2)	1708(2)	36(1)
C(47)	2274(3)	7656(2)	1945(2)	34(1)
C(48)	2341(2)	7457(2)	2763(2)	28(1)
C(49)	1329(2)	7071(2)	3375(2)	26(1)
C(50)	1252(3)	7699(3)	803(2)	45(1)
C(51)	42(6)	7551(6)	672(4)	54(2)
C(52)	2121(7)	6917(7)	223(4)	59(2)
C(51A)	1333(11)	6718(8)	284(6)	64(3)
C(52A)	2183(7)	8515(7)	296(5)	51(2)
N(43)	4228(11)	8152(16)	4203(7)	24(2)
C(61)	4710(12)	8496(19)	4777(8)	22(2)
C(62)	5830(11)	8891(17)	4558(8)	27(2)
C(63)	6471(10)	8930(13)	3732(8)	31(2)
C(64)	5996(8)	8614(7)	3081(5)	25(2)
C(65)	6565(6)	8660(6)	2202(4)	33(1)
C(66)	6025(6)	8342(6)	1619(4)	34(1)
C(67)	4885(7)	7968(7)	1902(6)	31(2)
C(68)	4286(12)	7890(19)	2762(7)	29(2)
C(69)	4857(8)	8249(10)	3360(7)	22(2)
C(70)	6645(5)	8374(6)	674(4)	41(2)
C(71)	5945(8)	8983(9)	179(5)	55(2)
C(72)	7004(8)	7265(7)	329(5)	62(2)
N(43A)	4411(11)	8076(15)	4091(8)	19(2)
C(61A)	4916(14)	8450(20)	4641(9)	26(3)
C(62A)	6050(13)	8817(17)	4384(9)	29(3)
C(63A)	6678(11)	8758(13)	3559(8)	33(2)
C(64A)	6185(8)	8360(8)	2951(6)	29(2)
C(65A)	6773(7)	8256(7)	2088(5)	35(2)
C(66A)	6232(6)	7899(7)	1526(4)	36(2)
C(67A)	5048(8)	7646(8)	1825(7)	34(2)
C(68A)	4394(11)	7810(20)	2656(8)	30(3)

Table 50 – continued from previous page

	x	y	z	U(eq)
C(69A)	5023(9)	8059(11)	3250(7)	21(2)
C(70A)	6834(6)	7757(8)	586(5)	46(2)
C(71A)	6386(9)	8607(10)	77(6)	60(3)
C(72A)	8149(6)	7734(7)	352(5)	52(2)
O(1S)	3717(10)	8093(10)	8046(7)	68(2)
C(1S)	4051(15)	8390(20)	7174(9)	48(3)
C(2S)	5234(12)	8858(13)	6987(8)	45(3)
C(3S)	5288(13)	9180(9)	7871(8)	57(3)
C(4S)	4299(18)	8644(15)	8449(8)	91(4)
O(1T)	4147(14)	7796(11)	7852(8)	73(3)
C(1T)	4288(18)	8340(20)	7062(11)	58(4)
C(2T)	5505(13)	8712(13)	6783(8)	47(3)
C(3T)	5762(13)	8860(11)	7631(8)	61(3)
C(4T)	4842(16)	8266(16)	8255(8)	87(4)

Table 51: Selected bond lengths [Å] and angles [°] for D19354_sq

Fe(1)-N(2)	1.848(16)
Fe(1)-N(43)	1.887(13)
Fe(1)-N(3)	1.922(12)
Fe(1)-N(42)	1.931(2)
Fe(1)-N(1)	1.944(14)
Fe(1)-N(41)	1.954(2)
Fe(1)-N(1A)	1.959(16)
Fe(1)-N(3A)	1.986(13)
Fe(1)-N(43A)	2.026(12)
Fe(1)-N(2A)	2.029(19)
N(2)-Fe(1)-N(43)	96.3(7)
N(2)-Fe(1)-N(3)	85.3(5)
N(43)-Fe(1)-N(3)	83.4(8)
N(2)-Fe(1)-N(42)	179.0(6)
N(43)-Fe(1)-N(42)	84.5(4)
N(3)-Fe(1)-N(42)	94.2(3)
N(2)-Fe(1)-N(1)	86.4(5)
N(43)-Fe(1)-N(1)	93.9(9)
N(3)-Fe(1)-N(1)	170.9(6)
N(42)-Fe(1)-N(1)	94.2(3)
N(2)-Fe(1)-N(41)	96.7(6)
N(43)-Fe(1)-N(41)	166.6(4)
N(3)-Fe(1)-N(41)	94.6(4)
N(42)-Fe(1)-N(41)	82.46(9)
N(1)-Fe(1)-N(41)	90.0(6)

Table 51 – continued from previous page

N(42)-Fe(1)-N(1A)	101.3(4)
N(41)-Fe(1)-N(1A)	88.2(7)
N(42)-Fe(1)-N(3A)	99.9(4)
N(41)-Fe(1)-N(3A)	89.1(5)
N(1A)-Fe(1)-N(3A)	158.0(5)
N(42)-Fe(1)-N(43A)	80.1(4)
N(41)-Fe(1)-N(43A)	162.4(3)
N(1A)-Fe(1)-N(43A)	93.5(9)
N(3A)-Fe(1)-N(43A)	95.7(7)
N(42)-Fe(1)-N(2A)	179.8(6)
N(41)-Fe(1)-N(2A)	97.3(6)
N(1A)-Fe(1)-N(2A)	78.6(6)
N(3A)-Fe(1)-N(2A)	80.1(5)
N(43A)-Fe(1)-N(2A)	100.2(7)

Table 52: Anisotropic displacement parameters ($Å^2 \times 10^3$) for D19354_sq. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	23(1)	19(1)	31(1)	-1(1)	-13(1)	0(1)
N(2)	35(4)	15(3)	30(5)	-3(2)	-13(3)	2(2)
N(1)	14(4)	25(3)	15(3)	1(2)	-2(3)	1(2)
C(1)	16(5)	28(3)	20(4)	-6(3)	0(4)	-1(3)
C(2)	21(4)	30(3)	21(3)	-7(3)	-5(3)	3(3)
C(3)	14(5)	22(3)	29(4)	-7(3)	-1(3)	1(3)
C(4)	10(5)	24(3)	20(3)	5(2)	0(3)	-6(2)
C(5)	19(4)	21(3)	26(3)	-4(3)	-3(4)	0(3)
C(6)	27(4)	23(3)	19(3)	1(2)	-4(3)	-7(3)
C(7)	27(4)	23(3)	20(4)	-5(3)	-2(5)	3(3)
C(8)	15(3)	26(3)	15(3)	2(2)	-5(3)	-4(2)
C(9)	8(4)	18(2)	19(4)	-1(2)	3(3)	-3(2)
C(10)	39(3)	25(3)	23(3)	-1(3)	-5(3)	-1(2)
C(11)	60(6)	56(6)	24(4)	15(4)	-19(4)	-5(4)
C(12)	48(5)	32(4)	40(6)	3(4)	12(4)	-1(4)
N(3)	10(4)	23(2)	27(3)	-1(2)	-1(2)	-6(2)
C(21)	26(4)	22(1)	34(3)	3(2)	-11(2)	1(2)
C(22)	26(4)	22(1)	34(3)	3(2)	-11(2)	1(2)
C(23)	20(3)	21(1)	37(3)	-2(2)	-11(2)	-1(2)
C(24)	20(3)	21(1)	37(3)	-2(2)	-11(2)	-1(2)
C(25)	21(4)	27(4)	40(4)	-5(3)	-11(3)	3(3)
C(26)	22(3)	36(4)	29(3)	-6(3)	-6(3)	-2(3)
C(27)	19(4)	24(4)	33(4)	7(3)	-4(3)	-10(3)
C(28)	9(4)	18(2)	27(3)	3(2)	-2(2)	-9(2)

Table 52 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(29)	12(4)	17(2)	29(3)	2(2)	-4(3)	-6(2)
C(30)	32(3)	52(5)	31(4)	-7(3)	-6(3)	1(3)
C(31)	34(3)	61(4)	39(3)	0(3)	-4(2)	3(3)
C(32)	46(5)	74(8)	29(4)	-7(4)	-8(3)	14(5)
N(2A)	16(4)	26(3)	17(3)	-1(2)	-8(2)	1(2)
N(1A)	14(4)	18(3)	22(5)	-2(3)	-1(4)	-4(2)
C(1A)	18(6)	27(4)	23(5)	-2(3)	2(4)	5(3)
C(2A)	28(5)	26(4)	43(7)	-9(5)	-5(7)	2(3)
C(3A)	14(5)	26(4)	45(6)	8(4)	0(5)	1(3)
C(4A)	8(5)	20(3)	36(5)	5(3)	1(5)	-4(3)
C(5A)	25(5)	36(6)	33(5)	20(4)	-5(5)	-5(5)
C(6A)	29(5)	44(6)	33(5)	11(4)	-14(5)	-5(4)
C(7A)	25(5)	40(5)	14(4)	4(3)	-2(4)	-6(4)
C(8A)	24(5)	20(3)	24(5)	1(3)	-6(5)	-2(3)
C(9A)	8(5)	28(3)	18(4)	9(3)	1(4)	-4(3)
C(10A)	66(7)	59(9)	31(5)	22(5)	-16(4)	-8(5)
C(11A)	63(8)	80(12)	51(8)	-12(6)	-20(6)	6(7)
C(12A)	65(7)	82(13)	36(6)	10(6)	-11(5)	-18(6)
N(3A)	7(5)	18(2)	30(4)	7(2)	-4(3)	-4(3)
C(21A)	26(4)	22(1)	34(3)	3(2)	-11(2)	1(2)
C(22A)	26(4)	22(1)	34(3)	3(2)	-11(2)	1(2)
C(23A)	20(3)	21(1)	37(3)	-2(2)	-11(2)	-1(2)
C(24A)	20(3)	21(1)	37(3)	-2(2)	-11(2)	-1(2)
C(25A)	26(5)	20(4)	32(4)	-7(3)	-7(4)	0(3)
C(26A)	28(5)	27(4)	29(4)	-2(3)	-4(3)	4(3)
C(27A)	16(4)	18(4)	22(3)	2(3)	3(3)	-5(3)
C(28A)	9(4)	18(2)	27(3)	3(2)	-2(2)	-9(2)
C(29A)	12(4)	17(2)	29(3)	2(2)	-4(3)	-6(2)
C(30A)	44(4)	41(5)	28(4)	-11(4)	7(3)	10(3)
C(31A)	37(4)	78(6)	42(4)	-7(4)	9(3)	-9(4)
C(32A)	66(7)	64(7)	29(4)	-6(4)	-9(4)	-14(5)
N(41)	23(1)	19(1)	34(1)	-2(1)	-10(1)	1(1)
N(42)	24(1)	29(1)	31(1)	1(1)	-12(1)	-6(1)
C(41)	26(1)	21(1)	38(1)	-1(1)	-9(1)	0(1)
C(42)	24(1)	27(1)	48(2)	-4(1)	-8(1)	-3(1)
C(43)	24(1)	41(2)	47(2)	-10(1)	-12(1)	-4(1)
C(44)	26(1)	33(1)	41(1)	-8(1)	-15(1)	0(1)
C(45)	32(1)	47(2)	43(2)	-8(1)	-18(1)	-3(1)
C(46)	38(1)	39(2)	37(1)	-6(1)	-20(1)	2(1)
C(47)	36(1)	36(1)	35(1)	1(1)	-17(1)	-5(1)
C(48)	28(1)	25(1)	34(1)	-1(1)	-14(1)	-4(1)
C(49)	24(1)	23(1)	34(1)	-3(1)	-12(1)	0(1)
C(50)	45(2)	58(2)	40(2)	-2(1)	-24(1)	-5(1)

Table 52 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(51)	64(4)	61(4)	50(4)	11(3)	-36(3)	-19(3)
C(52)	70(5)	70(5)	43(3)	-7(3)	-26(3)	1(4)
C(51A)	78(7)	74(6)	45(4)	-15(4)	-22(5)	-5(5)
C(52A)	44(4)	79(6)	35(4)	8(3)	-19(3)	-5(4)
N(43)	19(4)	25(4)	27(3)	-1(3)	-5(2)	8(3)
C(61)	17(4)	19(3)	32(4)	-6(3)	-10(3)	3(4)
C(62)	23(4)	26(4)	34(4)	-2(3)	-12(3)	0(3)
C(63)	23(4)	35(5)	39(4)	-3(3)	-14(3)	-7(3)
C(64)	22(3)	22(4)	29(3)	-2(2)	-7(2)	-1(3)
C(65)	25(3)	37(4)	34(3)	-1(3)	-4(2)	-8(3)
C(66)	30(3)	37(4)	29(2)	2(2)	-2(2)	-5(3)
C(67)	28(3)	34(5)	30(3)	2(3)	-8(2)	-8(3)
C(68)	31(4)	32(5)	23(3)	6(3)	-5(2)	-10(4)
C(69)	17(3)	16(5)	31(3)	-7(3)	-7(2)	4(3)
C(70)	35(3)	52(4)	32(3)	1(3)	-2(2)	-11(3)
C(71)	49(5)	80(6)	33(3)	14(4)	-8(3)	-8(4)
C(72)	76(6)	57(4)	40(4)	1(3)	4(4)	-9(4)
N(43A)	13(3)	12(3)	32(4)	-4(3)	-9(3)	3(3)
C(61A)	27(6)	24(4)	29(4)	-1(4)	-12(4)	5(5)
C(62A)	30(6)	24(4)	40(6)	1(4)	-19(4)	-5(5)
C(63A)	27(4)	32(6)	40(5)	4(4)	-12(4)	-10(4)
C(64A)	25(4)	25(5)	41(4)	-3(3)	-14(3)	-2(3)
C(65A)	22(3)	38(4)	41(3)	-2(3)	-3(2)	-6(3)
C(66A)	25(3)	39(4)	41(3)	-2(3)	-5(2)	-7(3)
C(67A)	30(3)	38(6)	34(3)	-3(4)	-9(3)	-7(3)
C(68A)	19(3)	40(6)	35(4)	-2(4)	-14(3)	-8(3)
C(69A)	22(3)	11(4)	27(3)	-3(3)	-6(3)	5(3)
C(70A)	41(4)	49(5)	42(4)	-8(3)	-2(3)	-16(4)
C(71A)	44(5)	91(8)	45(5)	10(5)	-11(4)	-12(4)
C(72A)	37(3)	60(5)	51(4)	5(3)	-3(3)	-7(3)
O(1S)	60(5)	93(6)	51(4)	6(4)	-16(3)	-6(4)
C(1S)	47(6)	50(6)	52(4)	6(4)	-23(4)	-17(5)
C(2S)	47(6)	37(5)	56(5)	3(4)	-21(4)	-4(4)
C(3S)	74(7)	46(5)	64(6)	9(4)	-39(5)	-20(4)
C(4S)	119(10)	106(9)	52(5)	3(5)	-27(6)	-53(8)
O(1T)	88(7)	72(6)	68(6)	21(4)	-31(5)	-44(5)
C(1T)	64(8)	45(6)	74(7)	20(6)	-35(6)	-17(6)
C(2T)	44(6)	40(5)	58(5)	2(4)	-18(4)	-5(4)
C(3T)	62(6)	60(6)	66(6)	-12(4)	-24(5)	-16(5)
C(4T)	94(9)	118(10)	55(6)	-6(6)	-24(6)	-43(7)

2.12 Fe-complex 2e

Table 53: Crystal data and structure refinement for **2e**

Identification code	D19244
Empirical formula	C114 H132 Fe2 N12 O2.50
Formula weight	1822.01
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 17.4469(6) Å α = 63.2290(10)°. b = 17.6298(7) Å β = 79.2240(10)°. c = 18.0962(6) Å γ = 88.9040(10)°.
Volume	4868.4(3) $Å^3$
Z	2
Density (calculated)	1.243 $Mg\,m^{-3}$
Absorption coefficient	0.357 mm^{-1}
F(000)	1944
Crystal size	0.544 x 0.311 x 0.256 mm^3
Theta range for data collection	2.295 to 26.372°.
Index ranges	-21<=h<=21, -22<=k<=22, -22<=l<=22
Reflections collected	214015
Independent reflections	19917 [R(int) = 0.0869]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	19917 / 3304 / 1374
Goodness-of-fit on F2	1.021
Final R indices [I>2sigma(I)]	R1 = 0.0459, wR2 = 0.1079
R indices (all data)	R1 = 0.0673, wR2 = 0.1197
Extinction coefficient	n/a
Largest diff. peak and hole	0.583 and -0.546 $e.Å^{-3}$

Table 54: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2e**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Fe(1)	2426(1)	-23(1)	5037(1)	14(1)
N(1)	3391(1)	312(1)	5237(1)	15(1)
N(2)	2975(1)	541(1)	3864(1)	16(1)
N(3)	1589(1)	-187(1)	4538(1)	16(1)
C(1)	3558(1)	213(1)	5959(1)	18(1)

Table 54 – continued from previous page

	x	y	z	U(eq)
C(2)	4275(1)	516(1)	6011(1)	20(1)
C(3)	4833(1)	929(1)	5296(1)	19(1)
C(4)	4681(1)	1054(1)	4508(1)	16(1)
C(5)	5217(1)	1490(1)	3737(1)	19(1)
C(6)	5027(1)	1610(1)	2986(1)	18(1)
C(7)	4283(1)	1299(1)	2989(1)	18(1)
C(8)	3722(1)	869(1)	3736(1)	15(1)
C(9)	3946(1)	739(1)	4504(1)	15(1)
C(10)	5624(1)	2094(1)	2153(1)	22(1)
C(11)	5828(1)	2986(2)	2050(2)	31(1)
C(12)	6373(1)	1618(2)	2189(2)	31(1)
C(13)	5318(1)	2190(2)	1380(1)	26(1)
C(21)	892(1)	-608(1)	4930(1)	19(1)
C(22)	328(1)	-650(1)	4488(1)	21(1)
C(23)	481(1)	-233(1)	3628(1)	21(1)
C(24)	1214(1)	226(1)	3183(1)	18(1)
C(25)	1425(1)	676(1)	2293(1)	20(1)
C(26)	2152(1)	1101(1)	1898(1)	20(1)
C(27)	2694(1)	1085(1)	2398(1)	19(1)
C(28)	2530(1)	643(1)	3278(1)	17(1)
C(29)	1762(1)	219(1)	3670(1)	15(1)
C(30)	2390(1)	1601(2)	932(1)	26(1)
C(31)	1833(2)	1383(2)	485(2)	32(1)
C(32)	3211(2)	1403(3)	624(2)	56(1)
C(33)	2388(2)	2554(2)	670(2)	59(1)
N(41)	2720(1)	-1182(1)	5326(1)	15(1)
N(42)	1892(1)	-553(1)	6213(1)	16(1)
N(43)	1984(1)	994(1)	5056(1)	16(1)
C(41)	3158(1)	-1472(1)	4836(1)	17(1)
C(42)	3322(1)	-2332(1)	5131(1)	20(1)
C(43)	3006(1)	-2908(1)	5938(1)	20(1)
C(44)	2513(1)	-2634(1)	6475(1)	18(1)
C(45)	2139(1)	-3188(1)	7316(1)	21(1)
C(46)	1673(1)	-2880(1)	7807(1)	20(1)
C(47)	1570(1)	-1998(1)	7470(1)	19(1)
C(48)	1924(1)	-1416(1)	6648(1)	16(1)
C(49)	2398(1)	-1756(1)	6142(1)	16(1)
C(50)	1279(1)	-3455(2)	8729(1)	25(1)
C(51)	1663(2)	-3220(2)	9300(2)	34(1)
C(52)	1373(2)	-4399(2)	8980(2)	43(1)
C(53)	402(1)	-3329(2)	8877(2)	40(1)
C(61)	2016(1)	1770(1)	4422(1)	19(1)
C(62)	1710(1)	2459(1)	4540(2)	24(1)

