

Figure S1. ^1H NMR Spectrum of SiPr(H)CCl_3 in C_6D_6 .

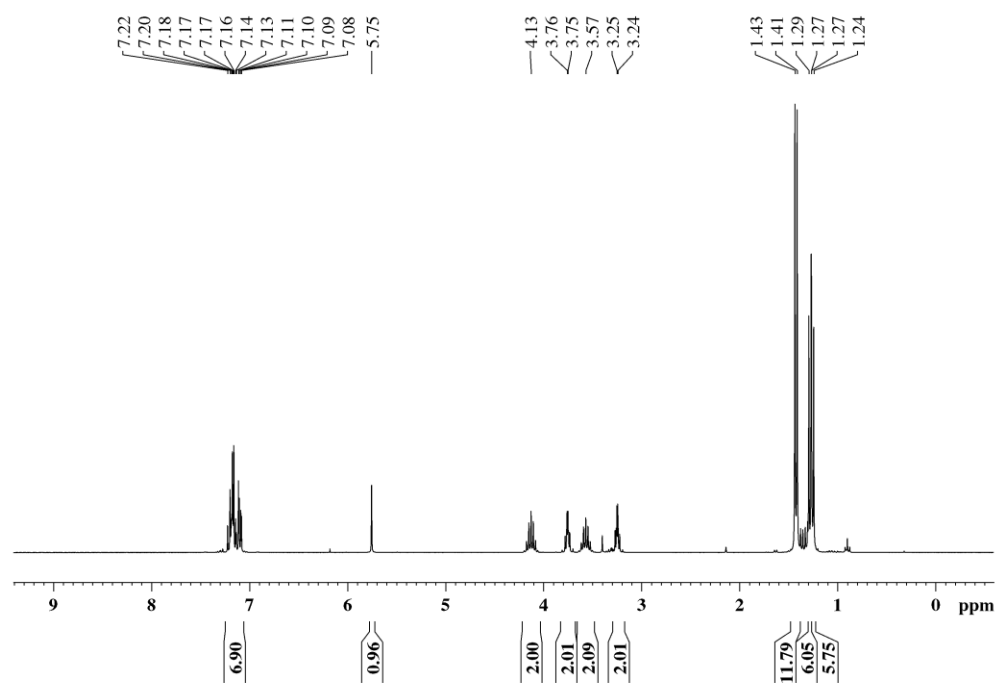


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR Spectrum of SiPr(H)CCl_3 in C_6D_6 .

