[3]rotaxanes composed of two dibenzo-24-crown-8 ether wheels and azamacrocyclic complex

M. Woźny, A. Więckowska, D. Trzybiński, S. Sutuła, S. Domagała and K. Woźniak

SUPPORTING INFORMATION

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Figure 1S. ^{1}H NMR spectrum (600 MHz, CD_3CN) of **4n**

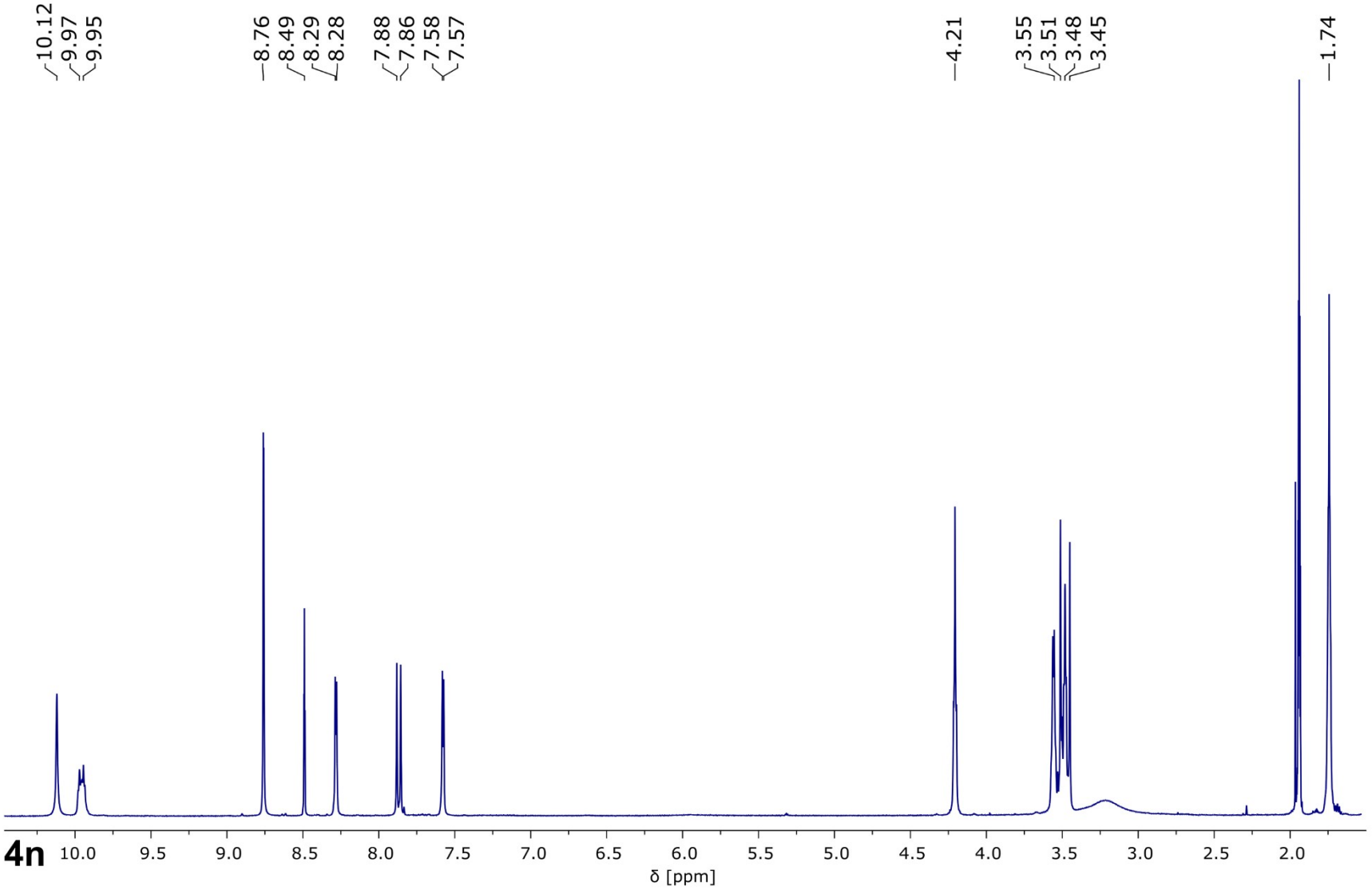


Figure 2S. ^{13}C NMR spectrum (125 MHz, CD_3CN) of **4n**

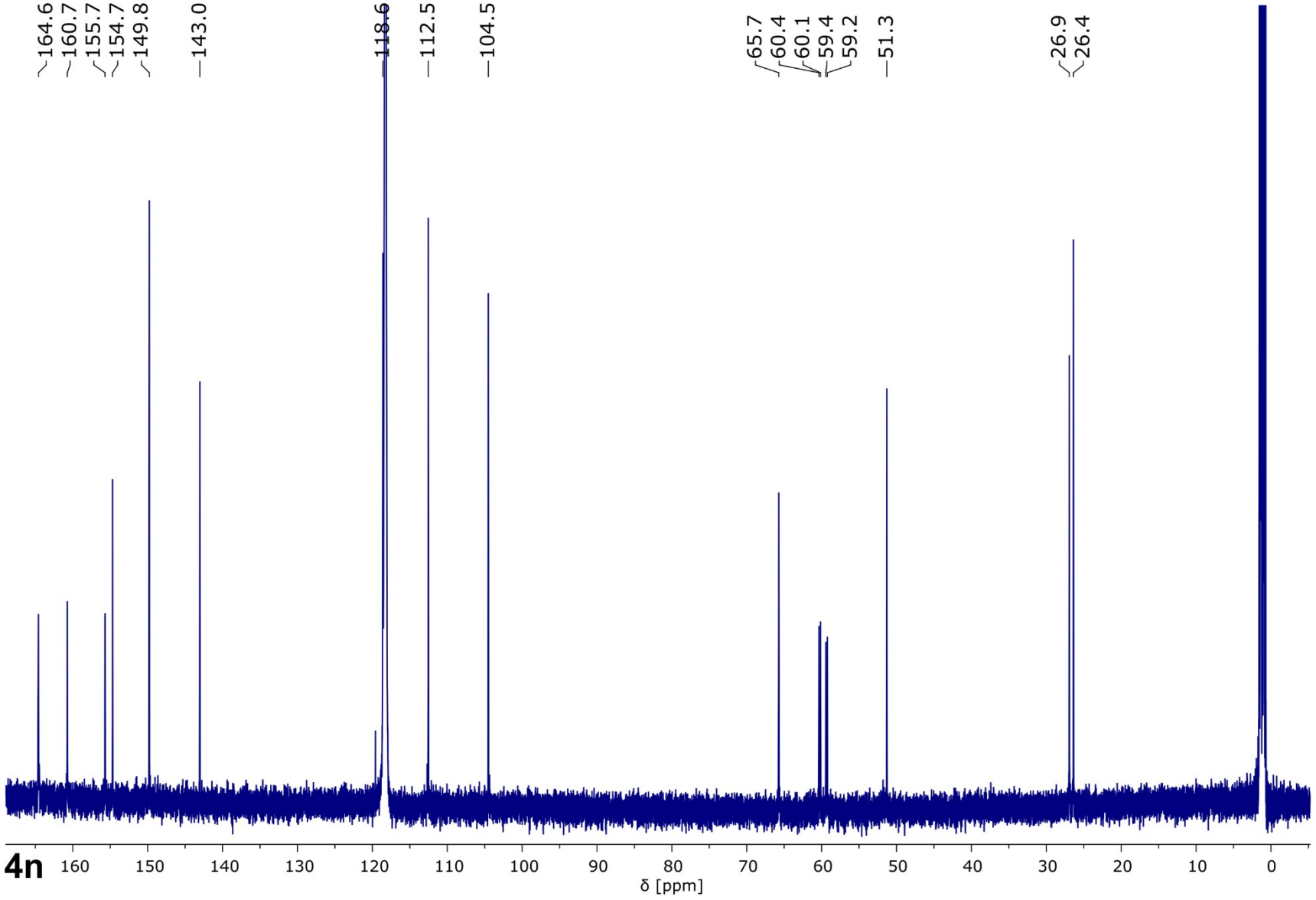
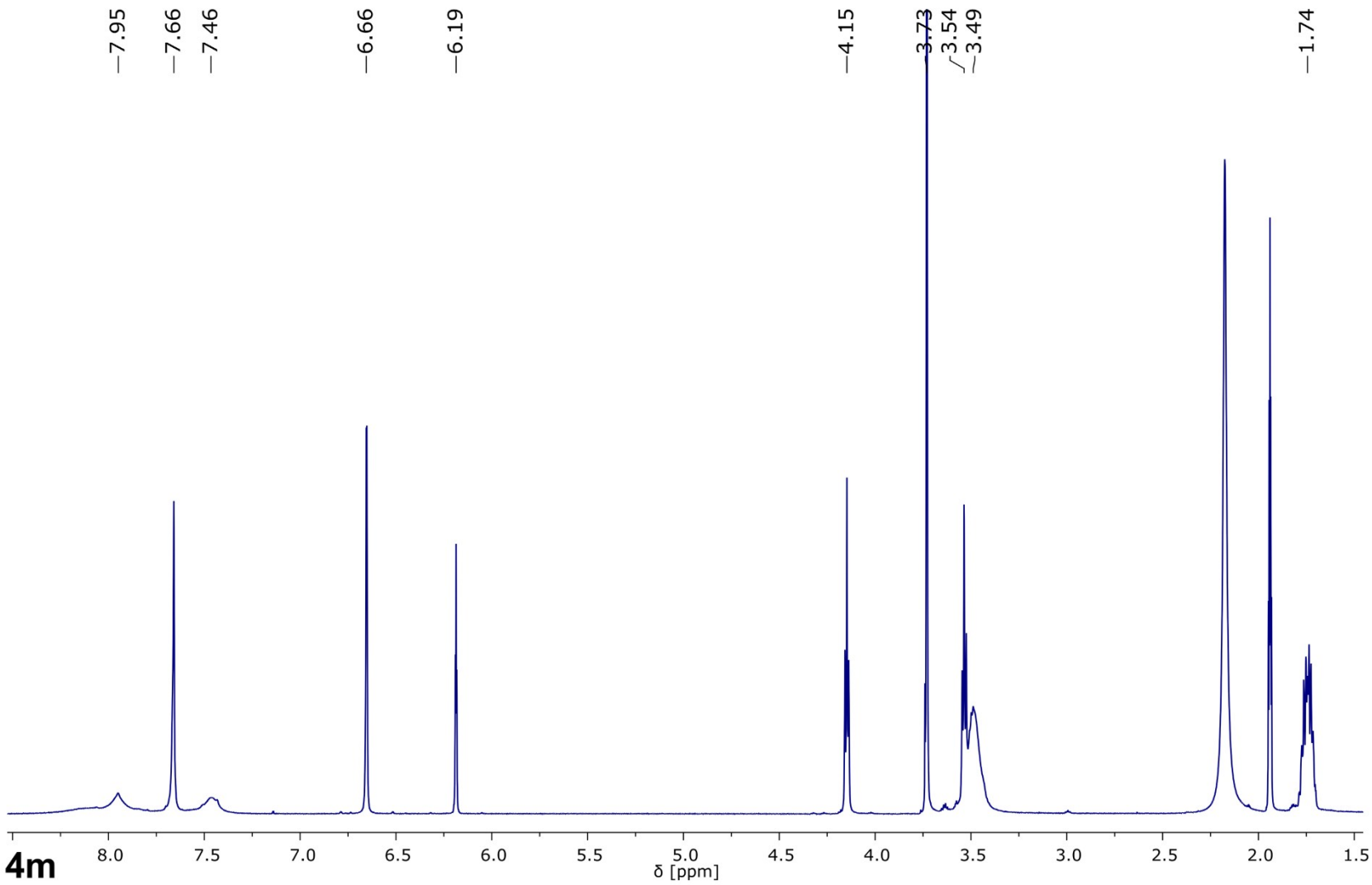


Figure 3S. ^{1}H NMR spectrum (600 MHz, CD_3CN) of **4m**



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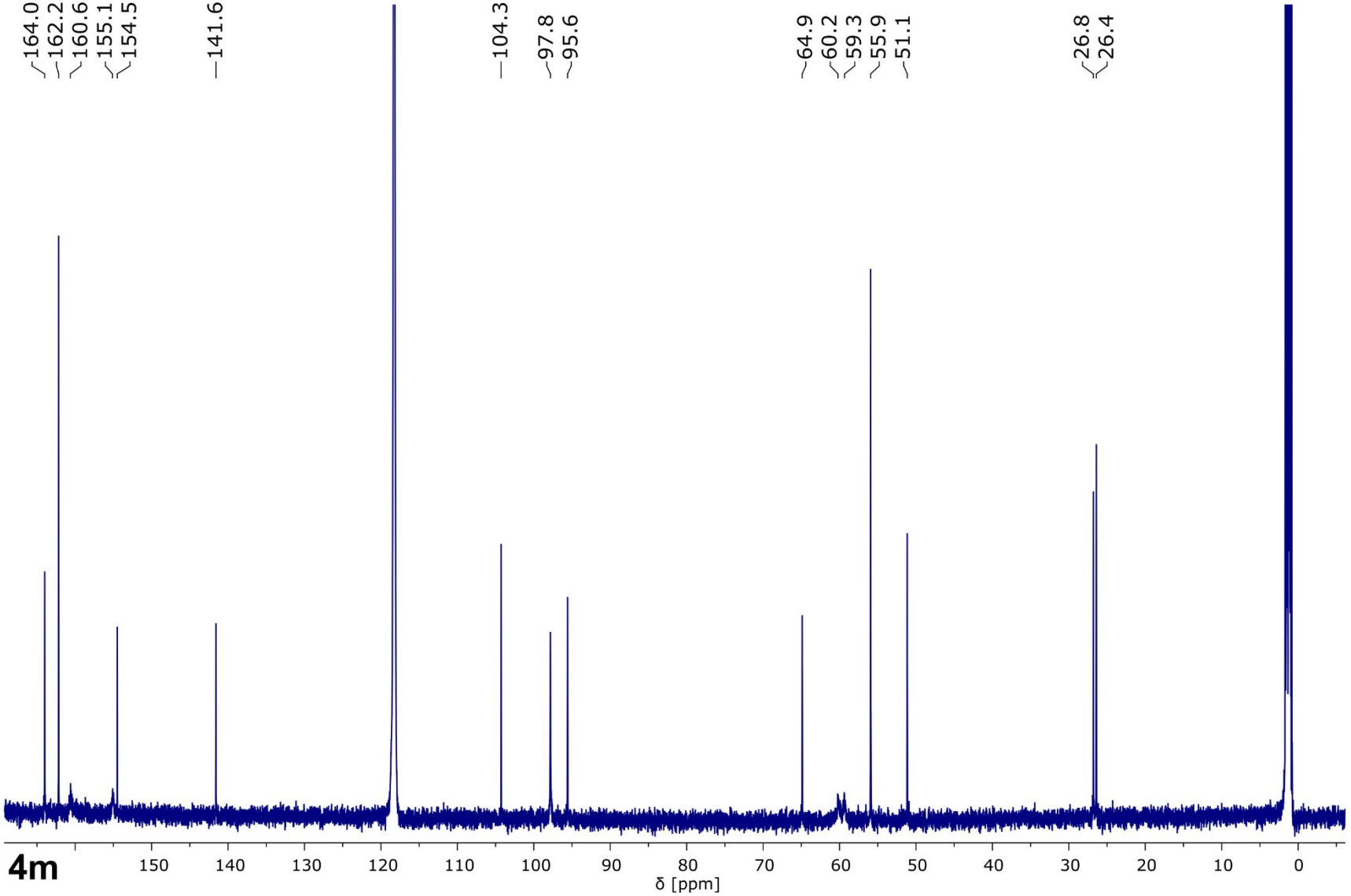

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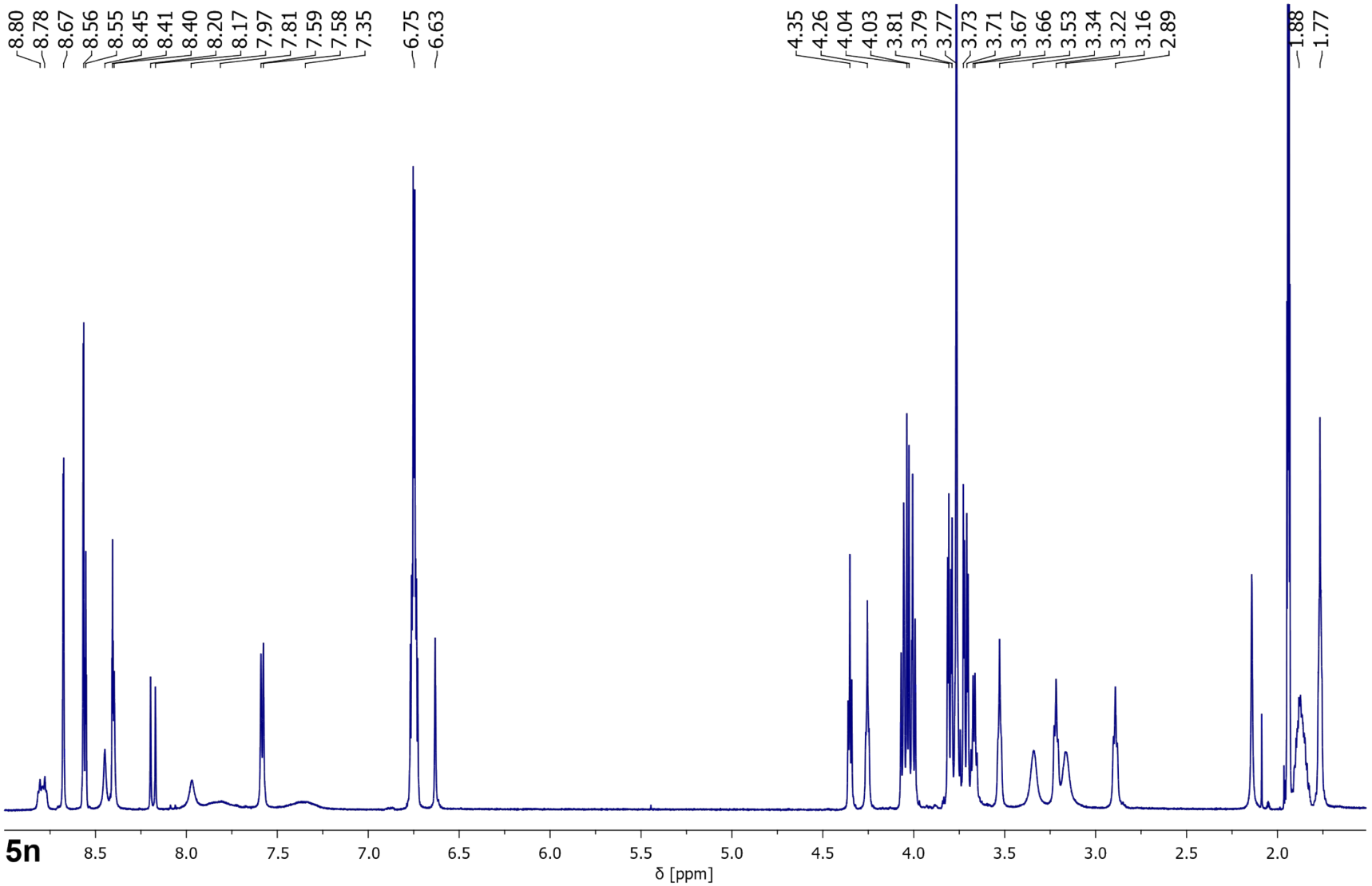