Table 54 – continued from previous page

	x	y	z	U(eq)
C(63)	1381(1)	2340(1)	5333(2)	23(1)
C(64)	1335(1)	1522(1)	6030(1)	19(1)
C(65)	1003(1)	1341(2)	6870(1)	23(1)
C(66)	974(1)	527(2)	7515(1)	22(1)
C(67)	1269(1)	-138(1)	7337(1)	20(1)
C(68)	1586(1)	-1(1)	6514(1)	17(1)
C(69)	1635(1)	858(1)	5856(1)	16(1)
C(70)	610(2)	346(2)	8428(2)	31(1)
C(71)	536(2)	-604(2)	9048(2)	44(1)
C(72)	-212(2)	672(2)	8453(2)	37(1)
C(73)	1121(2)	824(2)	8713(2)	48(1)
Fe(2)	2537(1)	5194(1)	4451(1)	15(1)
N(81)	2988(1)	4207(1)	4370(1)	16(1)
N(82)	2658(1)	5631(1)	3241(1)	17(1)
N(83)	2146(1)	6314(1)	4208(1)	18(1)
C(81)	3161(1)	3484(1)	4977(1)	19(1)
C(82)	3513(1)	2834(1)	4819(1)	22(1)
C(83)	3671(1)	2928(1)	4011(1)	20(1)
C(84)	3467(1)	3667(1)	3351(1)	17(1)
C(85)	3570(1)	3799(1)	2505(1)	19(1)
C(86)	3344(1)	4526(1)	1896(1)	18(1)
C(87)	3016(1)	5159(1)	2112(1)	17(1)
C(88)	2934(1)	5083(1)	2921(1)	16(1)
C(89)	3138(1)	4302(1)	3559(1)	15(1)
C(90)	3429(1)	4686(1)	975(1)	22(1)
C(91)	3826(2)	5575(2)	367(2)	35(1)
C(92)	3922(2)	4035(2)	804(2)	34(1)
C(93)	2616(1)	4630(2)	794(2)	31(1)
C(101)	1878(1)	6632(1)	4742(1)	20(1)
C(102)	1666(1)	7474(2)	4460(2)	26(1)
C(103)	1744(1)	8001(2)	3619(2)	27(1)
C(104)	2039(1)	7696(1)	3022(2)	23(1)
C(105)	2184(1)	8205(2)	2139(2)	29(1)
C(106)	2519(1)	7881(1)	1601(2)	25(1)
C(107)	2682(1)	7013(1)	1941(1)	21(1)
C(108)	2527(1)	6471(1)	2802(1)	17(1)
C(109)	2222(1)	6836(1)	3355(1)	18(1)
C(110)	2751(2)	8423(2)	640(2)	33(1)
C(111)	2393(3)	8032(3)	170(4)	39(1)
C(112)	3654(2)	8457(4)	375(3)	50(1)
C(113)	2523(4)	9342(3)	342(3)	53(2)
C(11A)	2584(16)	7875(14)	219(17)	39(1)
C(12A)	3575(8)	8788(13)	363(15)	50(1)

Table 54 – continued from previous page

	x	y	z	U(eq)
C(13A)	2133(12)	9106(12)	386(12)	53(2)
N(121)	3552(1)	5639(1)	4446(1)	16(1)
N(122)	2420(1)	4763(1)	5656(1)	15(1)
N(123)	1481(1)	4651(1)	4767(1)	18(1)
C(121)	4108(1)	6122(1)	3789(1)	19(1)
C(122)	4807(1)	6419(1)	3878(1)	22(1)
C(123)	4941(1)	6198(1)	4668(1)	20(1)
C(124)	4373(1)	5676(1)	5388(1)	16(1)
C(125)	4472(1)	5398(1)	6228(1)	18(1)
C(126)	3903(1)	4867(1)	6897(1)	17(1)
C(127)	3200(1)	4624(1)	6749(1)	17(1)
C(128)	3057(1)	4906(1)	5935(1)	15(1)
C(129)	3676(1)	5418(1)	5246(1)	14(1)
C(130)	4002(1)	4525(1)	7817(1)	21(1)
C(131)	3977(2)	3545(2)	8234(2)	29(1)
C(132)	3335(1)	4796(2)	8308(2)	27(1)
C(133)	4775(1)	4859(2)	7884(2)	30(1)
C(31A)	3291(12)	3995(17)	8513(14)	32(7)
C(32A)	4122(15)	5321(12)	7946(18)	26(6)
C(33A)	4726(12)	4019(18)	7962(19)	35(7)
C(141)	1032(1)	4590(1)	4276(1)	20(1)
C(142)	273(1)	4184(1)	4599(2)	24(1)
C(143)	-26(1)	3843(1)	5443(2)	24(1)
C(144)	426(1)	3901(1)	5993(1)	20(1)
C(145)	153(1)	3607(1)	6868(2)	22(1)
C(146)	611(1)	3726(1)	7358(1)	21(1)
C(147)	1381(1)	4109(1)	6981(1)	20(1)
C(148)	1695(1)	4382(1)	6129(1)	17(1)
C(149)	1188(1)	4302(1)	5626(1)	16(1)
C(150)	281(1)	3518(2)	8283(2)	26(1)
C(151)	-119(2)	4286(2)	8284(2)	48(1)
C(152)	928(2)	3341(3)	8803(2)	46(1)
C(153)	-294(2)	2737(2)	8735(2)	57(1)
C(51A)	430(30)	4324(17)	8360(20)	57(1)
C(52A)	710(20)	2800(20)	8850(20)	65(11)
C(53A)	-596(9)	3280(30)	8470(20)	46(1)
O(1S)	-39(1)	6427(1)	7105(1)	34(1)
C(1S)	117(3)	7286(3)	6464(3)	29(1)
C(2S)	-399(5)	7811(4)	6798(7)	30(1)
C(3S)	-1072(6)	7168(5)	7450(5)	31(1)
C(4S)	-858(3)	6319(4)	7448(4)	38(1)
O(1T)	-517(7)	6464(7)	6785(7)	33(3)
C(1T)	-15(15)	7174(15)	6637(19)	29(1)

Table 54 – continued from previous page

	x	y	z	U(eq)
C(2T)	-490(30)	7750(18)	6890(30)	25(4)
C(3T)	-1100(30)	7190(20)	7590(30)	33(5)
C(4T)	-1020(20)	6359(19)	7561(18)	40(4)
O(11S)	2679(2)	2040(3)	8175(2)	50(1)
C(11S)	2800(4)	2330(4)	7308(4)	39(1)
C(12S)	3158(3)	1680(3)	7096(3)	38(1)
C(13S)	3283(3)	960(3)	7912(3)	44(1)
C(14S)	3270(5)	1445(5)	8371(5)	58(2)
O(11T)	3040(9)	2150(10)	7336(9)	50(1)
C(11T)	3557(11)	1518(11)	7389(10)	56(3)
C(12T)	4025(9)	1181(11)	8052(10)	65(4)
C(13T)	3338(15)	1282(15)	8614(10)	68(5)
C(14T)	3384(13)	2222(11)	8005(11)	79(4)
O(21S)	4774(5)	9850(5)	1918(4)	80(2)
C(21S)	3967(6)	9371(6)	2429(7)	91(3)
C(22S)	4165(7)	8531(6)	2859(6)	91(3)
C(23S)	4494(5)	8489(4)	2077(4)	58(2)
C(24S)	4750(5)	9408(5)	1418(4)	61(2)
O(21T)	4229(6)	9520(7)	2584(7)	60(3)
C(21T)	4366(10)	8666(9)	2739(10)	68(3)
C(22T)	5188(10)	8662(11)	2439(10)	114(5)
C(23T)	5325(8)	9247(8)	1618(9)	74(3)
C(24T)	4689(14)	9816(13)	1689(11)	89(6)

Table 55: Selected bond lengths [Å] and angles [°] for D19354_sq

Fe(1)-N(42)	1.9420(17)
Fe(1)-N(3)	1.9420(17)
Fe(1)-N(1)	1.9424(17)
Fe(1)-N(2)	1.9461(17)
Fe(1)-N(43)	1.9490(17)
Fe(1)-N(41)	1.9526(17)
N(42)-Fe(1)-N(3)	98.80(7)
N(42)-Fe(1)-N(1)	95.67(7)
N(3)-Fe(1)-N(1)	165.41(7)
N(42)-Fe(1)-N(2)	178.00(7)
N(3)-Fe(1)-N(2)	82.63(7)
N(1)-Fe(1)-N(2)	82.86(7)
N(42)-Fe(1)-N(43)	82.56(7)
N(3)-Fe(1)-N(43)	91.27(7)
N(1)-Fe(1)-N(43)	88.76(7)
N(2)-Fe(1)-N(43)	96.04(7)

Table 55 – continued from previous page

N(42)-Fe(1)-N(41)	82.34(7)
N(3)-Fe(1)-N(41)	90.63(7)
N(1)-Fe(1)-N(41)	93.14(7)
N(2)-Fe(1)-N(41)	99.07(7)
N(43)-Fe(1)-N(41)	164.90(7)

Table 56: Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2e**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	13(1)	14(1)	16(1)	-7(1)	-4(1)	2(1)
N(1)	16(1)	13(1)	16(1)	-7(1)	-4(1)	4(1)
N(2)	16(1)	16(1)	17(1)	-8(1)	-4(1)	2(1)
N(3)	15(1)	14(1)	22(1)	-10(1)	-6(1)	3(1)
C(1)	18(1)	18(1)	19(1)	-8(1)	-5(1)	5(1)
C(2)	21(1)	21(1)	21(1)	-12(1)	-9(1)	5(1)
C(3)	17(1)	17(1)	26(1)	-10(1)	-10(1)	3(1)
C(4)	14(1)	13(1)	23(1)	-8(1)	-6(1)	3(1)
C(5)	15(1)	16(1)	25(1)	-7(1)	-7(1)	1(1)
C(6)	16(1)	14(1)	21(1)	-5(1)	-3(1)	2(1)
C(7)	17(1)	17(1)	18(1)	-6(1)	-5(1)	2(1)
C(8)	14(1)	11(1)	19(1)	-6(1)	-5(1)	3(1)
C(9)	15(1)	13(1)	18(1)	-7(1)	-5(1)	4(1)
C(10)	17(1)	22(1)	20(1)	-3(1)	-3(1)	-2(1)
C(11)	32(1)	25(1)	27(1)	-3(1)	-9(1)	-8(1)
C(12)	20(1)	35(1)	23(1)	-3(1)	1(1)	1(1)
C(13)	24(1)	27(1)	19(1)	-5(1)	-1(1)	-2(1)
C(21)	17(1)	18(1)	21(1)	-9(1)	-4(1)	3(1)
C(22)	16(1)	20(1)	29(1)	-12(1)	-6(1)	1(1)
C(23)	16(1)	24(1)	29(1)	-16(1)	-9(1)	3(1)
C(24)	17(1)	16(1)	25(1)	-12(1)	-8(1)	4(1)
C(25)	23(1)	19(1)	23(1)	-12(1)	-12(1)	4(1)
C(26)	26(1)	19(1)	20(1)	-10(1)	-8(1)	3(1)
C(27)	18(1)	20(1)	21(1)	-10(1)	-4(1)	-1(1)
C(28)	17(1)	15(1)	21(1)	-11(1)	-5(1)	3(1)
C(29)	18(1)	12(1)	18(1)	-9(1)	-6(1)	4(1)
C(30)	32(1)	29(1)	19(1)	-11(1)	-6(1)	-4(1)
C(31)	36(1)	38(2)	23(1)	-14(1)	-11(1)	-1(1)
C(32)	32(2)	110(3)	27(2)	-31(2)	-7(1)	4(2)
C(33)	117(3)	28(2)	26(2)	-8(1)	-11(2)	-18(2)
N(41)	11(1)	18(1)	19(1)	-10(1)	-6(1)	1(1)
N(42)	15(1)	17(1)	19(1)	-10(1)	-4(1)	3(1)
N(43)	12(1)	18(1)	20(1)	-10(1)	-6(1)	2(1)

Table 56 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(41)	15(1)	19(1)	20(1)	-11(1)	-4(1)	1(1)
C(42)	17(1)	23(1)	27(1)	-16(1)	-6(1)	4(1)
C(43)	22(1)	16(1)	28(1)	-12(1)	-10(1)	4(1)
C(44)	17(1)	16(1)	24(1)	-10(1)	-9(1)	2(1)
C(45)	25(1)	13(1)	23(1)	-6(1)	-9(1)	1(1)
C(46)	20(1)	20(1)	20(1)	-8(1)	-6(1)	-3(1)
C(47)	18(1)	21(1)	20(1)	-11(1)	-4(1)	1(1)
C(48)	15(1)	18(1)	19(1)	-9(1)	-7(1)	2(1)
C(49)	13(1)	18(1)	19(1)	-9(1)	-7(1)	1(1)
C(50)	26(1)	21(1)	22(1)	-5(1)	-4(1)	-4(1)
C(51)	38(1)	36(1)	21(1)	-7(1)	-4(1)	-7(1)
C(52)	64(2)	23(1)	30(1)	-4(1)	3(1)	-6(1)
C(53)	27(1)	45(2)	29(1)	-3(1)	0(1)	-5(1)
C(61)	17(1)	17(1)	24(1)	-9(1)	-6(1)	1(1)
C(62)	22(1)	17(1)	31(1)	-9(1)	-10(1)	3(1)
C(63)	20(1)	19(1)	35(1)	-16(1)	-9(1)	5(1)
C(64)	14(1)	22(1)	28(1)	-16(1)	-7(1)	3(1)
C(65)	21(1)	26(1)	32(1)	-21(1)	-7(1)	5(1)
C(66)	18(1)	32(1)	27(1)	-21(1)	-6(1)	3(1)
C(67)	18(1)	24(1)	21(1)	-12(1)	-5(1)	2(1)
C(68)	11(1)	21(1)	22(1)	-13(1)	-5(1)	2(1)
C(69)	12(1)	20(1)	21(1)	-12(1)	-6(1)	3(1)
C(70)	36(1)	38(1)	26(1)	-22(1)	-2(1)	2(1)
C(71)	62(2)	46(2)	22(1)	-18(1)	0(1)	11(1)
C(72)	34(1)	42(2)	40(2)	-29(1)	6(1)	-1(1)
C(73)	51(2)	69(2)	39(2)	-39(2)	-8(1)	-2(2)
Fe(2)	15(1)	18(1)	16(1)	-10(1)	-6(1)	4(1)
N(81)	12(1)	18(1)	17(1)	-9(1)	-6(1)	2(1)
N(82)	21(1)	16(1)	18(1)	-10(1)	-7(1)	7(1)
N(83)	13(1)	23(1)	24(1)	-16(1)	-7(1)	3(1)
C(81)	19(1)	21(1)	18(1)	-7(1)	-9(1)	2(1)
C(82)	20(1)	17(1)	27(1)	-6(1)	-10(1)	3(1)
C(83)	18(1)	14(1)	28(1)	-10(1)	-6(1)	4(1)
C(84)	14(1)	15(1)	23(1)	-9(1)	-3(1)	1(1)
C(85)	17(1)	19(1)	23(1)	-13(1)	-1(1)	2(1)
C(86)	17(1)	19(1)	19(1)	-10(1)	-1(1)	-2(1)
C(87)	20(1)	14(1)	17(1)	-8(1)	-4(1)	2(1)
C(88)	15(1)	15(1)	19(1)	-9(1)	-4(1)	1(1)
C(89)	13(1)	16(1)	16(1)	-7(1)	-2(1)	0(1)
C(90)	26(1)	24(1)	18(1)	-13(1)	-2(1)	3(1)
C(91)	45(2)	36(2)	20(1)	-12(1)	1(1)	-6(1)
C(92)	40(1)	49(2)	27(1)	-28(1)	-9(1)	17(1)
C(93)	31(1)	40(2)	29(1)	-21(1)	-10(1)	7(1)

Table 56 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(101)	14(1)	28(1)	28(1)	-20(1)	-6(1)	3(1)
C(102)	20(1)	33(1)	39(1)	-29(1)	-7(1)	6(1)
C(103)	26(1)	24(1)	42(1)	-23(1)	-11(1)	10(1)
C(104)	23(1)	21(1)	33(1)	-17(1)	-10(1)	7(1)
C(105)	33(1)	19(1)	36(1)	-13(1)	-12(1)	10(1)
C(106)	31(1)	17(1)	27(1)	-8(1)	-10(1)	4(1)
C(107)	27(1)	16(1)	23(1)	-10(1)	-9(1)	5(1)
C(108)	17(1)	17(1)	23(1)	-11(1)	-9(1)	5(1)
C(109)	17(1)	19(1)	24(1)	-12(1)	-9(1)	5(1)
C(110)	46(2)	16(1)	28(1)	-3(1)	-5(1)	5(1)
C(111)	57(3)	32(2)	21(2)	-3(2)	-13(2)	7(2)
C(112)	52(2)	29(3)	49(2)	-3(2)	0(2)	-7(2)
C(113)	85(4)	19(2)	36(2)	1(2)	-1(2)	11(2)
C(11A)	57(3)	32(2)	21(2)	-3(2)	-13(2)	7(2)
C(12A)	52(2)	29(3)	49(2)	-3(2)	0(2)	-7(2)
C(13A)	85(4)	19(2)	36(2)	1(2)	-1(2)	11(2)
N(121)	17(1)	15(1)	16(1)	-8(1)	-3(1)	4(1)
N(122)	15(1)	17(1)	16(1)	-10(1)	-5(1)	2(1)
N(123)	17(1)	17(1)	24(1)	-13(1)	-8(1)	6(1)
C(121)	19(1)	21(1)	16(1)	-8(1)	-2(1)	5(1)
C(122)	19(1)	23(1)	20(1)	-8(1)	2(1)	-1(1)
C(123)	15(1)	21(1)	24(1)	-11(1)	-3(1)	0(1)
C(124)	15(1)	16(1)	21(1)	-11(1)	-5(1)	4(1)
C(125)	16(1)	20(1)	23(1)	-13(1)	-9(1)	4(1)
C(126)	18(1)	20(1)	21(1)	-14(1)	-7(1)	6(1)
C(127)	16(1)	18(1)	16(1)	-8(1)	-2(1)	0(1)
C(128)	16(1)	16(1)	18(1)	-11(1)	-4(1)	3(1)
C(129)	15(1)	14(1)	16(1)	-8(1)	-4(1)	4(1)
C(130)	19(1)	27(1)	18(1)	-12(1)	-6(1)	2(1)
C(131)	37(2)	30(1)	20(1)	-9(1)	-10(1)	6(1)
C(132)	25(1)	41(2)	23(1)	-20(1)	-8(1)	5(1)
C(133)	24(1)	47(2)	24(1)	-18(1)	-11(1)	1(1)
C(31A)	29(10)	45(15)	19(9)	-13(10)	-7(8)	-4(10)
C(32A)	19(13)	41(11)	26(13)	-24(11)	3(11)	-3(9)
C(33A)	32(10)	56(16)	28(14)	-25(13)	-17(10)	19(11)
C(141)	24(1)	20(1)	26(1)	-16(1)	-14(1)	9(1)
C(142)	24(1)	20(1)	39(1)	-20(1)	-19(1)	9(1)
C(143)	18(1)	20(1)	42(1)	-18(1)	-12(1)	4(1)
C(144)	16(1)	18(1)	31(1)	-15(1)	-7(1)	5(1)
C(145)	13(1)	21(1)	33(1)	-14(1)	1(1)	0(1)
C(146)	17(1)	19(1)	25(1)	-12(1)	3(1)	0(1)
C(147)	18(1)	24(1)	23(1)	-14(1)	-3(1)	1(1)
C(148)	14(1)	18(1)	21(1)	-10(1)	-2(1)	1(1)

