Complexes obtained by electrophilic attack on a dinitrogen-derived terminal molybdenum nitride: Electronic structure analysis by CP MAS solid state ^{15}N NMR in combination with DFT calculations

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Contents

1. Single Crystal X-ray Structure Determination

1.1 ORTEP plot of 1-BF_3

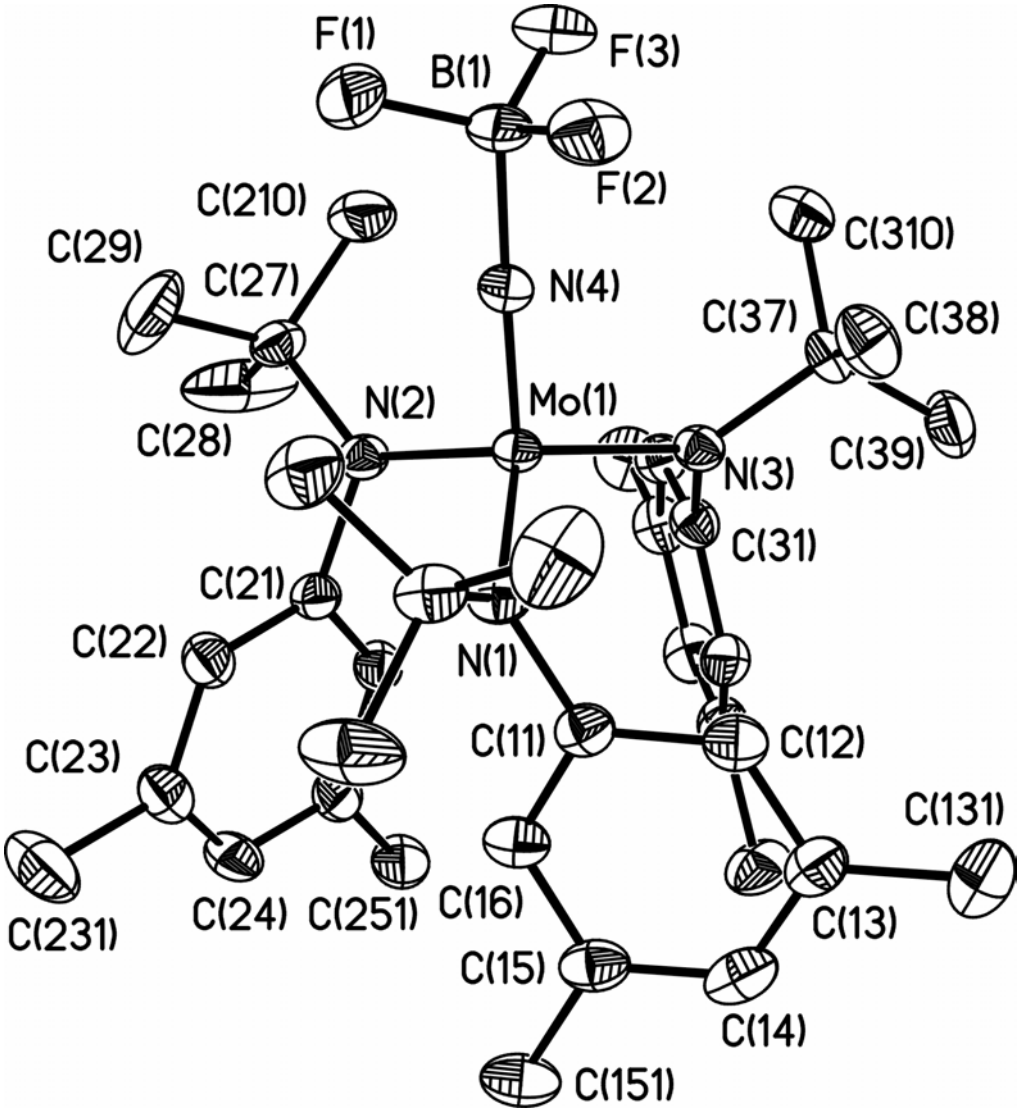


Figure 1. 35% thermal ellipsoid (ORTEP) representation of **1**-BF_3.. The CH_2Cl_2 molecule of solvation has been omitted.

1.2 ORTEP plot of 1-$GeCl_2$

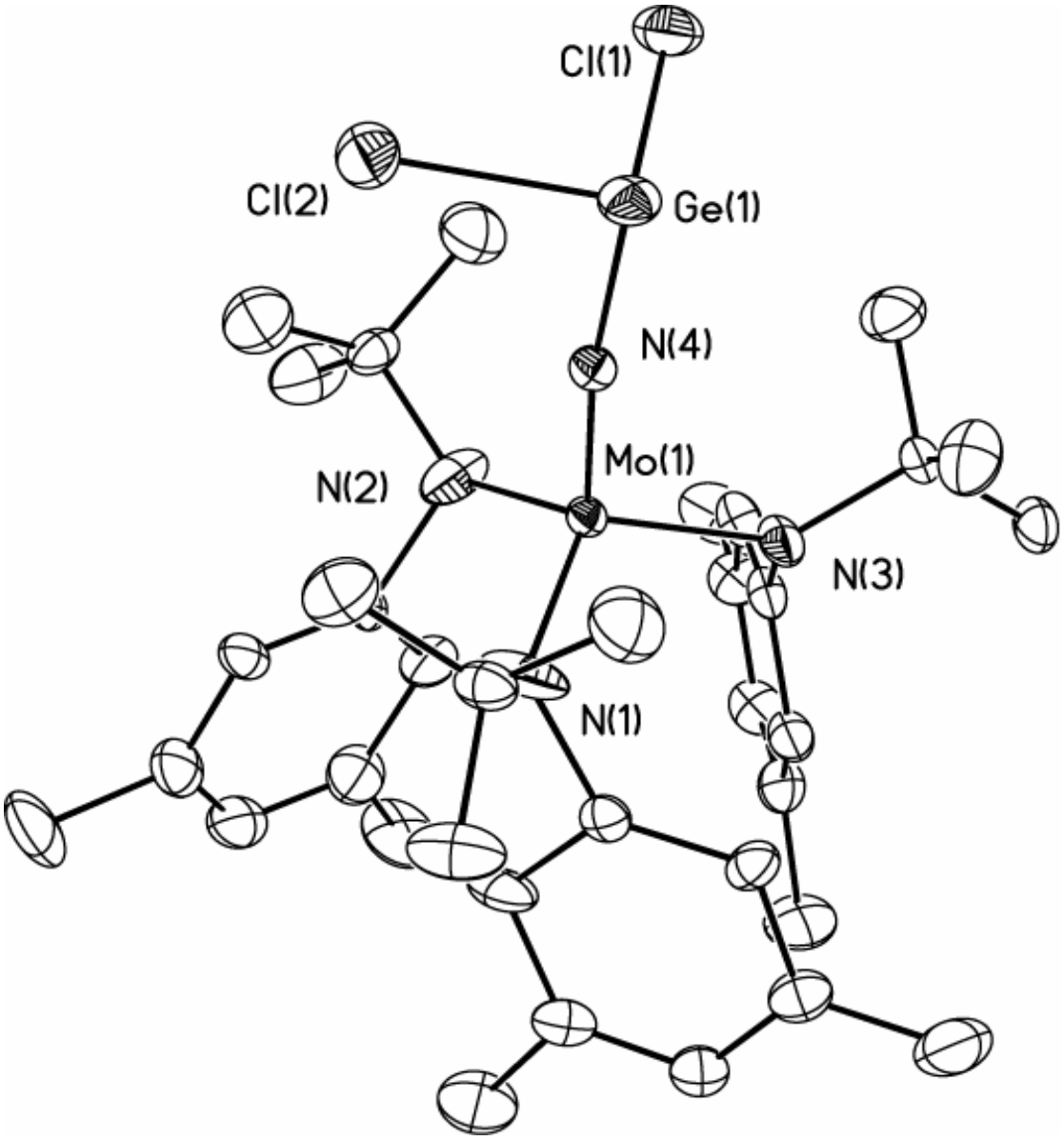


Figure 2. 35% thermal ellipsoid (ORTEP) representation of **1**-$GeCl_2$.

1.3 ORTEP plot of 1-$SnCl_2$

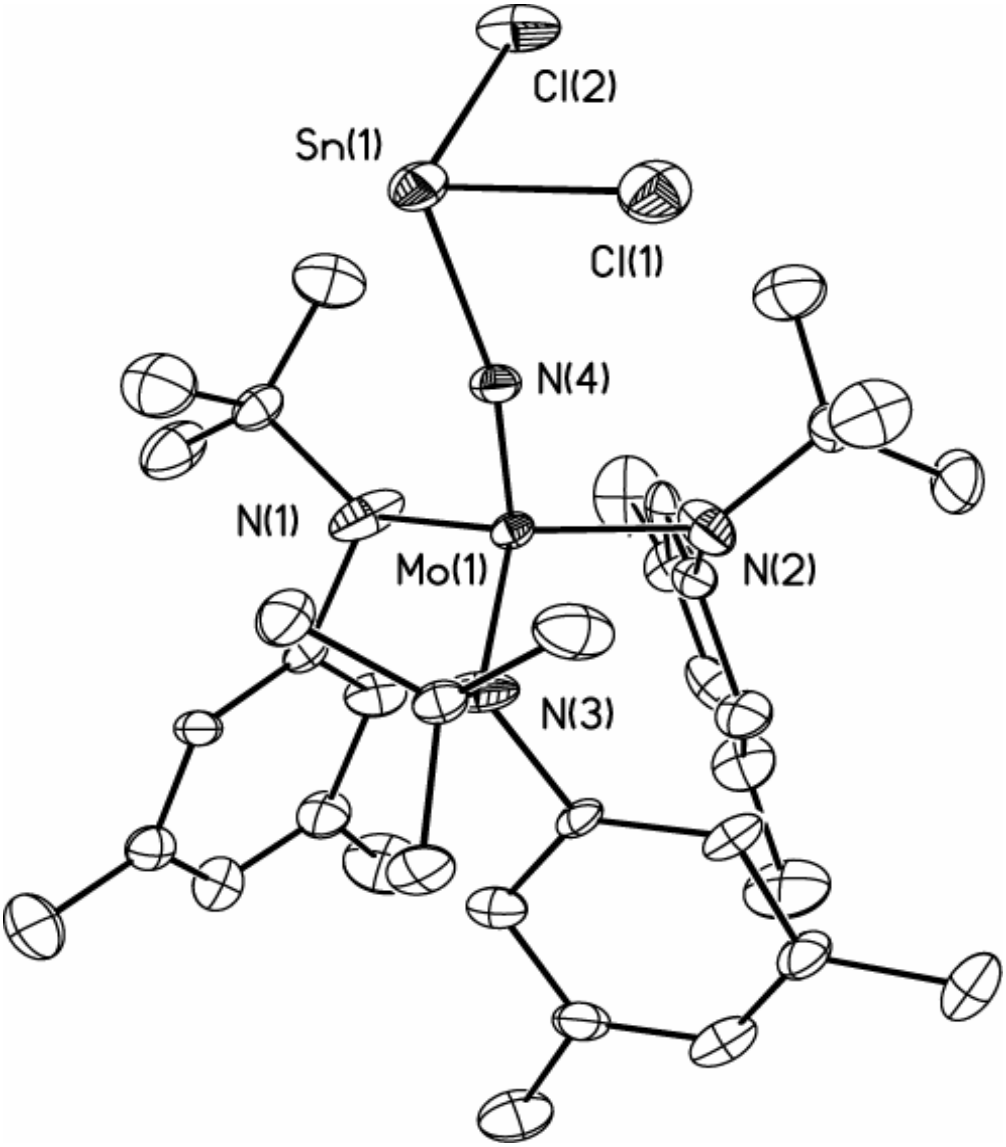


Figure 3: 35% thermal ellipsoid (ORTEP) representation of **1**-$SnCl_2$.

1.4 ORTEP plot of [**2b**]OTf

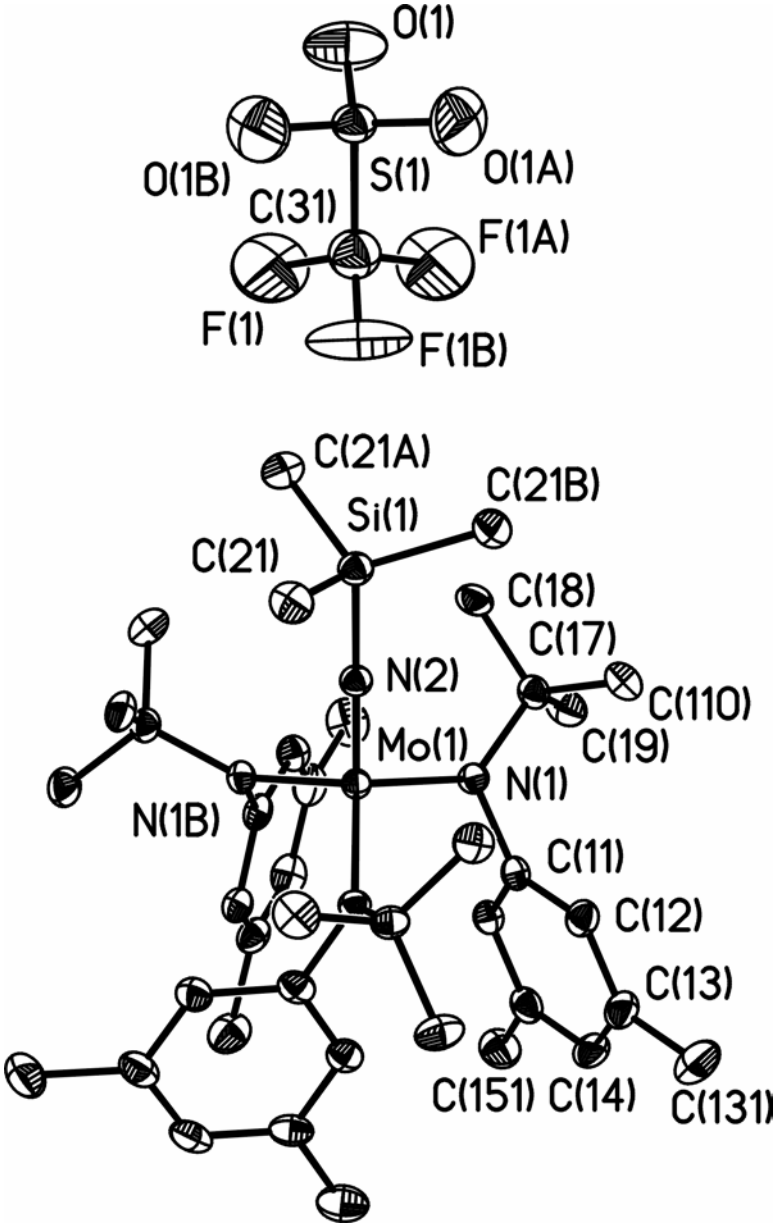


Figure 4. ORTEP diagram of $[(Me_3Si)NMo(N[^tBu]Ar)_3][SO_3CF_3]$ [**2b**]OTf with thermal ellipsoids at the 35% probability level.

1.5 ORTEP plot of [**2c**]OTf

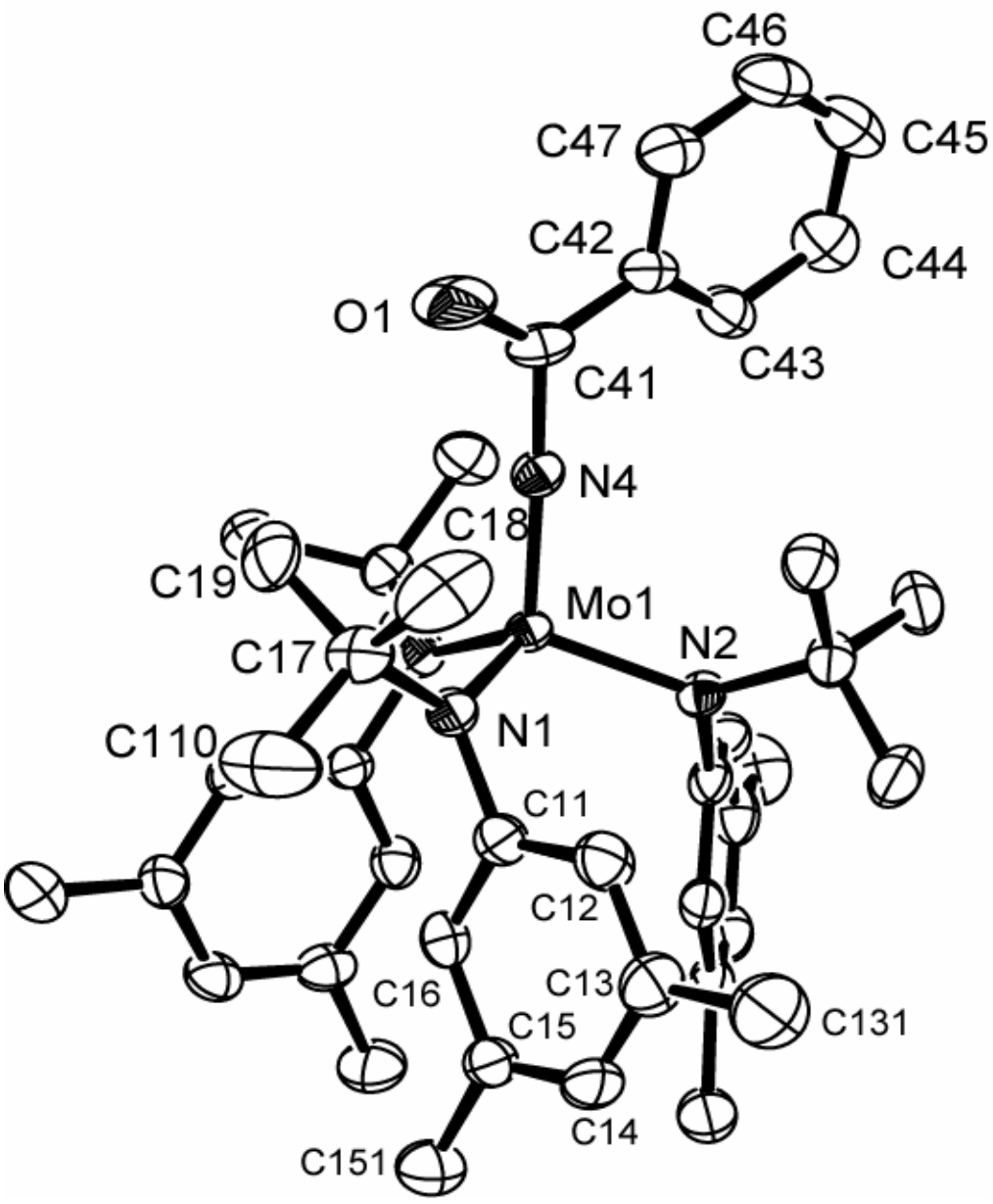


Figure 5. ORTEP diagram of [**2c**]OTf with thermal ellipsoids at the 50% probability level.

1.6 ORTEP plot of 3

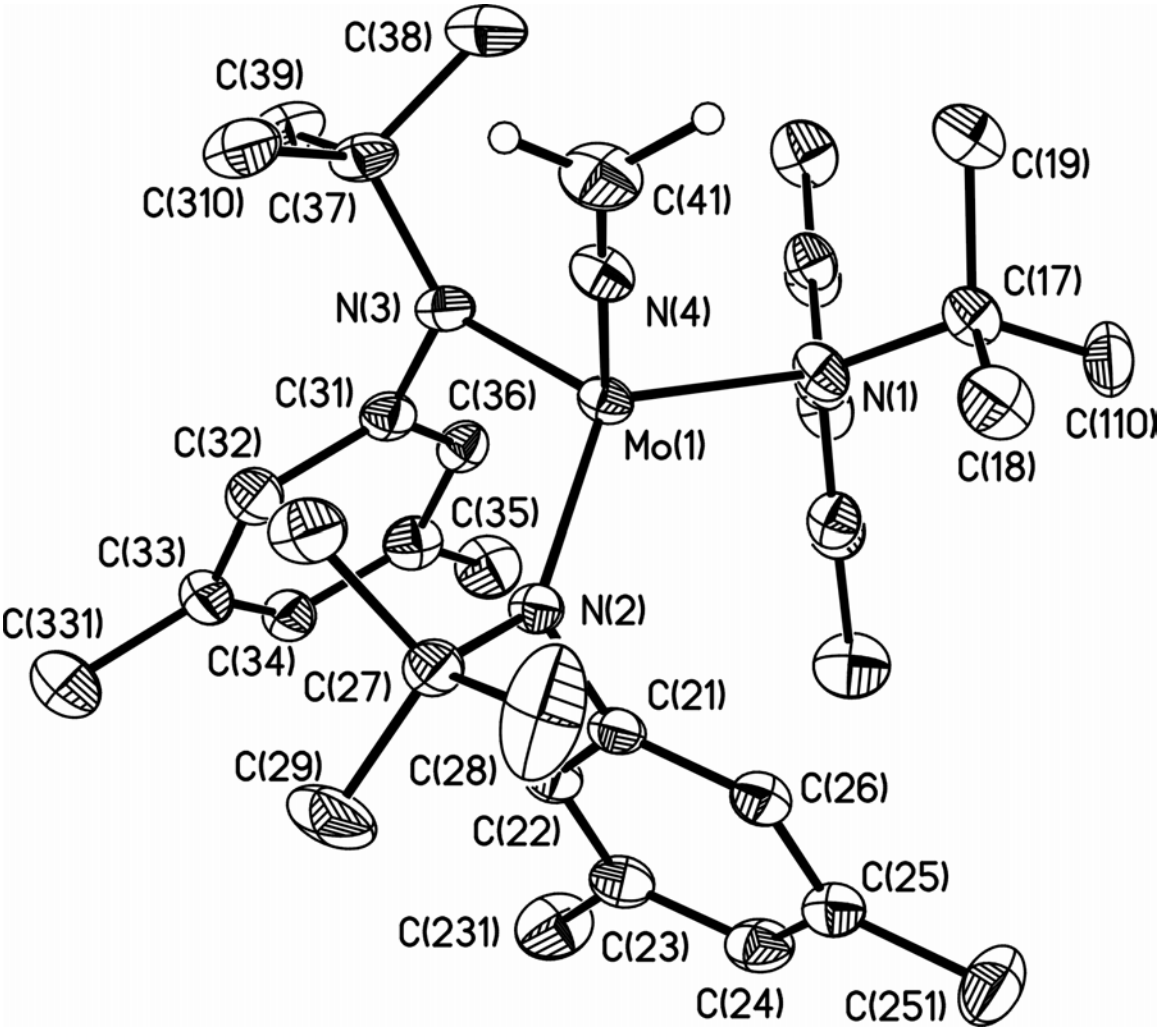


Figure 6. ORTEP diagram of **3** with thermal ellipsoids at the 35% probability level.

1.7 ORTEP plot of [**2d**]I

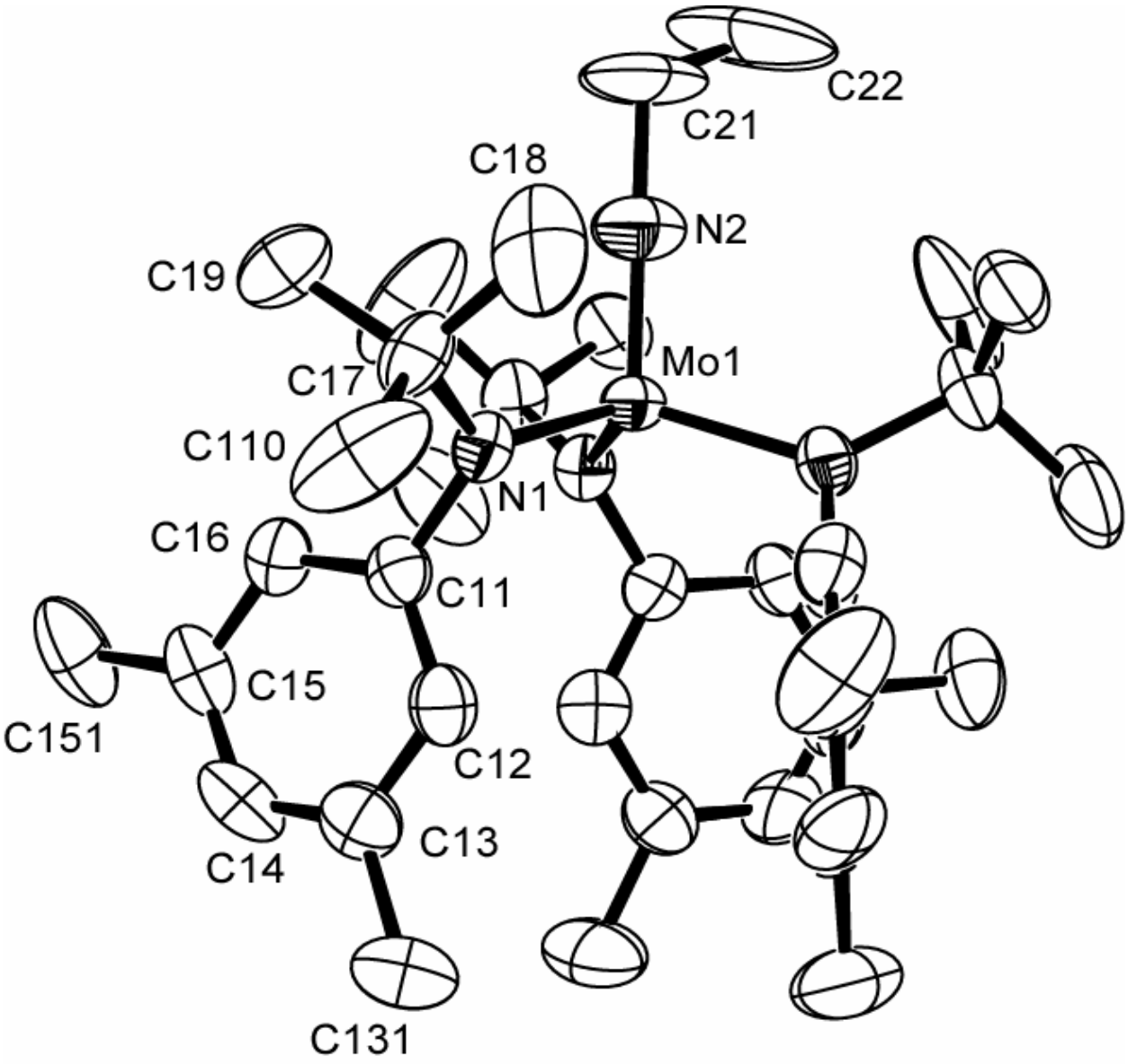


Figure 7. ORTEP diagram of $[(Me_3Si)NMo(N[^tBu]Ar)_3][SO_3CF_3]$ [**2d**]I with thermal ellipsoids at the 50% probability level.