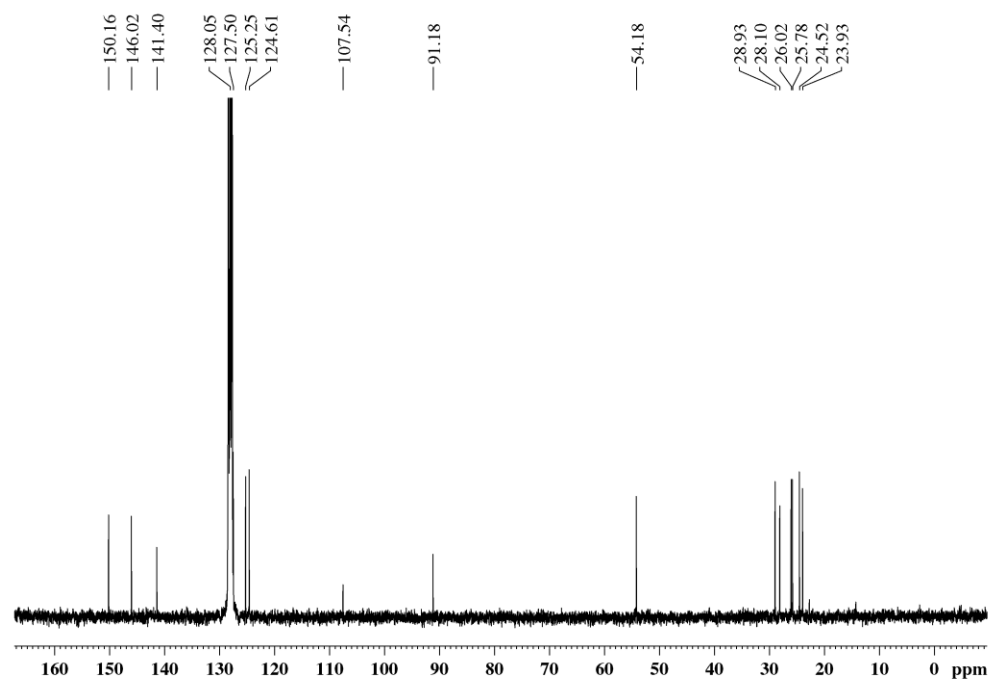


Figure S3. High resolution ESI mass spectrum of SIPr(H)CCl₃

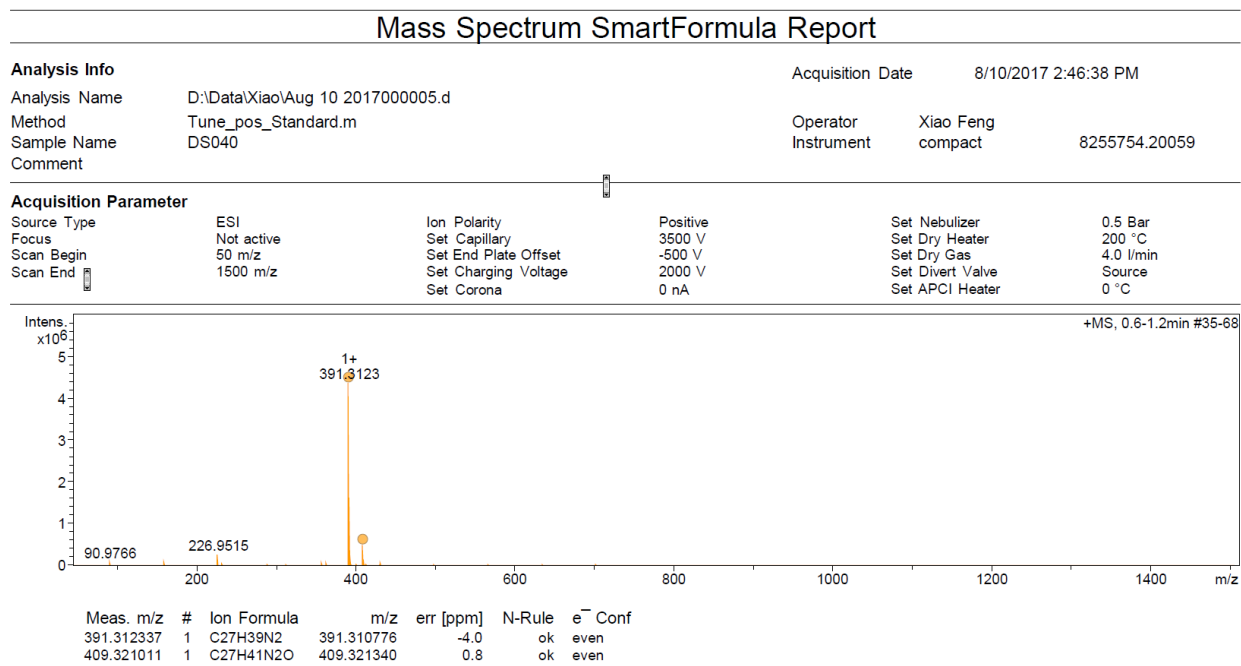


Table S1. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SiPr(H)(CCl₃). U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4141(1)	6873(1)	5020(1)	24(1)
C(1)	5252(2)	7582(1)	3778(1)	16(1)
N(1)	6917(2)	7377(1)	3947(1)	17(1)
Cl(2)	1984(1)	7336(1)	3792(1)	25(1)
C(2)	3977(2)	7027(1)	4048(1)	20(1)
N(2)	5123(2)	8260(1)	4159(1)	18(1)
Cl(3)	4245(1)	6205(1)	3572(1)	25(1)
C(3)	7733(2)	7876(1)	4471(1)	22(1)
C(4)	6736(2)	8547(1)	4359(1)	23(1)
C(5)	3849(2)	8777(1)	4013(1)	21(1)
C(6)	2976(3)	8995(1)	4627(1)	25(1)
C(8)	1330(3)	9759(2)	3799(2)	45(1)
C(7)	1729(3)	9488(2)	4504(1)	37(1)
C(10)	3511(3)	9076(1)	3305(1)	26(1)
C(9)	2230(3)	9556(2)	3210(1)	39(1)
C(11)	4503(3)	8910(1)	2637(1)	29(1)
C(12)	3535(3)	8461(2)	2054(1)	42(1)
C(13)	5133(4)	9590(2)	2276(1)	43(1)
C(16)	1903(3)	8365(1)	5738(1)	35(1)
C(15)	4020(3)	9326(1)	5920(1)	39(1)
C(14)	3371(3)	8724(1)	5412(1)	25(1)

C(17)	7826(2)	6829(1)	3603(1)	18(1)
C(18)	8430(2)	6256(1)	4043(1)	21(1)
C(19)	9426(2)	5750(1)	3726(1)	25(1)