Table 56 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(149)	16(1)	15(1)	22(1)	-12(1)	-5(1)	5(1)
C(150)	24(1)	28(1)	26(1)	-14(1)	5(1)	-3(1)
C(151)	67(2)	44(2)	30(2)	-20(1)	1(2)	22(2)
C(152)	38(2)	70(3)	22(2)	-14(2)	-2(1)	7(2)
C(153)	75(3)	51(2)	35(2)	-22(2)	22(2)	-36(2)
C(51A)	75(3)	51(2)	35(2)	-22(2)	22(2)	-36(2)
C(52A)	51(16)	69(15)	38(13)	3(16)	2(15)	15(16)
C(53A)	38(2)	70(3)	22(2)	-14(2)	-2(1)	7(2)
O(1S)	31(1)	29(1)	36(1)	-10(1)	-2(1)	5(1)
C(1S)	27(2)	32(2)	25(2)	-12(2)	2(2)	1(1)
C(2S)	27(3)	28(2)	29(3)	-10(2)	-1(2)	1(2)
C(3S)	27(2)	38(2)	23(3)	-11(2)	-4(2)	7(2)
C(4S)	34(3)	34(2)	37(3)	-10(2)	-1(2)	2(2)
O(1T)	36(5)	37(5)	27(5)	-15(4)	-2(4)	-1(4)
C(1T)	27(2)	32(2)	25(2)	-12(2)	2(2)	1(1)
C(2T)	26(8)	35(6)	23(7)	-20(6)	-7(6)	9(6)
C(3T)	27(7)	38(7)	28(8)	-12(6)	0(6)	5(6)
C(4T)	38(8)	44(6)	30(6)	-15(5)	7(6)	-3(6)
O(11S)	53(2)	52(2)	43(2)	-26(2)	6(2)	-10(2)
C(11S)	49(4)	30(3)	30(2)	-13(2)	5(2)	-1(2)
C(12S)	37(3)	38(3)	31(3)	-9(2)	-10(2)	7(2)
C(13S)	51(3)	46(3)	28(3)	-15(2)	2(2)	8(2)
C(14S)	79(4)	45(4)	58(4)	-23(3)	-40(3)	14(3)
O(11T)	53(2)	52(2)	43(2)	-26(2)	6(2)	-10(2)
C(11T)	63(7)	49(6)	39(6)	-12(5)	6(5)	0(5)
C(12T)	45(7)	58(7)	50(7)	9(6)	-4(5)	-18(6)
C(13T)	88(8)	76(7)	25(6)	-14(6)	2(6)	-6(7)
C(14T)	89(8)	77(7)	57(6)	-23(5)	-4(6)	-11(7)
O(21S)	104(4)	72(4)	67(4)	-40(3)	-4(3)	-1(3)
C(21S)	111(5)	67(4)	60(3)	-12(3)	12(3)	23(4)
C(22S)	111(5)	67(4)	60(3)	-12(3)	12(3)	23(4)
C(23S)	79(4)	49(3)	45(3)	-20(3)	-14(3)	4(3)
C(24S)	74(4)	64(4)	43(3)	-22(3)	-16(3)	-1(4)
O(21T)	66(5)	47(4)	60(5)	-22(4)	1(4)	-14(4)
C(21T)	107(7)	47(5)	78(6)	-45(5)	-38(5)	-8(5)
C(22T)	128(7)	79(7)	109(7)	-24(6)	-14(7)	9(6)
C(23T)	61(6)	48(6)	97(6)	-21(5)	-12(5)	-3(5)
C(24T)	88(8)	69(7)	69(7)	-6(6)	7(7)	17(6)

2.13 Fe-complex 2f

Table 57: Crystal data and structure refinement for **2f**

Identification code	D19338
Empirical formula	C52 H56 Fe N6
Formula weight	820.87
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 12.8536(16) Å α = 81.724(5)°. b = 13.1224(16) Å β = 74.463(5)°. c = 13.2718(16) Å γ = 75.050(5)°.
Volume	2077.0(4) $Å^3$
Z	2
Density (calculated)	1.313 $Mg\,m^{-3}$
Absorption coefficient	0.408 mm^{-1}
F(000)	872
Crystal size	0.211 x 0.063 x 0.057 mm^3
Theta range for data collection	1.598 to 27.102°.
Index ranges	-16<=h<=16, -16<=k<=16, -17<=l<=17
Reflections collected	80634
Independent reflections	9131 [R(int) = 0.0736]
Completeness to theta = 25.242°	99.7 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	9131 / 0 / 536
Goodness-of-fit on F2	1.135
Final R indices [I>2sigma(I)]	R1 = 0.0801, wR2 = 0.2323
R indices (all data)	R1 = 0.0955, wR2 = 0.2402
Extinction coefficient	n/a
Largest diff. peak and hole	2.207 and -0.654 $e.Å^{-3}$

Table 58: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **2f**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Fe(1)	5716(1)	2531(1)	7548(1)	11(1)
N(1)	7215(3)	2581(3)	7536(3)	13(1)
N(2)	5691(3)	1929(3)	8977(3)	13(1)
N(3)	6110(3)	3149(3)	6112(3)	14(1)
C(1)	4887(4)	1562(4)	9669(4)	16(1)

Table 58 – continued from previous page

	x	y	z	U(eq)
C(2)	4973(4)	1162(4)	10691(4)	18(1)
C(3)	5915(4)	1154(4)	10999(4)	18(1)
C(4)	6786(4)	1540(4)	10283(4)	15(1)
C(5)	7791(4)	1552(4)	10532(4)	14(1)
C(6)	8603(4)	1940(4)	9784(4)	15(1)
C(7)	8462(4)	2307(4)	8767(4)	16(1)
C(8)	7506(4)	2284(4)	8464(4)	13(1)
C(9)	6642(4)	1912(4)	9269(4)	14(1)
C(10)	9672(4)	1955(4)	10057(4)	16(1)
C(11)	10703(4)	1281(4)	9384(4)	18(1)
C(12)	11783(4)	1266(4)	9681(4)	18(1)
C(13)	11799(4)	805(4)	10803(4)	20(1)
C(21)	5486(4)	3467(4)	5420(4)	17(1)
C(22)	5897(4)	3874(4)	4392(4)	20(1)
C(23)	6989(4)	3925(4)	4063(4)	20(1)
C(24)	7686(4)	3569(4)	4767(4)	17(1)
C(25)	8840(4)	3531(4)	4474(4)	17(1)
C(26)	9479(4)	3130(4)	5192(4)	16(1)
C(27)	8988(4)	2808(4)	6236(4)	15(1)
C(28)	7848(4)	2859(4)	6577(4)	14(1)
C(29)	7210(4)	3210(4)	5798(4)	13(1)
C(30)	10726(4)	3016(4)	4847(4)	18(1)
C(31)	11159(4)	3658(4)	5445(4)	20(1)
C(32)	12413(4)	3581(4)	5089(4)	21(1)
C(33)	12796(5)	3995(5)	3955(4)	26(1)
N(41)	4233(3)	2478(3)	7518(3)	12(1)
N(42)	4960(3)	3916(3)	8072(3)	13(1)
N(43)	6084(3)	1117(3)	7070(3)	13(1)
C(41)	5382(4)	4611(4)	8369(4)	17(1)
C(42)	4727(4)	5558(4)	8798(4)	21(1)
C(43)	3601(4)	5783(4)	8905(4)	19(1)
C(44)	3111(4)	5067(4)	8591(4)	14(1)
C(45)	1964(4)	5253(4)	8647(4)	15(1)
C(46)	1559(4)	4529(4)	8301(4)	15(1)
C(47)	2274(4)	3585(4)	7910(4)	15(1)
C(48)	3410(4)	3345(3)	7844(3)	12(1)
C(49)	3830(4)	4131(4)	8181(4)	12(1)
C(50)	349(4)	4665(4)	8304(4)	18(1)
C(51)	-469(4)	5686(4)	8648(4)	17(1)
C(52)	-1623(4)	5657(4)	8560(4)	20(1)
C(53)	-2492(4)	6650(4)	8895(5)	26(1)
C(61)	7052(4)	407(4)	6947(4)	16(1)
C(62)	7200(4)	-602(4)	6603(4)	18(1)

Table 58 – continued from previous page

	x	y	z	U(eq)
C(63)	6330(4)	-864(4)	6364(4)	16(1)
C(64)	5292(4)	-136(4)	6502(4)	14(1)
C(65)	4345(4)	-362(4)	6299(4)	14(1)
C(66)	3341(4)	364(4)	6522(4)	15(1)
C(67)	3255(4)	1319(4)	6931(4)	15(1)
C(68)	4150(4)	1604(4)	7126(4)	13(1)
C(69)	5203(4)	836(4)	6885(4)	12(1)
C(70)	2284(4)	176(4)	6370(4)	19(1)
C(71)	2358(4)	-836(4)	5881(4)	19(1)
C(72)	1246(4)	-841(5)	5667(4)	25(1)
C(73)	373(5)	-1002(6)	6662(5)	38(2)

Table 59: Selected bond lengths [Å] and angles [°] for **2f**

Fe(1)-N(41)	1.936(4)
Fe(1)-N(1)	1.941(4)
Fe(1)-N(2)	1.941(4)
Fe(1)-N(43)	1.947(4)
Fe(1)-N(3)	1.948(4)
Fe(1)-N(42)	1.955(4)
N(41)-Fe(1)-N(1)	178.40(17)
N(41)-Fe(1)-N(2)	98.45(17)
N(1)-Fe(1)-N(2)	82.97(17)
N(41)-Fe(1)-N(43)	82.48(16)
N(1)-Fe(1)-N(43)	96.80(17)
N(2)-Fe(1)-N(43)	90.34(16)
N(41)-Fe(1)-N(3)	95.67(17)
N(1)-Fe(1)-N(3)	82.91(17)
N(2)-Fe(1)-N(3)	165.89(17)
N(43)-Fe(1)-N(3)	91.41(16)
N(41)-Fe(1)-N(42)	83.03(16)
N(1)-Fe(1)-N(42)	97.74(17)
N(2)-Fe(1)-N(42)	89.76(16)
N(43)-Fe(1)-N(42)	165.36(16)
N(3)-Fe(1)-N(42)	92.05(16)

Table 60: Anisotropic displacement parameters ($Å^2 \times 10^3$) for **2f**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	7(1)	12(1)	14(1)	-2(1)	-3(1)	0(1)
N(1)	10(2)	15(2)	13(2)	-1(2)	-4(2)	-2(2)
N(2)	11(2)	13(2)	15(2)	-5(2)	-2(2)	-1(2)
N(3)	11(2)	14(2)	15(2)	-4(2)	-3(2)	0(2)
C(1)	11(2)	17(2)	19(2)	-2(2)	-2(2)	-2(2)
C(2)	10(2)	24(3)	18(2)	0(2)	0(2)	-2(2)
C(3)	14(2)	20(2)	17(2)	1(2)	-2(2)	-1(2)
C(4)	11(2)	14(2)	17(2)	-2(2)	-4(2)	0(2)
C(5)	12(2)	13(2)	15(2)	-1(2)	-6(2)	1(2)
C(6)	10(2)	15(2)	19(2)	-6(2)	-4(2)	2(2)
C(7)	13(2)	17(2)	17(2)	-3(2)	-2(2)	-4(2)
C(8)	10(2)	13(2)	15(2)	-2(2)	-2(2)	0(2)
C(9)	11(2)	14(2)	16(2)	-3(2)	-3(2)	-1(2)
C(10)	11(2)	18(2)	19(2)	-4(2)	-6(2)	0(2)
C(11)	14(2)	19(2)	20(2)	-4(2)	-4(2)	-2(2)
C(12)	12(2)	23(3)	20(2)	0(2)	-7(2)	-3(2)
C(13)	14(2)	24(3)	21(3)	0(2)	-5(2)	-2(2)
C(21)	10(2)	20(2)	21(2)	-1(2)	-6(2)	0(2)
C(22)	16(2)	23(3)	19(2)	2(2)	-8(2)	0(2)
C(23)	21(3)	22(3)	16(2)	3(2)	-4(2)	-5(2)
C(24)	12(2)	17(2)	21(2)	1(2)	-5(2)	-3(2)
C(25)	16(2)	17(2)	18(2)	-1(2)	1(2)	-6(2)
C(26)	13(2)	14(2)	21(2)	-4(2)	-3(2)	-4(2)
C(27)	11(2)	17(2)	17(2)	0(2)	-6(2)	0(2)
C(28)	12(2)	15(2)	17(2)	-1(2)	-4(2)	-3(2)
C(29)	8(2)	13(2)	17(2)	-3(2)	-2(2)	-1(2)
C(30)	12(2)	21(2)	20(2)	-2(2)	-2(2)	-3(2)
C(31)	12(2)	22(3)	24(3)	-6(2)	-2(2)	0(2)
C(32)	12(2)	25(3)	26(3)	-1(2)	-6(2)	-2(2)
C(33)	18(3)	36(3)	25(3)	1(2)	-4(2)	-13(2)
N(41)	8(2)	10(2)	16(2)	-3(1)	-3(1)	2(1)
N(42)	10(2)	15(2)	14(2)	2(2)	-5(2)	-2(2)
N(43)	12(2)	17(2)	12(2)	0(2)	-5(2)	-2(2)
C(41)	12(2)	21(2)	21(2)	-2(2)	-6(2)	-3(2)
C(42)	20(3)	20(3)	26(3)	-5(2)	-9(2)	-7(2)
C(43)	18(2)	14(2)	24(3)	-6(2)	-6(2)	1(2)
C(44)	15(2)	14(2)	13(2)	0(2)	-6(2)	-2(2)
C(45)	12(2)	15(2)	14(2)	-5(2)	-1(2)	2(2)
C(46)	10(2)	17(2)	15(2)	-2(2)	-4(2)	1(2)
C(47)	10(2)	14(2)	19(2)	-2(2)	-4(2)	-1(2)

Table 60 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(48)	12(2)	9(2)	11(2)	-1(2)	-1(2)	1(2)
C(49)	9(2)	14(2)	12(2)	1(2)	-4(2)	1(2)
C(50)	11(2)	18(2)	25(3)	-8(2)	-5(2)	2(2)
C(51)	10(2)	18(2)	20(2)	-4(2)	-2(2)	0(2)
C(52)	13(2)	22(3)	23(3)	-4(2)	-8(2)	1(2)
C(53)	14(2)	24(3)	41(3)	-10(2)	-10(2)	4(2)
C(61)	12(2)	16(2)	18(2)	-3(2)	-3(2)	0(2)
C(62)	11(2)	15(2)	24(3)	-3(2)	-5(2)	5(2)
C(63)	16(2)	13(2)	18(2)	-5(2)	-2(2)	1(2)
C(64)	15(2)	14(2)	12(2)	0(2)	-3(2)	-2(2)
C(65)	13(2)	12(2)	17(2)	-3(2)	-4(2)	-1(2)
C(66)	15(2)	14(2)	16(2)	0(2)	-4(2)	-4(2)
C(67)	11(2)	16(2)	17(2)	1(2)	-5(2)	0(2)
C(68)	13(2)	14(2)	13(2)	-1(2)	-2(2)	-3(2)
C(69)	11(2)	15(2)	12(2)	0(2)	-3(2)	-3(2)
C(70)	13(2)	21(2)	25(3)	-7(2)	-4(2)	-4(2)
C(71)	15(2)	18(2)	25(3)	-5(2)	-6(2)	-2(2)
C(72)	20(3)	29(3)	29(3)	-6(2)	-8(2)	-7(2)
C(73)	24(3)	58(4)	39(4)	-12(3)	-3(3)	-19(3)

2.14 Fe-complex 2g

Table 61: Crystal data and structure refinement for **2g**

Identification code	D19368_sq
Empirical formula	C20 H15 Cl F2 Fe N3 O1.50
Formula weight	450.65
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Tetragonal
Space group	P4/mnc
Unit cell dimensions	a = 21.6101(5) Å $\alpha = 90°$
	b = 21.6101(5) Å $\beta = 90°$
	c = 21.4008(7) Å $\gamma = 90°$
Volume	9994.1(6) $Å^3$
Z	16
Density (calculated)	1.198 $Mg\,m^{-3}$
Absorption coefficient	0.739 mm^{-1}
F(000)	3664
Crystal size	0.934 x 0.066 x 0.052 mm^3
Theta range for data collection	1.333 to 25.678°.
Index ranges	-26<=h<=26, -25<=k<=26, -26<=l<=24
Reflections collected	61383
Independent reflections	4899 [R(int) = 0.1025]
Completeness to theta = 25.242°	99,90%
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	4899 / 1422 / 503
Goodness-of-fit on F2	1.039
Final R indices [I>2sigma(I)]	R1 = 0.0897, wR2 = 0.2362
R indices (all data)	R1 = 0.1130, wR2 = 0.2535
Extinction coefficient	n/a
Largest diff. peak and hole	1.517 and -0.783 $e.Å^{-3}$

Table 62: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for complex **2g**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Fe(1)	2189(1)	2811(1)	2500	29(1)
F(1)	3013(5)	5537(3)	1711(4)	79(3)
F(2)	4845(4)	3646(4)	3464(5)	58(2)
N(1)	1791(5)	3345(5)	1909(5)	34(2)