1.8 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**-BF_3. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	8622(1)	6619(1)	7238(1)	27(1)
F(1)	6919(3)	3586(2)	6399(2)	63(1)
N(1)	10459(4)	6309(3)	7698(3)	36(1)
B(1)	6859(6)	4212(5)	7092(4)	40(1)
Cl(1)	16185(3)	7345(2)	12079(3)	191(2)
F(2)	7419(3)	3731(2)	7822(2)	57(1)
N(2)	8241(4)	7111(3)	6108(2)	33(1)
Cl(2)	15025(5)	6604(6)	10363(3)	296(4)
F(3)	5569(3)	4411(3)	7016(2)	59(1)
N(3)	8011(4)	7578(3)	7992(2)	31(1)
N(4)	7705(4)	5395(3)	7143(2)	32(1)
C(11)	11309(5)	7231(4)	8249(3)	38(1)
C(12)	11423(5)	7348(4)	9106(3)	42(1)
C(13)	12225(5)	8220(5)	9638(3)	47(1)
C(14)	12947(5)	8963(5)	9296(4)	52(2)
C(15)	12868(5)	8877(4)	8445(4)	46(1)
C(16)	12028(5)	7996(4)	7918(3)	40(1)
C(17)	11089(5)	5236(4)	7697(3)	43(1)
C(18)	11156(8)	4676(5)	8494(4)	82(2)
C(19)	12490(6)	5510(5)	7609(5)	80(2)
C(21)	9365(5)	7790(4)	5996(3)	35(1)
C(22)	10346(5)	7328(4)	5729(3)	42(1)
C(23)	11421(6)	7986(5)	5634(3)	50(1)
C(24)	11492(5)	9125(5)	5808(3)	49(1)
C(25)	10541(5)	9621(4)	6079(3)	41(1)
C(26)	9466(5)	8941(4)	6173(3)	37(1)
C(27)	7087(5)	6753(4)	5315(3)	38(1)
C(28)	6834(7)	7711(7)	4774(5)	108(3)
C(29)	7391(7)	5774(7)	4846(5)	105(3)
C(31)	8062(5)	8737(4)	7804(3)	36(1)
C(32)	9225(5)	9443(4)	8187(3)	38(1)
C(33)	9283(5)	10561(4)	8021(3)	43(1)
C(34)	8178(6)	10948(4)	7478(3)	47(1)
C(35)	7020(5)	10254(4)	7083(3)	46(1)
C(36)	6978(5)	9143(4)	7253(3)	39(1)
C(37)	7235(5)	7297(4)	8598(3)	38(1)
C(38)	7829(6)	6338(5)	9084(4)	57(2)
C(39)	7369(6)	8293(5)	9222(4)	61(2)
C(41)	14981(9)	6406(8)	11326(7)	123(4)
C(110)	10304(6)	4461(5)	6936(4)	61(2)
C(131)	12307(7)	8353(6)	10552(4)	66(2)
C(151)	13662(6)	9687(5)	8082(4)	58(2)
C(210)	5848(5)	6438(5)	5551(4)	62(2)
C(231)	12468(7)	7476(6)	5331(5)	77(2)
C(251)	10641(6)	10858(4)	6261(4)	52(2)
C(310)	5773(5)	6969(5)	8120(4)	54(2)
C(331)	10540(6)	11321(4)	8457(4)	57(2)
C(351)	5837(6)	10693(5)	6494(4)	63(2)

1.9 Bond lengths [Å] and angles [°] for **1**-BF_3.

Mo(1)-N(4)	1.677(4)
Mo(1)-N(2)	1.945(4)
Mo(1)-N(1)	1.943(4)
Mo(1)-N(3)	1.946(4)
F(1)-B(1)	1.365(7)
N(1)-C(11)	1.458(6)
N(1)-C(17)	1.510(6)
B(1)-F(2)	1.371(7)
B(1)-F(3)	1.375(7)
B(1)-N(4)	1.611(7)
Cl(1)-C(41)	1.771(11)
N(2)-C(21)	1.455(6)
N(2)-C(27)	1.519(6)
Cl(2)-C(41)	1.651(10)
N(3)-C(31)	1.459(6)
N(3)-C(37)	1.516(6)
C(11)-C(12)	1.396(7)
C(11)-C(16)	1.391(7)
C(12)-C(13)	1.386(7)
C(13)-C(14)	1.388(8)
C(13)-C(131)	1.497(8)
C(14)-C(15)	1.393(8)
C(15)-C(16)	1.404(7)
C(15)-C(151)	1.507(7)
C(17)-C(110)	1.512(8)
C(17)-C(18)	1.512(8)
C(17)-C(19)	1.542(8)
C(21)-C(26)	1.398(7)
C(21)-C(22)	1.388(7)
C(22)-C(23)	1.389(7)
C(23)-C(24)	1.387(8)
C(23)-C(231)	1.507(8)
C(24)-C(25)	1.383(7)
C(25)-C(26)	1.402(7)
C(25)-C(251)	1.502(7)
C(27)-C(29)	1.495(8)
C(27)-C(28)	1.505(8)
C(27)-C(210)	1.503(7)
C(31)-C(36)	1.385(7)
C(31)-C(32)	1.396(7)
C(32)-C(33)	1.400(7)
C(33)-C(34)	1.384(7)
C(33)-C(331)	1.513(7)
C(34)-C(35)	1.388(8)
C(35)-C(36)	1.393(7)
C(35)-C(351)	1.501(7)
C(37)-C(310)	1.521(7)
C(37)-C(39)	1.516(7)
C(37)-C(38)	1.527(7)
N(4)-Mo(1)-N(2)	106.35(17)
N(4)-Mo(1)-N(1)	105.40(17)
N(2)-Mo(1)-N(1)	112.47(17)
N(4)-Mo(1)-N(3)	104.80(17)
N(2)-Mo(1)-N(3)	112.85(16)
N(1)-Mo(1)-N(3)	114.04(16)
C(11)-N(1)-C(17)	115.2(4)
C(11)-N(1)-Mo(1)	113.1(3)
C(17)-N(1)-Mo(1)	130.8(3)
F(1)-B(1)-F(2)	111.6(5)
F(1)-B(1)-F(3)	110.8(5)
F(2)-B(1)-F(3)	111.4(5)
F(1)-B(1)-N(4)	107.9(4)
F(2)-B(1)-N(4)	107.6(4)
F(3)-B(1)-N(4)	107.4(4)
C(21)-N(2)-C(27)	116.3(4)
C(21)-N(2)-Mo(1)	112.3(3)
C(27)-N(2)-Mo(1)	130.6(3)
C(31)-N(3)-C(37)	114.7(4)
C(31)-N(3)-Mo(1)	113.1(3)
C(37)-N(3)-Mo(1)	130.6(3)
B(1)-N(4)-Mo(1)	177.6(3)
C(12)-C(11)-C(16)	119.6(5)
C(12)-C(11)-N(1)	120.8(4)
C(16)-C(11)-N(1)	119.6(4)
C(13)-C(12)-C(11)	121.5(5)
C(12)-C(13)-C(14)	117.8(5)
C(12)-C(13)-C(131)	120.9(5)
C(14)-C(13)-C(131)	121.3(5)
C(15)-C(14)-C(13)	122.6(5)
C(14)-C(15)-C(16)	118.3(5)
C(14)-C(15)-C(151)	122.0(5)
C(16)-C(15)-C(151)	119.7(5)
C(11)-C(16)-C(15)	120.2(5)
C(110)-C(17)-N(1)	110.3(4)
C(110)-C(17)-C(18)	109.6(5)
N(1)-C(17)-C(18)	110.8(5)
C(110)-C(17)-C(19)	107.0(5)
N(1)-C(17)-C(19)	107.8(4)
C(18)-C(17)-C(19)	111.3(5)
C(26)-C(21)-C(22)	119.3(5)
C(26)-C(21)-N(2)	118.8(4)
C(22)-C(21)-N(2)	121.9(4)
C(23)-C(22)-C(21)	121.3(5)
C(22)-C(23)-C(24)	118.2(5)
C(22)-C(23)-C(231)	120.8(5)
C(24)-C(23)-C(231)	120.9(5)
C(25)-C(24)-C(23)	122.4(5)
C(24)-C(25)-C(26)	118.4(5)

C(24)-C(25)-C(251)	121.3(5)	C(34)-C(33)-C(331)	121.8(5)
C(26)-C(25)-C(251)	120.3(5)	C(32)-C(33)-C(331)	119.1(5)
C(21)-C(26)-C(25)	120.3(5)	C(33)-C(34)-C(35)	121.9(5)
C(29)-C(27)-C(28)	110.9(6)	C(36)-C(35)-C(34)	118.4(5)
C(29)-C(27)-C(210)	108.9(5)	C(36)-C(35)-C(351)	120.8(5)
C(28)-C(27)-C(210)	108.0(5)	C(34)-C(35)-C(351)	120.8(5)
C(29)-C(27)-N(2)	110.1(4)	C(31)-C(36)-C(35)	121.0(5)
C(28)-C(27)-N(2)	109.3(4)	C(310)-C(37)-N(3)	110.5(4)
C(210)-C(27)-N(2)	109.7(4)	C(310)-C(37)-C(39)	109.7(4)
C(36)-C(31)-C(32)	119.9(5)	N(3)-C(37)-C(39)	109.5(4)
C(36)-C(31)-N(3)	121.0(4)	C(310)-C(37)-C(38)	110.1(5)
C(32)-C(31)-N(3)	119.1(4)	N(3)-C(37)-C(38)	108.4(4)
C(31)-C(32)-C(33)	119.8(5)	C(39)-C(37)-C(38)	108.6(5)
C(34)-C(33)-C(32)	119.1(5)	Cl(2)-C(41)-Cl(1)	110.6(5)

1.10 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**-BF_3. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	26(1)	24(1)	31(1)	3(1)	9(1)	1(1)
F(1)	85(2)	38(2)	65(2)	-9(2)	31(2)	-15(2)
N(1)	32(2)	26(2)	49(3)	3(2)	10(2)	3(2)
B(1)	38(4)	29(3)	52(4)	5(3)	14(3)	-5(3)
Cl(1)	135(2)	52(1)	419(6)	24(2)	134(3)	5(1)
F(2)	63(2)	41(2)	63(2)	23(2)	13(2)	-2(2)
N(2)	34(2)	29(2)	33(2)	3(2)	9(2)	-2(2)
Cl(2)	219(4)	567(10)	223(4)	252(6)	165(4)	209(6)
F(3)	41(2)	49(2)	84(2)	10(2)	17(2)	-11(2)
N(3)	31(2)	27(2)	37(2)	2(2)	12(2)	2(2)
N(4)	30(2)	30(2)	36(2)	5(2)	10(2)	2(2)
C(11)	31(3)	36(3)	44(3)	0(2)	8(2)	7(2)
C(12)	37(3)	41(3)	48(3)	7(3)	10(3)	5(2)
C(13)	42(3)	47(3)	45(3)	-3(3)	5(3)	5(3)
C(14)	41(3)	42(3)	60(4)	-8(3)	-1(3)	4(3)
C(15)	33(3)	37(3)	62(4)	3(3)	7(3)	5(2)
C(16)	32(3)	33(3)	54(3)	9(2)	10(2)	5(2)
C(17)	37(3)	27(3)	61(3)	2(2)	10(3)	8(2)
C(18)	121(6)	40(4)	77(5)	12(3)	15(4)	20(4)
C(19)	40(4)	50(4)	151(7)	-4(4)	31(4)	14(3)
C(21)	34(3)	35(3)	33(3)	2(2)	9(2)	-3(2)
C(22)	47(3)	38(3)	45(3)	1(2)	21(3)	1(2)
C(23)	51(3)	55(4)	50(3)	5(3)	27(3)	1(3)
C(24)	46(3)	55(4)	50(3)	10(3)	23(3)	-11(3)
C(25)	48(3)	41(3)	36(3)	7(2)	17(2)	-1(3)
C(26)	44(3)	32(3)	37(3)	3(2)	16(2)	1(2)
C(27)	35(3)	38(3)	33(3)	3(2)	2(2)	-4(2)
C(28)	69(5)	114(6)	100(6)	74(5)	-37(4)	-41(4)

C(29)	53(4)	150(8)	86(5)	-79(5)	-4(4)	16(5)
C(31)	38(3)	33(3)	39(3)	5(2)	16(2)	6(2)
C(32)	40(3)	37(3)	38(3)	-2(2)	13(2)	4(2)
C(33)	51(3)	37(3)	43(3)	-2(2)	19(3)	3(3)
C(34)	62(4)	29(3)	54(3)	5(3)	24(3)	10(3)
C(35)	48(3)	41(3)	52(3)	6(3)	18(3)	16(3)
C(36)	35(3)	38(3)	44(3)	0(2)	13(2)	6(2)
C(37)	38(3)	46(3)	37(3)	3(2)	22(2)	2(2)
C(38)	62(4)	64(4)	56(4)	23(3)	28(3)	15(3)
C(39)	79(4)	59(4)	55(4)	-8(3)	44(3)	-5(3)
C(41)	88(6)	127(8)	185(10)	90(7)	69(7)	27(6)
C(110)	56(4)	44(3)	80(4)	-12(3)	16(3)	13(3)
C(131)	72(4)	71(4)	49(4)	-6(3)	9(3)	10(4)
C(151)	47(3)	44(3)	81(4)	14(3)	17(3)	-8(3)
C(210)	41(3)	80(5)	54(4)	1(3)	6(3)	-14(3)
C(231)	66(4)	74(5)	110(6)	6(4)	57(4)	8(4)
C(251)	64(4)	37(3)	59(4)	2(3)	28(3)	-11(3)
C(310)	39(3)	64(4)	62(4)	6(3)	22(3)	1(3)
C(331)	65(4)	35(3)	62(4)	-6(3)	12(3)	-12(3)
C(351)	59(4)	57(4)	73(4)	21(3)	14(3)	22(3)

1.11 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**-$GeCl_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2500(1)	-5314(1)	-8216(1)	24(1)
Ge(1)	2770(1)	-6478(1)	-9976(1)	38(1)
Cl(1)	3606(2)	-7168(2)	-10082(2)	49(1)
Ge(1')	2227(1)	-6478(1)	-9976(1)	37(1)
Cl(1')	1396(2)	-7169(2)	-10083(2)	50(1)
Cl(2)	2499(1)	-5135(1)	-10634(1)	59(1)
N(1)	3604(4)	-4551(4)	-8138(3)	56(2)
N(2)	1402(4)	-4547(4)	-8138(3)	58(2)
N(3)	2495(4)	-6420(3)	-7582(2)	40(1)
N(4)	2501(3)	-5796(3)	-9035(2)	28(1)
C(1)	4362(4)	-4390(4)	-8651(3)	36(1)
C(2)	5111(4)	-3818(6)	-8295(4)	65(2)
C(3)	4024(5)	-3842(5)	-9284(3)	62(2)
C(4)	4734(5)	-5371(5)	-8895(4)	68(2)
C(5)	4013(7)	-4608(8)	-7365(5)	29(2)
C(6)	4539(7)	-5364(8)	-7079(5)	34(3)
C(7)	4874(8)	-5268(10)	-6394(6)	42(3)
C(8)	4666(9)	-4410(9)	-6016(6)	45(3)
C(9)	4145(8)	-3700(9)	-6295(6)	45(3)
C(5')	3361(7)	-3592(8)	-7707(6)	35(3)
C(6')	2994(8)	-2723(8)	-7955(6)	40(3)
C(7')	2925(9)	-1914(9)	-7497(7)	49(3)
C(8')	3236(9)	-1991(9)	-6808(7)	54(4)
C(9')	3585(10)	-2859(10)	-6568(7)	55(3)

C(10)	3734(4)	-3734(5)	-6999(3)	47(2)
C(11)	5442(5)	-6041(6)	-6117(4)	69(2)
C(12)	3912(6)	-2851(6)	-5830(4)	82(3)
C(13)	634(4)	-4390(4)	-8651(3)	36(1)
C(14)	980(5)	-3834(6)	-9285(3)	67(2)
C(15)	260(6)	-5375(5)	-8891(4)	68(2)
C(16)	-108(5)	-3817(6)	-8296(4)	67(2)
C(17)	1628(7)	-3588(7)	-7708(6)	31(3)
C(18)	2012(7)	-2729(8)	-7963(6)	35(3)
C(19)	2070(9)	-1917(9)	-7500(7)	50(3)
C(20)	1762(9)	-1999(10)	-6805(7)	53(3)
C(21)	1420(10)	-2863(10)	-6566(7)	57(4)
C(17')	985(7)	-4609(8)	-7370(5)	31(2)
C(18')	455(7)	-5362(9)	-7086(5)	38(3)
C(19')	122(8)	-5263(10)	-6397(6)	42(3)
C(20')	326(8)	-4415(9)	-6014(6)	43(3)
C(21')	849(9)	-3696(9)	-6292(6)	46(3)
C(22)	1267(4)	-3730(5)	-6998(3)	45(2)
C(23)	2500(6)	-945(5)	-7761(5)	76(2)
C(24)	1084(7)	-2855(6)	-5831(4)	84(3)
C(25)	2500(4)	-7505(3)	-7717(3)	30(1)
C(26)	2498(4)	-8056(4)	-7025(3)	40(1)
C(27)	1658(4)	-7772(5)	-8137(3)	54(2)
C(28)	3346(5)	-7767(5)	-8135(3)	57(2)
C(29)	1908(7)	-6167(7)	-6927(6)	33(3)
C(30)	972(7)	-6202(8)	-6877(6)	35(3)
C(31)	548(9)	-5974(10)	-6235(6)	45(3)
C(32)	1082(9)	-5703(9)	-5659(6)	46(3)
C(33)	2009(8)	-5648(8)	-5695(6)	43(3)
C(29')	3090(7)	-6171(7)	-6926(6)	34(3)
C(30')	4027(7)	-6204(8)	-6877(6)	36(3)
C(31')	4451(8)	-5978(10)	-6240(6)	45(3)
C(32')	3922(9)	-5699(9)	-5655(6)	49(3)
C(33')	2992(9)	-5649(9)	-5701(6)	45(3)
C(34)	2497(4)	-5889(4)	-6340(3)	38(1)
C(35)	-436(5)	-6039(6)	-6115(4)	68(2)
C(36)	2497(5)	-5341(6)	-5057(3)	64(2)

1.12 Bond lengths [Å] and angles [°] for **1**-$GeCl_2$

Mo(1)-N(4)	1.700(4)
Mo(1)-N(3)	1.942(4)
Mo(1)-N(2)	1.942(5)
Mo(1)-N(1)	1.945(5)
Ge(1)-Cl(1)	1.572(3)
Ge(1)-N(4)	2.069(4)
Ge(1)-Cl(2)	2.264(2)
Ge(1')-Cl(1')	1.565(4)
Ge(1')-N(4)	2.069(4)
Ge(1')-Cl(2)	2.267(2)
N(1)-C(1)	1.510(7)
N(1)-C(5')	1.593(12)
N(1)-C(5)	1.598(11)
N(2)-C(13)	1.516(7)
N(2)-C(17)	1.587(11)
N(2)-C(17')	1.597(11)
N(3)-C(25)	1.510(6)
N(3)-C(29)	1.566(12)
N(3)-C(29')	1.571(12)
C(1)-C(3)	1.510(8)
C(1)-C(2)	1.518(8)

C(1)-C(4)	1.526(9)	N(4)-Mo(1)-N(3)	105.76(19)
C(5)-C(6)	1.407(15)	N(4)-Mo(1)-N(2)	106.5(2)
C(5)-C(10)	1.448(12)	N(3)-Mo(1)-N(2)	111.7(2)
C(6)-C(7)	1.407(15)	N(4)-Mo(1)-N(1)	106.1(2)
C(7)-C(8)	1.415(17)	N(3)-Mo(1)-N(1)	112.1(2)
C(7)-C(11)	1.452(14)	N(2)-Mo(1)-N(1)	114.0(3)
C(8)-C(9)	1.351(17)	Cl(1)-Ge(1)-N(4)	122.43(18)
C(9)-C(10)	1.478(13)	Cl(1)-Ge(1)-Cl(2)	123.84(16)
C(9)-C(12)	1.507(14)	N(4)-Ge(1)-Cl(2)	94.72(13)
C(5')-C(6')	1.393(16)	Cl(1')-Ge(1')-N(4)	122.70(18)
C(5')-C(10)	1.474(13)	Cl(1')-Ge(1')-Cl(2)	123.99(15)
C(6')-C(7')	1.417(16)	N(4)-Ge(1')-Cl(2)	94.67(13)
C(7')-C(8')	1.399(18)	Ge(1)-Cl(2)-Ge(1')	20.42(4)
C(7')-C(23)	1.554(15)	C(1)-N(1)-C(5')	112.6(5)
C(8')-C(9')	1.376(19)	C(1)-N(1)-C(5)	109.1(5)
C(9')-C(10)	1.472(14)	C(5')-N(1)-C(5)	69.3(6)
C(9')-C(12)	1.493(15)	C(1)-N(1)-Mo(1)	130.8(3)
C(11)-C(31')	1.487(14)	C(5')-N(1)-Mo(1)	107.1(5)
C(13)-C(16)	1.512(8)	C(5)-N(1)-Mo(1)	111.3(4)
C(13)-C(14)	1.521(9)	C(13)-N(2)-C(17)	112.0(5)
C(13)-C(15)	1.529(9)	C(13)-N(2)-C(17')	108.2(5)
C(17)-C(18)	1.396(16)	C(17)-N(2)-C(17')	69.4(6)
C(17)-C(22)	1.474(13)	C(13)-N(2)-Mo(1)	130.9(4)
C(18)-C(19)	1.426(16)	C(17)-N(2)-Mo(1)	108.2(5)
C(19)-C(20)	1.411(19)	C(17')-N(2)-Mo(1)	111.5(4)
C(19)-C(23)	1.559(15)	C(25)-N(3)-C(29)	111.0(5)
C(20)-C(21)	1.37(2)	C(25)-N(3)-C(29')	110.4(5)
C(21)-C(22)	1.465(15)	C(29)-N(3)-C(29')	67.8(6)
C(21)-C(24)	1.494(15)	C(25)-N(3)-Mo(1)	131.5(3)
C(17')-C(18')	1.407(15)	C(29)-N(3)-Mo(1)	109.3(4)
C(17')-C(22)	1.459(12)	C(29')-N(3)-Mo(1)	109.1(4)
C(18')-C(19')	1.416(15)	Mo(1)-N(4)-Ge(1')	167.8(3)
C(19')-C(20')	1.407(17)	Mo(1)-N(4)-Ge(1)	168.1(3)
C(19')-C(35)	1.451(14)	Ge(1')-N(4)-Ge(1)	22.39(6)
C(20')-C(21')	1.362(17)	N(1)-C(1)-C(3)	110.4(5)
C(21')-C(22)	1.489(13)	N(1)-C(1)-C(2)	109.1(5)
C(21')-C(24)	1.492(14)	C(3)-C(1)-C(2)	110.1(5)
C(25)-C(27)	1.526(8)	N(1)-C(1)-C(4)	109.8(5)
C(25)-C(26)	1.525(7)	C(3)-C(1)-C(4)	108.2(5)
C(25)-C(28)	1.528(8)	C(2)-C(1)-C(4)	109.2(6)
C(29)-C(30)	1.390(15)	C(6)-C(5)-C(10)	125.4(9)
C(29)-C(34)	1.470(12)	C(6)-C(5)-N(1)	127.2(9)
C(30)-C(31)	1.414(15)	C(10)-C(5)-N(1)	107.4(7)
C(31)-C(32)	1.406(17)	C(5)-C(6)-C(7)	119.2(10)
C(31)-C(35)	1.477(14)	C(6)-C(7)-C(8)	118.5(11)
C(32)-C(33)	1.376(17)	C(6)-C(7)-C(11)	118.3(10)
C(33)-C(34)	1.469(13)	C(8)-C(7)-C(11)	123.1(10)
C(33)-C(36)	1.478(14)	C(9)-C(8)-C(7)	121.4(11)
C(29')-C(30')	1.390(15)	C(8)-C(9)-C(10)	124.9(10)
C(29')-C(34)	1.476(13)	C(8)-C(9)-C(12)	117.0(10)
C(30')-C(31')	1.404(16)	C(10)-C(9)-C(12)	117.9(9)
C(31')-C(32')	1.420(18)	C(6')-C(5')-C(10)	124.8(9)
C(32')-C(33')	1.380(18)	C(6')-C(5')-N(1)	128.2(9)
C(33')-C(34)	1.462(13)	C(10)-C(5')-N(1)	106.4(8)
C(33')-C(36)	1.495(14)	C(5')-C(6')-C(7')	119.1(11)
		C(8')-C(7')-C(6')	120.0(12)