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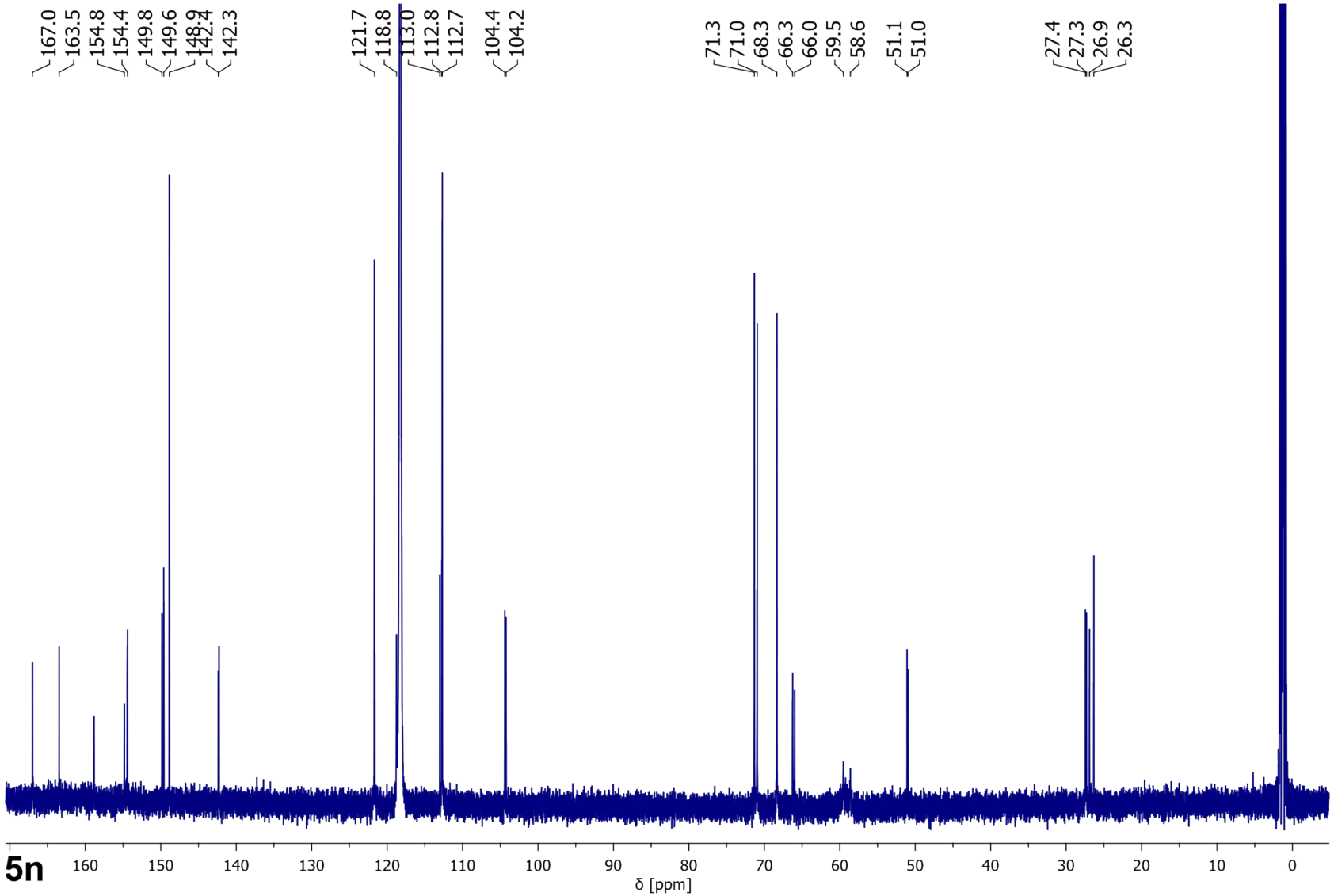

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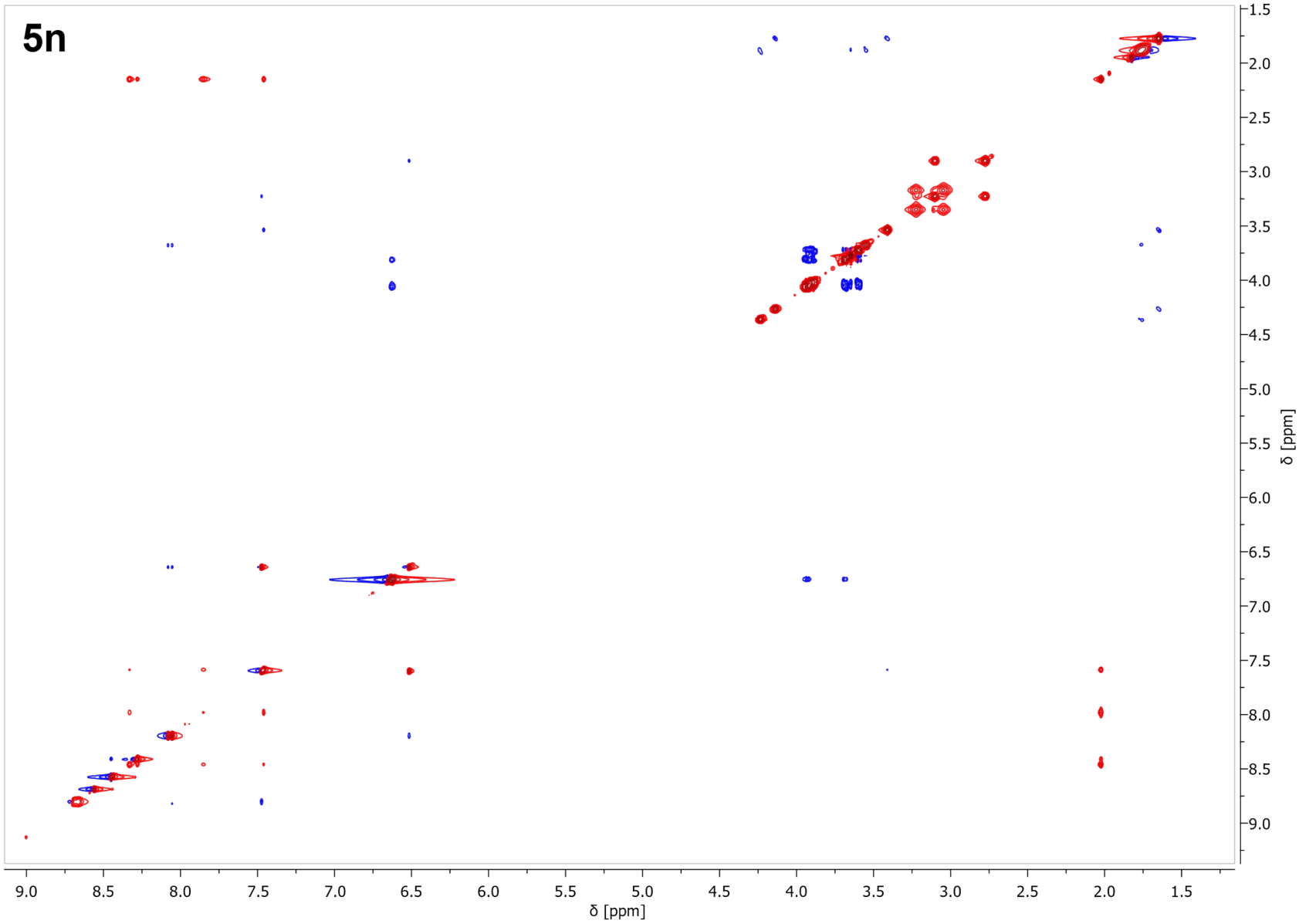

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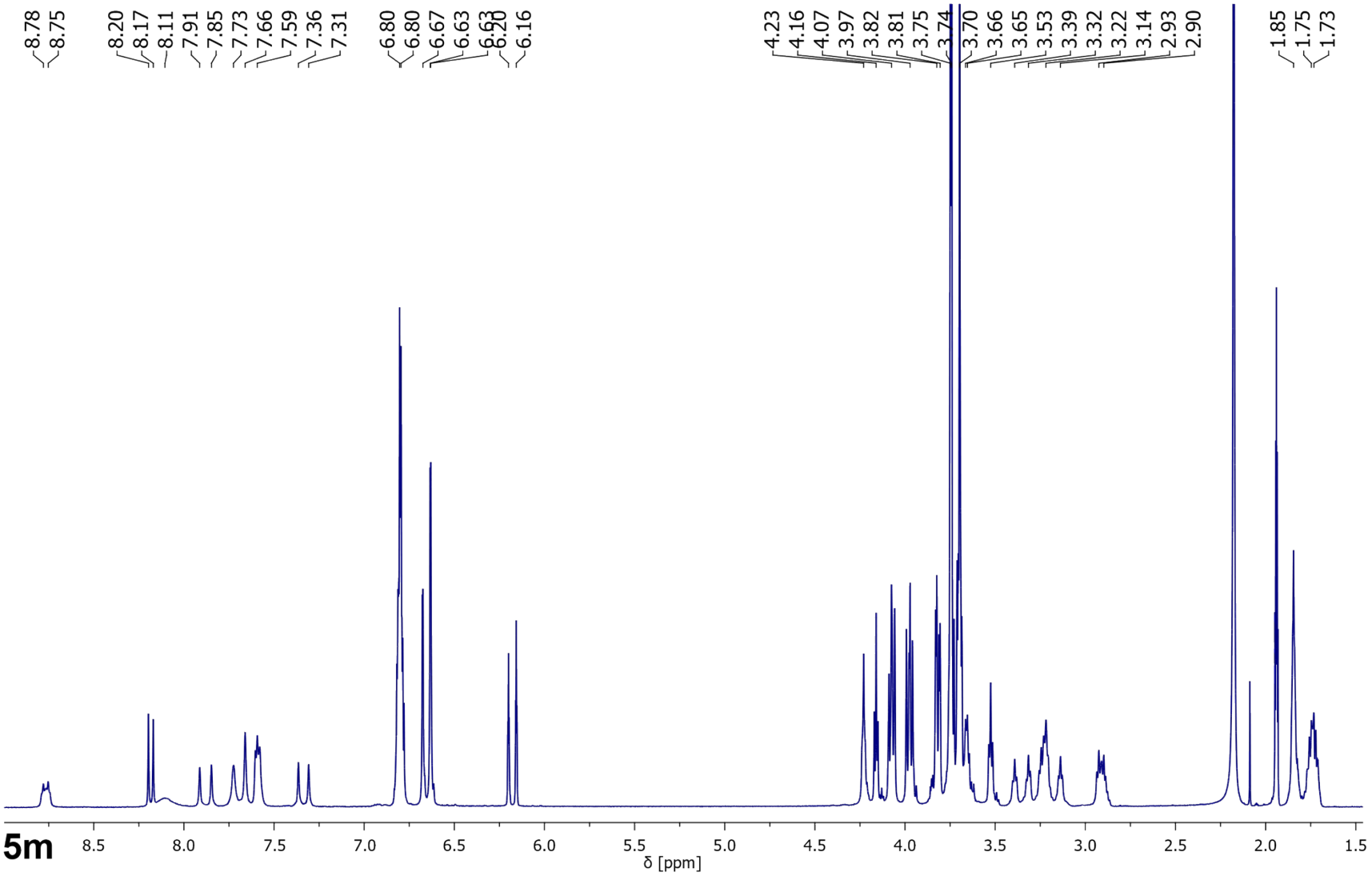

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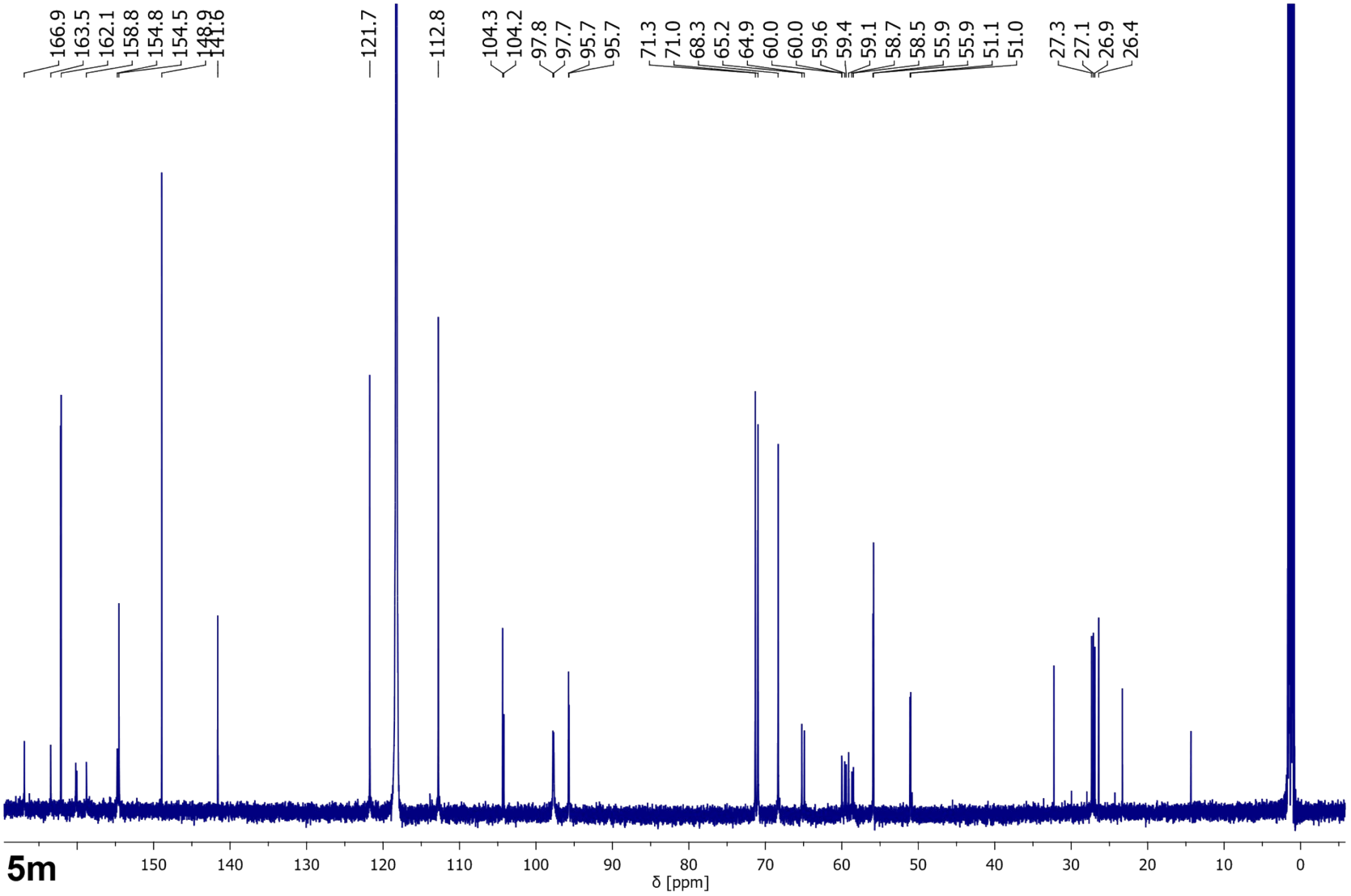

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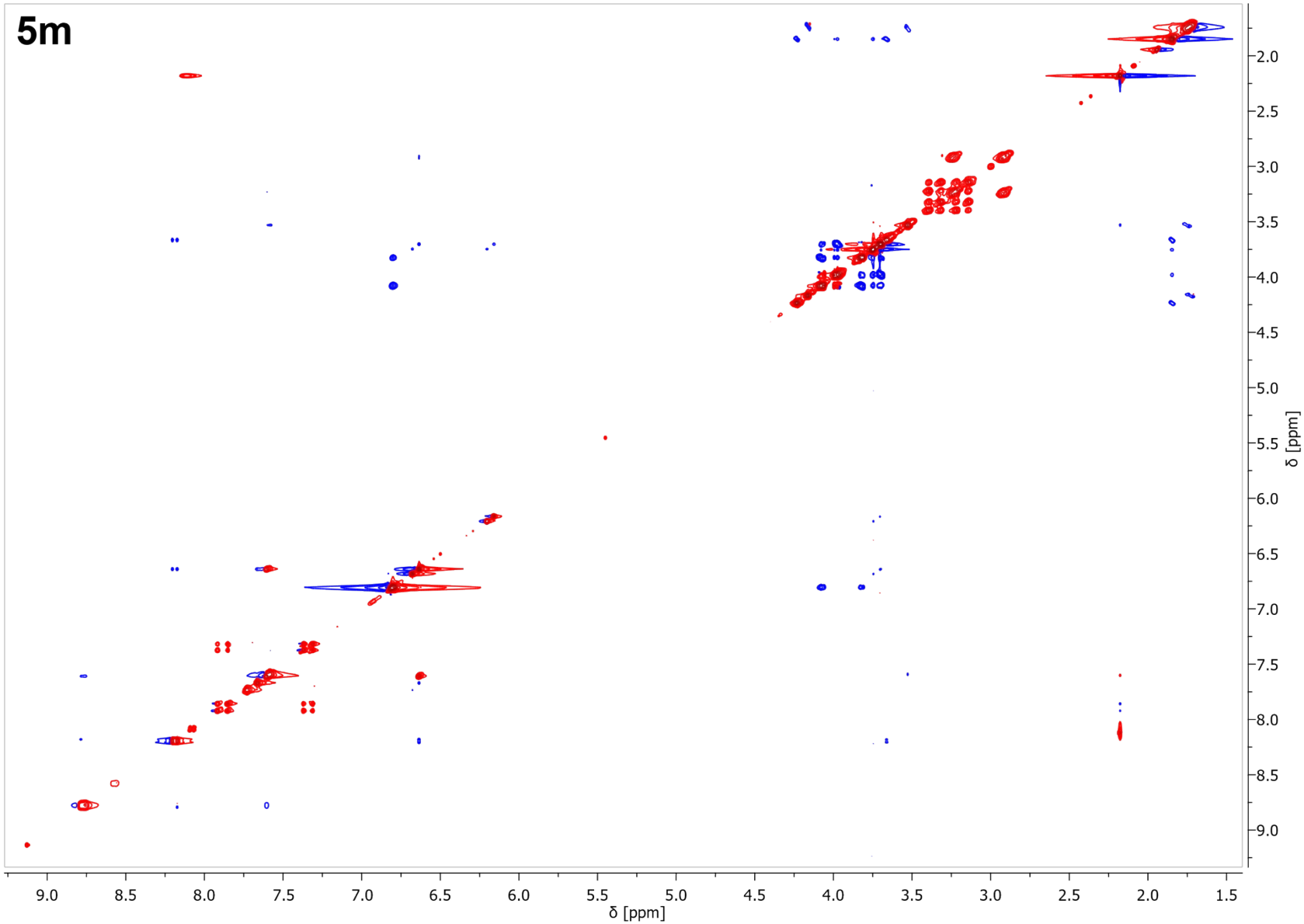