Table 62 – continued from previous page

	x	y	z	U(eq)
N(2)	2795(8)	3454(8)	2537(11)	33(3)
N(3)	2650(5)	2445(5)	3168(5)	36(2)
C(1)	1283(6)	3231(7)	1583(5)	45(3)
C(2)	1025(6)	3665(6)	1166(6)	60(3)
C(3)	1308(6)	4213(6)	1091(6)	64(3)
C(4)	1855(6)	4356(5)	1434(5)	57(3)
C(5)	2181(6)	4925(5)	1376(5)	65(3)
C(6)	2688(6)	4998(5)	1746(5)	59(3)
C(7)	2931(6)	4548(5)	2150(5)	49(3)
C(8)	2642(6)	3981(5)	2206(6)	42(3)
C(9)	2083(5)	3903(5)	1843(5)	44(3)
C(11)	2516(4)	1953(4)	3521(4)	40(2)
C(12)	2913(5)	1734(5)	3971(5)	57(3)
C(13)	3477(5)	2020(5)	4070(5)	56(3)
C(14)	3635(5)	2529(4)	3718(5)	40(2)
C(15)	4201(5)	2845(5)	3786(5)	43(2)
C(16)	4302(5)	3332(6)	3409(5)	40(2)
C(17)	3889(5)	3562(6)	2955(6)	37(3)
C(18)	3316(5)	3269(6)	2878(6)	34(1)
C(19)	3204(5)	2737(5)	3255(5)	33(2)
F(1A)	3372(6)	5349(6)	1539(7)	81(4)
F(2A)	4870(6)	3871(7)	3268(7)	54(3)
N(1A)	1872(8)	3332(8)	1792(8)	40(4)
N(2A)	2826(13)	3408(13)	2467(18)	35(4)
N(3A)	2792(7)	2435(7)	3084(7)	33(3)
C(1A)	1375(9)	3263(9)	1432(8)	46(4)
C(2A)	1209(8)	3697(9)	966(8)	50(4)
C(3A)	1556(8)	4204(8)	887(7)	52(4)
C(4A)	2099(7)	4305(7)	1254(7)	50(3)
C(5A)	2497(7)	4823(7)	1199(7)	54(3)
C(6A)	2987(7)	4855(7)	1588(7)	57(4)
C(7A)	3147(8)	4415(7)	2040(8)	47(4)
C(8A)	2761(8)	3916(8)	2090(8)	39(3)
C(9A)	2228(8)	3850(8)	1698(7)	40(3)
C(11A)	2767(8)	1885(7)	3370(7)	50(4)
C(12A)	3264(8)	1678(7)	3708(8)	66(4)
C(13A)	3798(8)	2011(7)	3784(8)	61(4)
C(14A)	3850(7)	2573(6)	3505(7)	46(3)
C(15A)	4373(7)	2956(7)	3542(7)	41(3)
C(16A)	4360(7)	3500(8)	3237(8)	40(3)
C(17A)	3866(8)	3732(9)	2883(9)	35(3)
C(18A)	3343(8)	3358(8)	2854(9)	34(1)
C(19A)	3329(7)	2773(7)	3145(8)	37(3)

Table 62 – continued from previous page

	x	y	z	U(eq)
Fe(2)	4473(1)	779(1)	5165(1)	45(1)
Cl(1)	3443(1)	615(1)	4996(5)	37(1)
Cl(2)	4892(1)	1735(1)	5005(6)	43(1)
O(1)	4922(4)	3(7)	5478(3)	43(1)
O(2)	4571(4)	541(4)	3806(5)	43(1)
O(2A)	4310(20)	1030(20)	3800(20)	43(1)
O(1S)	1050(7)	2053(6)	663(6)	105(4)
C(1S)	688(12)	1597(13)	334(11)	125(6)
C(2S)	1051(13)	1502(13)	-227(9)	142(7)
C(3S)	1575(13)	1936(13)	-257(9)	139(7)
C(4S)	1512(12)	2372(11)	262(8)	118(6)

Table 63: Selected bond lengths [Å] and angles [°] for complex **2g**

Fe(1)-N(2A)	1.888(19)
Fe(1)-N(2A)#1	1.888(19)
Fe(1)-N(2)	1.911(12)
Fe(1)-N(2)#1	1.911(12)
Fe(1)-N(3)	1.913(10)
Fe(1)-N(3)#1	1.913(10)
Fe(1)-N(1)	1.916(11)
Fe(1)-N(1)#1	1.916(11)
Fe(1)-N(3A)	1.980(14)
Fe(1)-N(3A)#1	1.980(14)
Fe(1)-N(1A)	2.007(16)
Fe(1)-N(1A)#1	2.007(16)
N(2A)-Fe(1)-N(2A)#1	176(2)
N(2A)-Fe(1)-N(2)#1	175.5(19)
N(2A)#1-Fe(1)-N(2)#1	6(2)
N(2)-Fe(1)-N(2)#1	176.7(12)
N(2)-Fe(1)-N(3)	85.0(4)
N(2)#1-Fe(1)-N(3)	97.2(9)
N(2A)-Fe(1)-N(3)#1	91.5(16)
N(2A)#1-Fe(1)-N(3)#1	86.0(5)
N(2)-Fe(1)-N(3)#1	97.2(9)
N(2)#1-Fe(1)-N(3)#1	85.0(4)
N(3)-Fe(1)-N(3)#1	97.3(6)
N(2)-Fe(1)-N(1)	84.1(4)
N(2)#1-Fe(1)-N(1)	93.4(9)
N(3)-Fe(1)-N(1)	167.4(5)
N(3)#1-Fe(1)-N(1)	90.4(5)
N(2A)-Fe(1)-N(1)#1	99.1(16)

Table 63 – continued from previous page

N(2A)#1-Fe(1)-N(1)#1	83.8(5)
N(2)-Fe(1)-N(1)#1	93.4(9)
N(2)#1-Fe(1)-N(1)#1	84.1(4)
N(3)-Fe(1)-N(1)#1	90.4(5)
N(3)#1-Fe(1)-N(1)#1	167.4(5)
N(1)-Fe(1)-N(1)#1	83.9(7)
N(2A)-Fe(1)-N(3A)	79.9(6)
N(2A)#1-Fe(1)-N(3A)	97.2(16)
N(2A)-Fe(1)-N(3A)#1	97.2(16)
N(2A)#1-Fe(1)-N(3A)#1	79.9(6)
N(2)-Fe(1)-N(3A)#1	102.8(10)
N(2)#1-Fe(1)-N(3A)#1	79.7(5)
N(3)-Fe(1)-N(3A)#1	89.1(4)
N(3)#1-Fe(1)-N(3A)#1	10.3(6)
N(1)-Fe(1)-N(3A)#1	99.5(6)
N(1)#1-Fe(1)-N(3A)#1	163.6(5)
N(3A)-Fe(1)-N(3A)#1	81.8(10)
N(2A)-Fe(1)-N(1A)	80.7(6)
N(2A)#1-Fe(1)-N(1A)	101.7(16)
N(3A)-Fe(1)-N(1A)	158.6(7)
N(3A)#1-Fe(1)-N(1A)	91.9(7)
N(2A)-Fe(1)-N(1A)#1	101.7(16)
N(2A)#1-Fe(1)-N(1A)#1	80.7(6)
N(2)-Fe(1)-N(1A)#1	96.0(11)
N(2)#1-Fe(1)-N(1A)#1	81.8(6)
N(3)-Fe(1)-N(1A)#1	82.5(6)
N(3)#1-Fe(1)-N(1A)#1	166.7(6)
N(1)-Fe(1)-N(1A)#1	92.3(4)
N(1)#1-Fe(1)-N(1A)#1	8.6(8)
N(3A)-Fe(1)-N(1A)#1	91.9(7)
N(3A)#1-Fe(1)-N(1A)#1	158.6(7)
N(1A)-Fe(1)-N(1A)#1	100.8(11)

Table 64: Anisotropic displacement parameters ($Å^2 \times 10^3$) for complex **2g**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	30(1)	30(1)	25(1)	-3(1)	-3(1)	1(1)
F(1)	118(7)	42(4)	77(5)	18(4)	-18(5)	-28(4)
F(2)	40(3)	70(6)	64(5)	4(4)	-10(3)	-18(4)
N(1)	45(4)	40(4)	18(4)	-7(3)	-8(3)	0(3)
N(2)	40(4)	41(4)	19(6)	-1(4)	-7(4)	-3(4)
N(3)	37(4)	38(4)	33(4)	4(3)	-5(4)	2(3)

Table 64 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	48(5)	51(5)	35(6)	4(4)	-18(4)	-3(4)
C(2)	70(7)	63(5)	49(7)	9(5)	-32(6)	-3(5)
C(3)	81(7)	62(5)	50(7)	14(5)	-35(6)	-1(6)
C(4)	81(6)	50(4)	40(6)	7(4)	-24(5)	-6(5)
C(5)	91(7)	51(5)	52(6)	12(5)	-17(5)	-9(5)
C(6)	85(7)	37(4)	55(6)	10(4)	-15(5)	-13(5)
C(7)	62(7)	42(5)	45(6)	-1(4)	-12(5)	-11(4)
C(8)	57(5)	41(4)	30(5)	0(4)	-9(4)	-10(4)
C(9)	60(6)	43(4)	28(5)	2(4)	-17(4)	-6(4)
C(11)	39(5)	35(4)	47(5)	10(4)	-12(4)	0(4)
C(12)	59(6)	48(5)	64(6)	25(5)	-27(5)	-13(4)
C(13)	55(5)	50(5)	61(6)	23(4)	-26(5)	-10(4)
C(14)	37(4)	42(4)	41(5)	6(4)	-14(4)	-2(3)
C(15)	36(5)	54(5)	39(5)	6(4)	-13(4)	-3(4)
C(16)	35(4)	44(6)	41(5)	-3(4)	-10(4)	-8(4)
C(17)	38(4)	41(6)	33(5)	3(4)	0(4)	-6(4)
C(18)	35(2)	38(3)	29(2)	-7(2)	-6(2)	-2(2)
C(19)	33(4)	34(4)	33(4)	0(3)	-8(4)	6(3)
F(1A)	73(8)	66(7)	103(10)	41(7)	-34(7)	-31(6)
F(2A)	37(5)	63(8)	63(8)	-15(6)	-16(5)	-9(5)
N(1A)	48(6)	43(6)	29(7)	7(5)	-14(5)	-6(5)
N(2A)	40(6)	44(6)	21(7)	0(5)	-9(5)	-6(5)
N(3A)	39(6)	29(5)	32(6)	-7(4)	-13(5)	2(4)
C(1A)	58(7)	46(6)	33(8)	5(6)	-24(6)	-9(6)
C(2A)	60(8)	56(6)	35(8)	8(6)	-23(6)	-4(6)
C(3A)	67(8)	51(6)	37(7)	17(6)	-21(6)	-2(6)
C(4A)	64(7)	51(6)	34(6)	11(5)	-16(5)	-8(5)
C(5A)	65(7)	50(6)	46(7)	18(6)	-9(6)	-9(6)
C(6A)	64(7)	47(6)	61(7)	15(6)	-15(6)	-17(6)
C(7A)	57(8)	47(6)	38(7)	4(5)	-15(6)	-15(6)
C(8A)	52(6)	42(5)	23(6)	0(5)	-9(5)	-9(5)
C(9A)	54(6)	40(5)	25(6)	5(5)	-14(5)	-9(5)
C(11A)	64(7)	40(6)	47(7)	3(5)	-19(6)	-8(6)
C(12A)	72(7)	53(7)	72(8)	24(6)	-19(7)	-1(6)
C(13A)	65(7)	51(6)	68(8)	11(6)	-21(7)	3(6)
C(14A)	43(6)	45(5)	51(7)	4(5)	-17(5)	2(5)
C(15A)	36(6)	44(6)	43(7)	-4(6)	-17(6)	5(5)
C(16A)	35(5)	44(6)	40(7)	-7(5)	-8(5)	-1(5)
C(17A)	36(5)	32(7)	36(7)	-9(5)	-8(5)	1(5)
C(18A)	35(2)	38(3)	29(2)	-7(2)	-6(2)	-2(2)
C(19A)	36(6)	35(5)	41(6)	-9(5)	-15(5)	0(4)
Fe(2)	42(1)	49(1)	45(2)	-13(1)	2(1)	2(1)
Cl(1)	46(1)	33(1)	32(1)	7(5)	-20(4)	-3(1)

Table 64 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cl(2)	28(1)	55(1)	48(1)	21(3)	9(3)	8(1)
O(1)	28(1)	55(1)	48(1)	21(3)	9(3)	8(1)
O(2)	28(1)	55(1)	48(1)	21(3)	9(3)	8(1)
O(2A)	28(1)	55(1)	48(1)	21(3)	9(3)	8(1)
O(1S)	152(11)	98(8)	65(6)	7(6)	-6(7)	8(8)
C(1S)	148(15)	143(13)	84(9)	-29(10)	-4(9)	15(11)
C(2S)	162(16)	180(15)	83(11)	-48(11)	-2(9)	-4(14)
C(3S)	178(15)	162(16)	76(9)	-19(9)	4(10)	0(14)
C(4S)	171(13)	118(13)	64(8)	2(7)	-6(9)	2(11)

2.15 Cr-complex 3

Table 65: Crystal data and structure refinement for $Cr(BQA)_2$

Identification code	D19081
Empirical formula	C44 H40 Cr N6 O2
Formula weight	736.82
Temperature	100(2) K
Wavelength	1.54178 Å
Crystal system	Triclinic
Space group	P-1
Unit cell dimensions	a = 9.0724(5) Å α = 81.026(4)°
	b = 12.7579(7) Å β = 75.685(4)°
	c = 16.0711(9) Å γ = 79.295(4)°
Volume	1759.15(17) $Å^3$
Z	2
Density (calculated)	1.391 $Mg\,m^{-3}$
Absorption coefficient	3.061 mm^{-1}
F(000)	772
Crystal size	0.096 x 0.077 x 0.054 mm^3
Theta range for data collection	3.549 to 66.586°.
Index ranges	-10<=h<=10, -15<=k<=15, -19<=l<=19
Reflections collected	47080
Independent reflections	6152 [R(int) = 0.1039]
Completeness to theta = 66.586°	99.2 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	6152 / 2210 / 724
Goodness-of-fit on F2	1.034
Final R indices [I>2sigma(I)]	R1 = 0.0570, wR2 = 0.1444
R indices (all data)	R1 = 0.0714, wR2 = 0.1548
Extinction coefficient	n/a
Largest diff. peak and hole	0.691 and -0.544 $e.Å^{-3}$

Table 66: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Cr(1)	3523(1)	6099(1)	2548(1)	29(1)
N(1)	1599(15)	5510(11)	3297(15)	28(3)
N(2)	4434(13)	4594(13)	2800(20)	33(3)
N(3)	5707(15)	6224(14)	1980(20)	30(2)
C(1)	162(18)	6031(13)	3489(17)	34(3)

Table 66 – continued from previous page

	x	y	z	U(eq)
C(2)	-1078(17)	5521(14)	3991(15)	41(3)
C(3)	-796(18)	4448(13)	4258(15)	41(3)
C(4)	675(16)	3854(11)	4032(17)	37(2)
C(5)	1056(18)	2742(10)	4290(12)	45(3)
C(6)	2506(18)	2246(11)	4021(12)	43(3)
C(7)	3698(18)	2799(11)	3531(18)	39(3)
C(8)	3439(13)	3895(10)	3286(10)	32(1)
C(9)	1876(14)	4416(9)	3532(10)	32(1)
C(10)	6293(17)	7093(12)	1524(15)	36(3)
C(11)	7895(17)	7093(13)	1255(14)	42(3)
C(12)	8881(16)	6211(13)	1407(13)	40(3)
C(13)	8326(14)	5260(12)	1853(16)	32(2)
C(14)	9279(14)	4288(12)	2027(12)	37(3)
C(15)	8645(12)	3411(12)	2443(13)	36(3)
C(16)	7049(11)	3458(10)	2760(8)	32(2)
C(17)	6029(13)	4387(12)	2604(16)	32(2)
C(18)	6697(14)	5306(14)	2130(20)	30(2)
N(1A)	1514(19)	5608(13)	3150(18)	29(3)
N(2A)	4322(15)	4552(14)	2900(20)	29(3)
N(3A)	5818(18)	6090(17)	2060(30)	31(4)
C(1A)	150(20)	6226(17)	3340(20)	37(4)
C(2A)	-1170(20)	5826(17)	3848(18)	44(4)
C(3A)	-1030(18)	4770(17)	4192(17)	41(4)
C(4A)	390(20)	4100(14)	4040(20)	38(3)
C(5A)	640(20)	2993(14)	4352(13)	42(3)
C(6A)	2050(20)	2427(13)	4183(14)	48(4)
C(7A)	3340(20)	2864(13)	3680(19)	42(3)
C(8A)	3196(16)	3939(12)	3346(12)	32(1)
C(9A)	1686(17)	4560(11)	3524(12)	32(1)
C(10A)	6510(20)	6946(15)	1684(17)	33(3)
C(11A)	8130(20)	6836(15)	1394(17)	44(4)
C(12A)	8999(19)	5880(14)	1518(15)	40(3)
C(13A)	8339(17)	4970(14)	1940(20)	35(3)
C(14A)	9181(17)	3954(14)	2101(14)	35(3)
C(15A)	8403(16)	3132(14)	2507(15)	40(3)
C(16A)	6803(14)	3247(11)	2730(10)	32(2)
C(17A)	5886(15)	4239(13)	2610(20)	32(2)
C(18A)	6697(17)	5112(16)	2200(30)	31(3)
N(21)	3077(3)	5982(2)	1391(2)	34(1)
N(22)	2625(3)	7616(2)	2261(2)	36(1)
N(23)	3723(3)	6723(2)	3579(2)	31(1)
C(21)	3283(3)	5110(3)	992(2)	39(1)
C(22)	3009(4)	5156(3)	163(2)	47(1)

Table 66 – continued from previous page

	x	y	z	U(eq)
C(23)	2527(4)	6121(3)	-259(2)	50(1)
C(24)	2304(4)	7064(3)	137(2)	46(1)
C(25)	1827(5)	8098(4)	-253(2)	58(1)
C(26)	1656(5)	8964(4)	174(3)	62(1)
C(27)	1899(5)	8881(3)	1014(2)	54(1)
C(28)	2318(4)	7879(3)	1442(2)	41(1)
C(29)	2570(3)	6962(3)	981(2)	37(1)
C(30)	4443(4)	6256(2)	4203(2)	35(1)
C(31)	4429(4)	6769(3)	4914(2)	40(1)
C(32)	3606(4)	7771(3)	5008(2)	44(1)
C(33)	2831(4)	8303(2)	4357(2)	40(1)
C(34)	1920(5)	9332(3)	4400(2)	53(1)
C(35)	1244(5)	9781(3)	3734(3)	59(1)
C(36)	1437(5)	9271(3)	2994(2)	51(1)
C(37)	2318(4)	8260(2)	2912(2)	38(1)
C(38)	2955(3)	7758(2)	3635(2)	34(1)
O(41)	2876(13)	9555(7)	6556(6)	69(2)
C(41)	3043(16)	10644(9)	6196(6)	81(3)
C(42)	3523(16)	11076(11)	6908(7)	90(3)
C(43)	2362(10)	10601(6)	7638(5)	59(2)
C(44)	2319(12)	9517(9)	7400(8)	64(2)
O(41A)	3421(14)	9351(8)	6637(8)	71(3)
C(41A)	4083(16)	10273(7)	6254(7)	73(3)
C(42A)	2922(16)	11229(9)	6730(8)	77(3)
C(43A)	3380(20)	10579(9)	7555(8)	95(3)
C(44A)	2820(20)	9559(11)	7466(9)	85(4)
O(51)	2899(9)	11280(6)	428(4)	85(2)
C(51)	1885(15)	11953(16)	992(9)	76(3)
C(52)	2633(16)	12051(13)	1718(8)	87(3)
C(53)	4116(15)	11333(15)	1507(10)	119(4)
C(54)	4289(12)	11078(12)	636(9)	110(3)
O(51A)	1646(7)	11502(5)	1554(4)	67(2)
C(51A)	2683(16)	11770(14)	1953(8)	83(3)
C(52A)	4207(12)	11900(11)	1327(8)	81(3)
C(53A)	3822(12)	11880(13)	491(7)	98(3)
C(54A)	2115(14)	11938(16)	706(8)	74(3)

