

Supporting Information

Mono- and Di-Cationic Hydrido Boron Compounds

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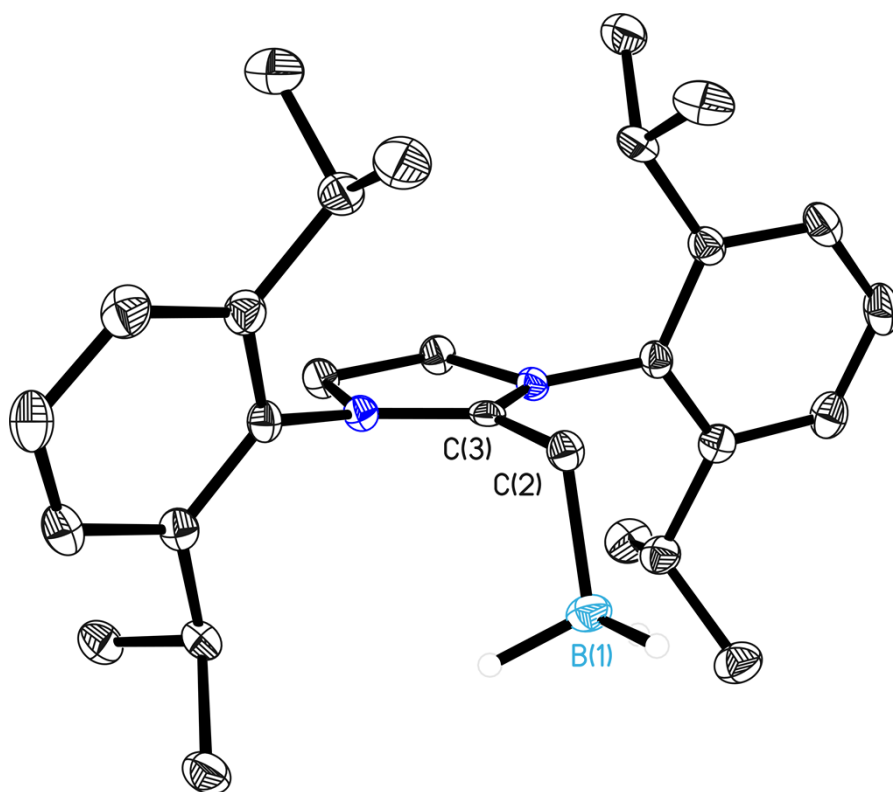


Fig. S1 Molecular structure of compound **4**. Thermal ellipsoids are represented at the 50 % probability level. Boron bound hydrogen atoms were refined without restraints.

Full list of bond distances and angles

Compound **4**

		C(8)-C(7)	1.5328(19)
		C(8)-H(8A)	0.9800
		C(8)-H(8B)	0.9800
		C(8)-H(8C)	0.9800
		C(7)-C(9)	1.5385(18)
		C(7)-H(7)	1.0000
		C(9)-H(9A)	0.9800
		C(9)-H(9B)	0.9800
		C(9)-H(9C)	0.9800
		C(10)-C(11)	1.381(2)
		C(10)-H(10)	0.9500
		C(11)-C(12)	1.382(2)
		C(11)-H(11)	0.9500
		C(12)-C(13)	1.3962(19)
		C(12)-H(12)	0.9500
		C(13)-C(14)	1.5176(19)
		C(14)-C(16)	1.526(2)
B(1)-C(2)	1.6767(19)		
B(1)-H(1)	1.132(13)		
B(1)-H(2)	1.147(12)		
B(1)-H(3)	1.138(12)		
C(2)-C(3)	1.4522(17)		
C(2)-H(2A)	0.9900		
C(2)-H(2B)	0.9900		
C(3)-N(4)	1.3361(16)		
C(3)-N(19)	1.3376(16)		
N(4)-C(5)	1.4427(16)		
N(4)-C(17)	1.4777(16)		
C(5)-C(13)	1.4051(18)		
C(5)-C(6)	1.4055(18)		
C(6)-C(10)	1.3974(19)		
C(6)-C(7)	1.5224(19)		

C(14)-C(15)	1.534(2)	C(29)-H(29)	1.0000
C(14)-H(14)	1.0000	C(30)-H(30A)	0.9800
C(15)-H(15A)	0.9800	C(30)-H(30B)	0.9800
C(15)-H(15B)	0.9800	C(30)-H(30C)	0.9800
C(15)-H(15C)	0.9800	C(31)-H(31A)	0.9800
C(16)-H(16A)	0.9800	C(31)-H(31B)	0.9800
C(16)-H(16B)	0.9800	C(31)-H(31C)	0.9800
C(16)-H(16C)	0.9800		
C(17)-C(18)	1.5280(18)	C(2)-B(1)-H(1)	109.2(8)
C(17)-H(17A)	0.9900	C(2)-B(1)-H(2)	107.4(8)
C(17)-H(17B)	0.9900	H(1)-B(1)-H(2)	110.0(11)
C(18)-N(19)	1.4752(16)	C(2)-B(1)-H(3)	109.3(8)
C(18)-H(18A)	0.9900	H(1)-B(1)-H(3)	111.1(11)
C(18)-H(18B)	0.9900	H(2)-B(1)-H(3)	109.7(11)
N(19)-C(20)	1.4414(16)	C(3)-C(2)-B(1)	109.68(10)
C(20)-C(21)	1.4052(19)	C(3)-C(2)-H(2A)	109.7
C(20)-C(28)	1.4071(18)	B(1)-C(2)-H(2A)	109.7
C(21)-C(25)	1.3953(19)	C(3)-C(2)-H(2B)	109.7
C(21)-C(22)	1.5190(19)	B(1)-C(2)-H(2B)	109.7
C(22)-C(23)	1.532(2)	H(2A)-C(2)-H(2B)	108.2
C(22)-C(24)	1.5319(19)	N(4)-C(3)-N(19)	110.49(11)
C(22)-H(22)	1.0000	N(4)-C(3)-C(2)	124.90(11)
C(23)-H(23A)	0.9800	N(19)-C(3)-C(2)	124.51(11)
C(23)-H(23B)	0.9800	C(3)-N(4)-C(5)	128.70(10)
C(23)-H(23C)	0.9800	C(3)-N(4)-C(17)	111.45(10)
C(24)-H(24A)	0.9800	C(5)-N(4)-C(17)	118.79(10)
C(24)-H(24B)	0.9800	C(13)-C(5)-C(6)	121.62(12)
C(24)-H(24C)	0.9800	C(13)-C(5)-N(4)	119.50(11)
C(25)-C(26)	1.381(2)	C(6)-C(5)-N(4)	118.47(11)
C(25)-H(25)	0.9500	C(10)-C(6)-C(5)	117.78(12)
C(26)-C(27)	1.384(2)	C(10)-C(6)-C(7)	119.36(12)
C(26)-H(26)	0.9500	C(5)-C(6)-C(7)	122.86(11)
C(27)-C(28)	1.3967(19)	C(7)-C(8)-H(8A)	109.5
C(27)-H(27)	0.9500	C(7)-C(8)-H(8B)	109.5
C(28)-C(29)	1.5206(19)	H(8A)-C(8)-H(8B)	109.5
C(29)-C(31)	1.5325(19)	C(7)-C(8)-H(8C)	109.5
C(29)-C(30)	1.534(2)	H(8A)-C(8)-H(8C)	109.5

H(8B)-C(8)-H(8C)	109.5	C(14)-C(16)-H(16A)	109.5
C(6)-C(7)-C(8)	110.87(11)	C(14)-C(16)-H(16B)	109.5
C(6)-C(7)-C(9)	110.71(11)	H(16A)-C(16)-H(16B)	109.5
C(8)-C(7)-C(9)	110.33(11)	C(14)-C(16)-H(16C)	109.5
C(6)-C(7)-H(7)	108.3	H(16A)-C(16)-H(16C)	109.5
C(8)-C(7)-H(7)	108.3	H(16B)-C(16)-H(16C)	109.5
C(9)-C(7)-H(7)	108.3	N(4)-C(17)-C(18)	103.27(10)
C(7)-C(9)-H(9A)	109.5	N(4)-C(17)-H(17A)	111.1
C(7)-C(9)-H(9B)	109.5	C(18)-C(17)-H(17A)	111.1
H(9A)-C(9)-H(9B)	109.5	N(4)-C(17)-H(17B)	111.1
C(7)-C(9)-H(9C)	109.5	C(18)-C(17)-H(17B)	111.1
H(9A)-C(9)-H(9C)	109.5	H(17A)-C(17)-H(17B)	109.1
H(9B)-C(9)-H(9C)	109.5	N(19)-C(18)-C(17)	102.85(10)
C(11)-C(10)-C(6)	121.61(13)	N(19)-C(18)-H(18A)	111.2
C(11)-C(10)-H(10)	119.2	C(17)-C(18)-H(18A)	111.2
C(6)-C(10)-H(10)	119.2	N(19)-C(18)-H(18B)	111.2
C(10)-C(11)-C(12)	119.50(13)	C(17)-C(18)-H(18B)	111.2
C(10)-C(11)-H(11)	120.3	H(18A)-C(18)-H(18B)	109.1
C(12)-C(11)-H(11)	120.3	C(3)-N(19)-C(20)	126.44(10)
C(11)-C(12)-C(13)	121.62(13)	C(3)-N(19)-C(18)	111.78(10)
C(11)-C(12)-H(12)	119.2	C(20)-N(19)-C(18)	120.61(10)
C(13)-C(12)-H(12)	119.2	C(21)-C(20)-C(28)	122.12(12)
C(12)-C(13)-C(5)	117.79(12)	C(21)-C(20)-N(19)	118.84(11)
C(12)-C(13)-C(14)	119.09(12)	C(28)-C(20)-N(19)	118.89(12)
C(5)-C(13)-C(14)	123.11(12)	C(25)-C(21)-C(20)	117.64(12)
C(13)-C(14)-C(16)	111.46(12)	C(25)-C(21)-C(22)	120.37(12)
C(13)-C(14)-C(15)	111.05(12)	C(20)-C(21)-C(22)	121.89(12)
C(16)-C(14)-C(15)	111.22(12)	C(21)-C(22)-C(23)	109.52(11)
C(13)-C(14)-H(14)	107.6	C(21)-C(22)-C(24)	113.01(12)
C(16)-C(14)-H(14)	107.6	C(23)-C(22)-C(24)	110.43(12)
C(15)-C(14)-H(14)	107.6	C(21)-C(22)-H(22)	107.9
C(14)-C(15)-H(15A)	109.5	C(23)-C(22)-H(22)	107.9
C(14)-C(15)-H(15B)	109.5	C(24)-C(22)-H(22)	107.9
H(15A)-C(15)-H(15B)	109.5	C(22)-C(23)-H(23A)	109.5
C(14)-C(15)-H(15C)	109.5	C(22)-C(23)-H(23B)	109.5
H(15A)-C(15)-H(15C)	109.5	H(23A)-C(23)-H(23B)	109.5
H(15B)-C(15)-H(15C)	109.5	C(22)-C(23)-H(23C)	109.5

H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(26)-C(25)-C(21)	121.48(13)
C(26)-C(25)-H(25)	119.3
C(21)-C(25)-H(25)	119.3
C(25)-C(26)-C(27)	119.79(13)
C(25)-C(26)-H(26)	120.1
C(27)-C(26)-H(26)	120.1
C(26)-C(27)-C(28)	121.55(13)
C(26)-C(27)-H(27)	119.2
C(28)-C(27)-H(27)	119.2
C(27)-C(28)-C(20)	117.41(13)
C(27)-C(28)-C(29)	119.71(12)
C(20)-C(28)-C(29)	122.87(12)
C(28)-C(29)-C(31)	111.43(12)
C(28)-C(29)-C(30)	111.58(12)
C(31)-C(29)-C(30)	110.32(12)
C(28)-C(29)-H(29)	107.8
C(31)-C(29)-H(29)	107.8
C(30)-C(29)-H(29)	107.8
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(29)-C(31)-H(31A)	109.5
C(29)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(29)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5

H(31B)-C(31)-H(31C)	109.5
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Compound 5

B(0)-C(0)	1.630(2)
B(0)-H(5B)	1.260(11)
B(0)-H(0BA)	1.120(13)
B(0)-H(0BB)	1.088(13)
C(0)-C(1)	1.4668(18)
C(0)-H(0A)	0.9900
C(0)-H(0B)	0.9900
C(1)-N(5)	1.3432(16)
C(1)-N(2)	1.3463(17)
N(2)-C(3)	1.3888(16)
N(2)-C(6)	1.4476(17)
C(3)-C(4)	1.338(2)
C(3)-H(3)	0.9500
C(4)-N(5)	1.3886(17)
C(4)-H(4)	0.9500
N(5)-C(18)	1.4472(17)
C(6)-C(11)	1.3969(19)
C(6)-C(7)	1.400(2)
C(8)-C(9)	1.380(2)
C(8)-C(7)	1.389(2)
C(8)-H(8)	0.9500
C(9)-C(10)	1.378(2)
C(9)-H(9)	0.9500
C(10)-C(11)	1.397(2)
C(10)-H(10)	0.9500
C(7)-C(12')	1.519(2)
C(7)-C(12)	1.519(2)
C(12)-C(13)	1.503(6)
C(12)-C(14)	1.547(5)
C(12)-H(12)	1.0000
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800

C(14)-H(14A)	0.9800	C(25)-H(25B)	0.9800
C(14)-H(14B)	0.9800	C(25)-H(25C)	0.9800
C(14)-H(14C)	0.9800	C(26)-H(26A)	0.9800
C(12')-C(14')	1.510(7)	C(26)-H(26B)	0.9800
C(12')-C(13')	1.568(8)	C(26)-H(26C)	0.9800
C(12')-H(12')	1.0000	C(24')-C(26')	1.454(6)
C(13')-H(13X)	0.9800	C(24')-C(25')	1.592(7)
C(13')-H(13Y)	0.9800	C(24')-H(24')	1.0000
C(13')-H(13Z)	0.9800	C(25')-H(25X)	0.9800
C(14')-H(14X)	0.9800	C(25')-H(25Y)	0.9800
C(14')-H(14Y)	0.9800	C(25')-H(25Z)	0.9800
C(14')-H(14Z)	0.9800	C(26')-H(26X)	0.9800
C(11)-C(15)	1.514(2)	C(26')-H(26Y)	0.9800
C(15)-C(16)	1.531(2)	C(26')-H(26Z)	0.9800
C(15)-C(17)	1.532(2)	C(23)-C(27)	1.5202(18)
C(15)-H(15)	1.0000	C(27)-C(29)	1.527(2)
C(16)-H(16A)	0.9800	C(27)-C(28)	1.527(2)
C(16)-H(16B)	0.9800	C(27)-H(27)	1.0000
C(16)-H(16C)	0.9800	C(28)-H(28A)	0.9800
C(17)-H(17A)	0.9800	C(28)-H(28B)	0.9800
C(17)-H(17B)	0.9800	C(28)-H(28C)	0.9800
C(17)-H(17C)	0.9800	C(29)-H(29A)	0.9800
C(18)-C(23)	1.3924(19)	C(29)-H(29B)	0.9800
C(18)-C(19)	1.4041(18)	C(29)-H(29C)	0.9800
C(20)-C(21)	1.377(2)	B(30)-C(30)	1.633(2)
C(20)-C(19)	1.392(2)	B(30)-H(5B)	1.268(11)
C(20)-H(20)	0.9500	B(30)-H(3BA)	1.102(12)
C(21)-C(22)	1.380(2)	B(30)-H(3BB)	1.101(12)
C(21)-H(21)	0.9500	C(30)-C(31)	1.4675(16)
C(22)-C(23)	1.398(2)	C(30)-H(30A)	0.9900
C(22)-H(22)	0.9500	C(30)-H(30B)	0.9900
C(19)-C(24')	1.517(2)	C(31)-N(35)	1.3429(16)
C(19)-C(24)	1.517(2)	C(31)-N(32)	1.3479(16)
C(24)-C(25)	1.472(5)	N(32)-C(33)	1.3873(16)
C(24)-C(26)	1.563(4)	N(32)-C(36)	1.4466(15)
C(24)-H(24)	1.0000	C(33)-C(34)	1.3459(18)
C(25)-H(25A)	0.9800	C(33)-H(33)	0.9500

C(34)-N(35)	1.3847(16)	C(51)-C(52)	1.388(2)
C(34)-H(34)	0.9500	C(51)-H(51)	0.9500
N(35)-C(48)	1.4485(15)	C(52)-C(53)	1.3944(19)
C(36)-C(37)	1.3986(17)	C(52)-H(52)	0.9500
C(36)-C(41)	1.3998(17)	C(49)-C(54)	1.5169(18)
C(38)-C(39)	1.387(2)	C(54)-C(55)	1.528(2)
C(38)-C(37)	1.3945(18)	C(54)-C(56)	1.531(2)
C(38)-H(38)	0.9500	C(54)-H(54)	1.0000
C(39)-C(40)	1.383(2)	C(55)-H(55A)	0.9800
C(39)-H(39)	0.9500	C(55)-H(55B)	0.9800
C(40)-C(41)	1.3973(18)	C(55)-H(55C)	0.9800
C(40)-H(40)	0.9500	C(56)-H(56A)	0.9800
C(37)-C(42)	1.5217(18)	C(56)-H(56B)	0.9800
C(42)-C(44)	1.5231(19)	C(56)-H(56C)	0.9800
C(42)-C(43)	1.5313(19)	C(53)-C(57)	1.5231(19)
C(42)-H(42)	1.0000	C(57)-C(59)	1.518(2)
C(43)-H(43A)	0.9800	C(57)-C(58)	1.522(2)
C(43)-H(43B)	0.9800	C(57)-H(57)	1.0000
C(43)-H(43C)	0.9800	C(58)-H(58A)	0.9800
C(44)-H(44A)	0.9800	C(58)-H(58B)	0.9800
C(44)-H(44B)	0.9800	C(58)-H(58C)	0.9800
C(44)-H(44C)	0.9800	C(59)-H(59A)	0.9800
C(41)-C(45)	1.5183(18)	C(59)-H(59B)	0.9800
C(45)-C(47)	1.5202(19)	C(59)-H(59C)	0.9800
C(45)-C(46)	1.525(2)	N(60)-S(61)	1.5775(12)
C(45)-H(45)	1.0000	N(60)-S(68)	1.5777(11)
C(46)-H(46A)	0.9800	S(61)-O(62)	1.4250(10)
C(46)-H(46B)	0.9800	S(61)-O(63)	1.4295(10)
C(46)-H(46C)	0.9800	S(61)-C(64)	1.8358(15)
C(47)-H(47A)	0.9800	C(64)-F(66)	1.3186(16)
C(47)-H(47B)	0.9800	C(64)-F(67)	1.3290(15)
C(47)-H(47C)	0.9800	C(64)-F(65)	1.3292(16)
C(48)-C(53)	1.3996(18)	S(68)-O(69)	1.4248(10)
C(48)-C(49)	1.3998(18)	S(68)-O(70)	1.4276(11)
C(50)-C(51)	1.383(2)	S(68)-C(71)	1.8194(16)
C(50)-C(49)	1.3977(18)	C(71)-F(72)	1.323(2)
C(50)-H(50)	0.9500	C(71)-F(74)	1.325(2)

C(71)-F(73)	1.3354(17)	C(8)-C(9)-H(9)	119.7
		C(9)-C(10)-C(11)	121.03(14)
C(0)-B(0)-H(5B)	101.2(8)	C(9)-C(10)-H(10)	119.5
C(0)-B(0)-H(0BA)	111.8(9)	C(11)-C(10)-H(10)	119.5
H(5B)-B(0)-H(0BA)	110.6(12)	C(8)-C(7)-C(6)	116.40(13)
C(0)-B(0)-H(0BB)	114.7(9)	C(8)-C(7)-C(12')	120.42(13)
H(5B)-B(0)-H(0BB)	103.0(12)	C(6)-C(7)-C(12')	123.17(13)
H(0BA)-B(0)-H(0BB)	114.3(13)	C(8)-C(7)-C(12)	120.42(13)
C(1)-C(0)-B(0)	111.08(11)	C(6)-C(7)-C(12)	123.17(13)
C(1)-C(0)-H(0A)	109.4	C(13)-C(12)-C(7)	114.3(4)
B(0)-C(0)-H(0A)	109.4	C(13)-C(12)-C(14)	110.2(4)
C(1)-C(0)-H(0B)	109.4	C(7)-C(12)-C(14)	110.0(3)
B(0)-C(0)-H(0B)	109.4	C(13)-C(12)-H(12)	107.4
H(0A)-C(0)-H(0B)	108.0	C(7)-C(12)-H(12)	107.4
N(5)-C(1)-N(2)	106.52(11)	C(14)-C(12)-H(12)	107.4
N(5)-C(1)-C(0)	126.37(12)	C(12)-C(13)-H(13A)	109.5
N(2)-C(1)-C(0)	127.09(12)	C(12)-C(13)-H(13B)	109.5
C(1)-N(2)-C(3)	109.58(11)	H(13A)-C(13)-H(13B)	109.5
C(1)-N(2)-C(6)	127.66(11)	C(12)-C(13)-H(13C)	109.5
C(3)-N(2)-C(6)	122.55(11)	H(13A)-C(13)-H(13C)	109.5
C(4)-C(3)-N(2)	107.10(12)	H(13B)-C(13)-H(13C)	109.5
C(4)-C(3)-H(3)	126.5	C(12)-C(14)-H(14A)	109.5
N(2)-C(3)-H(3)	126.5	C(12)-C(14)-H(14B)	109.5
C(3)-C(4)-N(5)	107.14(11)	H(14A)-C(14)-H(14B)	109.5
C(3)-C(4)-H(4)	126.4	C(12)-C(14)-H(14C)	109.5
N(5)-C(4)-H(4)	126.4	H(14A)-C(14)-H(14C)	109.5
C(1)-N(5)-C(4)	109.67(11)	H(14B)-C(14)-H(14C)	109.5
C(1)-N(5)-C(18)	126.63(11)	C(14')-C(12')-C(7)	112.8(4)
C(4)-N(5)-C(18)	123.70(11)	C(14')-C(12')-C(13')	108.9(5)
C(11)-C(6)-C(7)	124.02(13)	C(7)-C(12')-C(13')	109.6(4)
C(11)-C(6)-N(2)	118.18(12)	C(14')-C(12')-H(12')	108.5
C(7)-C(6)-N(2)	117.62(12)	C(7)-C(12')-H(12')	108.5
C(9)-C(8)-C(7)	121.38(15)	C(13')-C(12')-H(12')	108.5
C(9)-C(8)-H(8)	119.3	C(12')-C(13')-H(13X)	109.5
C(7)-C(8)-H(8)	119.3	C(12')-C(13')-H(13Y)	109.5
C(10)-C(9)-C(8)	120.61(14)	H(13X)-C(13')-H(13Y)	109.5
C(10)-C(9)-H(9)	119.7	C(12')-C(13')-H(13Z)	109.5