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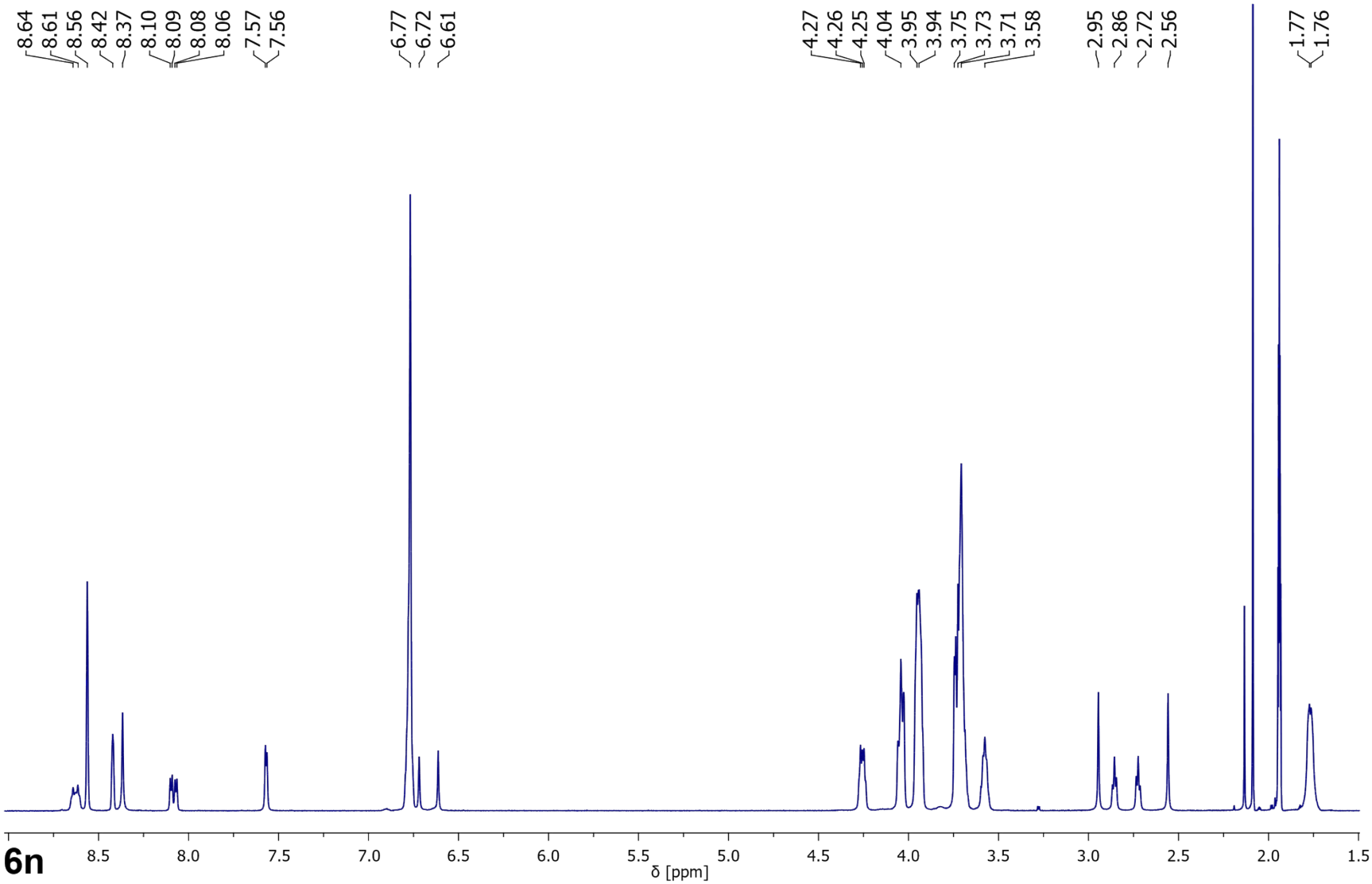
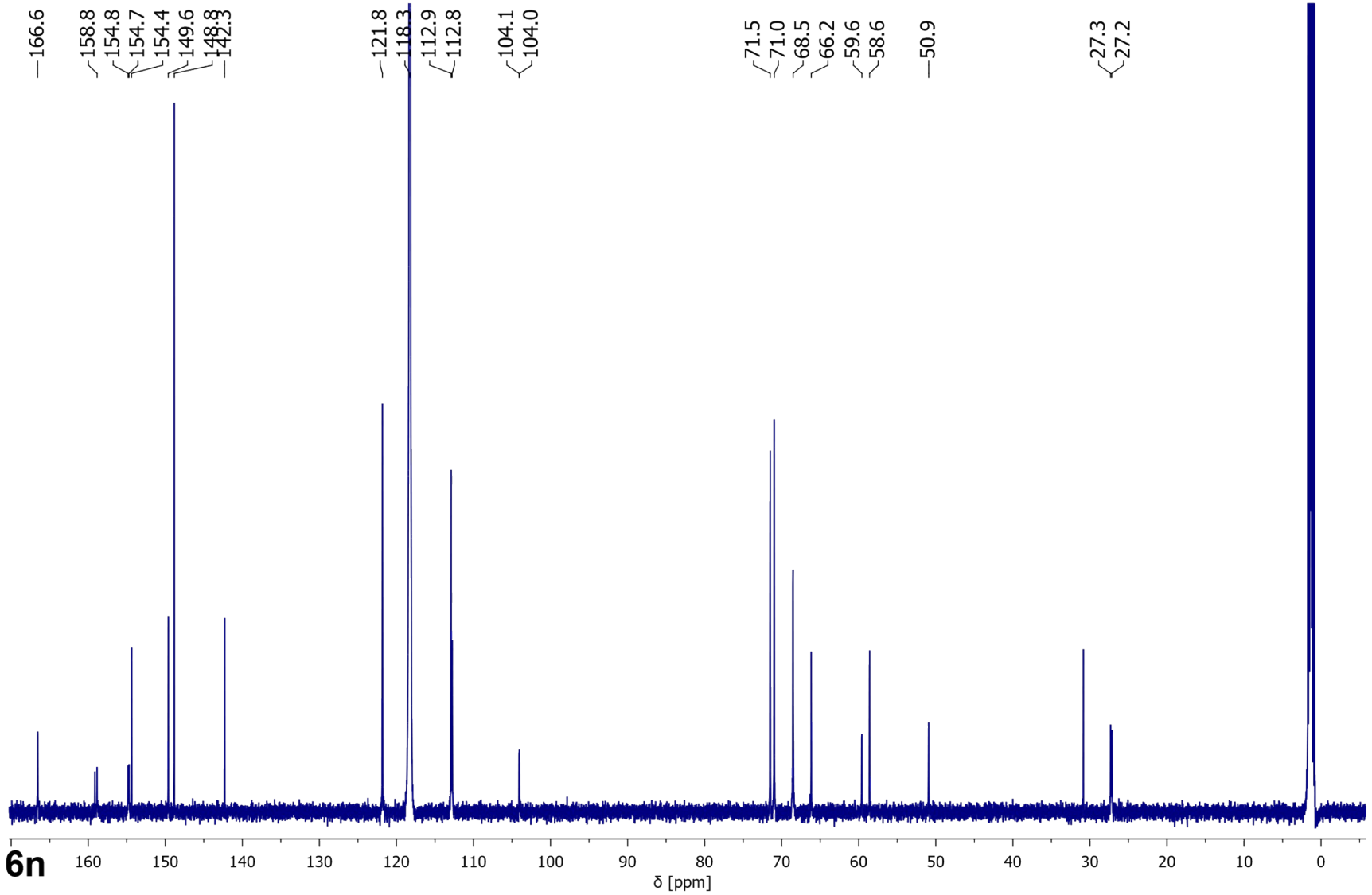


Figure 12S. ^{13}C NMR spectrum (125 MHz, CD_3CN) of **6n**



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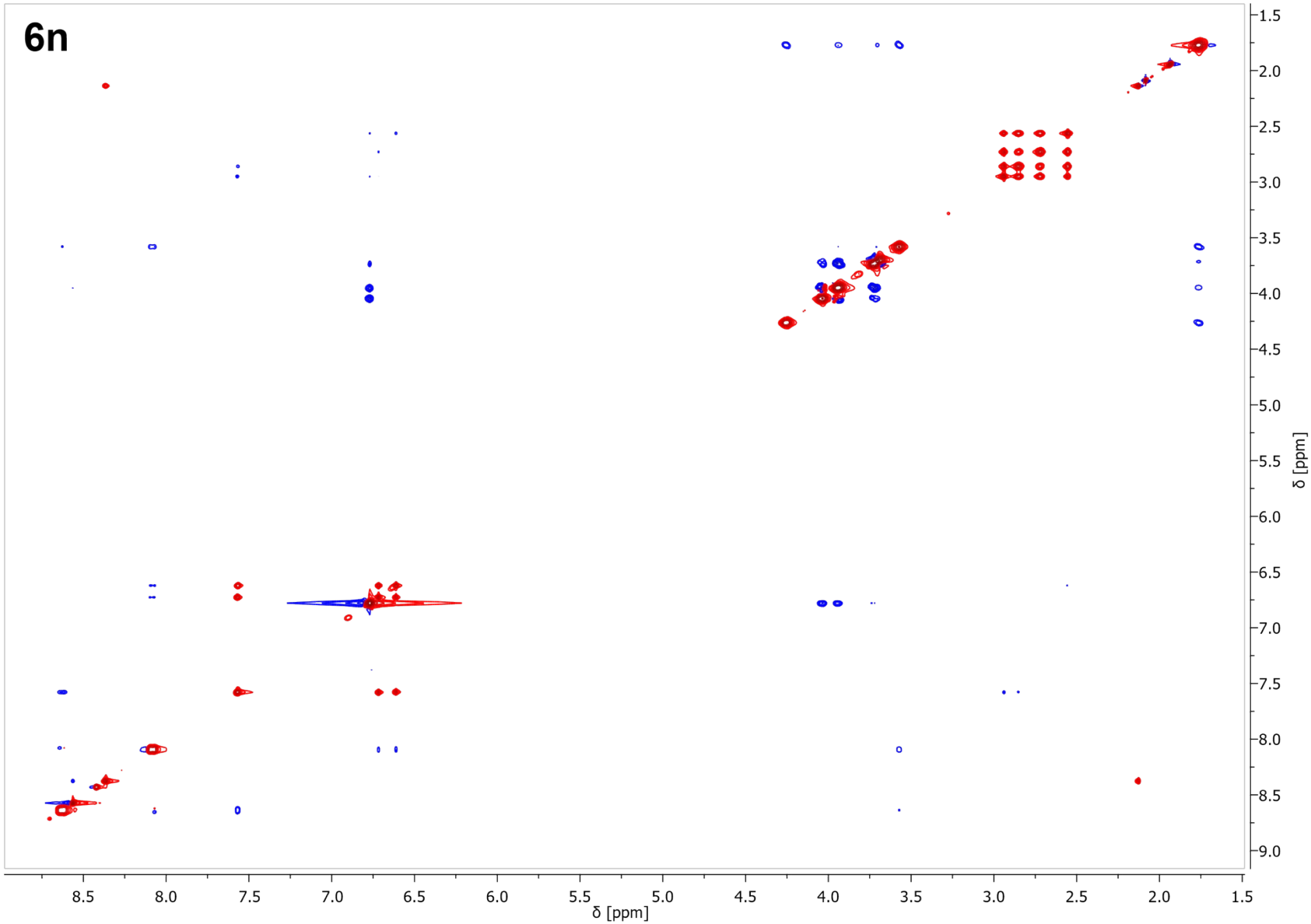

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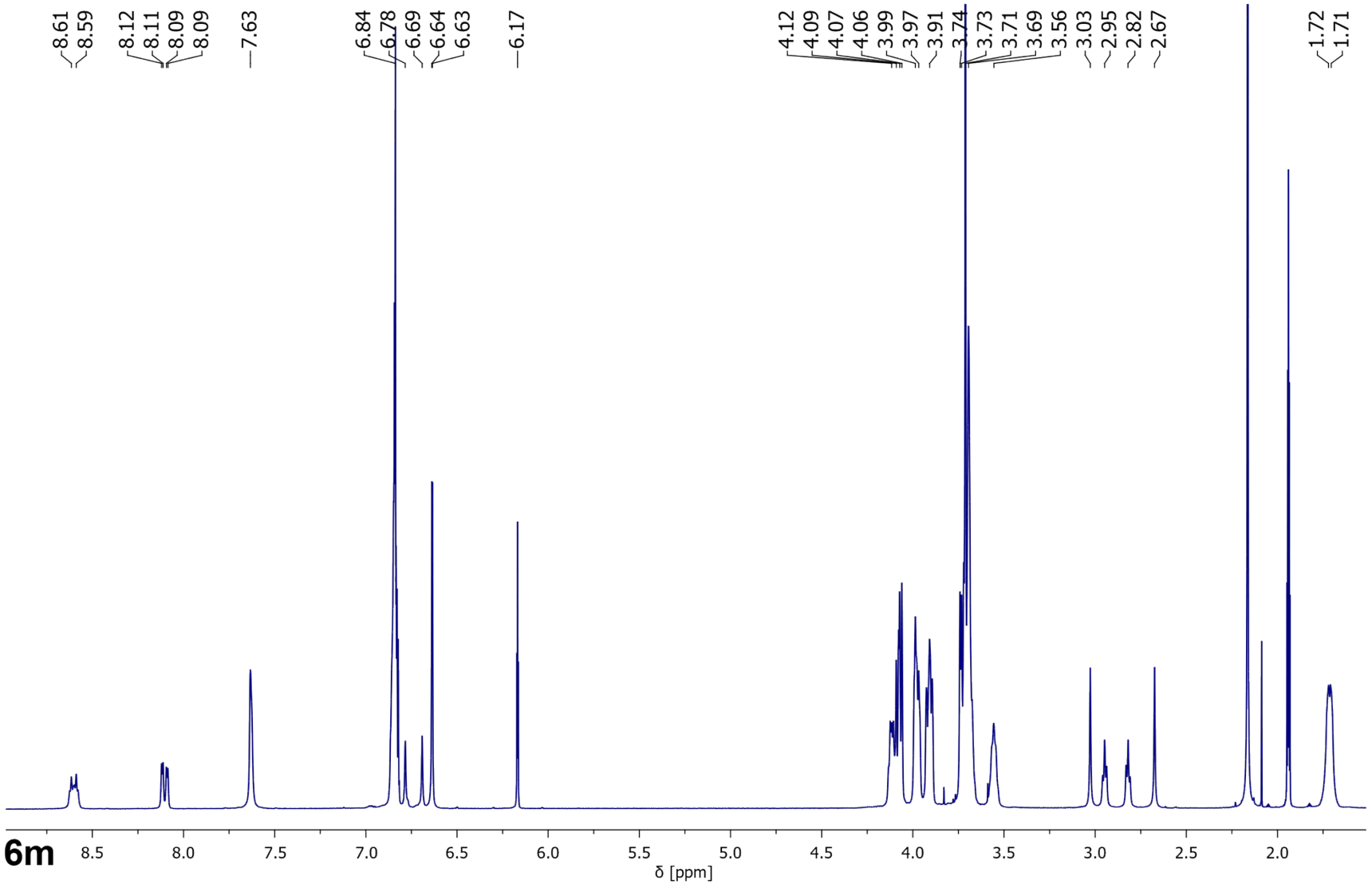


Figure 15S. ^{13}C NMR spectrum (125 MHz, CD_3CN) of **6m**

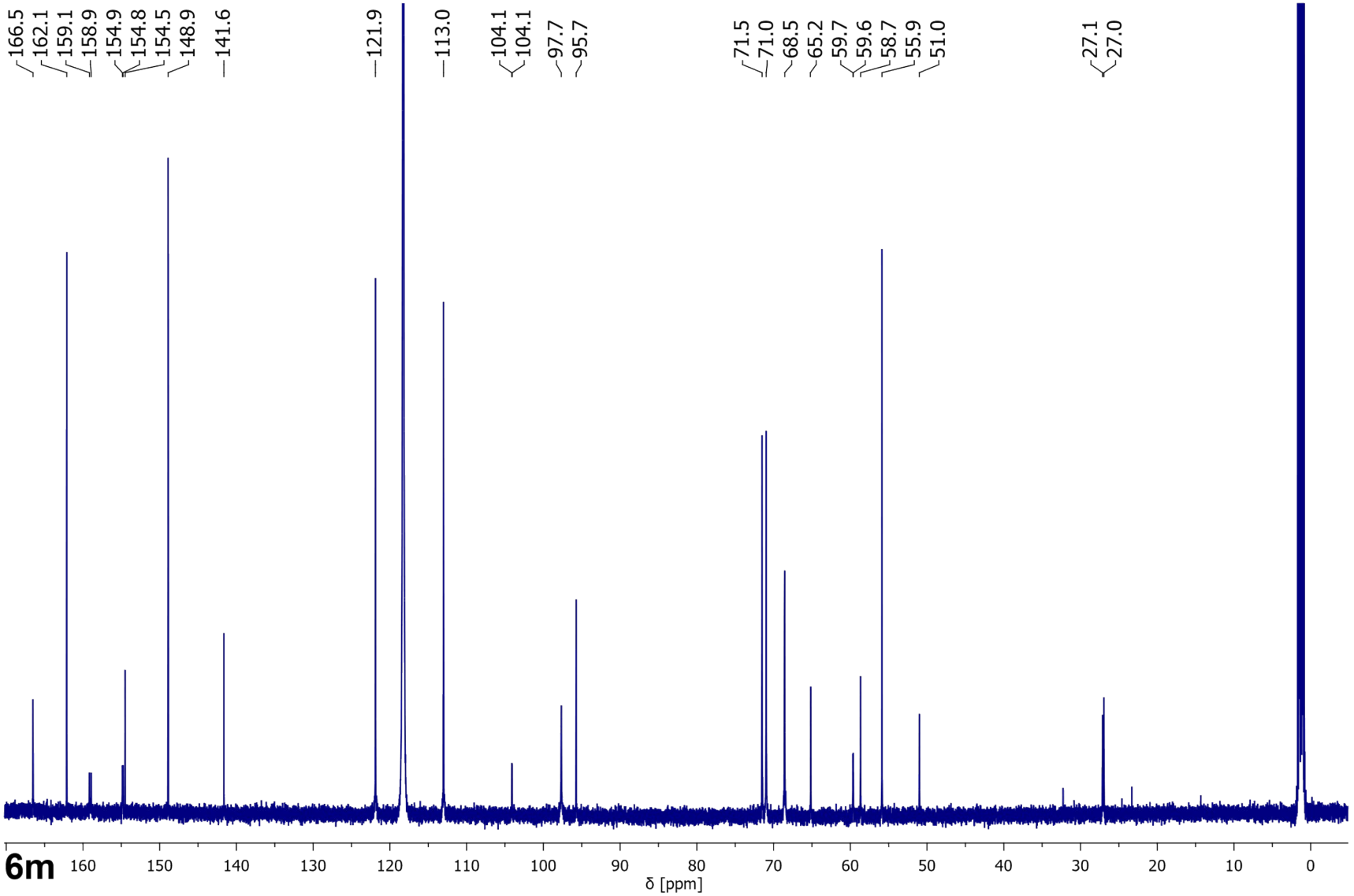
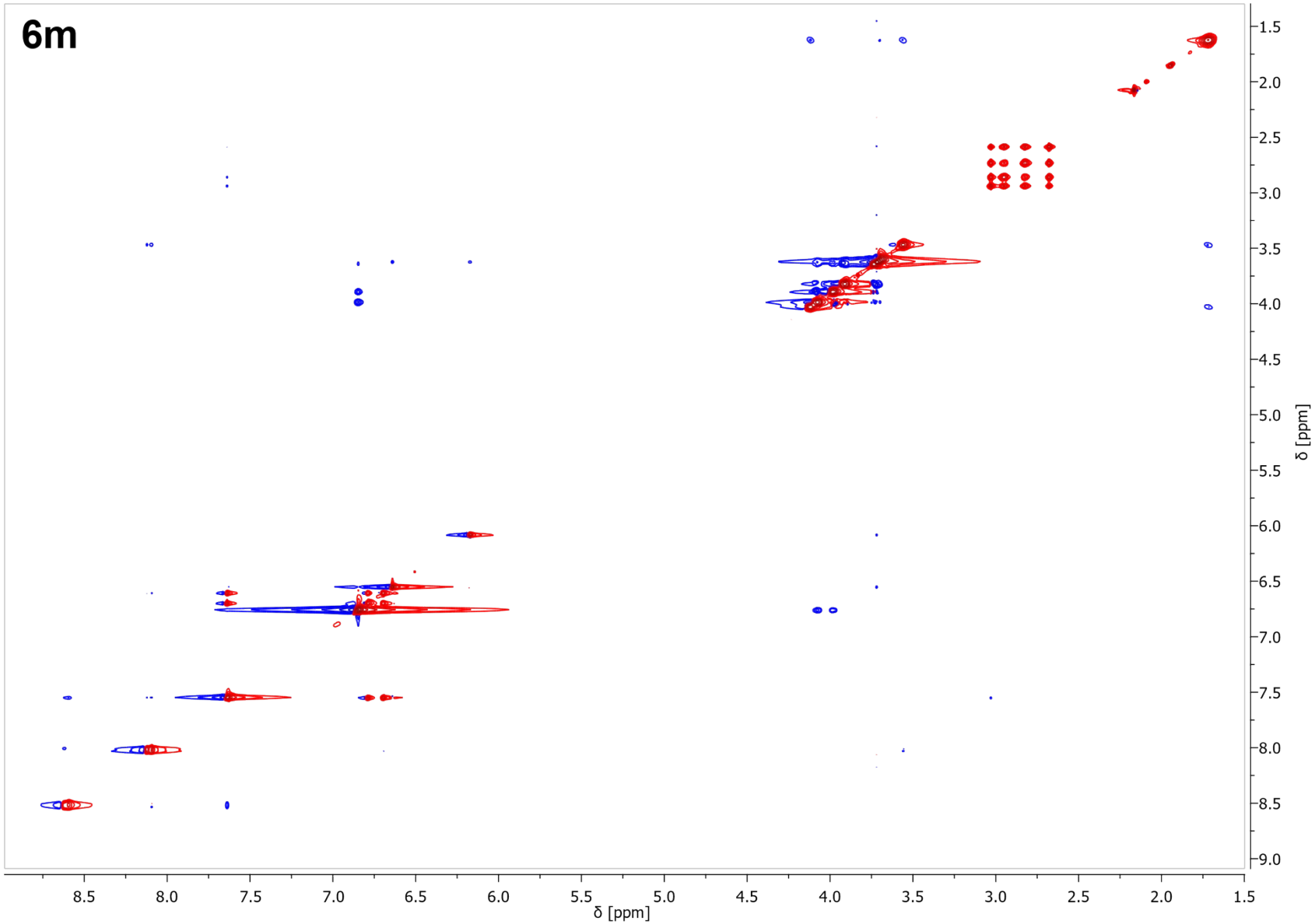