Table 67: Selected bond lengths [Å] and angles [°] for **3**

Cr(1)-N(2)	1.967(14)
Cr(1)-N(22)	1.986(3)
Cr(1)-N(3)	1.991(13)

Table 67 – continued from previous page

Cr(1)-N(1A)	2.003(15)
Cr(1)-N(23)	2.007(2)
Cr(1)-N(2A)	2.014(14)
Cr(1)-N(21)	2.030(3)
Cr(1)-N(3A)	2.034(15)
Cr(1)-N(1)	2.056(12)
N(2)-Cr(1)-N(22)	178.5(9)
N(2)-Cr(1)-N(3)	81.6(5)
N(22)-Cr(1)-N(3)	97.6(4)
N(22)-Cr(1)-N(1A)	95.5(4)
N(2)-Cr(1)-N(23)	100.8(10)
N(22)-Cr(1)-N(23)	80.44(10)
N(3)-Cr(1)-N(23)	90.5(13)
N(1A)-Cr(1)-N(23)	93.7(10)
N(22)-Cr(1)-N(2A)	176.6(6)
N(1A)-Cr(1)-N(2A)	81.3(5)
N(23)-Cr(1)-N(2A)	98.4(12)
N(2)-Cr(1)-N(21)	98.0(10)
N(22)-Cr(1)-N(21)	80.79(10)
N(3)-Cr(1)-N(21)	90.5(12)
N(1A)-Cr(1)-N(21)	89.6(9)
N(23)-Cr(1)-N(21)	161.17(10)
N(2A)-Cr(1)-N(21)	100.5(12)
N(22)-Cr(1)-N(3A)	103.2(5)
N(1A)-Cr(1)-N(3A)	161.3(6)
N(23)-Cr(1)-N(3A)	88.7(15)
N(2A)-Cr(1)-N(3A)	79.9(5)
N(21)-Cr(1)-N(3A)	94.1(15)
N(2)-Cr(1)-N(1)	80.6(4)
N(22)-Cr(1)-N(1)	100.3(3)
N(3)-Cr(1)-N(1)	161.7(5)
N(23)-Cr(1)-N(1)	88.7(8)
N(21)-Cr(1)-N(1)	96.1(8)

Table 68: Anisotropic displacement parameters ($Å^2 \times 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cr(1)	26(1)	32(1)	29(1)	-4(1)	-5(1)	-5(1)
N(1)	27(3)	41(4)	17(7)	-4(3)	-7(3)	-4(3)
N(2)	29(3)	42(5)	28(7)	-6(3)	-2(3)	-12(3)
N(3)	31(4)	31(5)	29(5)	-3(4)	-8(4)	-3(3)
C(1)	32(4)	40(5)	29(8)	-5(5)	-5(4)	-4(3)

Table 68 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(2)	29(4)	49(8)	40(8)	-6(6)	0(4)	-5(5)
C(3)	38(6)	44(6)	40(6)	-8(5)	2(5)	-14(4)
C(4)	35(5)	42(6)	36(4)	-7(5)	-7(4)	-11(4)
C(5)	42(7)	37(5)	49(5)	-1(5)	6(6)	-15(5)
C(6)	48(6)	32(4)	49(7)	-1(4)	-11(5)	-14(4)
C(7)	33(5)	39(4)	44(8)	-3(3)	-3(4)	-9(3)
C(8)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(9)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(10)	32(4)	33(5)	40(8)	1(4)	-7(4)	-7(4)
C(11)	32(5)	33(6)	55(7)	-1(4)	-1(4)	-6(4)
C(12)	28(4)	35(7)	55(5)	-4(6)	-2(4)	-11(5)
C(13)	32(3)	33(6)	33(5)	-8(6)	-9(3)	-4(3)
C(14)	30(4)	34(6)	47(5)	-9(5)	-9(3)	-4(4)
C(15)	32(4)	33(7)	47(6)	-3(5)	-15(4)	-2(3)
C(16)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(17)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(18)	28(4)	35(6)	27(5)	-4(6)	-7(4)	-8(3)
N(1A)	34(4)	38(4)	19(8)	-4(3)	-10(4)	-7(3)
N(2A)	34(4)	24(5)	25(7)	-2(4)	-7(4)	1(3)
N(3A)	28(4)	31(5)	35(9)	-5(5)	-6(5)	-5(4)
C(1A)	25(4)	48(7)	33(10)	-2(5)	1(4)	-6(4)
C(2A)	35(5)	56(8)	37(8)	-10(7)	2(5)	-9(5)
C(3A)	29(5)	55(10)	37(6)	0(9)	-2(4)	-12(5)
C(4A)	39(6)	46(7)	31(5)	-2(6)	-5(6)	-15(5)
C(5A)	43(7)	50(7)	37(6)	2(6)	-12(5)	-18(5)
C(6A)	49(9)	40(7)	52(8)	2(6)	-4(7)	-16(6)
C(7A)	47(8)	41(5)	44(10)	2(5)	-18(7)	-15(5)
C(8A)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(9A)	34(2)	37(2)	28(1)	-4(1)	-9(2)	-10(2)
C(10A)	32(5)	34(5)	34(8)	2(4)	-11(5)	-5(4)
C(11A)	31(6)	36(8)	63(9)	-4(7)	-5(6)	-8(5)
C(12A)	32(5)	32(8)	54(8)	-19(6)	-4(4)	1(5)
C(13A)	35(4)	33(7)	41(7)	-13(6)	-9(4)	-5(4)
C(14A)	32(5)	33(8)	46(7)	-13(6)	-18(4)	-2(4)
C(15A)	48(5)	36(7)	34(5)	-2(5)	-10(5)	1(4)
C(16A)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(17A)	37(2)	33(3)	30(1)	-8(3)	-13(2)	-6(2)
C(18A)	30(4)	30(5)	34(9)	-11(5)	-10(4)	2(3)
N(21)	27(1)	42(1)	32(1)	-6(1)	-3(1)	-6(1)
N(22)	39(1)	34(1)	35(1)	-2(1)	-8(1)	-2(1)
N(23)	31(1)	32(1)	29(1)	-2(1)	-4(1)	-8(1)
C(21)	30(2)	49(2)	38(2)	-12(1)	-3(1)	-6(1)
C(22)	36(2)	67(2)	42(2)	-19(2)	-3(2)	-10(2)

Table 68 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(23)	39(2)	81(2)	32(2)	-10(2)	-6(1)	-11(2)
C(24)	34(2)	67(2)	35(2)	-3(2)	-6(1)	-6(2)
C(25)	53(2)	80(3)	36(2)	8(2)	-15(2)	-3(2)
C(26)	67(3)	64(2)	46(2)	12(2)	-14(2)	5(2)
C(27)	61(2)	47(2)	46(2)	4(2)	-10(2)	4(2)
C(28)	38(2)	46(2)	34(2)	1(1)	-5(1)	-4(1)
C(29)	28(2)	50(2)	31(2)	1(1)	-4(1)	-5(1)
C(30)	35(2)	36(2)	34(2)	-1(1)	-6(1)	-10(1)
C(31)	48(2)	44(2)	32(2)	2(1)	-10(1)	-17(1)
C(32)	61(2)	44(2)	31(2)	-6(1)	-6(2)	-21(2)
C(33)	51(2)	35(2)	35(2)	-5(1)	-2(1)	-16(1)
C(34)	74(3)	36(2)	46(2)	-10(2)	-3(2)	-12(2)
C(35)	76(3)	34(2)	61(2)	-8(2)	-9(2)	1(2)
C(36)	66(2)	34(2)	48(2)	-2(2)	-13(2)	4(2)
C(37)	42(2)	33(2)	38(2)	-1(1)	-7(1)	-7(1)
C(38)	35(2)	31(2)	34(2)	-2(1)	-3(1)	-9(1)
O(41)	102(6)	66(4)	52(3)	-4(3)	-33(4)	-27(4)
C(41)	103(6)	90(5)	58(4)	-6(4)	-10(5)	-47(5)
C(42)	105(7)	95(6)	78(6)	-18(5)	5(5)	-61(5)
C(43)	45(4)	63(4)	70(4)	-25(3)	5(4)	-18(3)
C(44)	46(4)	60(4)	81(4)	-20(4)	3(4)	-12(4)
O(41A)	83(6)	44(4)	70(5)	-2(3)	12(5)	-13(4)
C(41A)	89(6)	48(5)	75(5)	-9(4)	8(5)	-29(4)
C(42A)	82(7)	55(5)	93(6)	13(5)	-26(5)	-16(5)
C(43A)	128(8)	70(5)	83(6)	-7(5)	-19(6)	-10(6)
C(44A)	114(9)	61(5)	71(5)	6(4)	-21(6)	-2(6)
O(51)	95(5)	64(4)	79(4)	-5(3)	-3(4)	8(4)
C(51)	69(5)	74(6)	77(6)	-6(6)	-14(5)	2(5)
C(52)	70(5)	98(7)	91(6)	-12(6)	-29(5)	2(5)
C(53)	71(6)	148(9)	128(7)	7(7)	-31(6)	-2(6)
C(54)	70(5)	101(7)	137(7)	-27(6)	13(5)	1(5)
O(51A)	65(4)	61(4)	70(4)	1(3)	-11(3)	-12(3)
C(51A)	72(5)	100(8)	80(6)	-2(6)	-17(4)	-24(5)
C(52A)	58(4)	82(6)	101(6)	-1(5)	-25(4)	-3(5)
C(53A)	73(5)	121(7)	81(5)	12(6)	-8(4)	-2(6)
C(54A)	67(5)	69(6)	79(6)	1(6)	-15(5)	-6(5)

2.16 oxidized Cr-complex $[Cr(BQA)_2]Cl$

The unit cell of $[Cr(BQA)_2]Cl$ was determined using 9988 reflections and the structure was solved in the triclinic space group $P\bar{1}$. The asymmetric unit contains one $[Cr(BQA)_2]$, the chloride anion and two dichloromethane molecules. One of the solvent molecules was

found to be disordered over three positions. The disorder was refined with the help of similarity restraints on 1,2- and 1,3 distances and ADP similarity restraints. The thermal displacement parameters of equivalent atoms of the disordered solvent molecule were set to the same parameters.[7, 8] The disorder ratio was allowed to refine and converged to 0.593(2), 0.337(2) and 0.071(2).

Table 69: Crystal data and structure refinement for $[Cr(BQA)_2]Cl$

Identification code	D19050
Empirical formula	C38 H28 Cl5 Cr N6
Formula weight	797.91
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 10.7738(4) Å α = 80.5576(14)°. b = 11.6879(5) Å β = 78.3853(14)°. c = 15.3294(6) Å γ = 68.2652(14)°.
Volume	1747.86(12) $Å^3$
Z	2
Density (calculated)	1.516 $Mg\,m^{-3}$
Absorption coefficient	0.749 mm^{-1}
F(000)	814
Crystal size	0.982 x 0.032 x 0.028 mm^3
Theta range for data collection	2.215 to 27.103°.
Index ranges	-13<=h<=13, -14<=k<=14, -19<=l<=19
Reflections collected	89998
Independent reflections	7699 [R(int) = 0.1164]
Completeness to theta = 25.242°	99.9 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	7699 / 157 / 478
Goodness-of-fit on F2	1.045
Final R indices [I>2sigma(I)]	R1 = 0.0543, wR2 = 0.1228
R indices (all data)	R1 = 0.0766, wR2 = 0.1323
Extinction coefficient	n/a
Largest diff. peak and hole	0.942 and -1.309 $e.Å^{-3}$

Table 70: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for $[Cr(BQA)_2]Cl$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Cr(1)	4635(1)	7507(1)	7468(1)	11(1)
N(1)	6637(2)	6448(2)	7278(2)	14(1)
N(2)	5425(2)	8789(2)	7464(2)	14(1)
N(3)	2899(2)	9010(2)	7651(2)	16(1)
N(21)	4601(2)	7630(2)	6126(2)	14(1)
N(22)	3761(2)	6277(2)	7475(2)	14(1)
N(23)	4379(3)	6968(2)	8808(2)	16(1)
C(1)	7180(3)	5244(3)	7196(2)	16(1)
C(2)	8569(3)	4633(3)	7001(2)	22(1)
C(3)	9412(3)	5300(3)	6867(2)	24(1)
C(4)	8883(3)	6589(3)	6936(2)	19(1)
C(5)	9671(3)	7360(3)	6761(2)	24(1)
C(6)	9034(3)	8610(3)	6794(2)	24(1)
C(7)	7626(3)	9156(3)	7029(2)	19(1)
C(8)	6811(3)	8438(3)	7236(2)	14(1)
C(9)	7466(3)	7136(3)	7155(2)	15(1)
C(10)	4523(3)	9949(3)	7664(2)	14(1)
C(11)	4768(3)	10984(3)	7813(2)	18(1)
C(12)	3693(3)	12095(3)	7990(2)	21(1)
C(13)	2376(3)	12212(3)	8037(2)	22(1)
C(14)	2063(3)	11180(3)	7924(2)	19(1)
C(15)	739(3)	11192(3)	7974(2)	26(1)
C(16)	524(3)	10144(3)	7867(2)	26(1)
C(17)	1635(3)	9058(3)	7717(2)	21(1)
C(18)	3134(3)	10058(3)	7745(2)	15(1)
C(21)	5097(3)	8315(3)	5475(2)	19(1)
C(22)	4992(3)	8331(3)	4575(2)	22(1)
C(23)	4360(3)	7622(3)	4355(2)	21(1)
C(24)	3853(3)	6853(3)	5028(2)	18(1)
C(25)	3279(3)	6025(3)	4846(2)	21(1)
C(26)	2968(3)	5218(3)	5523(2)	22(1)
C(27)	3137(3)	5219(3)	6415(2)	18(1)
C(28)	3589(3)	6078(3)	6645(2)	15(1)
C(29)	4007(3)	6873(3)	5920(2)	14(1)
C(30)	3201(3)	5881(3)	8309(2)	16(1)
C(31)	2305(3)	5243(3)	8535(2)	23(1)
C(32)	1836(4)	4935(3)	9437(2)	30(1)
C(33)	2221(4)	5263(3)	10129(2)	31(1)
C(34)	3096(3)	5957(3)	9938(2)	23(1)

Table 70 – continued from previous page

	x	y	z	U(eq)
C(35)	3506(4)	6402(3)	10594(2)	32(1)
C(36)	4337(4)	7075(3)	10355(2)	31(1)
C(37)	4763(3)	7345(3)	9447(2)	24(1)
C(38)	3569(3)	6261(3)	9033(2)	18(1)
Cl(41)	1542(1)	10044(1)	5440(1)	41(1)
Cl(42)	1192(1)	12615(1)	5515(1)	57(1)
C(41)	353(4)	11565(3)	5563(3)	33(1)
Cl(51)	869(3)	11889(3)	10629(2)	67(1)
Cl(52)	3701(2)	10448(2)	10131(1)	56(1)
C(51)	2120(9)	10339(10)	10520(8)	51(2)
Cl(53)	1451(3)	9502(3)	9963(2)	32(1)
Cl(54)	1595(5)	11692(5)	10614(4)	67(1)
C(51A)	2511(16)	10165(16)	10339(16)	51(2)
Cl(55)	166(18)	11637(17)	10149(13)	67(1)
Cl(56)	2755(19)	10723(17)	10593(12)	56(1)
C(51B)	1620(30)	10230(30)	10220(50)	51(2)
Cl(1)	-2585(1)	12180(1)	7434(1)	19(1)

Table 71: Selected bond lengths [Å] and angles [°] for $[Cr(BQA)_2]Cl$

Cr(1)-N(2)	1.978(2)
Cr(1)-N(22)	1.986(2)
Cr(1)-N(1)	2.039(2)
Cr(1)-N(23)	2.042(2)
Cr(1)-N(3)	2.045(2)
Cr(1)-N(21)	2.045(2)
N(2)-Cr(1)-N(22)	177.44(10)
N(2)-Cr(1)-N(1)	80.51(10)
N(22)-Cr(1)-N(1)	102.04(10)
N(2)-Cr(1)-N(23)	99.77(10)
N(22)-Cr(1)-N(23)	80.39(10)
N(1)-Cr(1)-N(23)	93.73(10)
N(2)-Cr(1)-N(3)	80.42(10)
N(22)-Cr(1)-N(3)	97.03(10)
N(1)-Cr(1)-N(3)	160.92(10)
N(23)-Cr(1)-N(3)	89.76(10)
N(2)-Cr(1)-N(21)	99.04(10)
N(22)-Cr(1)-N(21)	80.78(10)
N(1)-Cr(1)-N(21)	90.08(9)
N(23)-Cr(1)-N(21)	161.17(10)
N(3)-Cr(1)-N(21)	92.64(10)

Table 72: Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Cr(BQA)_2]Cl$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2 U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Cr(1)	16(1)	10(1)	10(1)	-1(1)	-3(1)	-6(1)
N(1)	19(1)	13(1)	11(1)	-1(1)	-3(1)	-7(1)
N(2)	19(1)	11(1)	14(1)	-1(1)	-4(1)	-6(1)
N(3)	19(1)	12(1)	15(1)	-1(1)	-2(1)	-5(1)
N(21)	17(1)	14(1)	12(1)	-2(1)	-2(1)	-6(1)
N(22)	19(1)	15(1)	12(1)	-1(1)	-1(1)	-8(1)
N(23)	21(1)	13(1)	14(1)	-1(1)	-4(1)	-6(1)
C(1)	24(2)	14(1)	13(1)	1(1)	-4(1)	-10(1)
C(2)	23(2)	13(2)	26(2)	-3(1)	-5(1)	-3(1)
C(3)	20(2)	19(2)	31(2)	-2(1)	-5(1)	-4(1)
C(4)	20(2)	17(2)	21(2)	-2(1)	-6(1)	-6(1)
C(5)	16(2)	23(2)	34(2)	-7(1)	-1(1)	-9(1)
C(6)	21(2)	25(2)	31(2)	-6(1)	-2(1)	-14(1)
C(7)	24(2)	13(1)	22(2)	-4(1)	-4(1)	-7(1)
C(8)	20(2)	14(1)	10(1)	-2(1)	-5(1)	-6(1)
C(9)	19(2)	15(1)	13(1)	-1(1)	-4(1)	-7(1)
C(10)	21(2)	13(1)	7(1)	-1(1)	-2(1)	-6(1)
C(11)	24(2)	16(2)	16(1)	0(1)	-6(1)	-8(1)
C(12)	31(2)	14(2)	21(2)	-2(1)	-6(1)	-11(1)
C(13)	25(2)	13(2)	27(2)	-4(1)	-4(1)	-3(1)
C(14)	24(2)	14(2)	16(1)	-2(1)	-3(1)	-5(1)
C(15)	21(2)	21(2)	30(2)	-3(1)	-2(1)	-2(1)
C(16)	17(2)	28(2)	35(2)	-4(2)	-4(1)	-8(1)
C(17)	21(2)	17(2)	25(2)	-3(1)	-3(1)	-6(1)
C(18)	21(2)	12(1)	11(1)	1(1)	-4(1)	-5(1)
C(21)	23(2)	18(2)	17(2)	1(1)	-3(1)	-9(1)
C(22)	28(2)	22(2)	12(1)	3(1)	-2(1)	-8(1)
C(23)	24(2)	22(2)	13(1)	-2(1)	-4(1)	-2(1)
C(24)	17(2)	16(2)	17(1)	-4(1)	-4(1)	-1(1)
C(25)	20(2)	24(2)	18(2)	-8(1)	-6(1)	-4(1)
C(26)	21(2)	22(2)	27(2)	-12(1)	-4(1)	-8(1)
C(27)	19(2)	17(2)	20(2)	-4(1)	-2(1)	-6(1)
C(28)	15(1)	13(1)	16(1)	-5(1)	-1(1)	-4(1)
C(29)	14(1)	14(1)	13(1)	-2(1)	-2(1)	-3(1)
C(30)	18(1)	12(1)	16(1)	-3(1)	1(1)	-4(1)
C(31)	26(2)	19(2)	25(2)	-7(1)	3(1)	-11(1)
C(32)	34(2)	25(2)	31(2)	-4(1)	10(2)	-19(2)
C(33)	45(2)	26(2)	19(2)	1(1)	7(2)	-17(2)
C(34)	33(2)	16(2)	16(2)	0(1)	1(1)	-6(1)
C(35)	54(2)	25(2)	13(2)	1(1)	-2(2)	-12(2)