H(13X)-C(13')-H(13Z)	109.5	C(22)-C(21)-H(21)	119.6
H(13Y)-C(13')-H(13Z)	109.5	C(21)-C(22)-C(23)	121.03(14)
C(12')-C(14')-H(14X)	109.5	C(21)-C(22)-H(22)	119.5
C(12')-C(14')-H(14Y)	109.5	C(23)-C(22)-H(22)	119.5
H(14X)-C(14')-H(14Y)	109.5	C(20)-C(19)-C(18)	116.81(13)
C(12')-C(14')-H(14Z)	109.5	C(20)-C(19)-C(24')	121.22(13)
H(14X)-C(14')-H(14Z)	109.5	C(18)-C(19)-C(24')	121.93(13)
H(14Y)-C(14')-H(14Z)	109.5	C(20)-C(19)-C(24)	121.22(13)
C(6)-C(11)-C(10)	116.46(14)	C(18)-C(19)-C(24)	121.93(13)
C(6)-C(11)-C(15)	123.08(13)	C(25)-C(24)-C(19)	110.9(3)
C(10)-C(11)-C(15)	120.44(14)	C(25)-C(24)-C(26)	112.2(3)
C(11)-C(15)-C(16)	110.14(14)	C(19)-C(24)-C(26)	108.9(2)
C(11)-C(15)-C(17)	112.22(13)	C(25)-C(24)-H(24)	108.2
C(16)-C(15)-C(17)	110.26(14)	C(19)-C(24)-H(24)	108.2
C(11)-C(15)-H(15)	108.0	C(26)-C(24)-H(24)	108.2
C(16)-C(15)-H(15)	108.0	C(24)-C(25)-H(25A)	109.5
C(17)-C(15)-H(15)	108.0	C(24)-C(25)-H(25B)	109.5
C(15)-C(16)-H(16A)	109.5	H(25A)-C(25)-H(25B)	109.5
C(15)-C(16)-H(16B)	109.5	C(24)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16B)	109.5	H(25A)-C(25)-H(25C)	109.5
C(15)-C(16)-H(16C)	109.5	H(25B)-C(25)-H(25C)	109.5
H(16A)-C(16)-H(16C)	109.5	C(24)-C(26)-H(26A)	109.5
H(16B)-C(16)-H(16C)	109.5	C(24)-C(26)-H(26B)	109.5
C(15)-C(17)-H(17A)	109.5	H(26A)-C(26)-H(26B)	109.5
C(15)-C(17)-H(17B)	109.5	C(24)-C(26)-H(26C)	109.5
H(17A)-C(17)-H(17B)	109.5	H(26A)-C(26)-H(26C)	109.5
C(15)-C(17)-H(17C)	109.5	H(26B)-C(26)-H(26C)	109.5
H(17A)-C(17)-H(17C)	109.5	C(26')-C(24')-C(19)	118.3(4)
H(17B)-C(17)-H(17C)	109.5	C(26')-C(24')-C(25')	110.2(4)
C(23)-C(18)-C(19)	123.64(13)	C(19)-C(24')-C(25')	111.8(3)
C(23)-C(18)-N(5)	117.67(11)	C(26')-C(24')-H(24')	105.1
C(19)-C(18)-N(5)	118.60(12)	C(19)-C(24')-H(24')	105.1
C(21)-C(20)-C(19)	121.02(14)	C(25')-C(24')-H(24')	105.1
C(21)-C(20)-H(20)	119.5	C(24')-C(25')-H(25X)	109.5
C(19)-C(20)-H(20)	119.5	C(24')-C(25')-H(25Y)	109.5
C(20)-C(21)-C(22)	120.74(14)	H(25X)-C(25')-H(25Y)	109.5
C(20)-C(21)-H(21)	119.6	C(24')-C(25')-H(25Z)	109.5

H(25X)-C(25')-H(25Z)	109.5	B(30)-C(30)-H(30A)	109.6
H(25Y)-C(25')-H(25Z)	109.5	C(31)-C(30)-H(30B)	109.6
C(24')-C(26')-H(26X)	109.5	B(30)-C(30)-H(30B)	109.6
C(24')-C(26')-H(26Y)	109.5	H(30A)-C(30)-H(30B)	108.1
H(26X)-C(26')-H(26Y)	109.5	N(35)-C(31)-N(32)	106.68(10)
C(24')-C(26')-H(26Z)	109.5	N(35)-C(31)-C(30)	127.06(11)
H(26X)-C(26')-H(26Z)	109.5	N(32)-C(31)-C(30)	126.23(11)
H(26Y)-C(26')-H(26Z)	109.5	C(31)-N(32)-C(33)	109.53(10)
C(18)-C(23)-C(22)	116.72(13)	C(31)-N(32)-C(36)	124.91(10)
C(18)-C(23)-C(27)	122.52(12)	C(33)-N(32)-C(36)	124.94(10)
C(22)-C(23)-C(27)	120.75(13)	C(34)-C(33)-N(32)	106.94(11)
C(23)-C(27)-C(29)	110.97(12)	C(34)-C(33)-H(33)	126.5
C(23)-C(27)-C(28)	111.18(12)	N(32)-C(33)-H(33)	126.5
C(29)-C(27)-C(28)	111.17(12)	C(33)-C(34)-N(35)	107.16(11)
C(23)-C(27)-H(27)	107.8	C(33)-C(34)-H(34)	126.4
C(29)-C(27)-H(27)	107.8	N(35)-C(34)-H(34)	126.4
C(28)-C(27)-H(27)	107.8	C(31)-N(35)-C(34)	109.69(10)
C(27)-C(28)-H(28A)	109.5	C(31)-N(35)-C(48)	127.59(10)
C(27)-C(28)-H(28B)	109.5	C(34)-N(35)-C(48)	122.63(10)
H(28A)-C(28)-H(28B)	109.5	C(37)-C(36)-C(41)	124.19(11)
C(27)-C(28)-H(28C)	109.5	C(37)-C(36)-N(32)	118.56(11)
H(28A)-C(28)-H(28C)	109.5	C(41)-C(36)-N(32)	117.25(11)
H(28B)-C(28)-H(28C)	109.5	C(39)-C(38)-C(37)	121.17(13)
C(27)-C(29)-H(29A)	109.5	C(39)-C(38)-H(38)	119.4
C(27)-C(29)-H(29B)	109.5	C(37)-C(38)-H(38)	119.4
H(29A)-C(29)-H(29B)	109.5	C(40)-C(39)-C(38)	120.82(12)
C(27)-C(29)-H(29C)	109.5	C(40)-C(39)-H(39)	119.6
H(29A)-C(29)-H(29C)	109.5	C(38)-C(39)-H(39)	119.6
H(29B)-C(29)-H(29C)	109.5	C(39)-C(40)-C(41)	120.65(13)
C(30)-B(30)-H(5B)	110.3(8)	C(39)-C(40)-H(40)	119.7
C(30)-B(30)-H(3BA)	114.1(8)	C(41)-C(40)-H(40)	119.7
H(5B)-B(30)-H(3BA)	108.0(11)	C(38)-C(37)-C(36)	116.35(12)
C(30)-B(30)-H(3BB)	113.7(8)	C(38)-C(37)-C(42)	121.82(12)
H(5B)-B(30)-H(3BB)	95.8(11)	C(36)-C(37)-C(42)	121.79(11)
H(3BA)-B(30)-H(3BB)	113.3(12)	C(37)-C(42)-C(44)	112.97(12)
C(31)-C(30)-B(30)	110.16(10)	C(37)-C(42)-C(43)	110.92(11)
C(31)-C(30)-H(30A)	109.6	C(44)-C(42)-C(43)	109.86(12)

C(37)-C(42)-H(42)	107.6	C(53)-C(48)-N(35)	117.91(11)
C(44)-C(42)-H(42)	107.6	C(49)-C(48)-N(35)	118.17(11)
C(43)-C(42)-H(42)	107.6	C(51)-C(50)-C(49)	120.95(13)
C(42)-C(43)-H(43A)	109.5	C(51)-C(50)-H(50)	119.5
C(42)-C(43)-H(43B)	109.5	C(49)-C(50)-H(50)	119.5
H(43A)-C(43)-H(43B)	109.5	C(50)-C(51)-C(52)	120.79(13)
C(42)-C(43)-H(43C)	109.5	C(50)-C(51)-H(51)	119.6
H(43A)-C(43)-H(43C)	109.5	C(52)-C(51)-H(51)	119.6
H(43B)-C(43)-H(43C)	109.5	C(51)-C(52)-C(53)	120.69(13)
C(42)-C(44)-H(44A)	109.5	C(51)-C(52)-H(52)	119.7
C(42)-C(44)-H(44B)	109.5	C(53)-C(52)-H(52)	119.7
H(44A)-C(44)-H(44B)	109.5	C(50)-C(49)-C(48)	116.75(12)
C(42)-C(44)-H(44C)	109.5	C(50)-C(49)-C(54)	120.79(12)
H(44A)-C(44)-H(44C)	109.5	C(48)-C(49)-C(54)	122.45(11)
H(44B)-C(44)-H(44C)	109.5	C(49)-C(54)-C(55)	111.24(12)
C(40)-C(41)-C(36)	116.80(12)	C(49)-C(54)-C(56)	111.34(12)
C(40)-C(41)-C(45)	120.57(12)	C(55)-C(54)-C(56)	110.12(12)
C(36)-C(41)-C(45)	122.62(11)	C(49)-C(54)-H(54)	108.0
C(41)-C(45)-C(47)	110.79(11)	C(55)-C(54)-H(54)	108.0
C(41)-C(45)-C(46)	112.01(12)	C(56)-C(54)-H(54)	108.0
C(47)-C(45)-C(46)	109.85(12)	C(54)-C(55)-H(55A)	109.5
C(41)-C(45)-H(45)	108.0	C(54)-C(55)-H(55B)	109.5
C(47)-C(45)-H(45)	108.0	H(55A)-C(55)-H(55B)	109.5
C(46)-C(45)-H(45)	108.0	C(54)-C(55)-H(55C)	109.5
C(45)-C(46)-H(46A)	109.5	H(55A)-C(55)-H(55C)	109.5
C(45)-C(46)-H(46B)	109.5	H(55B)-C(55)-H(55C)	109.5
H(46A)-C(46)-H(46B)	109.5	C(54)-C(56)-H(56A)	109.5
C(45)-C(46)-H(46C)	109.5	C(54)-C(56)-H(56B)	109.5
H(46A)-C(46)-H(46C)	109.5	H(56A)-C(56)-H(56B)	109.5
H(46B)-C(46)-H(46C)	109.5	C(54)-C(56)-H(56C)	109.5
C(45)-C(47)-H(47A)	109.5	H(56A)-C(56)-H(56C)	109.5
C(45)-C(47)-H(47B)	109.5	H(56B)-C(56)-H(56C)	109.5
H(47A)-C(47)-H(47B)	109.5	C(52)-C(53)-C(48)	117.05(12)
C(45)-C(47)-H(47C)	109.5	C(52)-C(53)-C(57)	120.66(12)
H(47A)-C(47)-H(47C)	109.5	C(48)-C(53)-C(57)	122.25(12)
H(47B)-C(47)-H(47C)	109.5	C(59)-C(57)-C(58)	110.59(15)
C(53)-C(48)-C(49)	123.74(12)	C(59)-C(57)-C(53)	112.65(13)

C(58)-C(57)-C(53)	110.51(13)	F(74)-C(71)-F(73)	107.72(14)
C(59)-C(57)-H(57)	107.6	F(72)-C(71)-S(68)	111.17(11)
C(58)-C(57)-H(57)	107.6	F(74)-C(71)-S(68)	111.82(12)
C(53)-C(57)-H(57)	107.6	F(73)-C(71)-S(68)	109.31(11)
C(57)-C(58)-H(58A)	109.5		
C(57)-C(58)-H(58B)	109.5	Compound 8	
H(58A)-C(58)-H(58B)	109.5		
C(57)-C(58)-H(58C)	109.5	B(1)-C(2)	1.601(4)
H(58A)-C(58)-H(58C)	109.5	B(1)-B(1)#1	1.755(7)
H(58B)-C(58)-H(58C)	109.5	B(1)-H(2)	1.28(3)
C(57)-C(59)-H(59A)	109.5	B(1)-H(1)	1.07(3)
C(57)-C(59)-H(59B)	109.5	C(8)-C(7)	1.540(4)
H(59A)-C(59)-H(59B)	109.5	C(8)-H(8A)	0.9800
C(57)-C(59)-H(59C)	109.5	C(8)-H(8B)	0.9800
H(59A)-C(59)-H(59C)	109.5	C(8)-H(8C)	0.9800
H(59B)-C(59)-H(59C)	109.5	C(2)-C(3)	1.488(3)
S(61)-N(60)-S(68)	125.05(7)	C(2)-H(2A)	0.9900
O(62)-S(61)-O(63)	118.58(6)	C(2)-H(2B)	0.9900
O(62)-S(61)-N(60)	116.61(6)	C(3)-N(19)	1.322(3)
O(63)-S(61)-N(60)	108.27(6)	C(3)-N(4)	1.326(3)
O(62)-S(61)-C(64)	104.53(7)	N(4)-C(5)	1.449(3)
O(63)-S(61)-C(64)	104.54(6)	N(4)-C(17)	1.477(3)
N(60)-S(61)-C(64)	102.14(6)	C(5)-C(6)	1.402(4)
F(66)-C(64)-F(67)	107.96(12)	C(5)-C(13)	1.405(4)
F(66)-C(64)-F(65)	108.34(11)	C(6)-C(10)	1.395(4)
F(67)-C(64)-F(65)	107.97(11)	C(6)-C(7)	1.521(4)
F(66)-C(64)-S(61)	111.00(9)	C(7)-C(9)	1.535(4)
F(67)-C(64)-S(61)	111.15(9)	C(7)-H(7)	1.0000
F(65)-C(64)-S(61)	110.31(10)	C(9)-H(9A)	0.9800
O(69)-S(68)-O(70)	118.67(6)	C(9)-H(9B)	0.9800
O(69)-S(68)-N(60)	116.71(6)	C(9)-H(9C)	0.9800
O(70)-S(68)-N(60)	109.20(6)	C(10)-C(11)	1.382(5)
O(69)-S(68)-C(71)	104.96(7)	C(10)-H(10)	0.9500
O(70)-S(68)-C(71)	103.56(8)	C(11)-C(12)	1.371(5)
N(60)-S(68)-C(71)	101.14(7)	C(11)-H(11)	0.9500
F(72)-C(71)-F(74)	108.00(14)	C(17)-C(18)	1.526(4)
F(72)-C(71)-F(73)	108.71(14)	C(17)-H(17A)	0.9900

C(17)-H(17B)	0.9900	C(29)-H(29)	1.0000
C(16)-C(14)	1.526(6)	C(28)-C(27)	1.399(4)
C(16)-H(16A)	0.9800	C(27)-H(27)	0.9500
C(16)-H(16B)	0.9800	C(30)-H(30A)	0.9800
C(16)-H(16C)	0.9800	C(30)-H(30B)	0.9800
C(15)-C(14)	1.518(6)	C(30)-H(30C)	0.9800
C(15)-H(15A)	0.9800	C(31)-H(31A)	0.9800
C(15)-H(15B)	0.9800	C(31)-H(31B)	0.9800
C(15)-H(15C)	0.9800	C(31)-H(31C)	0.9800
C(14)-C(13)	1.520(5)	N(32)-S(33)	1.533(8)
C(14)-H(14)	1.0000	N(32)-S(40)	1.614(11)
C(13)-C(12)	1.397(5)	S(33)-O(35)	1.395(10)
C(12)-H(12)	0.9500	S(33)-O(34)	1.459(8)
C(18)-N(19)	1.479(3)	S(33)-C(36)	1.832(10)
C(18)-H(18A)	0.9900	C(36)-F(39)	1.277(12)
C(18)-H(18B)	0.9900	C(36)-F(38)	1.320(12)
N(19)-C(20)	1.447(3)	C(36)-F(37)	1.333(12)
C(20)-C(28)	1.401(4)	S(40)-O(41)	1.369(10)
C(20)-C(21)	1.412(4)	S(40)-O(42)	1.438(11)
C(21)-C(25)	1.397(4)	S(40)-C(43)	1.848(14)
C(21)-C(22)	1.521(4)	C(43)-F(46)	1.306(15)
C(22)-C(24)	1.530(5)	C(43)-F(45)	1.329(15)
C(22)-C(23)	1.540(4)	C(43)-F(44)	1.340(15)
C(22)-H(22)	1.0000	N(32')-S(40')	1.588(16)
C(23)-H(23A)	0.9800	N(32')-S(33')	1.595(16)
C(23)-H(23B)	0.9800	S(33')-O(35')	1.389(15)
C(23)-H(23C)	0.9800	S(33')-O(34')	1.450(17)
C(24)-H(24A)	0.9800	S(33')-C(36')	1.844(17)
C(24)-H(24B)	0.9800	C(36')-F(37')	1.299(18)
C(24)-H(24C)	0.9800	C(36')-F(39')	1.346(19)
C(26)-C(27)	1.378(5)	C(36')-F(38')	1.350(18)
C(26)-C(25)	1.378(5)	S(40')-O(42')	1.405(17)
C(26)-H(26)	0.9500	S(40')-O(41')	1.456(18)
C(25)-H(25)	0.9500	S(40')-C(43')	1.817(17)
C(29)-C(28)	1.521(4)	C(43')-F(46')	1.318(19)
C(29)-C(30)	1.532(4)	C(43')-F(44')	1.328(19)
C(29)-C(31)	1.540(4)	C(43')-F(45')	1.331(19)

N(47)-S(48)	1.559(15)	B(1)#1-B(1)-H(1)	108.8(18)
N(47)-S(55)	1.570(13)	H(2)-B(1)-H(1)	103(2)
S(48)-O(50)	1.411(16)	C(7)-C(8)-H(8A)	109.5
S(48)-O(49)	1.437(16)	C(7)-C(8)-H(8B)	109.5
S(48)-C(51)	1.864(17)	H(8A)-C(8)-H(8B)	109.5
C(51)-F(53)	1.280(18)	C(7)-C(8)-H(8C)	109.5
C(51)-F(54)	1.318(18)	H(8A)-C(8)-H(8C)	109.5
C(51)-F(52)	1.351(18)	H(8B)-C(8)-H(8C)	109.5
S(55)-O(56)	1.393(9)	C(3)-C(2)-B(1)	118.6(2)
S(55)-O(57)	1.433(9)	C(3)-C(2)-H(2A)	107.7
S(55)-C(58)	1.949(15)	B(1)-C(2)-H(2A)	107.7
C(58)-F(59)	1.259(16)	C(3)-C(2)-H(2B)	107.7
C(58)-F(60)	1.314(16)	B(1)-C(2)-H(2B)	107.7
C(58)-F(61)	1.323(16)	H(2A)-C(2)-H(2B)	107.1
N(47')-S(48')	1.582(17)	N(19)-C(3)-N(4)	111.9(2)
N(47')-S(55')	1.595(13)	N(19)-C(3)-C(2)	124.1(2)
S(48')-O(50')	1.434(16)	N(4)-C(3)-C(2)	124.0(2)
S(48')-O(49')	1.455(16)	C(3)-N(4)-C(5)	125.4(2)
S(48')-C(51')	1.849(18)	C(3)-N(4)-C(17)	110.9(2)
C(51')-F(52')	1.270(18)	C(5)-N(4)-C(17)	123.2(2)
C(51')-F(53')	1.326(18)	C(6)-C(5)-C(13)	123.0(3)
C(51')-F(54')	1.340(18)	C(6)-C(5)-N(4)	118.8(2)
S(55')-O(57')	1.425(9)	C(13)-C(5)-N(4)	118.2(2)
S(55')-O(56')	1.428(11)	C(10)-C(6)-C(5)	116.8(3)
S(55')-C(58')	1.826(15)	C(10)-C(6)-C(7)	120.1(3)
C(58')-F(60')	1.305(16)	C(5)-C(6)-C(7)	123.0(2)
C(58')-F(59')	1.318(17)	C(6)-C(7)-C(9)	113.1(3)
C(58')-F(61')	1.387(18)	C(6)-C(7)-C(8)	109.8(2)
C(1)-Cl(2)	1.698(13)	C(9)-C(7)-C(8)	109.5(2)
C(1)-Cl(3)	1.740(14)	C(6)-C(7)-H(7)	108.1
C(1)-H(1A)	0.9900	C(9)-C(7)-H(7)	108.1
C(1)-H(1B)	0.9900	C(8)-C(7)-H(7)	108.1
		C(7)-C(9)-H(9A)	109.5
C(2)-B(1)-B(1)#1	123.6(3)	C(7)-C(9)-H(9B)	109.5
C(2)-B(1)-H(2)	111.0(15)	H(9A)-C(9)-H(9B)	109.5
B(1)#1-B(1)-H(2)	47.0(15)	C(7)-C(9)-H(9C)	109.5
C(2)-B(1)-H(1)	127.6(18)	H(9A)-C(9)-H(9C)	109.5