Figure 16S. ^{1}H-^{1}H ROESY NMR spectrum (600 MHz, CD_3CN) of **6m**



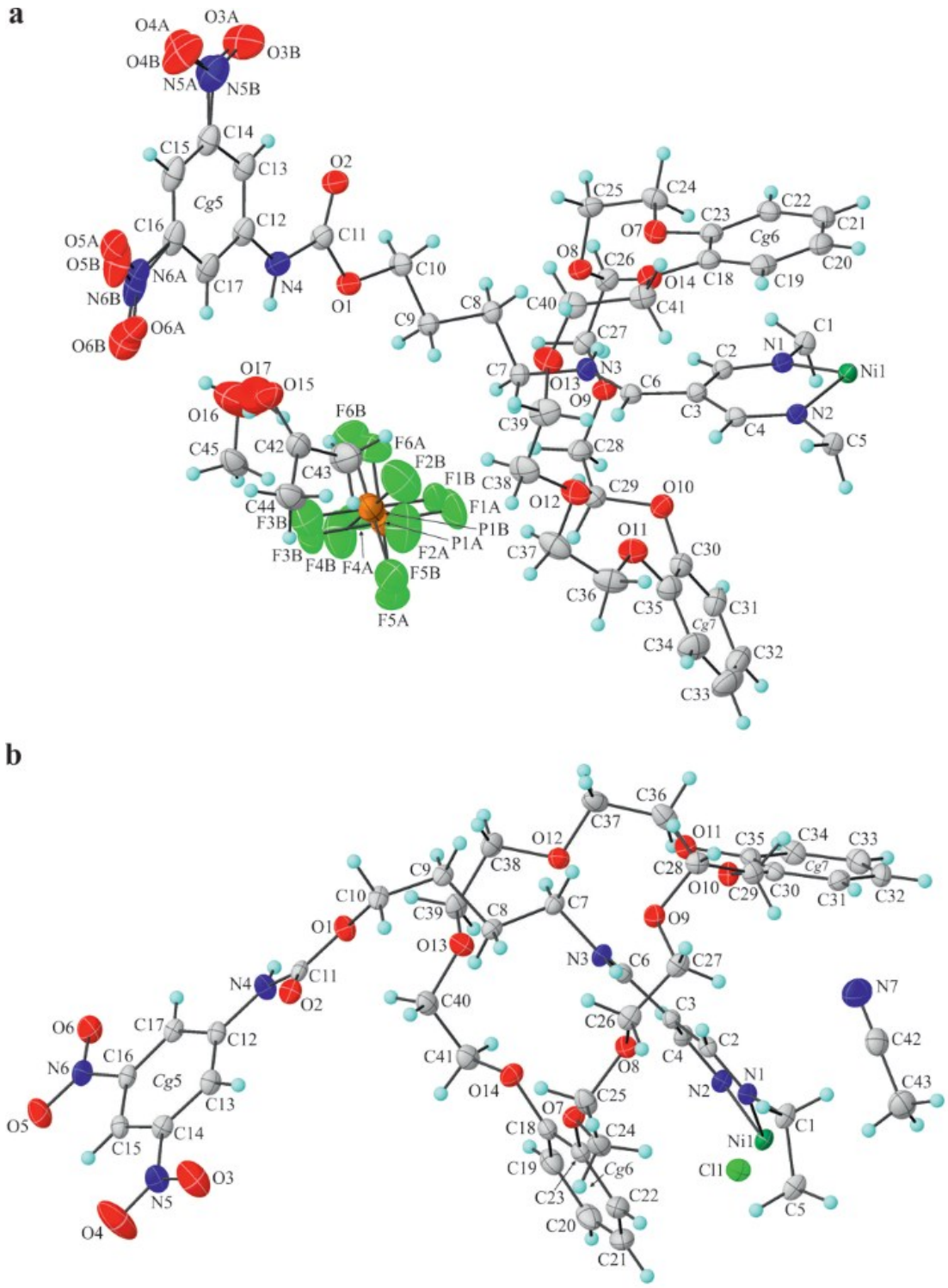


Figure 17S. Contents of the asymmetric part of the crystal lattice of 6n (a) and 6nCl (b). Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as small spheres of arbitrary radius. The Cg5, Cg6 and Cg7 denote the geometric centers of gravity of the aromatic rings defined by the C12−C17, C18−C23 and C30−35 atoms for both structures, respectively.

Table 1S. Bond lengths for **6n**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni(1)	N(1)[1]	1.8589(13)	C(24)	C(25)	1.509(2)
Ni(1)	N(1)	1.8588(13)	C(26)	C(27)	1.502(2)
Ni(1)	N(2)	1.8586(12)	C(28)	C(29)	1.507(2)
Ni(1)	N(2)[1]	1.8586(12)	C(30)	C(31)	1.387(2)
O(1)	C(10)	1.4549(17)	C(30)	C(35)	1.408(2)
O(1)	C(11)	1.341(2)	C(31)	C(32)	1.390(3)
O(2)	C(11)	1.207(2)	C(32)	C(33)	1.376(3)
O(7)	C(23)	1.3700(19)	C(33)	C(34)	1.390(3)
O(7)	C(24)	1.4302(18)	C(34)	C(35)	1.397(3)
O(8)	C(25)	1.4303(18)	C(36)	C(37)	1.495(3)
O(8)	C(26)	1.4340(17)	C(38)	C(39)	1.495(3)
O(9)	C(27)	1.4263(18)	C(40)	C(41)	1.508(2)
O(9)	C(28)	1.4263(18)	O(3A)	N(5A)	1.229(7)
O(10)	C(29)	1.4379(19)	O(4A)	N(5A)	1.233(7)
O(10)	C(30)	1.381(2)	O(5A)	N(6A)	1.229(7)
O(11)	C(35)	1.366(2)	O(6A)	N(6A)	1.227(6)
O(11)	C(36)	1.438(2)	O(3B)	N(5B)	1.220(11)
O(12)	C(37)	1.428(2)	O(4B)	N(5B)	1.222(11)
O(12)	C(38)	1.433(2)	O(5B)	N(6B)	1.233(10)
O(13)	C(39)	1.419(2)	O(6B)	N(6B)	1.231(10)
O(13)	C(40)	1.427(2)	P(1A)	F(1A)	1.591(2)
O(14)	C(18)	1.3705(19)	P(1A)	F(2A)	1.5853(17)
O(14)	C(41)	1.4361(18)	P(1A)	F(3A)	1.5978(16)
N(1)	C(1)	1.4734(17)	P(1A)	F(4A)	1.5965(15)
N(1)	C(2)	1.2958(19)	P(1A)	F(5A)	1.5979(16)
N(2)	C(4)	1.300(2)	P(1A)	F(6A)	1.5976(19)
N(2)	C(5)	1.4774(18)	P(1A)	P(1B)	0.553(9)
N(3)	C(6)	1.306(2)	P(1A)	F(1B)	1.289(10)
N(3)	C(7)	1.4614(18)	P(1A)	F(2B)	1.968(11)
N(4)	C(11)	1.375(2)	P(1A)	F(4B)	1.306(10)
N(4)	C(12)	1.395(2)	P(1A)	F(5B)	1.425(9)
C(1)	C(5)[1]	1.516(2)	P(1A)	F(6B)	1.885(10)
C(2)	C(3)	1.4238(19)	F(1A)	P(1B)	1.937(8)
C(3)	C(4)	1.424(2)	F(2A)	P(1B)	1.382(7)
C(3)	C(6)	1.406(2)	F(2A)	F(2B)	1.019(13)
C(5)	C(1)[1]	1.516(2)	F(2A)	F(5B)	1.271(13)
C(7)	C(8)	1.526(2)	F(3A)	P(1B)	1.399(7)
C(8)	C(9)	1.530(2)	F(3A)	F(3B)	0.810(12)
C(9)	C(10)	1.509(2)	F(3A)	F(4B)	1.504(13)
C(12)	C(13)	1.388(3)	F(4A)	P(1B)	1.937(8)
C(12)	C(17)	1.402(2)	F(4A)	F(4B)	0.809(14)
C(13)	C(14)	1.386(2)	F(5A)	P(1B)	2.020(8)
C(14)	C(15)	1.378(3)	F(5A)	F(5B)	1.101(16)

C(14)	N(5A)	1.497(7)	F(6A)	P(1B)	1.290(7)
C(14)	N(5B)	1.446(11)	F(6A)	F(6B)	0.527(11)
C(15)	C(16)	1.374(3)	P(1B)	F(1B)	1.578(7)
C(16)	C(17)	1.381(3)	P(1B)	F(2B)	1.576(7)
C(16)	N(6A)	1.466(7)	P(1B)	F(3B)	1.576(7)
C(16)	N(6B)	1.521(11)	P(1B)	F(4B)	1.577(7)
C(18)	C(19)	1.384(2)	P(1B)	F(5B)	1.577(7)
C(18)	C(23)	1.413(2)	P(1B)	F(6B)	1.577(7)
C(19)	C(20)	1.399(2)	O(16)	C(45)	1.343(7)
C(20)	C(21)	1.379(3)	O(15)	C(42)	1.225(3)
C(21)	C(22)	1.400(2)	C(42)	C(43)	1.501(4)
C(22)	C(23)	1.393(2)	C(42)	C(44)	1.495(3)

[1]-X,2-Y,-Z

Table 2S. Valence angles for **6n**.

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
N(1)	Ni(1)	N(1)[1]	180.0	F(1B)	P(1A)	F(4A)	88.6(5)
N(2)	Ni(1)	N(1)[1]	86.12(5)	F(1B)	P(1A)	F(5A)	102.8(5)
N(2)[1]	Ni(1)	N(1)	86.12(5)	F(1B)	P(1A)	F(6A)	76.7(5)
N(2)[1]	Ni(1)	N(1)[1]	93.88(5)	F(1B)	P(1A)	F(2B)	83.6(4)
N(2)	Ni(1)	N(1)	93.88(5)	F(1B)	P(1A)	F(4B)	118.5(7)
N(2)[1]	Ni(1)	N(2)	180.0	F(1B)	P(1A)	F(5B)	110.4(5)
C(11)	O(1)	C(10)	115.23(13)	F(1B)	P(1A)	F(6B)	87.2(4)
C(23)	O(7)	C(24)	116.82(12)	F(4B)	P(1A)	F(1A)	117.8(6)
C(25)	O(8)	C(26)	113.07(11)	F(4B)	P(1A)	F(2A)	148.5(6)
C(28)	O(9)	C(27)	111.71(12)	F(4B)	P(1A)	F(3A)	61.4(6)
C(30)	O(10)	C(29)	115.84(12)	F(4B)	P(1A)	F(4A)	30.3(6)
C(35)	O(11)	C(36)	115.63(14)	F(4B)	P(1A)	F(5A)	78.5(5)
C(37)	O(12)	C(38)	109.83(15)	F(4B)	P(1A)	F(6A)	100.6(6)
C(39)	O(13)	C(40)	111.95(14)	F(4B)	P(1A)	F(2B)	148.0(6)
C(18)	O(14)	C(41)	117.04(13)	F(4B)	P(1A)	F(5B)	109.4(5)
C(1)	N(1)	Ni(1)	113.10(10)	F(4B)	P(1A)	F(6B)	86.7(4)
C(2)	N(1)	Ni(1)	127.43(10)	F(5B)	P(1A)	F(1A)	99.8(5)
C(2)	N(1)	C(1)	119.46(13)	F(5B)	P(1A)	F(2A)	49.6(6)
C(4)	N(2)	Ni(1)	126.74(10)	F(5B)	P(1A)	F(3A)	80.5(4)
C(4)	N(2)	C(5)	119.64(12)	F(5B)	P(1A)	F(4A)	130.1(6)
C(5)	N(2)	Ni(1)	113.59(9)	F(5B)	P(1A)	F(5A)	42.2(6)
C(6)	N(3)	C(7)	122.42(13)	F(5B)	P(1A)	F(6A)	139.0(6)
C(11)	N(4)	C(12)	125.55(15)	F(5B)	P(1A)	F(2B)	80.4(4)
N(1)	C(1)	C(5)[1]	106.67(12)	F(5B)	P(1A)	F(6B)	144.3(6)
N(1)	C(2)	C(3)	123.77(14)	F(6B)	P(1A)	F(2B)	70.7(3)
C(2)	C(3)	C(4)	121.58(13)	P(1A)	F(1A)	P(1B)	14.1(2)
C(6)	C(3)	C(2)	122.24(14)	P(1B)	F(2A)	P(1A)	20.0(3)
C(6)	C(3)	C(4)	116.16(13)	F(2B)	F(2A)	P(1A)	95.7(6)
N(2)	C(4)	C(3)	124.35(13)	F(2B)	F(2A)	P(1B)	80.5(6)
N(2)	C(5)	C(1)[1]	106.05(12)	F(2B)	F(2A)	F(5B)	153.3(9)

N(3)	C(6)	C(3)	127.08(14)	F(5B)	F(2A)	P(1A)	58.6(5)
N(3)	C(7)	C(8)	112.23(12)	F(5B)	F(2A)	P(1B)	72.8(6)
C(7)	C(8)	C(9)	109.61(12)	P(1B)	F(3A)	P(1A)	19.9(3)
C(10)	C(9)	C(8)	111.68(13)	P(1B)	F(3A)	F(4B)	65.7(5)
O(1)	C(10)	C(9)	106.11(12)	F(3B)	F(3A)	P(1A)	105.9(7)
O(1)	C(11)	N(4)	108.17(14)	F(3B)	F(3A)	P(1B)	86.7(7)
O(2)	C(11)	O(1)	125.08(15)	F(3B)	F(3A)	F(4B)	147.3(10)
O(2)	C(11)	N(4)	126.74(16)	F(4B)	F(3A)	P(1A)	49.7(4)
N(4)	C(12)	C(17)	117.24(17)	P(1A)	F(4A)	P(1B)	14.2(2)
C(13)	C(12)	N(4)	123.46(15)	F(4B)	F(4A)	P(1A)	54.5(7)
C(13)	C(12)	C(17)	119.29(16)	F(4B)	F(4A)	P(1B)	52.2(6)
C(14)	C(13)	C(12)	118.39(16)	P(1A)	F(5A)	P(1B)	11.4(2)
C(13)	C(14)	N(5A)	116.5(3)	F(5B)	F(5A)	P(1A)	60.5(5)
C(13)	C(14)	N(5B)	120.1(6)	F(5B)	F(5A)	P(1B)	50.9(4)
C(15)	C(14)	C(13)	124.38(19)	P(1B)	F(6A)	P(1A)	18.4(4)
C(15)	C(14)	N(5A)	119.1(4)	F(6B)	F(6A)	P(1A)	115.4(13)
C(15)	C(14)	N(5B)	115.2(7)	F(6B)	F(6A)	P(1B)	113.6(14)
C(16)	C(15)	C(14)	115.22(17)	P(1A)	P(1B)	F(1A)	44.5(6)
C(15)	C(16)	C(17)	123.82(17)	P(1A)	P(1B)	F(2A)	101.3(7)
C(15)	C(16)	N(6A)	113.9(4)	P(1A)	P(1B)	F(3A)	100.8(8)
C(15)	C(16)	N(6B)	125.9(9)	P(1A)	P(1B)	F(4A)	45.2(6)
C(17)	C(16)	N(6A)	122.2(4)	P(1A)	P(1B)	F(6A)	114.1(10)
C(17)	C(16)	N(6B)	110.2(10)	P(1A)	P(1B)	F(1B)	49.5(8)
C(16)	C(17)	C(12)	118.89(19)	P(1A)	P(1B)	F(2B)	128.5(7)
O(14)	C(18)	C(19)	125.42(15)	P(1A)	P(1B)	F(3B)	130.4(8)
O(14)	C(18)	C(23)	114.71(14)	P(1A)	P(1B)	F(4B)	51.4(7)
C(19)	C(18)	C(23)	119.88(15)	P(1A)	P(1B)	F(5B)	64.1(8)
C(18)	C(19)	C(20)	120.11(16)	P(1A)	P(1B)	F(6B)	115.8(8)
C(21)	C(20)	C(19)	120.25(16)	F(2A)	P(1B)	F(1A)	84.5(3)
C(20)	C(21)	C(22)	120.25(16)	F(2A)	P(1B)	F(3A)	107.5(5)
C(23)	C(22)	C(21)	119.95(16)	F(2A)	P(1B)	F(4A)	146.5(6)
O(7)	C(23)	C(18)	115.44(14)	F(2A)	P(1B)	F(1B)	89.5(4)
O(7)	C(23)	C(22)	125.02(15)	F(2A)	P(1B)	F(2B)	39.6(5)
C(22)	C(23)	C(18)	119.54(15)	F(2A)	P(1B)	F(3B)	90.5(4)
O(7)	C(24)	C(25)	107.96(12)	F(2A)	P(1B)	F(4B)	140.3(5)
O(8)	C(25)	C(24)	113.04(13)	F(2A)	P(1B)	F(5B)	50.4(5)
O(8)	C(26)	C(27)	108.14(12)	F(2A)	P(1B)	F(6B)	129.7(5)
O(9)	C(27)	C(26)	108.39(12)	F(3A)	P(1B)	F(1A)	145.4(6)
O(9)	C(28)	C(29)	110.04(13)	F(3A)	P(1B)	F(4A)	82.8(3)
O(10)	C(29)	C(28)	109.24(13)	F(3A)	P(1B)	F(1B)	149.1(5)
O(10)	C(30)	C(31)	117.95(16)	F(3A)	P(1B)	F(2B)	119.7(5)
O(10)	C(30)	C(35)	122.43(15)	F(3A)	P(1B)	F(3B)	30.9(5)
C(31)	C(30)	C(35)	119.59(16)	F(3A)	P(1B)	F(4B)	60.4(5)
C(30)	C(31)	C(32)	121.23(18)	F(3A)	P(1B)	F(5B)	82.1(4)
C(33)	C(32)	C(31)	119.30(19)	F(3A)	P(1B)	F(6B)	97.9(4)

C(32)	C(33)	C(34)	120.50(19)	F(4A) P(1B) F(1A)	71.2(3)
C(33)	C(34)	C(35)	120.75(19)	F(6A) P(1B) F(1A)	85.9(4)
O(11)	C(35)	C(30)	117.07(15)	F(6A) P(1B) F(2A)	116.1(5)
O(11)	C(35)	C(34)	124.30(17)	F(6A) P(1B) F(3A)	115.1(5)
C(34)	C(35)	C(30)	118.61(17)	F(6A) P(1B) F(4A)	85.6(4)
O(11)	C(36)	C(37)	110.66(15)	F(6A) P(1B) F(1B)	77.5(5)
O(12)	C(37)	C(36)	110.93(17)	F(6A) P(1B) F(2B)	77.6(5)
O(12)	C(38)	C(39)	109.97(16)	F(6A) P(1B) F(3B)	102.6(5)
O(13)	C(39)	C(38)	110.00(16)	F(6A) P(1B) F(4B)	102.5(5)
O(13)	C(40)	C(41)	112.15(14)	F(6A) P(1B) F(5B)	162.2(5)
O(14)	C(41)	C(40)	106.86(14)	F(6A) P(1B) F(6B)	17.8(5)
O(3A)	N(5A)	C(14)	119.0(7)	F(1B) P(1B) F(1A)	8.5(4)
O(3A)	N(5A)	O(4A)	122.4(8)	F(1B) P(1B) F(4A)	69.6(4)
O(4A)	N(5A)	C(14)	118.5(6)	F(2B) P(1B) F(1A)	90.6(4)
O(5A)	N(6A)	C(16)	121.1(6)	F(2B) P(1B) F(4A)	156.1(5)
O(6A)	N(6A)	C(16)	114.3(6)	F(2B) P(1B) F(1B)	90.0
O(6A)	N(6A)	O(5A)	124.6(6)	F(2B) P(1B) F(4B)	179.96(7)
O(3B)	N(5B)	C(14)	116.4(13)	F(2B) P(1B) F(5B)	90.0
O(3B)	N(5B)	O(4B)	127.6(15)	F(2B) P(1B) F(6B)	90.0
O(4B)	N(5B)	C(14)	115.7(12)	F(3B) P(1B) F(1A)	171.4(4)
O(5B)	N(6B)	C(16)	110.4(12)	F(3B) P(1B) F(4A)	110.4(4)
O(6B)	N(6B)	C(16)	124.4(13)	F(3B) P(1B) F(1B)	180.0
O(6B)	N(6B)	O(5B)	125.2(11)	F(3B) P(1B) F(2B)	90.0
F(1A)	P(1A)	F(3A)	179.21(13)	F(3B) P(1B) F(4B)	90.0
F(1A)	P(1A)	F(4A)	90.03(12)	F(3B) P(1B) F(5B)	90.0
F(1A)	P(1A)	F(5A)	89.87(12)	F(3B) P(1B) F(6B)	90.0
F(1A)	P(1A)	F(6A)	89.73(12)	F(4B) P(1B) F(1A)	89.4(4)
F(1A)	P(1A)	F(2B)	89.0(4)	F(4B) P(1B) F(4A)	23.9(5)
F(1A)	P(1A)	F(6B)	100.2(4)	F(4B) P(1B) F(1B)	90.0
F(2A)	P(1A)	F(1A)	91.19(12)	F(4B) P(1B) F(5B)	90.0
F(2A)	P(1A)	F(3A)	89.55(10)	F(4B) P(1B) F(6B)	90.0
F(2A)	P(1A)	F(4A)	178.77(12)	F(5B) P(1B) F(1A)	81.5(4)
F(2A)	P(1A)	F(5A)	90.39(12)	F(5B) P(1B) F(4A)	102.0(5)
F(2A)	P(1A)	F(6A)	90.82(13)	F(5B) P(1B) F(1B)	90.0
F(2A)	P(1A)	F(2B)	31.0(4)	F(5B) P(1B) F(6B)	180.0
F(2A)	P(1A)	F(6B)	100.7(4)	F(6B) P(1B) F(1A)	98.5(4)
F(3A)	P(1A)	F(5A)	89.86(10)	F(6B) P(1B) F(4A)	78.0(5)
F(3A)	P(1A)	F(2B)	91.8(3)	F(6B) P(1B) F(1B)	90.0
F(3A)	P(1A)	F(6B)	79.9(4)	P(1A) F(1B) P(1B)	19.0(4)
F(4A)	P(1A)	F(3A)	89.22(10)	F(2A) F(2B) P(1A)	53.3(5)
F(4A)	P(1A)	F(5A)	89.56(9)	F(2A) F(2B) P(1B)	59.8(5)
F(4A)	P(1A)	F(6A)	89.23(10)	P(1B) F(2B) P(1A)	12.7(2)
F(4A)	P(1A)	F(2B)	149.1(4)	F(3A) F(3B) P(1A)	50.9(6)
F(4A)	P(1A)	F(6B)	79.1(4)	F(3A) F(3B) P(1B)	62.4(6)
F(5A)	P(1A)	F(2B)	121.3(4)	P(1B) F(3B) P(1A)	12.3(2)