Table 72 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(36)	52(2)	30(2)	16(2)	-2(1)	-12(2)	-16(2)
C(37)	33(2)	23(2)	18(2)	-2(1)	-8(1)	-11(1)
C(38)	22(2)	12(1)	16(1)	-1(1)	-1(1)	-4(1)
Cl(41)	32(1)	42(1)	35(1)	-2(1)	-1(1)	1(1)
Cl(42)	62(1)	69(1)	52(1)	-29(1)	18(1)	-42(1)
C(41)	28(2)	38(2)	33(2)	-8(2)	0(2)	-11(2)
Cl(51)	67(2)	54(1)	62(1)	4(1)	19(2)	-20(2)
Cl(52)	71(1)	52(1)	48(1)	2(1)	-7(1)	-30(1)
C(51)	56(5)	56(4)	48(5)	0(3)	-1(4)	-33(4)
Cl(53)	36(1)	42(2)	14(1)	2(1)	-4(1)	-8(1)
Cl(54)	67(2)	54(1)	62(1)	4(1)	19(2)	-20(2)
C(51A)	56(5)	56(4)	48(5)	0(3)	-1(4)	-33(4)
Cl(55)	67(2)	54(1)	62(1)	4(1)	19(2)	-20(2)
Cl(56)	71(1)	52(1)	48(1)	2(1)	-7(1)	-30(1)
C(51B)	56(5)	56(4)	48(5)	0(3)	-1(4)	-33(4)
Cl(1)	21(1)	17(1)	21(1)	-4(1)	-5(1)	-9(1)

2.17 Mn-complex 4

The unit cell of **4** was determined using 9975 reflections and the structure was solved in the hexagonal space group $P6_5$. The asymmetric unit contains one molecule of **4** as well as heavily disordered solvent molecules. SQUEEZE as implemented in Platon was used to include a model for the disordered solvent in the refinement. One independent void at 0.0 0.0 0.0 with a volume of 1156 $Å^3$ was found in the unit cell. The equivalent of 278 electrons were found in the void which corresponds to 6 to 7 molecules of the used solvents (THF and n-hexane). The obtained model was added as .fab-file to the refinement using SHELXL.

Table 73: Crystal data and structure refinement for **4**

Identification code	D18079_sq
Empirical formula	C36 H24 Mn N6
Formula weight	595.55
Temperature	100(2) K
Wavelength	0.71073 Å
Crystal system	Hexagonal
Space group	$P6_5$
Unit cell dimensions	a = 20.5446(5) Å $\alpha = 90°$.
	b = 20.5446(5) Å $\beta = 90°$.
	c = 13.8346(4) Å $\gamma = 120°$.
Volume	5057.0(3) $Å^3$
Z	6
Density (calculated)	1.173 $Mg\,m^{-3}$
Absorption coefficient	0.423 mm^{-1}
F(000)	1842
Crystal size	0.420 x 0.038 x 0.034 mm^3
Theta range for data collection	2.289 to 29.127°.
Index ranges	-28<=h<=28, -28<=k<=28, -18<=l<=18
Reflections collected	396141
Independent reflections	9056 [R(int) = 0.1489]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Refinement method	Full-matrix least-squares on F2
Data / restraints / parameters	9056 / 1 / 388
Goodness-of-fit on F2	1.029
Final R indices [I>2sigma(I)]	R1 = 0.0330, wR2 = 0.0638
R indices (all data)	R1 = 0.0414, wR2 = 0.0665
Absolute structure parameter	0.012(5)
Extinction coefficient	n/a
Largest diff. peak and hole	0.198 and -0.250 $e.Å^{-3}$

Table 74: Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor

	x	y	z	U(eq)
Mn(1)	5082(1)	739(1)	783(1)	17(1)
N(1)	5903(1)	391(1)	314(1)	21(1)
N(2)	5903(1)	1076(1)	1948(1)	19(1)
N(3)	4740(1)	1308(1)	1885(1)	19(1)
N(21)	5568(1)	1722(1)	-250(1)	17(1)
N(22)	4241(1)	481(1)	-323(1)	18(1)
N(23)	4101(1)	-381(1)	1195(1)	20(1)

Table 74 – continued from previous page

	x	y	z	U(eq)
C(1)	5880(1)	57(1)	-515(2)	29(1)
C(2)	6451(1)	-83(1)	-811(2)	36(1)
C(3)	7052(2)	127(1)	-220(2)	35(1)
C(4)	7111(1)	495(1)	659(2)	27(1)
C(5)	6512(1)	622(1)	908(2)	21(1)
C(6)	6528(1)	1013(1)	1782(2)	20(1)
C(7)	7194(1)	1309(1)	2326(2)	26(1)
C(8)	7783(1)	1180(2)	2064(2)	31(1)
C(9)	7747(2)	773(2)	1270(2)	33(1)
C(10)	5746(1)	1321(1)	2790(2)	17(1)
C(11)	6064(1)	1401(1)	3710(2)	21(1)
C(12)	5843(1)	1673(1)	4501(2)	23(1)
C(13)	5308(1)	1886(1)	4419(2)	24(1)
C(14)	4943(1)	1784(1)	3528(2)	20(1)
C(15)	5135(1)	1478(1)	2733(2)	18(1)
C(16)	4360(1)	1957(1)	3384(2)	26(1)
C(17)	3983(1)	1793(1)	2530(2)	27(1)
C(18)	4179(1)	1444(1)	1796(2)	25(1)
C(21)	6223(1)	2346(1)	-158(2)	21(1)
C(22)	6531(1)	2899(1)	-882(2)	23(1)
C(23)	6148(1)	2775(1)	-1729(2)	23(1)
C(24)	5453(1)	2106(1)	-1871(2)	20(1)
C(25)	5174(1)	1596(1)	-1084(2)	17(1)
C(26)	5055(1)	1924(1)	-2747(2)	25(1)
C(27)	4407(1)	1244(1)	-2836(2)	25(1)
C(28)	4108(1)	739(1)	-2060(2)	22(1)
C(29)	4454(1)	902(1)	-1148(2)	18(1)
C(30)	3529(1)	-113(1)	-154(2)	20(1)
C(31)	2863(1)	-286(1)	-619(2)	29(1)
C(32)	2179(1)	-937(2)	-372(2)	37(1)
C(33)	2132(2)	-1421(2)	334(2)	39(1)
C(34)	2775(1)	-1248(1)	876(2)	29(1)
C(35)	3470(1)	-585(1)	655(2)	22(1)
C(36)	2775(2)	-1684(1)	1655(2)	35(1)
C(37)	3408(2)	-1464(1)	2197(2)	37(1)
C(38)	4065(2)	-800(1)	1941(2)	28(1)

Table 75: Selected bond lengths [Å] and angles [°] for **4**

Mn(1)-N(22)	2.1663(19)
Mn(1)-N(2)	2.1806(19)
Mn(1)-N(1)	2.2321(19)

Table 75 – continued from previous page

Mn(1)-N(3)	2.2366(19)
Mn(1)-N(23)	2.2454(18)
Mn(1)-N(21)	2.2589(18)
N(22)-Mn(1)-N(2)	174.66(7)
N(22)-Mn(1)-N(1)	110.72(7)
N(2)-Mn(1)-N(1)	74.24(7)
N(22)-Mn(1)-N(3)	100.89(7)
N(2)-Mn(1)-N(3)	74.08(7)
N(1)-Mn(1)-N(3)	148.27(7)
N(22)-Mn(1)-N(23)	74.38(7)
N(2)-Mn(1)-N(23)	107.06(7)
N(1)-Mn(1)-N(23)	100.40(7)
N(3)-Mn(1)-N(23)	90.41(7)
N(22)-Mn(1)-N(21)	73.39(7)
N(2)-Mn(1)-N(21)	104.93(7)
N(1)-Mn(1)-N(21)	91.98(7)
N(3)-Mn(1)-N(21)	94.49(6)
N(23)-Mn(1)-N(21)	147.75(7)

Table 76: Anisotropic displacement parameters ($Å^2 \times 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a*^2U_{11} + ... + 2hka*b*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Mn(1)	21(1)	17(1)	13(1)	0(1)	-1(1)	9(1)
N(1)	24(1)	15(1)	22(1)	0(1)	2(1)	7(1)
N(2)	21(1)	20(1)	14(1)	2(1)	0(1)	10(1)
N(3)	25(1)	18(1)	16(1)	2(1)	0(1)	12(1)
N(21)	22(1)	16(1)	14(1)	-3(1)	-1(1)	9(1)
N(22)	20(1)	17(1)	15(1)	0(1)	0(1)	7(1)
N(23)	26(1)	17(1)	17(1)	1(1)	4(1)	11(1)
C(1)	28(1)	20(1)	31(1)	-7(1)	4(1)	6(1)
C(2)	32(1)	25(1)	42(2)	-13(1)	9(1)	8(1)
C(3)	31(1)	22(1)	50(2)	-4(1)	13(1)	13(1)
C(4)	29(1)	20(1)	32(1)	6(1)	6(1)	13(1)
C(5)	23(1)	14(1)	24(1)	4(1)	2(1)	8(1)
C(6)	21(1)	16(1)	21(1)	6(1)	3(1)	8(1)
C(7)	24(1)	28(1)	23(1)	5(1)	2(1)	11(1)
C(8)	20(1)	38(1)	33(1)	8(1)	0(1)	14(1)
C(9)	28(1)	36(1)	42(2)	10(1)	8(1)	20(1)
C(10)	21(1)	11(1)	16(1)	2(1)	-1(1)	5(1)
C(11)	24(1)	20(1)	16(1)	2(1)	-2(1)	9(1)
C(12)	29(1)	22(1)	13(1)	0(1)	-2(1)	8(1)
C(13)	29(1)	20(1)	19(1)	-1(1)	3(1)	10(1)

Table 76 – continued from previous page

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(14)	26(1)	15(1)	16(1)	3(1)	4(1)	9(1)
C(15)	26(1)	13(1)	14(1)	3(1)	1(1)	7(1)
C(16)	37(1)	24(1)	22(1)	-1(1)	4(1)	19(1)
C(17)	38(1)	30(1)	24(1)	1(1)	0(1)	24(1)
C(18)	34(1)	28(1)	20(1)	2(1)	-3(1)	19(1)
C(21)	21(1)	19(1)	19(1)	-2(1)	-2(1)	9(1)
C(22)	21(1)	16(1)	28(1)	1(1)	2(1)	6(1)
C(23)	28(1)	18(1)	25(1)	6(1)	6(1)	13(1)
C(24)	26(1)	16(1)	18(1)	3(1)	4(1)	12(1)
C(25)	22(1)	16(1)	15(1)	-1(1)	1(1)	11(1)
C(26)	35(1)	25(1)	16(1)	6(1)	2(1)	16(1)
C(27)	33(1)	29(1)	15(1)	-2(1)	-4(1)	16(1)
C(28)	26(1)	20(1)	18(1)	-4(1)	-4(1)	10(1)
C(29)	22(1)	15(1)	18(1)	-2(1)	0(1)	10(1)
C(30)	22(1)	17(1)	19(1)	-3(1)	2(1)	8(1)
C(31)	25(1)	32(1)	24(1)	0(1)	0(1)	10(1)
C(32)	20(1)	43(2)	32(1)	-6(1)	-3(1)	3(1)
C(33)	25(1)	30(1)	40(2)	-3(1)	7(1)	-2(1)
C(34)	32(1)	20(1)	27(1)	-1(1)	10(1)	6(1)
C(35)	23(1)	18(1)	22(1)	-1(1)	7(1)	9(1)
C(36)	41(2)	23(1)	37(2)	8(1)	19(1)	13(1)
C(37)	48(2)	31(1)	37(2)	17(1)	20(1)	25(1)
C(38)	36(1)	30(1)	24(1)	9(1)	10(1)	22(1)

3 DFT calculations

Table 77: Absolute energies (a.u.) computed with method/Def2TZVP

Molecule	Multiplicity	Method	Absolute energy
1a	1	PBEPBE	-3492.5578851
2a	1	PBEPBE	-2976.9923581
2a	3	PBEPBE	-2976.9532000
2a	5	PBEPBE	-2976.9038425
2a	1	BLYP	-2978.7464030
2a	1	OLYP	-2978.9492766
3	1	PBEPBE	Does not converge
3	3	PBEPBE	-2757.7576040
3	5	PBEPBE	-2757.7346991
$[Cr(BQA)_2]^+$	2	PBEPBE	-2757.5661227
$[Cr(BQA)_2]^+$	4	PBEPBE	-2757.5883125
4	2	PBEPBE	-2864.2641805
4	4	PBEPBE	-2864.2397968
4	6	PBEPBE	-2864.2369049

Table 78: Average metal to nitrogen bonding length of the complexes as determined by XRD and computed at PBEPBE/Def2TZVP

	Av. Len. M—N_{amide} / Å		Av. Len. M–$N_{quinolinyl}$ / Å	
Molecule	XRD	Calc.	XRD	Calc.
1a[a]	2.07	2.10	2.18	2.22
2a[a]	1.93	1.95	1.94	1.95
3[b]	1.98	2.01	2.04	2.03
4[c]	2.17	2.18	2.24	2.26

[a] Multiplicity for the calculation was set to 1
[b] Multiplicity for the calculation was set to 3
[c] Multiplicity for the calculation was set to 6

Table 79: XYZ-coordinates of optimized specie for **1a**, PBEPBE/ Def2TZVP, multiplicity = 1

a.n.	x	y	z
7	2.101049	-0.000064	-0.000211
6	2.705588	-1.039497	-0.645106
6	2.705890	1.039269	0.644558
6	4.045176	1.464745	0.552761
6	4.527845	2.570755	1.275867

Table 79 – continued from previous page

a.n.	x	y	z
6	3.721353	3.304709	2.125419
6	2.350091	2.96541	2.226889
6	1.833814	1.859486	1.475761
7	0.511110	1.550091	1.498774
6	-0.326269	2.249335	2.253754
6	0.098371	3.324532	3.058425
6	1.430749	3.681278	3.034047
6	1.833219	-1.859542	-1.476169
6	4.044811	-1.465216	-0.553539
6	4.527157	-2.571305	-1.276741
6	3.720386	-3.305100	-2.126165
6	2.349168	-2.965551	-2.227396
6	1.429559	-3.681243	-3.034406
1	4.727871	-0.955542	0.121695
1	5.577887	-2.847210	-1.160104
1	4.728030	0.954938	-0.122581
1	5.578605	2.846467	1.159047
1	4.114394	4.144713	2.700574
1	-0.624759	3.864366	3.670738
1	1.794883	4.523981	3.627118
1	-1.377911	1.952751	2.212673
1	4.113176	-4.145170	-2.701396
6	0.097242	-3.324255	-3.058551
7	0.510569	-1.549904	-1.498952
6	-0.327064	-2.248988	-2.253795
1	-1.378646	-1.952217	-2.212526
1	1.793439	-4.524007	-3.627549
1	-0.626092	-3.863951	-3.670745
30	0.000000	0.000139	0.000003
1	-1.793602	-4.523941	3.627555
1	0.625948	-3.863956	3.67077
6	-1.429692	-3.681189	3.034413
6	-0.097365	-3.32424	3.058569
1	-4.113320	-4.145039	2.701383
6	-3.720501	-3.304981	2.126153
6	-2.349274	-2.965472	2.227395
6	0.326979	-2.248987	2.253814
6	-4.527243	-2.571165	1.276721
1	1.378570	-1.952247	2.212552
6	-1.833287	-1.859480	1.476169
1	-5.57798	-2.847039	1.160076
7	-0.510628	-1.549880	1.498962
6	-4.044859	-1.465091	0.553521

Table 79 – continued from previous page

a.n.	x	y	z
6	-2.705625	-1.039410	0.645098
1	-4.728001	0.955093	0.122565
7	-2.101049	0.000004	0.000206
1	-4.727899	-0.955400	-0.121721
6	-4.045127	1.464877	-0.552774
6	-2.705854	1.039358	-0.644565
6	-4.527756	2.570904	-1.275881
1	-5.578508	2.846650	-1.159066
6	-1.833747	1.859549	-1.475761
7	-0.511053	1.550112	-1.498766
6	-3.721236	3.304833	-2.125429
6	-2.349984	2.965490	-2.22689
6	0.326353	2.249330	-2.253741
1	-4.114247	4.144850	-2.700584
6	-1.430615	3.681329	-3.034043
1	1.377986	1.952713	-2.212654
6	-0.098248	3.324541	-3.058413
1	-1.794719	4.524045	-3.627116
1	0.624903	3.864352	-3.670721

Table 80: XYZ-coordinates of optimized specie for **2a**, PBEPBE/ Def2TZVP, multiplicity = 1

a.n.	x	y	z
7	-1.945946	-0.000217	0.000810
6	-2.534341	0.945365	-0.799694
6	-2.533304	-0.946121	0.801698
6	-3.885824	-1.305960	0.955721
6	-4.261811	-2.320030	1.854750
6	-3.340172	-3.006588	2.626705
6	-1.962048	-2.706881	2.493292
6	-1.569432	-1.691252	1.571482
7	-0.250504	-1.370669	1.361636
6	0.694268	-2.010967	2.061046
6	0.384723	-3.009631	3.000470
6	-0.931708	-3.362708	3.215948
6	-1.571345	1.690952	-1.570143
6	-3.887137	1.304558	-0.952812
6	-4.264186	2.318518	-1.851524
6	-3.343381	3.005614	-2.623997
6	-1.965023	2.706560	-2.491520
6	-0.935446	3.363061	-3.214648
1	-4.662520	0.830314	-0.360108