C(8')-C(7')-C(23)	120.2(10)	C(17')-C(22)-C(21')	110.5(8)
C(6')-C(7')-C(23)	119.8(11)	C(21)-C(22)-C(21')	61.7(8)
C(9')-C(8')-C(7')	120.1(11)	C(17)-C(22)-C(21')	170.0(8)
C(8')-C(9')-C(10)	125.1(11)	C(7')-C(23)-C(19)	48.0(6)
C(8')-C(9')-C(12)	115.4(11)	C(21')-C(24)-C(21)	61.0(8)
C(10)-C(9')-C(12)	119.2(10)	N(3)-C(25)-C(27)	108.8(5)
C(5)-C(10)-C(9')	171.1(9)	N(3)-C(25)-C(26)	109.8(4)
C(5)-C(10)-C(9)	110.4(8)	C(27)-C(25)-C(26)	109.6(5)
C(9')-C(10)-C(9)	61.7(7)	N(3)-C(25)-C(28)	109.0(5)
C(5)-C(10)-C(5')	76.8(6)	C(27)-C(25)-C(28)	109.8(5)
C(9')-C(10)-C(5')	110.5(8)	C(26)-C(25)-C(28)	109.9(5)
C(9)-C(10)-C(5')	170.4(8)	C(30)-C(29)-C(34)	123.1(9)
C(7)-C(11)-C(31')	48.0(7)	C(30)-C(29)-N(3)	127.0(9)
C(9')-C(12)-C(9)	60.6(7)	C(34)-C(29)-N(3)	109.9(7)
C(16)-C(13)-N(2)	109.1(5)	C(29)-C(30)-C(31)	119.8(11)
C(16)-C(13)-C(14)	110.1(6)	C(32)-C(31)-C(30)	119.3(11)
N(2)-C(13)-C(14)	109.5(5)	C(32)-C(31)-C(35)	116.5(10)
C(16)-C(13)-C(15)	109.3(6)	C(30)-C(31)-C(35)	124.2(10)
N(2)-C(13)-C(15)	109.8(5)	C(33)-C(32)-C(31)	122.3(11)
C(14)-C(13)-C(15)	109.0(5)	C(32)-C(33)-C(34)	121.5(10)
C(18)-C(17)-C(22)	125.7(9)	C(32)-C(33)-C(36)	117.4(10)
C(18)-C(17)-N(2)	127.1(9)	C(34)-C(33)-C(36)	121.2(9)
C(22)-C(17)-N(2)	106.9(7)	C(30')-C(29')-C(34)	123.5(9)
C(17)-C(18)-C(19)	117.7(11)	C(30')-C(29')-N(3)	127.2(9)
C(20)-C(19)-C(18)	120.3(12)	C(34)-C(29')-N(3)	109.3(7)
C(20)-C(19)-C(23)	120.2(11)	C(29')-C(30')-C(31')	119.7(11)
C(18)-C(19)-C(23)	119.5(11)	C(30')-C(31')-C(32')	119.8(11)
C(21)-C(20)-C(19)	120.3(12)	C(30')-C(31')-C(11)	124.3(11)
C(20)-C(21)-C(22)	124.9(11)	C(32')-C(31')-C(11)	115.9(10)
C(20)-C(21)-C(24)	115.7(11)	C(33')-C(32')-C(31')	121.0(11)
C(22)-C(21)-C(24)	119.1(11)	C(32')-C(33')-C(34)	122.7(11)
C(18')-C(17')-C(22)	125.3(9)	C(32')-C(33')-C(36)	116.9(10)
C(18')-C(17')-N(2)	127.6(9)	C(34)-C(33')-C(36)	120.5(10)
C(22)-C(17')-N(2)	107.1(7)	C(33')-C(34)-C(33)	59.5(7)
C(17')-C(18')-C(19')	119.0(11)	C(33')-C(34)-C(29)	173.0(8)
C(20')-C(19')-C(18')	119.3(11)	C(33)-C(34)-C(29)	114.1(8)
C(20')-C(19')-C(35)	122.3(10)	C(33')-C(34)-C(29')	113.3(8)
C(18')-C(19')-C(35)	118.4(10)	C(33)-C(34)-C(29')	172.1(8)
C(21')-C(20')-C(19')	121.1(11)	C(29)-C(34)-C(29')	72.9(6)
C(20')-C(21')-C(22)	124.7(10)	C(19')-C(35)-C(31)	48.4(7)
C(20')-C(21')-C(24)	117.4(10)	C(33)-C(36)-C(33')	58.6(7)
C(22)-C(21')-C(24)	117.7(9)		
C(17')-C(22)-C(21)	171.2(9)		
C(17')-C(22)-C(17)	76.4(6)		
C(21)-C(22)-C(17)	110.9(8)		

Symmetry transformations used to generate equivalent atoms:

1.13 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**-$GeCl_2$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	30(1)	20(1)	21(1)	-1(1)	0(1)	0(1)
Ge(1)	43(1)	41(1)	29(1)	-11(1)	-1(1)	6(1)
Cl(1)	59(2)	49(2)	38(2)	-8(1)	6(1)	11(2)
Ge(1')	40(1)	42(1)	30(1)	-11(1)	0(1)	-6(1)
Cl(1')	60(2)	50(2)	40(2)	-8(1)	-6(1)	-11(2)

Cl(2)	100(1)	46(1)	31(1)	2(1)	0(1)	0(1)
N(1)	68(4)	68(4)	33(3)	-21(3)	15(3)	-43(3)
N(2)	67(4)	70(4)	35(3)	-21(3)	-15(3)	43(3)
N(3)	76(3)	23(2)	20(2)	-2(2)	0(2)	-1(2)
N(4)	32(2)	26(2)	27(2)	-2(2)	-1(2)	1(2)
C(1)	36(3)	40(3)	32(3)	-1(3)	2(2)	-13(3)
C(2)	50(4)	90(6)	56(4)	-19(4)	2(3)	-24(4)
C(3)	73(5)	68(5)	45(4)	3(4)	-6(4)	1(4)
C(4)	93(6)	55(5)	56(5)	-8(4)	-1(4)	5(4)
C(5)	26(5)	31(6)	31(6)	2(5)	3(5)	-6(5)
C(6)	32(6)	40(7)	30(6)	9(5)	-4(5)	-4(5)
C(7)	47(7)	52(8)	27(6)	-1(6)	-3(5)	0(7)
C(8)	54(8)	42(7)	38(7)	-4(6)	-9(6)	-2(6)
C(9)	45(7)	47(8)	43(7)	-10(6)	-6(6)	-7(6)
C(5')	36(6)	26(6)	42(7)	-2(5)	4(5)	-14(5)
C(6')	37(7)	27(6)	56(8)	-6(6)	1(6)	-6(5)
C(7')	56(9)	31(7)	61(9)	-9(6)	5(7)	-6(6)
C(8')	65(9)	37(8)	59(9)	-14(7)	15(7)	-18(7)
C(9')	71(9)	46(8)	47(8)	-8(7)	1(7)	-7(7)
C(10)	62(4)	49(4)	29(3)	-14(3)	-1(3)	-20(3)
C(11)	59(5)	78(5)	69(5)	-17(4)	-26(4)	14(4)
C(12)	121(7)	70(5)	53(5)	-30(4)	-19(5)	3(5)
C(13)	35(3)	42(3)	32(3)	-3(3)	-6(2)	12(3)
C(14)	88(6)	69(5)	45(4)	3(4)	1(4)	-1(4)
C(15)	96(6)	53(4)	53(4)	-7(4)	-2(4)	-3(4)
C(16)	51(4)	89(6)	60(5)	-16(4)	-4(3)	24(4)
C(17)	32(6)	19(6)	43(7)	-4(5)	-9(5)	10(5)
C(18)	30(6)	27(6)	50(7)	-9(5)	-7(5)	5(5)
C(19)	47(8)	32(7)	70(10)	-2(6)	-7(7)	8(6)
C(20)	54(8)	43(8)	61(9)	-17(7)	-12(7)	13(7)
C(21)	76(10)	49(9)	47(8)	-8(7)	-3(7)	15(8)
C(17')	32(6)	29(6)	32(6)	-1(5)	0(5)	11(5)
C(18')	35(6)	51(7)	27(6)	8(5)	3(5)	1(6)
C(19')	48(7)	48(8)	30(7)	-1(6)	3(5)	0(7)
C(20')	45(7)	39(7)	45(7)	-1(6)	8(6)	3(6)
C(21')	53(8)	44(7)	43(7)	-5(6)	10(6)	2(6)
C(22)	58(4)	50(4)	27(3)	-13(3)	-1(3)	18(3)
C(23)	85(6)	24(4)	119(7)	-7(4)	-1(5)	-2(4)
C(24)	134(8)	67(5)	50(4)	-30(4)	17(5)	-2(5)
C(25)	37(3)	19(3)	33(3)	0(2)	-2(2)	0(2)
C(26)	60(4)	27(3)	34(3)	6(3)	1(3)	1(3)
C(27)	62(4)	58(4)	41(4)	8(3)	-9(3)	-10(4)
C(28)	67(5)	60(4)	44(4)	8(3)	11(3)	16(4)
C(29)	42(7)	20(6)	37(6)	3(5)	5(5)	2(5)
C(30)	41(7)	27(6)	37(7)	2(5)	17(5)	-2(5)
C(31)	51(8)	48(8)	35(7)	1(6)	9(6)	-4(7)
C(32)	63(9)	44(7)	31(7)	1(6)	13(6)	-8(6)
C(33)	49(8)	36(7)	44(7)	9(6)	1(6)	-2(6)
C(29')	40(7)	20(6)	41(7)	6(5)	-4(5)	2(5)
C(30')	40(7)	30(6)	40(7)	-2(5)	-14(5)	2(5)
C(31')	45(7)	50(8)	41(8)	8(6)	-11(6)	3(7)
C(32')	54(8)	50(8)	42(7)	3(6)	-12(6)	3(6)
C(33')	57(9)	37(7)	42(7)	4(6)	2(6)	5(6)
C(34)	63(4)	27(3)	24(3)	0(2)	1(3)	0(3)
C(35)	56(4)	78(5)	72(5)	-17(4)	25(4)	-14(4)
C(36)	87(5)	77(5)	28(4)	-14(3)	-2(3)	-1(4)

1.14 Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**-$SnCl_2$. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Mo(1)	2500(1)	-5320(1)	-8186(1)	20(1)
Sn(1)	2806(1)	-6569(1)	-10023(1)	35(1)
Cl(1')	3699(2)	-7258(3)	-10088(2)	41(1)
Sn(1')	2182(1)	-6570(1)	-10023(1)	29(1)
Cl(1)	1305(3)	-7258(3)	-10091(2)	49(1)
Cl(2)	2498(2)	-5097(2)	-10676(1)	53(1)
N(1)	3607(5)	-4561(5)	-8113(3)	51(2)
N(2)	1399(4)	-4547(5)	-8123(3)	50(2)
N(3)	2490(5)	-6424(4)	-7552(3)	38(2)
N(4)	2503(3)	-5814(4)	-8996(3)	26(1)
C(1)	4356(4)	-4395(5)	-8636(3)	32(2)
C(2)	5100(6)	-3793(8)	-8302(4)	60(3)
C(3)	3996(7)	-3875(7)	-9262(4)	59(2)
C(4)	4748(7)	-5382(7)	-8866(5)	64(3)
C(5)	4012(8)	-4600(9)	-7363(6)	21(3)
C(6)	4547(8)	-5330(10)	-7077(6)	27(3)
C(7)	4907(9)	-5239(11)	-6395(7)	32(3)
C(8)	4697(9)	-4391(10)	-6016(7)	34(3)
C(9)	4124(10)	-3665(12)	-6285(7)	39(4)
C(5')	3384(9)	-3599(10)	-7698(7)	30(3)
C(6')	3013(9)	-2720(10)	-7940(8)	39(4)
C(7')	2959(11)	-1916(12)	-7488(9)	46(4)
C(8')	3280(13)	-1978(14)	-6812(10)	59(5)
C(9')	3631(12)	-2854(14)	-6544(9)	54(4)
C(10)	3747(5)	-3735(6)	-6986(3)	38(2)
C(11)	5462(6)	-6027(7)	-6105(5)	57(2)
C(12)	3913(8)	-2840(8)	-5837(5)	70(3)
C(13)	650(4)	-4394(5)	-8636(3)	33(2)
C(14)	983(7)	-3882(7)	-9276(4)	58(2)

C(15)	270(7)	-5399(7)	-8867(5)	63(3)
C(16)	-104(5)	-3802(8)	-8300(4)	59(2)
C(17)	1611(8)	-3603(9)	-7696(7)	27(3)
C(18)	1973(8)	-2738(10)	-7939(7)	30(3)
C(19)	2048(9)	-1922(10)	-7487(8)	37(3)
C(20)	1726(11)	-2005(12)	-6810(8)	46(4)
C(21)	1383(12)	-2879(12)	-6558(8)	47(4)
C(17')	986(9)	-4593(10)	-7358(6)	29(3)
C(18')	450(8)	-5344(11)	-7083(7)	34(3)
C(19')	97(11)	-5252(14)	-6392(7)	48(4)
C(20')	318(10)	-4386(12)	-6026(7)	40(4)
C(21')	879(11)	-3667(13)	-6285(8)	49(4)
C(22)	1263(5)	-3740(6)	-6991(4)	40(2)
C(23)	2501(7)	-962(6)	-7732(6)	69(3)
C(24)	1072(8)	-2862(8)	-5835(5)	75(3)
C(25)	2495(4)	-7508(5)	-7697(3)	27(1)
C(26)	2498(5)	-8070(5)	-7009(3)	36(2)
C(27)	1666(6)	-7780(7)	-8113(4)	52(2)
C(28)	3350(5)	-7760(7)	-8109(4)	49(2)
C(29)	1920(8)	-6186(9)	-6895(6)	25(3)
C(30)	974(9)	-6214(9)	-6852(6)	25(3)
C(31)	554(9)	-6000(11)	-6213(7)	35(3)
C(32)	1104(10)	-5711(10)	-5657(7)	35(3)
C(33)	2014(10)	-5635(10)	-5694(7)	34(3)
C(29')	3094(10)	-6175(10)	-6903(6)	32(3)
C(30')	4010(10)	-6234(10)	-6856(7)	35(3)
C(31')	4458(10)	-6005(13)	-6216(8)	45(4)
C(32')	3902(10)	-5695(11)	-5647(8)	41(4)
C(33')	2989(10)	-5631(10)	-5692(7)	36(3)
C(34)	2497(5)	-5874(5)	-6332(3)	34(2)
C(35)	-461(5)	-6029(7)	-6116(4)	51(2)
C(36)	2504(6)	-5290(7)	-5068(4)	56(2)

1.15 Bond lengths [Å] and angles [°] for **1**-$SnCl_2$

Mo(1)-N(4)	1.692(5)
Mo(1)-N(3)	1.941(6)
Mo(1)-N(2)	1.948(6)
Mo(1)-N(1)	1.946(6)
Sn(1)-Sn(1')	0.9226(12)
Sn(1)-Cl(1')	1.630(4)
Sn(1)-N(4)	2.266(5)
Sn(1)-Cl(2)	2.417(2)
Sn(1)-Cl(1)	2.417(4)
Cl(1')-Sn(1')	2.438(4)
Sn(1')-Cl(1)	1.610(4)
Sn(1')-N(4)	2.271(5)
Sn(1')-Cl(2)	2.421(2)
N(1)-C(1)	1.512(8)
N(1)-C(5')	1.574(15)
N(1)-C(5)	1.555(13)
N(2)-C(13)	1.494(9)
N(2)-C(17)	1.562(14)
N(2)-C(17')	1.588(13)
N(3)-C(25)	1.512(8)
N(3)-C(29)	1.549(12)
N(3)-C(29')	1.566(14)
C(1)-C(3)	1.493(11)
C(1)-C(2)	1.516(10)
C(1)-C(4)	1.537(11)
C(5)-C(6)	1.388(17)
C(5)-C(10)	1.444(14)
C(6)-C(7)	1.414(17)
C(7)-C(8)	1.41(2)
C(7)-C(11)	1.465(16)
C(8)-C(9)	1.40(2)
C(9)-C(12)	1.455(17)
C(9)-C(10)	1.454(15)
C(5')-C(6')	1.40(2)
C(5')-C(10)	1.475(15)
C(6')-C(7')	1.40(2)
C(7')-C(8')	1.38(2)
C(7')-C(23)	1.545(19)
C(8')-C(9')	1.41(3)
C(9')-C(12)	1.415(18)
C(9')-C(10)	1.484(19)
C(11)-C(31')	1.500(17)
C(13)-C(14)	1.496(10)
C(13)-C(16)	1.523(10)
C(13)-C(15)	1.551(11)
C(17)-C(18)	1.381(19)
C(17)-C(22)	1.458(14)
C(18)-C(19)	1.418(19)
C(19)-C(20)	1.39(2)
C(19)-C(23)	1.550(17)
C(20)-C(21)	1.39(2)
C(21)-C(24)	1.459(17)
C(21)-C(22)	1.452(17)
C(17')-C(18')	1.403(19)
C(17')-C(22)	1.425(15)
C(18')-C(19')	1.428(18)
C(19')-C(20')	1.42(2)
C(19')-C(35)	1.448(19)
C(20')-C(21')	1.38(2)
C(21')-C(24)	1.428(19)
C(21')-C(22)	1.470(16)
C(25)-C(27)	1.508(10)
C(25)-C(28)	1.532(9)
C(25)-C(26)	1.526(9)
C(29)-C(30)	1.403(18)
C(29)-C(34)	1.437(15)
C(30)-C(31)	1.404(17)
C(31)-C(32)	1.39(2)
C(31)-C(35)	1.515(15)

C(32)-C(33)	1.35(2)	N(4)-Sn(1')-Cl(1')	91.69(16)
C(33)-C(34)	1.453(15)	Cl(2)-Sn(1')-Cl(1')	96.78(12)
C(33)-C(36)	1.477(16)	Sn(1')-Cl(1)-Sn(1)	13.01(7)
C(29')-C(30')	1.36(2)	Sn(1)-Cl(2)-Sn(1')	21.99(3)
C(29')-C(34)	1.466(15)	C(1)-N(1)-C(5')	111.3(6)
C(30')-C(31')	1.43(2)	C(1)-N(1)-C(5)	109.5(6)
C(31')-C(32')	1.43(2)	C(5')-N(1)-C(5)	69.2(7)
C(32')-C(33')	1.36(2)	C(1)-N(1)-Mo(1)	130.7(4)
C(33')-C(34)	1.462(17)	C(5')-N(1)-Mo(1)	107.9(6)
C(33')-C(36)	1.471(15)	C(5)-N(1)-Mo(1)	111.7(5)
		C(13)-N(2)-C(17)	112.0(7)
N(4)-Mo(1)-N(3)	105.1(2)	C(13)-N(2)-C(17')	108.9(7)
N(4)-Mo(1)-N(2)	106.2(2)	C(17)-N(2)-C(17')	68.2(7)
N(3)-Mo(1)-N(2)	112.2(3)	C(13)-N(2)-Mo(1)	131.0(4)
N(4)-Mo(1)-N(1)	106.0(2)	C(17)-N(2)-Mo(1)	108.4(6)
N(3)-Mo(1)-N(1)	112.4(3)	C(17')-N(2)-Mo(1)	111.1(6)
N(2)-Mo(1)-N(1)	114.1(3)	C(25)-N(3)-C(29)	111.0(6)
Sn(1')-Sn(1)-Cl(1')	144.10(19)	C(25)-N(3)-C(29')	110.9(7)
Sn(1')-Sn(1)-N(4)	78.57(16)	C(29)-N(3)-C(29')	67.8(7)
Cl(1')-Sn(1)-N(4)	119.51(19)	C(25)-N(3)-Mo(1)	130.7(4)
Sn(1')-Sn(1)-Cl(2)	79.28(11)	C(29)-N(3)-Mo(1)	110.4(6)
Cl(1')-Sn(1)-Cl(2)	126.65(15)	C(29')-N(3)-Mo(1)	108.7(6)
N(4)-Sn(1)-Cl(2)	91.68(14)	Mo(1)-N(4)-Sn(1)	168.0(3)
Sn(1')-Sn(1)-Cl(1)	23.12(13)	Mo(1)-N(4)-Sn(1')	167.1(3)
Cl(1')-Sn(1)-Cl(1)	120.98(18)	Sn(1)-N(4)-Sn(1')	23.47(6)
N(4)-Sn(1)-Cl(1)	92.40(17)	C(3)-C(1)-N(1)	110.0(6)
Cl(2)-Sn(1)-Cl(1)	97.26(13)	C(3)-C(1)-C(2)	109.6(7)
Sn(1)-Cl(1')-Sn(1')	12.82(7)	N(1)-C(1)-C(2)	109.7(6)
Sn(1)-Sn(1')-Cl(1)	143.9(2)	C(3)-C(1)-C(4)	109.0(7)
Sn(1)-Sn(1')-N(4)	77.96(16)	N(1)-C(1)-C(4)	109.6(6)
Cl(1)-Sn(1')-N(4)	120.27(19)	C(2)-C(1)-C(4)	109.0(7)
Sn(1)-Sn(1')-Cl(2)	78.73(11)	C(6)-C(5)-C(10)	123.4(10)
Cl(1)-Sn(1')-Cl(2)	127.14(17)	C(6)-C(5)-N(1)	127.5(10)
N(4)-Sn(1')-Cl(2)	91.44(14)	C(10)-C(5)-N(1)	109.1(9)
Sn(1)-Sn(1')-Cl(1')	23.08(12)	C(5)-C(6)-C(7)	120.9(12)
Cl(1)-Sn(1')-Cl(1')	120.79(19)	C(8)-C(7)-C(6)	117.8(13)

C(8)-C(7)-C(11)	122.6(11)	C(20)-C(19)-C(23)	120.2(13)
C(6)-C(7)-C(11)	119.6(12)	C(18)-C(19)-C(23)	121.3(12)
C(9)-C(8)-C(7)	122.1(12)	C(19)-C(20)-C(21)	121.5(14)
C(8)-C(9)-C(12)	117.7(12)	C(20)-C(21)-C(24)	115.6(13)
C(8)-C(9)-C(10)	121.5(12)	C(20)-C(21)-C(22)	123.2(13)
C(12)-C(9)-C(10)	120.9(12)	C(24)-C(21)-C(22)	121.0(13)
C(6')-C(5')-C(10)	123.7(12)	C(18')-C(17')-C(22)	125.4(11)
C(6')-C(5')-N(1)	129.4(12)	C(18')-C(17')-N(2)	126.5(11)
C(10)-C(5')-N(1)	106.6(9)	C(22)-C(17')-N(2)	108.1(9)
C(5')-C(6')-C(7')	119.7(14)	C(17')-C(18')-C(19')	119.4(14)
C(8')-C(7')-C(6')	120.6(16)	C(18')-C(19')-C(20')	116.5(15)
C(8')-C(7')-C(23)	119.0(14)	C(18')-C(19')-C(35)	118.8(14)
C(6')-C(7')-C(23)	120.3(14)	C(20')-C(19')-C(35)	124.7(12)
C(7')-C(8')-C(9')	121.4(16)	C(21')-C(20')-C(19')	124.1(13)
C(8')-C(9')-C(12)	116.4(15)	C(20')-C(21')-C(24)	117.1(12)
C(8')-C(9')-C(10)	122.0(14)	C(20')-C(21')-C(22)	120.9(14)
C(12)-C(9')-C(10)	121.5(14)	C(24)-C(21')-C(22)	121.9(13)
C(5)-C(10)-C(9)	114.2(10)	C(17')-C(22)-C(21')	113.5(10)
C(5)-C(10)-C(9')	170.2(11)	C(17')-C(22)-C(17)	75.6(8)
C(9)-C(10)-C(9')	57.7(9)	C(21')-C(22)-C(17)	168.5(10)
C(5)-C(10)-C(5')	75.0(8)	C(17')-C(22)-C(21)	169.6(10)
C(9)-C(10)-C(5')	169.0(10)	C(21')-C(22)-C(21)	57.9(10)
C(9')-C(10)-C(5')	112.5(10)	C(17)-C(22)-C(21)	112.3(10)
C(7)-C(11)-C(31')	51.5(9)	C(7')-C(23)-C(19)	51.6(8)
C(9')-C(12)-C(9)	59.2(10)	C(21')-C(24)-C(21)	58.7(9)
C(14)-C(13)-N(2)	110.9(6)	C(27)-C(25)-N(3)	109.6(6)
C(14)-C(13)-C(16)	109.8(7)	C(27)-C(25)-C(28)	110.1(6)
N(2)-C(13)-C(16)	109.9(6)	N(3)-C(25)-C(28)	108.8(6)
C(14)-C(13)-C(15)	107.6(6)	C(27)-C(25)-C(26)	109.4(6)
N(2)-C(13)-C(15)	109.3(7)	N(3)-C(25)-C(26)	109.8(5)
C(16)-C(13)-C(15)	109.2(7)	C(28)-C(25)-C(26)	109.2(6)
C(18)-C(17)-C(22)	124.1(11)	C(30)-C(29)-C(34)	123.7(10)
C(18)-C(17)-N(2)	127.8(11)	C(30)-C(29)-N(3)	125.9(11)
C(22)-C(17)-N(2)	107.8(9)	C(34)-C(29)-N(3)	110.3(9)
C(17)-C(18)-C(19)	120.1(12)	C(31)-C(30)-C(29)	119.3(12)
C(20)-C(19)-C(18)	118.5(13)	C(32)-C(31)-C(30)	117.7(12)

C(32)-C(31)-C(35)	119.5(11)	C(32')-C(33')-C(34)	122.2(12)
C(30)-C(31)-C(35)	122.8(12)	C(32')-C(33')-C(36)	117.2(13)
C(33)-C(32)-C(31)	124.1(12)	C(34)-C(33')-C(36)	120.6(11)
C(32)-C(33)-C(34)	121.2(12)	C(29)-C(34)-C(33)	113.8(9)
C(32)-C(33)-C(36)	118.0(12)	C(29)-C(34)-C(33')	171.5(9)
C(34)-C(33)-C(36)	120.8(11)	C(33)-C(34)-C(33')	59.4(8)
C(30')-C(29')-C(34)	124.7(11)	C(29)-C(34)-C(29')	73.5(7)
C(30')-C(29')-N(3)	127.4(12)	C(33)-C(34)-C(29')	171.1(10)
C(34)-C(29')-N(3)	107.9(10)	C(33')-C(34)-C(29')	112.9(9)
C(29')-C(30')-C(31')	120.4(14)	C(19')-C(35)-C(31)	50.9(8)
C(32')-C(31')-C(30')	116.8(13)	C(33)-C(36)-C(33')	58.6(8)
C(32')-C(31')-C(11)	118.0(12)		
C(30')-C(31')-C(11)	125.2(13)	Symmetry transformations used to generate	
C(33')-C(32')-C(31')	123.1(14)	equivalent atoms:	

1.16 Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**-$SnCl_2$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	26(1)	16(1)	18(1)	-1(1)	4(1)	0(1)
Sn(1)	45(1)	35(1)	26(1)	-9(1)	5(1)	5(1)
Cl(1')	45(2)	43(2)	34(2)	-5(2)	7(2)	9(2)
Sn(1')	29(1)	33(1)	26(1)	-8(1)	3(1)	-3(1)
Cl(1)	54(2)	53(3)	39(2)	-11(2)	-1(2)	-8(2)
Cl(2)	90(2)	38(1)	30(1)	4(1)	3(1)	0(1)
N(1)	63(4)	61(5)	29(3)	-24(3)	18(3)	-43(4)
N(2)	58(4)	63(5)	29(3)	-21(3)	-9(3)	36(4)
N(3)	78(4)	18(3)	18(3)	-1(2)	5(3)	3(3)
N(4)	31(3)	23(3)	23(3)	0(2)	5(2)	2(2)
C(1)	31(3)	34(4)	32(4)	0(3)	7(3)	-9(3)
C(2)	48(5)	81(7)	50(5)	-18(5)	8(4)	-25(5)
C(3)	76(6)	52(6)	47(5)	6(4)	-6(4)	-5(5)
C(4)	87(7)	51(6)	53(5)	-8(4)	0(5)	12(5)
C(5)	24(6)	18(7)	21(6)	-2(5)	4(5)	-3(5)
C(6)	32(7)	31(8)	17(6)	4(5)	-1(5)	2(6)
C(7)	31(7)	39(9)	24(7)	1(6)	3(5)	-7(6)