F(5A)	P(1A)	F(6B)	164.8(4)	P(1A)	F(4B)	F(3A)	68.9(5)
F(6A)	P(1A)	F(3A)	90.53(11)	P(1A)	F(4B)	P(1B)	19.3(4)
F(6A)	P(1A)	F(5A)	178.73(11)	F(3A)	F(4B)	P(1B)	53.9(3)
F(6A)	P(1A)	F(2B)	59.9(4)	F(4A)	F(4B)	P(1A)	95.1(9)
F(6A)	P(1A)	F(6B)	14.6(4)	F(4A)	F(4B)	F(3A)	150.5(11)
P(1B)	P(1A)	F(1A)	121.4(7)	F(4A)	F(4B)	P(1B)	103.9(8)
P(1B)	P(1A)	F(2A)	58.7(6)	P(1A)	F(5B)	P(1B)	20.4(4)
P(1B)	P(1A)	F(3A)	59.3(7)	F(2A)	F(5B)	P(1A)	71.8(4)
P(1B)	P(1A)	F(4A)	120.6(7)	F(2A)	F(5B)	P(1B)	56.8(4)
P(1B)	P(1A)	F(5A)	133.7(7)	F(5A)	F(5B)	P(1A)	77.3(8)
P(1B)	P(1A)	F(6A)	47.5(7)	F(5A)	F(5B)	F(2A)	144.3(9)
P(1B)	P(1A)	F(1B)	111.4(9)	F(5A)	F(5B)	P(1B)	96.3(7)
P(1B)	P(1A)	F(2B)	38.8(6)	F(6A)	F(6B)	P(1A)	50.0(11)
P(1B)	P(1A)	F(4B)	109.2(9)	F(6A)	F(6B)	P(1B)	48.5(11)
P(1B)	P(1A)	F(5B)	95.4(10)	P(1B)	F(6B)	P(1A)	15.3(3)
P(1B)	P(1A)	F(6B)	48.8(6)	O(15)	C(42)	C(43)	122.5(2)
F(1B)	P(1A)	F(1A)	13.1(6)	O(15)	C(42)	C(44)	121.7(2)
F(1B)	P(1A)	F(2A)	92.6(5)	C(44)	C(42)	C(43)	115.8(2)
F(1B)	P(1A)	F(3A)	167.1(5)				

[1]-X,2-Y,-Z

Table 3S. Torsion angles for **6n**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ni(1)	N(1)	C(1)	C(5)[1]	-33.21(14)	F(5A)	P(1A)	P(1B)	F(4B)	-92.3(11)
Ni(1)	N(1)	C(2)	C(3)	-5.6(2)	F(5A)	P(1A)	P(1B)	F(5B)	20.4(5)
Ni(1)	N(2)	C(4)	C(3)	4.8(2)	F(5A)	P(1A)	P(1B)	F(6B)	-159.6(5)
Ni(1)	N(2)	C(5)	C(1)[1]	31.76(14)	F(5A)	P(1A)	F(1B)	P(1B)	-148.2(9)
O(7)	C(24)	C(25)	O(8)	-71.69(16)	F(5A)	P(1A)	F(4B)	F(3A)	96.2(4)
O(8)	C(26)	C(27)	O(9)	-58.66(15)	F(5A)	P(1A)	F(4B)	F(4A)	-109.4(9)
O(9)	C(28)	C(29)	O(10)	-66.63(16)	F(5A)	P(1A)	F(4B)	P(1B)	132.5(8)
O(10)	C(30)	C(31)	C(32)	177.46(17)	F(5A)	P(1A)	F(5B)	F(2A)	162.1(8)
O(10)	C(30)	C(35)	O(11)	5.2(2)	F(5A)	P(1A)	F(5B)	P(1B)	-158.0(6)
O(10)	C(30)	C(35)	C(34)	-176.42(17)	F(5A)	P(1A)	F(6B)	F(6A)	-175.6(5)
O(11)	C(36)	C(37)	O(12)	-81.20(19)	F(5A)	P(1A)	F(6B)	P(1B)	106.3(16)
O(12)	C(38)	C(39)	O(13)	73.8(2)	F(6A)	P(1A)	F(1A)	P(1B)	37.4(8)
O(13)	C(40)	C(41)	O(14)	72.44(17)	F(6A)	P(1A)	F(2A)	P(1B)	36.9(8)
O(14)	C(18)	C(19)	C(20)	-178.73(14)	F(6A)	P(1A)	F(2A)	F(2B)	-3.7(7)
O(14)	C(18)	C(23)	O(7)	-2.79(19)	F(6A)	P(1A)	F(2A)	F(5B)	168.4(6)
O(14)	C(18)	C(23)	C(22)	177.59(13)	F(6A)	P(1A)	F(3A)	P(1B)	-37.6(8)
N(1)	Ni(1)	N(2)	C(4)	-13.36(13)	F(6A)	P(1A)	F(3A)	F(3B)	-53.2(8)
N(1)[1]	Ni(1)	N(2)	C(4)	166.64(13)	F(6A)	P(1A)	F(3A)	F(4B)	101.8(7)
N(1)	Ni(1)	N(2)	C(5)	168.52(10)	F(6A)	P(1A)	F(4A)	P(1B)	-37.5(8)
N(1)[1]	Ni(1)	N(2)	C(5)	-11.48(10)	F(6A)	P(1A)	F(4A)	F(4B)	-112.9(10)
N(1)	C(2)	C(3)	C(4)	-8.1(2)	F(6A)	P(1A)	P(1B)	F(1A)	-55.5(8)
N(1)	C(2)	C(3)	C(6)	173.67(14)	F(6A)	P(1A)	P(1B)	F(2A)	-125.5(8)
N(2)	Ni(1)	N(1)	C(1)	-166.91(10)	F(6A)	P(1A)	P(1B)	F(3A)	124.0(8)

N(2)[1]	Ni(1)	N(1)	C(1)	13.08(10)	F(6A)	P(1A)	P(1B)	F(4A)	55.7(9)
N(2)	Ni(1)	N(1)	C(2)	13.82(13)	F(6A)	P(1A)	P(1B)	F(1B)	-46.0(11)
N(2)[1]	Ni(1)	N(1)	C(2)	-166.18(13)	F(6A)	P(1A)	P(1B)	F(2B)	-93.1(10)
N(3)	C(7)	C(8)	C(9)	-164.63(13)	F(6A)	P(1A)	P(1B)	F(3B)	134.0(11)
N(4)	C(12)	C(13)	C(14)	-179.54(17)	F(6A)	P(1A)	P(1B)	F(4B)	86.9(10)
N(4)	C(12)	C(17)	C(16)	179.30(17)	F(6A)	P(1A)	P(1B)	F(5B)	-160.4(5)
C(1)	N(1)	C(2)	C(3)	175.19(13)	F(6A)	P(1A)	P(1B)	F(6B)	19.6(5)
C(2)	N(1)	C(1)	C(5)[1]	146.12(13)	F(6A)	P(1A)	F(1B)	P(1B)	33.0(9)
C(2)	C(3)	C(4)	N(2)	8.5(2)	F(6A)	P(1A)	F(4B)	F(3A)	-84.7(4)
C(2)	C(3)	C(6)	N(3)	-7.8(2)	F(6A)	P(1A)	F(4B)	F(4A)	69.6(9)
C(4)	N(2)	C(5)	C(1)[1]	-146.51(13)	F(6A)	P(1A)	F(4B)	P(1B)	-48.5(8)
C(4)	C(3)	C(6)	N(3)	173.92(14)	F(6A)	P(1A)	F(5B)	F(2A)	-17.8(8)
C(5)	N(2)	C(4)	C(3)	-177.14(13)	F(6A)	P(1A)	F(5B)	F(5A)	-179.87(18)
C(6)	N(3)	C(7)	C(8)	108.00(16)	F(6A)	P(1A)	F(5B)	P(1B)	22.2(6)
C(6)	C(3)	C(4)	N(2)	-173.19(14)	F(6A)	P(1A)	F(6B)	P(1B)	-78.1(18)
C(7)	N(3)	C(6)	C(3)	178.64(14)	F(6A)	P(1B)	F(1B)	P(1A)	-137.7(11)
C(7)	C(8)	C(9)	C(10)	176.31(14)	F(6A)	P(1B)	F(2B)	P(1A)	-111.1(12)
C(8)	C(9)	C(10)	O(1)	-168.12(13)	F(6A)	P(1B)	F(2B)	F(2A)	-166.4(10)
C(10)	O(1)	C(11)	O(2)	4.9(3)	F(6A)	P(1B)	F(3B)	P(1A)	137.8(11)
C(10)	O(1)	C(11)	N(4)	-174.93(14)	F(6A)	P(1B)	F(3B)	F(3A)	118.3(9)
C(11)	O(1)	C(10)	C(9)	173.38(14)	F(6A)	P(1B)	F(4B)	P(1A)	111.0(12)
C(11)	N(4)	C(12)	C(13)	9.3(3)	F(6A)	P(1B)	F(4B)	F(3A)	-112.0(6)
C(11)	N(4)	C(12)	C(17)	-170.66(17)	F(6A)	P(1B)	F(4B)	F(4A)	46.2(10)
C(12)	N(4)	C(11)	O(1)	173.98(16)	F(6A)	P(1B)	F(5B)	P(1A)	-88.6(19)
C(12)	N(4)	C(11)	O(2)	-5.8(3)	F(6A)	P(1B)	F(5B)	F(2A)	44.6(18)
C(12)	C(13)	C(14)	C(15)	0.3(3)	F(6A)	P(1B)	F(5B)	F(5A)	-110.2(18)
C(12)	C(13)	C(14)	N(5A)	-176.9(6)	F(6A)	P(1B)	F(6B)	P(1A)	88.7(19)
C(12)	C(13)	C(14)	N(5B)	172.6(13)	P(1B)	P(1A)	F(2A)	F(2B)	-40.6(8)
C(13)	C(12)	C(17)	C(16)	-0.7(3)	P(1B)	P(1A)	F(2A)	F(5B)	131.5(11)
C(13)	C(14)	C(15)	C(16)	-0.7(3)	P(1B)	P(1A)	F(3A)	F(3B)	-15.5(8)
C(13)	C(14)	N(5A)	O(3A)	-0.5(14)	P(1B)	P(1A)	F(3A)	F(4B)	139.5(12)
C(13)	C(14)	N(5A)	O(4A)	-177.9(9)	P(1B)	P(1A)	F(4A)	F(4B)	-75.4(12)
C(13)	C(14)	N(5B)	O(3B)	9(2)	P(1B)	P(1A)	F(5A)	F(5B)	-31.1(8)
C(13)	C(14)	N(5B)	O(4B)	-177.6(13)	P(1B)	P(1A)	F(6A)	F(6B)	-88.8(19)
C(14)	C(15)	C(16)	C(17)	0.4(3)	P(1B)	P(1A)	F(4B)	F(3A)	-36.3(11)
C(14)	C(15)	C(16)	N(6A)	177.7(5)	P(1B)	P(1A)	F(4B)	F(4A)	118.1(11)
C(14)	C(15)	C(16)	N(6B)	-174.9(10)	P(1B)	P(1A)	F(5B)	F(2A)	-40.0(9)
C(15)	C(14)	N(5A)	O(3A)	-177.8(9)	P(1B)	P(1A)	F(5B)	F(5A)	158.0(6)
C(15)	C(14)	N(5A)	O(4A)	4.8(14)	P(1B)	P(1A)	F(6B)	F(6A)	78.1(18)
C(15)	C(14)	N(5B)	O(3B)	-178.3(15)	P(1B)	F(2A)	F(2B)	P(1A)	-13.0(3)
C(15)	C(14)	N(5B)	O(4B)	-5(2)	P(1B)	F(2A)	F(5B)	P(1A)	15.5(4)
C(15)	C(16)	C(17)	C(12)	0.2(3)	P(1B)	F(2A)	F(5B)	F(5A)	46.6(15)
C(15)	C(16)	N(6A)	O(5A)	-5.6(12)	P(1B)	F(3A)	F(3B)	P(1A)	-5.2(3)
C(15)	C(16)	N(6A)	O(6A)	173.8(7)	P(1B)	F(3A)	F(4B)	P(1A)	14.0(4)
C(15)	C(16)	N(6B)	O(5B)	-20.3(18)	P(1B)	F(3A)	F(4B)	F(4A)	-47(2)

C(15)	C(16)	N(6B)	O(6B)	162.7(11)	P(1B)	F(4A)	F(4B)	P(1A)	-17.5(3)
C(17)	C(12)	C(13)	C(14)	0.4(3)	P(1B)	F(4A)	F(4B)	F(3A)	37.5(18)
C(17)	C(16)	N(6A)	O(5A)	171.7(8)	P(1B)	F(5A)	F(5B)	P(1A)	-7.6(2)
C(17)	C(16)	N(6A)	O(6A)	-8.8(10)	P(1B)	F(5A)	F(5B)	F(2A)	-37.7(12)
C(17)	C(16)	N(6B)	O(5B)	163.8(12)	P(1B)	F(6A)	F(6B)	P(1A)	-20.2(5)
C(17)	C(16)	N(6B)	O(6B)	-13.2(16)	F(1B)	P(1A)	F(1A)	P(1B)	43(2)
C(18)	O(14)	C(41)	C(40)	172.27(13)	F(1B)	P(1A)	F(2A)	P(1B)	113.6(10)
C(18)	C(19)	C(20)	C(21)	0.5(2)	F(1B)	P(1A)	F(2A)	F(2B)	73.1(6)
C(19)	C(18)	C(23)	O(7)	177.50(13)	F(1B)	P(1A)	F(2A)	F(5B)	-114.8(6)
C(19)	C(18)	C(23)	C(22)	-2.1(2)	F(1B)	P(1A)	F(3A)	P(1B)	-46(2)
C(19)	C(20)	C(21)	C(22)	-0.7(2)	F(1B)	P(1A)	F(3A)	F(3B)	-62(3)
C(20)	C(21)	C(22)	C(23)	-0.5(2)	F(1B)	P(1A)	F(3A)	F(4B)	93(2)
C(21)	C(22)	C(23)	O(7)	-177.70(14)	F(1B)	P(1A)	F(4A)	P(1B)	-114.3(10)
C(21)	C(22)	C(23)	C(18)	1.9(2)	F(1B)	P(1A)	F(4A)	F(4B)	170.4(13)
C(23)	O(7)	C(24)	C(25)	175.93(12)	F(1B)	P(1A)	F(5A)	P(1B)	137.4(12)
C(23)	C(18)	C(19)	C(20)	0.9(2)	F(1B)	P(1A)	F(5A)	F(5B)	106.3(8)
C(24)	O(7)	C(23)	C(18)	172.60(13)	F(1B)	P(1A)	F(6A)	P(1B)	-136.5(12)
C(24)	O(7)	C(23)	C(22)	-7.8(2)	F(1B)	P(1A)	F(6A)	F(6B)	134.7(18)
C(25)	O(8)	C(26)	C(27)	-171.50(12)	F(1B)	P(1A)	P(1B)	F(1A)	-9.5(5)
C(26)	O(8)	C(25)	C(24)	-82.02(15)	F(1B)	P(1A)	P(1B)	F(2A)	-79.5(8)
C(27)	O(9)	C(28)	C(29)	-172.26(12)	F(1B)	P(1A)	P(1B)	F(3A)	170.0(5)
C(28)	O(9)	C(27)	C(26)	175.05(12)	F(1B)	P(1A)	P(1B)	F(4A)	101.7(9)
C(29)	O(10)	C(30)	C(31)	116.04(17)	F(1B)	P(1A)	P(1B)	F(6A)	46.0(11)
C(29)	O(10)	C(30)	C(35)	-65.9(2)	F(1B)	P(1A)	P(1B)	F(2B)	-47.2(12)
C(30)	O(10)	C(29)	C(28)	-149.07(14)	F(1B)	P(1A)	P(1B)	F(3B)	-180.0
C(30)	C(31)	C(32)	C(33)	-0.3(3)	F(1B)	P(1A)	P(1B)	F(4B)	132.8(12)
C(31)	C(30)	C(35)	O(11)	-176.79(16)	F(1B)	P(1A)	P(1B)	F(5B)	-114.4(9)
C(31)	C(30)	C(35)	C(34)	1.6(3)	F(1B)	P(1A)	P(1B)	F(6B)	65.6(9)
C(31)	C(32)	C(33)	C(34)	0.3(3)	F(1B)	P(1A)	F(4B)	F(3A)	-165.3(6)
C(32)	C(33)	C(34)	C(35)	0.7(3)	F(1B)	P(1A)	F(4B)	F(4A)	-11.0(15)
C(33)	C(34)	C(35)	O(11)	176.64(19)	F(1B)	P(1A)	F(4B)	P(1B)	-129.1(13)
C(33)	C(34)	C(35)	C(30)	-1.6(3)	F(1B)	P(1A)	F(5B)	F(2A)	75.3(8)
C(35)	O(11)	C(36)	C(37)	-160.59(15)	F(1B)	P(1A)	F(5B)	F(5A)	-86.7(9)
C(35)	C(30)	C(31)	C(32)	-0.7(3)	F(1B)	P(1A)	F(5B)	P(1B)	115.3(11)
C(36)	O(11)	C(35)	C(30)	167.21(16)	F(1B)	P(1A)	F(6B)	F(6A)	-43.9(18)
C(36)	O(11)	C(35)	C(34)	-11.1(3)	F(1B)	P(1A)	F(6B)	P(1B)	-121.9(10)
C(37)	O(12)	C(38)	C(39)	-177.91(16)	F(1B)	P(1B)	F(2B)	P(1A)	-33.9(11)
C(38)	O(12)	C(37)	C(36)	-164.09(15)	F(1B)	P(1B)	F(2B)	F(2A)	-89.2(7)
C(39)	O(13)	C(40)	C(41)	96.65(17)	F(1B)	P(1B)	F(4B)	P(1A)	33.9(11)
C(40)	O(13)	C(39)	C(38)	-174.81(15)	F(1B)	P(1B)	F(4B)	F(3A)	170.9(5)
C(41)	O(14)	C(18)	C(19)	7.2(2)	F(1B)	P(1B)	F(4B)	F(4A)	-30.9(11)
C(41)	O(14)	C(18)	C(23)	-172.46(13)	F(1B)	P(1B)	F(5B)	P(1A)	-43.8(8)
N(5A)	C(14)	C(15)	C(16)	176.4(7)	F(1B)	P(1B)	F(5B)	F(2A)	89.3(6)
N(6A)	C(16)	C(17)	C(12)	-176.8(5)	F(1B)	P(1B)	F(5B)	F(5A)	-65.4(7)
N(5B)	C(14)	C(15)	C(16)	-173.4(12)	F(1B)	P(1B)	F(6B)	P(1A)	43.8(8)