H(9B)-C(9)-H(9C)	109.5	N(19)-C(18)-C(17)	103.0(2)
C(11)-C(10)-C(6)	121.5(3)	N(19)-C(18)-H(18A)	111.2
C(11)-C(10)-H(10)	119.3	C(17)-C(18)-H(18A)	111.2
C(6)-C(10)-H(10)	119.3	N(19)-C(18)-H(18B)	111.2
C(12)-C(11)-C(10)	120.2(3)	C(17)-C(18)-H(18B)	111.2
C(12)-C(11)-H(11)	119.9	H(18A)-C(18)-H(18B)	109.1
C(10)-C(11)-H(11)	119.9	C(3)-N(19)-C(20)	126.7(2)
N(4)-C(17)-C(18)	103.0(2)	C(3)-N(19)-C(18)	110.8(2)
N(4)-C(17)-H(17A)	111.2	C(20)-N(19)-C(18)	121.9(2)
C(18)-C(17)-H(17A)	111.2	C(28)-C(20)-C(21)	122.5(3)
N(4)-C(17)-H(17B)	111.2	C(28)-C(20)-N(19)	118.8(2)
C(18)-C(17)-H(17B)	111.2	C(21)-C(20)-N(19)	118.6(2)
H(17A)-C(17)-H(17B)	109.1	C(25)-C(21)-C(20)	117.1(3)
C(14)-C(16)-H(16A)	109.5	C(25)-C(21)-C(22)	119.2(3)
C(14)-C(16)-H(16B)	109.5	C(20)-C(21)-C(22)	123.7(3)
H(16A)-C(16)-H(16B)	109.5	C(21)-C(22)-C(24)	111.0(3)
C(14)-C(16)-H(16C)	109.5	C(21)-C(22)-C(23)	112.0(3)
H(16A)-C(16)-H(16C)	109.5	C(24)-C(22)-C(23)	109.9(3)
H(16B)-C(16)-H(16C)	109.5	C(21)-C(22)-H(22)	107.9
C(14)-C(15)-H(15A)	109.5	C(24)-C(22)-H(22)	107.9
C(14)-C(15)-H(15B)	109.5	C(23)-C(22)-H(22)	107.9
H(15A)-C(15)-H(15B)	109.5	C(22)-C(23)-H(23A)	109.5
C(14)-C(15)-H(15C)	109.5	C(22)-C(23)-H(23B)	109.5
H(15A)-C(15)-H(15C)	109.5	H(23A)-C(23)-H(23B)	109.5
H(15B)-C(15)-H(15C)	109.5	C(22)-C(23)-H(23C)	109.5
C(15)-C(14)-C(13)	113.1(4)	H(23A)-C(23)-H(23C)	109.5
C(15)-C(14)-C(16)	111.0(3)	H(23B)-C(23)-H(23C)	109.5
C(13)-C(14)-C(16)	110.0(3)	C(22)-C(24)-H(24A)	109.5
C(15)-C(14)-H(14)	107.5	C(22)-C(24)-H(24B)	109.5
C(13)-C(14)-H(14)	107.5	H(24A)-C(24)-H(24B)	109.5
C(16)-C(14)-H(14)	107.5	C(22)-C(24)-H(24C)	109.5
C(12)-C(13)-C(5)	116.9(3)	H(24A)-C(24)-H(24C)	109.5
C(12)-C(13)-C(14)	119.8(3)	H(24B)-C(24)-H(24C)	109.5
C(5)-C(13)-C(14)	123.3(3)	C(27)-C(26)-C(25)	120.8(3)
C(11)-C(12)-C(13)	121.6(3)	C(27)-C(26)-H(26)	119.6
C(11)-C(12)-H(12)	119.2	C(25)-C(26)-H(26)	119.6
C(13)-C(12)-H(12)	119.2	C(26)-C(25)-C(21)	121.1(3)

C(26)-C(25)-H(25)	119.4	F(38)-C(36)-S(33)	110.0(7)
C(21)-C(25)-H(25)	119.4	F(37)-C(36)-S(33)	110.6(8)
C(28)-C(29)-C(30)	109.9(2)	O(41)-S(40)-O(42)	121.4(8)
C(28)-C(29)-C(31)	112.2(2)	O(41)-S(40)-N(32)	120.2(7)
C(30)-C(29)-C(31)	109.3(3)	O(42)-S(40)-N(32)	107.8(8)
C(28)-C(29)-H(29)	108.5	O(41)-S(40)-C(43)	102.8(8)
C(30)-C(29)-H(29)	108.5	O(42)-S(40)-C(43)	98.8(9)
C(31)-C(29)-H(29)	108.5	N(32)-S(40)-C(43)	100.9(8)
C(27)-C(28)-C(20)	117.5(3)	F(46)-C(43)-F(45)	100.6(13)
C(27)-C(28)-C(29)	119.2(3)	F(46)-C(43)-F(44)	108.1(13)
C(20)-C(28)-C(29)	123.3(3)	F(45)-C(43)-F(44)	111.4(14)
C(26)-C(27)-C(28)	120.9(3)	F(46)-C(43)-S(40)	113.9(12)
C(26)-C(27)-H(27)	119.5	F(45)-C(43)-S(40)	111.3(11)
C(28)-C(27)-H(27)	119.5	F(44)-C(43)-S(40)	111.0(11)
C(29)-C(30)-H(30A)	109.5	S(40')-N(32')-S(33')	129.0(15)
C(29)-C(30)-H(30B)	109.5	O(35')-S(33')-O(34')	117.6(15)
H(30A)-C(30)-H(30B)	109.5	O(35')-S(33')-N(32')	116.2(14)
C(29)-C(30)-H(30C)	109.5	O(34')-S(33')-N(32')	107.8(16)
H(30A)-C(30)-H(30C)	109.5	O(35')-S(33')-C(36')	106.0(14)
H(30B)-C(30)-H(30C)	109.5	O(34')-S(33')-C(36')	97.3(16)
C(29)-C(31)-H(31A)	109.5	N(32')-S(33')-C(36')	110.2(12)
C(29)-C(31)-H(31B)	109.5	F(37')-C(36')-F(39')	108(2)
H(31A)-C(31)-H(31B)	109.5	F(37')-C(36')-F(38')	110(2)
C(29)-C(31)-H(31C)	109.5	F(39')-C(36')-F(38')	110(2)
H(31A)-C(31)-H(31C)	109.5	F(37')-C(36')-S(33')	117(2)
H(31B)-C(31)-H(31C)	109.5	F(39')-C(36')-S(33')	100.9(18)
S(33)-N(32)-S(40)	121.9(6)	F(38')-C(36')-S(33')	110.8(16)
O(35)-S(33)-O(34)	115.6(7)	O(42')-S(40')-O(41')	114(2)
O(35)-S(33)-N(32)	119.1(8)	O(42')-S(40')-N(32')	107.8(16)
O(34)-S(33)-N(32)	103.6(5)	O(41')-S(40')-N(32')	111(2)
O(35)-S(33)-C(36)	107.5(7)	O(42')-S(40')-C(43')	111.8(18)
O(34)-S(33)-C(36)	104.9(5)	O(41')-S(40')-C(43')	101.0(19)
N(32)-S(33)-C(36)	104.8(5)	N(32')-S(40')-C(43')	111.5(13)
F(39)-C(36)-F(38)	111.1(11)	F(46')-C(43')-F(44')	105(2)
F(39)-C(36)-F(37)	108.4(10)	F(46')-C(43')-F(45')	103(2)
F(38)-C(36)-F(37)	105.8(10)	F(44')-C(43')-F(45')	105(2)
F(39)-C(36)-S(33)	111.0(8)	F(46')-C(43')-S(40')	119(2)

F(44')-C(43')-S(40')	118(2)	F(52')-C(51')-S(48')	102.2(16)
F(45')-C(43')-S(40')	104.5(18)	F(53')-C(51')-S(48')	98.3(15)
S(48)-N(47)-S(55)	115.7(11)	F(54')-C(51')-S(48')	103.1(15)
O(50)-S(48)-O(49)	119.3(16)	O(57')-S(55')-O(56')	114.9(9)
O(50)-S(48)-N(47)	110.8(14)	O(57')-S(55')-N(47')	111.8(10)
O(49)-S(48)-N(47)	120.3(15)	O(56')-S(55')-N(47')	110.6(11)
O(50)-S(48)-C(51)	106.0(14)	O(57')-S(55')-C(58')	100.2(9)
O(49)-S(48)-C(51)	99.5(14)	O(56')-S(55')-C(58')	109.8(10)
N(47)-S(48)-C(51)	95.7(12)	N(47')-S(55')-C(58')	108.9(10)
F(53)-C(51)-F(54)	109.5(19)	F(60')-C(58')-F(59')	110.7(17)
F(53)-C(51)-F(52)	117(2)	F(60')-C(58')-F(61')	97.6(17)
F(54)-C(51)-F(52)	108.4(19)	F(59')-C(58')-F(61')	105.2(17)
F(53)-C(51)-S(48)	105.6(16)	F(60')-C(58')-S(55')	124.0(16)
F(54)-C(51)-S(48)	104.8(15)	F(59')-C(58')-S(55')	111.6(12)
F(52)-C(51)-S(48)	110.4(15)	F(61')-C(58')-S(55')	104.9(12)
O(56)-S(55)-O(57)	118.4(7)	Cl(2)-C(1)-Cl(3)	114.4(11)
O(56)-S(55)-N(47)	111.9(8)	Cl(2)-C(1)-H(1A)	108.7
O(57)-S(55)-N(47)	119.9(7)	Cl(3)-C(1)-H(1A)	108.7
O(56)-S(55)-C(58)	99.5(8)	Cl(2)-C(1)-H(1B)	108.7
O(57)-S(55)-C(58)	105.0(8)	Cl(3)-C(1)-H(1B)	108.7
N(47)-S(55)-C(58)	96.7(9)	H(1A)-C(1)-H(1B)	107.6
F(59)-C(58)-F(60)	111.7(15)		
F(59)-C(58)-F(61)	113.3(15)	Compound 9	
F(60)-C(58)-F(61)	112.8(16)		
F(59)-C(58)-S(55)	110.8(13)	B(1)-C(2)	1.690(3)
F(60)-C(58)-S(55)	101.1(12)	B(1)-C(32)	1.692(3)
F(61)-C(58)-S(55)	106.4(12)	B(1)-H(1)	1.116(19)
S(48')-N(47')-S(55')	121.0(14)	B(1)-H(2)	1.120(19)
O(50')-S(48')-O(49')	117.5(15)	C(2)-C(3)	1.454(3)
O(50')-S(48')-N(47')	118.2(14)	C(2)-H(2A)	0.9900
O(49')-S(48')-N(47')	111.4(15)	C(2)-H(2B)	0.9900
O(50')-S(48')-C(51')	104.3(14)	C(3)-N(4)	1.335(3)
O(49')-S(48')-C(51')	94.9(14)	C(3)-N(7)	1.337(3)
N(47')-S(48')-C(51')	106.7(13)	N(4)-C(8)	1.443(3)
F(52')-C(51')-F(53')	114(2)	N(4)-C(5)	1.471(3)
F(52')-C(51')-F(54')	113(2)	C(5)-C(6)	1.535(3)
F(53')-C(51')-F(54')	123(2)	C(5)-H(5A)	0.9900

C(5)-H(5B)	0.9900	C(21)-C(26)	1.522(3)
C(6)-N(7)	1.481(3)	C(22)-C(23)	1.386(3)
C(6)-H(6A)	0.9900	C(22)-H(22)	0.9500
C(6)-H(6B)	0.9900	C(23)-C(24)	1.386(4)
N(7)-C(20)	1.442(3)	C(23)-H(23)	0.9500
C(8)-C(9)	1.406(3)	C(24)-C(25)	1.398(4)
C(8)-C(13)	1.409(3)	C(24)-H(24)	0.9500
C(9)-C(10)	1.392(4)	C(25)-C(29)	1.518(3)
C(9)-C(14)	1.526(3)	C(26)-C(28)	1.530(4)
C(10)-C(11)	1.388(4)	C(26)-C(27)	1.538(3)
C(10)-H(10)	0.9500	C(26)-H(26)	1.0000
C(11)-C(12)	1.383(4)	C(27)-H(27A)	0.9800
C(11)-H(11)	0.9500	C(27)-H(27B)	0.9800
C(12)-C(13)	1.393(4)	C(27)-H(27C)	0.9800
C(12)-H(12)	0.9500	C(28)-H(28A)	0.9800
C(13)-C(17)	1.524(4)	C(28)-H(28B)	0.9800
C(14)-C(15)	1.530(3)	C(28)-H(28C)	0.9800
C(14)-C(16)	1.534(4)	C(29)-C(30)	1.527(4)
C(14)-H(14)	1.0000	C(29)-C(31)	1.540(4)
C(15)-H(15A)	0.9800	C(29)-H(29)	1.0000
C(15)-H(15B)	0.9800	C(30)-H(30A)	0.9800
C(15)-H(15C)	0.9800	C(30)-H(30B)	0.9800
C(16)-H(16A)	0.9800	C(30)-H(30C)	0.9800
C(16)-H(16B)	0.9800	C(31)-H(31A)	0.9800
C(16)-H(16C)	0.9800	C(31)-H(31B)	0.9800
C(17)-C(18)	1.521(4)	C(31)-H(31C)	0.9800
C(17)-C(19)	1.533(4)	C(32)-C(33)	1.458(3)
C(17)-H(17)	1.0000	C(32)-H(32A)	0.9900
C(18)-H(18A)	0.9800	C(32)-H(32B)	0.9900
C(18)-H(18B)	0.9800	C(33)-N(34)	1.329(3)
C(18)-H(18C)	0.9800	C(33)-N(37)	1.342(3)
C(19)-H(19A)	0.9800	N(34)-C(38)	1.451(3)
C(19)-H(19B)	0.9800	N(34)-C(35)	1.481(3)
C(19)-H(19C)	0.9800	C(35)-C(36)	1.533(3)
C(20)-C(25)	1.406(3)	C(35)-H(35A)	0.9900
C(20)-C(21)	1.412(3)	C(35)-H(35B)	0.9900
C(21)-C(22)	1.389(3)	C(36)-N(37)	1.467(3)

C(36)-H(36A)	0.9900	C(52)-H(52)	0.9500
C(36)-H(36B)	0.9900	C(53)-C(54)	1.389(4)
N(37)-C(50)	1.440(3)	C(53)-H(53)	0.9500
C(38)-C(39)	1.398(3)	C(54)-C(55)	1.398(3)
C(38)-C(43)	1.408(3)	C(54)-H(54)	0.9500
C(39)-C(40)	1.405(3)	C(55)-C(59)	1.517(3)
C(39)-C(44)	1.522(3)	C(56)-C(58)	1.528(4)
C(40)-C(41)	1.387(4)	C(56)-C(57)	1.541(4)
C(40)-H(40)	0.9500	C(56)-H(56)	1.0000
C(41)-C(42)	1.378(4)	C(57)-H(57A)	0.9800
C(41)-H(41)	0.9500	C(57)-H(57B)	0.9800
C(42)-C(43)	1.401(3)	C(57)-H(57C)	0.9800
C(42)-H(42)	0.9500	C(58)-H(58A)	0.9800
C(43)-C(47)	1.524(4)	C(58)-H(58B)	0.9800
C(44)-C(46)	1.530(4)	C(58)-H(58C)	0.9800
C(44)-C(45)	1.532(4)	C(59)-C(61)	1.529(3)
C(44)-H(44)	1.0000	C(59)-C(60)	1.535(3)
C(45)-H(45A)	0.9800	C(59)-H(59)	1.0000
C(45)-H(45B)	0.9800	C(60)-H(60A)	0.9800
C(45)-H(45C)	0.9800	C(60)-H(60B)	0.9800
C(46)-H(46A)	0.9800	C(60)-H(60C)	0.9800
C(46)-H(46B)	0.9800	C(61)-H(61A)	0.9800
C(46)-H(46C)	0.9800	C(61)-H(61B)	0.9800
C(47)-C(49)	1.526(4)	C(61)-H(61C)	0.9800
C(47)-C(48)	1.527(4)	F(62)-C(62)	1.314(4)
C(47)-H(47)	1.0000	C(62)-C(63)	1.346(4)
C(48)-H(48A)	0.9800	C(62)-C(67)	1.366(4)
C(48)-H(48B)	0.9800	C(63)-C(64)	1.363(5)
C(48)-H(48C)	0.9800	C(63)-H(63)	0.9500
C(49)-H(49A)	0.9800	C(64)-C(65)	1.391(5)
C(49)-H(49B)	0.9800	C(64)-H(64)	0.9500
C(49)-H(49C)	0.9800	C(65)-C(66)	1.388(5)
C(50)-C(55)	1.401(3)	C(65)-H(65)	0.9500
C(50)-C(51)	1.402(3)	C(66)-C(67)	1.369(5)
C(51)-C(52)	1.398(3)	C(66)-H(66)	0.9500
C(51)-C(56)	1.525(3)	C(67)-H(67)	0.9500
C(52)-C(53)	1.383(4)	F(69)-C(69)	1.208(5)

C(69)-C(71)	1.363(5)	C(3)-N(4)-C(8)	125.99(19)
C(69)-C(70)	1.369(5)	C(3)-N(4)-C(5)	111.52(19)
C(69)-H(69)	0.9500	C(8)-N(4)-C(5)	122.04(18)
C(70)-C(71)#1	1.364(5)	N(4)-C(5)-C(6)	102.87(18)
C(70)-H(70)	0.9500	N(4)-C(5)-H(5A)	111.2
C(71)-C(70)#1	1.364(5)	C(6)-C(5)-H(5A)	111.2
C(71)-H(71)	0.9500	N(4)-C(5)-H(5B)	111.2
N(73)-S(74)	1.576(2)	C(6)-C(5)-H(5B)	111.2
N(73)-S(81)	1.578(2)	H(5A)-C(5)-H(5B)	109.1
S(74)-O(76)	1.420(2)	N(7)-C(6)-C(5)	102.68(18)
S(74)-O(75)	1.434(2)	N(7)-C(6)-H(6A)	111.2
S(74)-C(77)	1.836(3)	C(5)-C(6)-H(6A)	111.2
C(77)-F(78)	1.313(3)	N(7)-C(6)-H(6B)	111.2
C(77)-F(79)	1.322(3)	C(5)-C(6)-H(6B)	111.2
C(77)-F(80)	1.341(3)	H(6A)-C(6)-H(6B)	109.1
S(81)-O(82)	1.424(2)	C(3)-N(7)-C(20)	124.76(19)
S(81)-O(83)	1.425(2)	C(3)-N(7)-C(6)	110.85(19)
S(81)-C(84)	1.824(3)	C(20)-N(7)-C(6)	123.41(19)
C(84)-F(87)	1.311(3)	C(9)-C(8)-C(13)	122.4(2)
C(84)-F(86)	1.346(3)	C(9)-C(8)-N(4)	119.4(2)
C(84)-F(85)	1.348(3)	C(13)-C(8)-N(4)	118.2(2)
		C(10)-C(9)-C(8)	117.6(2)
C(2)-B(1)-C(32)	109.21(18)	C(10)-C(9)-C(14)	119.8(2)
C(2)-B(1)-H(1)	110.1(12)	C(8)-C(9)-C(14)	122.6(2)
C(32)-B(1)-H(1)	110.5(12)	C(11)-C(10)-C(9)	121.2(2)
C(2)-B(1)-H(2)	111.7(13)	C(11)-C(10)-H(10)	119.4
C(32)-B(1)-H(2)	107.3(12)	C(9)-C(10)-H(10)	119.4
H(1)-B(1)-H(2)	108.1(17)	C(12)-C(11)-C(10)	120.0(2)
C(3)-C(2)-B(1)	112.01(18)	C(12)-C(11)-H(11)	120.0
C(3)-C(2)-H(2A)	109.2	C(10)-C(11)-H(11)	120.0
B(1)-C(2)-H(2A)	109.2	C(11)-C(12)-C(13)	121.6(2)
C(3)-C(2)-H(2B)	109.2	C(11)-C(12)-H(12)	119.2
B(1)-C(2)-H(2B)	109.2	C(13)-C(12)-H(12)	119.2
H(2A)-C(2)-H(2B)	107.9	C(12)-C(13)-C(8)	117.2(2)
N(4)-C(3)-N(7)	110.9(2)	C(12)-C(13)-C(17)	120.1(2)
N(4)-C(3)-C(2)	124.8(2)	C(8)-C(13)-C(17)	122.7(2)
N(7)-C(3)-C(2)	124.3(2)	C(9)-C(14)-C(15)	112.0(2)

C(9)-C(14)-C(16)	110.1(2)	C(21)-C(20)-N(7)	118.9(2)
C(15)-C(14)-C(16)	110.6(2)	C(22)-C(21)-C(20)	117.8(2)
C(9)-C(14)-H(14)	108.0	C(22)-C(21)-C(26)	120.0(2)
C(15)-C(14)-H(14)	108.0	C(20)-C(21)-C(26)	122.1(2)
C(16)-C(14)-H(14)	108.0	C(23)-C(22)-C(21)	121.5(2)
C(14)-C(15)-H(15A)	109.5	C(23)-C(22)-H(22)	119.2
C(14)-C(15)-H(15B)	109.5	C(21)-C(22)-H(22)	119.2
H(15A)-C(15)-H(15B)	109.5	C(24)-C(23)-C(22)	120.0(2)
C(14)-C(15)-H(15C)	109.5	C(24)-C(23)-H(23)	120.0
H(15A)-C(15)-H(15C)	109.5	C(22)-C(23)-H(23)	120.0
H(15B)-C(15)-H(15C)	109.5	C(23)-C(24)-C(25)	121.0(2)
C(14)-C(16)-H(16A)	109.5	C(23)-C(24)-H(24)	119.5
C(14)-C(16)-H(16B)	109.5	C(25)-C(24)-H(24)	119.5
H(16A)-C(16)-H(16B)	109.5	C(24)-C(25)-C(20)	118.0(2)
C(14)-C(16)-H(16C)	109.5	C(24)-C(25)-C(29)	119.3(2)
H(16A)-C(16)-H(16C)	109.5	C(20)-C(25)-C(29)	122.6(2)
H(16B)-C(16)-H(16C)	109.5	C(21)-C(26)-C(28)	109.27(19)
C(18)-C(17)-C(13)	111.7(2)	C(21)-C(26)-C(27)	112.7(2)
C(18)-C(17)-C(19)	111.2(2)	C(28)-C(26)-C(27)	110.5(2)
C(13)-C(17)-C(19)	110.8(2)	C(21)-C(26)-H(26)	108.1
C(18)-C(17)-H(17)	107.6	C(28)-C(26)-H(26)	108.1
C(13)-C(17)-H(17)	107.6	C(27)-C(26)-H(26)	108.1
C(19)-C(17)-H(17)	107.6	C(26)-C(27)-H(27A)	109.5
C(17)-C(18)-H(18A)	109.5	C(26)-C(27)-H(27B)	109.5
C(17)-C(18)-H(18B)	109.5	H(27A)-C(27)-H(27B)	109.5
H(18A)-C(18)-H(18B)	109.5	C(26)-C(27)-H(27C)	109.5
C(17)-C(18)-H(18C)	109.5	H(27A)-C(27)-H(27C)	109.5
H(18A)-C(18)-H(18C)	109.5	H(27B)-C(27)-H(27C)	109.5
H(18B)-C(18)-H(18C)	109.5	C(26)-C(28)-H(28A)	109.5
C(17)-C(19)-H(19A)	109.5	C(26)-C(28)-H(28B)	109.5
C(17)-C(19)-H(19B)	109.5	H(28A)-C(28)-H(28B)	109.5
H(19A)-C(19)-H(19B)	109.5	C(26)-C(28)-H(28C)	109.5
C(17)-C(19)-H(19C)	109.5	H(28A)-C(28)-H(28C)	109.5
H(19A)-C(19)-H(19C)	109.5	H(28B)-C(28)-H(28C)	109.5
H(19B)-C(19)-H(19C)	109.5	C(25)-C(29)-C(30)	112.6(2)
C(25)-C(20)-C(21)	121.7(2)	C(25)-C(29)-C(31)	109.3(2)
C(25)-C(20)-N(7)	119.4(2)	C(30)-C(29)-C(31)	110.5(2)