C(8)	36(7)	30(9)	37(8)	-8(6)	-3(6)	-6(6)
C(9)	48(8)	44(10)	24(7)	-13(6)	1(6)	-3(7)
C(5')	39(7)	14(7)	38(8)	1(6)	2(6)	-13(6)
C(6')	30(7)	20(8)	66(10)	-5(7)	11(7)	-8(6)
C(7')	50(9)	30(10)	58(10)	-6(7)	-2(8)	-13(7)
C(8')	73(12)	44(12)	62(12)	-3(9)	32(10)	-11(9)
C(9')	65(11)	50(12)	45(9)	-4(8)	-2(8)	-2(9)
C(10)	56(5)	32(4)	26(4)	-11(3)	-1(3)	-15(3)
C(11)	47(5)	65(6)	58(5)	-4(5)	-14(4)	0(4)
C(12)	105(8)	59(6)	47(5)	-22(5)	-10(5)	-7(6)
C(13)	32(3)	37(4)	30(4)	-4(3)	1(3)	10(3)
C(14)	78(6)	52(6)	44(5)	5(4)	11(4)	7(5)
C(15)	83(7)	49(6)	58(6)	-10(4)	6(5)	-15(5)
C(16)	43(5)	81(7)	53(5)	-16(5)	2(4)	23(4)
C(17)	32(7)	15(7)	35(7)	-6(5)	0(5)	9(5)
C(18)	22(6)	22(8)	47(8)	5(6)	-2(5)	10(5)
C(19)	38(8)	21(8)	52(9)	-2(6)	-1(7)	8(6)
C(20)	63(10)	30(10)	44(9)	-12(7)	-18(8)	17(8)
C(21)	64(10)	35(10)	42(9)	-10(7)	-2(7)	-2(8)
C(17')	35(7)	28(8)	24(7)	5(6)	4(5)	7(6)
C(18')	28(7)	48(10)	25(7)	5(6)	4(5)	1(6)
C(19')	48(9)	69(13)	25(7)	4(8)	2(6)	11(9)
C(20')	51(9)	40(10)	30(8)	-4(7)	9(6)	2(7)
C(21')	49(9)	55(11)	43(9)	-7(8)	20(7)	3(8)
C(22)	53(4)	37(5)	30(4)	-11(3)	5(3)	16(4)
C(23)	85(7)	19(5)	104(8)	-10(5)	-2(6)	1(4)
C(24)	119(9)	62(7)	45(5)	-24(5)	20(5)	11(6)
C(25)	37(3)	17(4)	27(3)	-2(3)	6(3)	0(3)
C(26)	55(4)	18(4)	34(4)	10(3)	11(3)	3(3)
C(27)	63(5)	55(6)	40(4)	11(4)	-6(4)	-17(4)
C(28)	47(4)	61(6)	37(4)	8(4)	14(3)	17(4)
C(29)	35(7)	18(7)	22(6)	1(5)	11(5)	5(5)
C(30)	39(7)	8(7)	29(7)	-3(5)	16(5)	2(5)
C(31)	39(8)	34(9)	33(8)	-2(6)	18(6)	-6(6)
C(32)	54(9)	26(8)	26(7)	-2(6)	10(6)	4(6)
C(33)	45(8)	29(8)	27(7)	6(6)	1(6)	-2(6)

C(29')	54(9)	24(8)	19(6)	7(5)	-7(6)	-13(6)
C(30')	47(8)	13(7)	44(8)	3(6)	-18(6)	5(6)
C(31')	35(8)	60(12)	41(9)	-12(8)	-5(6)	7(8)
C(32')	49(9)	33(9)	40(8)	-1(7)	-5(7)	6(7)
C(33')	47(8)	26(8)	35(8)	10(6)	12(6)	6(6)
C(34)	55(4)	25(4)	21(3)	2(3)	3(3)	2(3)
C(35)	39(4)	54(6)	60(5)	-2(4)	19(4)	-6(4)
C(36)	82(6)	62(6)	23(4)	-12(4)	6(4)	-5(5)

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

	x	y	z	U(eq)
Mo(1)	6071(1)	8929(1)	11071(1)	23(1)
N(1)	5334(2)	8235(2)	10485(2)	25(1)
Si(1)	7295(1)	7705(1)	12295(1)	29(1)
F(1)	9332(3)	6526(3)	13433(3)	135(2)
O(1)	10001(3)	4993(3)	13995(3)	93(2)
S(1)	9550(1)	5450(1)	14550(1)	38(1)
N(2)	6669(2)	8331(2)	11669(2)	26(1)
C(11)	4529(2)	8580(2)	10358(3)	30(1)
C(12)	3942(3)	8503(2)	10940(3)	33(1)
C(13)	3179(2)	8842(3)	10838(3)	40(1)
C(14)	3023(3)	9253(3)	10117(3)	41(1)
C(15)	3603(3)	9332(3)	9527(3)	36(1)
C(16)	4365(3)	8995(2)	9650(3)	31(1)
C(17)	5423(3)	7353(2)	10273(3)	30(1)
C(18)	6305(2)	7111(3)	10229(3)	35(1)
C(19)	4989(3)	6831(3)	10898(3)	44(1)
C(21)	7518(3)	8276(3)	13227(3)	40(1)
C(31)	8923(3)	6077(3)	13923(3)	58(2)
C(110)	5047(3)	7208(3)	9435(3)	42(1)
C(131)	2543(3)	8759(4)	11493(3)	56(2)
C(151)	3410(3)	9766(3)	8744(3)	52(1)

1.18 Bond lengths [Å] and angles [°] for [**2b**]OTf.

Mo(1)-N(2)	1.715(6)	C(11)-C(12)	1.374(6)
Mo(1)-N(1)	1.936(3)	C(11)-C(16)	1.385(6)
Mo(1)-N(1)#1	1.936(3)	C(12)-C(13)	1.393(6)
Mo(1)-N(1)#2	1.936(3)	C(13)-C(14)	1.397(6)
N(1)-C(17)	1.510(5)	C(13)-C(131)	1.517(6)
N(1)-C(11)	1.466(5)	C(14)-C(15)	1.376(6)
Si(1)-N(2)	1.795(6)	C(15)-C(16)	1.394(6)
Si(1)-C(21)	1.848(4)		
Si(1)-C(21)#1	1.848(4)	C(15)-C(151)	1.518(6)
Si(1)-C(21)#2	1.847(4)	C(17)-C(110)	1.540(6)
F(1)-C(31)	1.289(5)	C(17)-C(18)	1.517(6)
O(1)-S(1)	1.405(4)	C(17)-C(19)	1.527(6)
S(1)-O(1)#1	1.405(4)	C(31)-F(1)#1	1.291(5)
S(1)-O(1)#2	1.406(4)	C(31)-F(1)#2	1.291(5)
S(1)-C(31)	1.801(9)		

N(2)-Mo(1)-N(1)	108.08(10)	O(1)-S(1)-C(31)	103.9(2)
N(2)-Mo(1)-N(1)#1	108.02(10)	O(1)#1-S(1)-C(31)	103.9(2)
N(1)-Mo(1)-N(1)#1	110.84(9)	O(1)#2-S(1)-C(31)	103.9(2)
N(2)-Mo(1)-N(1)#2	108.08(10)	Mo(1)-N(2)-Si(1)	179.94(13)
N(1)-Mo(1)-N(1)#2	110.85(9)	C(12)-C(11)-C(16)	120.0(4)
N(1)#1-Mo(1)-N(1)#2	110.84(9)	C(12)-C(11)-N(1)	120.5(4)
C(17)-N(1)-C(11)	115.6(3)	C(16)-C(11)-N(1)	119.5(4)
C(17)-N(1)-Mo(1)	129.0(3)	C(11)-C(12)-C(13)	121.3(4)
C(11)-N(1)-Mo(1)	114.4(2)	C(14)-C(13)-C(12)	117.8(4)
N(2)-Si(1)-C(21)	107.65(16)	C(14)-C(13)-C(131)	121.8(4)
N(2)-Si(1)-C(21)#1	107.67(16)	C(12)-C(13)-C(131)	120.4(4)
C(21)-Si(1)-C(21)#1	111.22(15)	C(15)-C(14)-C(13)	121.6(4)
N(2)-Si(1)-C(21)#2	107.63(16)	C(14)-C(15)-C(16)	119.3(4)
C(21)-Si(1)-C(21)#2	111.25(15)	C(14)-C(15)-C(151)	120.4(4)
C(21)#1-Si(1)-C(21)#2	111.23(15)	C(16)-C(15)-C(151)	120.3(4)
O(1)-S(1)-O(1)#1	114.47(16)	C(15)-C(16)-C(11)	120.0(4)
O(1)-S(1)-O(1)#2	114.43(16)	N(1)-C(17)-C(110)	108.7(3)
O(1)#1-S(1)-O(1)#2	114.43(16)	N(1)-C(17)-C(18)	111.1(3)

C(110)-C(17)-C(18)	107.7(4)
N(1)-C(17)-C(19)	110.2(3)
C(110)-C(17)-C(19)	109.5(4)
C(18)-C(17)-C(19)	109.7(4)
F(1)#1-C(31)-F(1)#2	105.6(5)
F(1)#1-C(31)-F(1)	105.8(5)
F(1)#2-C(31)-F(1)	105.8(5)
F(1)#1-C(31)-S(1)	113.0(4)
F(1)#2-C(31)-S(1)	113.0(4)
F(1)-C(31)-S(1)	113.1(4)

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	23(1)	23(1)	23(1)	-1(1)	1(1)	-1(1)
N(1)	24(2)	26(2)	25(2)	-4(2)	-2(2)	0(2)
Si(1)	29(1)	29(1)	29(1)	2(1)	-2(1)	2(1)
F(1)	126(4)	142(4)	136(4)	106(3)	4(3)	12(3)
O(1)	104(3)	99(3)	76(3)	-11(3)	14(3)	54(3)
S(1)	38(1)	38(1)	38(1)	4(1)	-4(1)	4(1)
N(2)	26(1)	26(1)	26(1)	1(2)	-1(2)	1(2)
C(11)	28(2)	25(2)	38(3)	-6(2)	-3(2)	-6(2)
C(12)	29(2)	36(2)	35(3)	-3(2)	-2(2)	-4(2)
C(13)	27(2)	41(3)	51(3)	-9(3)	-2(2)	-5(2)
C(14)	25(3)	43(3)	54(3)	-8(2)	-9(2)	2(2)
C(15)	37(3)	28(2)	44(3)	-1(2)	-13(2)	-5(2)
C(16)	31(2)	27(2)	35(3)	-3(2)	-2(2)	-4(2)
C(17)	32(2)	27(2)	31(3)	-4(2)	-5(2)	-3(2)
C(18)	39(3)	25(2)	41(3)	-8(2)	-2(2)	5(2)
C(19)	48(3)	28(3)	54(3)	4(2)	1(2)	-1(2)
C(21)	45(3)	40(3)	34(3)	0(2)	-7(2)	2(2)
C(31)	58(2)	58(2)	58(2)	3(4)	-3(4)	3(4)
C(110)	52(3)	35(3)	39(3)	-6(2)	-15(2)	2(2)
C(131)	34(3)	73(4)	61(3)	-10(3)	7(2)	3(3)
C(151)	51(3)	45(3)	61(4)	7(3)	-19(3)	3(2)

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

	x	y	z	U(eq)
Mo(1)	5283(1)	2027(1)	9563(1)	23(1)
N(1)	4947(2)	1362(1)	9983(2)	28(1)
O(1)	2248(2)	2377(1)	9495(3)	64(1)
S(1)	8352(2)	-923(1)	6752(2)	54(1)

F(1)	9815(6)	-230(2)	6552(6)	141(3)
O(2)	8229(6)	-1284(2)	7483(5)	106(2)
C(5)	9540(18)	-607(8)	7122(8)	83(6)
S(1A)	8500(7)	-723(3)	6502(6)	54(1)
F(1A)	9147(15)	-1095(6)	7990(15)	141(3)
O(2A)	8807(18)	-282(6)	6077(13)	106(2)
C(5A)	9480(60)	-710(30)	7500(30)	83(6)
N(2)	5796(3)	1998(1)	8328(2)	27(1)
F(2)	10406(3)	-879(2)	7172(3)	122(2)
N(3)	6318(2)	2325(1)	10398(2)	26(1)
O(3)	7547(4)	-568(2)	6753(4)	121(2)
F(3)	9417(4)	-363(2)	7926(3)	127(2)
N(4)	4083(2)	2370(1)	9591(2)	28(1)
O(4)	8670(3)	-1157(1)	5947(2)	58(1)
O(5)	3288(3)	937(1)	6786(2)	60(1)
C(11)	5815(3)	1114(1)	10495(3)	30(1)
C(12)	5830(4)	1132(2)	11433(3)	40(1)
C(13)	6638(4)	895(2)	11926(3)	48(1)
C(14)	7444(4)	640(2)	11456(3)	44(1)
C(15)	7445(3)	612(1)	10531(3)	34(1)
C(16)	6618(3)	853(1)	10042(3)	31(1)
C(17)	3846(3)	1091(2)	9975(3)	38(1)
C(18)	4078(4)	527(2)	9931(5)	92(2)
C(19)	3205(4)	1228(2)	10817(3)	67(2)
C(21)	6368(3)	1538(1)	8089(3)	26(1)
C(22)	5787(3)	1116(2)	7820(3)	31(1)
C(23)	6324(3)	675(2)	7599(3)	35(1)
C(24)	7455(3)	673(2)	7619(3)	36(1)
C(25)	8050(3)	1091(2)	7858(3)	35(1)
C(26)	7490(3)	1528(2)	8115(3)	32(1)
C(27)	5562(3)	2342(2)	7520(3)	32(1)
C(28)	6646(3)	2488(2)	7089(3)	43(1)
C(29)	4980(4)	2815(2)	7830(3)	40(1)
C(31)	7425(3)	2336(1)	10069(3)	28(1)
C(32)	8141(3)	1953(2)	10288(3)	32(1)
C(33)	9211(3)	1969(2)	9979(3)	37(1)

C(34)	9523(3)	2373(2)	9439(3)	41(1)
C(35)	8817(3)	2756(2)	9213(3)	36(1)
C(36)	7756(3)	2736(2)	9529(3)	32(1)
C(37)	6146(3)	2585(2)	11308(3)	31(1)
C(38)	4954(3)	2546(2)	11578(3)	36(1)
C(39)	6468(4)	3137(2)	11235(3)	42(1)
C(41)	3061(3)	2617(2)	9632(3)	35(1)
C(42)	3064(3)	3156(2)	9860(3)	31(1)
C(43)	3983(4)	3454(2)	9832(3)	37(1)
C(44)	3940(4)	3952(2)	10078(3)	46(1)
C(45)	2967(4)	4157(2)	10350(3)	51(1)
C(46)	2041(4)	3868(2)	10357(3)	51(1)
C(47)	2080(4)	3372(2)	10104(3)	39(1)
C(61)	3650(4)	879(2)	5867(4)	64(2)
C(62)	3216(5)	392(2)	5539(4)	72(2)
C(63)	2143(5)	370(2)	6030(4)	75(2)
C(64)	2423(4)	595(2)	6939(4)	62(2)
C(110)	3203(3)	1234(2)	9144(3)	49(1)
C(131)	6649(5)	913(2)	12954(3)	71(2)
C(151)	8328(4)	331(2)	10032(3)	50(1)
C(210)	4848(4)	2064(2)	6839(3)	40(1)
C(231)	5684(4)	215(2)	7344(3)	50(1)
C(251)	9282(3)	1088(2)	7829(3)	50(1)
C(310)	6859(3)	2332(2)	12018(3)	43(1)
C(331)	10003(3)	1563(2)	10237(4)	54(1)
C(351)	9189(4)	3198(2)	8659(3)	54(1)

1.21 Bond lengths [Å] and angles [°] for [**2c**]OTf

Mo(1)-N(4)	1.739(3)
Mo(1)-N(1)	1.928(3)
Mo(1)-N(2)	1.935(3)
Mo(1)-N(3)	1.938(3)
N(1)-C(11)	1.463(5)
N(1)-C(17)	1.537(5)
O(1)-C(41)	1.204(5)
S(1)-O(3)	1.371(5)
S(1)-O(4)	1.402(4)
S(1)-O(2)	1.455(7)
S(1)-C(5)	1.77(2)
F(1)-C(5)	1.355(18)
C(5)-F(2)	1.29(2)
C(5)-F(3)	1.362(17)
S(1A)-O(3)	1.301(9)

S(1A)-O(2A)	1.388(17)	C(31)-C(36)	1.395(6)
S(1A)-O(4)	1.435(9)	C(32)-C(33)	1.399(6)
S(1A)-C(5A)	1.89(6)	C(33)-C(34)	1.398(6)
F(1A)-C(5A)	1.32(7)	C(33)-C(331)	1.504(6)
C(5A)-F(3)	1.12(7)	C(34)-C(35)	1.382(6)
C(5A)-F(2)	1.33(7)	C(35)-C(36)	1.393(5)
N(2)-C(21)	1.459(5)	C(35)-C(351)	1.508(6)
N(2)-C(27)	1.531(5)	C(37)-C(310)	1.521(6)
N(3)-C(31)	1.452(5)	C(37)-C(38)	1.528(5)
N(3)-C(37)	1.527(5)	C(37)-C(39)	1.532(6)
N(4)-C(41)	1.422(5)	C(41)-C(42)	1.479(6)
O(5)-C(64)	1.424(6)	C(42)-C(43)	1.384(6)
O(5)-C(61)	1.440(6)	C(42)-C(47)	1.392(6)
C(11)-C(12)	1.385(6)	C(43)-C(44)	1.380(6)
C(11)-C(16)	1.386(5)	C(44)-C(45)	1.380(6)
C(12)-C(13)	1.383(6)	C(45)-C(46)	1.377(7)
C(13)-C(14)	1.393(6)	C(46)-C(47)	1.377(6)
C(13)-C(131)	1.519(6)	C(61)-C(62)	1.486(7)
C(14)-C(15)	1.367(6)	C(62)-C(63)	1.513(7)
C(15)-C(16)	1.400(6)	C(63)-C(64)	1.507(7)
C(15)-C(151)	1.517(6)		
C(17)-C(110)	1.504(6)	N(4)-Mo(1)-N(1)	107.03(13)
C(17)-C(19)	1.523(6)	N(4)-Mo(1)-N(2)	109.17(14)
C(17)-C(18)	1.536(6)	N(1)-Mo(1)-N(2)	109.75(13)
C(21)-C(26)	1.383(5)	N(4)-Mo(1)-N(3)	108.88(14)
C(21)-C(22)	1.392(5)	N(1)-Mo(1)-N(3)	108.37(13)
C(22)-C(23)	1.389(5)	N(2)-Mo(1)-N(3)	113.42(13)
C(23)-C(24)	1.393(6)	C(11)-N(1)-C(17)	115.6(3)
C(23)-C(231)	1.506(6)	C(11)-N(1)-Mo(1)	115.3(2)
C(24)-C(25)	1.379(6)	C(17)-N(1)-Mo(1)	128.5(2)
C(25)-C(26)	1.409(5)	O(3)-S(1)-O(4)	121.0(3)
C(25)-C(251)	1.518(6)	O(3)-S(1)-O(2)	112.1(4)
C(27)-C(29)	1.525(6)	O(4)-S(1)-O(2)	111.3(3)
C(27)-C(210)	1.524(6)	O(3)-S(1)-C(5)	105.5(7)
C(27)-C(28)	1.534(5)	O(4)-S(1)-C(5)	103.8(6)
C(31)-C(32)	1.387(5)	O(2)-S(1)-C(5)	100.2(6)

F(2)-C(5)-F(1)	104.0(14)	C(14)-C(13)-C(131)	120.8(4)
F(2)-C(5)-F(3)	108.4(11)	C(15)-C(14)-C(13)	122.0(4)
F(1)-C(5)-F(3)	102.6(14)	C(14)-C(15)-C(16)	118.9(4)
F(2)-C(5)-S(1)	115.4(14)	C(14)-C(15)-C(151)	121.2(4)
F(1)-C(5)-S(1)	111.8(10)	C(16)-C(15)-C(151)	119.9(4)
F(3)-C(5)-S(1)	113.5(13)	C(11)-C(16)-C(15)	120.1(4)
O(3)-S(1A)-O(2A)	96.3(9)	C(110)-C(17)-C(19)	109.4(4)
O(3)-S(1A)-O(4)	123.7(7)	C(110)-C(17)-N(1)	110.2(3)
O(2A)-S(1A)-O(4)	112.6(9)	C(19)-C(17)-N(1)	110.1(4)
O(3)-S(1A)-C(5A)	110(2)	C(110)-C(17)-C(18)	108.2(4)
O(2A)-S(1A)-C(5A)	99(3)	C(19)-C(17)-C(18)	111.5(4)
O(4)-S(1A)-C(5A)	111(2)	N(1)-C(17)-C(18)	107.3(3)
F(3)-C(5A)-F(1A)	108(4)	C(26)-C(21)-C(22)	120.2(4)
F(3)-C(5A)-F(2)	123(6)	C(26)-C(21)-N(2)	119.6(3)
F(1A)-C(5A)-F(2)	102(5)	C(22)-C(21)-N(2)	120.2(3)
F(3)-C(5A)-S(1A)	114(4)	C(21)-C(22)-C(23)	120.6(4)
F(1A)-C(5A)-S(1A)	102(4)	C(24)-C(23)-C(22)	118.4(4)
F(2)-C(5A)-S(1A)	105(3)	C(24)-C(23)-C(231)	121.6(4)
C(21)-N(2)-C(27)	113.9(3)	C(22)-C(23)-C(231)	120.0(4)
C(21)-N(2)-Mo(1)	115.0(2)	C(25)-C(24)-C(23)	122.2(4)
C(27)-N(2)-Mo(1)	130.4(2)	C(24)-C(25)-C(26)	118.5(4)
C(5)-F(2)-C(5A)	28(3)	C(24)-C(25)-C(251)	121.2(4)
C(31)-N(3)-C(37)	115.0(3)	C(26)-C(25)-C(251)	120.2(4)
C(31)-N(3)-Mo(1)	114.2(2)	C(21)-C(26)-C(25)	120.1(4)
C(37)-N(3)-Mo(1)	130.6(2)	C(29)-C(27)-C(210)	109.4(4)
S(1A)-O(3)-S(1)	29.1(3)	C(29)-C(27)-N(2)	110.5(3)
C(5A)-F(3)-C(5)	27(3)	C(210)-C(27)-N(2)	109.1(3)
C(41)-N(4)-Mo(1)	175.7(3)	C(29)-C(27)-C(28)	109.1(3)
S(1)-O(4)-S(1A)	27.4(3)	C(210)-C(27)-C(28)	110.5(3)
C(64)-O(5)-C(61)	108.5(4)	N(2)-C(27)-C(28)	108.4(3)
C(12)-C(11)-C(16)	119.8(4)	C(32)-C(31)-C(36)	120.7(4)
C(12)-C(11)-N(1)	120.3(4)	C(32)-C(31)-N(3)	120.3(4)
C(16)-C(11)-N(1)	119.9(4)	C(36)-C(31)-N(3)	119.0(3)
C(11)-C(12)-C(13)	120.8(4)	C(31)-C(32)-C(33)	120.1(4)
C(12)-C(13)-C(14)	118.4(4)	C(32)-C(33)-C(34)	118.2(4)
C(12)-C(13)-C(131)	120.8(4)	C(32)-C(33)-C(331)	120.4(4)

C(34)-C(33)-C(331)	121.4(4)	C(43)-C(42)-C(47)	118.9(4)
C(35)-C(34)-C(33)	122.3(4)	C(43)-C(42)-C(41)	123.6(4)
C(34)-C(35)-C(36)	118.7(4)	C(47)-C(42)-C(41)	117.5(4)
C(34)-C(35)-C(351)	121.1(4)	C(44)-C(43)-C(42)	120.8(4)
C(36)-C(35)-C(351)	120.2(4)	C(43)-C(44)-C(45)	119.7(5)
C(31)-C(36)-C(35)	120.0(4)	C(46)-C(45)-C(44)	120.0(4)
C(310)-C(37)-N(3)	108.7(3)	C(45)-C(46)-C(47)	120.5(4)
C(310)-C(37)-C(38)	109.9(3)	C(46)-C(47)-C(42)	120.1(4)
N(3)-C(37)-C(38)	109.8(3)	O(5)-C(61)-C(62)	106.7(4)
C(310)-C(37)-C(39)	109.1(3)	C(61)-C(62)-C(63)	101.0(4)
N(3)-C(37)-C(39)	109.8(3)	C(64)-C(63)-C(62)	102.5(4)
C(38)-C(37)-C(39)	109.5(3)	O(5)-C(64)-C(63)	106.3(5)
O(1)-C(41)-N(4)	118.7(4)		
O(1)-C(41)-C(42)	123.9(4)		
N(4)-C(41)-C(42)	117.4(4)		

Symmetry transformations used to generate equivalent atoms

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	17(1)	25(1)	26(1)	0(1)	1(1)	0(1)
N(1)	22(2)	29(2)	33(2)	-3(2)	1(2)	-1(1)
O(1)	20(2)	55(2)	119(3)	-7(2)	-4(2)	0(2)
S(1)	48(1)	56(2)	58(2)	-12(1)	8(1)	8(1)
F(1)	138(6)	81(4)	206(7)	-16(4)	45(5)	-44(4)
O(2)	149(6)	73(4)	97(5)	8(4)	68(4)	-1(4)
C(5)	74(6)	86(11)	87(13)	-47(11)	-25(11)	23(7)
S(1A)	48(1)	56(2)	58(2)	-12(1)	8(1)	8(1)
F(1A)	138(6)	81(4)	206(7)	-16(4)	45(5)	-44(4)
O(2A)	149(6)	73(4)	97(5)	8(4)	68(4)	-1(4)
C(5A)	74(6)	86(11)	87(13)	-47(11)	-25(11)	23(7)
N(2)	25(2)	27(2)	29(2)	1(2)	-3(2)	-1(1)
F(2)	62(2)	154(4)	149(4)	-75(3)	-41(2)	26(2)
N(3)	18(2)	31(2)	29(2)	-2(2)	2(2)	-2(1)
O(3)	85(3)	134(4)	144(5)	-74(4)	-34(3)	65(3)