C(26)	8079(2)	6173(1)	4859(1)	25(1)
C(20)	9815(2)	5802(1)	2993(1)	28(1)
C(28)	7280(3)	5455(1)	5018(1)	36(1)
C(21)	9205(2)	6362(1)	2562(1)	29(1)
C(27)	9631(3)	6283(1)	5359(1)	32(1)
C(22)	8224(2)	6889(1)	2854(1)	24(1)
C(23)	7713(3)	7528(2)	2379(1)	32(1)
C(25)	7448(4)	7349(2)	1550(1)	54(1)
C(24)	8929(4)	8128(2)	2485(2)	52(1)

Table S2. Bond lengths [Å] and angles [°] for SIPr(H)(CCl₃).

Cl(1)-C(2)	1.770(2)
C(1)-N(1)	1.443(2)
C(1)-N(2)	1.450(3)
C(1)-C(2)	1.576(3)
N(1)-C(17)	1.432(2)
N(1)-C(3)	1.464(2)
Cl(2)-C(2)	1.7800(19)
C(2)-Cl(3)	1.780(2)
N(2)-C(5)	1.442(3)
N(2)-C(4)	1.462(3)
C(3)-C(4)	1.509(3)
C(5)-C(10)	1.404(3)
C(5)-C(6)	1.415(3)
C(6)-C(7)	1.391(3)
C(6)-C(14)	1.519(3)
C(8)-C(9)	1.384(4)
C(8)-C(7)	1.388(3)
C(10)-C(9)	1.391(3)
C(10)-C(11)	1.526(3)
C(11)-C(13)	1.533(3)
C(11)-C(12)	1.534(3)
C(16)-C(14)	1.532(3)
C(15)-C(14)	1.529(3)

C(17)-C(18)	1.408(3)
C(17)-C(22)	1.410(3)
C(18)-C(19)	1.398(3)
C(18)-C(26)	1.520(3)
C(19)-C(20)	1.378(3)
C(26)-C(28)	1.532(3)
C(26)-C(27)	1.538(3)
C(20)-C(21)	1.383(3)
C(21)-C(22)	1.397(3)
C(22)-C(23)	1.516(3)
C(23)-C(24)	1.512(4)
C(23)-C(25)	1.533(3)