N(6B)	C(16)	C(17)	C(12)	176.2(8)	F(1B)	P(1B)	F(6B)	F(6A)	-44.8(18)
P(1A)	F(2A)	P(1B)	F(1A)	-41.5(6)	F(2B)	P(1A)	F(1A)	P(1B)	-22.5(8)
P(1A)	F(2A)	P(1B)	F(3A)	105.3(9)	F(2B)	P(1A)	F(2A)	P(1B)	40.6(8)
P(1A)	F(2A)	P(1B)	F(4A)	1.51(18)	F(2B)	P(1A)	F(2A)	F(5B)	172.1(10)
P(1A)	F(2A)	P(1B)	F(6A)	-124.2(12)	F(2B)	P(1A)	F(3A)	P(1B)	22.2(8)
P(1A)	F(2A)	P(1B)	F(1B)	-48.4(8)	F(2B)	P(1A)	F(3A)	F(3B)	6.7(8)
P(1A)	F(2A)	P(1B)	F(2B)	-139.0(8)	F(2B)	P(1A)	F(3A)	F(4B)	161.7(5)
P(1A)	F(2A)	P(1B)	F(3B)	131.5(8)	F(2B)	P(1A)	F(4A)	P(1B)	-39.1(8)
P(1A)	F(2A)	P(1B)	F(4B)	40.9(8)	F(2B)	P(1A)	F(4A)	F(4B)	-114.5(11)
P(1A)	F(2A)	P(1B)	F(5B)	42.0(10)	F(2B)	P(1A)	F(5A)	P(1B)	47.1(8)
P(1A)	F(2A)	P(1B)	F(6B)	-138.0(10)	F(2B)	P(1A)	F(5A)	F(5B)	16.0(7)
P(1A)	F(2A)	F(2B)	P(1B)	13.0(3)	F(2B)	P(1A)	F(6A)	P(1B)	-46.3(8)
P(1A)	F(2A)	F(5B)	F(5A)	31.0(13)	F(2B)	P(1A)	F(6A)	F(6B)	-135.1(18)
P(1A)	F(2A)	F(5B)	P(1B)	-15.5(4)	F(2B)	P(1A)	P(1B)	F(1A)	37.7(11)
P(1A)	F(3A)	P(1B)	F(1A)	0.63(17)	F(2B)	P(1A)	P(1B)	F(2A)	-32.3(6)
P(1A)	F(3A)	P(1B)	F(2A)	-105.6(9)	F(2B)	P(1A)	P(1B)	F(3A)	-142.8(11)
P(1A)	F(3A)	P(1B)	F(4A)	41.6(7)	F(2B)	P(1A)	P(1B)	F(4A)	148.8(6)
P(1A)	F(3A)	P(1B)	F(6A)	123.3(12)	F(2B)	P(1A)	P(1B)	F(6A)	93.1(10)
P(1A)	F(3A)	P(1B)	F(1B)	14.9(7)	F(2B)	P(1A)	P(1B)	F(1B)	47.2(12)
P(1A)	F(3A)	P(1B)	F(2B)	-147.0(10)	F(2B)	P(1A)	P(1B)	F(3B)	-132.8(12)
P(1A)	F(3A)	P(1B)	F(3B)	-165.1(7)	F(2B)	P(1A)	P(1B)	F(4B)	180.0
P(1A)	F(3A)	P(1B)	F(4B)	32.9(10)	F(2B)	P(1A)	P(1B)	F(5B)	-67.3(9)
P(1A)	F(3A)	P(1B)	F(5B)	-61.6(9)	F(2B)	P(1A)	P(1B)	F(6B)	112.7(9)
P(1A)	F(3A)	P(1B)	F(6B)	118.4(9)	F(2B)	P(1A)	F(1B)	P(1B)	-27.5(8)
P(1A)	F(3A)	F(3B)	P(1B)	5.2(3)	F(2B)	P(1A)	F(4B)	F(3A)	-36.3(11)
P(1A)	F(3A)	F(4B)	F(4A)	-61(2)	F(2B)	P(1A)	F(4B)	F(4A)	118.1(11)
P(1A)	F(3A)	F(4B)	P(1B)	-14.0(4)	F(2B)	P(1A)	F(4B)	P(1B)	0.0
P(1A)	F(4A)	F(4B)	F(3A)	55.0(18)	F(2B)	P(1A)	F(5B)	F(2A)	-4.1(5)
P(1A)	F(4A)	F(4B)	P(1B)	17.5(3)	F(2B)	P(1A)	F(5B)	F(5A)	-166.2(6)
P(1A)	F(5A)	F(5B)	F(2A)	-30.1(12)	F(2B)	P(1A)	F(5B)	P(1B)	35.9(6)
P(1A)	F(5A)	F(5B)	P(1B)	7.6(2)	F(2B)	P(1A)	F(6B)	F(6A)	40.3(17)
P(1A)	F(6A)	P(1B)	F(1A)	35.4(7)	F(2B)	P(1A)	F(6B)	P(1B)	-37.7(7)
P(1A)	F(6A)	P(1B)	F(2A)	117.2(11)	F(2B)	F(2A)	P(1B)	P(1A)	139.0(8)
P(1A)	F(6A)	P(1B)	F(3A)	-116.0(11)	F(2B)	F(2A)	P(1B)	F(1A)	97.6(7)
P(1A)	F(6A)	P(1B)	F(4A)	-36.0(7)	F(2B)	F(2A)	P(1B)	F(3A)	-115.7(6)
P(1A)	F(6A)	P(1B)	F(1B)	34.1(9)	F(2B)	F(2A)	P(1B)	F(4A)	140.5(8)
P(1A)	F(6A)	P(1B)	F(2B)	126.9(9)	F(2B)	F(2A)	P(1B)	F(6A)	14.8(11)
P(1A)	F(6A)	P(1B)	F(3B)	-145.9(9)	F(2B)	F(2A)	P(1B)	F(1B)	90.6(5)
P(1A)	F(6A)	P(1B)	F(4B)	-53.1(9)	F(2B)	F(2A)	P(1B)	F(3B)	-89.5(5)
P(1A)	F(6A)	P(1B)	F(5B)	80.2(19)	F(2B)	F(2A)	P(1B)	F(4B)	179.9
P(1A)	F(6A)	P(1B)	F(6B)	-99.7(19)	F(2B)	F(2A)	P(1B)	F(5B)	-179.0(9)
P(1A)	F(6A)	F(6B)	P(1B)	20.2(5)	F(2B)	F(2A)	P(1B)	F(6B)	1.0(9)
P(1A)	P(1B)	F(2B)	F(2A)	-55.3(10)	F(2B)	F(2A)	F(5B)	P(1A)	18(2)
P(1A)	P(1B)	F(3B)	F(3A)	-19.4(10)	F(2B)	F(2A)	F(5B)	F(5A)	49(3)
P(1A)	P(1B)	F(4B)	F(3A)	137.0(13)	F(2B)	F(2A)	F(5B)	P(1B)	2.2(19)

P(1A)	P(1B)	F(4B)	F(4A)	-64.8(11)	F(2B)	P(1B)	F(1B) P(1A) 145.0(10)
P(1A)	P(1B)	F(5B)	F(2A)	133.2(10)	F(2B)	P(1B)	F(3B) P(1A) -145.0(10)
P(1A)	P(1B)	F(5B)	F(5A)	-21.6(6)	F(2B)	P(1B)	F(3B) F(3A) -164.4(9)
P(1A)	P(1B)	F(6B)	F(6A)	-88.7(19)	F(2B)	P(1B)	F(5B) P(1A) -133.8(8)
F(1A)	P(1A)	F(2A)	P(1B)	126.6(8)	F(2B)	P(1B)	F(5B) F(2A) -0.6(6)
F(1A)	P(1A)	F(2A)	F(2B)	86.1(7)	F(2B)	P(1B)	F(5B) F(5A) -155.4(7)
F(1A)	P(1A)	F(2A)	F(5B)	-101.8(6)	F(2B)	P(1B)	F(6B) P(1A) 133.8(8)
F(1A)	P(1A)	F(4A)	P(1B)	-127.2(8)	F(2B)	P(1B)	F(6B) F(6A) 45.1(18)
F(1A)	P(1A)	F(4A)	F(4B)	157.4(10)	F(3B)	F(3A)	P(1B) P(1A) 165.1(7)
F(1A)	P(1A)	F(5A)	P(1B)	135.8(9)	F(3B)	F(3A)	P(1B) F(1A) 165.7(8)
F(1A)	P(1A)	F(5A)	F(5B)	104.8(6)	F(3B)	F(3A)	P(1B) F(2A) 59.4(10)
F(1A)	P(1A)	F(6A)	P(1B)	-135.3(8)	F(3B)	F(3A)	P(1B) F(4A) -153.3(8)
F(1A)	P(1A)	F(6A)	F(6B)	135.9(17)	F(3B)	F(3A)	P(1B) F(6A) -71.6(11)
F(1A)	P(1A)	P(1B)	F(2A)	-70.0(7)	F(3B)	F(3A)	P(1B) F(1B) 179.9
F(1A)	P(1A)	P(1B)	F(3A)	179.49(14)	F(3B)	F(3A)	P(1B) F(2B) 18.0(10)
F(1A)	P(1A)	P(1B)	F(4A)	111.2(7)	F(3B)	F(3A)	P(1B) F(4B) -162.0(10)
F(1A)	P(1A)	P(1B)	F(6A)	55.5(8)	F(3B)	F(3A)	P(1B) F(5B) 103.4(8)
F(1A)	P(1A)	P(1B)	F(1B)	9.5(5)	F(3B)	F(3A)	P(1B) F(6B) -76.6(8)
F(1A)	P(1A)	P(1B)	F(2B)	-37.7(11)	F(3B)	F(3A)	F(4B) P(1A) 48.8(19)
F(1A)	P(1A)	P(1B)	F(3B)	-170.5(5)	F(3B)	F(3A)	F(4B) F(4A) -12(4)
F(1A)	P(1A)	P(1B)	F(4B)	142.3(11)	F(3B)	F(3A)	F(4B) P(1B) 34.8(16)
F(1A)	P(1A)	P(1B)	F(5B)	-104.9(7)	F(3B)	P(1B)	F(2B) P(1A) 146.1(11)
F(1A)	P(1A)	P(1B)	F(6B)	75.1(7)	F(3B)	P(1B)	F(2B) F(2A) 90.8(7)
F(1A)	P(1A)	F(1B)	P(1B)	-141(2)	F(3B)	P(1B)	F(4B) P(1A) -146.1(11)
F(1A)	P(1A)	F(4B)	F(3A)	179.89(14)	F(3B)	P(1B)	F(4B) F(3A) -9.1(5)
F(1A)	P(1A)	F(4B)	F(4A)	-25.8(12)	F(3B)	P(1B)	F(4B) F(4A) 149.1(11)
F(1A)	P(1A)	F(4B)	P(1B)	-143.9(11)	F(3B)	P(1B)	F(5B) P(1A) 136.1(8)
F(1A)	P(1A)	F(5B)	F(2A)	83.2(4)	F(3B)	P(1B)	F(5B) F(2A) -90.7(6)
F(1A)	P(1A)	F(5B)	F(5A)	-78.9(5)	F(3B)	P(1B)	F(5B) F(5A) 114.5(7)
F(1A)	P(1A)	F(5B)	P(1B)	123.2(7)	F(3B)	P(1B)	F(6B) P(1A) -136.1(8)
F(1A)	P(1A)	F(6B)	F(6A)	-45.0(16)	F(3B)	P(1B)	F(6B) F(6A) 135.2(18)
F(1A)	P(1A)	F(6B)	P(1B)	-123.0(7)	F(4B)	P(1A)	F(1A) P(1B) 139.3(12)
F(1A)	P(1B)	F(1B)	P(1A)	51(3)	F(4B)	P(1A)	F(2A) P(1B) -75.3(11)
F(1A)	P(1B)	F(2B)	P(1A)	-25.4(9)	F(4B)	P(1A)	F(2A) F(2B) -115.8(11)
F(1A)	P(1B)	F(2B)	F(2A)	-80.7(7)	F(4B)	P(1A)	F(2A) F(5B) 56.3(10)
F(1A)	P(1B)	F(4B)	P(1A)	25.4(9)	F(4B)	P(1A)	F(3A) P(1B) -139.5(12)
F(1A)	P(1B)	F(4B)	F(3A)	162.3(6)	F(4B)	P(1A)	F(3A) F(3B) -155.0(12)
F(1A)	P(1B)	F(4B)	F(4A)	-39.5(9)	F(4B)	P(1A)	F(4A) P(1B) 75.4(12)
F(1A)	P(1B)	F(5B)	P(1A)	-43.2(6)	F(4B)	P(1A)	F(5A) P(1B) -105.7(12)
F(1A)	P(1B)	F(5B)	F(2A)	89.9(5)	F(4B)	P(1A)	F(5A) F(5B) -136.8(9)
F(1A)	P(1B)	F(5B)	F(5A)	-64.9(6)	F(4B)	P(1A)	F(6A) P(1B) 106.4(11)
F(1A)	P(1B)	F(6B)	P(1A)	43.2(6)	F(4B)	P(1A)	F(6A) F(6B) 17.7(16)
F(1A)	P(1B)	F(6B)	F(6A)	-45.4(17)	F(4B)	P(1A)	P(1B) F(1A) -142.3(11)
F(2A)	P(1A)	F(1A)	P(1B)	-53.4(8)	F(4B)	P(1A)	P(1B) F(2A) 147.7(6)
F(2A)	P(1A)	F(3A)	P(1B)	53.2(8)	F(4B)	P(1A)	P(1B) F(3A) 37.2(11)

F(2A)	P(1A)	F(3A)	F(3B)	37.6(8)	F(4B)	P(1A)	P(1B) F(4A) -31.2(6)
F(2A)	P(1A)	F(3A)	F(4B)	-167.3(6)	F(4B)	P(1A)	P(1B) F(6A) -86.9(10)
F(2A)	P(1A)	F(5A)	P(1B)	44.7(9)	F(4B)	P(1A)	P(1B) F(1B) -132.8(12)
F(2A)	P(1A)	F(5A)	F(5B)	13.6(6)	F(4B)	P(1A)	P(1B) F(2B) 180.0
F(2A)	P(1A)	F(6A)	P(1B)	-44.1(8)	F(4B)	P(1A)	P(1B) F(3B) 47.2(12)
F(2A)	P(1A)	F(6A)	F(6B)	-132.9(17)	F(4B)	P(1A)	P(1B) F(5B) 112.7(9)
F(2A)	P(1A)	P(1B)	F(1A)	70.0(7)	F(4B)	P(1A)	P(1B) F(6B) -67.3(9)
F(2A)	P(1A)	P(1B)	F(3A)	-110.5(7)	F(4B)	P(1A)	F(1B) P(1B) 128.0(13)
F(2A)	P(1A)	P(1B)	F(4A)	-178.82(13)	F(4B)	P(1A)	F(5B) F(2A) -152.6(6)
F(2A)	P(1A)	P(1B)	F(6A)	125.5(8)	F(4B)	P(1A)	F(5B) F(5A) 45.4(10)
F(2A)	P(1A)	P(1B)	F(1B)	79.5(8)	F(4B)	P(1A)	F(5B) P(1B) -112.6(11)
F(2A)	P(1A)	P(1B)	F(2B)	32.3(6)	F(4B)	P(1A)	F(6B) F(6A) -162.6(16)
F(2A)	P(1A)	P(1B)	F(3B)	-100.5(8)	F(4B)	P(1A)	F(6B) P(1B) 119.3(10)
F(2A)	P(1A)	P(1B)	F(4B)	-147.7(6)	F(4B)	F(3A)	P(1B) P(1A) -32.9(10)
F(2A)	P(1A)	P(1B)	F(5B)	-34.9(7)	F(4B)	F(3A)	P(1B) F(1A) -32.3(10)
F(2A)	P(1A)	P(1B)	F(6B)	145.1(7)	F(4B)	F(3A)	P(1B) F(2A) -138.5(7)
F(2A)	P(1A)	F(1B)	P(1B)	-57.3(8)	F(4B)	F(3A)	P(1B) F(4A) 8.7(6)
F(2A)	P(1A)	F(4B)	F(3A)	24.8(11)	F(4B)	F(3A)	P(1B) F(6A) 90.4(7)
F(2A)	P(1A)	F(4B)	F(4A)	179.2(2)	F(4B)	F(3A)	P(1B) F(1B) -18.0(10)
F(2A)	P(1A)	F(4B)	P(1B)	61.1(10)	F(4B)	F(3A)	P(1B) F(2B) -180.0
F(2A)	P(1A)	F(5B)	F(5A)	-162.1(8)	F(4B)	F(3A)	P(1B) F(3B) 162.0(10)
F(2A)	P(1A)	F(5B)	P(1B)	40.0(9)	F(4B)	F(3A)	P(1B) F(5B) -94.5(3)
F(2A)	P(1A)	F(6B)	F(6A)	48.2(17)	F(4B)	F(3A)	P(1B) F(6B) 85.4(3)
F(2A)	P(1A)	F(6B)	P(1B)	-29.9(7)	F(4B)	F(3A)	F(3B) P(1A) -36.6(14)
F(2A)	P(1B)	F(1B)	P(1A)	105.4(10)	F(4B)	F(3A)	F(3B) P(1B) -31.4(14)
F(2A)	P(1B)	F(2B)	P(1A)	55.3(10)	F(4B)	P(1B)	F(1B) P(1A) -35.0(10)
F(2A)	P(1B)	F(3B)	P(1A)	-105.4(10)	F(4B)	P(1B)	F(3B) P(1A) 35.0(10)
F(2A)	P(1B)	F(3B)	F(3A)	-124.8(9)	F(4B)	P(1B)	F(3B) F(3A) 15.6(9)
F(2A)	P(1B)	F(4B)	P(1A)	-55.3(10)	F(4B)	P(1B)	F(5B) P(1A) 46.1(8)
F(2A)	P(1B)	F(4B)	F(3A)	81.7(7)	F(4B)	P(1B)	F(5B) F(2A) 179.3(6)
F(2A)	P(1B)	F(4B)	F(4A)	-120.1(11)	F(4B)	P(1B)	F(5B) F(5A) 24.5(7)
F(2A)	P(1B)	F(5B)	P(1A)	-133.2(10)	F(4B)	P(1B)	F(6B) P(1A) -46.1(8)
F(2A)	P(1B)	F(5B)	F(5A)	-154.8(10)	F(4B)	P(1B)	F(6B) F(6A) -134.8(18)
F(2A)	P(1B)	F(6B)	P(1A)	133.2(10)	F(5B)	P(1A)	F(1A) P(1B) -102.6(11)
F(2A)	P(1B)	F(6B)	F(6A)	44.5(18)	F(5B)	P(1A)	F(2A) P(1B) -131.5(11)
F(3A)	P(1A)	F(2A)	P(1B)	-53.6(8)	F(5B)	P(1A)	F(2A) F(2B) -172.1(10)
F(3A)	P(1A)	F(2A)	F(2B)	-94.2(7)	F(5B)	P(1A)	F(3A) P(1B) 102.2(11)
F(3A)	P(1A)	F(2A)	F(5B)	77.9(6)	F(5B)	P(1A)	F(3A) F(3B) 86.7(10)
F(3A)	P(1A)	F(4A)	P(1B)	53.0(8)	F(5B)	P(1A)	F(3A) F(4B) -118.3(6)
F(3A)	P(1A)	F(4A)	F(4B)	-22.3(10)	F(5B)	P(1A)	F(4A) P(1B) 129.9(12)
F(3A)	P(1A)	F(5A)	P(1B)	-44.9(9)	F(5B)	P(1A)	F(4A) F(4B) 54.6(11)
F(3A)	P(1A)	F(5A)	F(5B)	-76.0(6)	F(5B)	P(1A)	F(5A) P(1B) 31.1(8)
F(3A)	P(1A)	F(6A)	P(1B)	45.4(8)	F(5B)	P(1A)	F(6A) P(1B) -30.6(8)
F(3A)	P(1A)	F(6A)	F(6B)	-43.3(17)	F(5B)	P(1A)	F(6A) F(6B) -119.4(17)
F(3A)	P(1A)	P(1B)	F(1A)	-179.49(14)	F(5B)	P(1A)	P(1B) F(1A) 104.9(7)