F(3)	145(4)	130(3)	107(3)	-74(3)	-53(3)	45(3)
N(4)	23(2)	31(2)	30(2)	1(2)	1(2)	-1(2)
O(4)	55(2)	57(2)	62(2)	-20(2)	1(2)	9(2)
O(5)	56(2)	61(2)	64(3)	-2(2)	-9(2)	-6(2)
C(11)	32(2)	23(2)	35(3)	3(2)	-2(2)	-3(2)
C(12)	51(3)	39(3)	30(3)	-1(2)	1(2)	7(2)
C(13)	63(3)	46(3)	34(3)	5(2)	-10(3)	6(3)
C(14)	49(3)	31(3)	51(3)	4(2)	-18(3)	7(2)
C(15)	32(2)	25(2)	46(3)	1(2)	-8(2)	-2(2)
C(16)	34(2)	28(2)	31(2)	-3(2)	2(2)	-5(2)
C(17)	25(2)	31(2)	58(3)	7(2)	4(2)	-9(2)
C(18)	42(3)	32(3)	202(8)	5(4)	-16(4)	-11(3)
C(19)	37(3)	117(5)	46(3)	20(3)	14(3)	-7(3)
C(21)	25(2)	31(2)	21(2)	-1(2)	1(2)	4(2)
C(22)	27(2)	37(2)	28(2)	-1(2)	-1(2)	1(2)
C(23)	43(3)	33(2)	30(3)	-4(2)	-4(2)	3(2)
C(24)	38(3)	40(3)	31(3)	-4(2)	6(2)	10(2)
C(25)	29(2)	45(3)	30(3)	4(2)	5(2)	8(2)
C(26)	33(3)	35(2)	29(2)	-4(2)	2(2)	-2(2)
C(27)	33(2)	35(2)	28(2)	2(2)	0(2)	-1(2)
C(28)	45(3)	47(3)	36(3)	9(2)	8(2)	-3(2)
C(29)	50(3)	34(2)	34(3)	10(2)	3(2)	7(2)
C(31)	20(2)	34(2)	30(2)	-7(2)	-1(2)	-5(2)
C(32)	28(2)	36(2)	33(3)	-10(2)	-4(2)	0(2)
C(33)	24(2)	42(3)	43(3)	-19(2)	-4(2)	1(2)
C(34)	20(2)	54(3)	50(3)	-21(3)	3(2)	-5(2)
C(35)	33(3)	42(3)	33(3)	-8(2)	5(2)	-12(2)
C(36)	25(2)	36(2)	34(3)	-7(2)	0(2)	-1(2)
C(37)	26(2)	39(2)	28(2)	-6(2)	3(2)	-5(2)
C(38)	32(2)	43(3)	33(3)	-5(2)	3(2)	-3(2)
C(39)	37(3)	44(3)	44(3)	-17(2)	4(2)	-6(2)
C(41)	19(2)	45(3)	40(3)	7(2)	4(2)	6(2)
C(42)	29(2)	34(2)	31(3)	3(2)	1(2)	8(2)
C(43)	42(3)	35(3)	34(3)	-2(2)	4(2)	8(2)
C(44)	53(3)	41(3)	43(3)	7(2)	3(2)	1(2)
C(45)	74(4)	39(3)	39(3)	2(2)	8(3)	20(3)

C(46)	50(3)	61(3)	41(3)	4(3)	11(2)	25(3)
C(47)	36(3)	52(3)	30(3)	4(2)	5(2)	9(2)
C(61)	56(3)	62(4)	73(4)	4(3)	3(3)	5(3)
C(62)	82(4)	67(4)	67(4)	-14(3)	-18(3)	14(3)
C(63)	72(4)	64(4)	88(5)	3(3)	-25(4)	-16(3)
C(64)	62(4)	48(3)	75(4)	7(3)	-5(3)	-5(3)
C(110)	29(3)	60(3)	59(3)	-17(3)	1(2)	-13(2)
C(131)	107(5)	71(4)	36(3)	4(3)	-13(3)	25(3)
C(151)	38(3)	50(3)	63(3)	-5(3)	-2(2)	9(2)
C(210)	43(3)	42(3)	36(3)	3(2)	-5(2)	6(2)
C(231)	53(3)	36(3)	61(3)	-8(2)	-4(3)	3(2)
C(251)	31(3)	61(3)	59(3)	-4(3)	4(2)	9(2)
C(310)	35(3)	59(3)	33(3)	-7(2)	-6(2)	-2(2)
C(331)	30(3)	60(3)	71(4)	-25(3)	-7(2)	9(2)
C(351)	45(3)	62(3)	55(3)	-3(3)	19(3)	-16(3)

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

	x	y	z	U(eq)
Mo(1)	3636(1)	2970(1)	2693(1)	27(1)
N(1)	3895(4)	1556(4)	1918(3)	33(1)
N(2)	3034(3)	2745(4)	3895(3)	29(1)
N(3)	2931(4)	4409(4)	2077(3)	33(1)
N(4)	5131(4)	3439(4)	2991(3)	35(1)
C(11)	2931(5)	1426(5)	1223(4)	34(1)
C(12)	2994(5)	1906(5)	367(3)	35(1)
C(13)	2051(5)	1759(5)	-308(4)	41(1)
C(14)	1050(5)	1113(5)	-98(4)	43(1)
C(15)	969(5)	617(6)	770(4)	45(1)
C(16)	1919(5)	777(5)	1433(4)	36(1)
C(17)	4970(5)	767(5)	1842(4)	37(1)
C(18)	5470(5)	448(6)	2793(4)	51(2)
C(19)	5914(5)	1425(6)	1343(4)	48(1)
C(21)	2179(4)	1750(5)	3860(3)	32(1)
C(22)	980(4)	1969(5)	3608(3)	34(1)
C(23)	155(5)	1049(5)	3564(4)	39(1)
C(24)	540(5)	-131(5)	3769(4)	44(2)
C(25)	1729(5)	-384(5)	4033(4)	38(1)
C(26)	2538(5)	574(5)	4070(4)	35(1)

C(27)	3379(5)	3248(4)	4820(3)	34(1)
C(28)	4269(8)	2445(7)	5336(5)	89(3)
C(29)	2256(7)	3414(7)	5332(5)	74(2)
C(31)	1654(5)	4452(5)	2122(3)	33(1)
C(32)	1150(5)	5118(5)	2817(4)	39(1)
C(33)	-58(5)	5138(5)	2899(5)	47(2)
C(34)	-801(5)	4488(5)	2259(4)	40(1)
C(35)	-339(5)	3820(5)	1573(4)	41(1)
C(36)	891(5)	3805(5)	1523(4)	34(1)
C(37)	3533(5)	5516(5)	1739(4)	38(1)
C(38)	4543(5)	5092(6)	1165(4)	52(2)
C(39)	2629(6)	6262(6)	1109(5)	55(2)
C(41)	6224(5)	3758(7)	3234(5)	48(2)
C(110)	4609(5)	-409(5)	1339(5)	51(2)
C(131)	2148(6)	2277(6)	-1238(4)	56(2)
C(151)	-100(6)	-106(7)	998(5)	61(2)
C(210)	3917(6)	4489(6)	4721(4)	51(2)
C(231)	-1150(5)	1293(6)	3314(6)	61(2)
C(251)	2130(6)	-1654(5)	4267(6)	62(2)
C(310)	4042(6)	6300(6)	2515(4)	52(2)
C(331)	-590(6)	5833(7)	3648(5)	61(2)
C(351)	-1173(5)	3128(8)	898(4)	56(2)

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

Mo(1)-N(4)	1.777(4)	C(17)-C(110)	1.535(8)
Mo(1)-N(2)	1.963(4)	C(21)-C(26)	1.388(8)
Mo(1)-N(3)	1.968(4)	C(21)-C(22)	1.388(7)
Mo(1)-N(1)	1.971(4)	C(22)-C(23)	1.373(8)
N(1)-C(11)	1.441(7)	C(23)-C(24)	1.399(8)
N(1)-C(17)	1.498(7)	C(23)-C(231)	1.506(8)
N(2)-C(21)	1.458(6)	C(24)-C(25)	1.390(8)
N(2)-C(27)	1.497(6)	C(25)-C(26)	1.392(8)
N(3)-C(31)	1.439(7)	C(25)-C(251)	1.505(8)
N(3)-C(37)	1.501(7)	C(27)-C(28)	1.500(9)
N(4)-C(41)	1.300(7)	C(27)-C(210)	1.509(8)
C(11)-C(12)	1.378(8)	C(27)-C(29)	1.529(8)
C(11)-C(16)	1.397(8)	C(31)-C(36)	1.383(7)
C(12)-C(13)	1.407(7)	C(31)-C(32)	1.415(8)
C(13)-C(14)	1.385(8)	C(32)-C(33)	1.369(8)
C(13)-C(131)	1.500(8)	C(33)-C(34)	1.408(9)
C(14)-C(15)	1.404(9)	C(33)-C(331)	1.507(9)
C(15)-C(16)	1.402(8)	C(34)-C(35)	1.386(8)
C(15)-C(151)	1.500(9)	C(35)-C(36)	1.388(8)
C(17)-C(18)	1.515(8)	C(35)-C(351)	1.520(9)
C(17)-C(19)	1.521(8)	C(37)-C(310)	1.514(8)
		C(37)-C(38)	1.538(8)
		C(37)-C(39)	1.558(8)

N(4)-Mo(1)-N(2)	101.27(18)	N(2)-Mo(1)-N(1)	120.10(18)
N(4)-Mo(1)-N(3)	102.56(18)	N(3)-Mo(1)-N(1)	116.33(18)
N(2)-Mo(1)-N(3)	111.50(17)	C(11)-N(1)-C(17)	116.9(4)
N(4)-Mo(1)-N(1)	101.36(19)	C(11)-N(1)-Mo(1)	110.9(3)

C(17)-N(1)-Mo(1)	131.3(3)	C(22)-C(23)-C(231)	121.2(5)
C(21)-N(2)-C(27)	115.8(4)	C(24)-C(23)-C(231)	119.9(5)
C(21)-N(2)-Mo(1)	109.5(3)	C(25)-C(24)-C(23)	121.5(5)
C(27)-N(2)-Mo(1)	134.1(3)	C(24)-C(25)-C(26)	117.8(5)
C(31)-N(3)-C(37)	117.6(4)	C(24)-C(25)-C(251)	121.0(5)
C(31)-N(3)-Mo(1)	111.8(3)	C(26)-C(25)-C(251)	121.2(5)
C(37)-N(3)-Mo(1)	129.5(3)	C(21)-C(26)-C(25)	121.7(5)
C(41)-N(4)-Mo(1)	178.0(4)	N(2)-C(27)-C(28)	111.1(4)
C(12)-C(11)-C(16)	120.1(5)	N(2)-C(27)-C(210)	109.0(4)
C(12)-C(11)-N(1)	121.8(5)	C(28)-C(27)-C(210)	109.3(5)
C(16)-C(11)-N(1)	118.1(5)	N(2)-C(27)-C(29)	109.3(4)
C(11)-C(12)-C(13)	121.2(5)	C(28)-C(27)-C(29)	111.2(6)
C(14)-C(13)-C(12)	118.6(5)	C(210)-C(27)-C(29)	106.8(5)
C(14)-C(13)-C(131)	121.2(5)	C(36)-C(31)-C(32)	118.1(5)
C(12)-C(13)-C(131)	120.2(5)	C(36)-C(31)-N(3)	121.5(5)
C(13)-C(14)-C(15)	121.0(5)	C(32)-C(31)-N(3)	120.4(5)
C(14)-C(15)-C(16)	119.4(5)	C(33)-C(32)-C(31)	121.7(5)
C(14)-C(15)-C(151)	121.4(5)	C(32)-C(33)-C(34)	118.1(5)
C(16)-C(15)-C(151)	119.2(6)	C(32)-C(33)-C(331)	121.5(6)
C(11)-C(16)-C(15)	119.7(5)	C(34)-C(33)-C(331)	120.4(5)
N(1)-C(17)-C(18)	108.0(4)	C(35)-C(34)-C(33)	121.8(5)
N(1)-C(17)-C(19)	110.6(5)	C(34)-C(35)-C(36)	118.3(5)
C(18)-C(17)-C(19)	109.8(5)	C(34)-C(35)-C(351)	120.1(5)
N(1)-C(17)-C(110)	110.2(4)	C(36)-C(35)-C(351)	121.5(5)
C(18)-C(17)-C(110)	108.5(5)	C(35)-C(36)-C(31)	121.9(5)
C(19)-C(17)-C(110)	109.8(5)	N(3)-C(37)-C(310)	111.6(4)
C(26)-C(21)-C(22)	118.8(5)	N(3)-C(37)-C(38)	107.7(5)
		C(310)-C(37)-C(38)	109.9(5)
C(26)-C(21)-N(2)	121.3(4)	N(3)-C(37)-C(39)	109.9(4)
C(22)-C(21)-N(2)	119.9(4)	C(310)-C(37)-C(39)	109.9(5)
C(23)-C(22)-C(21)	121.3(5)	C(38)-C(37)-C(39)	107.8(5)
C(22)-C(23)-C(24)	118.9(5)		

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Mo(1)	25(1)	34(1)	21(1)	-2(1)	2(1)	-3(1)
N(1)	39(3)	41(2)	18(2)	-12(2)	1(2)	-1(2)
N(2)	29(2)	30(3)	26(2)	0(2)	4(2)	-2(2)
N(3)	33(3)	36(3)	30(3)	3(2)	6(2)	-8(2)
N(4)	32(3)	44(3)	28(2)	-1(2)	5(2)	0(2)
C(11)	34(3)	40(3)	29(3)	-2(2)	2(2)	5(2)
C(12)	40(3)	41(3)	24(3)	-8(2)	1(2)	2(2)
C(13)	49(3)	49(4)	23(3)	-8(2)	-3(2)	2(3)
C(14)	47(3)	53(4)	28(3)	-10(3)	-9(3)	6(3)
C(15)	38(3)	50(4)	46(4)	-11(3)	-1(3)	-4(3)

C(16)	39(3)	35(3)	33(3)	-1(3)	-1(2)	0(2)
C(17)	32(3)	42(3)	36(3)	-2(3)	4(2)	4(2)
C(18)	46(3)	64(4)	43(4)	6(3)	0(3)	11(3)
C(19)	40(3)	63(4)	42(4)	1(3)	9(3)	5(3)
C(21)	33(3)	36(3)	27(3)	0(2)	9(2)	-4(2)
C(22)	32(3)	41(3)	29(3)	3(2)	3(2)	0(2)
C(23)	35(3)	51(4)	30(3)	3(3)	2(2)	-3(3)
C(24)	43(4)	49(4)	42(3)	-3(3)	8(3)	-17(3)
C(25)	40(3)	41(3)	33(3)	2(2)	5(2)	-3(2)
C(26)	33(3)	41(3)	29(3)	1(2)	4(2)	1(2)
C(27)	48(3)	34(4)	20(2)	-1(2)	2(2)	-4(2)
C(28)	137(8)	62(4)	58(5)	-17(4)	-66(5)	17(4)
C(29)	96(5)	88(6)	41(4)	-32(3)	36(4)	-44(4)
C(31)	39(3)	35(3)	25(3)	8(2)	2(2)	1(2)
C(32)	47(3)	40(3)	31(3)	-1(3)	1(2)	-2(2)
C(33)	53(4)	40(3)	50(4)	3(3)	21(3)	9(3)
C(34)	39(3)	38(3)	45(3)	3(3)	9(3)	2(2)
C(35)	37(3)	44(3)	40(3)	8(3)	-1(3)	1(2)
C(36)	39(3)	31(3)	30(3)	2(2)	-1(2)	-2(2)
C(37)	44(3)	43(3)	26(3)	8(2)	2(2)	-12(2)
C(38)	49(4)	67(4)	41(4)	6(3)	11(3)	-17(3)
C(39)	53(4)	53(4)	59(4)	23(3)	-1(3)	-10(3)
C(41)	25(3)	63(5)	55(4)	-4(3)	-1(3)	-11(3)
C(110)	51(4)	36(3)	66(4)	-11(3)	8(3)	10(3)
C(131)	64(4)	70(4)	32(3)	-3(3)	-5(3)	5(3)
C(151)	44(4)	76(5)	62(4)	-2(4)	-7(3)	-16(3)
C(210)	75(4)	54(4)	24(3)	-10(3)	5(3)	-25(3)
C(231)	35(3)	69(5)	80(5)	14(4)	-1(3)	-5(3)
C(251)	60(4)	36(4)	90(5)	6(3)	4(4)	-2(3)
C(310)	67(4)	54(4)	36(3)	-1(3)	6(3)	-25(3)
C(331)	51(4)	72(4)	62(4)	-4(4)	17(3)	6(3)
C(351)	39(3)	64(5)	64(4)	-5(4)	-2(2)	-9(4)

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

	x	y	z	U(eq)
I(1)	-5196(1)	-9804(1)	-196(1)	42(1)
Mo(1)	-10797(1)	-10797(1)	-797(1)	34(1)
N(1)	-10002(2)	-11519(2)	-287(3)	37(1)
Cl(1)	-8759(4)	-11629(4)	2499(3)	171(2)
N(2)	-11401(3)	-11401(3)	-1401(3)	67(3)
C(11)	-9195(3)	-11151(3)	-206(3)	39(1)
C(12)	-8628(3)	-11235(3)	-828(4)	44(1)
C(13)	-7847(4)	-10902(4)	-749(4)	61(2)
C(14)	-7655(4)	-10479(4)	-35(4)	62(2)

C(15)	-8220(4)	-10395(4)	587(4)	55(2)
C(16)	-9001(3)	-10730(4)	505(3)	48(2)
C(17)	-10048(4)	-12429(3)	-132(4)	49(2)
C(18)	-10934(5)	-12681(4)	13(7)	115(4)
C(19)	-9715(4)	-12906(3)	-857(4)	59(2)
C(21)	-11917(4)	-11917(4)	-1917(4)	108(6)
C(22)	-12580(20)	-11449(19)	-2320(20)	160(17)
C(31)	-8479(5)	-11521(5)	3479(5)	115(6)
C(110)	-9559(7)	-12626(4)	633(4)	99(3)
C(131)	-7227(4)	-10985(6)	-1441(4)	84(3)
C(151)	-7980(4)	-9936(5)	1366(4)	86(2)

1.27 Bond lengths [Å] and angles [°] for [**2d**]I.

Mo(1)-N(2)	1.708(9)
Mo(1)-N(1)#1	1.939(4)
Mo(1)-N(1)	1.939(4)
Mo(1)-N(1)#2	1.939(4)
N(1)-C(11)	1.453(6)
N(1)-C(17)	1.508(6)
Cl(1)-C(31)	1.671(8)
N(2)-C(21)	1.457(15)
C(11)-C(12)	1.380(7)
C(11)-C(16)	1.384(8)
C(12)-C(13)	1.391(8)
C(13)-C(14)	1.390(9)
C(13)-C(131)	1.521(9)
C(14)-C(15)	1.378(8)
C(15)-C(16)	1.392(8)
C(15)-C(151)	1.526(9)
C(17)-C(19)	1.517(8)
C(17)-C(110)	1.515(10)
C(17)-C(18)	1.521(9)
C(21)-C(22)	1.48(3)
C(21)-C(22)#2	1.48(3)
C(21)-C(22)#1	1.48(3)
C(31)-Cl(1)#3	1.671(8)
C(31)-Cl(1)#4	1.671(8)
N(2)-Mo(1)-N(1)#1	106.44(12)
N(2)-Mo(1)-N(1)	106.44(12)
N(1)#1-Mo(1)-N(1)	112.32(11)
N(2)-Mo(1)-N(1)#2	106.44(12)
N(1)#1-Mo(1)-N(1)#2	112.32(11)
N(1)-Mo(1)-N(1)#2	112.32(11)
C(11)-N(1)-C(17)	115.8(4)
C(11)-N(1)-Mo(1)	113.2(3)
C(17)-N(1)-Mo(1)	129.6(3)
C(21)-N(2)-Mo(1)	180.0(4)
C(12)-C(11)-C(16)	120.9(5)
C(12)-C(11)-N(1)	119.9(5)
C(16)-C(11)-N(1)	119.2(5)
C(11)-C(12)-C(13)	120.4(6)
C(14)-C(13)-C(12)	118.6(6)
C(14)-C(13)-C(131)	121.0(6)
C(12)-C(13)-C(131)	120.4(7)
C(15)-C(14)-C(13)	121.0(6)
C(14)-C(15)-C(16)	120.1(6)
C(14)-C(15)-C(151)	119.4(6)
C(16)-C(15)-C(151)	120.5(6)
C(11)-C(16)-C(15)	119.0(5)
N(1)-C(17)-C(19)	110.9(4)
N(1)-C(17)-C(110)	108.7(5)
C(19)-C(17)-C(110)	110.2(5)
N(1)-C(17)-C(18)	109.8(4)
C(19)-C(17)-C(18)	108.8(6)
C(110)-C(17)-C(18)	108.4(7)
N(2)-C(21)-C(22)	112.3(12)
N(2)-C(21)-C(22)#2	112.3(12)
C(22)-C(21)-C(22)#2	106.5(13)
N(2)-C(21)-C(22)#1	112.3(12)
C(22)-C(21)-C(22)#1	106.5(13)
C(22)#2-C(21)-C(22)#1	106.5(13)
Cl(1)#3-C(31)-Cl(1)	100.9(6)
Cl(1)#3-C(31)-Cl(1)#4	100.9(6)
Cl(1)-C(31)-Cl(1)#4	100.9(6)

Symmetry transformations used to generate equivalent atoms:
#1 y,z-1,x+1 #2 z-1,x,y+1 #3 -z-1/2,-x-2,y+3/2
#4 -y-2,z-3/2,-x-1/2

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

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
I(1)	42(1)	42(1)	42(1)	2(1)	-2(1)	2(1)
Mo(1)	34(1)	34(1)	34(1)	-3(1)	-3(1)	-3(1)
N(1)	40(3)	32(2)	40(2)	0(2)	6(2)	7(2)
Cl(1)	190(5)	209(6)	115(4)	58(4)	-36(3)	35(5)
N(2)	67(3)	67(3)	67(3)	-14(3)	-14(3)	-14(3)
C(11)	38(3)	32(3)	45(3)	7(3)	0(3)	5(2)
C(12)	46(3)	48(3)	37(3)	4(3)	3(3)	11(3)
C(13)	38(3)	74(4)	69(4)	18(4)	7(3)	10(3)
C(14)	35(3)	83(5)	69(5)	16(4)	-13(3)	-6(3)
C(15)	56(4)	62(4)	46(4)	9(3)	-13(3)	9(3)
C(16)	44(4)	46(3)	54(4)	7(3)	0(3)	13(3)
C(17)	68(4)	27(3)	52(3)	5(3)	12(3)	10(2)
C(18)	94(6)	30(3)	220(12)	25(5)	63(7)	-1(4)
C(19)	87(5)	37(3)	54(4)	0(3)	2(4)	4(3)
C(21)	108(6)	108(6)	108(6)	-42(4)	-42(4)	-42(4)
C(22)	150(30)	120(20)	210(40)	10(20)	-150(30)	-50(20)
C(31)	115(6)	115(6)	115(6)	-37(5)	37(5)	37(5)
C(110)	202(11)	36(4)	60(4)	12(3)	-15(6)	14(5)
C(131)	39(4)	144(8)	70(5)	29(5)	12(3)	13(4)
C(151)	71(5)	106(7)	80(5)	-20(5)	-28(4)	-7(4)

2 Density Functional Theory calculations

2.1 Representative input file for $^{15}NMo(NH_2)_3$, 1-m

```
#! /bin/sh

nohup $ADFBIN/adf <<EOR > adf.out
Title NMo_nh2_3

SYMMETRY nosym

ATOMS
 N     0.000000     0.000000     0.000000
Mo     0.000000     0.000000     1.660000
 N     1.912533     0.000000     2.172462
 N    -0.956267     1.656302     2.172462
 N    -0.956267    -1.656302     2.172462
 H    -1.378108     2.234788     1.462907
 H    -1.021252     1.921025     3.142906
 H     2.624437     0.076083     1.462907
 H     2.174282    -0.076083     3.142906
 H    -1.246329    -2.310871     1.462907
 H    -1.153031    -1.844942     3.142906
END

BASIS
  type TZ2P
  core none
END

GEOMETRY
  sp
END
RELATIVISTIC ZORA SpinOrbit

charge 0

XC
  LDA VWN
  GGA Becke Perdew
END

SCF
  DIIS
END

end input
EOR
```

2.2 Optimized geometry for $^{15}NMo(NH_2)_3$, 1m

```
N         0.000273   -0.000374    0.011827
Mo       -0.000112    0.000273    1.663469
N         1.904387    0.001685    2.159868
N        -0.955178    1.648290    2.159832
```

N	-0.948821	-1.651117	2.160007
H	-1.338378	2.317686	1.496960
H	-1.111237	1.966529	3.116064
H	2.675064	-0.002888	1.497448
H	2.257033	-0.022920	3.116079
H	-1.337223	-2.317045	1.496870
H	-1.143554	-1.946794	3.116252

2.3 Optimized geometry for $F_3BNMo(NH_2)_3$, 1m-BF_3

N	0.055495	0.007750	-0.002036
Mo	0.014467	0.000346	1.668265
N	-0.938570	-1.633336	2.138379
N	1.890153	0.000863	2.195411
N	-0.941169	1.631122	2.141964
H	-1.307640	2.299598	1.463613
H	-1.127416	1.938423	3.097018
H	2.668475	0.015517	1.537721
H	2.225972	-0.023338	3.158685
H	-1.310270	-2.300994	1.465841
H	-1.142815	-1.925394	3.094738
B	0.121545	0.061459	-1.684336
F	-0.532909	-1.086355	-2.091417
F	-0.541676	1.230918	-2.011937
F	1.470440	0.074212	-1.970352

2.4 Optimized geometry for $Cl_3BNMo(NH_2)_3$, 1m-BCl_3

N	1.856833	0.013810	2.142056
Mo	-0.025622	0.000975	1.658484
N	-0.003417	0.013894	-0.022729
B	0.017057	0.023563	-1.575637
Cl	-0.852866	-1.528951	-2.085917
N	-0.958547	-1.647112	2.095398
N	-0.992537	1.622956	2.120111
Cl	-0.884369	1.563417	-2.068912
Cl	1.809448	0.044282	-2.039936
H	-1.195106	1.932316	3.071591
H	-1.365918	2.277411	1.433577
H	2.216841	0.010418	3.097216
H	2.616805	0.027227	1.462452
H	-1.152840	-1.975766	3.042116
H	-1.320506	-2.297174	1.398619

2.5 Optimized geometry for $Cl_2GeNMo(NH_2)_3$, 1m-$GeCl_2$

N	-0.022949	-0.004136	-0.088800
Mo	0.011369	-0.063509	1.579132
Ge	-0.069608	0.046318	-2.251946
N	1.913421	-0.072831	2.000406
N	-0.918341	1.539364	2.211796
N	-0.911241	-1.720499	2.030103
H	2.645265	-0.078075	1.288222
H	2.312484	-0.117016	2.937949
H	-1.337200	2.259385	1.627844

H	-1.045218	1.765189	3.199206
H	-1.273365	-2.376245	1.336611
H	-1.057547	-2.071485	2.976756
Cl	2.181962	-0.284597	-2.370218
Cl	-0.859892	-2.083020	-2.393800

2.6 Optimized geometry for $Cl_2SnNMo(NH_2)_3$, 1m-$SnCl_2$

N	-0.038458	-0.011444	-0.015785
Mo	0.011478	-0.061378	1.650534
Sn	-0.100824	0.100367	-2.364838
N	1.917010	-0.065721	2.057303
N	-0.921311	1.547179	2.265199
N	-0.899743	-1.720955	2.118474
H	2.639607	-0.076642	1.341929
H	2.323608	-0.107213	2.991527
H	-1.347381	2.252689	1.665470
H	-1.046961	1.793486	3.247350
H	-1.259866	-2.376183	1.430648
H	-1.039955	-2.071784	3.065891
Cl	2.321613	-0.285994	-2.393610
Cl	-0.933213	-2.205652	-2.451313