C(25)-C(29)-H(29)	108.1	C(35)-C(36)-H(36B)	111.1
C(30)-C(29)-H(29)	108.1	H(36A)-C(36)-H(36B)	109.1
C(31)-C(29)-H(29)	108.1	C(33)-N(37)-C(50)	126.22(19)
C(29)-C(30)-H(30A)	109.5	C(33)-N(37)-C(36)	111.78(18)
C(29)-C(30)-H(30B)	109.5	C(50)-N(37)-C(36)	121.00(17)
H(30A)-C(30)-H(30B)	109.5	C(39)-C(38)-C(43)	123.0(2)
C(29)-C(30)-H(30C)	109.5	C(39)-C(38)-N(34)	119.0(2)
H(30A)-C(30)-H(30C)	109.5	C(43)-C(38)-N(34)	118.0(2)
H(30B)-C(30)-H(30C)	109.5	C(38)-C(39)-C(40)	117.0(2)
C(29)-C(31)-H(31A)	109.5	C(38)-C(39)-C(44)	123.3(2)
C(29)-C(31)-H(31B)	109.5	C(40)-C(39)-C(44)	119.6(2)
H(31A)-C(31)-H(31B)	109.5	C(41)-C(40)-C(39)	121.1(2)
C(29)-C(31)-H(31C)	109.5	C(41)-C(40)-H(40)	119.5
H(31A)-C(31)-H(31C)	109.5	C(39)-C(40)-H(40)	119.5
H(31B)-C(31)-H(31C)	109.5	C(42)-C(41)-C(40)	120.6(2)
C(33)-C(32)-B(1)	110.50(19)	C(42)-C(41)-H(41)	119.7
C(33)-C(32)-H(32A)	109.6	C(40)-C(41)-H(41)	119.7
B(1)-C(32)-H(32A)	109.6	C(41)-C(42)-C(43)	120.9(2)
C(33)-C(32)-H(32B)	109.6	C(41)-C(42)-H(42)	119.6
B(1)-C(32)-H(32B)	109.6	C(43)-C(42)-H(42)	119.6
H(32A)-C(32)-H(32B)	108.1	C(42)-C(43)-C(38)	117.4(2)
N(34)-C(33)-N(37)	110.56(19)	C(42)-C(43)-C(47)	119.8(2)
N(34)-C(33)-C(32)	125.3(2)	C(38)-C(43)-C(47)	122.7(2)
N(37)-C(33)-C(32)	124.0(2)	C(39)-C(44)-C(46)	113.9(2)
C(33)-N(34)-C(38)	125.53(19)	C(39)-C(44)-C(45)	109.8(2)
C(33)-N(34)-C(35)	111.64(18)	C(46)-C(44)-C(45)	109.6(2)
C(38)-N(34)-C(35)	122.54(18)	C(39)-C(44)-H(44)	107.8
N(34)-C(35)-C(36)	102.85(18)	C(46)-C(44)-H(44)	107.8
N(34)-C(35)-H(35A)	111.2	C(45)-C(44)-H(44)	107.8
C(36)-C(35)-H(35A)	111.2	C(44)-C(45)-H(45A)	109.5
N(34)-C(35)-H(35B)	111.2	C(44)-C(45)-H(45B)	109.5
C(36)-C(35)-H(35B)	111.2	H(45A)-C(45)-H(45B)	109.5
H(35A)-C(35)-H(35B)	109.1	C(44)-C(45)-H(45C)	109.5
N(37)-C(36)-C(35)	103.09(17)	H(45A)-C(45)-H(45C)	109.5
N(37)-C(36)-H(36A)	111.1	H(45B)-C(45)-H(45C)	109.5
C(35)-C(36)-H(36A)	111.1	C(44)-C(46)-H(46A)	109.5
N(37)-C(36)-H(36B)	111.1	C(44)-C(46)-H(46B)	109.5

H(46A)-C(46)-H(46B)	109.5	C(54)-C(55)-C(50)	117.2(2)
C(44)-C(46)-H(46C)	109.5	C(54)-C(55)-C(59)	119.9(2)
H(46A)-C(46)-H(46C)	109.5	C(50)-C(55)-C(59)	122.9(2)
H(46B)-C(46)-H(46C)	109.5	C(51)-C(56)-C(58)	112.2(2)
C(43)-C(47)-C(49)	113.8(2)	C(51)-C(56)-C(57)	110.8(2)
C(43)-C(47)-C(48)	110.2(2)	C(58)-C(56)-C(57)	110.7(2)
C(49)-C(47)-C(48)	110.4(2)	C(51)-C(56)-H(56)	107.6
C(43)-C(47)-H(47)	107.4	C(58)-C(56)-H(56)	107.6
C(49)-C(47)-H(47)	107.4	C(57)-C(56)-H(56)	107.6
C(48)-C(47)-H(47)	107.4	C(56)-C(57)-H(57A)	109.5
C(47)-C(48)-H(48A)	109.5	C(56)-C(57)-H(57B)	109.5
C(47)-C(48)-H(48B)	109.5	H(57A)-C(57)-H(57B)	109.5
H(48A)-C(48)-H(48B)	109.5	C(56)-C(57)-H(57C)	109.5
C(47)-C(48)-H(48C)	109.5	H(57A)-C(57)-H(57C)	109.5
H(48A)-C(48)-H(48C)	109.5	H(57B)-C(57)-H(57C)	109.5
H(48B)-C(48)-H(48C)	109.5	C(56)-C(58)-H(58A)	109.5
C(47)-C(49)-H(49A)	109.5	C(56)-C(58)-H(58B)	109.5
C(47)-C(49)-H(49B)	109.5	H(58A)-C(58)-H(58B)	109.5
H(49A)-C(49)-H(49B)	109.5	C(56)-C(58)-H(58C)	109.5
C(47)-C(49)-H(49C)	109.5	H(58A)-C(58)-H(58C)	109.5
H(49A)-C(49)-H(49C)	109.5	H(58B)-C(58)-H(58C)	109.5
H(49B)-C(49)-H(49C)	109.5	C(55)-C(59)-C(61)	112.0(2)
C(55)-C(50)-C(51)	122.9(2)	C(55)-C(59)-C(60)	110.46(19)
C(55)-C(50)-N(37)	118.2(2)	C(61)-C(59)-C(60)	110.6(2)
C(51)-C(50)-N(37)	118.77(19)	C(55)-C(59)-H(59)	107.9
C(52)-C(51)-C(50)	117.7(2)	C(61)-C(59)-H(59)	107.9
C(52)-C(51)-C(56)	119.0(2)	C(60)-C(59)-H(59)	107.9
C(50)-C(51)-C(56)	123.4(2)	C(59)-C(60)-H(60A)	109.5
C(53)-C(52)-C(51)	120.6(2)	C(59)-C(60)-H(60B)	109.5
C(53)-C(52)-H(52)	119.7	H(60A)-C(60)-H(60B)	109.5
C(51)-C(52)-H(52)	119.7	C(59)-C(60)-H(60C)	109.5
C(52)-C(53)-C(54)	120.6(2)	H(60A)-C(60)-H(60C)	109.5
C(52)-C(53)-H(53)	119.7	H(60B)-C(60)-H(60C)	109.5
C(54)-C(53)-H(53)	119.7	C(59)-C(61)-H(61A)	109.5
C(53)-C(54)-C(55)	121.0(2)	C(59)-C(61)-H(61B)	109.5
C(53)-C(54)-H(54)	119.5	H(61A)-C(61)-H(61B)	109.5
C(55)-C(54)-H(54)	119.5	C(59)-C(61)-H(61C)	109.5

H(61A)-C(61)-H(61C)	109.5	N(73)-S(74)-C(77)	102.89(13)
H(61B)-C(61)-H(61C)	109.5	F(78)-C(77)-F(79)	109.0(2)
F(62)-C(62)-C(63)	117.3(3)	F(78)-C(77)-F(80)	107.1(2)
F(62)-C(62)-C(67)	118.3(3)	F(79)-C(77)-F(80)	108.2(2)
C(63)-C(62)-C(67)	124.4(3)	F(78)-C(77)-S(74)	111.54(18)
C(62)-C(63)-C(64)	117.8(3)	F(79)-C(77)-S(74)	109.9(2)
C(62)-C(63)-H(63)	121.1	F(80)-C(77)-S(74)	110.98(19)
C(64)-C(63)-H(63)	121.1	O(82)-S(81)-O(83)	119.30(14)
C(63)-C(64)-C(65)	120.6(3)	O(82)-S(81)-N(73)	116.45(12)
C(63)-C(64)-H(64)	119.7	O(83)-S(81)-N(73)	109.01(14)
C(65)-C(64)-H(64)	119.7	O(82)-S(81)-C(84)	104.31(12)
C(66)-C(65)-C(64)	119.4(4)	O(83)-S(81)-C(84)	103.60(12)
C(66)-C(65)-H(65)	120.3	N(73)-S(81)-C(84)	101.53(13)
C(64)-C(65)-H(65)	120.3	F(87)-C(84)-F(86)	107.6(2)
C(67)-C(66)-C(65)	120.1(3)	F(87)-C(84)-F(85)	108.7(2)
C(67)-C(66)-H(66)	120.0	F(86)-C(84)-F(85)	105.4(2)
C(65)-C(66)-H(66)	120.0	F(87)-C(84)-S(81)	113.32(19)
C(62)-C(67)-C(66)	117.7(3)	F(86)-C(84)-S(81)	110.45(18)
C(62)-C(67)-H(67)	121.1	F(85)-C(84)-S(81)	111.12(17)
C(66)-C(67)-H(67)	121.1		
F(69)-C(69)-C(71)	117.1(4)		
F(69)-C(69)-C(70)	119.4(4)		
C(71)-C(69)-C(70)	123.3(4)		
C(71)-C(69)-H(69)	118.4		
C(70)-C(69)-H(69)	118.4		
C(71)#1-C(70)-C(69)	118.2(3)		
C(71)#1-C(70)-H(70)	120.9		
C(69)-C(70)-H(70)	120.9		
C(69)-C(71)-C(70)#1	118.6(3)		
C(69)-C(71)-H(71)	120.7		
C(70)#1-C(71)-H(71)	120.7		
S(74)-N(73)-S(81)	123.93(15)		
O(76)-S(74)-O(75)	118.80(14)		
O(76)-S(74)-N(73)	108.37(13)		
O(75)-S(74)-N(73)	116.66(12)		
O(76)-S(74)-C(77)	103.38(13)		
O(75)-S(74)-C(77)	104.47(12)		

Computational details

The geometries of the compounds **5-9** have been optimized using the functional M06-2X¹ combined with the def2-SVP basis set.² Stationary points were located with the Berny algorithm³ using redundant coordinates. Analytical Hessians were computed to determine the nature of the stationary points.⁴ All geometry optimizations were performed using the Gaussian 09 suite of programs.⁵ The NBO⁶ analyses have been carried out with the GENNBO 5.9⁷ program at the M06-2X/def2-TZVPP level of theory.

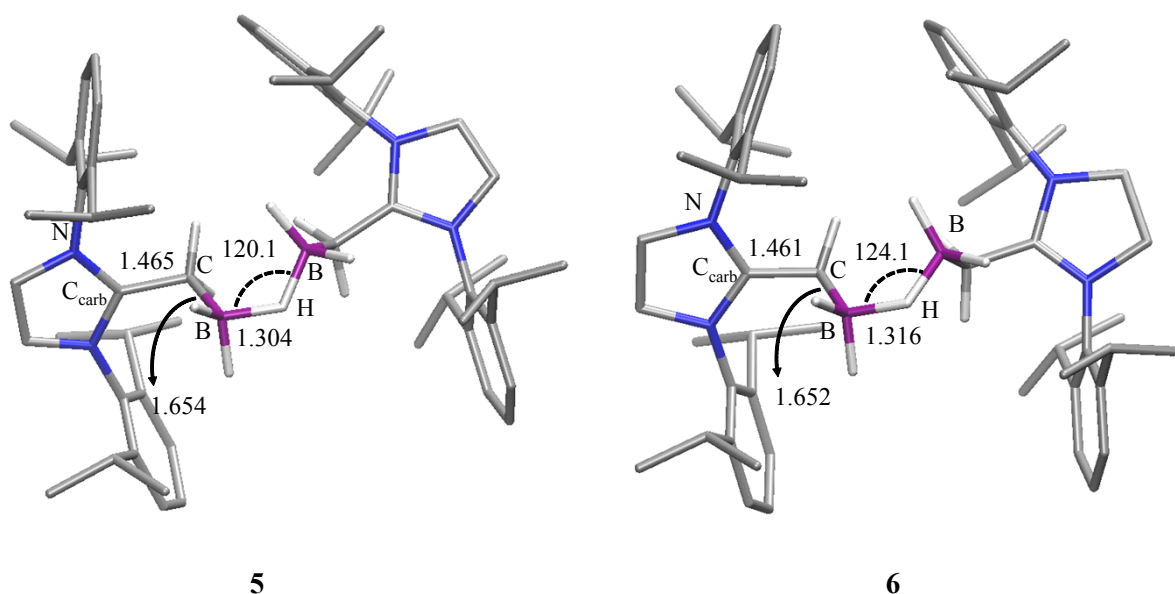


Fig. S2 Optimized structure (M06-2X/def2-SVP) of compounds **5** and **6**. Hydrogen atoms, except on the CH₂-H₂B-H-BH₂-CH₂ moiety, have been omitted for clarity. Bond distances and angles are in [Å] and [°], respectively.

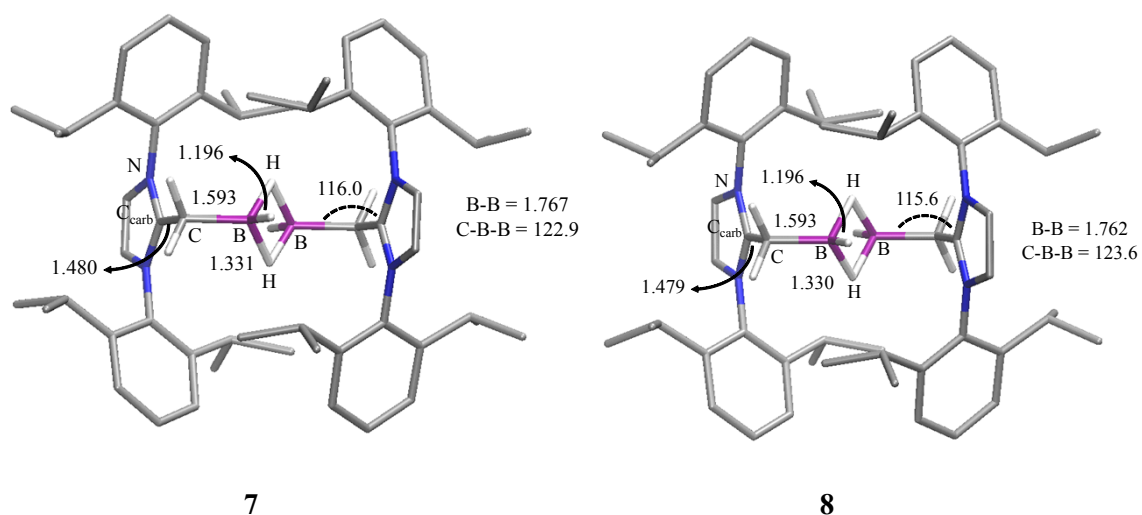


Fig. S3 Optimized structure (M06-2X/def2-SVP) of compounds **7** and **8**. Hydrogen atoms, except on the CH₂-HBH₂BH-CH₂ moiety, have been omitted for clarity. Bond distances and angles are in [Å] and [°], respectively.

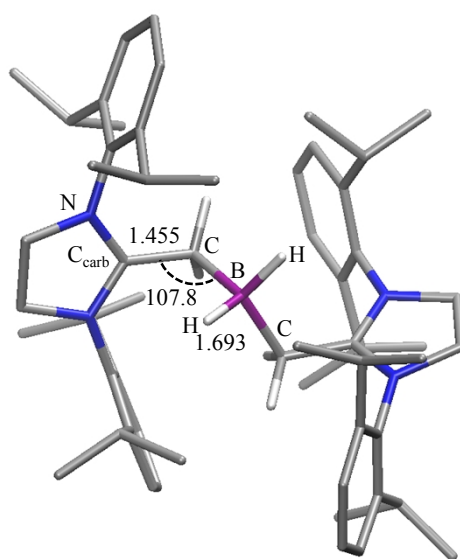


Fig. S4 Optimized structure (M06-2X/def2-SVP) of compound **9**. Hydrogen atoms, except on the CH₂-BH₂-CH₂ moiety, have been omitted for clarity. Bond distances and angles are in [Å] and [°], respectively.

Table S1 NPA charges and Wiberg Bond Order values at the M06-2X/def2- TZVPP of compounds **5-9**.

Comp.	Q(B)	Q(μH)	Q(C)	Q(C _{carb})	Q(N)	WBO(B-μH)	WBO(C-B)	WBO(B-B)	WBO(C-C _{carb})
5	-0.10	+0.05	-0.73	+0.57	-0.35	0.49	0.83	0.29	1.08
6	-0.10	+0.03	-0.75	+0.69	-0.42	0.50	0.81	0.29	1.10
7	+0.11	+0.13	-0.78	+0.53/	-0.33	0.46	0.91	0.64	1.05
8	+0.11	+0.13	-0.80	+0.66	-0.39	0.46	0.90	0.65	1.05
9	-0.08	---	-0.74	+0.69	-0.42	---	0.78	---	1.11

Table S2 NBO results at the M06-2X/def2- TZVPP//M06-2X/def2-SVP of compound **5**.

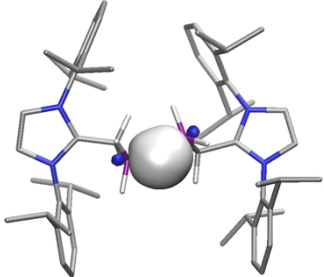
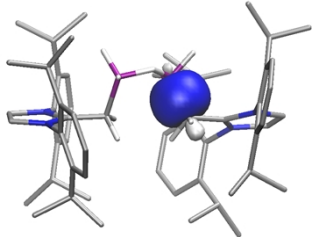
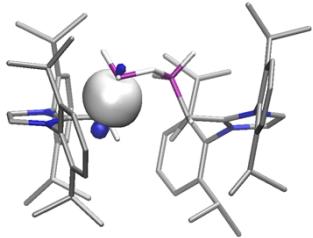
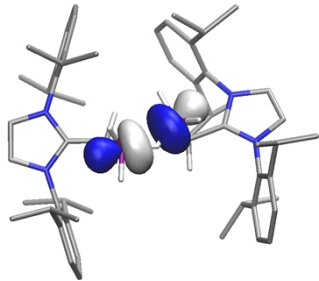
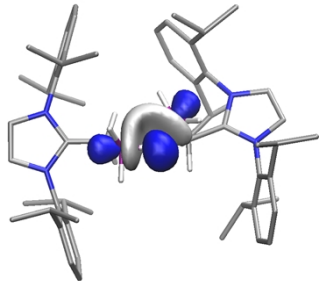
Orbital	Occ.	Contribution from atoms to the orbitals	Atomic orbitals
	1.98	B (26.79%) - H (47.42%) – B (25.80%)	B: s (17.49%) p (82.44%) H: s (99.52%) p (0.47%) B: s (17.43%) p (82.49%)
	1.92	B (31.84%) – C (68.16%)	B: s (25.71%) p (74.25%) C: s (30.85%) p (69.06%)
	1.92	B (32.10%) – C (67.90%)	B: s (26.20%) p (73.76%) C: s (30.84%) p (69.06%)
	0.03	B (49.47%) - H (0.00%) – B (50.53%)	B: s (17.49%) p (82.44%) H: s (0.00%) p (0.00%) B: s (17.43%) p (82.49%)
	0.02	B (23.74%) - H (52.58%) – B (23.67%)	B: s (17.49%) p (82.44%) H: s (99.52%) p (0.47%) B: s (17.43%) p (82.49%)

Table S3 NBO results at the M06-2X/def2- TZVPP//M06-2X/def2-SVP of compound **6**.

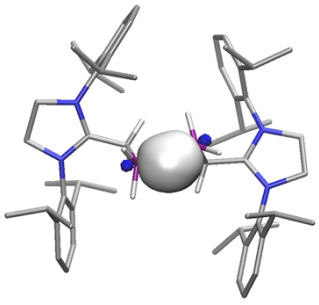
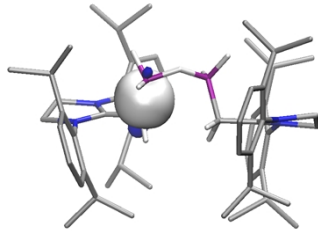
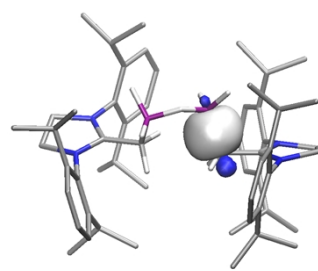
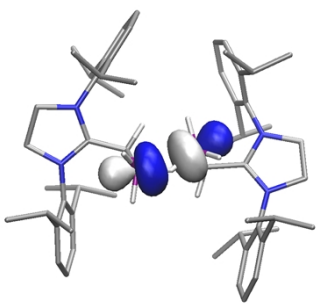
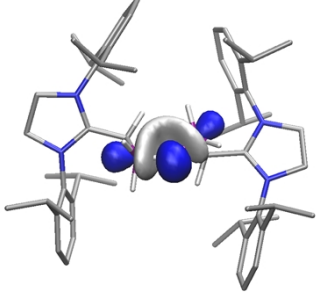
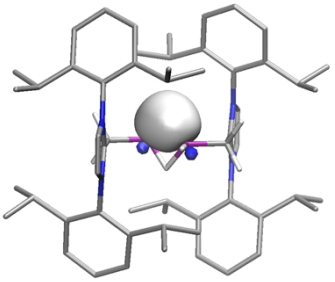
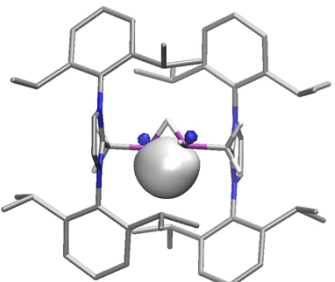
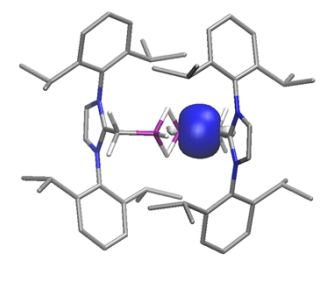
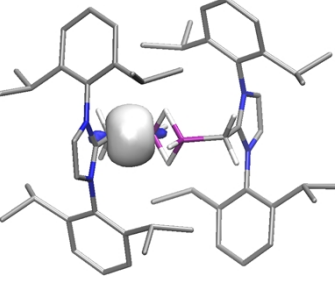
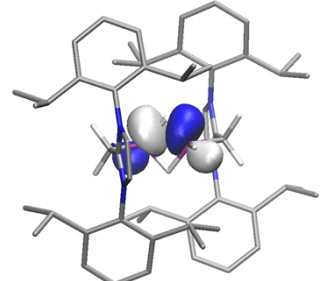
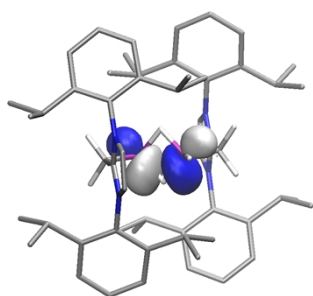
Orbital	Occ.	Contribution from atoms to the orbitals	Atomic orbitals
	1.98	B (26.53%) - H (48.31%) – B (25.16%)	B: s (17.00%) p (82.93%) H: s (99.60%) p (0.40%) B: s (16.70%) p (83.23%)
	1.90	B (31.51%) – C (68.49%)	B: s (25.69%) p (74.27%) C: s (29.17%) p (70.71%)
	1.91	B (31.80%) – C (68.20%)	B: s (26.20%) p (73.77%) C: s (29.38%) p (70.51%)
	0.03	B (51.84%) - H (0.11%) – B (48.05%)	B: s (17.00%) p (82.93%) H: s (99.60%) p (0.40%) B: s (16.70%) p (83.23%)
	0.02	B (21.63%) – H(51.58%)- B 26.79% ()	B: s (17.00%) p (82.93%) H: s (99.60%) p (0.40%) B: s (16.70%) p (83.23%)

Table S4 NBO results at the M06-2X/def2- TZVPP//M06-2X/def2-SVP of compound **7**.