Table 80 – continued from previous page

a.n.	x	y	z
1	-5.325095	2.563942	-1.936927
1	-4.661815	-0.832098	0.363508
1	-5.322545	-2.565959	1.940859
1	-3.655293	-3.782049	3.326634
1	1.197287	-3.496131	3.541151
1	-1.195369	-4.143447	3.932560
1	1.724134	-1.719339	1.858080
1	-3.659337	3.781027	-3.323603
6	0.381298	3.010627	-3.000004
7	-0.252145	1.370886	-1.361262
6	0.691905	2.011864	-2.061040
1	1.722027	1.720616	-1.858816
1	-1.199923	4.143827	-3.930929
1	1.193293	3.497696	-3.541027
26	0.000001	0.000113	-0.000018
1	1.199286	4.143954	3.930977
1	-1.193833	3.497475	3.541063
6	0.934926	3.363151	3.214692
6	-0.381765	3.010526	3.000042
1	3.658747	3.781533	3.323650
6	3.342913	3.006076	2.624038
6	1.964603	2.706807	2.491562
6	-0.692221	2.011720	2.061073
6	4.263823	2.319136	1.851551
1	-1.722300	1.720321	1.858847
6	1.571076	1.691144	1.570180
1	5.324692	2.564732	1.936945
7	0.251924	1.370880	1.361301
6	3.886926	1.305127	0.952831
6	2.534187	0.945718	0.799720
1	4.661928	-0.831551	-0.363339
7	1.945946	0.000054	-0.000799
1	4.662374	0.831020	0.360103
6	3.886019	-1.305480	-0.955608
6	2.533454	-0.945775	-0.801665
6	4.262157	-2.319503	-1.854627
1	5.322920	-2.565331	-1.940675
6	1.569702	-1.691001	-1.571508
7	0.250732	-1.370554	-1.361724
6	3.340632	-3.006137	-2.626651
6	1.962470	-2.706571	-2.493318
6	-0.693939	-2.010916	-2.061215
1	3.655875	-3.781555	-3.326575

Table 80 – continued from previous page

a.n.	x	y	z
6	0.932235	-3.362475	-3.216054
1	-1.723844	-1.719392	-1.858298
6	-0.384241	-3.009521	-3.000651
1	1.196010	-4.143173	-3.932669
1	-1.196726	-3.496081	-3.541398

Table 81: XYZ-coordinates of optimized specie for **2a**, PBEPBE/ Def2TZVP, multiplicity = 3

a.n.	x	y	z
7	-1.914733	0.000084	-0.000005
6	-2.507687	1.033923	-0.690253
6	-2.507785	-1.033700	0.690244
6	-3.854679	-1.446337	0.716532
6	-4.246369	-2.531891	1.516220
6	-3.343702	-3.237308	2.300351
6	-1.969818	-2.887539	2.279420
6	-1.563703	-1.795428	1.457326
7	-0.250586	-1.418648	1.344452
6	0.684920	-2.072802	2.051436
6	0.361781	-3.142679	2.896027
6	-0.956197	-3.557302	3.011855
6	-1.563535	1.795560	-1.457338
6	-3.854543	1.446685	-0.716541
6	-4.246136	2.532263	-1.516243
6	-3.343405	3.237588	-2.300383
6	-1.969552	2.887700	-2.279442
6	-0.955868	3.557373	-3.011874
1	-4.598020	0.956327	-0.093924
1	-5.297702	2.826773	-1.513666
1	-4.598115	-0.955900	0.093928
1	-5.297961	-2.826307	1.513638
1	-3.673095	-4.071404	2.922080
1	1.160490	-3.639656	3.447291
1	-1.225938	-4.396876	3.655561
1	1.712070	-1.731867	1.927555
1	-3.672723	4.071704	-2.922125
6	0.362074	3.142639	-2.896034
7	-0.250450	1.418669	-1.344452
6	0.685116	2.072740	-2.051434
1	1.712235	1.731714	-1.927546
1	-1.225533	4.396965	-3.655586
1	1.160829	3.639547	-3.447293

Table 81 – continued from previous page

a.n.	x	y	z
26	-0.000156	-0.000001	-0.000001
1	1.225838	4.396861	3.655501
1	-1.160640	3.639948	3.446701
6	0.956089	3.557395	3.011653
6	-0.361863	3.142963	2.895543
1	3.673055	4.071151	2.922622
6	3.343706	3.237178	2.300710
6	1.969795	2.887587	2.279351
6	-0.684971	2.073220	2.050685
6	4.246433	2.531622	1.516818
1	-1.712165	1.732551	1.926477
6	1.563734	1.795619	1.457061
1	5.298089	2.825817	1.514541
7	0.250568	1.419123	1.343791
6	3.854810	1.446107	0.717009
6	2.507883	1.033644	0.690232
1	4.598351	-0.955923	-0.094707
7	1.914921	-0.000082	0.000007
1	4.598437	0.955525	0.094752
6	3.854691	-1.446434	-0.716980
6	2.507798	-1.033859	-0.690212
6	4.246231	-2.531971	-1.516800
1	5.297864	-2.826251	-1.514521
6	1.563589	-1.795751	-1.457051
7	0.250452	-1.419152	-1.343782
6	3.343451	-3.237446	-2.300703
6	1.969567	-2.887748	-2.279343
6	-0.685136	-2.073177	-2.050676
1	3.672736	-4.071439	-2.922623
6	0.955809	-3.557478	-3.011645
1	-1.712303	-1.732424	-1.926469
6	-0.362111	-3.142945	-2.895533
1	1.225493	-4.396963	-3.655494
1	-1.160927	-3.639871	-3.446688

Table 82: XYZ-coordinates of optimized specie for **2a**, PBEPBE/ Def2TZVP, multiplicity = 5

a.n.	x	y	z
7	1.903933	0.000014	0.000070
6	2.504712	0.995653	0.745172
6	2.504797	-0.995595	-0.745006
6	3.861376	-1.403789	-0.764221

Table 82 – continued from previous page

a.n.	x	y	z
6	4.263037	-2.442308	-1.609119
6	3.362863	-3.108099	-2.439671
6	1.982238	-2.778329	-2.409015
6	1.567062	-1.732700	-1.532418
7	0.252556	-1.388035	-1.383943
6	-0.685985	-2.023715	-2.120428
6	-0.353672	-3.032375	-3.021581
6	0.977180	-3.423719	-3.170326
6	1.566900	1.732723	1.532528
6	3.861272	1.403904	0.764464
6	4.262842	2.442440	1.609386
6	3.362593	3.108190	2.439890
6	1.981985	2.778362	2.409155
6	0.976858	3.423703	3.170418
1	4.589126	0.950514	0.097788
1	5.312913	2.740957	1.609301
1	4.589173	-0.950369	-0.097503
1	5.313121	-2.740781	-1.608976
1	3.701922	-3.911135	-3.096396
1	-1.148300	-3.508985	-3.595953
1	1.253488	-4.223250	-3.859803
1	-1.717206	-1.708706	-1.968065
1	3.701583	3.911238	3.096637
6	-0.353968	3.032298	3.021602
7	0.252416	1.388006	1.383973
6	-0.686190	2.023635	2.120419
1	-1.717389	1.708584	1.968000
1	1.253095	4.223239	3.859917
1	-1.148648	3.508866	3.595939
26	0.000007	-0.000013	-0.000001
1	-1.253155	4.223297	-3.859830
1	1.148615	3.509031	-3.595795
6	-0.976903	3.423745	-3.170357
6	0.353937	3.032399	-3.021509
1	-3.701653	3.911148	-3.096651
6	-3.362649	3.108096	-2.439917
6	-1.982025	2.778326	-2.409155
6	0.686174	2.023691	-2.120380
6	-4.262895	2.442275	-1.609465
1	1.717379	1.708658	-1.967966
6	-1.566920	1.732674	-1.532554
1	-5.312984	2.740731	-1.609416
7	-0.252430	1.387969	-1.384011

Table 82 – continued from previous page

a.n.	x	y	z
6	-3.861300	1.403745	-0.764547
6	-2.504717	0.995581	-0.745209
1	-4.589178	-0.950252	0.097635
7	-1.903917	-0.000010	-0.000070
1	-4.589153	0.950290	-0.097909
6	-3.861369	-1.403720	0.764313
6	-2.504778	-0.995582	0.745046
6	-4.263029	-2.442243	1.609208
1	-5.313124	-2.740678	1.609104
6	-1.567037	-1.732690	1.532444
7	-0.252533	-1.388006	1.383978
6	-3.362838	-3.108085	2.439705
6	-1.982207	-2.778342	2.409016
6	0.686023	-2.023761	2.120379
1	-3.701893	-3.911134	3.096417
6	-0.977135	-3.423789	3.170260
1	1.717242	-1.708746	1.968019
6	0.353721	-3.032474	3.021478
1	-1.253439	-4.223343	3.859712
1	1.148361	-3.509133	3.595794

Table 83: XYZ-coordinates of optimized specie for **2a**, BLYP/ Def2TZVP, multiplicity = 1

a.n.	x	y	z
7	1.976144	0.000238	0.001077
6	2.564582	-0.944778	-0.811054
6	2.563295	0.945608	0.813731
6	3.921299	1.298742	0.974215
6	4.307340	2.307858	1.880171
6	3.389076	2.999616	2.655392
6	2.004624	2.709782	2.520246
6	1.599686	1.697060	1.591150
7	0.269883	1.391777	1.386216
6	-0.666774	2.042677	2.093756
6	-0.343462	3.037267	3.038172
6	0.979966	3.374918	3.250362
6	1.602051	-1.696807	-1.589258
6	3.922920	-1.297146	-0.970410
6	4.310241	-2.306216	-1.875876
6	3.392989	-2.998706	-2.651642
6	2.008259	-2.709632	-2.517674
6	0.984529	-3.375698	-3.248243

Table 83 – continued from previous page

a.n.	x	y	z
1	4.694679	-0.820531	-0.380936
1	5.371151	-2.541107	-1.962469
1	4.693786	0.822641	0.385281
1	5.368045	2.543344	1.967642
1	3.709872	3.767781	3.357206
1	-1.146884	3.529828	3.582624
1	1.252873	4.148202	3.968012
1	-1.698575	1.765719	1.896743
1	3.714784	-3.766902	-3.352964
6	-0.339262	-3.038789	-3.037101
7	0.271929	-1.392067	-1.385570
6	-0.663850	-2.043919	-2.093427
1	-1.695947	-1.767358	-1.897389
1	1.258412	-4.149129	-3.965361
1	-1.141998	-3.532126	-3.581862
26	0.000039	-0.000157	-0.000014
1	-1.258258	-4.148670	3.965915
1	1.142142	-3.531625	3.582406
6	-0.984384	-3.375312	3.248714
6	0.339403	-3.038378	3.037569
1	-3.714634	-3.766603	3.353408
6	-3.392850	-2.998483	2.651999
6	-2.008123	-2.709371	2.518045
6	0.663980	-2.043596	2.093793
6	-4.310113	-2.306115	1.876125
1	1.696071	-1.767014	1.897756
6	-1.601917	-1.696643	1.589524
1	-5.371019	-2.541022	1.962722
7	-0.271805	-1.391856	1.385849
6	-3.922798	-1.297137	0.970554
6	-2.564468	-0.944774	0.811198
1	-4.693766	0.822226	-0.385210
7	-1.976089	0.000168	-0.001014
1	-4.694537	-0.820568	0.380996
6	-3.921352	1.298335	-0.974256
6	-2.563318	0.945337	-0.813798
6	-4.307497	2.307293	-1.880344
1	-5.368222	2.542694	-1.967806
6	-1.599785	1.696695	-1.591391
7	-0.269961	1.391467	-1.386494
6	-3.389306	2.998989	-2.655720
6	-2.004824	2.709246	-2.520622
6	0.666632	2.042272	-2.094211

Table 83 – continued from previous page

a.n.	x	y	z
1	-3.710184	3.767024	-3.357637
6	-0.980234	3.374295	-3.250911
1	1.698454	1.765371	-1.897233
6	0.343220	3.036703	-3.038763
1	-1.253212	4.147457	-3.968665
1	1.146590	3.529195	-3.583354

Table 84: XYZ-coordinates of optimized specie for **2a**, OLYP/ Def2TZVP, multiplicity = 1

a.n.	x	y	z
7	1.951745	0.000028	-0.000147
6	2.540282	0.968757	0.770265
6	2.540191	-0.968682	-0.770656
6	3.888551	-1.360233	-0.875443
6	4.276887	-2.389369	-1.749163
6	3.370883	-3.063969	-2.546749
6	1.994886	-2.741029	-2.457292
6	1.586787	-1.713281	-1.553764
7	0.267324	-1.382324	-1.376919
6	-0.658648	-2.015217	-2.104424
6	-0.336072	-3.017710	-3.033428
6	0.979894	-3.388263	-3.207520
6	1.586941	1.713400	1.553412
6	3.888654	1.360293	0.874952
6	4.277042	2.389512	1.748555
6	3.371088	3.064216	2.546108
6	1.995081	2.741281	2.456764
6	0.980124	3.388667	3.206908
1	4.650671	0.902757	0.261110
1	5.331893	2.655532	1.793528
1	4.650599	-0.902751	-0.261598
1	5.331733	-2.655401	-1.794214
1	3.695624	-3.846003	-3.228388
1	-1.136710	-3.493226	-3.594174
1	1.251827	-4.173724	-3.909663
1	-1.688238	-1.721541	-1.938836
1	3.695873	3.846340	3.227623
6	-0.335857	3.018121	3.032901
7	0.267471	1.382383	1.376710
6	-0.658476	2.015450	2.104107
1	-1.688071	1.721720	1.938644
1	1.252091	4.174246	3.908905

Table 84 – continued from previous page

a.n.	x	y	z
1	-1.136474	3.493768	3.593566
26	0.000002	0.000009	-0.000013
1	-1.252649	4.174174	-3.908845
1	1.136002	3.493971	-3.593569
6	-0.980576	3.388603	-3.206878
6	0.335452	3.018209	-3.032907
1	-3.696379	3.845957	-3.227539
6	-3.371491	3.063851	-2.546052
6	-1.995445	2.741075	-2.456738
6	0.658204	2.015545	-2.104150
6	-4.277353	2.389015	-1.748504
1	1.687835	1.721926	-1.938715
6	-1.587167	1.713216	-1.553422
1	-5.332238	2.654908	-1.793456
7	-0.267656	1.382347	-1.376762
6	-3.888829	1.359819	-0.874936
6	-2.540407	0.968445	-0.770273
1	-4.650489	-0.903323	0.261621
7	-1.951748	-0.000238	0.000101
1	-4.650783	0.902169	-0.261101
6	-3.888379	-1.360700	0.875465
6	-2.540066	-0.968992	0.770651
6	-4.276578	-2.389867	1.749211
1	-5.331391	-2.656023	1.794285
6	-1.586562	-1.713456	1.553763
7	-0.267142	-1.382334	1.376898
6	-3.370479	-3.064348	2.546790
6	-1.994522	-2.741246	2.457305
6	0.658919	-2.015120	2.104386
1	-3.695115	-3.846414	3.228443
6	-0.979440	-3.388357	3.207517
1	1.688470	-1.721318	1.938787
6	0.336479	-3.017651	3.033397
1	-1.251267	-4.173848	3.909668
1	1.137185	-3.493072	3.594126

Table 85: XYZ-coordinates of optimized specie for **3**, PBEPBE/ Def2TZVP, multiplicity = 3

a.n.	x	y	z
7	2.007345	-0.000013	-0.000073
6	2.603639	-0.990009	-0.752463
6	2.603734	0.989936	0.752302

Table 85 – continued from previous page

a.n.	x	y	z
6	3.952659	1.378790	0.814735
6	4.364727	2.425424	1.660985
6	3.476092	3.116859	2.463231
6	2.095786	2.797743	2.409501
6	1.667405	1.750422	1.540884
7	0.336047	1.424688	1.400084
6	-0.576460	2.089377	2.127534
6	-0.226313	3.111454	3.020761
6	1.100772	3.473347	3.162511
6	1.667223	-1.750467	-1.540970
6	3.952542	-1.378928	-0.814975
6	4.364505	-2.425600	-1.661229
6	3.475786	-3.117010	-2.463403
6	2.095499	-2.797826	-2.409592
6	1.100405	-3.473399	-3.162525
1	4.696941	-0.902782	-0.184289
1	5.423827	-2.691035	-1.678191
1	4.696994	0.902626	0.183987
1	5.424063	2.690809	1.677886
1	3.815065	3.916430	3.123945
1	-1.013088	3.612723	3.585471
1	1.396842	4.276384	3.840391
1	-1.615535	1.793833	1.979726
1	3.814679	-3.916612	-3.124121
6	-0.226653	-3.111439	-3.020699
7	0.335889	-1.424668	-1.400090
6	-0.576695	-2.089327	-2.127470
1	-1.615747	-1.793731	-1.979604
1	1.396394	-4.276464	-3.840407
1	-1.013488	-3.612681	-3.585349
24	0.000000	0.000023	0.000004
1	-1.396540	-4.276424	3.840405
1	1.013362	-3.612710	3.585363
6	-1.100525	-3.473366	3.162526
6	0.226545	-3.111445	3.020708
1	-3.814811	-3.916502	3.124105
6	-3.475891	-3.116909	2.463390
6	-2.095594	-2.797765	2.409587
6	0.576621	-2.089342	2.127482
6	-4.364586	-2.425471	1.661212
1	1.615683	-1.793776	1.979622
6	-1.667284	-1.750416	1.540969
1	-5.423915	-2.690877	1.678168

Table 85 – continued from previous page

a.n.	x	y	z
7	-0.335940	-1.424656	1.400098
6	-3.952587	-1.378810	0.814963
6	-2.603673	-0.989929	0.752459
1	-4.696967	0.902771	-0.184002
7	-2.007346	0.000052	0.000077
1	-4.696969	-0.902642	0.184274
6	-3.952615	1.378912	-0.814746
6	-2.603701	0.990017	-0.752305
6	-4.364646	2.425556	-1.661000
1	-5.423974	2.690973	-1.677907
6	-1.667345	1.750474	-1.540883
7	-0.335997	1.424701	-1.400075
6	-3.475986	3.116964	-2.463241
6	-2.095690	2.797807	-2.409503
6	0.576534	2.089364	-2.127519
1	-3.814932	3.916545	-3.123958
6	-1.100652	3.473383	-3.162507
1	1.615599	1.793790	-1.979705
6	0.226422	3.111452	-3.020748
1	-1.396694	4.276429	-3.840388
1	1.013215	3.612699	-3.585452