2.7 Optimized geometry for $[CH_3NMo(NH_2)_3]^+$, [2a-m]

N	-0.013631	0.027029	0.068536
Mo	0.006004	-0.005736	1.768658
N	-0.882425	1.603491	2.358478
N	1.872727	-0.052408	2.256183
N	-0.946544	-1.609842	2.262356
C	-0.008810	0.015270	-1.364944
H	-0.550994	-0.870484	-1.725931
H	-0.498680	0.923492	-1.743952
H	1.028584	-0.018969	-1.727635
H	2.664490	-0.066032	1.613458
H	2.200365	-0.065857	3.225793
H	-1.282964	2.340504	1.779276
H	-1.005327	1.824483	3.351333
H	-1.359898	-2.289497	1.623846
H	-1.103059	-1.892110	3.233608

2.8 Optimized geometry for $[(CH_3)_3SiNMo(NH_2)_3]^+$, [2b-m]

N	0.0017	0.0017	0.0057
N	-0.9267	-1.6058	2.2509
N	1.8538	-0.0001	2.2522
N	-0.9277	1.6053	2.2515
Mo	0.0001	0.0001	1.7022
H	-1.3360	2.2976	1.6245
H	-1.0637	1.8820	3.2267
H	2.6580	0.0080	1.6258
H	2.1607	-0.0230	3.2275
H	-1.3218	-2.3060	1.6242
H	-1.0990	-1.8612	3.2261
H	1.9097	0.0327	-3.3935

H	2.3403	0.9130	-1.9134
H	2.3443	-0.8748	-1.9311
H	-0.9233	-1.6196	-3.4186
H	-0.3792	-2.4560	-1.9505
H	-1.9282	-1.5635	-1.9566
H	-0.9407	1.6589	-3.3947
H	-1.9360	1.5828	-1.9268
H	-0.3893	2.4797	-1.9207
Si	0.0087	0.0125	-1.8270
C	-0.8912	-1.5567	-2.3193
C	-0.9013	1.5832	-2.2964
C	1.8240	0.0216	-2.2953

2.9 Optimized geometry for $[PhC(O)NMo(NH_2)_3]^+$, [2c-m]

N	0.006488	-0.031329	-0.031230
Mo	-0.046566	0.010830	1.673002
N	-1.020312	1.599339	2.155442
N	-0.935293	-1.602091	2.234423
N	1.799633	0.078068	2.245918
H	-1.399579	2.291733	1.506786
H	-1.176526	1.888064	3.125143
H	-1.273449	-2.326754	1.599284
H	-1.206577	-1.811033	3.198749
H	2.597641	0.254694	1.635004
H	2.098413	0.034847	3.223086
O	-0.808032	0.522041	-2.098564
C	0.041318	-0.097053	-1.506359
C	1.120792	-0.929996	-2.050439
C	1.197294	-1.041195	-3.453566
C	2.205645	-1.805356	-4.028301
C	3.145352	-2.453397	-3.217204
C	3.071785	-2.349041	-1.824411
C	2.058087	-1.597985	-1.238761
H	0.462881	-0.524447	-4.067591
H	2.264188	-1.896159	-5.111712
H	3.937463	-3.044539	-3.672437
H	3.802447	-2.854809	-1.196411
H	1.996506	-1.530713	-0.153598

2.10 Optimized geometry for $H_2CNMo(N[CH_3]Ph)_3$, 3m-C_3

C	-0.077798	-0.257055	-0.038200
C	-0.031999	-0.266111	1.357612
C	1.196032	-0.215979	2.022227
C	2.397091	-0.137091	1.296317
C	2.341596	-0.145010	-0.108812
C	1.114180	-0.203656	-0.769349
N	3.649450	-0.024830	1.976530
C	4.408522	-1.266709	2.125422
H	3.783652	-2.060915	2.572254
H	-0.953355	-0.307249	1.934987
H	1.085788	-0.194670	-1.857172
Mo	4.196791	1.793376	2.566630
N	3.906512	3.338402	1.351623
C	2.678616	4.053519	1.492425
C	2.655306	5.338405	2.073518

C	1.452262	6.012970	2.264934
C	0.242117	5.424285	1.879087
C	0.254899	4.157211	1.294443
C	1.460779	3.477763	1.095909
H	1.456683	6.999378	2.728970
H	-0.678053	3.693222	0.976784
C	4.972265	4.071132	0.655715
H	5.849984	3.427178	0.572071
H	5.272142	4.996058	1.169654
H	4.635766	4.344882	-0.357539
N	3.946981	2.304822	4.453100
C	2.687282	1.915718	5.012771
C	1.515200	2.633063	4.726838
C	0.280895	2.199749	5.219961
C	0.201841	1.059652	6.021163
C	1.369400	0.351176	6.331218
C	2.599806	0.774752	5.833550
H	-0.618805	2.764296	4.979452
H	1.317429	-0.540888	6.954515
C	4.884392	2.935050	5.384884
H	5.063941	2.314298	6.277737
H	5.839980	3.102506	4.876756
H	4.491828	3.908252	5.727739
N	5.974661	1.703245	2.544632
C	7.270734	1.601269	2.578634
H	5.269914	-1.095308	2.783988
H	4.784256	-1.634983	1.152866
H	3.589806	5.792541	2.401914
H	7.893169	2.487155	2.736733
H	-0.697735	5.954755	2.029670
H	1.578281	3.532683	4.114427
H	7.756901	0.631275	2.435788
H	3.508289	0.213250	6.053851
H	1.467995	2.498356	0.618149
H	-0.760666	0.722790	6.406168
H	1.237377	-0.221393	3.112327
H	3.272657	-0.078260	-0.671586
H	-1.036140	-0.288964	-0.555934

2.11 Optimized geometry for $H_2CNMo(N[CH_3]Ph)_3$, 3m-C_s

N	0.0150	-0.2453	0.1226
N	-0.6464	1.3580	-2.2606
N	-0.0782	-1.8161	-2.3580
N	2.4391	0.2599	-1.7866
C	0.0065	-0.2773	1.4173
C	-0.4002	1.8949	-3.6083
C	-1.7724	1.9172	-1.5765
C	-1.5803	2.9769	-0.6789
C	-2.6575	3.5174	0.0232
C	-3.9461	3.0113	-0.1647
C	-4.1476	1.9667	-1.0716
C	-3.0696	1.4254	-1.7759
C	-1.1195	-2.6814	-1.7854
C	0.1379	-1.9925	-3.7671
C	1.3452	-2.5334	-4.2386

C	1.5752	-2.6874	-5.6076
C	0.6032	-2.3018	-6.5338
C	-0.6067	-1.7715	-6.0776
C	-0.8407	-1.6237	-4.7097
C	3.4590	-0.7907	-1.7309
C	2.9031	1.5991	-1.8239
C	3.8055	2.0443	-2.8105
C	4.1895	3.3837	-2.8681
C	3.6873	4.3097	-1.9477
C	2.8060	3.8747	-0.9555
C	2.4272	2.5336	-0.8857
H	0.9295	-0.1563	1.9955
H	-0.9359	-0.4230	1.9558
H	0.4598	1.3821	-4.0634
H	-1.2708	1.7536	-4.2698
H	-0.1648	2.9699	-3.5652
H	-2.4905	4.3355	0.7241
H	-5.1508	1.5632	-1.2313
H	-1.1224	-2.5531	-0.6992
H	-2.1267	-2.4405	-2.1654
H	-0.9137	-3.7369	-2.0239
H	-1.3697	-1.4643	-6.7925
H	2.5170	-3.1145	-5.9525
H	2.9711	-1.7583	-1.5649
H	4.0356	-0.8644	-2.6667
H	4.1647	-0.6170	-0.9023
H	2.4235	4.5785	-0.2164
H	4.8767	3.7105	-3.6485
H	3.9861	5.3557	-2.0000
H	1.7695	2.1853	-0.0885
H	4.1828	1.3394	-3.5512
H	2.0984	-2.8397	-3.5148
H	-1.7846	-1.2072	-4.3586
H	0.7873	-2.4125	-7.6017
H	-4.7859	3.4277	0.3925
H	-0.5715	3.3610	-0.5359
H	-3.2246	0.6057	-2.4784
Mo	0.4881	-0.0833	-1.6129

2.12 Optimized geometry for $[CH_3CH_2NMo(NH_2)_3]^+$, [2d-m]

N	1.828992	0.014545	2.192469
Mo	-0.024516	0.002681	1.649339
N	-0.975190	1.599082	2.175734
N	-0.000183	0.024315	-0.050127
C	0.018116	0.022853	-1.493189
N	-0.945444	-1.621518	2.144071
H	-1.143728	1.850535	3.153539
H	-1.372914	2.303171	1.554912
H	2.125367	0.004047	3.172005
H	2.641797	0.032342	1.575949
H	-1.111932	-1.893430	3.116751
H	-1.328375	-2.321985	1.510154
H	0.168822	1.065735	-1.816932
H	0.903383	-0.555182	-1.805091
C	-1.266512	-0.563805	-2.087278

```
H        -1.192794   -0.528779   -3.181505
H        -1.400460   -1.609237   -1.784602
H        -2.144518    0.016278   -1.779343
```

2.13 NMR calculations: Representative input and output files

```
NMR
  OUT iso tens refs info
  CALC all
  U1K best
  NUC 1
  MAXMEMORYUSAGE 960
  ANALYSIS
END

End Input

 *******************************************************************************
 *                                                                             *
 *  -------------------------------------                                      *
 *   Amsterdam Density Functional  (ADF)        2002.03   6 December, 2002    *
 *  -------------------------------------                                      *
 *                                                                             *
 *                                                                             *
 *                             =================                               *
 *                             |               |                               *
 *                             |     N M R     |                               *
 *                             |               |                               *
 *                             =================                               *
 *                                                                             *
 *                                                                             *
 *   Online information and documentation:  http://www.scm.com                 *
 *   E-mail:  support@scm.com   info@scm.com                                   *
 *                                                                             *
 *   Scientific publications using ADF results must be properly referenced     *
 *   See the User Manuals (or the web site) for recommended citations          *
 *                                                                             *
 *****************************  pentium_linux  ******************************

                     **********************************
                     ||******************************||
                     ||                              ||
                     ||  ##   ##  ###  ###  ######   ||
                     ||  ###  ##  ########  ##   ##  ||
                     ||  #### ##  ## ## ##  ######   ||
                     ||  ## ####  ##    ##  ## ##    ||
                     ||  ##  ###  ##    ##  ##  ##   ||
                     ||  ##   ##  ##    ##  ##   ##  ||
                     ||                              ||
                     | ****************************** |
                     **********************************

                           Written for ADF by

                   Stephen K. Wolff & Georg Schreckenbach

                     The research group of Tom Ziegler
                   University of Calgary, Alberta, Canada
                   ---------------------------------------
                            Date last modified:
                            18 June, 1999 (GS)
                                References:
                                ===========

                   1. G. Schreckenbach and T. ZIegler,
                      J. Phys. Chem. 99 (1995) 606
```

```
                  2. G. Schreckenbach and T. Ziegler
                     Int. J. Quantum CHem. 61 (1997) 899

                  3. S. K. Wolff and T. Ziegler
                     J. Chem. Phys. 109 (1998) 895

                  ---------------------------------------


################################################################################


=== INFO:

NMR was mostly written by S. K. Wolff and G. Schreckenbach in
the research group of T. Zielger at the University of Calgary
for the Amsterdam Density Functional package.

Schreckenbach and Ziegler developed a GIAO-DFT formulation for
calculating NMR shielding tensors, with the incorporation
a frozen core approximation.  This formulation was extended by
Wolff to include spin-orbit coupling.  This program is based
on those formulations.

--- REF: G. Schreckenbach and T. Ziegler
         J. Int. J. Quantum Chem. 61 (1997) 899.

--- REF: G. Schreckenbach and T. Ziegler
         J. Phys. Chem. 99 (1995) 606.

--- REF: S. K. Wolff and T. Ziegler
         J. Chem. Phys. 109 (1998) 895.


################################################################################

              <><><><><><><><><><><><><><><><><><><><><><><><><>

                 GENERAL ADF INFORMATION:
                 ------------------------

                 TITLE:    NMo_nh2_3
                 JOB ID:   ADF 2002.03  RunTime: Jul08-2003 15:29:58
                 NONLXC:   Becke88 Perdew86
                 SYMMETRY: NOSYM

                 IOPREL:   3
                 ------>  Scalar ZORA + core pot. (Re MOs)
                 ------>  Core pot used in K, Full pot used in V

              <><><><><><><><><><><><><><><><><><><><><><><><><>

              ==================================================

                 NUCLEAR COORDINATES (ANGSTROMS):
                 --------------------------------

                 N  (  1):       0.0003     -0.0004      0.0118
                 N  (  2):       1.9044      0.0017      2.1599
                 N  (  3):      -0.9552      1.6483      2.1598
                 N  (  4):      -0.9488     -1.6511      2.1600
                 Mo (  5):      -0.0001      0.0003      1.6635
                 H  (  6):      -1.3384      2.3177      1.4970
                 H  (  7):      -1.1112      1.9665      3.1161
                 H  (  8):       2.6751     -0.0029      1.4975
                 H  (  9):       2.2570     -0.0229      3.1161
                 H  ( 10):      -1.3372     -2.3171      1.4969
                 H  ( 11):      -1.1436     -1.9468      3.1163

              ==================================================
```

```
<><><><><><><><><><><><><><><><><><><><><><><><><>

   NUMBERS:
   --------

   number of virtual electrons:     76.00

   ---   AOs   ---          ---   MOs   ---
   ncor =     0             nocc =    38
   nval =   274             nvir =   205
   nbas =   274             nmo  =   243

<><><><><><><><><><><><><><><><><><><><><><><><><>

==================================================

   FRAGMENT TYPES:
   ---------------

   Nitrogen (V)
   Molybdenum (V, all electron)
   Hydrogen (V)

==================================================
==================================================

   --------------------------
       ATOM TYPE: N
   --------------------------
   === BASIS
     1S    8.74     VALENCE
     1S    5.90     VALENCE
     2S    5.15     VALENCE
     2S    2.50     VALENCE
     2S    1.50     VALENCE
     2P    3.68     VALENCE
     2P    1.88     VALENCE
     2P    1.00     VALENCE
     3D    2.20     VALENCE
     4F    3.30     VALENCE

   --------------------------
       ATOM TYPE: H
   --------------------------
   === BASIS
     1S    0.69     VALENCE
     1S    0.92     VALENCE
     1S    1.58     VALENCE
     2P    1.25     VALENCE
     3D    2.50     VALENCE


   --------------------------
       ATOM TYPE: Mo
   --------------------------
      === BASIS
     1S  269.00     VALENCE
     1S   67.10     VALENCE
     1S   41.50     VALENCE
     2S   49.50     VALENCE
     2S   17.55     VALENCE
     3S    9.00     VALENCE
     3S    5.90     VALENCE
     4S    5.10     VALENCE
     4S    3.30     VALENCE
     5S    2.15     VALENCE
     5S    1.35     VALENCE
     5S    0.87     VALENCE
     2P   25.80     VALENCE
     2P   16.75     VALENCE
     3P   10.15     VALENCE
     3P    7.05     VALENCE
     4P    4.95     VALENCE
     4P    3.30     VALENCE
     4P    2.30     VALENCE
     3D   15.30     VALENCE
     3D    9.00     VALENCE
     3D    5.75     VALENCE
     4D    3.50     VALENCE
     4D    1.85     VALENCE
     4D    0.97     VALENCE
     5P    1.35     VALENCE
     4F    2.00     VALENCE
```

```
            ==================================================
            <><><><><><><><><><><><><><><><><><><><><><><><><>

               TENSOR INFORMATION:
               -------------------

                            CALC                   U1K

               paramagnetic  = T     mass-velocity = F
               diamagnetic   = T     Darwin        = F
               Fermi-cont.   = F     Zeeman        = F
               ZORA SO       = F     ZORA SO       = F
               ZORA SCALE    = T     ZORA SO FULL  = F
                                     E IN U1 SCL   = F

            <><><><><><><><><><><><><><><><><><><><><><><><><>

            <><><><><><><><><><><><><><><><><><><><><><><><><>

               OUTPUT SWITCHES:
               ----------------

                         ISO = T                F1 = F
                        TENS = T                S1 = F
                         EIG = F                U1 = F
                         AOP = F                B1 = F
                         AOD = F                F  = F
                         AOF = F                 S = F
                        INFO = T              REFS = T

            <><><><><><><><><><><><><><><><><><><><><><><><><>

            --------------------------------------------------

               CALCULATE THE POTENTIAL? T

               ---> Potential is NOT on TAPE10.
                    So it will be calculated.

            --------------------------------------------------

===================================================
Numerical Integration : Atomic Polyhedra (Te Velde)  ***  (parameters, tests)  ***
===================================================

General Accuracy Parameter :                          4.00

Symmetry used in the points section:  NOSYM


Summary of the Symmetry Unique Points:
--------------------------------------
   Nr. of used Symmetry Operators                    1

   Points in the Atomic Spheres                   7166
   Points in the Atomic Polyhedra                63774
   Points in the Outer Region                     6969
   ---------------------------------------------------
   Total                                         77909

   Sum of Weights                              100262.772697

Total nr. of points:      77909
Nr. of blocks:              609
Block length:               128
Nr. of dummy points:         43


Test of Precision of the Numerical Integration Grid
===================================================
```

```
 Integral of the Total Core Density:                  0.00000000000000
################################################################################
********************************************************************************

****  N U C L E U S :   N  (  1)

=== INFO:
When an external magnetic field interacts with electron density,
it induces electronic currents to flow.  The currents produce a
magnetic field.  This induced magnetic field may re-enforce the
external magnetic field, or reduce it.

=== INFO:
The paramagnetic shielding results from currents induced by the
external magnetic field, which re-enforce the external magnetic
field.

--- REF: H. Fukui Mag. Res. Rev. 11 (1987) 205.

 ==============================================================================

===  PARAMAGNETIC NMR SHIELDING TENSORS (ppm)

    ===     paramagnetic b^(1) tensor       ===     paramagnetic u^(1) tensor
    ----------------------------------      ----------------------------------
           0.000     0.000     0.000           -1270.704     2.012    -0.185
           0.000     0.000     0.000               2.012 -1270.776     0.437
           0.000     0.000     0.000              -0.185     0.437  -240.799
    ----------------------------------      ----------------------------------
    isotropic shielding =      0.000        isotropic shielding =   -927.426

    ===     paramagnetic s^(1) tensor       ===     paramagnetic gauge tensor
    ----------------------------------      ----------------------------------
          45.776     0.047    -0.008              3.678     0.003    -0.001
           0.047    45.764    -0.007              0.003     3.677    -0.001
          -0.008    -0.007    -3.937             -0.001    -0.001    -0.084
    ----------------------------------      ----------------------------------
    isotropic shielding =     29.201        isotropic shielding =      2.423

                        **********************************
                        CARTESIAN AXIS REPRESENTATION

                        ==== total paramagnetic tensor
                        ----------------------------------
                           -1221.250     2.062    -0.194
                               2.062 -1221.335     0.428
                              -0.194     0.428  -244.820
                        ----------------------------------
                        isotropic shielding =   -895.802

                        **********************************
                        ----------------------------------
                        PRINCIPAL AXIS REPRESENTATION

                        ==== Shieldings:

                           -1223.356 -1219.230  -244.820

                        ==== Principal Axis System:

                               0.700     0.714     0.000
                              -0.714     0.700     0.000
                               0.000     0.000     1.000
                        ----------------------------------
=== INFO:
When an external magnetic field interacts with electron density,
it induces electronic currents to flow.  The currents produce a
magnetic field.  This induced magnetic field may re-enforce the
external magnetic field, or reduce it.

=== INFO:
```

The diamagnetic shielding results from currents induced by the
external magnetic field, which reduce the external magnetic
field.
--- REF: H. Fukui
         Mag. Res. Rev. 11 (1987) 205.

```
================================================================================
===  DIAMAGNETIC NMR SHIELDING TENSORS (ppm)

    ===       diamagnetic core tensor       ===    diamagnetic valence tensor
    ------------------------------------     ------------------------------------
           0.000     0.000     0.000              316.865    -0.012    -0.008
           0.000     0.000     0.000               -0.012   316.870     0.013
           0.000     0.000     0.000               -0.008     0.013   350.242
    ------------------------------------     ------------------------------------
    isotropic shielding =      0.000        isotropic shielding =    327.992

                         ************************************
                         CARTESIAN AXIS REPRESENTATION

                         ==== total diamaginetic NMR tensor
                         ------------------------------------
                              316.865    -0.012    -0.008
                               -0.012   316.870     0.013
                               -0.008     0.013   350.242
                         ------------------------------------
                         isotropic shielding =    327.992

                         ************************************
                         ------------------------------------
                         PRINCIPAL AXIS REPRESENTATION

                         ==== Shieldings:

                              316.856   316.879   350.242

                         ==== Principal Axis System:

                                0.787     0.616     0.000
                                0.616    -0.787     0.000
                                0.000     0.000     1.000
                         ------------------------------------

================================================================================
====  TOTAL NMR SHIELDING TENSOR (ppm)

                         ************************************
                         CARTESIAN AXIS REPRESENTATION

                         ==== total shielding tensor
                         ------------------------------------
                             -904.386     2.051    -0.202
                                2.051  -904.465     0.441
                               -0.202     0.441   105.422
                         ------------------------------------
                         isotropic shielding =   -567.809

                         ************************************
                         ------------------------------------
                         PRINCIPAL AXIS REPRESENTATION

                         ==== Shieldings:

                             -906.477  -902.374   105.423

                         ==== Principal Axis System:

                                0.700     0.714     0.000
                               -0.714     0.700     0.000
                                0.000     0.000     1.000
                         ------------------------------------
```

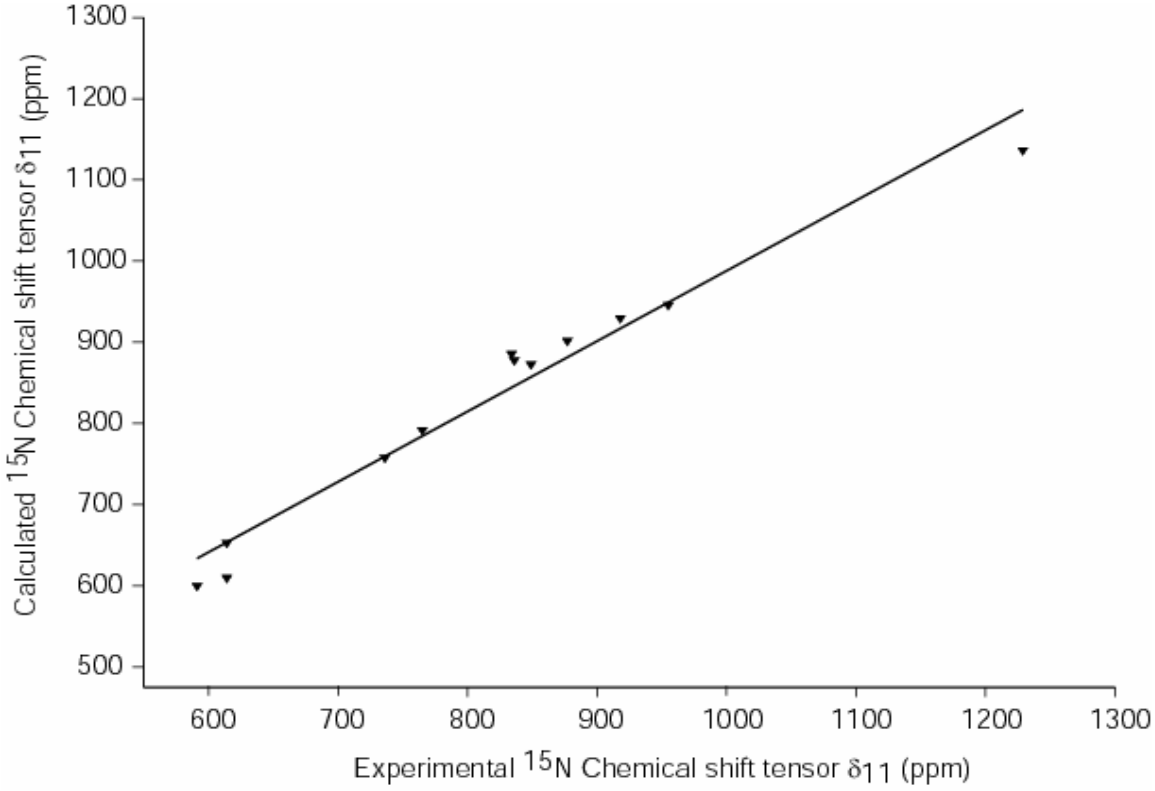
```
*****************************************************************************
*** MO ANALYSIS OF CONTRIBUTIONS TO U^(1)
 === INFO:
Calculations reveal that in general the paramagnetic shielding
is very sensitive to electronic changes within the molecule.
The magnitude of the paramagnetic shielding is largly dependent
on the components of the u^(1) matrix.  These components are
proportional to the coupling of occupied and virtual orbitals
by the magnetic field, and inversely proportional to the energy
difference between these orbitals.
Following, a simple orbtial picture is presented, then a table.
The orbital picture includes the LUMO, HOMO and HOMO-LUMO GAP (HLG).
In the table that follows, k = 1, 2, 3 is the magnetic field
component, "vir" is the virtual orbital number, "occ" is the
occupied orbital number, "sym" is the representation, "cmp" is
the component of the representation, "<M_k>" is the coupling
due to the k-th component of the magnetic field,
"e(vir)-e(occ)" is the energy difference, and "u1k~" is
half*<M_k>/[e(vir)-e(occ)], which is the main contribution to
"u^(1)".  Note that "<M_k> = < vir | [ r_{mu} x grad ]_k | occ >"
Only the five major components are listed.

--- REF: G. Schreckenbach
         Relativity and Magnetic Properties. A Density Functional Study
         Ph.D. Thesis 1996.

--- REF: Y. Ruiz-Morales
         The Calculation and Interpretation of NMR Chemical Shifts
         in Compounds of Transition Metals and Heavy Elements
         Ph.D. Thesis 1997.

--- REF: J. Gerratt and I. M. Mills
         J. Chem. Phys. 49 (1968) 1719.

                        MO                                ENERGY (eV)
                        ========================================

                        243   nmo   - - - - - - - - - -  **********
                         39   LUMO  - - - - - - - - - -      -1.904
                                                |
                                                |  HLG --->     3.847
                                                |
                         38   HOMO  ------------------      -5.751
                          1   1     ------------------  -20282.190


    ------------------------------------------------------------------------------------------------
    k   R/I    vir ( sym,cmp)    occ ( sym,cmp)         u1k~            <M_k>        e(vir)-e(occ)
    ------------------------------------------------------------------------------------------------
    1  real     39 (A   , 39)     35 (A   , 35)    -0.160151D+01    -0.587081D+00       4.988
    1  real     42 (A   , 42)     35 (A   , 35)     0.119527D+01     0.554337D+00       6.310
    1  real     44 (A   , 44)     34 (A   , 34)     0.115709D+01     0.623591D+00       7.332
    1  real     42 (A   , 42)     33 (A   , 33)    -0.565803D+00    -0.282290D+00       6.788
    1  real     43 (A   , 43)     34 (A   , 34)     0.565710D+00     0.282214D+00       6.787


    2  real     40 (A   , 40)     35 (A   , 35)    -0.159751D+01    -0.586057D+00       4.991
    2  real     43 (A   , 43)     35 (A   , 35)     0.119477D+01     0.554200D+00       6.311
    2  real     44 (A   , 44)     33 (A   , 33)    -0.115721D+01    -0.623804D+00       7.334
    2  real     42 (A   , 42)     34 (A   , 34)     0.564095D+00     0.281364D+00       6.786
    2  real     43 (A   , 43)     33 (A   , 33)     0.562078D+00     0.280476D+00       6.789


    3  real     39 (A   , 39)     31 (A   , 31)    -0.113197D+01    -0.655671D+00       7.881
    3  real     40 (A   , 40)     32 (A   , 32)    -0.113023D+01    -0.654847D+00       7.883
    3  real     39 (A   , 39)     33 (A   , 33)    -0.832438D+00    -0.334410D+00       5.466
    3  real     40 (A   , 40)     34 (A   , 34)    -0.831574D+00    -0.334184D+00       5.468
    3  real     42 (A   , 42)     37 (A   , 37)     0.626748D+00     0.280671D+00       6.093

*****************************************************************************
```