Orbital	Occ.	Contribution from atoms to the orbitals	Atomic orbitals
	1.97	B (28.42%) - H (43.20%) – B (28.38%)	B: s (17.92%) p (81.91%) H: s (98.95%) p (1.03%) B: s (17.81%) p (82.02%)
	1.97	B (28.38%) - H (43.20%) – B (28.42%)	B: s (17.85%) p (81.98%) H: s (98.95%) p (1.03%) B: s (17.92%) p (81.92%)
	1.95	B (34.75%) – C (65.25%)	B: s (32.10%) p (67.86%) C: s (32.27%) p (67.58%)
	1.95	B (34.72%) – C (65.28%)	B: s (32.17%) p (67.79%) C: s (32.26%) p (67.60%)
	0.04	B (48.02%) - H (0.05%) – B (51.93%)	B: s (17.92%) p (81.91%) H: s (98.95%) p (1.03%) B: s (17.81%) p (82.02%)

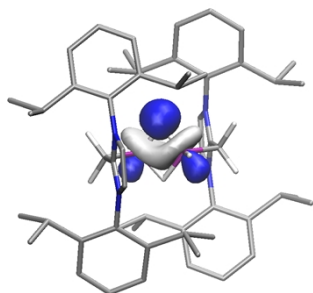


0.03 B (23.56%) - H (56.75%) – B (19.69%)

B: s (17.92%) p (81.91%)

H: s (98.95%) p (1.03%)

B: s (17.81%) p (82.02%)

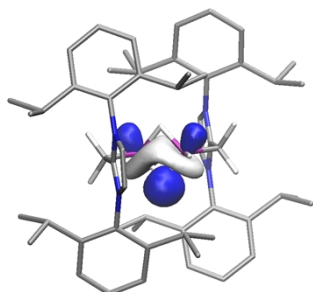


0.04 B (51.03%) - H (0.01%) – B (48.96%)

B: s (17.85%) p (81.98%)

H: s (98.95%) p (1.03%)

B: s (17.92%) p (81.92%)



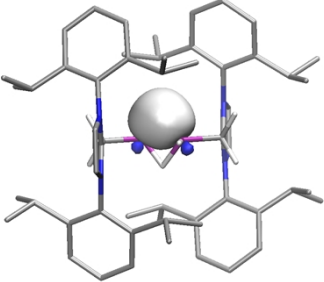
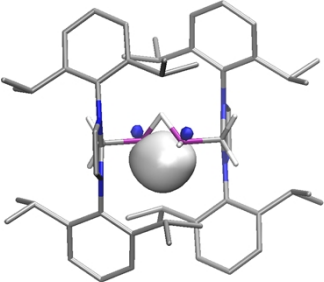
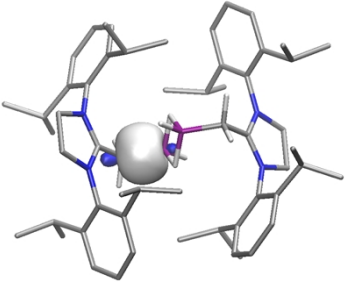
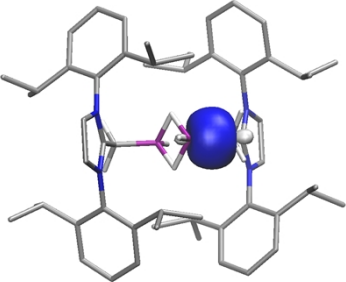
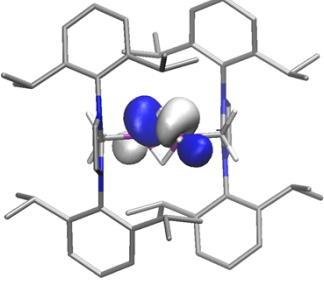
0.03 B (20.59%) - H (56.79%) – B (22.62%)

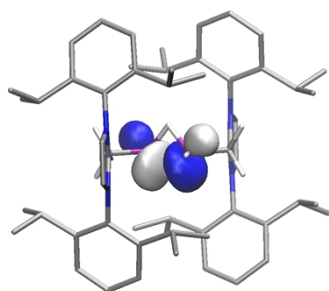
B: s (17.85%) p (81.98%)

H: s (98.95%) p (1.03%)

B: s (17.92%) p (81.92%)

Table S5 NBO results at the M06-2X/def2- TZVPP//M06-2X/def2-SVP of compound **8**.

Orbital	Occ.	Contribution from atoms to the orbitals	Atomic orbitals
	1.97	B (28.50%) - H (43.00%) – B (28.50%)	B: s (17.99%) p (81.85%) H: s (98.92%) p (1.06%) B: s (17.98%) p (81.85%)
	1.97	B (28.50%) - H (43.00%) – B (28.50%)	B: s (17.98%) p (81.85%) H: s (98.92%) p (1.06%) B: s (17.98%) p (81.85%)
	1.94	B (34.54%) – C (65.46%)	B: s (32.00%) p (67.96%) C: s (31.20%) p (68.66%)
	1.94	B (34.54%) – C (65.46%)	B: s (31.99%) p (67.96%) C: s (31.20%) p (68.66%)
	0.04	B (49.93%) - H (0.00%) – B (50.07%)	B: s (17.99%) p (81.85%) H: s (0.00%) p (0.00%) B: s (17.98%) p (81.85%)

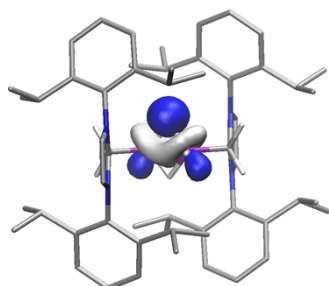


0.03 B (21.57%) - H (57.00%) - B (21.43%)

B: s (17.99%) p (81.85%)

H: s (98.92%) p (1.06%)

B: s (17.98%) p (81.85%)

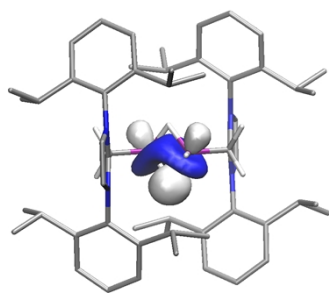


0.04 B (50.04%) - H (0.00%) - B (49.96%)

B: s (17.98%) p (81.85%)

H: s (0.00%) p (0.00%)

B: s (17.98%) p (81.85%)



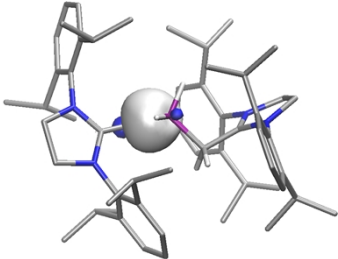
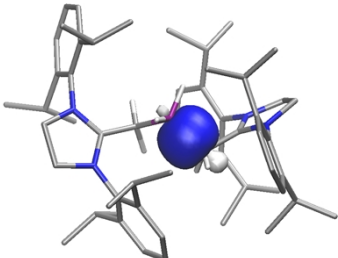
0.03 B (21.46%) - H (57.00%) - B (21.54%)

B: s (17.98%) p (81.85%)

H: s (98.92%) p (1.06%)

B: s (17.98%) p (81.85%)

Table S6. NBO results at the M06-2X/def2- TZVPP//M06-2X/def2-S of compound **9**.

Orbital	Occ.	Contribution from atoms to the orbitals	Atomic orbitals
	1.89	B (30.94%) – C (69.06%)	B: s (23.40%) p (76.57%) C: s (28.80%) p (71.10%)
	1.89	B (30.95%) – C (69.05%)	B: s (23.43%) p (76.54%) C: s (28.86%) p (71.05%)

M06-2X/def2-SVP Cartesian coordinates (in Å) and Electronic Energies (in Hartrees) of the calculated structures.

5				C	0.881495000000	-3.824076000000	-2.614057000000
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H	1.844815000000	0.186010000000	-2.487546000000	C	4.309639000000	3.920860000000	0.360757000000
C	1.613147000000	0.221728000000	-0.102152000000	H	4.204954000000	4.642163000000	1.170752000000
H	1.684490000000	1.298335000000	0.107889000000	C	4.628345000000	4.373697000000	-0.918481000000
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C	1.120851000000	-3.626868000000	2.518780000000	C	3.093302000000	3.079367000000	2.884682000000
H	0.888669000000	-3.687906000000	3.584106000000	H	3.741389000000	3.928525000000	3.146640000000
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H	-0.784917000000	2.050109000000	3.403176000000

6

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C	3.786875000000	2.727172000000	0.670884000000
H	2.861103000000	1.241827000000	1.890083000000
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H	4.674141000000	1.023169000000	3.577928000000
H	5.604806000000	2.301142000000	2.755590000000
C	2.909170000000	3.020922000000	3.044990000000
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H	1.995589000000	3.479418000000	2.639549000000
C	3.561938000000	2.080149000000	2.032842000000
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H	-3.829756000000	-1.359923000000	1.969727000000

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C	3.498482000000	-4.259394000000	-0.764040000000
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B	0.463781000000	-0.002339000000	-0.784455000000
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9

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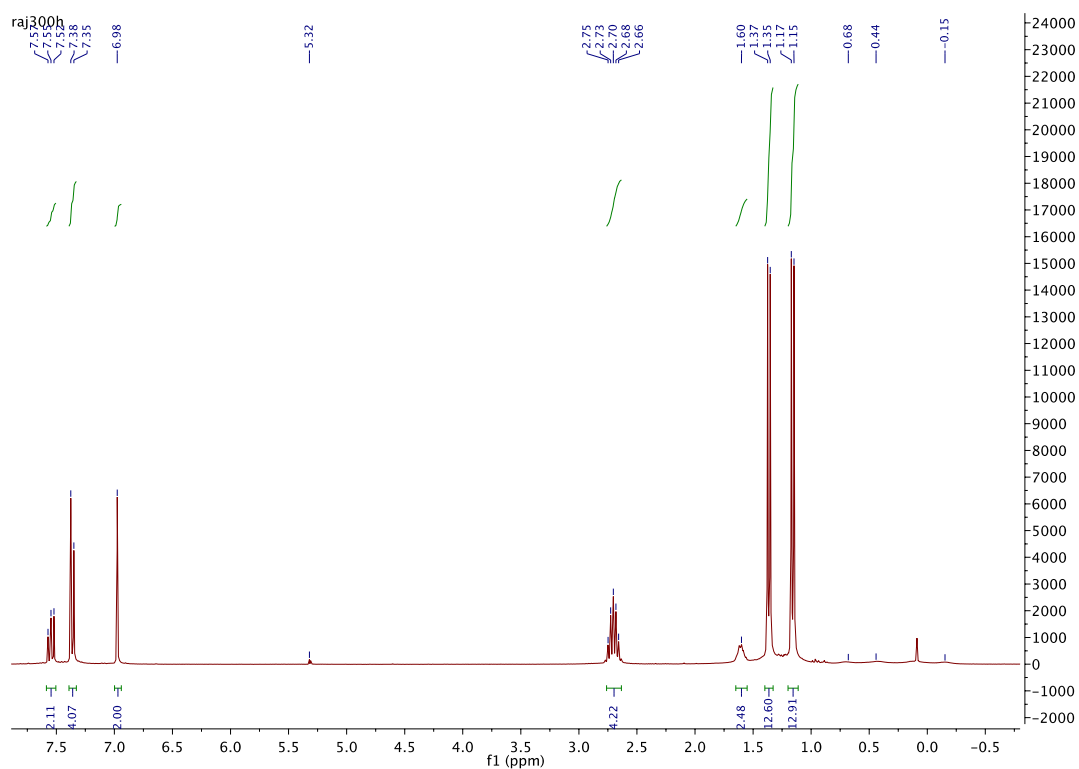
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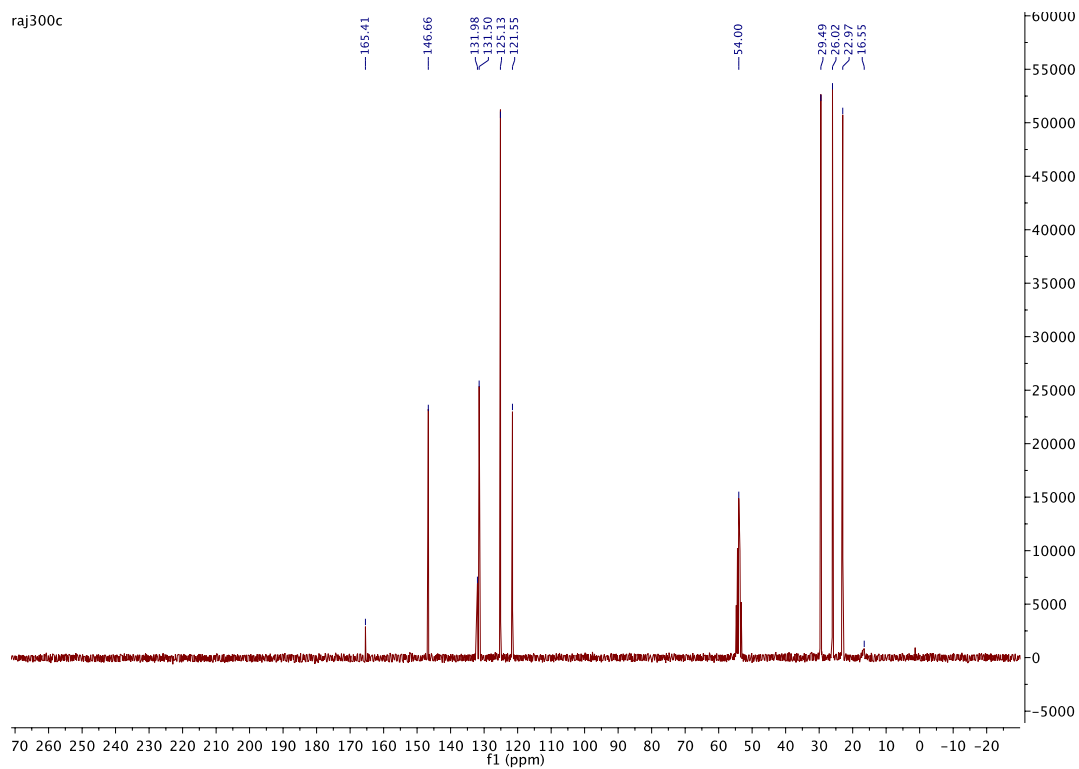
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H	-5.916370000000	2.488284000000	-2.898257000000
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C	-2.826244000000	3.552768000000	0.455848000000
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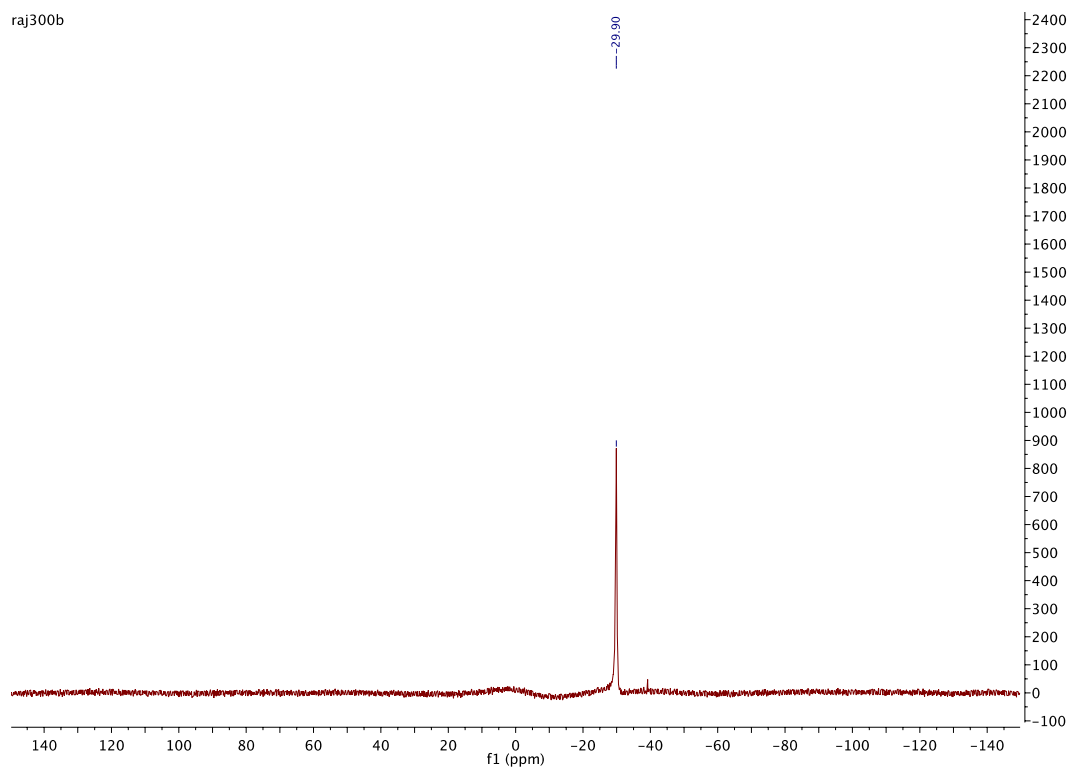
Plots of NMR Spectra:



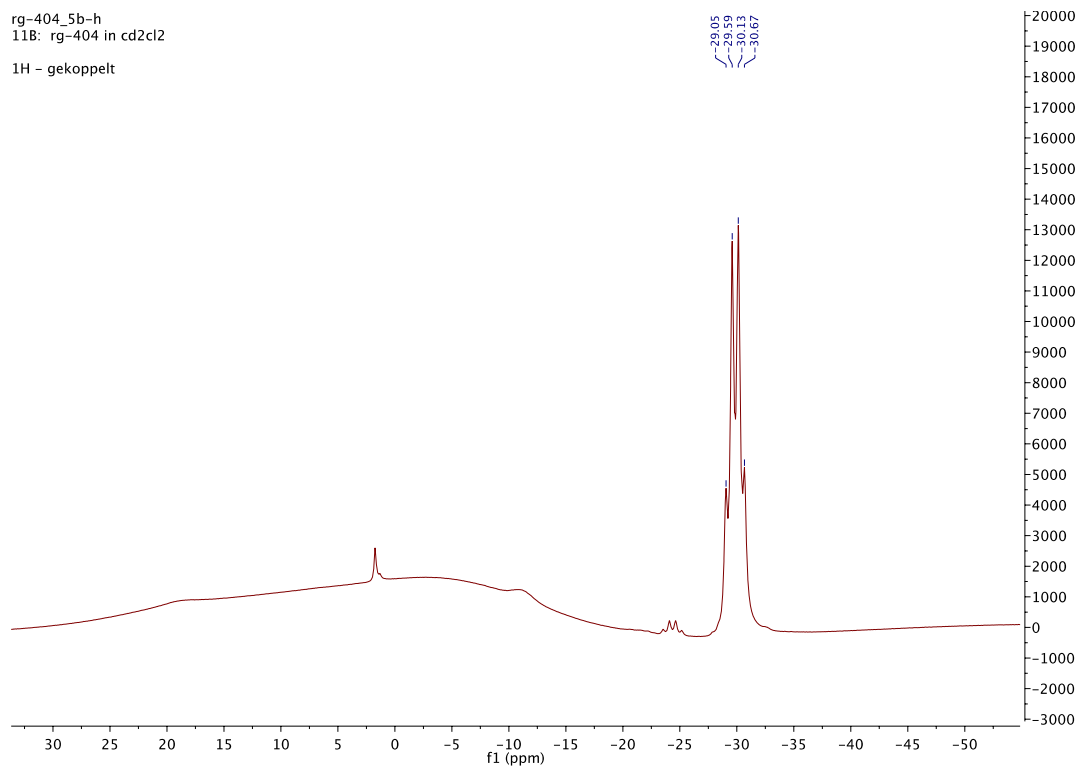
Plot 1. ^1H NMR spectrum of compound **3**.