N(1)-C(1)-N(2)	103.21(15)
N(1)-C(1)-C(2)	113.99(16)
N(2)-C(1)-C(2)	111.22(15)
C(17)-N(1)-C(1)	128.06(15)
C(17)-N(1)-C(3)	120.08(15)
C(1)-N(1)-C(3)	111.36(15)
C(1)-C(2)-Cl(1)	113.44(13)
C(1)-C(2)-Cl(2)	109.36(14)
Cl(1)-C(2)-Cl(2)	108.96(10)
C(1)-C(2)-Cl(3)	108.47(13)
Cl(1)-C(2)-Cl(3)	109.28(11)
Cl(2)-C(2)-Cl(3)	107.14(10)

C(5)-N(2)-C(1)	125.00(15)
C(5)-N(2)-C(4)	116.38(17)
C(1)-N(2)-C(4)	110.26(15)
N(1)-C(3)-C(4)	102.55(15)
N(2)-C(4)-C(3)	102.15(17)
C(10)-C(5)-C(6)	120.60(19)
C(10)-C(5)-N(2)	122.59(18)
C(6)-C(5)-N(2)	116.77(18)
C(7)-C(6)-C(5)	118.3(2)
C(7)-C(6)-C(14)	119.15(19)
C(5)-C(6)-C(14)	122.56(19)
C(9)-C(8)-C(7)	119.3(2)
C(8)-C(7)-C(6)	121.5(2)
C(9)-C(10)-C(5)	118.7(2)
C(9)-C(10)-C(11)	118.25(19)
C(5)-C(10)-C(11)	123.05(19)
C(8)-C(9)-C(10)	121.5(2)
C(10)-C(11)-C(13)	112.1(2)
C(10)-C(11)-C(12)	111.59(19)
C(13)-C(11)-C(12)	110.0(2)
C(6)-C(14)-C(15)	111.0(2)
C(6)-C(14)-C(16)	111.73(19)
C(15)-C(14)-C(16)	110.60(19)
C(18)-C(17)-C(22)	120.17(18)
C(18)-C(17)-N(1)	118.72(17)

C(22)-C(17)-N(1)	120.92(18)
C(19)-C(18)-C(17)	118.99(19)
C(19)-C(18)-C(26)	118.39(19)
C(17)-C(18)-C(26)	122.60(18)
C(20)-C(19)-C(18)	121.3(2)
C(18)-C(26)-C(28)	112.22(19)
C(18)-C(26)-C(27)	110.64(17)
C(28)-C(26)-C(27)	111.15(19)
C(19)-C(20)-C(21)	119.5(2)
C(20)-C(21)-C(22)	121.63(19)
C(21)-C(22)-C(17)	118.5(2)
C(21)-C(22)-C(23)	119.54(19)
C(17)-C(22)-C(23)	121.87(19)
C(24)-C(23)-C(22)	110.73(19)
C(24)-C(23)-C(25)	109.9(2)
C(22)-C(23)-C(25)	113.3(2)

Table S3. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for SIPr(H)(CCl₃). The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U^{11} + \dots + 2hka^*b^*U^{12}]$.

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
Cl(1)	22(1)	27(1)	22(1)	4(1)	3(1)	0(1)
C(1)	13(1)	19(1)	16(1)	1(1)	-1(1)	2(1)
N(1)	12(1)	19(1)	18(1)	-3(1)	-4(1)	2(1)
Cl(2)	13(1)	29(1)	32(1)	-1(1)	-2(1)	1(1)
C(2)	14(1)	22(1)	22(1)	-2(1)	-2(1)	2(1)
N(2)	15(1)	15(1)	22(1)	-2(1)	-2(1)	2(1)
Cl(3)	21(1)	21(1)	35(1)	-8(1)	-1(1)	-1(1)
C(3)	18(1)	26(1)	21(1)	-4(1)	-5(1)	0(1)
C(4)	20(1)	21(1)	28(1)	-6(1)	-1(1)	-2(1)
C(5)	19(1)	18(1)	25(1)	2(1)	1(1)	3(1)
C(6)	25(1)	23(1)	27(1)	1(1)	4(1)	5(1)
C(8)	43(2)	46(2)	45(2)	12(1)	4(1)	29(1)
C(7)	37(1)	38(2)	36(1)	3(1)	9(1)	19(1)
C(10)	31(1)	22(1)	25(1)	3(1)	2(1)	6(1)
C(9)	46(1)	38(2)	33(1)	10(1)	-1(1)	17(1)
C(11)	37(1)	27(1)	22(1)	5(1)	2(1)	2(1)
C(12)	50(2)	48(2)	26(1)	-1(1)	-2(1)	-1(1)
C(13)	63(2)	32(2)	36(1)	8(1)	14(1)	0(1)
C(16)	38(1)	35(1)	35(1)	5(1)	13(1)	7(1)
C(15)	54(2)	31(2)	32(1)	-7(1)	2(1)	6(1)
C(14)	30(1)	23(1)	23(1)	0(1)	4(1)	6(1)