2.14 Generation of spectra from calculated chemical shielding tensors

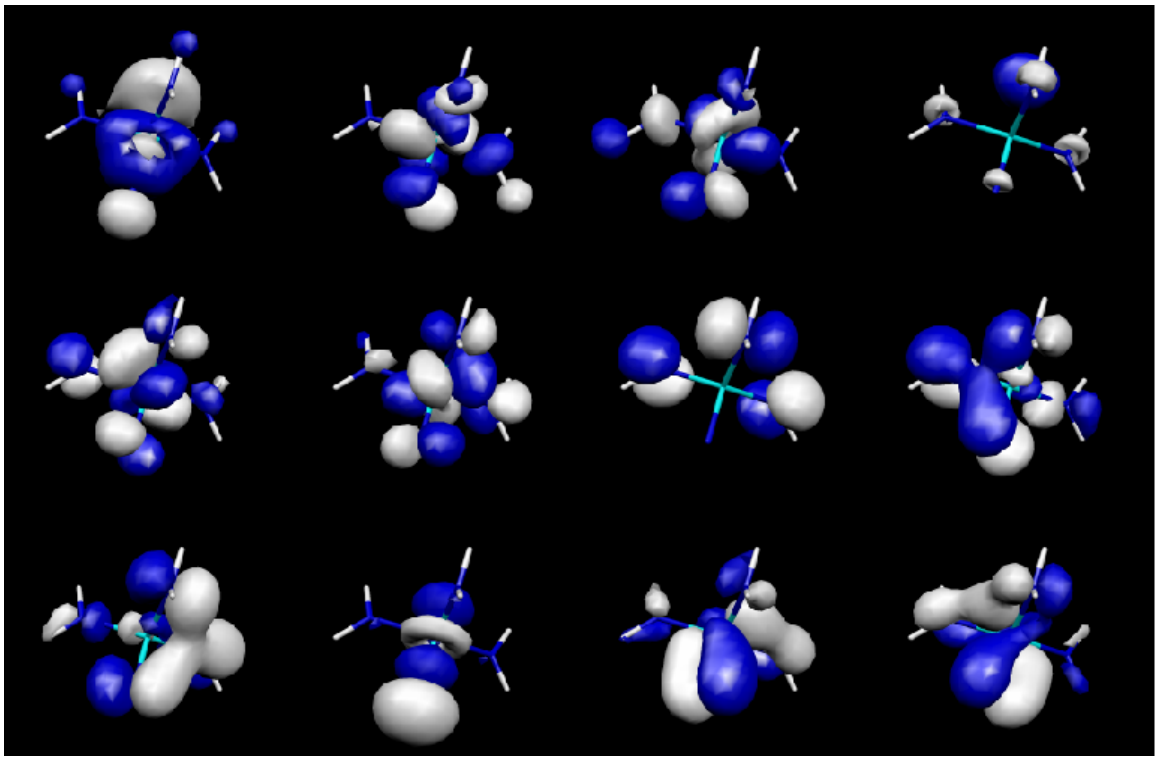
Generation of spectra from calculated values of the chemical shielding tensor was achieved using the Simpson program. A representative input file is included below. 'Shift 1' values are taken from the calculated shielding tensors; '448p' being the calculated isotropic shift (δ_{iso}); '-130p' the reduced anisotropy ($\delta_{33}-\delta_{iso}$) and '0.3553' being the asymmetry ($[\delta_{11}-\delta_{22}]/\ \delta_{33}$). 'Spin rate' and line broadening (`faddlb`) must be set according to those used in acquisition of the experimental spectrum to which the calculated values are being compared. Two output files are created (calc.fid and calc.spe) upon successful simulation of the desired spectrum.

```
# MAS CSA spectrum
# Uses the gcompute method


spinsys {
    nuclei 15N
    channels 15N
    shift 1 448p -130p 0.3553 0 0 0 0
}

par {
    method           gcompute
    start_operator   Inx
    detect_operator  Inp
    spin_rate        3500
    gamma_angles     40
    sw               gamma_angles*spin_rate
    crystal_file     rep168
    np               2048
    proton_frequency 501e6
}

proc pulseq {} {
    maxdt 1
    delay 9999
}

proc main {} {
    global par

    set f [fsimpson]
    fsave $f calc.fid
    fzerofill $f 4096
    faddlb $f 100 0
    fft $f
    fsave $f calc.spe
}
```

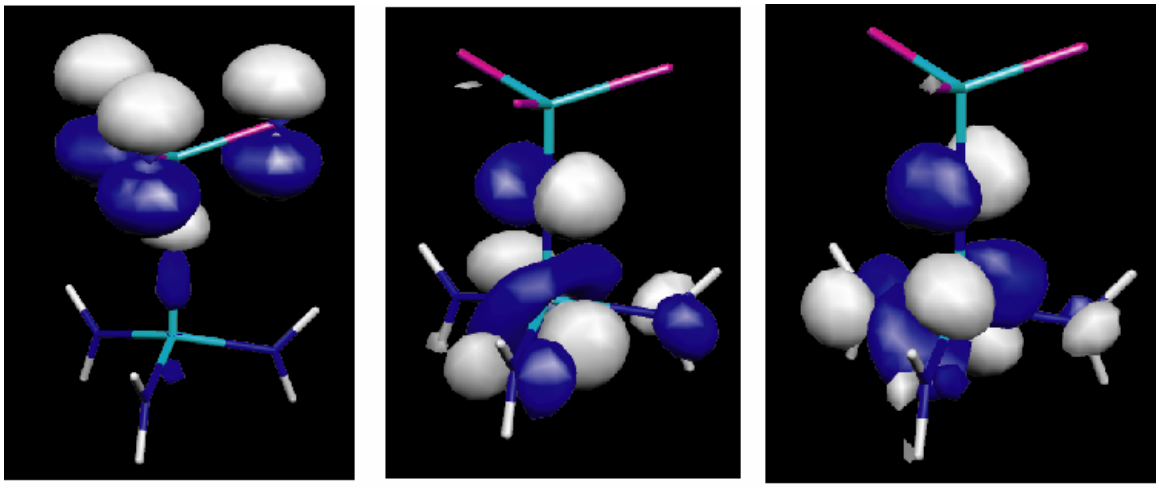
2.15 Plot of the Experimental ^{15}N chemical shift tensor (δ_{11}) (ppm) versus calculated ^{15}N chemical shift tensor (δ_{11}) (ppm).



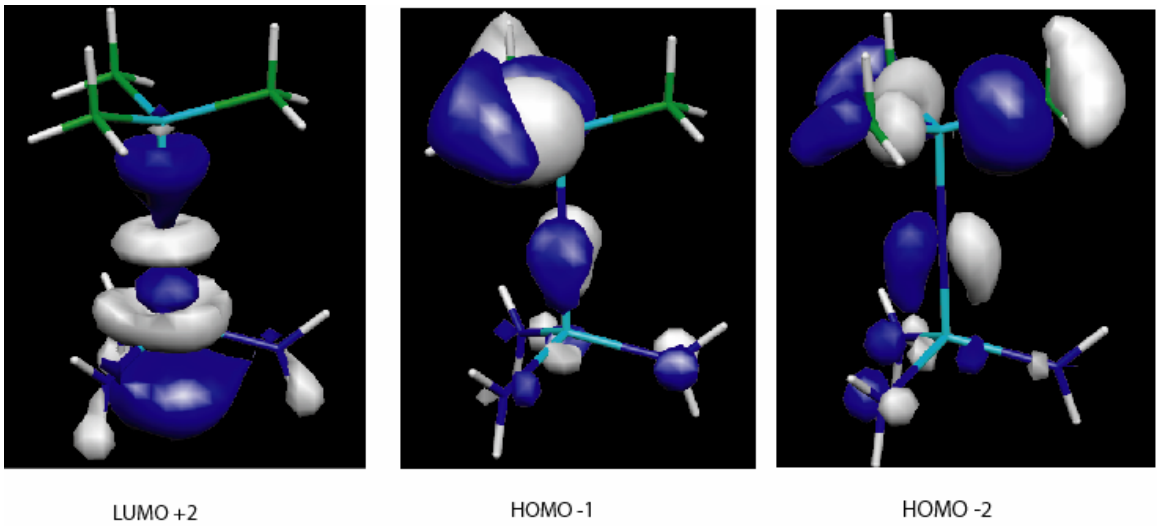
2.16 Selected orbitals [LUMO+5 (top left)→HOMO−5 (bottom right)] of $NMo(NH_2)_3$, (1m)



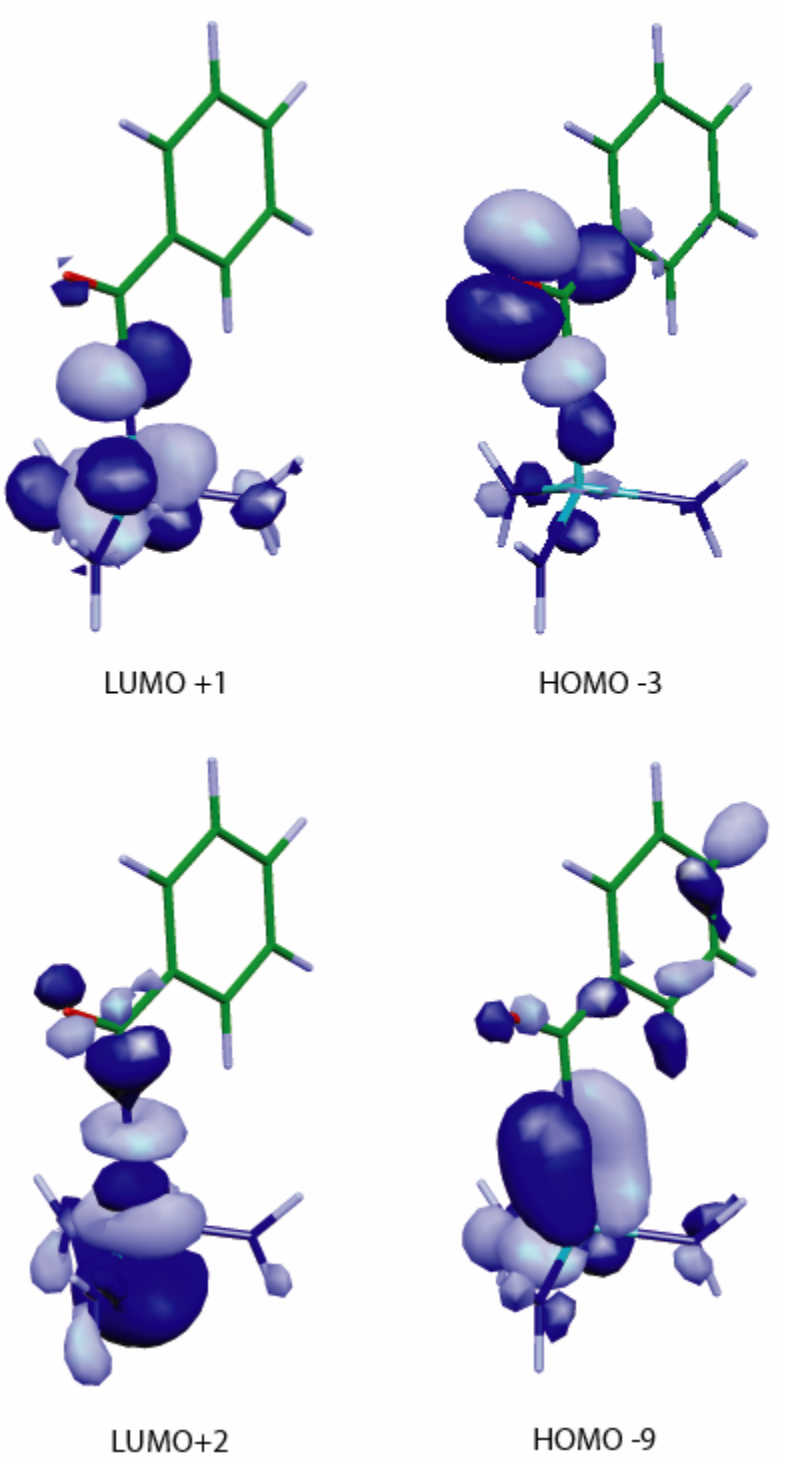
2.17 Selected orbitals (HOMO-4, LUMO+1 and LUMO) of $Cl_3B{-}NMo(NH_2)_3$ (1m−BCl_3)



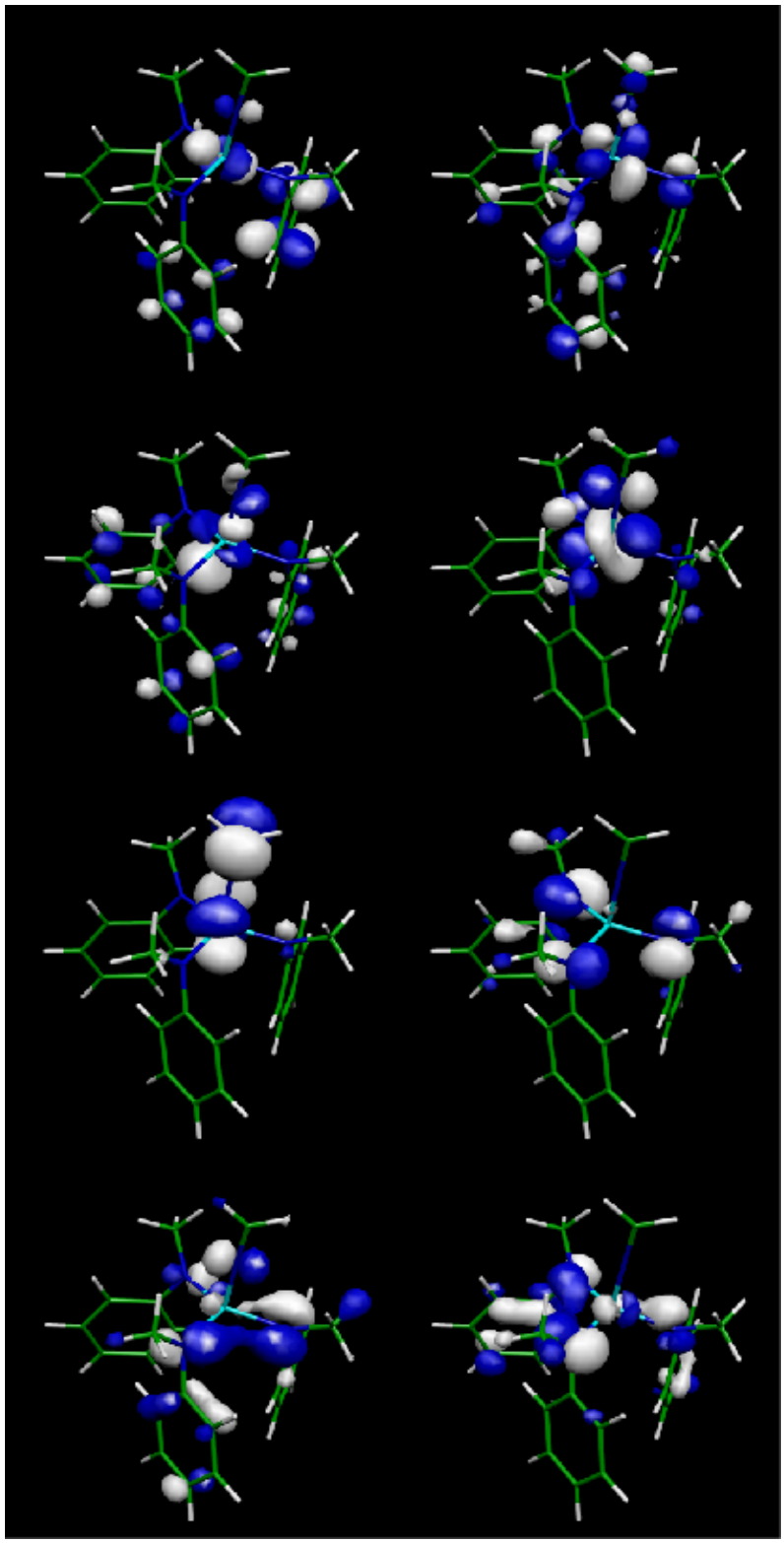
2.18 Selected orbitals (LUMO+2, HOMO-1 and HOMO-2) of $[(CH_3)_3SiNMo(NH_2)_3]^+$ [2b-m]



2.19 Selected orbitals (LUMO+1, HOMO−3, LUMO+2 and HOMO −9) of $[PhC(O)NMo(NH_2)_3]^+$ [2c-m]



2.20 Selected orbitals (LUMO+3 (top left)→HOMO−3 (bottom right)] of H_2C=NMo(N[CH_3]Ph)$_3$ (3m-C_3)



3. ^{15}N Solid State CP MAS NMR Spectroscopy: Experimental Information and Representative Spectra

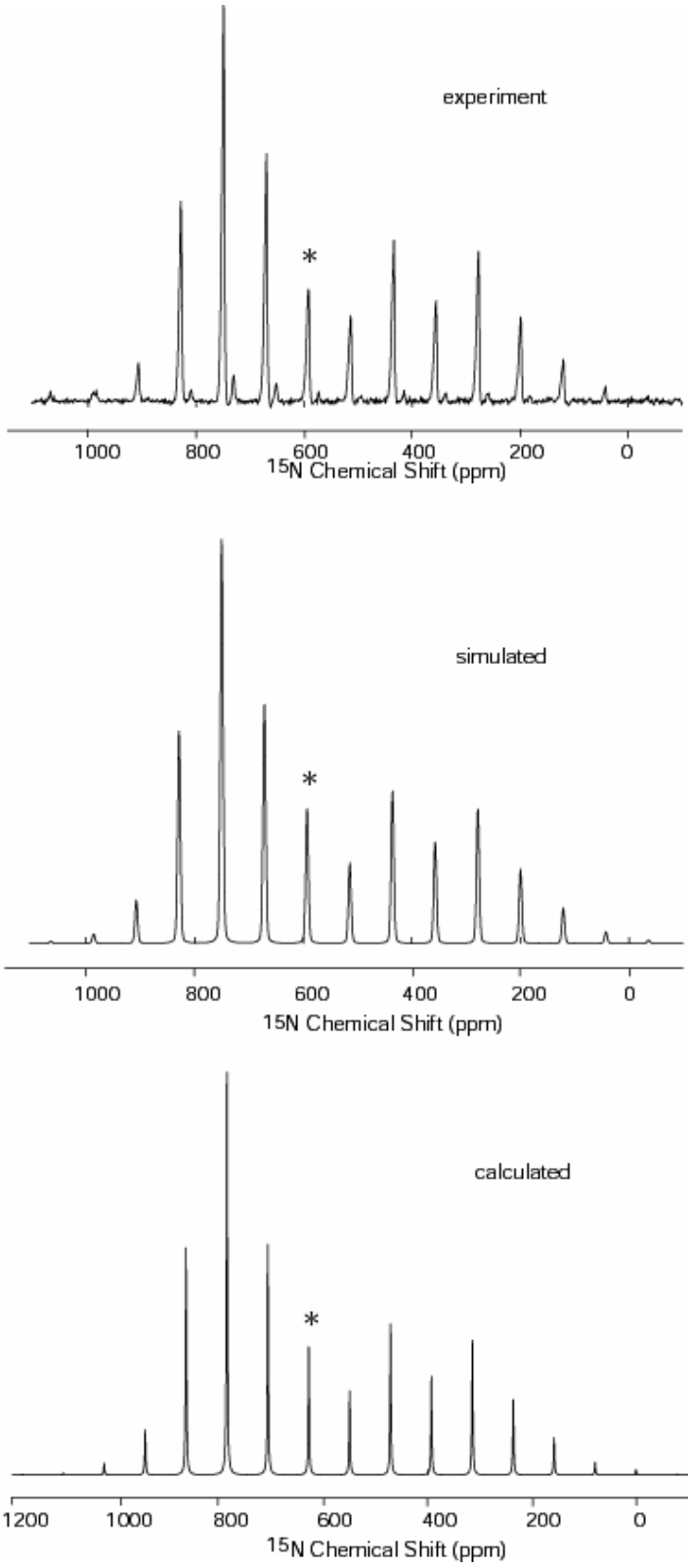
3.1 Solid-state ^{15}N CPMAS NMR: Experimental Information

The sample temperature was maintained at 25 ºC for all solid-state NMR experiments. Solid-state NMR spectra were acquired using a custom-designed spectrometer (courtesy of Dr. David J. Ruben) operating at 501 MHz for ^{1}H (50.8 MHz for ^{15}N). All spectra were acquired using a triple-resonance (^{1}H/^{13}C/^{15}N) magic-angle spinning (MAS) probe from Chemagnetics (Fort Collins, CO). The samples were packed in a glove box into 4.0 mm zirconium rotors; the packed rotors were made air tight by adding layers of vacuum grease above and below the sample, and by inserting a screw made of Vespel into the top spacer. Depending on the sample, spinning frequencies of between 3 and 5 kHz were used; this frequency was regulated to better than ±3 Hz using a Bruker spinning frequency controller. Samples were referenced indirectly to the ^{13}C CPMAS spectra of adamantane (acquired prior to each sample acquisition).

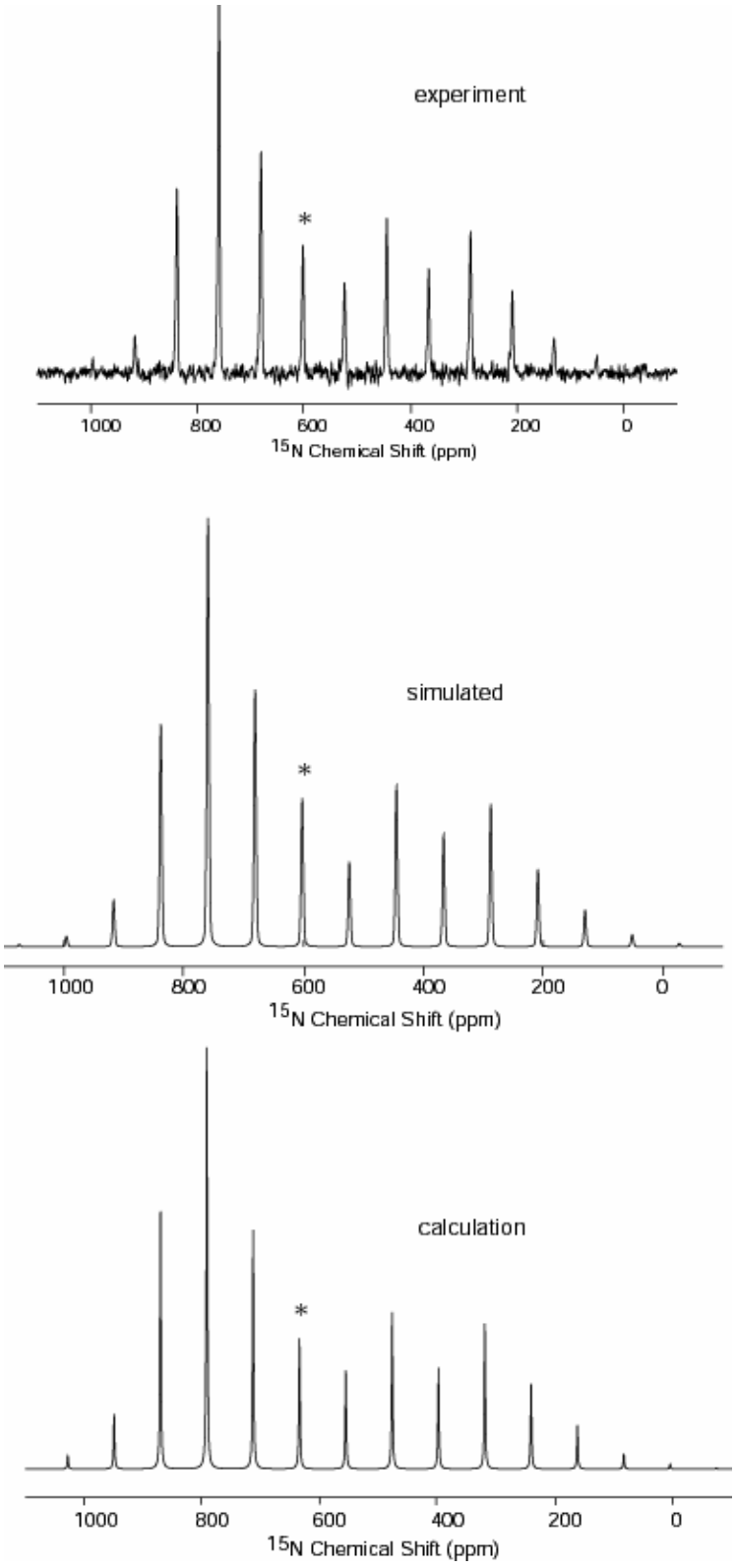
Proton-nitrogen cross-polarization under the Hartmann-Hahn match was used to enhance the sensitivity of all ^{15}N NMR spectra. Cross polarization times of 4 ms were used for samples for which the ^{1}H-^{15}N distance was expected to be relatively short (2-3 Å); longer polarization times of up to 10 ms were used for samples in which the ^{1}H-^{15}N distances were expected to be larger. The RF field strength used for the cross-polarization step was 50 kHz on the ^{1}H channel and ramped between 45 and 55 kHz on the ^{15}N channel. Two pulse phase modulation (TPPM)[1] decoupling at ~83 kHz was used during signal acquisition. A recycle delay of 3 s was employed for each sample. Acquisition times varied between 0.5 and 21 h (between 512 and 24,500 scans (depending on the sample) were used in acquiring the spectra).