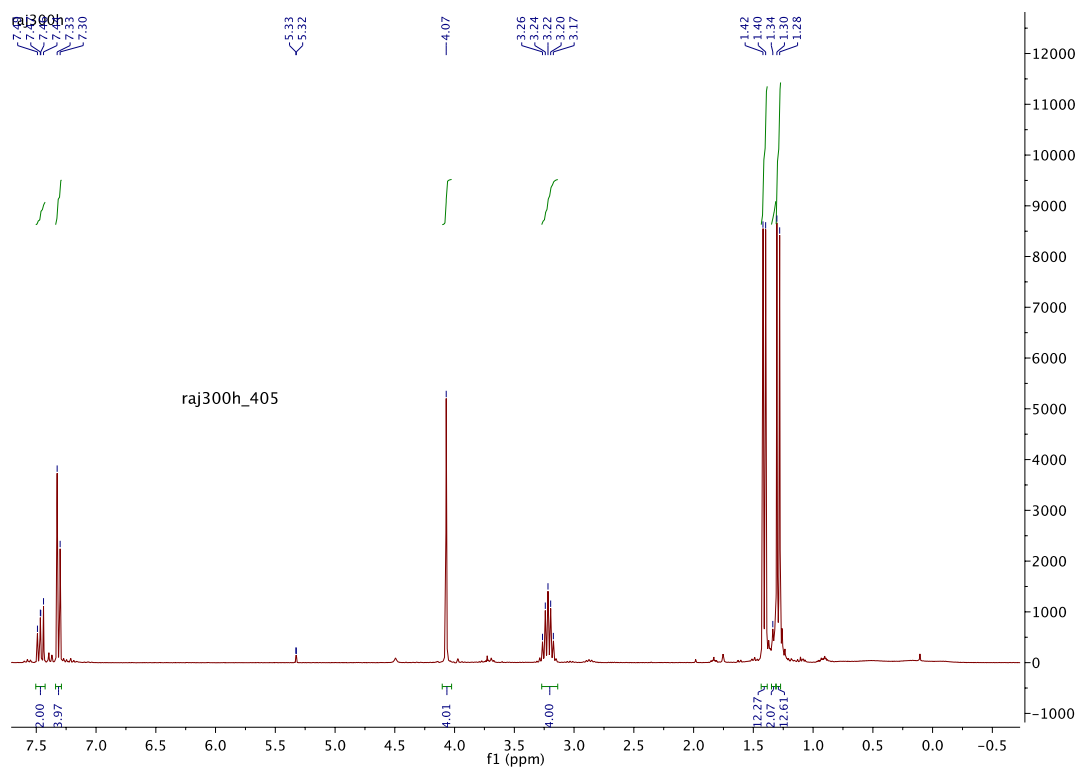
Plot 2. ^{13}C NMR spectrum of compound **3**.



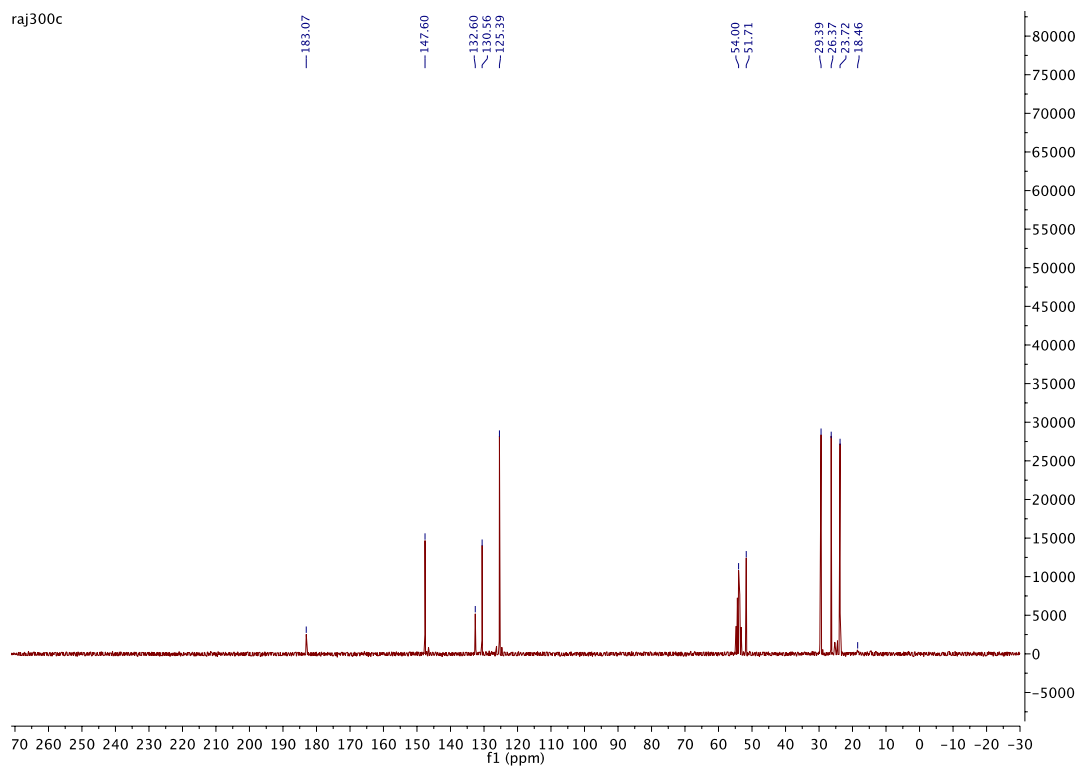
Plot 3. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **3**.



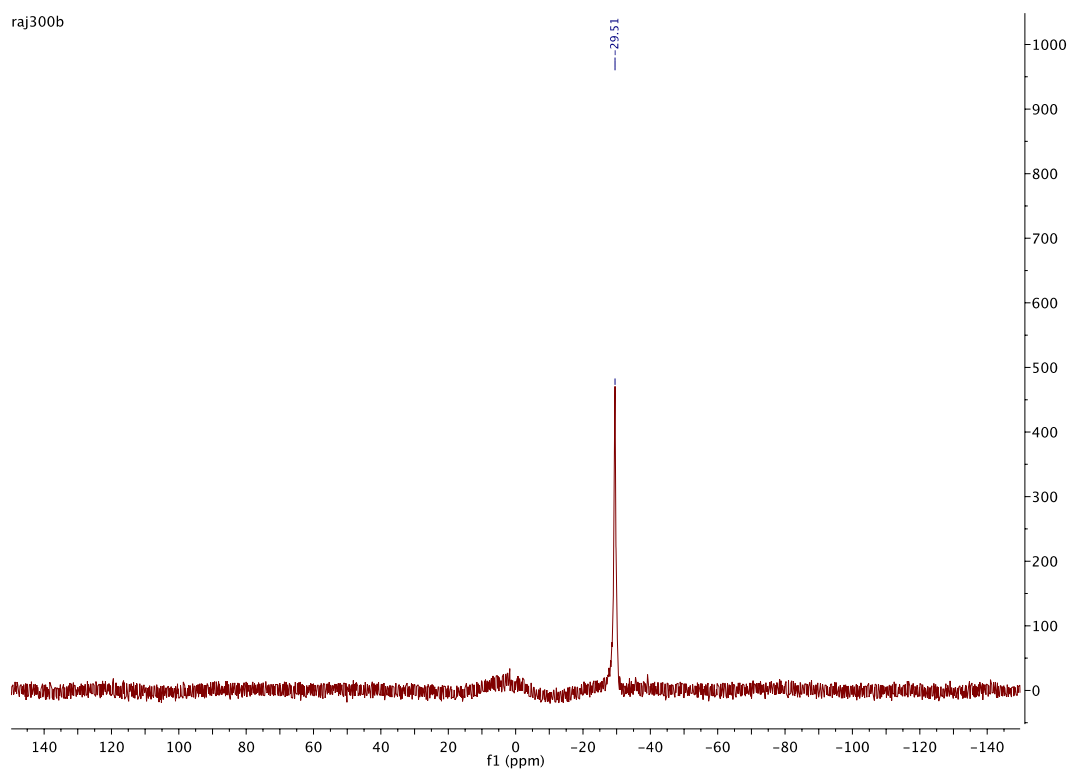
Plot 4. ^{11}B NMR spectrum of compound **3**.



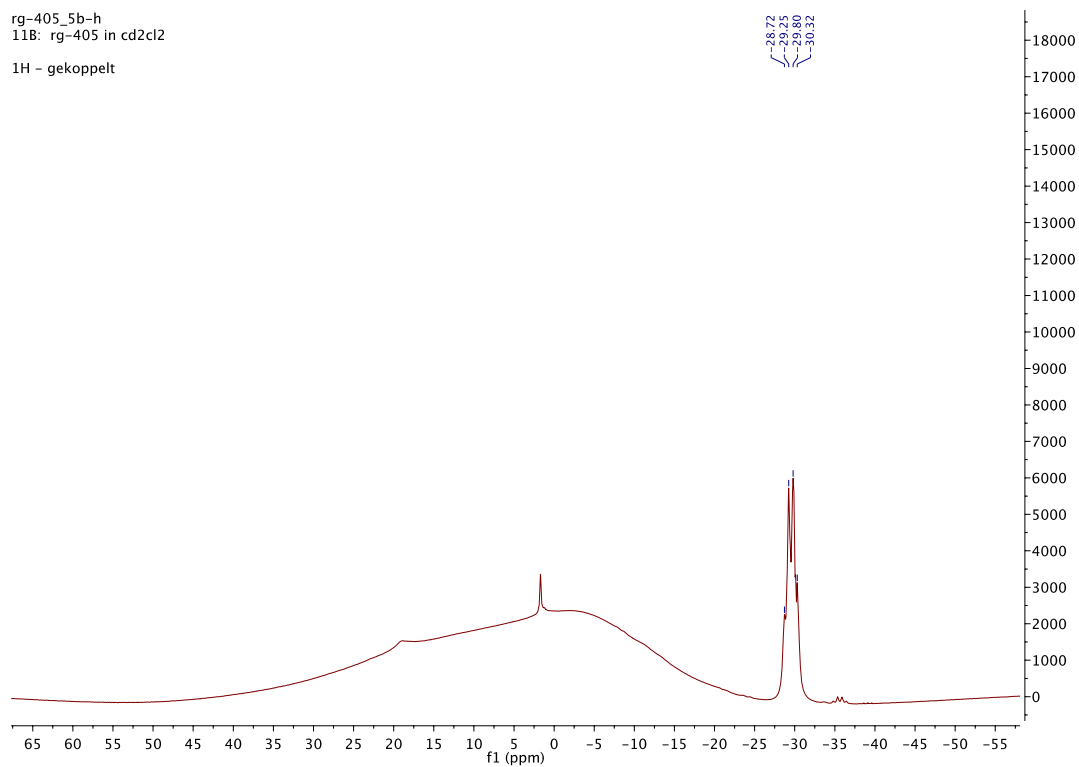
Plot 5. ^1H NMR spectrum of compound **4**.



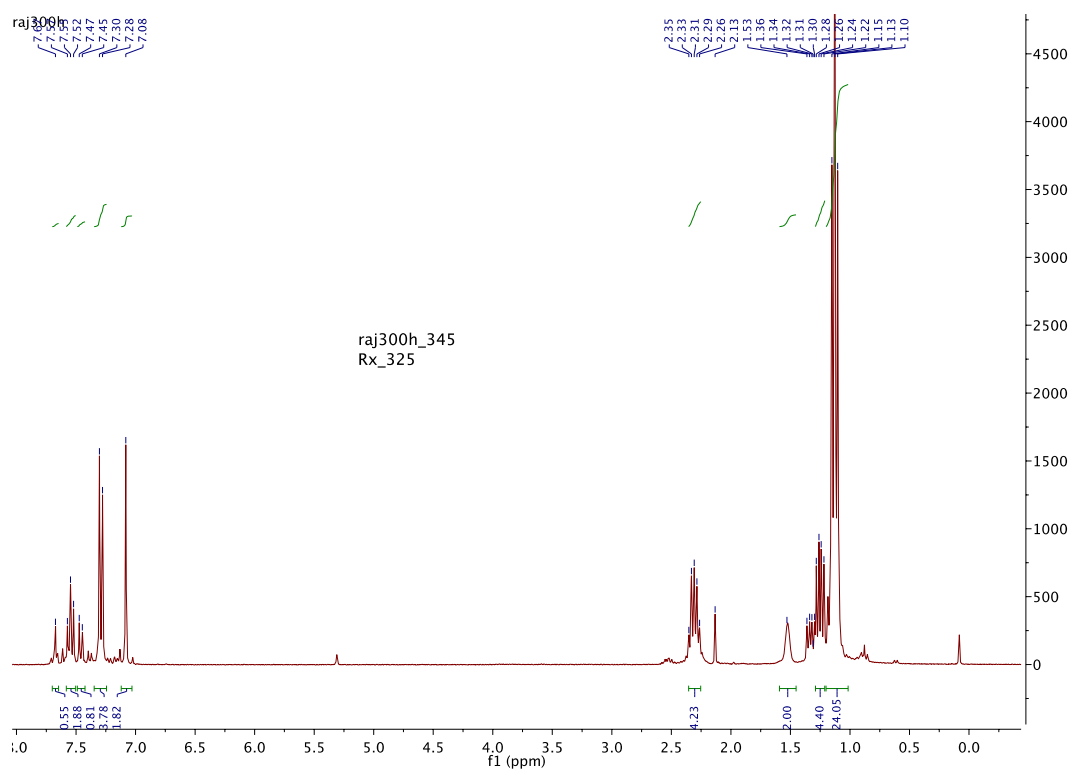
Plot 6. ^{13}C NMR spectrum of compound **4**.



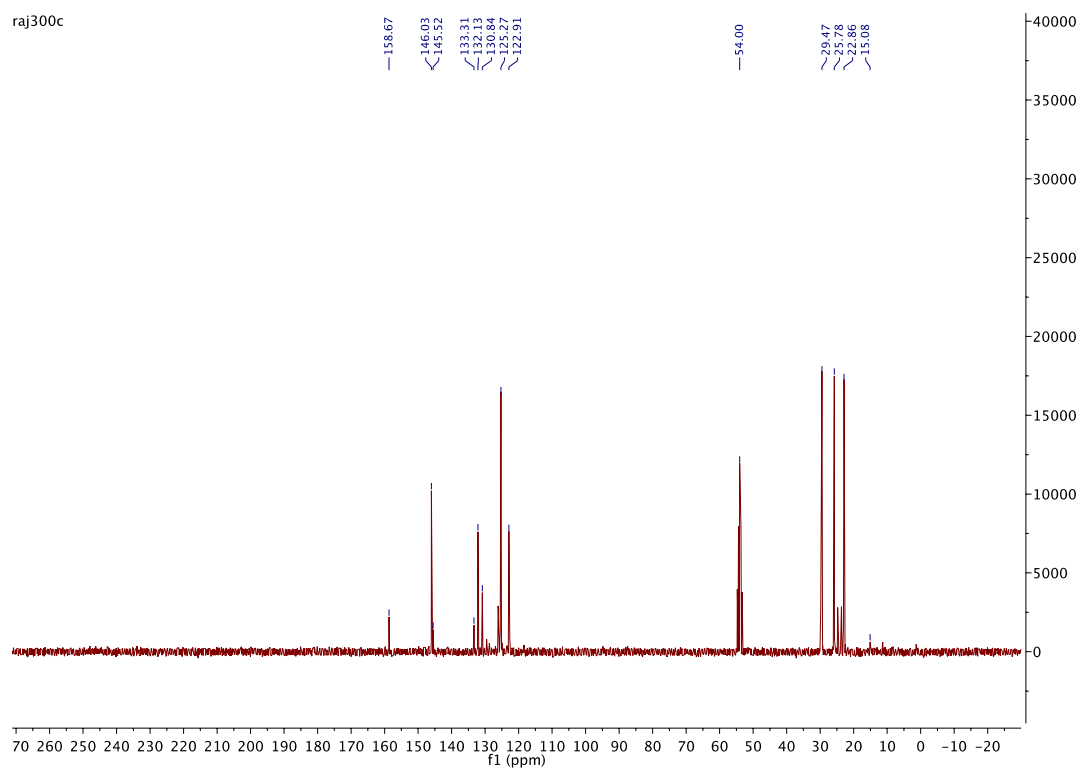
Plot 7. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **4**.



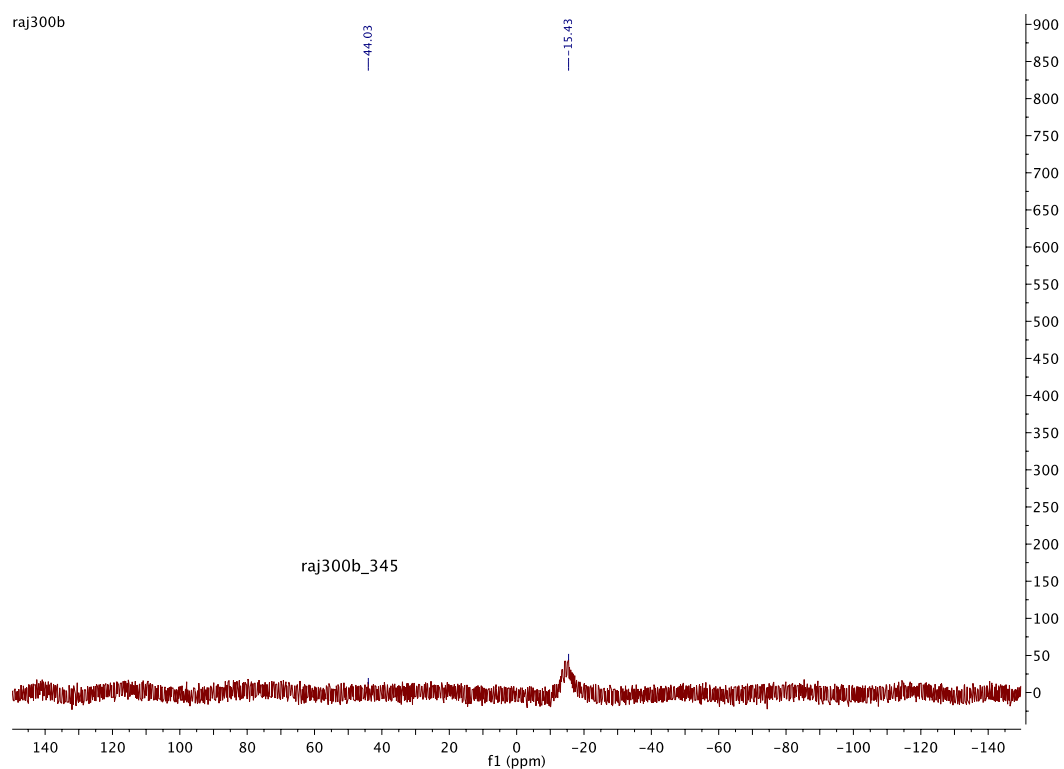
Plot 8. ^{11}B NMR spectrum of compound **4**.



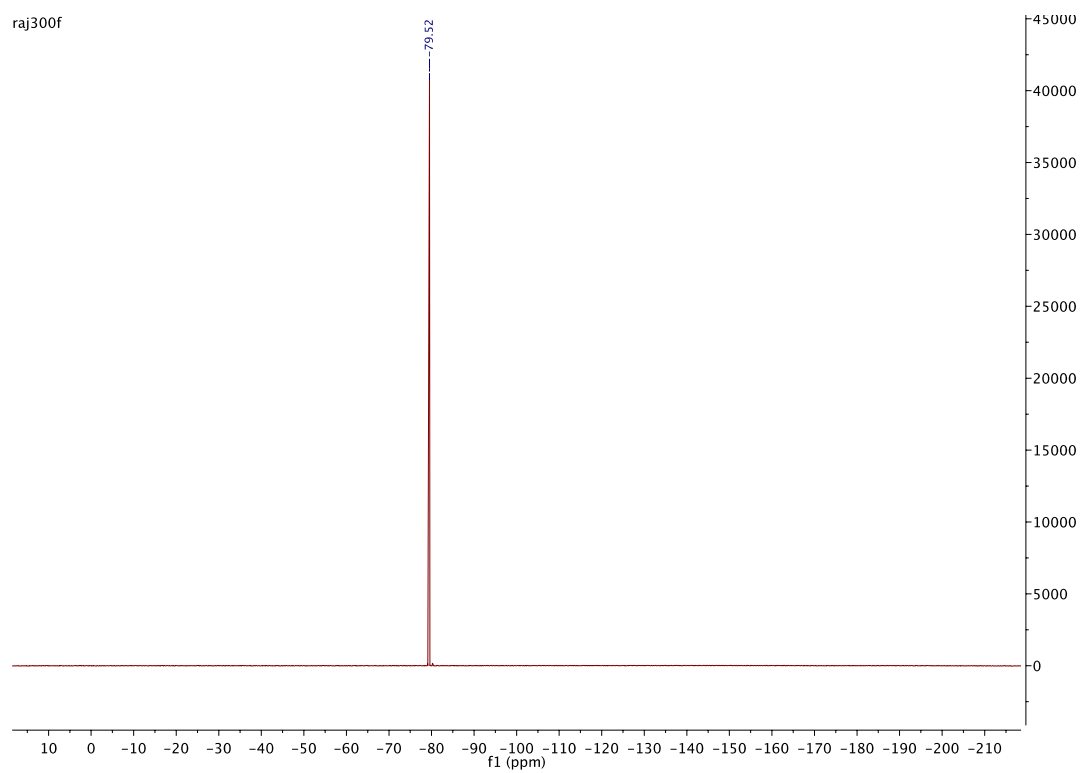
Plot 9. ^1H NMR spectrum of compound **5** (traces of 1,2- $\text{Cl}_2\text{C}_6\text{H}_4$).



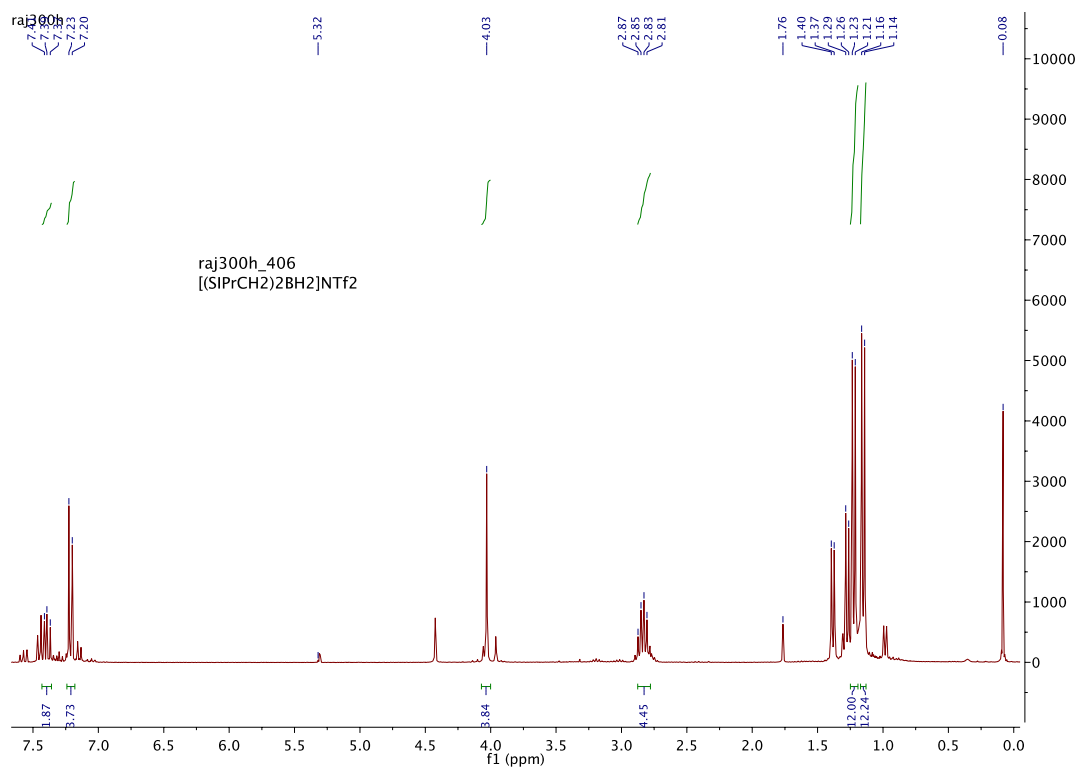
Plot 10. ^{13}C NMR spectrum of compound **5** (traces of 1,2- $\text{Cl}_2\text{C}_6\text{H}_4$).