F(3A)	P(1A)	P(1B)	F(2A)	110.5(7)	F(5B)	P(1A)	P(1B) F(2A) 34.9(7)
F(3A)	P(1A)	P(1B)	F(4A)	-68.3(7)	F(5B)	P(1A)	P(1B) F(3A) -75.6(7)
F(3A)	P(1A)	P(1B)	F(6A)	-124.0(8)	F(5B)	P(1A)	P(1B) F(4A) -143.9(8)
F(3A)	P(1A)	P(1B)	F(1B)	-170.0(5)	F(5B)	P(1A)	P(1B) F(6A) 160.4(5)
F(3A)	P(1A)	P(1B)	F(2B)	142.8(11)	F(5B)	P(1A)	P(1B) F(1B) 114.4(9)
F(3A)	P(1A)	P(1B)	F(3B)	10.0(5)	F(5B)	P(1A)	P(1B) F(2B) 67.3(9)
F(3A)	P(1A)	P(1B)	F(4B)	-37.2(11)	F(5B)	P(1A)	P(1B) F(3B) -65.6(9)
F(3A)	P(1A)	P(1B)	F(5B)	75.6(7)	F(5B)	P(1A)	P(1B) F(4B) -112.7(9)
F(3A)	P(1A)	P(1B)	F(6B)	-104.4(7)	F(5B)	P(1A)	P(1B) F(6B) -180.0
F(3A)	P(1A)	F(1B)	P(1B)	42.0(19)	F(5B)	P(1A)	F(1B) P(1B) -104.8(13)
F(3A)	P(1A)	F(4B)	F(4A)	154.4(12)	F(5B)	P(1A)	F(4B) F(3A) 67.0(7)
F(3A)	P(1A)	F(4B)	P(1B)	36.3(11)	F(5B)	P(1A)	F(4B) F(4A) -138.6(10)
F(3A)	P(1A)	F(5B)	F(2A)	-97.6(4)	F(5B)	P(1A)	F(4B) P(1B) 103.3(13)
F(3A)	P(1A)	F(5B)	F(5A)	100.4(5)	F(5B)	P(1A)	F(6B) F(6A) 78.1(18)
F(3A)	P(1A)	F(5B)	P(1B)	-57.6(7)	F(5B)	P(1A)	F(6B) P(1B) 0.0
F(3A)	P(1A)	F(6B)	F(6A)	135.8(17)	F(5B)	F(2A)	P(1B) P(1A) -42.0(10)
F(3A)	P(1A)	F(6B)	P(1B)	57.7(7)	F(5B)	F(2A)	P(1B) F(1A) -83.4(5)
F(3A)	P(1B)	F(1B)	P(1A)	-19.4(10)	F(5B)	F(2A)	P(1B) F(3A) 63.3(8)
F(3A)	P(1B)	F(2B)	P(1A)	136.9(13)	F(5B)	F(2A)	P(1B) F(4A) -40.5(10)
F(3A)	P(1B)	F(2B)	F(2A)	81.6(7)	F(5B)	F(2A)	P(1B) F(6A) -166.2(6)
F(3A)	P(1B)	F(3B)	P(1A)	19.4(10)	F(5B)	F(2A)	P(1B) F(1B) -90.4(4)
F(3A)	P(1B)	F(4B)	P(1A)	-137.0(13)	F(5B)	F(2A)	P(1B) F(2B) 179.0(9)
F(3A)	P(1B)	F(4B)	F(4A)	158.2(13)	F(5B)	F(2A)	P(1B) F(3B) 89.5(4)
F(3A)	P(1B)	F(5B)	P(1A)	106.2(9)	F(5B)	F(2A)	P(1B) F(4B) -1.1(9)
F(3A)	P(1B)	F(5B)	F(2A)	-120.6(8)	F(5B)	F(2A)	P(1B) F(6B) -180.0
F(3A)	P(1B)	F(5B)	F(5A)	84.6(7)	F(5B)	F(2A)	F(2B) P(1A) -15(2)
F(3A)	P(1B)	F(6B)	P(1A)	-106.2(9)	F(5B)	F(2A)	F(2B) P(1B) -2.1(19)
F(3A)	P(1B)	F(6B)	F(6A)	165(2)	F(5B)	P(1B)	F(1B) P(1A) 55.0(10)
F(4A)	P(1A)	F(1A)	P(1B)	126.6(8)	F(5B)	P(1B)	F(2B) P(1A) 56.1(11)
F(4A)	P(1A)	F(3A)	P(1B)	-126.9(8)	F(5B)	P(1B)	F(2B) F(2A) 0.8(7)
F(4A)	P(1A)	F(3A)	F(3B)	-142.4(8)	F(5B)	P(1B)	F(3B) P(1A) -55.0(10)
F(4A)	P(1A)	F(3A)	F(4B)	12.6(6)	F(5B)	P(1B)	F(3B) F(3A) -74.4(9)
F(4A)	P(1A)	F(5A)	P(1B)	-134.1(9)	F(5B)	P(1B)	F(4B) P(1A) -56.1(11)
F(4A)	P(1A)	F(5A)	F(5B)	-165.2(6)	F(5B)	P(1B)	F(4B) F(3A) 80.9(5)
F(4A)	P(1A)	F(6A)	P(1B)	134.7(9)	F(5B)	P(1B)	F(4B) F(4A) -120.9(11)
F(4A)	P(1A)	F(6A)	F(6B)	45.9(17)	F(6B)	P(1A)	F(1A) P(1B) 47.7(8)
F(4A)	P(1A)	P(1B)	F(1A)	-111.2(7)	F(6B)	P(1A)	F(2A) P(1B) 26.0(6)
F(4A)	P(1A)	P(1B)	F(2A)	178.82(13)	F(6B)	P(1A)	F(2A) F(2B) -14.5(6)
F(4A)	P(1A)	P(1B)	F(3A)	68.3(7)	F(6B)	P(1A)	F(2A) F(5B) 157.6(6)
F(4A)	P(1A)	P(1B)	F(6A)	-55.7(9)	F(6B)	P(1A)	F(3A) P(1B) -47.8(8)
F(4A)	P(1A)	P(1B)	F(1B)	-101.7(9)	F(6B)	P(1A)	F(3A) F(3B) -63.3(8)
F(4A)	P(1A)	P(1B)	F(2B)	-148.8(6)	F(6B)	P(1A)	F(3A) F(4B) 91.7(5)
F(4A)	P(1A)	P(1B)	F(3B)	78.3(9)	F(6B)	P(1A)	F(4A) P(1B) -26.9(7)
F(4A)	P(1A)	P(1B)	F(4B)	31.2(6)	F(6B)	P(1A)	F(4A) F(4B) -102.2(11)
F(4A)	P(1A)	P(1B)	F(5B)	143.9(8)	F(6B)	P(1A)	F(5A) P(1B) -92.4(17)

F(4A)	P(1A)	P(1B)	F(6B)	-36.1(7)	F(6B)	P(1A)	F(5A)	F(5B)	-123.5(15)
F(4A)	P(1A)	F(1B)	P(1B)	122.5(8)	F(6B)	P(1A)	F(6A)	P(1B)	88.8(19)
F(4A)	P(1A)	F(4B)	F(3A)	-154.4(12)	F(6B)	P(1A)	P(1B)	F(1A)	-75.1(7)
F(4A)	P(1A)	F(4B)	P(1B)	-118.1(11)	F(6B)	P(1A)	P(1B)	F(2A)	-145.1(7)
F(4A)	P(1A)	F(5B)	F(2A)	-178.45(15)	F(6B)	P(1A)	P(1B)	F(3A)	104.4(7)
F(4A)	P(1A)	F(5B)	F(5A)	19.5(8)	F(6B)	P(1A)	P(1B)	F(4A)	36.1(8)
F(4A)	P(1A)	F(5B)	P(1B)	-138.5(9)	F(6B)	P(1A)	P(1B)	F(6A)	-19.6(5)
F(4A)	P(1A)	F(6B)	F(6A)	-133.0(17)	F(6B)	P(1A)	P(1B)	F(1B)	-65.6(9)
F(4A)	P(1A)	F(6B)	P(1B)	148.9(7)	F(6B)	P(1A)	P(1B)	F(2B)	-112.7(9)
F(4A)	P(1B)	F(1B)	P(1A)	-47.8(8)	F(6B)	P(1A)	P(1B)	F(3B)	114.4(9)
F(4A)	P(1B)	F(2B)	P(1A)	-64.7(11)	F(6B)	P(1A)	P(1B)	F(4B)	67.3(9)
F(4A)	P(1B)	F(2B)	F(2A)	-120.0(11)	F(6B)	P(1A)	P(1B)	F(5B)	180.0
F(4A)	P(1B)	F(3B)	P(1A)	47.8(8)	F(6B)	P(1A)	F(1B)	P(1B)	43.4(8)
F(4A)	P(1B)	F(3B)	F(3A)	28.4(8)	F(6B)	P(1A)	F(4B)	F(3A)	-80.3(5)
F(4A)	P(1B)	F(4B)	P(1A)	64.8(11)	F(6B)	P(1A)	F(4B)	F(4A)	74.0(11)
F(4A)	P(1B)	F(4B)	F(3A)	-158.2(13)	F(6B)	P(1A)	F(4B)	P(1B)	-44.1(8)
F(4A)	P(1B)	F(5B)	P(1A)	25.3(6)	F(6B)	P(1A)	F(5B)	F(2A)	-40.0(9)
F(4A)	P(1B)	F(5B)	F(2A)	158.5(6)	F(6B)	P(1A)	F(5B)	F(5A)	158.0(6)
F(4A)	P(1B)	F(5B)	F(5A)	3.7(6)	F(6B)	P(1A)	F(5B)	P(1B)	0.0
F(4A)	P(1B)	F(6B)	P(1A)	-25.3(6)	F(6B)	F(6A)	P(1B)	P(1A)	99.7(19)
F(4A)	P(1B)	F(6B)	F(6A)	-114.0(19)	F(6B)	F(6A)	P(1B)	F(1A)	135.1(17)
F(5A)	P(1A)	F(1A)	P(1B)	-143.8(8)	F(6B)	F(6A)	P(1B)	F(2A)	-143.1(15)
F(5A)	P(1A)	F(2A)	P(1B)	-143.5(8)	F(6B)	F(6A)	P(1B)	F(3A)	-16(2)
F(5A)	P(1A)	F(2A)	F(2B)	175.9(7)	F(6B)	F(6A)	P(1B)	F(4A)	63.7(19)
F(5A)	P(1A)	F(2A)	F(5B)	-12.0(6)	F(6B)	F(6A)	P(1B)	F(1B)	133.8(18)
F(5A)	P(1A)	F(3A)	P(1B)	143.6(8)	F(6B)	F(6A)	P(1B)	F(2B)	-133.5(18)
F(5A)	P(1A)	F(3A)	F(3B)	128.0(8)	F(6B)	F(6A)	P(1B)	F(3B)	-46.2(18)
F(5A)	P(1A)	F(3A)	F(4B)	-76.9(6)	F(6B)	F(6A)	P(1B)	F(4B)	46.6(18)
F(5A)	P(1A)	F(4A)	P(1B)	142.9(8)	F(6B)	F(6A)	P(1B)	F(5B)	179.9
F(5A)	P(1A)	F(4A)	F(4B)	67.5(10)	F(6B)	P(1B)	F(1B)	P(1A)	-125.0(10)
F(5A)	P(1A)	P(1B)	F(1A)	125.3(9)	F(6B)	P(1B)	F(2B)	P(1A)	-123.9(11)
F(5A)	P(1A)	P(1B)	F(2A)	55.3(9)	F(6B)	P(1B)	F(2B)	F(2A)	-179.2(7)
F(5A)	P(1A)	P(1B)	F(3A)	-55.2(9)	F(6B)	P(1B)	F(3B)	P(1A)	125.0(10)
F(5A)	P(1A)	P(1B)	F(4A)	-123.5(9)	F(6B)	P(1B)	F(3B)	F(3A)	105.5(9)
F(5A)	P(1A)	P(1B)	F(6A)	-179.21(17)	F(6B)	P(1B)	F(4B)	P(1A)	123.9(11)
F(5A)	P(1A)	P(1B)	F(1B)	134.8(12)	F(6B)	P(1B)	F(4B)	F(3A)	-99.1(5)
F(5A)	P(1A)	P(1B)	F(2B)	87.7(11)	F(6B)	P(1B)	F(4B)	F(4A)	59.1(11)
F(5A)	P(1A)	P(1B)	F(3B)	-45.2(12)					

[1]-X,2-Y,-Z

Table 4S. Bond lengths for **6nCl**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Ni1	N1	1.8526(14)	O7	C24	1.432(2)
Ni1	N1[1]	1.8526(14)	O8	C25	1.423(2)
Ni1	N2[1]	1.8566(14)	O8	C26	1.422(2)
Ni1	N2	1.8567(14)	O9	C27	1.424(2)

O1	C10	1.456(2)	O9	C28	1.424(2)
O1	C11	1.343(2)	O10	C29	1.438(2)
O2	C11	1.210(2)	O10	C30	1.375(2)
O3	N5	1.2041(19)	O11	C35	1.374(2)
O4	N5	1.208(2)	O11	C36	1.433(2)
O5	N6	1.2241(19)	O12	C37	1.415(2)
O6	N6	1.2281(19)	O12	C38	1.420(2)
N1	C1	1.474(2)	O13	C39	1.417(2)
N1	C2	1.294(2)	O13	C40	1.424(2)
N2	C4	1.299(2)	O14	C18	1.370(2)
N2	C5[1]	1.472(2)	O14	C41	1.434(2)
N3	C6	1.300(2)	C18	C19	1.382(3)
N3	C7	1.457(2)	C18	C23	1.404(3)
N4	C11	1.363(2)	C19	C20	1.390(3)
N4	C12	1.397(2)	C20	C21	1.373(3)
N5	C14	1.477(2)	C21	C22	1.390(3)
N6	C16	1.476(2)	C22	C23	1.387(3)
C1	C5	1.510(2)	C24	C25	1.490(3)
C2	C3	1.422(2)	C26	C27	1.492(2)
C3	C4	1.419(2)	C28	C29	1.500(2)
C3	C6	1.402(2)	C30	C31	1.381(2)
C5	N2[1]	1.472(2)	C30	C35	1.404(2)
C7	C8	1.516(2)	C31	C32	1.393(3)
C8	C9	1.521(2)	C32	C33	1.368(3)
C9	C10	1.506(2)	C33	C34	1.386(3)
C12	C13	1.395(2)	C34	C35	1.383(2)
C12	C17	1.400(2)	C36	C37	1.491(3)
C13	C14	1.377(2)	C38	C39	1.492(3)
C14	C15	1.379(2)	C40	C41	1.499(3)
C15	C16	1.382(2)	N7	C42	1.134(3)
C16	C17	1.371(2)	C42	C43	1.442(3)
O7	C23	1.371(2)			

[1]1-X,1-Y,1-Z

Table 5S. Valence angles for **6nCl**.

Atom	**Atom**	**Atom**	**Angle/°**	**Atom**	**Atom**	**Atom**	**Angle/°**
N1	Ni1	N1[1]	180.0	C17	C16	N6	118.27(15)
N1[1]	Ni1	N2[1]	93.69(6)	C17	C16	C15	123.76(16)
N1	Ni1	N2[1]	86.31(6)	C16	C17	C12	119.07(16)
N1	Ni1	N2	93.68(6)	C23	O7	C24	116.27(14)
N1[1]	Ni1	N2	86.32(6)	C26	O8	C25	110.57(13)
N2[1]	Ni1	N2	180.0	C27	O9	C28	112.49(13)
C11	O1	C10	116.36(13)	C30	O10	C29	115.99(13)
C1	N1	Ni1	113.09(11)	C35	O11	C36	115.20(13)
C2	N1	Ni1	127.54(12)	C37	O12	C38	111.37(14)
C2	N1	C1	119.36(14)	C39	O13	C40	112.60(13)

C4	N2	Ni1	126.78(12)	C18	O14	C41	116.76(14)
C4	N2	C5[1]	120.06(14)	O14	C18	C19	124.72(17)
C5[1]	N2	Ni1	113.11(11)	O14	C18	C23	115.52(16)
C6	N3	C7	123.74(15)	C19	C18	C23	119.75(17)
C11	N4	C12	125.01(15)	C18	C19	C20	120.16(19)
O3	N5	O4	122.78(16)	C21	C20	C19	120.26(19)
O3	N5	C14	118.63(16)	C20	C21	C22	120.17(19)
O4	N5	C14	118.57(15)	C23	C22	C21	120.14(19)
O5	N6	O6	124.26(15)	O7	C23	C18	115.88(15)
O5	N6	C16	117.74(15)	O7	C23	C22	124.61(17)
O6	N6	C16	118.00(14)	C22	C23	C18	119.51(17)
N1	C1	C5	106.38(13)	O7	C24	C25	108.89(15)
N1	C2	C3	124.12(15)	O8	C25	C24	111.11(15)
C4	C3	C2	121.15(15)	O8	C26	C27	108.39(14)
C6	C3	C2	121.50(15)	O9	C27	C26	108.30(14)
C6	C3	C4	117.35(15)	O9	C28	C29	114.52(15)
N2	C4	C3	124.56(15)	O10	C29	C28	108.16(14)
N2[1]	C5	C1	106.58(14)	O10	C30	C31	124.42(16)
N3	C6	C3	127.00(16)	O10	C30	C35	115.98(15)
N3	C7	C8	112.14(14)	C31	C30	C35	119.57(16)
C7	C8	C9	111.15(14)	C30	C31	C32	119.99(17)
C10	C9	C8	113.51(15)	C33	C32	C31	120.44(17)
O1	C10	C9	107.89(14)	C32	C33	C34	120.06(18)
O1	C11	N4	109.03(15)	C35	C34	C33	120.41(18)
O2	C11	O1	124.82(15)	O11	C35	C30	116.12(15)
O2	C11	N4	126.15(17)	O11	C35	C34	124.32(16)
N4	C12	C17	117.51(16)	C34	C35	C30	119.53(16)
C13	C12	N4	123.22(15)	O11	C36	C37	109.68(15)
C13	C12	C17	119.24(16)	O12	C37	C36	109.27(15)
C14	C13	C12	118.36(16)	O12	C38	C39	109.19(15)
C13	C14	N5	117.56(15)	O13	C39	C38	108.81(14)
C13	C14	C15	124.38(16)	O13	C40	C41	112.94(15)
C15	C14	N5	118.07(16)	O14	C41	C40	107.75(15)
C14	C15	C16	115.19(16)	N7	C42	C43	179.5(2)
C15	C16	N6	117.97(15)				

[1]1-X,1-Y,1-Z

Table 6S. Torsion angles for **6nCl**.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
Ni1	N1	C1	C5	-32.96(16)	C15	C16	C17	C12	0.3(3)
Ni1	N1	C2	C3	-4.0(2)	C17	C12	C13	C14	0.6(2)
Ni1	N2	C4	C3	6.8(3)	O7	C24	C25	O8	-73.88(18)
O3	N5	C14	C13	1.7(3)	O8	C26	C27	O9	67.13(18)
O3	N5	C14	C15	-178.75(18)	O9	C28	C29	O10	69.53(18)
O4	N5	C14	C13	-176.68(19)	O10	C30	C31	C32	-178.32(16)
O4	N5	C14	C15	2.9(3)	O10	C30	C35	O11	0.7(2)