[1] Bennett, A. E.; Rienstra, C. M.; Auger, M.; Lakshmi, K. V.; Griffin, R. G. *J. Chem. Phys*, **1995**, *103*, 6951.

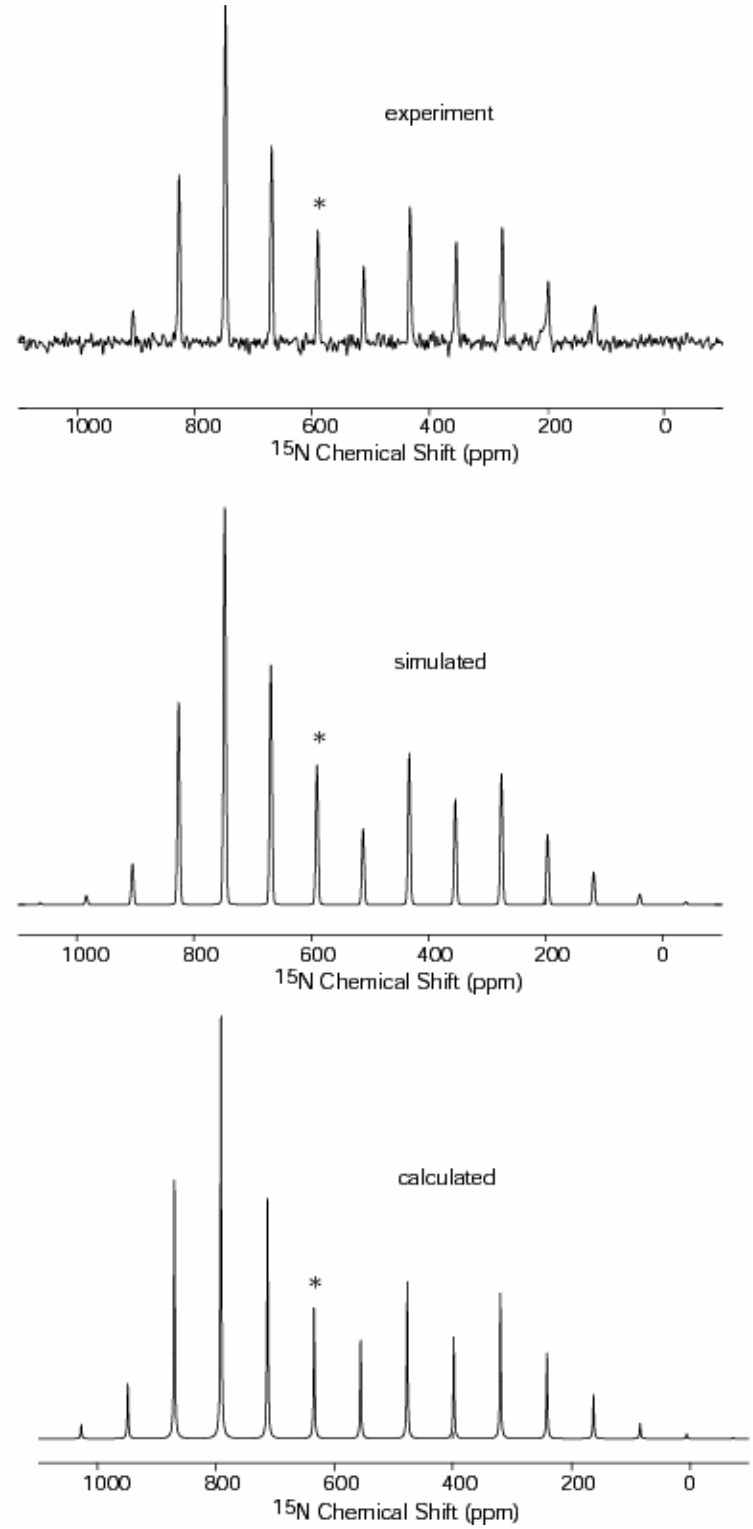
3.2 Experimental, simulated and calculated ^{15}N CPMAS spectra for $F_3B{-}^{15}NMo(N[^tBu]Ar)_3$, 1−$BF_3$ (Calculated spectrum of 1m-BF_3)



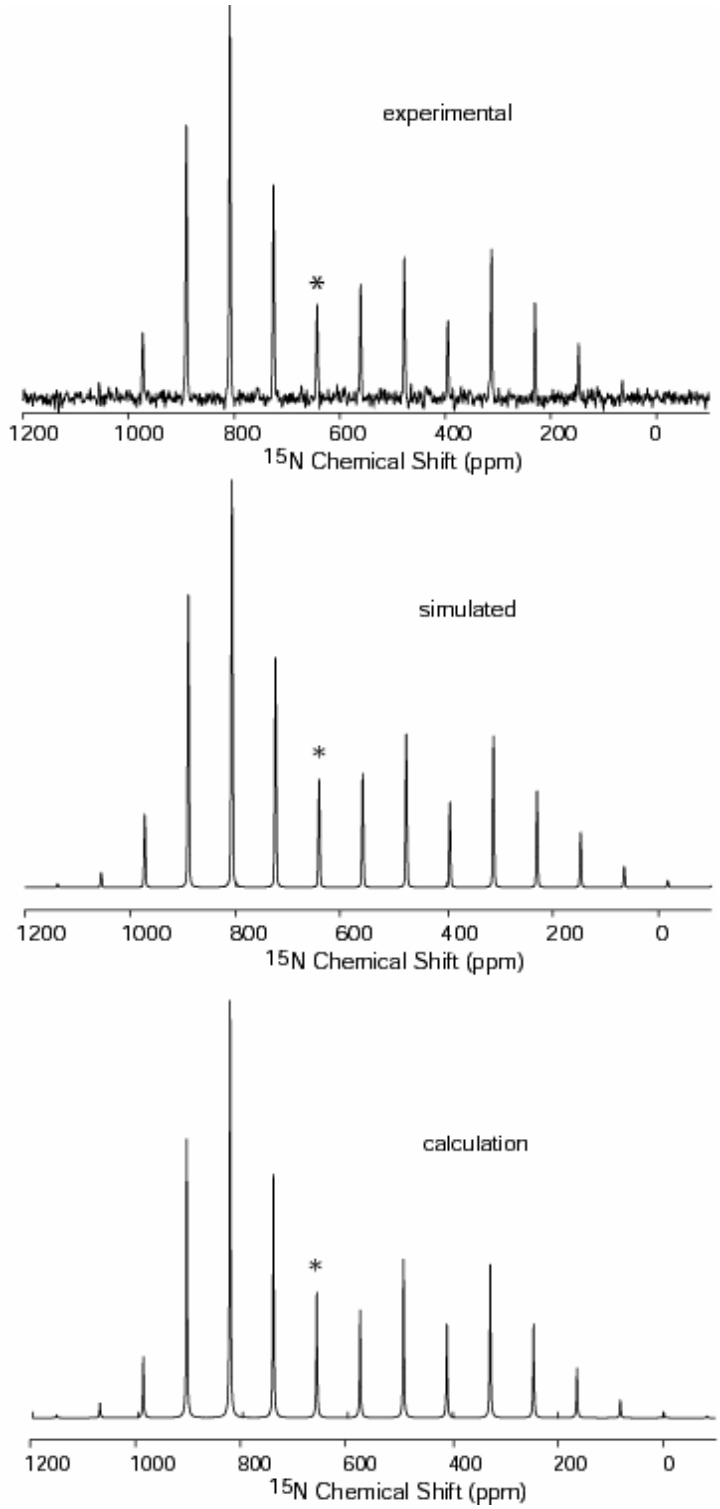
3.3 Experimental, simulated and calculated ^{15}N CPMAS spectra for $Cl_3Al–^{15}NMo(N[^tBu]Ar)_3$, 1−$AlCl_3$ (Calculated spectrum of 1m-$AlCl_3$)



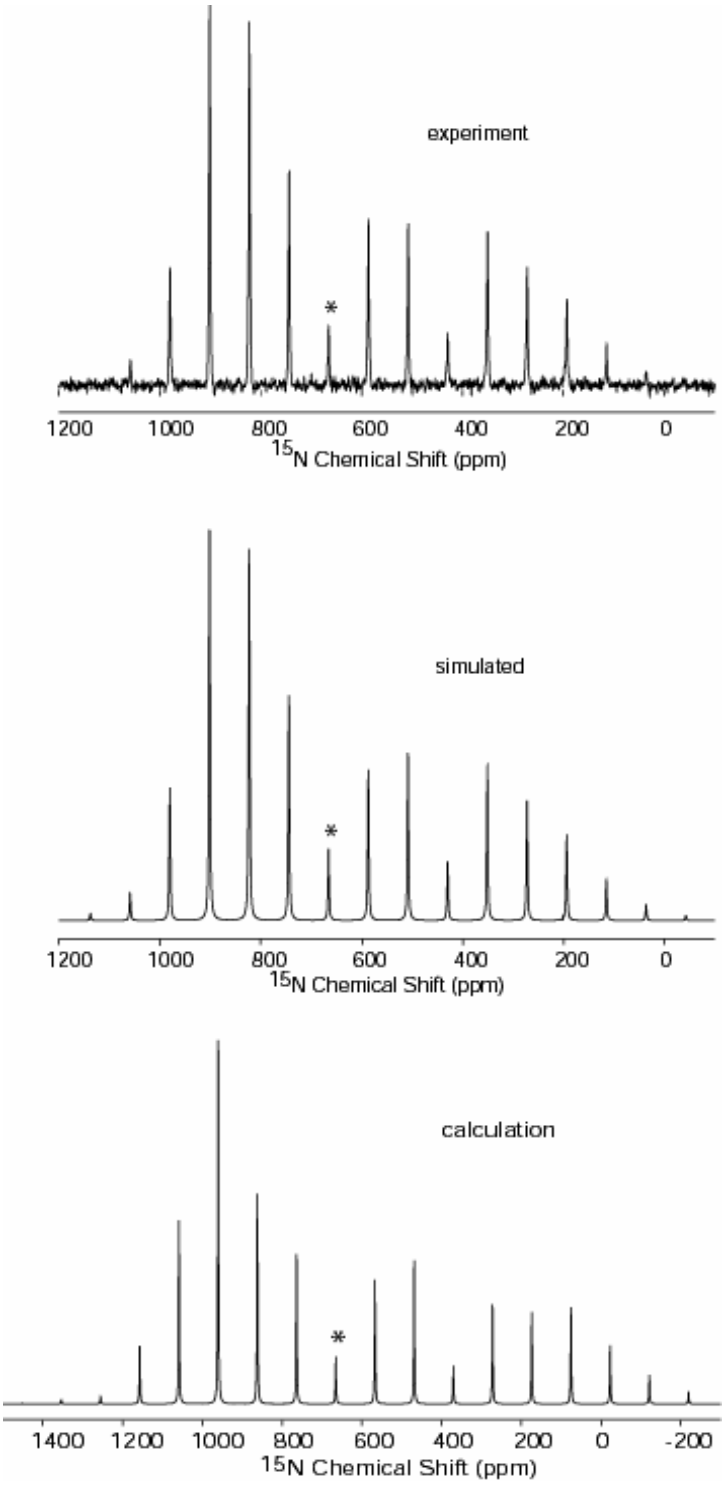
3.4 Experimental, simulated and calculated ^{15}N CPMAS spectra for $Cl_3Ga{-}^{15}NMo(N[^tBu]Ar)_3$, 1−$GaCl_3$ (Calculated spectrum of 1m-$GaCl_3$)



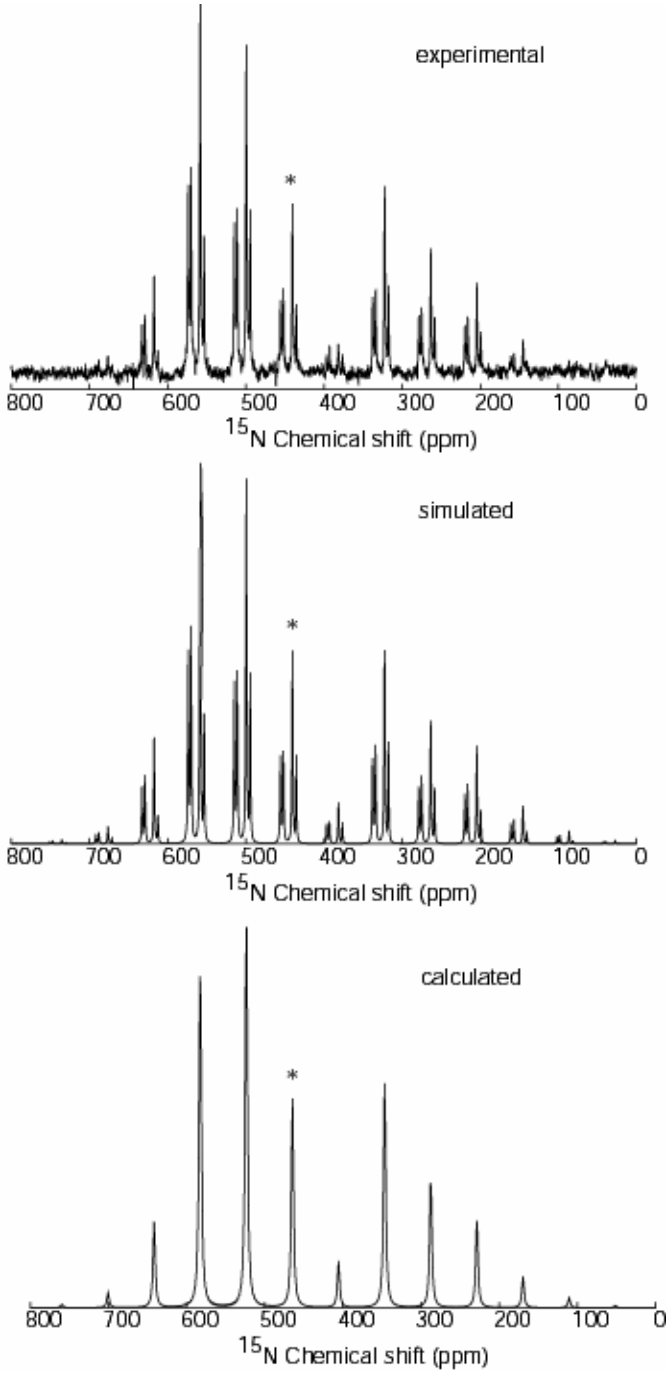
3.5 Experimental, simulated and calculated ^{15}N CPMAS spectra for $Cl_2Ge{-}^{15}NMo(N[^tBu]Ar)_3$, 1−$GeCl_2$ (Calculated spectrum of 1m-$GeCl_2$)



3.6 Experimental, simulated and calculated ^{15}N CPMAS spectra for $Cl_2Sn-^{15}NMo(N[^tBu]Ar)_3$, 1−$SnCl_2$ (Calculated spectrum of 1m-$SnCl_2$)

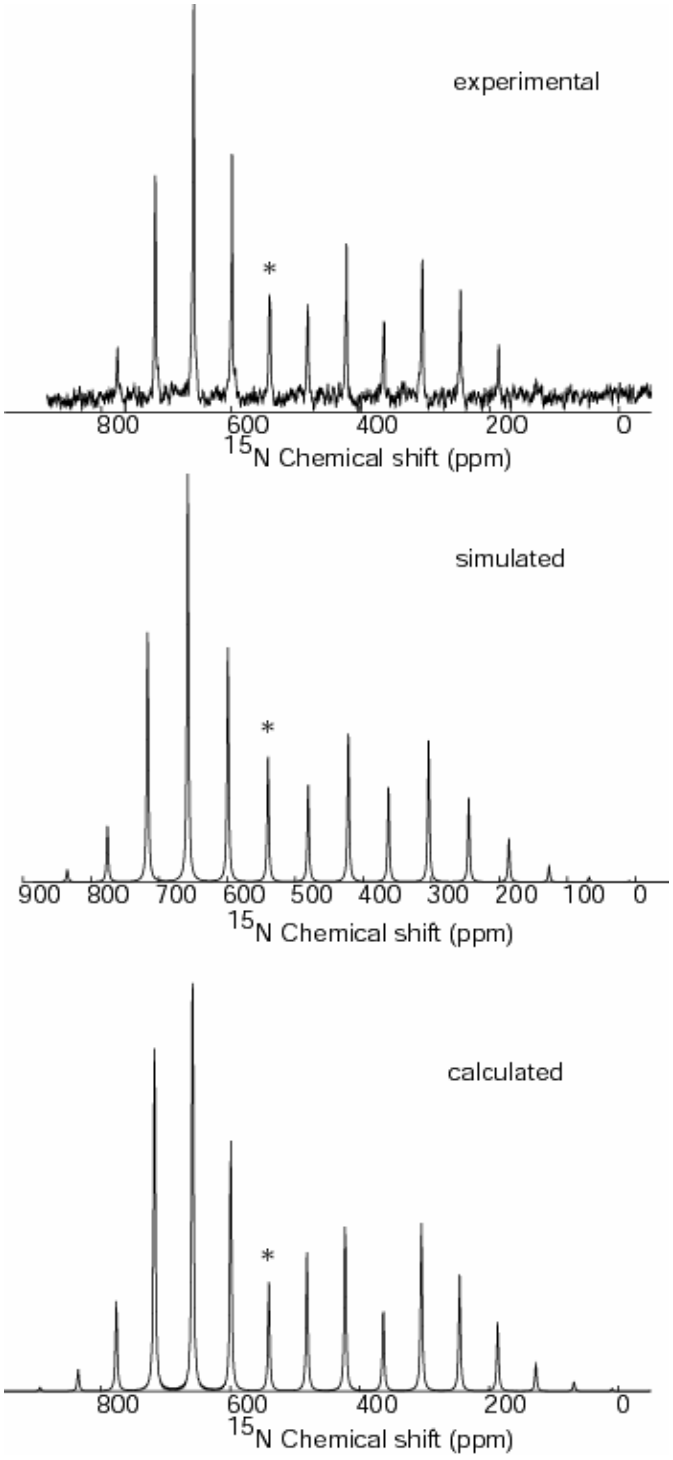


3.7 Experimental, simulated and calculated ^{15}N CPMAS spectra for $[CH_3{}^{15}NMo(N[^tBu]Ar)_3]I$ [2a]I (Calculated spectrum of [2a-m]I)

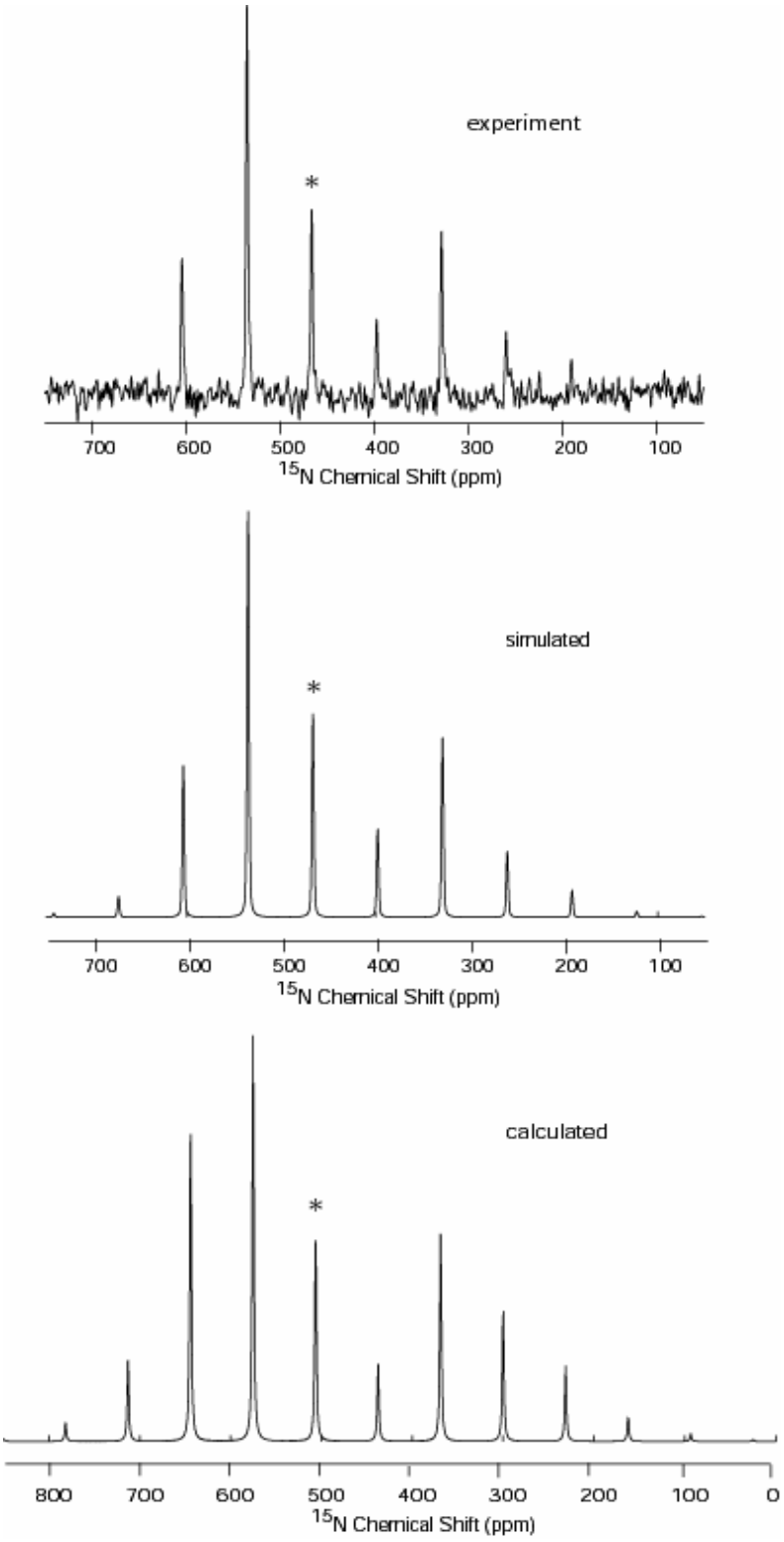


The group of four peaks seen for each spinning sideband indicates that there are four electronically distinct forms of this complex in the unit cell.

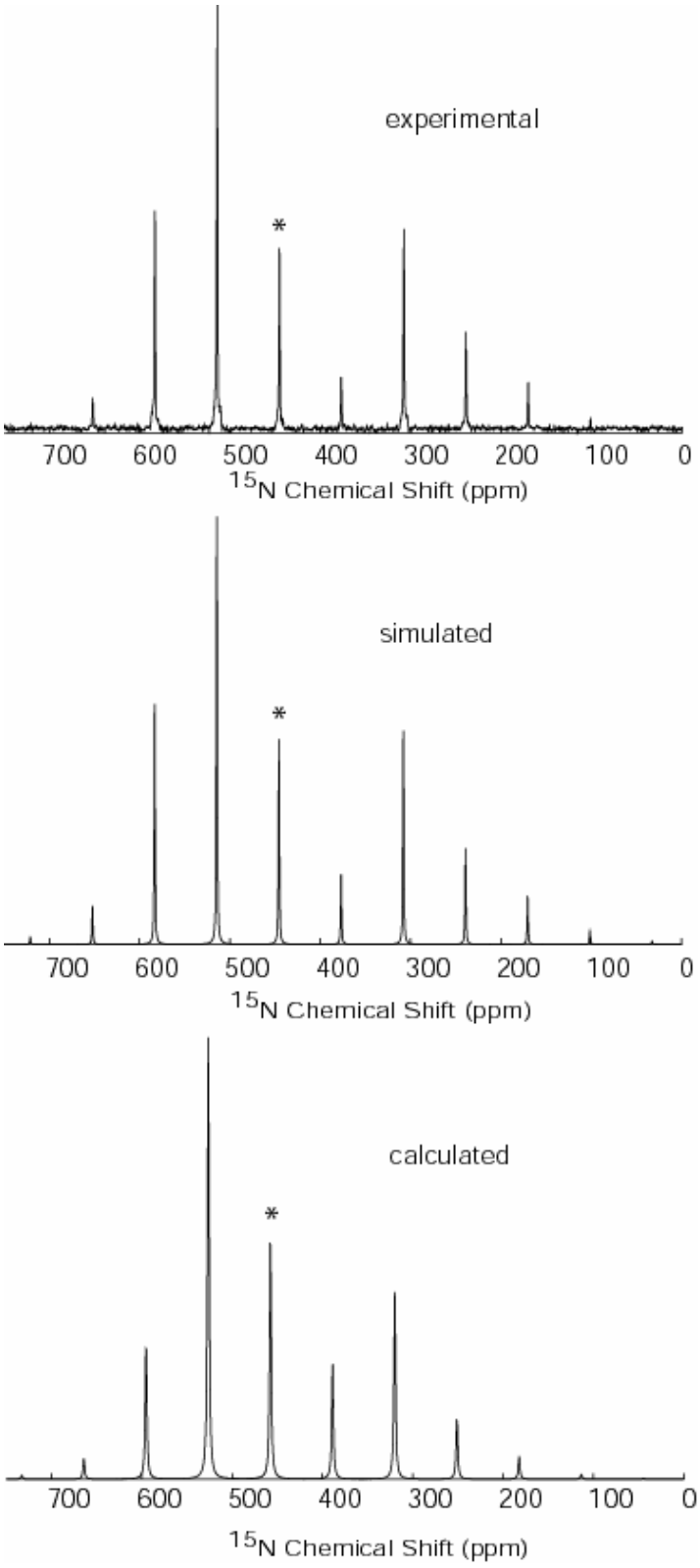
3.8 Experimental, simulated and calculated ^{15}N CPMAS spectra for $[(CH_3)_3Si^{15}NMo(N[^tBu]Ar)_3]OTf$ [2b]OTf (Calculated spectrum of [2b-m]OTf)



3.9 Experimental, simulated and calculated ^{15}N CPMAS spectra for [PhC(O)^{15}NMo(N[^{t}Bu]Ar)$_3$]OTf [2c]OTf (Calculated spectrum of [2c-m]OTf)



3.10 Experimental, simulated and calculated ^{15}N CPMAS spectra for $H_2C=^{15}NMo(N[^tBu]Ar)_3$ (3) (calculated spectrum of 3m-C_3)



3.11 Experimental, simulated and calculated ^{15}N CPMAS spectra for $H_2C=^{15}NMo(N[^tBu]Ar)_3$ (3) (calculated spectrum of 3m-C_s)