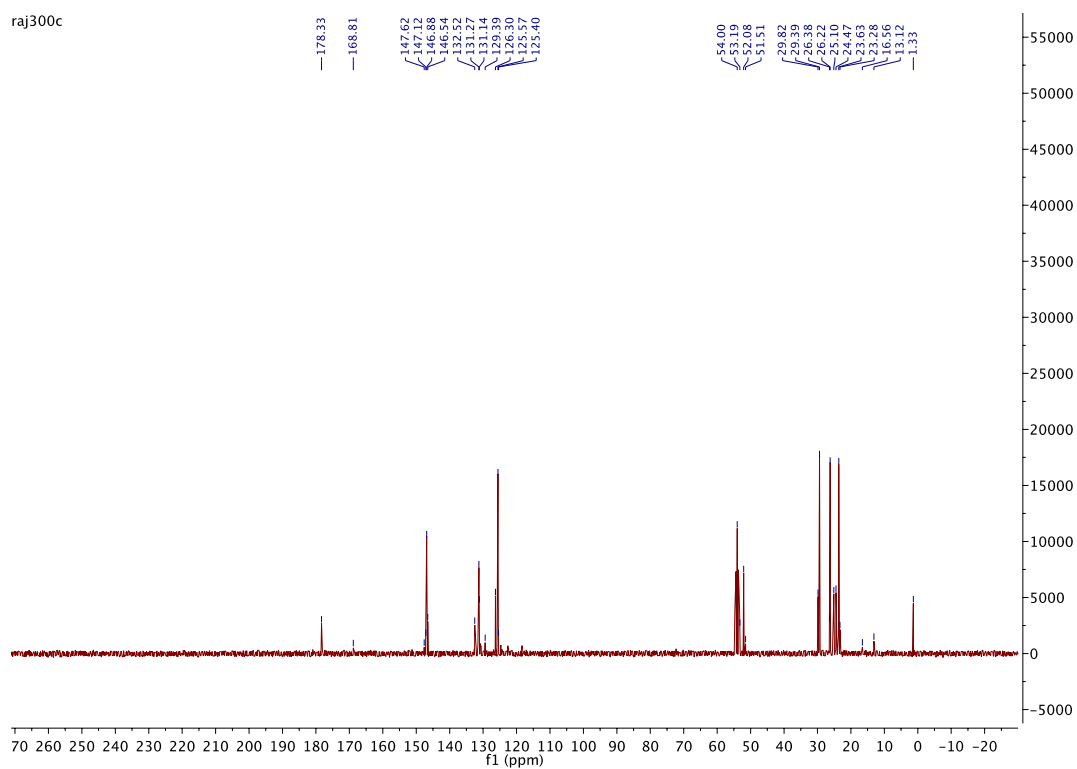
Plot 11. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **5**.



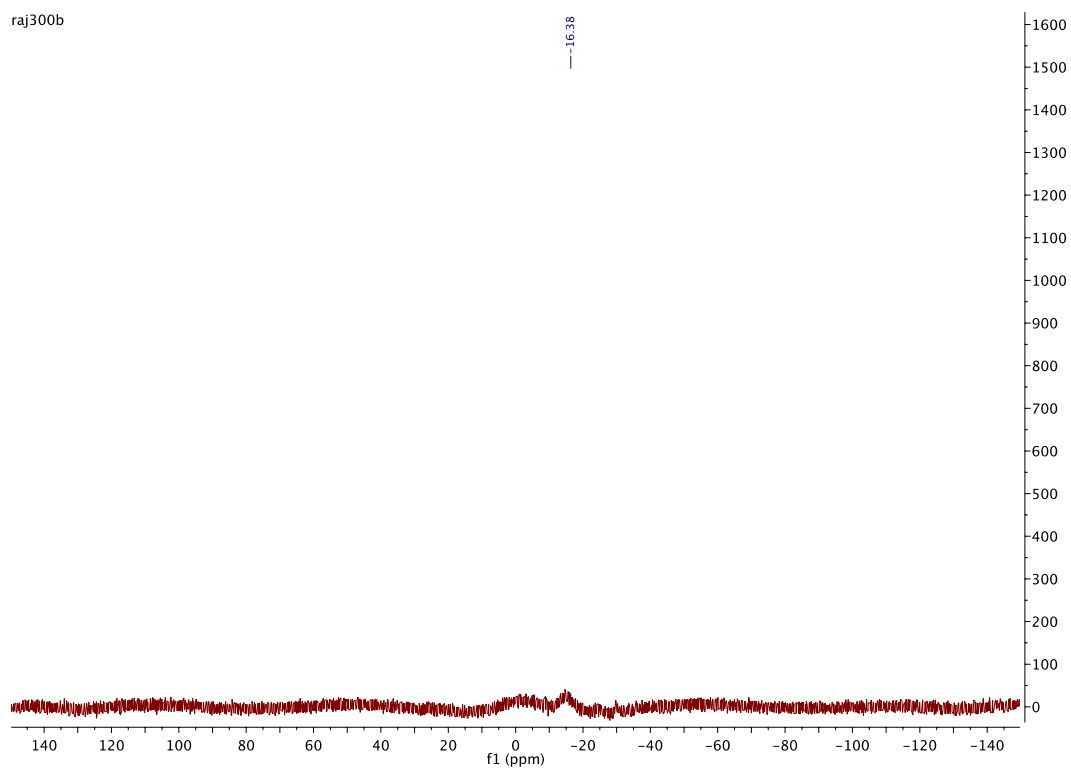
Plot 12. ^{19}F NMR spectrum of compound **5**.



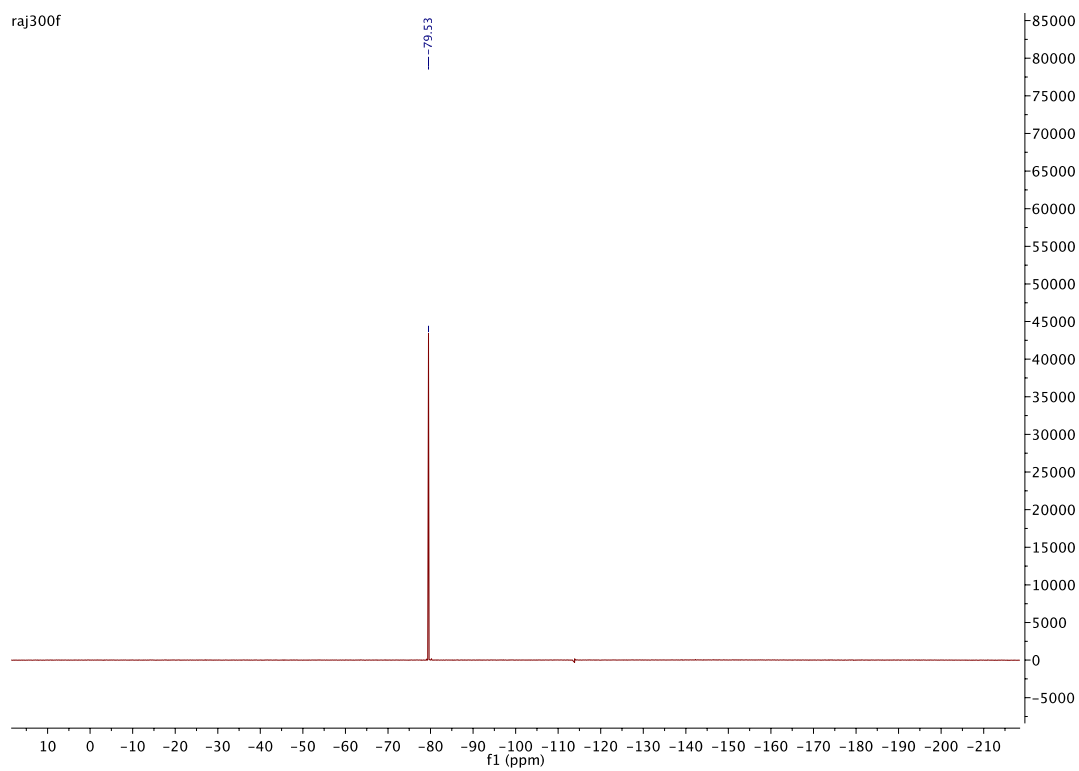
Plot 13. ¹H NMR spectrum of compound **6**.



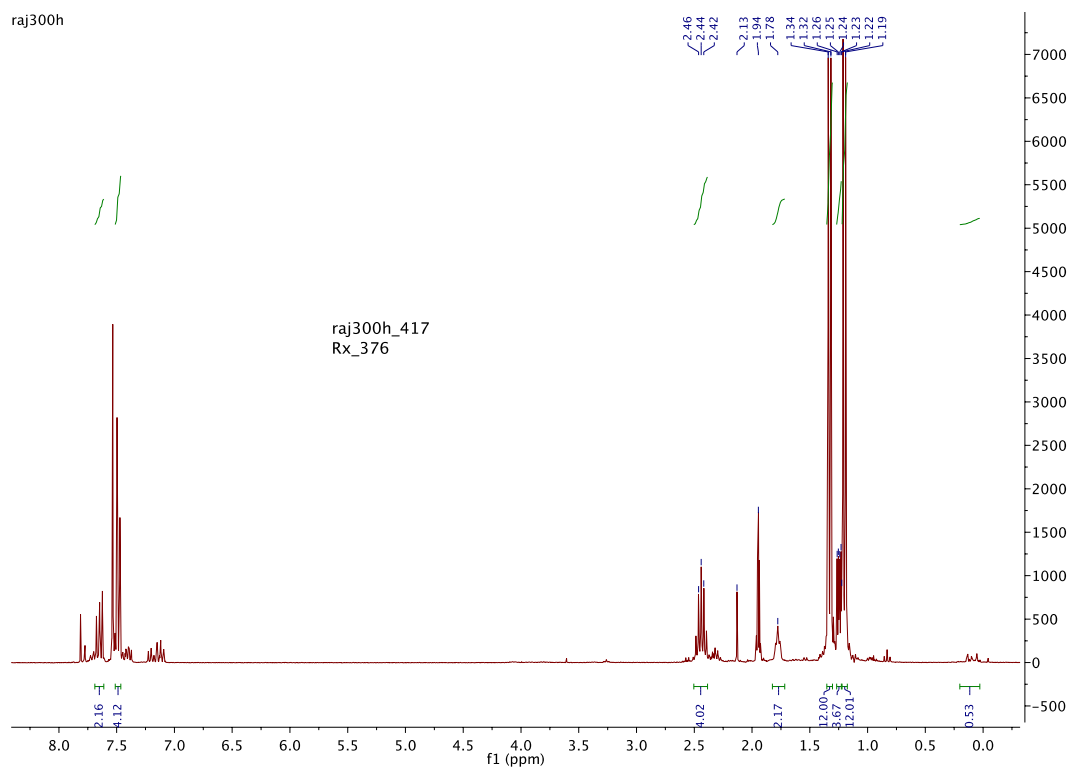
Plot 14. ¹³C NMR spectrum of compound **6**.



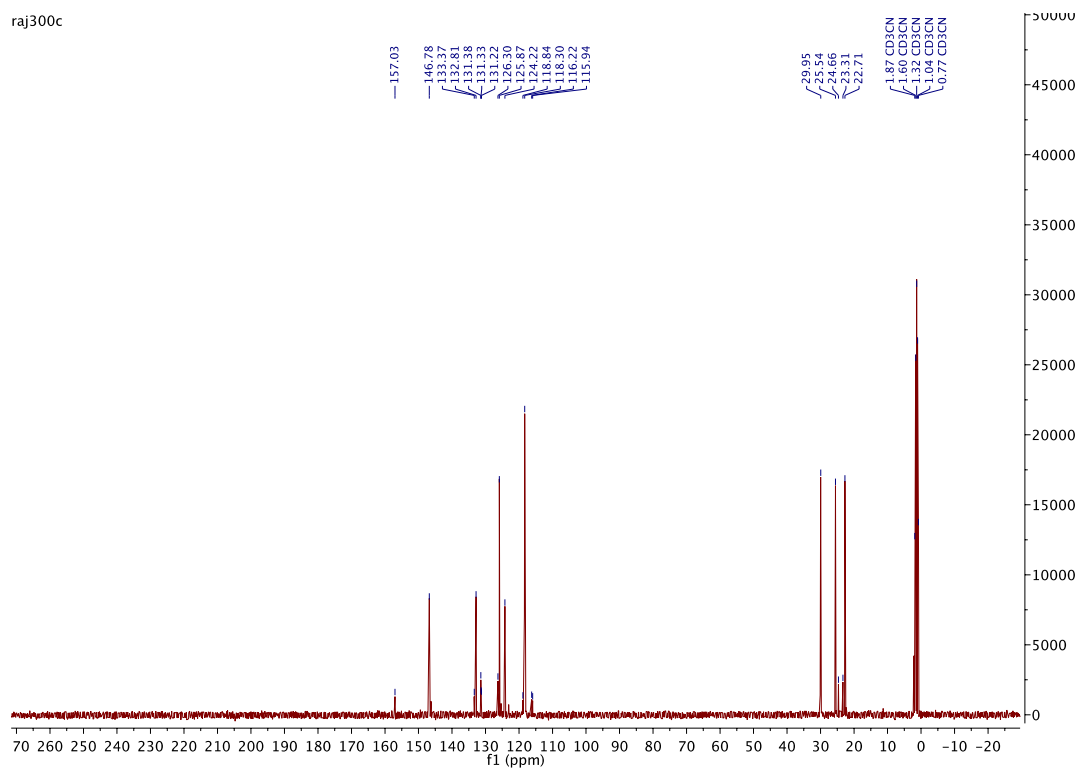
Plot 15. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **6**.



Plot 16. ^{19}F NMR spectrum of compound **6**.

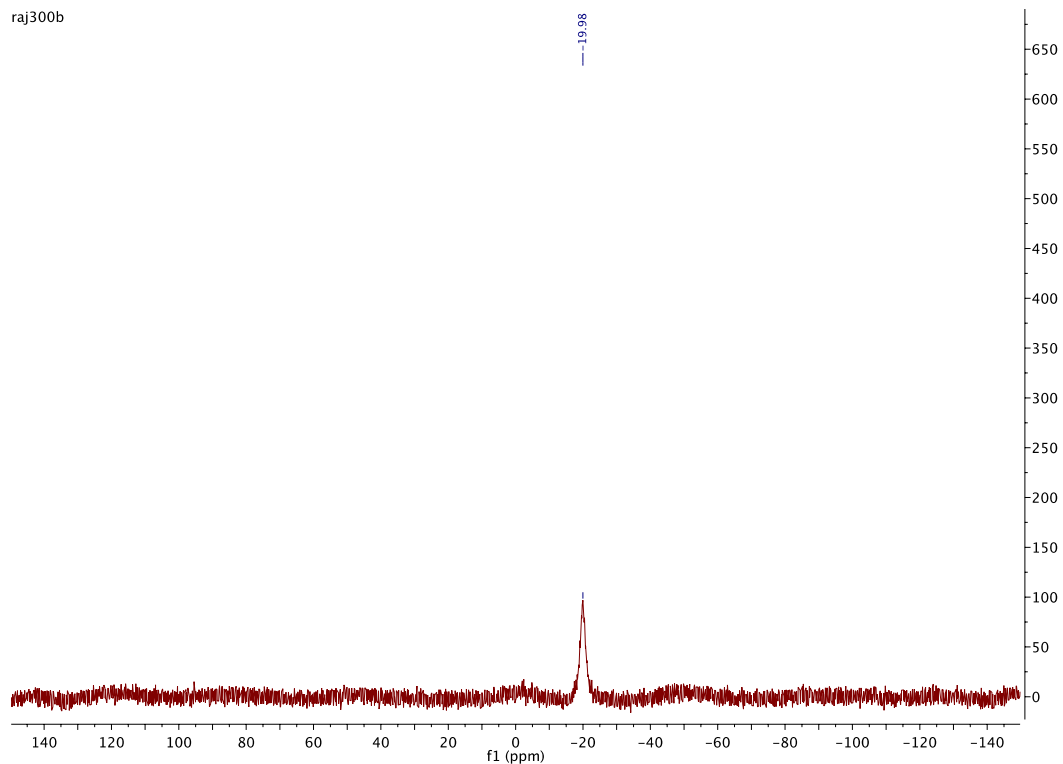


Plot 17. ^1H NMR spectrum of compound **7**.



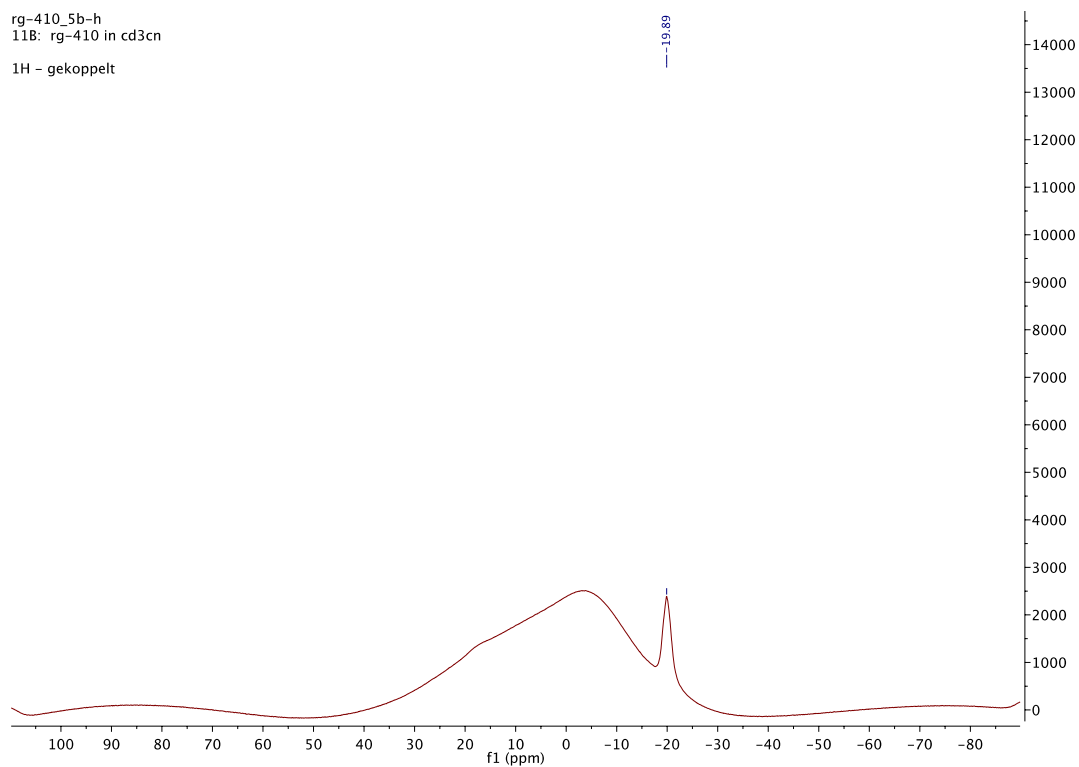
Plot 18. ^{13}C NMR spectrum of compound **7**.

raj300b

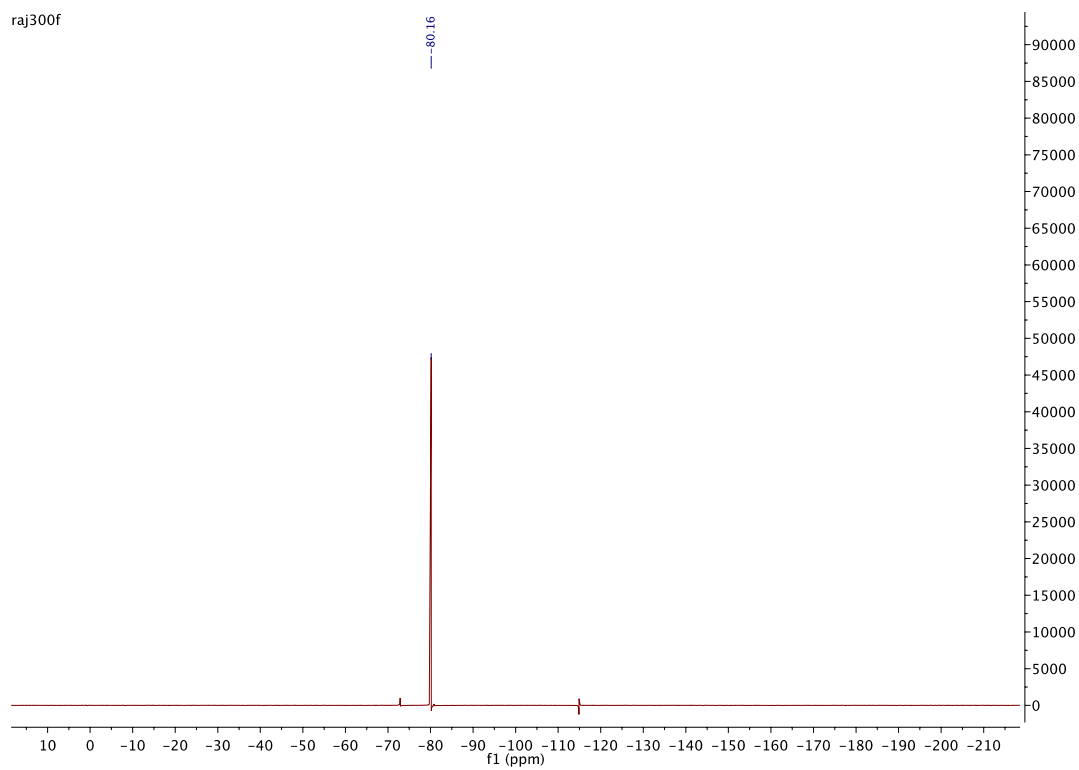


Plot 19. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **7**.