C(17)	12(1)	20(1)	20(1)	-5(1)	-2(1)	-1(1)
C(18)	14(1)	21(1)	27(1)	-2(1)	-1(1)	0(1)
C(19)	18(1)	22(1)	36(1)	-4(1)	-2(1)	2(1)
C(26)	21(1)	25(1)	29(1)	6(1)	2(1)	8(1)
C(20)	17(1)	29(1)	38(1)	-16(1)	-1(1)	1(1)
C(28)	32(1)	33(1)	43(1)	14(1)	6(1)	7(1)
C(21)	20(1)	46(2)	21(1)	-10(1)	0(1)	0(1)
C(27)	30(1)	40(2)	26(1)	2(1)	-3(1)	11(1)
C(22)	14(1)	36(1)	21(1)	-3(1)	-3(1)	1(1)
C(23)	23(1)	51(2)	23(1)	8(1)	4(1)	10(1)
C(25)	55(2)	75(2)	30(1)	9(1)	-15(1)	-7(2)
C(24)	71(2)	42(2)	40(2)	12(1)	-15(1)	-1(2)

Table S4. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for $\text{SiPr(H)(CCl}_3\text{)}$.

	x	y	z	U(eq)
H(1)	5070	7657	3230	19
H(3A)	8872	7956	4349	26
H(3B)	7712	7700	4989	26
H(4A)	6740	8834	4822	28
H(4B)	7136	8845	3954	28
H(8)	448	10082	3723	54
H(7)	1137	9642	4911	44
H(9)	1967	9748	2729	47
H(11)	5466	8623	2820	34
H(12A)	2608	8738	1847	62
H(12B)	3143	8026	2288	62
H(12C)	4233	8330	1653	62
H(13A)	5789	9460	1860	65
H(13B)	5799	9862	2646	65
H(13C)	4213	9884	2092	65
H(16A)	1051	8722	5797	53
H(16B)	2228	8158	6224	53
H(16C)	1492	7987	5400	53
H(15A)	4990	9533	5717	58
H(15B)	4297	9135	6418	58
H(15C)	3188	9697	5952	58

H(14)	4244	8356	5387	31
H(19)	9843	5364	4021	30
H(26)	7299	6559	4981	30
H(20)	10497	5454	2786	34
H(28A)	6275	5407	4705	54
H(28B)	7033	5433	5544	54
H(28C)	8022	5066	4907	54
H(21)	9459	6391	2055	35
H(27A)	10436	5922	5240	48
H(27B)	9378	6235	5882	48
H(27C)	10069	6761	5275	48
H(23)	6658	7704	2555	39
H(25A)	6942	7758	1286	81
H(25B)	6739	6931	1489	81
H(25C)	8495	7245	1343	81
H(24A)	9958	7984	2285	78
H(24B)	9103	8235	3017	78
H(24C)	8514	8555	2222	78

Table S5. XYZ atomic coordinates for SIPr(H)CCl₃ optimized at the B3LYP/6-311G(2d,p) level of theory