Table 86: XYZ-coordinates of optimized specie for **3**, PBEPBE/ Def2TZVP, multiplicity = 5

a.n.	x	y	z
7	-2.000587	0.000009	-0.000018
6	-2.599815	1.005852	-0.731708
6	-2.599843	-1.005818	0.731670
6	-3.950468	-1.407032	0.757718
6	-4.374017	-2.463284	1.580813
6	-3.498060	-3.159739	2.399437
6	-2.120216	-2.833259	2.378643
6	-1.677155	-1.772797	1.528572
7	-0.348480	-1.452205	1.423146
6	0.562474	-2.113409	2.155081
6	0.201872	-3.141184	3.032965
6	-1.132026	-3.50646	3.142250
6	-1.677102	1.772819	-1.528592
6	-3.950433	1.407090	-0.757773
6	-4.373951	2.463355	-1.580866
6	-3.497970	3.159800	-2.399473
6	-2.120132	2.833295	-2.378662

Table 86 – continued from previous page

a.n.	x	y	z
6	-1.131918	3.506483	-3.142250
1	-4.680702	0.928166	-0.112176
1	-5.431123	2.737278	-1.569230
1	-4.680719	-0.928101	0.112106
1	-5.431194	-2.737188	1.569163
1	-3.847920	-3.968325	3.043093
1	0.976606	-3.646587	3.609836
1	-1.436476	-4.316794	3.808050
1	1.601057	-1.80909	2.021297
1	-3.847806	3.968397	-3.043128
6	0.201971	3.141183	-3.032948
7	-0.348434	1.452203	-1.423149
6	0.562542	2.113395	-2.155067
1	1.601118	1.809056	-2.021270
1	-1.436345	4.316828	-3.808048
1	0.976722	3.646576	-3.609805
24	0.000000	-0.000004	0.000001
1	1.436412	4.316808	3.808046
1	-0.976665	3.646588	3.609810
6	1.131973	3.506467	3.142250
6	-0.201922	3.141184	3.032953
1	3.847866	3.968344	3.043122
6	3.498018	3.159751	2.399469
6	2.120175	2.833264	2.378661
6	-0.562508	2.113399	2.155074
6	4.373988	2.463293	1.58086
1	-1.601088	1.809072	2.021282
6	1.677130	1.772794	1.528593
1	5.431164	2.737202	1.569222
7	0.348457	1.452193	1.423155
6	3.950454	1.407034	0.757768
6	2.599831	1.005814	0.731706
1	4.680707	-0.928163	-0.112116
7	2.000587	-0.000020	0.000018
1	4.680716	0.928100	0.11217
6	3.950448	-1.407086	-0.757725
6	2.599828	-1.005854	-0.731673
6	4.373980	-2.463343	-1.580821
1	5.431154	-2.737261	-1.569175
6	1.677127	-1.772821	-1.528573
7	0.348457	-1.452210	-1.423144
6	3.498012	-3.159788	-2.399442
6	2.120172	-2.833289	-2.378644

Table 86 – continued from previous page

a.n.	x	y	z
6	-0.562508	-2.113404	-2.155076
1	3.847859	-3.968379	-3.043098
6	1.131970	-3.506478	-3.142247
1	-1.601087	-1.809070	-2.02129
6	-0.201922	-3.141185	-3.032958
1	1.436409	-4.316818	-3.808046
1	-0.976664	-3.646579	-3.609826

Table 87: XYZ-coordinates of optimized specie for $[Cr(BQA)_2]^+$, PBEPBE/ Def2TZVP, multiplicity = 2

a.n.	x	y	z
7	1.955333	0.000189	-0.000001
6	2.574804	-1.072026	-0.626413
6	2.574595	1.072522	0.626416
6	3.903726	1.498883	0.547430
6	4.337503	2.616633	1.289912
6	3.478420	3.326541	2.107473
6	2.108757	2.961179	2.181029
6	1.666615	1.846627	1.417127
7	0.348839	1.453901	1.378307
6	-0.538439	2.127859	2.125382
6	-0.174902	3.222211	2.926533
6	1.139898	3.647669	2.955598
6	1.666975	-1.846308	-1.417125
6	3.904017	-1.498131	-0.547422
6	4.338011	-2.615799	-1.289901
6	3.479067	-3.325874	-2.107462
6	2.109334	-2.960776	-2.181024
6	1.140609	-3.647456	-2.955593
1	4.611115	-0.994915	0.108184
1	5.382685	-2.920593	-1.210935
1	4.610924	0.995805	-0.108176
1	5.382118	2.921629	1.210949
1	3.834283	4.181207	2.684644
1	-0.944622	3.726098	3.511077
1	1.441003	4.504547	3.560697
1	-1.572896	1.787159	2.074660
1	3.835096	-4.180474	-2.684631
6	-0.174272	-3.222251	-2.926533
7	0.349124	-1.453836	-1.378311
6	-0.538023	-2.127967	-2.125387

Table 87 – continued from previous page

a.n.	x	y	z
1	-1.572545	-1.787464	-2.074669
1	1.441882	-4.504277	-3.560689
1	-0.943893	-3.726287	-3.511078
24	-0.000001	0.000000	-0.000003
1	-1.441006	-4.504548	3.560694
1	0.944618	-3.726098	3.511075
6	-1.139901	-3.647670	2.955596
6	0.174898	-3.222212	2.926531
1	-3.834284	-4.181212	2.684637
6	-3.478421	-3.326544	2.107468
6	-2.108759	-2.961180	2.181026
6	0.538436	-2.127860	2.125381
6	-4.337504	-2.616638	1.289904
1	1.572893	-1.787159	2.074659
6	-1.666618	-1.846627	1.417125
1	-5.382118	-2.921638	1.210938
7	-0.348843	-1.453901	1.378306
6	-3.903728	-1.498888	0.547423
6	-2.574598	-1.072522	0.626413
1	-4.611114	0.994932	0.108190
7	-1.955336	-0.000188	-0.000002
1	-4.610924	-0.995815	-0.108187
6	-3.904015	1.498142	-0.547420
6	-2.574804	1.072029	-0.626414
6	-4.338006	2.615810	-1.289900
1	-5.382678	2.920610	-1.210931
6	-1.666974	1.846308	-1.417128
7	-0.349123	1.453834	-1.378313
6	-3.479061	3.325880	-2.107465
6	-2.109330	2.960777	-2.181027
6	0.538025	2.127962	-2.125390
1	-3.835088	4.180480	-2.684633
6	-1.140604	3.647453	-2.955599
1	1.572547	1.787457	-2.074672
6	0.174277	3.222245	-2.926539
1	-1.441874	4.504274	-3.560695
1	0.943899	3.726279	-3.511084

Table 88: XYZ-coordinates of optimized specie for $[Cr(BQA)_2]^+$, PBEPBE/ Def2TZVP, multiplicity = 4

a.n.	x	y	z
7	1.997990	0.000016	0.000091
6	2.601156	-0.99610	-0.746049
6	2.601035	0.996178	0.746266
6	3.944828	1.390911	0.791463
6	4.369418	2.440558	1.632546
6	3.493912	3.130091	2.447346
6	2.11509	2.805798	2.408795
6	1.676718	1.757538	1.545085
7	0.346633	1.441925	1.426506
6	-0.559651	2.098200	2.154669
6	-0.202354	3.119498	3.050533
6	1.126484	3.475067	3.171188
6	1.676948	-1.757507	-1.54495
6	3.944975	-1.390753	-0.791143
6	4.369695	-2.440367	-1.632202
6	3.494293	-3.129947	-2.447076
6	2.115450	-2.805737	-2.40863
6	1.126941	-3.475064	-3.1711
1	4.685001	-0.91646	-0.15361
1	5.428448	-2.705121	-1.632471
1	4.684932	0.916654	0.153995
1	5.428155	2.705375	1.632896
1	3.840761	3.928734	3.10394
1	-0.979638	3.621002	3.626479
1	1.429739	4.276812	3.847808
1	-1.600316	1.803856	2.012931
1	3.841242	-3.928566	-3.103647
6	-0.201928	-3.119576	-3.050545
7	0.346835	-1.44197	-1.426476
6	-0.559355	-2.0983	-2.154709
1	-1.600047	-1.804016	-2.013052
1	1.430297	-4.276788	-3.847699
1	-0.979137	-3.621128	-3.62655
24	0.000001	-0.00003	-0.000007
1	-1.430187	-4.276802	3.847714
1	0.979231	-3.621085	3.626558
6	-1.126852	-3.475074	3.17111
6	0.202009	-3.119555	3.05055
1	-3.841142	-3.928641	3.103663
6	-3.494213	-3.130018	2.447086

Table 88 – continued from previous page

a.n.	x	y	z
6	-2.115377	-2.805776	2.408637
6	0.559410	-2.098276	2.154707
6	-4.369632	-2.440463	1.63221
1	1.600096	-1.803967	2.013047
6	-1.676901	-1.757541	1.54495
1	-5.428379	-2.705242	1.632483
7	-0.346796	-1.441972	1.426472
6	-3.944939	-1.390845	0.791144
6	-2.601129	-0.996161	0.746046
1	-4.684956	0.916529	-0.154003
7	-1.997988	-0.000036	-0.000102
1	-4.684976	-0.916572	0.153609
6	-3.944864	1.390811	-0.791466
6	-2.601061	0.996114	-0.746271
6	-4.369482	2.440450	-1.632544
1	-5.428226	2.705238	-1.632893
6	-1.676764	1.757502	-1.545088
7	-0.34667	1.441922	-1.426511
6	-3.493994	3.130012	-2.447341
6	-2.115164	2.805754	-2.408792
6	0.559597	2.098225	-2.154672
1	-3.840865	3.928649	-3.103930
6	-1.126575	3.475053	-3.171182
1	1.600269	1.803907	-2.012936
6	0.202272	3.119518	-3.050529
1	-1.429852	4.276794	-3.847797
1	0.979543	3.621046	-3.626474

Table 89: XYZ-coordinates of optimized specie for **4**, BPEBPE/ Def2TZVP, multiplicity = 2

a.n.	x	y	z
7	1.965265	0.000000	0.000040
6	2.562241	0.971981	0.772001
6	2.562286	-0.971964	-0.771908
6	3.91165	-1.356810	-0.861968
6	4.306195	-2.387369	-1.734984
6	3.404368	-3.056488	-2.544015
6	2.026785	-2.731609	-2.470051
6	1.615304	-1.714550	-1.559799
7	0.292449	-1.378850	-1.390152
6	-0.633414	-1.989889	-2.145445
6	-0.300435	-2.975631	-3.087624

Table 89 – continued from previous page

a.n.	x	y	z
6	1.017296	-3.359648	-3.245600
6	1.615217	1.714558	1.559850
6	3.911596	1.356850	0.862109
6	4.306090	2.387424	1.735129
6	3.404222	3.056536	2.544121
6	2.026646	2.731633	2.470109
6	1.017118	3.359662	3.245614
1	4.667912	0.889900	0.238903
1	5.364109	2.655620	1.773784
1	4.667935	-0.889855	-0.238728
1	5.364219	-2.655548	-1.773601
1	3.733885	-3.839191	-3.229216
1	-1.097393	-3.436046	-3.672611
1	1.295922	-4.139472	-3.957173
1	-1.666986	-1.688368	-1.977465
1	3.733700	3.839251	3.229327
6	-0.300601	2.975622	3.087594
7	0.292373	1.378835	1.390157
6	-0.633528	1.989864	2.145411
1	-1.667089	1.688324	1.977396
1	1.295705	4.139498	3.957191
1	-1.097588	3.436028	3.672547
25	-0.000001	-0.000012	-0.000002
1	-1.295740	4.139497	-3.957183
1	1.097558	3.436044	-3.672543
6	-1.017148	3.359661	-3.245608
6	0.300574	2.97563	-3.087591
1	-3.733731	3.839232	-3.229316
6	-3.404247	3.056517	-2.544113
6	-2.026670	2.731623	-2.470104
6	0.633509	1.989872	-2.145411
6	-4.306110	2.387397	-1.735123
1	1.667073	1.688339	-1.977399
6	-1.615232	1.714549	-1.559849
1	-5.364130	2.655586	-1.773775
7	-0.292386	1.378834	-1.390158
6	-3.911607	1.356824	-0.862105
6	-2.562250	0.971963	-0.772001
1	-4.667928	-0.889898	0.238726
7	-1.965266	-0.000017	-0.000043
1	-4.667920	0.889868	-0.238900
6	-3.911639	-1.356845	0.861966
6	-2.562278	-0.971986	0.771906

Table 89 – continued from previous page

a.n.	x	y	z
6	-4.306174	-2.387407	1.734983
1	-5.364196	-2.655596	1.773600
6	-1.615289	-1.714564	1.559797
7	-0.292437	-1.378852	1.390149
6	-3.404341	-3.056518	2.544014
6	-2.026760	-2.731627	2.470050
6	0.633432	-1.989884	2.145441
1	-3.733850	-3.839224	3.229215
6	-1.017266	-3.359657	3.245597
1	1.667002	-1.688354	1.977460
6	0.300463	-2.97563	3.087621
1	-1.295884	-4.139484	3.957171
1	1.097425	-3.436038	3.672607

Table 90: XYZ-coordinates of optimized specie for **4**, PBEPBE/ Def2TZVP, multiplicity = 4

a.n.	x	y	z
7	1.943118	0.000018	0.000143
6	2.542736	0.995730	0.751596
6	2.542910	-0.995622	-0.751266
6	3.892277	-1.391086	-0.799903
6	4.297380	-2.435033	-1.649625
6	3.403843	-3.115923	-2.461625
6	2.024307	-2.790457	-2.413527
6	1.606669	-1.743804	-1.539576
7	0.284326	-1.409293	-1.389452
6	-0.645764	-2.054967	-2.114832
6	-0.308283	-3.071085	-3.015696
6	1.018165	-3.448396	-3.165931
6	1.606337	1.743855	1.539773
6	3.892065	1.391302	0.800393
6	4.296979	2.435300	1.650141
6	3.403288	3.116136	2.462017
6	2.023784	2.790556	2.413756
6	1.017499	3.448427	3.166029
1	4.633868	0.922315	0.160934
1	5.353462	2.711192	1.664753
1	4.633963	-0.922058	-0.160338
1	5.353886	-2.710841	-1.664112
1	3.741605	-3.914753	-3.123792
1	-1.102212	-3.560158	-3.580697
1	1.299837	-4.250358	-3.850953

Table 90 – continued from previous page

a.n.	x	y	z
1	-1.679765	-1.749611	-1.957328
1	3.740904	3.915005	3.124209
6	-0.308899	3.071002	3.015644
7	0.284038	1.409236	1.389493
6	-0.646190	2.054843	2.114754
1	-1.680148	1.749402	1.957132
1	1.299024	4.250424	3.851071
1	-1.102936	3.560017	3.580544
25	-0.000002	-0.000039	-0.000003
1	-1.299178	4.250401	-3.851048
1	1.102806	3.560074	-3.580528
6	-1.017625	3.448407	-3.166013
6	0.308786	3.071026	-3.015632
1	-3.741045	3.914895	-3.124188
6	-3.403402	3.116031	-2.462002
6	-2.023888	2.790496	-2.413746
6	0.646111	2.054869	-2.114753
6	-4.297069	2.435162	-1.650128
1	1.680079	1.749460	-1.957137
6	-1.606405	1.743802	-1.539771
1	-5.353561	2.711020	-1.664736
7	-0.284095	1.409224	-1.389498
6	-3.892119	1.391173	-0.800386
6	-2.542777	0.995643	-0.751593
1	-4.633936	-0.922226	0.160356
7	-1.943123	-0.000051	-0.000144
1	-4.633906	0.922163	-0.160927
6	-3.892229	-1.391226	0.799916
6	-2.542876	-0.995712	0.751270
6	-4.297289	-2.435189	1.649638
1	-5.353786	-2.711034	1.664131
6	-1.606605	-1.743863	1.539574
7	-0.284273	-1.409304	1.389445
6	-3.403724	-3.116050	2.461629
6	-2.024199	-2.790536	2.413521
6	0.645844	-2.054956	2.114808
1	-3.741452	-3.914896	3.123793
6	-1.018029	-3.448449	3.165911
1	1.679834	-1.749563	1.957300
6	0.308405	-3.071094	3.015665
1	-1.299670	-4.250426	3.850929
1	1.102356	-3.560148	3.580653

Table 91: XYZ-coordinates of optimized specie for **4**, PBEPBE/ Def2TZVP, multiplicity = 6

a.n.	x	y	z
7	2.175426	-0.001795	-0.001064
6	2.793718	-1.058798	-0.609796
6	2.796756	1.053837	0.606947
6	4.128767	1.485720	0.460135
6	4.625145	2.610935	1.142713
6	3.839572	3.356221	2.003085
6	2.475413	3.008117	2.157335
6	1.946486	1.882408	1.446119
7	0.624907	1.559733	1.512128
6	-0.192857	2.270626	2.281939
6	0.248002	3.363914	3.051705
6	1.575731	3.732269	2.979008
6	1.940635	-1.885535	-1.447922
6	4.124957	-1.493574	-0.464575
6	4.618078	-2.619859	-1.147755
6	3.829862	-3.363423	-2.007193
6	2.466271	-3.012370	-2.159788
6	1.564033	-3.734572	-2.980374
1	4.790277	-0.970889	0.219373
1	5.661633	-2.904078	-0.992836
1	4.792126	0.961588	-0.224607
1	5.669127	2.892892	0.986539
1	4.243734	4.211558	2.547072
1	-0.460969	3.909280	3.675644
1	1.949848	4.590011	3.543584
1	-1.243582	1.967571	2.280615
1	4.231516	-4.219623	-2.551680
6	0.237008	-3.363371	-3.051426
7	0.619673	-1.560032	-1.512291
6	-0.200563	-2.269162	-2.281092
1	-1.250640	-1.963885	-2.278415
1	1.935617	-4.593099	-3.545427
1	-0.473897	-3.907208	-3.674499
25	0.000002	0.000667	0.000203
1	-1.943709	-4.589821	3.545606
1	0.466683	-3.907246	3.675837
6	-1.570664	-3.731830	2.980700
6	-0.243163	-3.362458	3.052389
1	-4.238617	-4.213182	2.550758
6	-3.835511	-3.357569	2.006422
6	-2.471502	-3.008415	2.159645

Table 91 – continued from previous page

a.n.	x	y	z
6	0.196295	-2.268883	2.282226
6	-4.622286	-2.612937	1.146589
1	1.246793	-1.965049	2.280068
6	-1.943956	-1.882347	1.447977
1	-5.666168	-2.895698	0.991200
7	-0.622579	-1.558657	1.512987
6	-4.127267	-1.487379	0.463583
6	-2.795484	-1.054472	0.609393
1	-4.790866	0.968656	0.223273
7	-2.175421	0.001611	0.000862
1	-4.791534	-0.963788	-0.220695
6	-4.126456	1.491899	-0.461131
6	-2.794983	1.058159	-0.607354
6	-4.620943	2.617842	-1.143879
1	-5.664603	2.901247	-0.988176
6	-1.943162	1.885598	-1.446067
7	-0.621995	1.561113	-1.511441
6	-3.833932	3.362073	-2.003849
6	-2.470186	3.012079	-2.157473
6	0.197128	2.270920	-2.280811
1	-4.236645	4.217999	-2.547982
6	-1.569106	3.735029	-2.978674
1	1.247435	1.966423	-2.278974
6	-0.241850	3.364849	-3.050739
1	-1.941767	4.593311	-3.543390
1	0.468178	3.909272	-3.674300

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