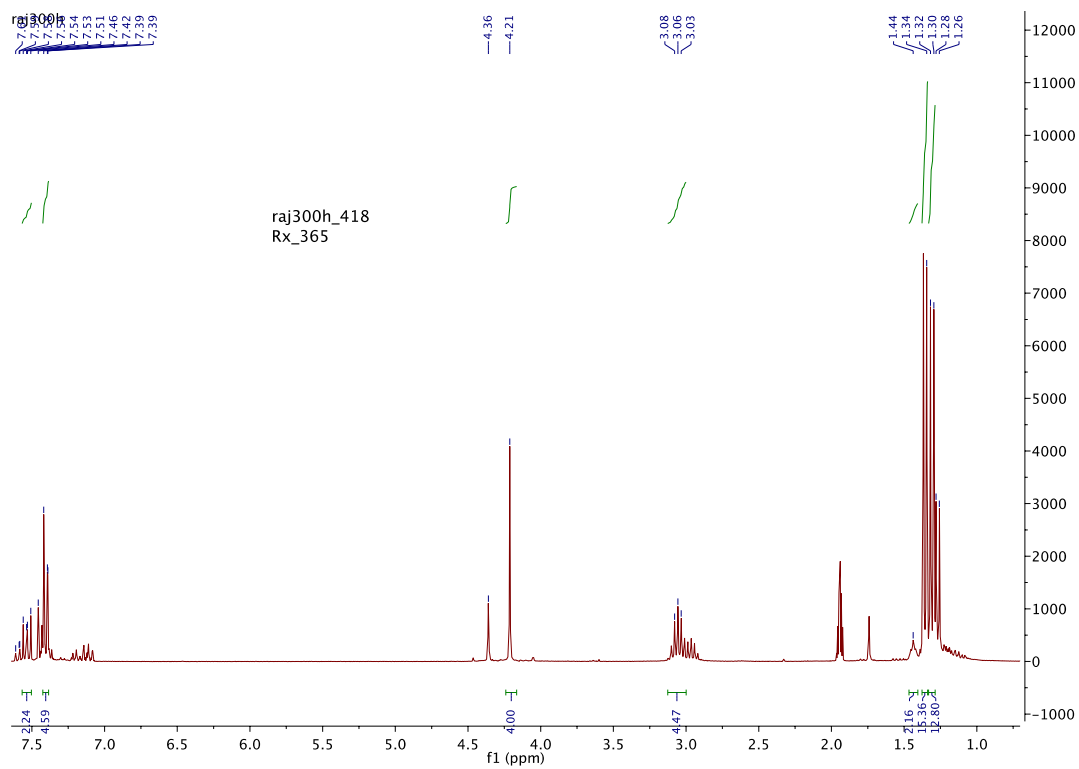
rg-410_5b-h
11B: rg-410 in cd3cn
1H – gekoppelt



Plot 20. ^{11}B NMR spectrum of compound **7**.

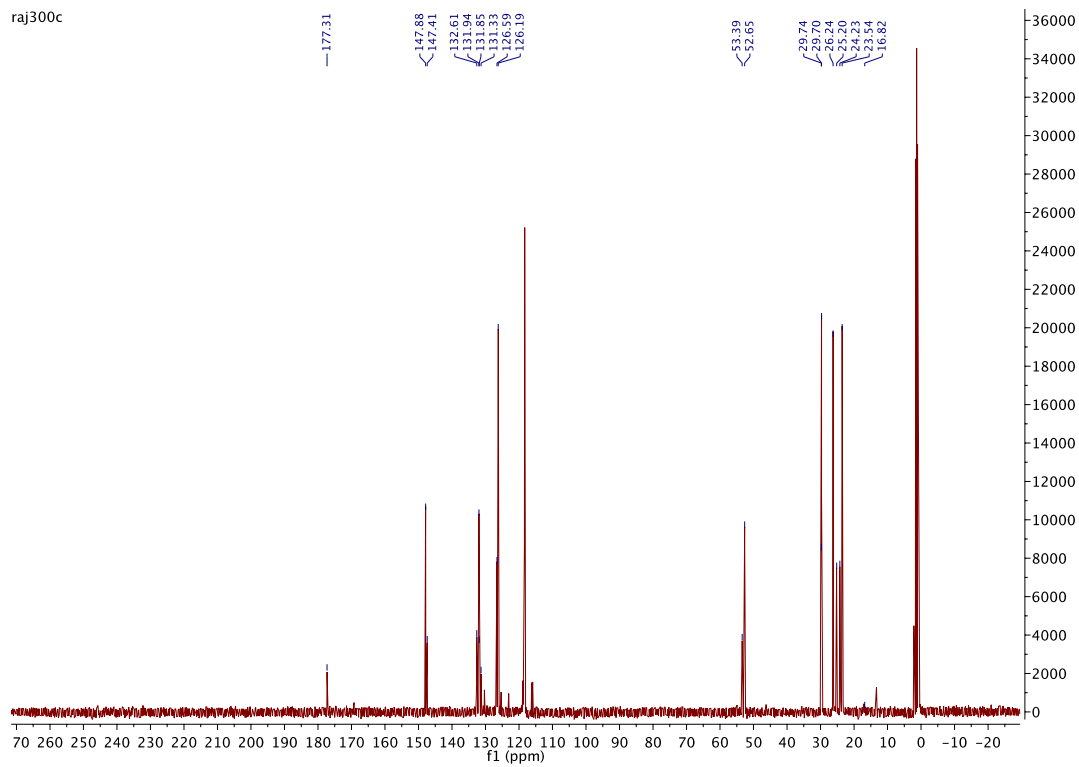


Plot 21. ^{19}F NMR spectrum of compound **7**.



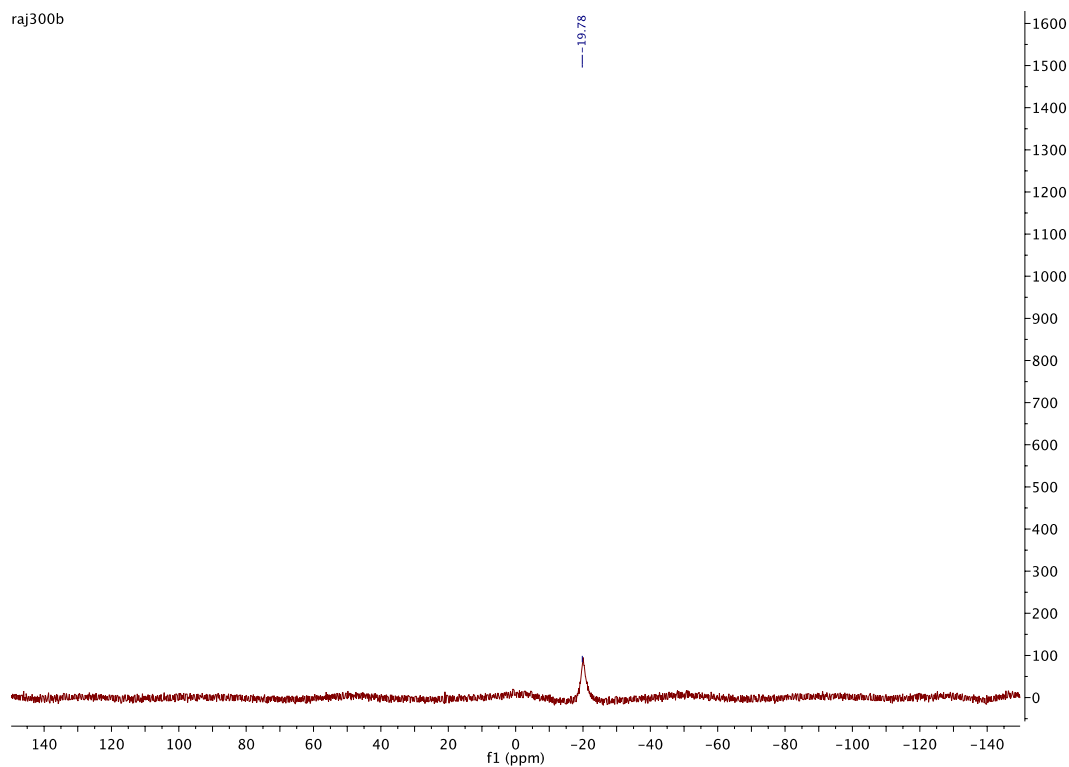
Plot 22. ^1H NMR spectrum of compound **8**.

raj300c

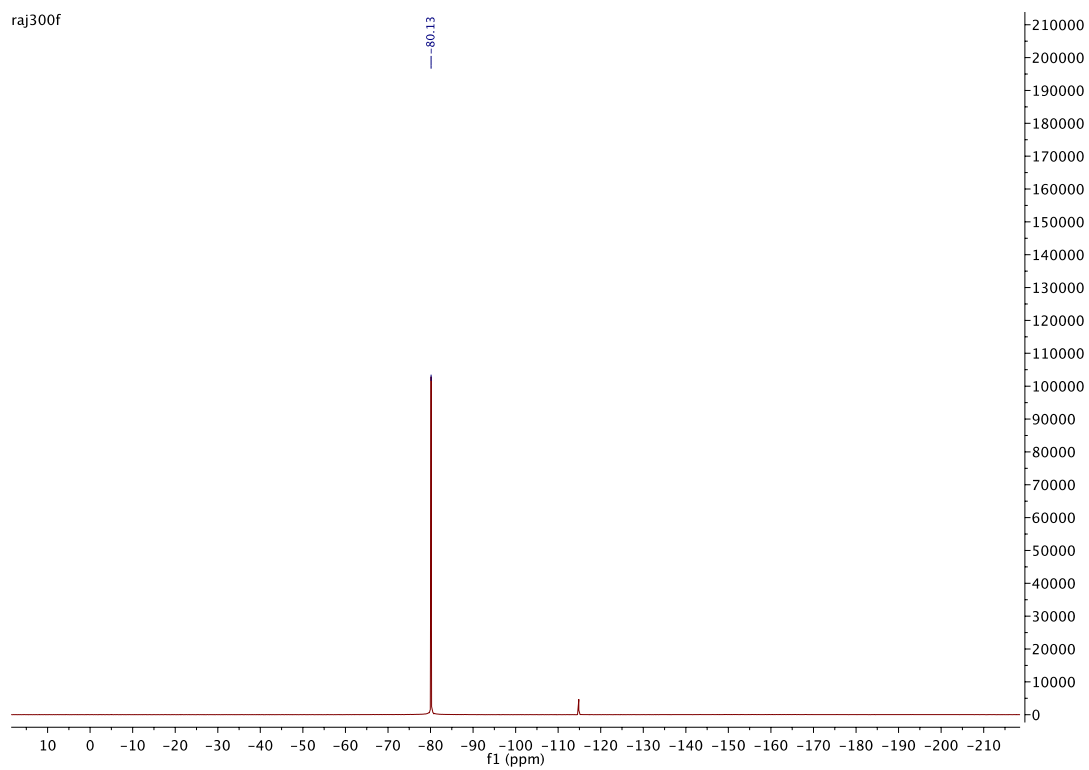


Plot 23. ^{13}C NMR spectrum of compound 8.

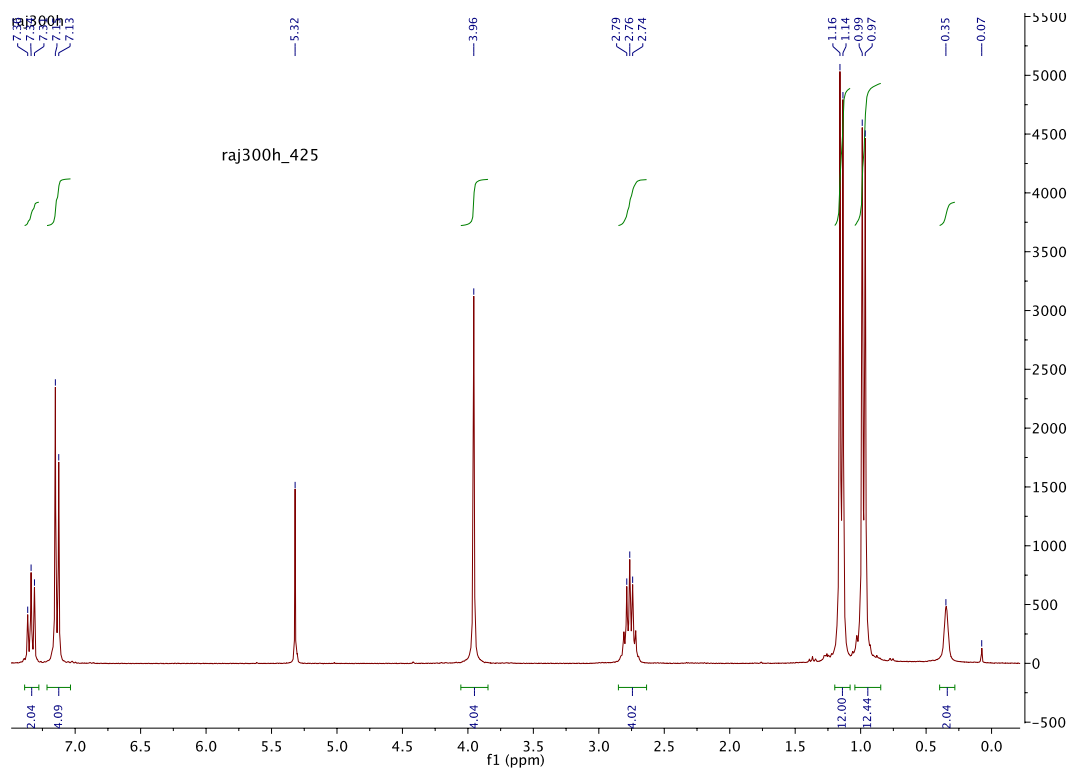
raj300b



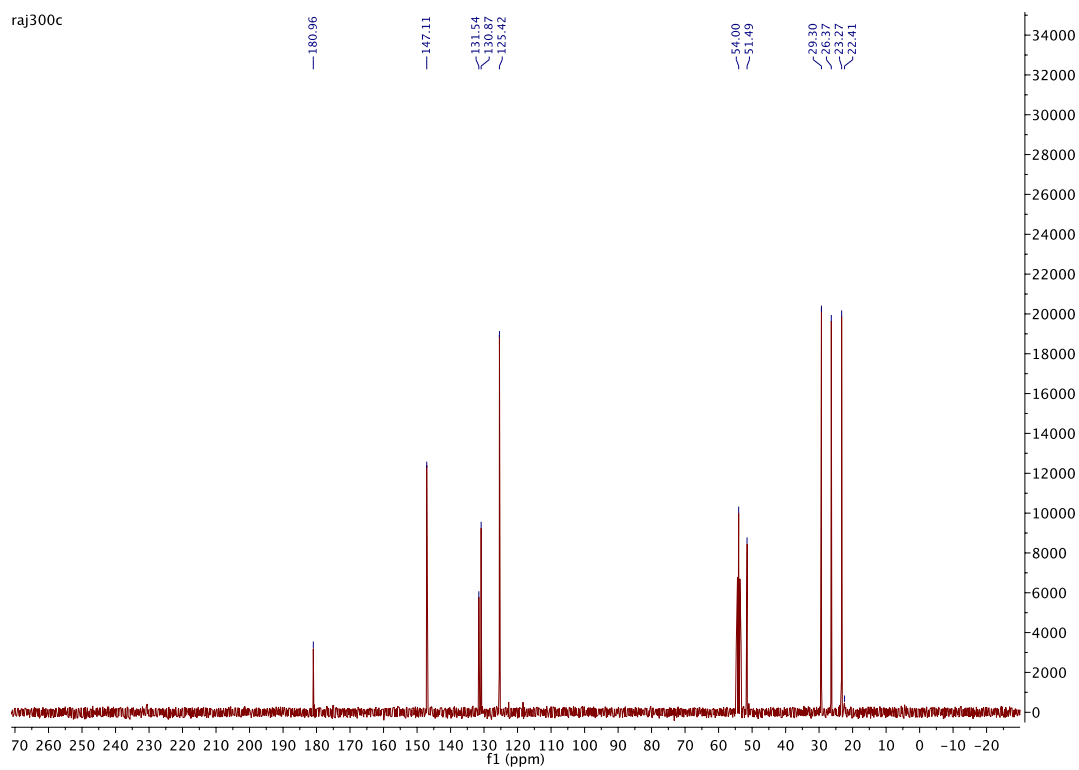
Plot 24. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound 8.



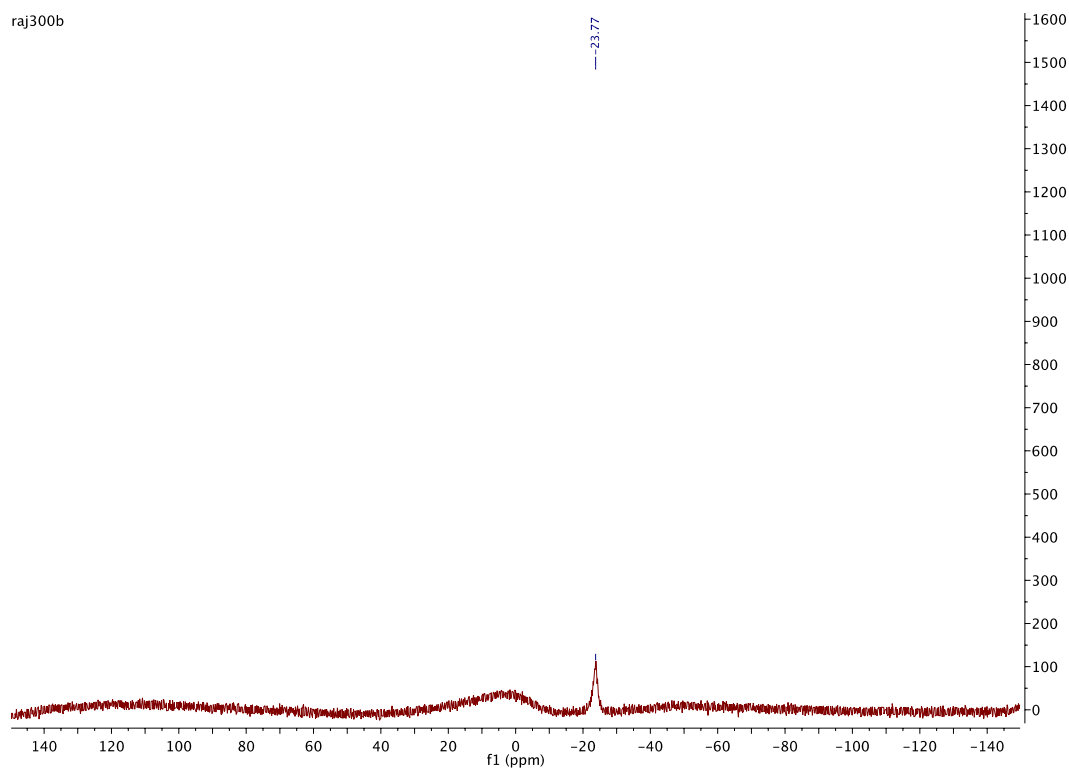
Plot 25. ^{19}F NMR spectrum of compound **8**.



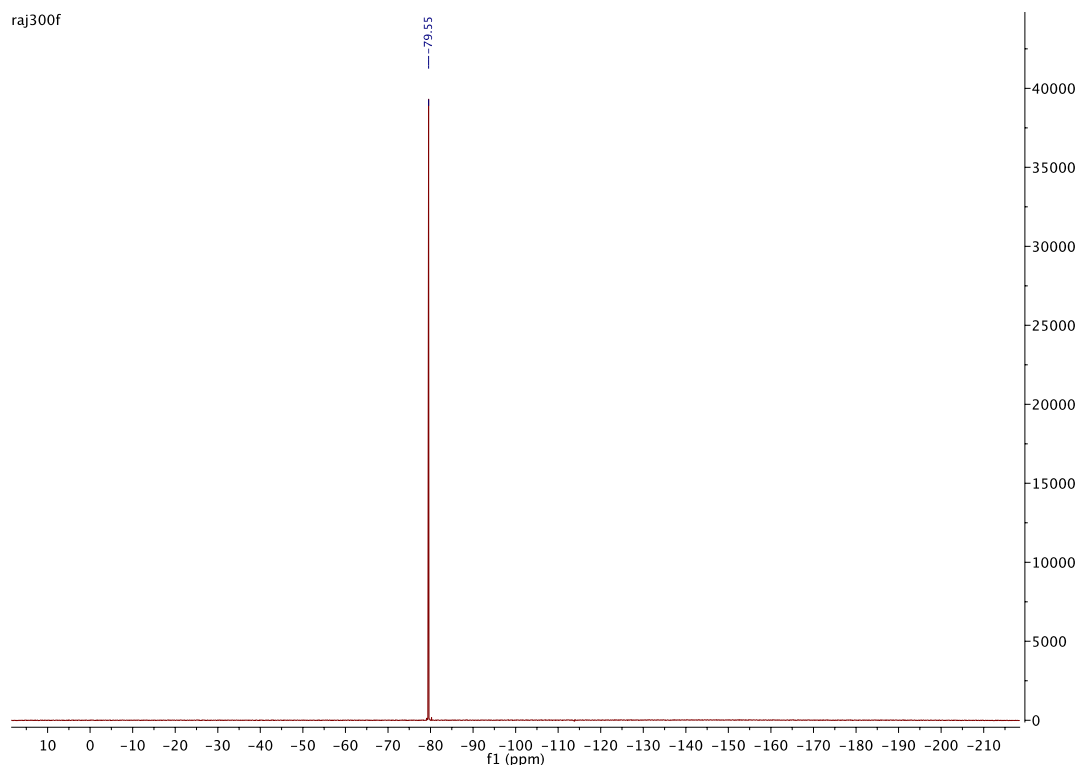
Plot 26. ^1H NMR spectrum of compound **9**.



Plot 27. ^{13}C NMR spectrum of compound **9**.



Plot 28. $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of compound **9**.



Plot 29. ^{19}F NMR spectrum of compound **9**.

References

1. Y. Zhao and D. G. Truhlar, *Theor. Chem. Acc.*, 2008, **120**, 215-241.
2. F. Weigend and R. Ahlrichs, *Phys. Chem. Chem. Phys.*, 2005, **7**, 3297-3305.
3. C. Y. Peng, P. Y. Ayala, H. B. Schlegel and M. J. Frisch, *J. Comput. Chem.*, 1996, **17**, 49-56.
4. J. W. McIver and A. Komornicki, *J. Am. Chem. Soc.*, 1972, **94**, 2625-2633.
5. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. J. A. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski and D. J. Fox, Gaussian 09, Revision C.01. Gaussian, Inc., Wallingford CT, 2009.
6. (a) A. E. Reed, L. A. Curtiss and F. Weinhold, *Chem. Rev.*, 1988, **88**, 899-926; (b) A. E. Reed and F. Weinhold, *J. Chem. Phys.*, 1985, **83**, 1736-1740; (c) A. E. Reed, R. B. Weinstock and F. Weinhold, *J. Chem. Phys.*, 1985, **83**, 735-746; (d) J. P. Foster and F. Weinhold, *J. Am. Chem. Soc.*, 1980, **102**, 7211-7218.
7. E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales and F. Weinhold, Theoretical Chemistry Institute, University of Wisconsin, Madison, WI, GENNBO 5.9 edn., 2009.