N	1.11543900	-0.06858500	-0.66556900
N	-1.16904200	-0.13990900	-0.63763900
C	-0.74513800	-0.49745100	-1.99239600
C	0.67382500	0.03934700	-2.05475000
C	2.49733000	0.23057200	-0.38819400
C	3.44360100	-0.80361800	-0.58907900
C	4.79211600	-0.54163500	-0.35472600
C	5.22299900	0.70335800	0.07039800
C	4.29884600	1.71966100	0.23109700
C	2.93957300	1.51824200	-0.01423600
C	3.05757400	-2.19558600	-1.07408500
C	3.51010200	-3.29740000	-0.10128500
C	3.60965300	-2.46954500	-2.48523500
C	2.01713200	2.72228900	0.11450700
C	1.98268300	3.26842300	1.55238300
C	2.39504000	3.83184500	-0.88352900
C	-2.52153100	0.27778900	-0.39557700
C	-2.86289300	1.64402600	-0.28517500
C	-4.19121500	1.99010400	-0.03242100
C	-5.18473500	1.03120700	0.05153400
C	-4.85709400	-0.30123300	-0.13430300
C	-3.54085800	-0.70326700	-0.35432000
C	-1.86614100	2.77292500	-0.50151600

C	-1.72434000	3.67350900	0.73576600
C	-2.23218900	3.60679600	-1.74318700
C	-3.26484000	-2.18339800	-0.58187800
C	-3.82163900	-3.07502500	0.53970900
C	-3.80481300	-2.63956400	-1.95022000
H	-0.76251300	-1.58063400	-2.16297500
H	-1.40130700	-0.02709300	-2.72572600
H	1.31662400	-0.55353400	-2.70654300
H	0.69405500	1.07798000	-2.41614100
H	5.51780200	-1.33282200	-0.50120400
H	6.27447900	0.88413800	0.26135600
H	4.64014300	2.70129400	0.53758500
H	1.97112900	-2.23422200	-1.12330300
H	3.13475900	-3.11610300	0.90605000
H	4.59950900	-3.36593600	-0.04874200
H	3.13591400	-4.26984900	-0.43198400
H	3.29300400	-1.70701900	-3.20034500
H	4.70251600	-2.48474900	-2.48731200
H	3.26365700	-3.44033400	-2.85010200
H	1.01044600	2.40465400	-0.14479200
H	1.28788300	4.10753100	1.63087700
H	2.96786300	3.62551400	1.86111800
H	1.67244100	2.50111200	2.26383400
H	3.38387000	4.24428400	-0.67119200
H	2.40640700	3.45618900	-1.90882600

H	1.67604600	4.65353200	-0.82941300
H	-4.45449800	3.03604100	0.07248300
H	-6.21162400	1.32197100	0.24044500
H	-5.63978200	-1.04966600	-0.10011400
H	-0.89624300	2.32459600	-0.70721400
H	-2.18622800	-2.31667600	-0.58834200
H	-1.42232000	3.10300300	1.61609300
H	-2.66822200	4.16959200	0.97334400
H	-0.97902700	4.45329500	0.56170400
H	-3.18537600	4.12364800	-1.61132700
H	-2.31717100	2.97801800	-2.63194300
H	-1.46660400	4.36356900	-1.93359000
H	-3.44240300	-2.76882600	1.51514100
H	-3.52482000	-4.11377900	0.37391600
H	-4.91338600	-3.04937400	0.57697400
H	-4.89295600	-2.54616400	-1.99623600
H	-3.55208000	-3.68762700	-2.13178200
H	-3.38890800	-2.04473700	-2.76620600
C	-0.02620700	0.05471600	0.23171300
H	-0.08546400	1.00863100	0.77262400
C	0.02667100	-0.98496600	1.43352300
Cl	-1.40914500	-0.71226800	2.49561800
Cl	0.03358300	-2.69279600	0.89032400
Cl	1.48594700	-0.69744900	2.45918400