O5	N6	C16	C15	1.8(2)	O10	C30	C35	C34	178.75(15)
O5	N6	C16	C17	-177.63(16)	O11	C36	C37	O12	-76.16(19)
O6	N6	C16	C15	-178.37(15)	O12	C38	C39	O13	67.79(19)
O6	N6	C16	C17	2.2(2)	O13	C40	C41	O14	71.99(18)
N1	Ni1	N2	C4	-14.08(15)	O14	C18	C19	C20	-178.96(17)
N1[1]	Ni1	N2	C4	165.92(15)	O14	C18	C23	O7	-1.1(2)
N1[1]	Ni1	N2	C51	-11.64(12)	O14	C18	C23	C22	179.09(16)
N1	Ni1	N2	C51	168.36(12)	C18	O14	C41	C40	172.12(14)
N1	C1	C5	N21	40.00(18)	C18	C19	C20	C21	0.0(3)
N1	C2	C3	C4	-8.4(3)	C19	C18	C23	O7	-179.71(16)
N1	C2	C3	C6	172.06(16)	C19	C18	C23	C22	0.5(3)
N2	Ni1	N1	C1	-167.13(12)	C19	C20	C21	C22	0.6(3)
N2[1]	Ni1	N1	C1	12.87(12)	C20	C21	C22	C23	-0.6(3)
N2[1]	Ni1	N1	C2	-167.23(15)	C21	C22	C23	O7	-179.74(17)
N2	Ni1	N1	C2	12.77(15)	C21	C22	C23	C18	0.0(3)
N3	C7	C8	C9	-178.28(14)	C23	O7	C24	C25	-178.32(14)
N4	C12	C13	C14	-177.03(17)	C23	C18	C19	C20	-0.5(3)
N4	C12	C17	C16	176.85(16)	C24	O7	C23	C18	170.94(15)
N5	C14	C15	C16	179.50(15)	C24	O7	C23	C22	-9.3(2)
N6	C16	C17	C12	179.72(15)	C25	O8	C26	C27	173.60(14)
C1	N1	C2	C3	175.91(15)	C26	O8	C25	C24	-159.94(15)
C2	N1	C1	C5	147.13(15)	C27	O9	C28	C29	79.63(18)
C2	C3	C4	N2	7.0(3)	C28	O9	C27	C26	178.92(14)
C2	C3	C6	N3	-6.6(3)	C29	O10	C30	C31	13.0(2)
C4	C3	C6	N3	173.87(16)	C29	O10	C30	C35	-165.39(15)
C5[1]	N2	C4	C3	-175.81(16)	C30	O10	C29	C28	168.97(14)
C6	N3	C7	C8	115.83(18)	C30	C31	C32	C33	-0.1(3)
C6	C3	C4	N2	-173.53(16)	C31	C30	C35	O11	-177.74(15)
C7	N3	C6	C3	175.49(16)	C31	C30	C35	C34	0.3(3)
C7	C8	C9	C10	176.89(14)	C31	C32	C33	C34	-0.2(3)
C8	C9	C10	O1	-77.04(18)	C32	C33	C34	C35	0.5(3)
C10	O1	C11	O2	-10.2(2)	C33	C34	C35	O11	177.35(16)
C10	O1	C11	N4	169.62(14)	C33	C34	C35	C30	-0.5(3)
C11	O1	C10	C9	156.23(14)	C35	O11	C36	C37	-173.18(14)
C11	N4	C12	C13	-21.6(3)	C35	C30	C31	C32	0.0(3)
C11	N4	C12	C17	160.76(17)	C36	O11	C35	C30	164.99(15)
C12	N4	C11	O1	175.90(16)	C36	O11	C35	C34	-13.0(2)
C12	N4	C11	O2	-4.3(3)	C37	O12	C38	C39	178.44(15)
C12	C13	C14	N5	179.91(15)	C38	O12	C37	C36	-173.53(15)
C12	C13	C14	C15	0.4(3)	C39	O13	C40	C41	92.77(18)
C13	C12	C17	C16	-0.9(2)	C40	O13	C39	C38	178.28(15)
C13	C14	C15	C16	-0.9(3)	C41	O14	C18	C19	10.1(2)
C14	C15	C16	N6	-178.81(15)	C41	O14	C18	C23	-168.40(15)
C14	C15	C16	C17	0.6(3)					

[1]1-X,1-Y,1-Z

Table 7S. The geometry of hydrogen bonds in the crystal of **6n**.

D–H	A	d(D···A) (Å)	< D–H···A (°)
N3–H3	O8	2.971(2)	148
N3–H3	O9^{i}	2.999(2)	127
N4–H4	O15	2.894(2)	150
C1–H1A	O6A^{ii}	3.195(8)	133
C2–H2	O9	3.374(2)	149
C6–H6	O12	3.250(8)	160
C13–H13	O2*	2.830(2)	122
C17–H17	O15	3.225(3)	138
C24–H24A	O5A^{ii}	3.202(10)	123
C29–H29A	O11*	2.968(2)	104
C39–H39A	O4A^{iii}	3.503(8)	158
C39–H39B	O4A^{iv}	3.274(8)	148
C39–H39B	N5A^{iv}	3.495(12)	152
C43–H43C	O4A^{iii}	3.174(8)	125

Symmetry codes: (ii) $x, y + 1, z - 1$; (iii) $-x, -y, -z + 1$; (iv) $x, y + 1, z$; (*) intramolecular interaction.

Table 8S. The geometry of π–π interactions in the crystal of **6n**.

*Cg*I	*Cg*J	*Cg*I···*Cg*J (Å)	Dihedral angle (°)	Interplanar distance (Å)	Offset (Å)
5	5^{iii}	3.730(2)	0	3.445(2)	1.430(2)

Symmetry code: (iii) $-x, -y, -z + 1$.
*Cg*5 represents the centre of gravity of the C12–C17 aromatic ring (Figs 1Sa and 2a).
*Cg*I···*Cg*J is the distance between ring centroids.
The dihedral angle is the angle between the mean planes of *Cg*I and *Cg*J.
The interplanar distance is the perpendicular distance from *Cg*I to ring J.
The offset is the perpendicular distance from ring I to ring J.

Table 9S. The geometry of Ni···π interactions in the crystal of **6n**.

*Cg*I	MeJ	*Cg*I···MeJ (Å)	MeJ_Perp	Beta (°)
6	Ni1	3.639	3.446	18.72
6	Ni1^{i}	3.639	3.446	18.72

Symmetry code: (i) $-x, -y + 2, -z$.
*Cg*6 represents the centre of gravity of the C18–C23 aromatic ring (Figs 1Sa and 2a).
*Cg*I···MeJ is the distance between ring centroid and the atom of metal.
MeJ_Perp is the perpendicular distance from the atom of metal to ring centroid.
Beta is the angle between CgI→Me vector and normal to plane J.

Table 10S. The geometry of the P−F···π interactions in the crystal of **6n**.

Y−X	*Cg*I	d(X··· *Cg*I) (Å)	< Y−X···*Cg*I (°)
P1A−F3A	5^{v}	3.483(2)	152.5(2)
P1B−F3B	5^{v}	3.639(11)	129.4(6)

Symmetry code: (v) $-x + 1, -y, -z + 1$.
*Cg*5 represents the centre of gravity of the C12–C17 aromatic ring (Figs 1Sa and 2a).

Table 11S. The geometry of hydrogen bonds in the crystal of **6nCl**.

D–H	A	d(D···A) (Å)	< D–H···A (°)
N3–H3	O8	3.107(2)	157(2)
N3–H3	O9	3.097(2)	128.8(19)
N4–H4A	Cl1^{ii}	3.133(2)	165(2)
C1–H1A	Cl1	3.474(2)	137
C2–H2	O8	3.226(2)	136
C4–H4	O3^{iii}	3.360(2)	156
C5–H5A	O3^{iv}	3.462(2)	152
C13–H13	O2*	2.856(2)	117
C17–H17	Cl1^{ii}	3.476(2)	134
C25–H25A	O11^{v}	3.337(2)	138
C25–H25B	O10^{v}	3.237(2)	128
C29–H29B	N7	3.487(3)	161
C32–H32	O4^{vi}	3.160(3)	121
C36–H36A	O2^{iii}	3.213(2)	128
C40–H40A	Cl1^{ii}	3.566(2)	142

Symmetry codes: (ii) $x + 1/2, -y + 1/2, z - 1/2$; (iii) $x - 1/2, -y + 1/2, z - 1/2$; (iv) $-x + 3/2, y + 1/2, -z + 3/2$; (v) $x + 1/2, -y + 1/2, z + 1/2$; (vi) $x - 3/2, -y + 1/2, z - 1/2$; (*) intramolecular interaction.

Table 12S. The geometry of Ni···π interactions in the crystal of **6nCl**.

***Cg*I**	**MeJ**	***Cg*I···MeJ (Å)**	**MeJ_Perp**	**Beta (°)**
6	Ni1	3.852	–3.415	27.55
6	Ni1^{i}	3.852	–3.415	27.55

Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.
*Cg*6 represents the centre of gravity of the C18–C23 aromatic ring (Figs 1Sb and 2b).
*Cg*I···MeJ is the distance between ring centroid and the atom of metal.
MeJ_Perp is the perpendicular distance from the atom of metal to ring centroid.
Beta is the angle between CgI→Me vector and normal to plane J.

Table 13S. The geometry of the Y−X···π interactions in the crystal of **6nCl**.

Y−X	***Cg*I**	**d(X··· *Cg*I) (Å)**	**< Y−X···*Cg*I (°)**
C11−O2	5^{vii}	3.162(2)	110.45(11)

Symmetry code: (vii) $-x + 2, -y, -z + 1$.
*Cg*5 represents the centre of gravity of the C12–C17 aromatic ring (Figs 1Sb and 2b).

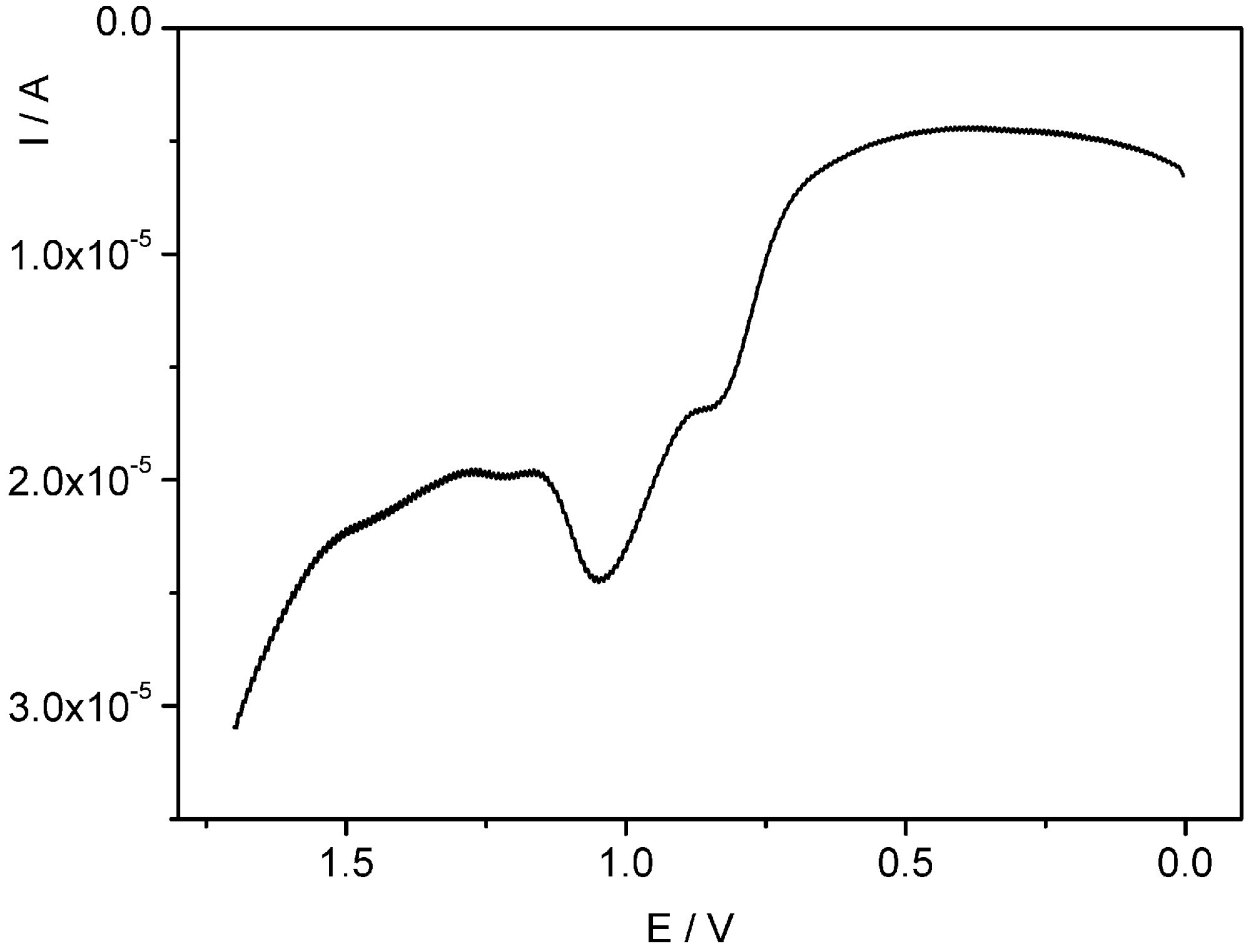


Figure 18S. Square wave voltammogram recorded on GCE in 0.1 M TBAHFP/DMF solution of **5n** ($4.5 \cdot 10^{-4}$ mol·dm^3) in the presence of excess of triethylamine, frequency = 100 Hz, reference electrode: Ag/AgCl in methanol.

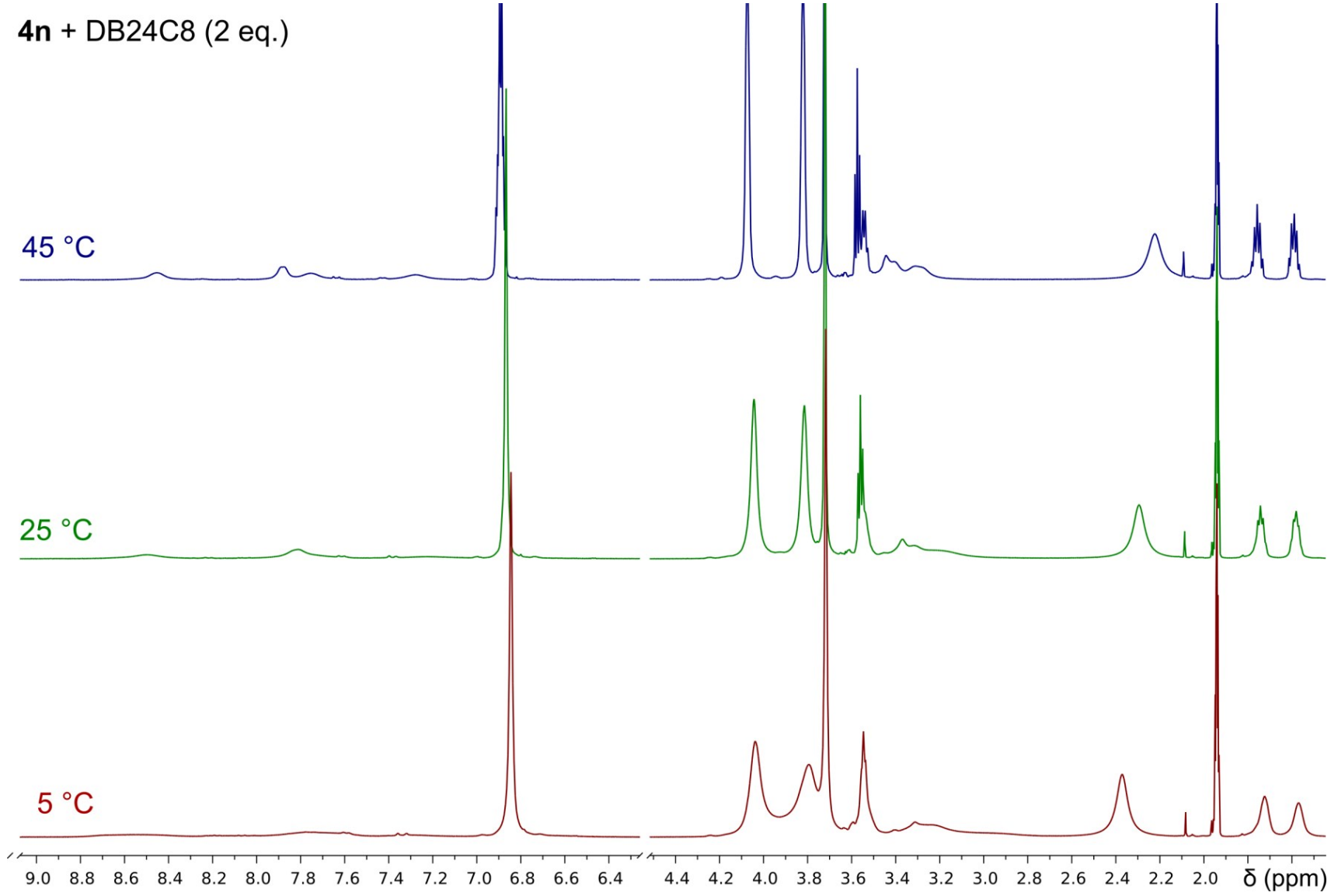


Figure 19S. ^{1}H NMR spectra (600 MHz) of a mixture of **4n** and DB24C8 (1:2 molar ratio, C_{DB24C8} = 19 g/l) in CD_3CN. The signals are broadened and averaged, proving that the mixture of substrates is in dynamic equilibrium with products: [2]- and [3]pseudorotaxane (see also: Figure 20S).

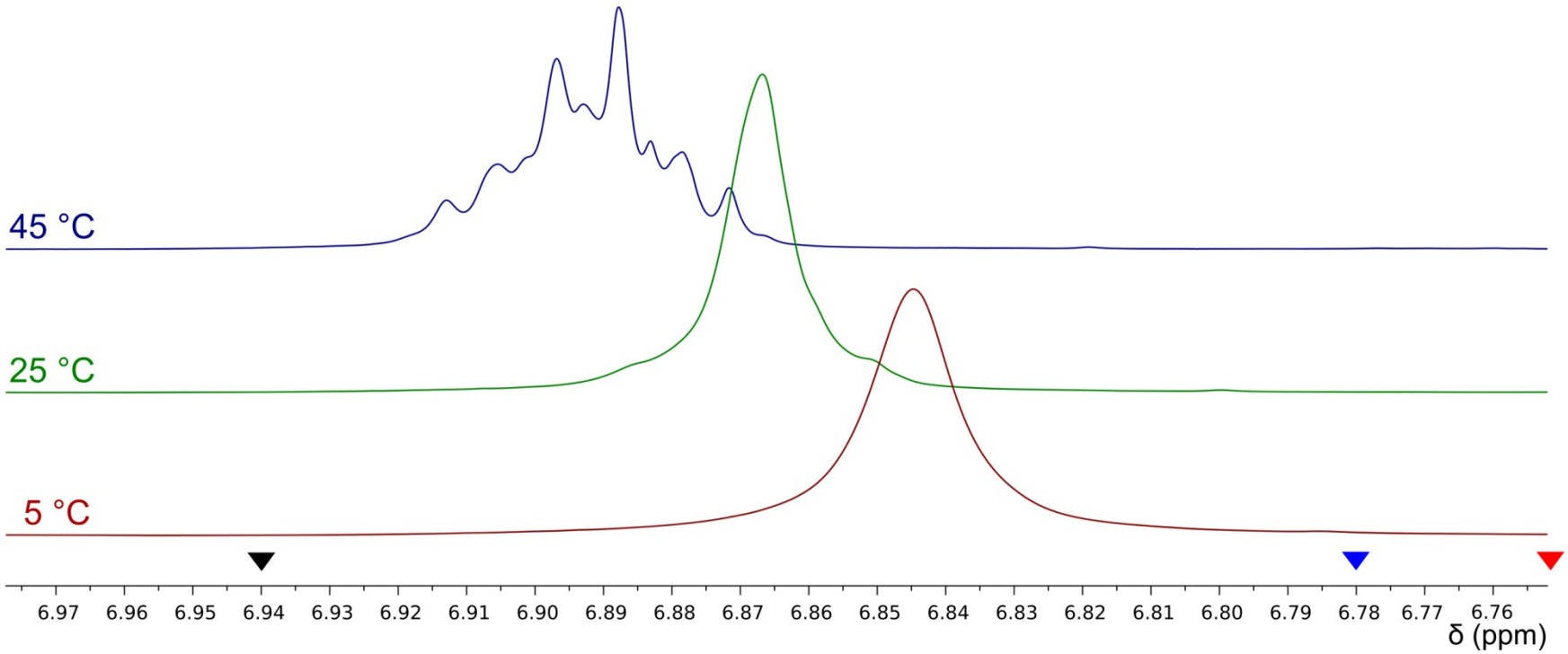


Figure 20S. The signals of aromatic protons of DB24C8 from Figure 19S. The amount of pseudorotaxanes rises when temperature decreases, as evidenced by the progressive broadening and shift of DB24C8 aromatic signal. Black triangle marks the chemical shift of H_{Ar} signal of pure DB24C8 in CD_3CN. Blue and red triangles mark the position of H_{Ar} signals in [3]rotaxane **6n**, and [2]rotaxane **5n**, respectively.